Full wwPDB X-ray Structure Validation Report ⓘ

Dec 12, 2023 – 08:23 pm GMT

PDB ID	:	2YKS
Title	:	PENTAMERIC LIGAND GATED ION CHANNEL ELIC MUTANT F246A
Authors	:	Zimmermann, I.; Dutzler, R.
Deposited on	:	2011-05-30
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:

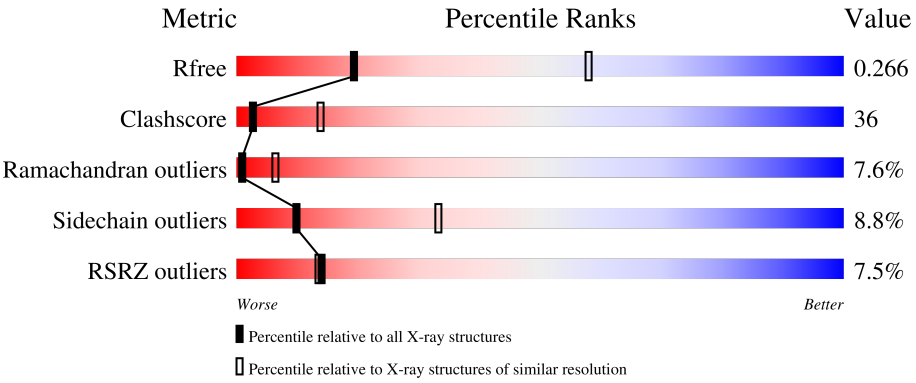
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 <=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	8% 41% 45% 9% • 5%
1	B	321	7% 44% 42% 8% • 5%
1	C	321	6% 43% 42% 9% • 5%
1	D	321	7% 42% 44% 8% • 5%
1	E	321	6% 43% 44% 8% • 5%

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Mol	Chain	Length	Quality of chain
1	F	321	7% 42% 44% 9% • 5%
1	G	321	6% 45% 42% 8% • 5%
1	H	321	9% 42% 44% 8% • 5%
1	I	321	6% 42% 44% 8% • 5%
1	J	321	10% 42% 43% 9% • 5%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 24950 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
			2495	1625	415	449	6			
1	B	306	Total	C	N	O	S	0	0	0
			2495	1625	415	449	6			
1	C	306	Total	C	N	O	S	0	0	0
			2495	1625	415	449	6			
1	D	306	Total	C	N	O	S	0	0	0
			2495	1625	415	449	6			
1	E	306	Total	C	N	O	S	0	0	0
			2495	1625	415	449	6			
1	F	306	Total	C	N	O	S	0	0	0
			2495	1625	415	449	6			
1	G	306	Total	C	N	O	S	0	0	0
			2495	1625	415	449	6			
1	H	306	Total	C	N	O	S	0	0	0
			2495	1625	415	449	6			
1	I	306	Total	C	N	O	S	0	0	0
			2495	1625	415	449	6			
1	J	306	Total	C	N	O	S	0	0	0
			2495	1625	415	449	6			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	246	ALA	PHE	engineered mutation	UNP P0C7B7
A	288	ASN	MET	conflict	UNP P0C7B7
B	246	ALA	PHE	engineered mutation	UNP P0C7B7
B	288	ASN	MET	conflict	UNP P0C7B7
C	246	ALA	PHE	engineered mutation	UNP P0C7B7
C	288	ASN	MET	conflict	UNP P0C7B7
D	246	ALA	PHE	engineered mutation	UNP P0C7B7
D	288	ASN	MET	conflict	UNP P0C7B7
E	246	ALA	PHE	engineered mutation	UNP P0C7B7

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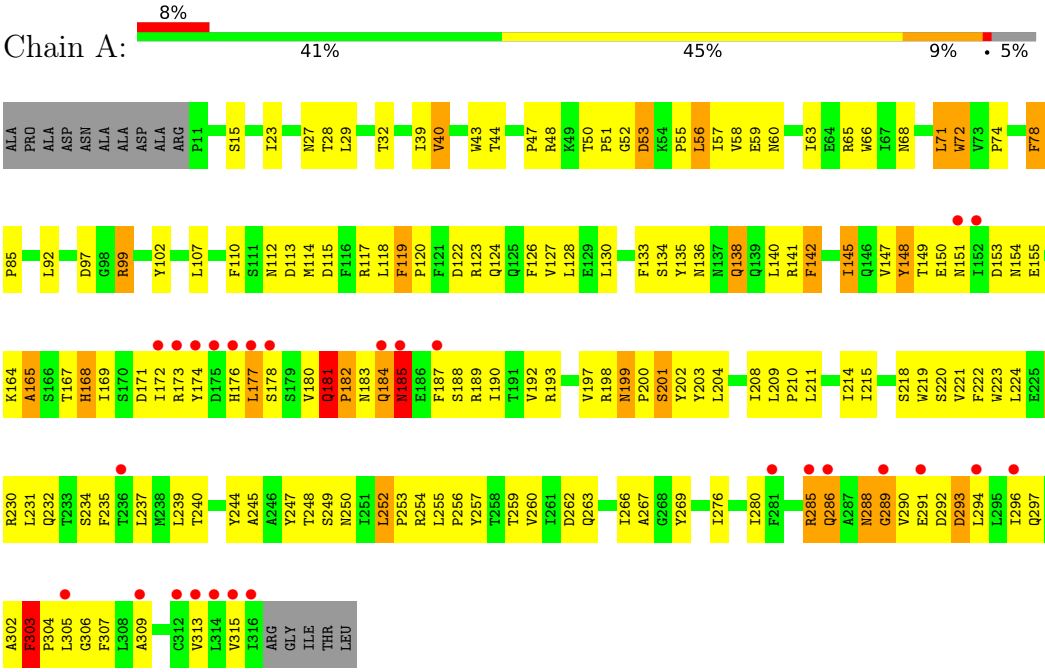
Chain	Residue	Modelled	Actual	Comment	Reference
E	288	ASN	MET	conflict	UNP P0C7B7
F	246	ALA	PHE	engineered mutation	UNP P0C7B7
F	288	ASN	MET	conflict	UNP P0C7B7
G	246	ALA	PHE	engineered mutation	UNP P0C7B7
G	288	ASN	MET	conflict	UNP P0C7B7
H	246	ALA	PHE	engineered mutation	UNP P0C7B7
H	288	ASN	MET	conflict	UNP P0C7B7
I	246	ALA	PHE	engineered mutation	UNP P0C7B7
I	288	ASN	MET	conflict	UNP P0C7B7
J	246	ALA	PHE	engineered mutation	UNP P0C7B7
J	288	ASN	MET	conflict	UNP P0C7B7

3 Residue-property plots (i)

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.

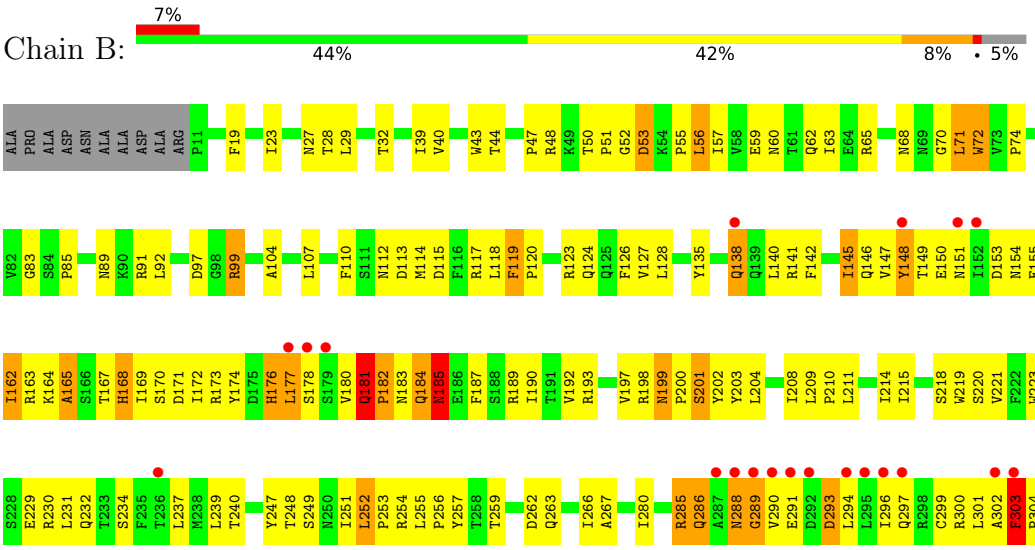
• Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL

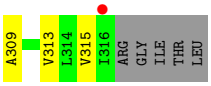
Chain A:



• Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL

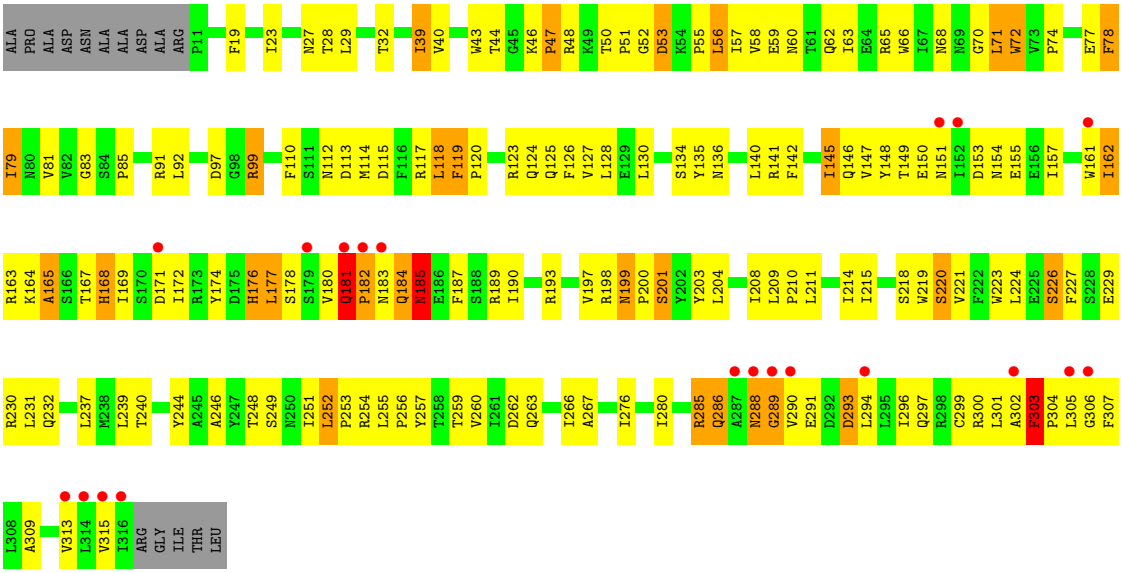
Chain B:





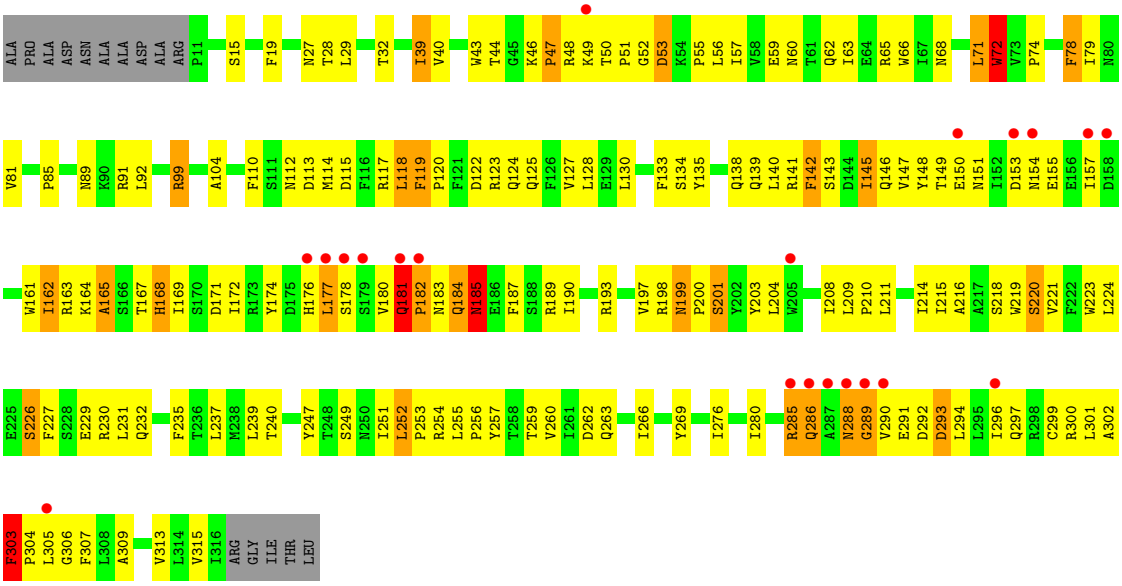
• Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL

Chain C:



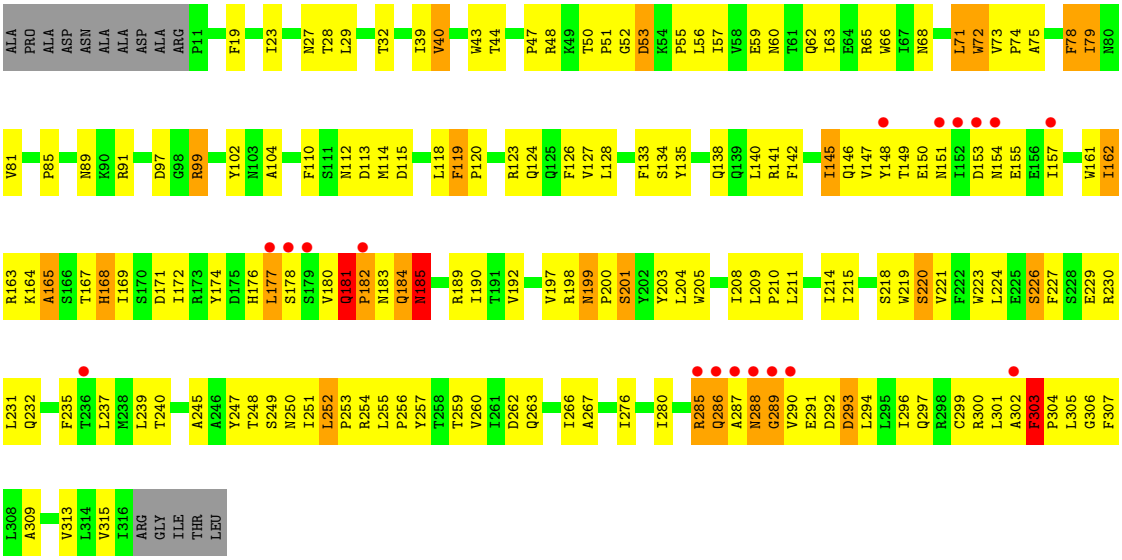
• Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL

Chain D:



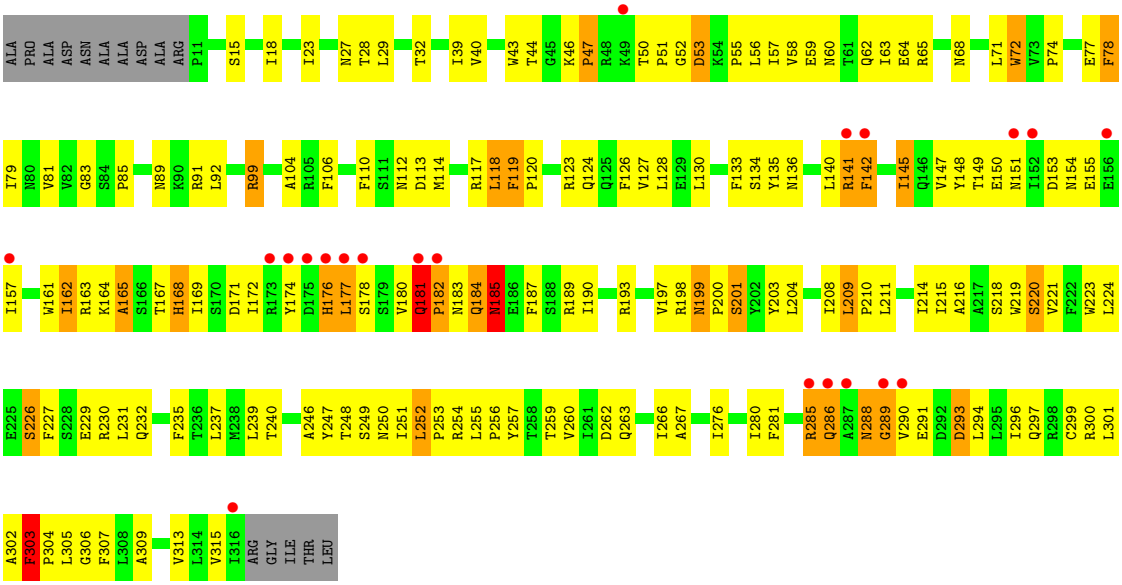
• Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL

Chain E:



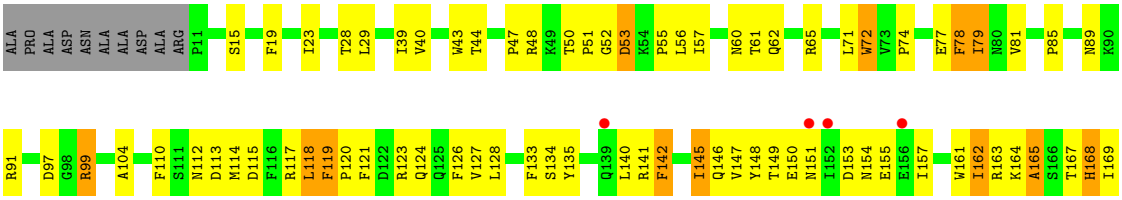
• Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL

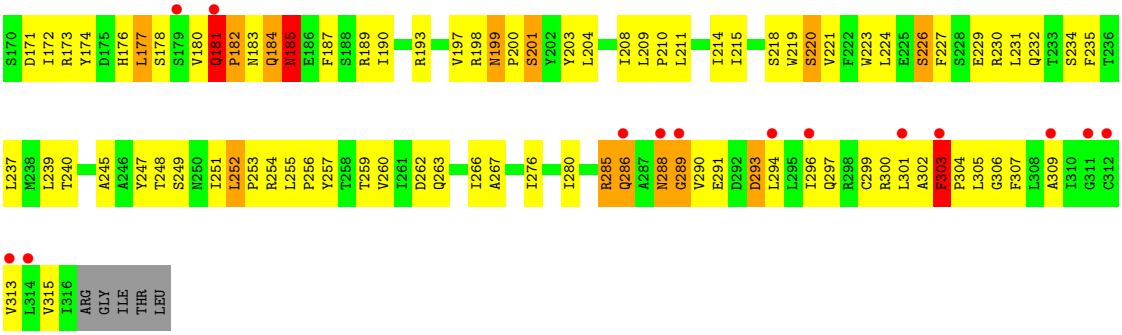
Chain F:



• Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL

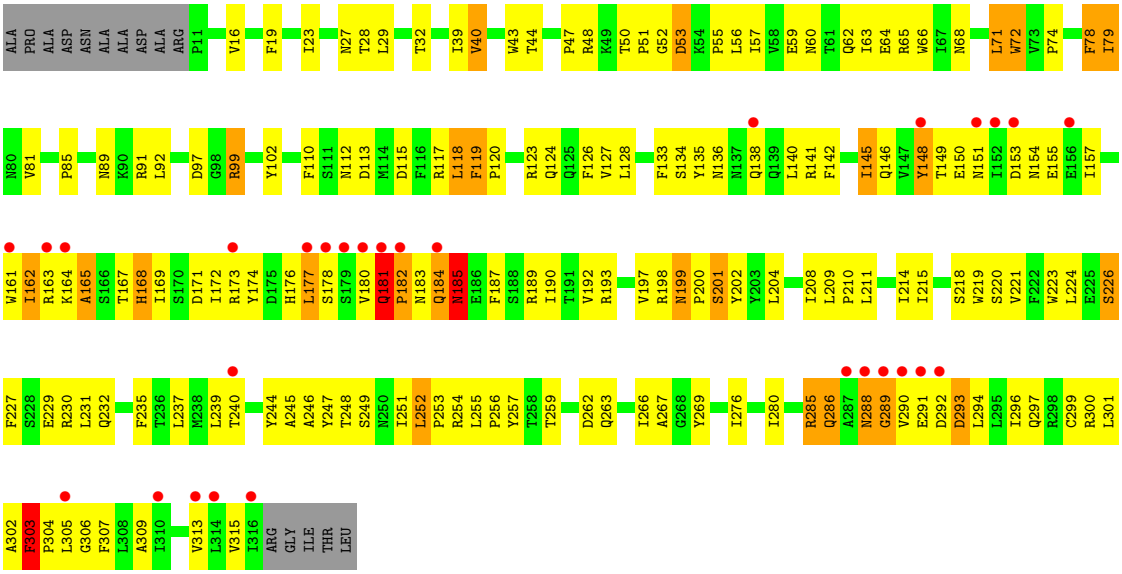
Chain G:





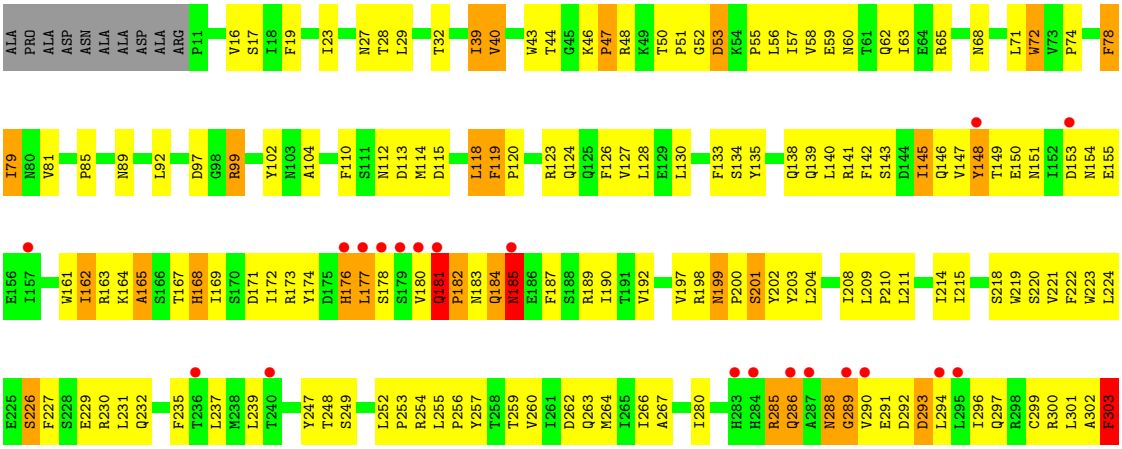
• Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL

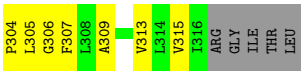
Chain H:



• Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL

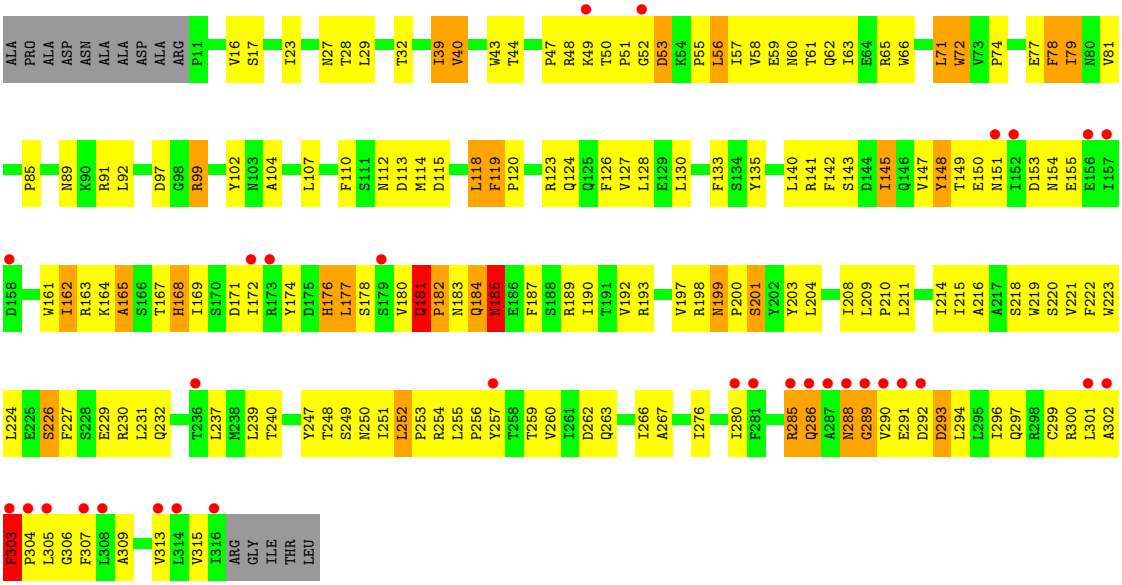
Chain I:





• Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL

Chain J:



4 Data and refinement statistics (i)

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)	19.97 – 3.30 40.48 – 3.28	Depositor EDS
% Data completeness (in resolution range)	98.2 (19.97-3.30) 96.6 (40.48-3.28)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.16 (at 3.25Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7_650)	Depositor
R, R_{free}	0.242 , 0.265 0.246 , 0.266	Depositor DCC
R_{free} test set	4322 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	103.0	Xtriage
Anisotropy	0.353	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 76.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	24950	wwPDB-VP
Average B, all atoms (Å^2)	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.66	0/2562	0.75	1/3493 (0.0%)
1	B	0.73	0/2562	0.78	1/3493 (0.0%)
1	C	0.72	0/2562	0.77	1/3493 (0.0%)
1	D	0.75	2/2562 (0.1%)	0.77	1/3493 (0.0%)
1	E	0.69	0/2562	0.76	0/3493
1	F	0.67	0/2562	0.78	0/3493
1	G	0.75	0/2562	0.79	0/3493
1	H	0.70	0/2562	0.76	0/3493
1	I	0.77	0/2562	0.78	1/3493 (0.0%)
1	J	0.70	0/2562	0.77	1/3493 (0.0%)
All	All	0.71	2/25620 (0.0%)	0.77	6/34930 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	72	TRP	CD2-CE2	5.75	1.48	1.41
1	D	72	TRP	CZ3-CH2	5.25	1.48	1.40

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	39	ILE	CG1-CB-CG2	-5.91	98.40	111.40
1	I	39	ILE	CG1-CB-CG2	-5.89	98.44	111.40
1	C	39	ILE	CG1-CB-CG2	-5.67	98.92	111.40
1	B	138	GLN	N-CA-C	-5.12	97.17	111.00
1	J	39	ILE	CG1-CB-CG2	-5.07	100.25	111.40
1	A	138	GLN	N-CA-C	-5.02	97.45	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2495	0	2471	204	1
1	B	2495	0	2471	204	0
1	C	2495	0	2471	200	0
1	D	2495	0	2471	196	2
1	E	2495	0	2471	196	1
1	F	2495	0	2471	198	1
1	G	2495	0	2471	209	2
1	H	2495	0	2471	193	0
1	I	2495	0	2471	208	0
1	J	2495	0	2471	196	1
All	All	24950	0	24710	1786	4

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 36.

All (1786) 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:B:164:LYS:HG2	1:I:163:ARG:HB3	1.28	1.16
1:I:164:LYS:NZ	1:I:165:ALA:H	1.52	1.06
1:D:164:LYS:NZ	1:D:165:ALA:H	1.54	1.05
1:B:164:LYS:NZ	1:B:165:ALA:H	1.52	1.05
1:G:164:LYS:NZ	1:G:165:ALA:H	1.58	1.01
1:B:173:ARG:HH22	1:I:139:GLN:NE2	1.62	0.97
1:B:164:LYS:HZ2	1:B:165:ALA:H	1.02	0.97
1:J:164:LYS:HZ2	1:J:165:ALA:H	1.12	0.97
1:J:164:LYS:NZ	1:J:165:ALA:H	1.65	0.95
1:F:164:LYS:HZ2	1:F:165:ALA:N	1.65	0.95
1:F:164:LYS:NZ	1:F:165:ALA:H	1.66	0.93
1:A:164:LYS:NZ	1:A:165:ALA:H	1.67	0.92
1:H:223:TRP:HE1	1:H:300:ARG:HB3	1.33	0.92
1:J:223:TRP:HE1	1:J:300:ARG:HB3	1.35	0.92
1:H:164:LYS:NZ	1:H:165:ALA:H	1.67	0.91
1:B:164:LYS:HZ2	1:B:165:ALA:N	1.69	0.91
1:A:164:LYS:HZ2	1:A:165:ALA:N	1.69	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:164:LYS:HZ2	1:C:165:ALA:H	0.91	0.90
1:C:223:TRP:HE1	1:C:300:ARG:HB3	1.33	0.90
1:A:223:TRP:HE1	1:A:300:ARG:HB3	1.36	0.90
1:E:164:LYS:NZ	1:E:165:ALA:H	1.70	0.90
1:H:164:LYS:HZ2	1:H:165:ALA:H	1.18	0.89
1:J:145:ILE:H	1:J:145:ILE:HD12	1.36	0.89
1:A:249:SER:HB3	1:E:251:ILE:HG13	1.53	0.89
1:H:162:ILE:HG22	1:H:163:ARG:H	1.37	0.89
1:E:167:THR:HG22	1:E:168:HIS:H	1.37	0.89
1:A:167:THR:HG22	1:A:168:HIS:H	1.38	0.89
1:I:167:THR:HG22	1:I:168:HIS:H	1.36	0.89
1:I:145:ILE:H	1:I:145:ILE:HD12	1.36	0.89
1:I:223:TRP:HE1	1:I:300:ARG:HB3	1.38	0.89
1:I:164:LYS:HZ1	1:I:165:ALA:H	1.12	0.89
1:G:223:TRP:HE1	1:G:300:ARG:HB3	1.36	0.88
1:E:223:TRP:HE1	1:E:300:ARG:HB3	1.39	0.88
1:B:167:THR:HG22	1:B:168:HIS:H	1.39	0.88
1:D:164:LYS:HZ1	1:D:165:ALA:N	1.71	0.87
1:E:164:LYS:HZ2	1:E:165:ALA:H	1.18	0.87
1:H:167:THR:HG22	1:H:168:HIS:H	1.37	0.87
1:D:164:LYS:HZ1	1:D:165:ALA:H	0.87	0.87
1:B:145:ILE:H	1:B:145:ILE:HD12	1.39	0.87
1:D:223:TRP:HE1	1:D:300:ARG:HB3	1.40	0.87
1:A:140:LEU:HD13	1:A:190:ILE:HG13	1.56	0.87
1:G:164:LYS:HZ1	1:G:165:ALA:N	1.73	0.86
1:B:181:GLN:HG3	1:B:182:PRO:HD3	1.57	0.86
1:C:164:LYS:NZ	1:C:165:ALA:H	1.73	0.86
1:E:181:GLN:HG3	1:E:182:PRO:HD3	1.57	0.86
1:B:168:HIS:ND1	1:I:167:THR:HB	1.91	0.86
1:D:72:TRP:CZ2	1:D:74:PRO:HG3	2.11	0.86
1:F:181:GLN:HG3	1:F:182:PRO:HD3	1.58	0.86
1:H:145:ILE:HD12	1:H:145:ILE:H	1.40	0.86
1:B:173:ARG:HH22	1:I:139:GLN:HE22	1.22	0.85
1:F:237:LEU:HD13	1:G:235:PHE:CD2	2.09	0.85
1:I:224:LEU:HD21	1:J:231:LEU:HD22	1.58	0.85
1:D:181:GLN:HG3	1:D:182:PRO:HD3	1.59	0.85
1:C:145:ILE:HD12	1:C:145:ILE:H	1.41	0.85
1:G:181:GLN:HG3	1:G:182:PRO:HD3	1.57	0.85
1:A:72:TRP:CZ2	1:A:74:PRO:HG3	2.11	0.85
1:A:164:LYS:HZ2	1:A:165:ALA:H	0.85	0.84
1:A:181:GLN:HG3	1:A:182:PRO:HD3	1.58	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:181:GLN:HG3	1:H:182:PRO:HD3	1.59	0.84
1:G:164:LYS:HZ1	1:G:165:ALA:H	0.88	0.84
1:J:167:THR:HG22	1:J:168:HIS:H	1.42	0.84
1:A:288:ASN:CG	1:A:289:GLY:H	1.81	0.84
1:C:181:GLN:HG3	1:C:182:PRO:HD3	1.59	0.83
1:I:215:ILE:O	1:I:218:SER:HB3	1.78	0.83
1:E:145:ILE:H	1:E:145:ILE:HD12	1.43	0.83
1:F:145:ILE:H	1:F:145:ILE:HD12	1.41	0.83
1:G:294:LEU:HA	1:G:297:GLN:HE21	1.43	0.83
1:E:162:ILE:HG22	1:E:163:ARG:H	1.44	0.83
1:I:181:GLN:HG3	1:I:182:PRO:HD3	1.58	0.83
1:J:181:GLN:HG3	1:J:182:PRO:HD3	1.58	0.83
1:A:145:ILE:H	1:A:145:ILE:HD12	1.43	0.83
1:F:256:PRO:HG2	1:F:257:TYR:HD1	1.43	0.82
1:H:256:PRO:HG2	1:H:257:TYR:HD1	1.44	0.82
1:F:215:ILE:O	1:F:218:SER:HB3	1.80	0.82
1:A:162:ILE:HG22	1:A:163:ARG:H	1.44	0.82
1:F:167:THR:HG22	1:F:168:HIS:H	1.43	0.82
1:G:162:ILE:HG22	1:G:163:ARG:H	1.44	0.82
1:B:223:TRP:HE1	1:B:300:ARG:HB3	1.43	0.82
1:C:164:LYS:HZ2	1:C:165:ALA:N	1.76	0.82
1:F:198:ARG:O	1:F:200:PRO:HD3	1.80	0.82
1:B:164:LYS:HD3	1:I:163:ARG:HD2	1.61	0.82
1:C:256:PRO:HG2	1:C:257:TYR:HD1	1.45	0.82
1:D:44:THR:HA	1:D:99:ARG:HA	1.62	0.81
1:G:288:ASN:CG	1:G:289:GLY:H	1.83	0.81
1:A:293:ASP:HB2	1:A:296:ILE:HG22	1.61	0.81
1:C:288:ASN:CG	1:C:289:GLY:H	1.84	0.81
1:F:72:TRP:CZ2	1:F:74:PRO:HG3	2.14	0.81
1:H:223:TRP:NE1	1:H:300:ARG:HB3	1.95	0.81
1:I:198:ARG:O	1:I:200:PRO:HD3	1.79	0.81
1:I:288:ASN:CG	1:I:289:GLY:H	1.84	0.81
1:J:215:ILE:O	1:J:218:SER:HB3	1.80	0.81
1:J:288:ASN:CG	1:J:289:GLY:H	1.83	0.81
1:G:145:ILE:H	1:G:145:ILE:HD12	1.43	0.81
1:H:140:LEU:HD13	1:H:190:ILE:HG13	1.63	0.81
1:C:218:SER:HA	1:C:237:LEU:HD21	1.62	0.81
1:H:288:ASN:CG	1:H:289:GLY:H	1.83	0.81
1:J:72:TRP:CZ2	1:J:74:PRO:HG3	2.15	0.81
1:B:288:ASN:CG	1:B:289:GLY:H	1.84	0.81
1:E:288:ASN:CG	1:E:289:GLY:H	1.84	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:119:PHE:HB3	1:J:120:PRO:HD3	1.61	0.81
1:B:119:PHE:HB3	1:B:120:PRO:HD3	1.63	0.81
1:I:256:PRO:HG2	1:I:257:TYR:HD1	1.44	0.81
1:J:294:LEU:HA	1:J:297:GLN:HE21	1.46	0.81
1:B:140:LEU:HD13	1:B:190:ILE:HG13	1.62	0.81
1:D:162:ILE:HG22	1:D:163:ARG:H	1.44	0.81
1:D:237:LEU:HD13	1:E:235:PHE:CD2	2.15	0.81
1:F:288:ASN:CG	1:F:289:GLY:H	1.83	0.80
1:I:164:LYS:HZ2	1:I:164:LYS:HA	1.45	0.80
1:J:293:ASP:HB2	1:J:296:ILE:HG22	1.63	0.80
1:C:119:PHE:HB3	1:C:120:PRO:HD3	1.63	0.80
1:D:288:ASN:CG	1:D:289:GLY:H	1.85	0.80
1:F:223:TRP:HE1	1:F:300:ARG:HB3	1.46	0.80
1:J:140:LEU:HD13	1:J:190:ILE:HG13	1.61	0.80
1:I:256:PRO:HG2	1:I:257:TYR:CD1	2.16	0.80
1:A:294:LEU:HA	1:A:297:GLN:HE21	1.46	0.80
1:D:198:ARG:O	1:D:200:PRO:HD3	1.81	0.80
1:A:256:PRO:HG2	1:A:257:TYR:HD1	1.45	0.80
1:D:167:THR:HG22	1:D:168:HIS:H	1.47	0.80
1:E:256:PRO:HG2	1:E:257:TYR:HD1	1.46	0.80
1:G:167:THR:HG22	1:G:168:HIS:H	1.47	0.80
1:D:256:PRO:HG2	1:D:257:TYR:HD1	1.47	0.79
1:I:72:TRP:CZ2	1:I:74:PRO:HG3	2.17	0.79
1:G:119:PHE:HB3	1:G:120:PRO:HD3	1.64	0.79
1:G:256:PRO:HG2	1:G:257:TYR:HD1	1.46	0.79
1:D:140:LEU:HD13	1:D:190:ILE:HG13	1.64	0.79
1:D:215:ILE:O	1:D:218:SER:HB3	1.81	0.79
1:F:119:PHE:HB3	1:F:120:PRO:HD3	1.65	0.79
1:G:223:TRP:NE1	1:G:300:ARG:HB3	1.97	0.79
1:B:224:LEU:HD21	1:C:231:LEU:HD22	1.62	0.79
1:F:294:LEU:HA	1:F:297:GLN:HE21	1.46	0.79
1:D:294:LEU:HA	1:D:297:GLN:HE21	1.46	0.79
1:A:223:TRP:NE1	1:A:300:ARG:HB3	1.96	0.79
1:J:198:ARG:O	1:J:200:PRO:HD3	1.83	0.79
1:G:140:LEU:HD13	1:G:190:ILE:HG13	1.65	0.79
1:H:44:THR:HA	1:H:99:ARG:HA	1.63	0.79
1:C:293:ASP:HB2	1:C:296:ILE:HG22	1.65	0.79
1:H:218:SER:HA	1:H:237:LEU:HD21	1.64	0.79
1:E:294:LEU:HA	1:E:297:GLN:HE21	1.46	0.78
1:F:140:LEU:HD13	1:F:190:ILE:HG13	1.64	0.78
1:C:167:THR:HG22	1:C:168:HIS:H	1.48	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:ILE:HG22	1:B:163:ARG:H	1.48	0.78
1:A:239:LEU:HD23	1:E:240:THR:HA	1.65	0.78
1:F:256:PRO:HG2	1:F:257:TYR:CD1	2.19	0.78
1:H:294:LEU:HA	1:H:297:GLN:HE21	1.48	0.78
1:C:198:ARG:O	1:C:200:PRO:HD3	1.84	0.78
1:J:223:TRP:NE1	1:J:300:ARG:HB3	1.99	0.78
1:A:235:PHE:CD2	1:E:237:LEU:HD13	2.19	0.78
1:F:249:SER:HB3	1:J:251:ILE:HG13	1.65	0.78
1:H:256:PRO:HG2	1:H:257:TYR:CD1	2.19	0.78
1:D:91:ARG:HB2	1:E:133:PHE:HE2	1.47	0.78
1:H:119:PHE:HB3	1:H:120:PRO:HD3	1.65	0.78
1:H:198:ARG:O	1:H:200:PRO:HD3	1.84	0.77
1:C:162:ILE:HG22	1:C:163:ARG:H	1.48	0.77
1:E:140:LEU:HD13	1:E:190:ILE:HG13	1.64	0.77
1:I:294:LEU:HA	1:I:297:GLN:HE21	1.49	0.77
1:C:223:TRP:NE1	1:C:300:ARG:HB3	1.98	0.77
1:G:256:PRO:HG2	1:G:257:TYR:CD1	2.20	0.77
1:I:293:ASP:HB2	1:I:296:ILE:HG22	1.65	0.77
1:F:68:ASN:ND2	1:J:65:ARG:HD2	1.99	0.77
1:H:224:LEU:HD21	1:I:231:LEU:HD22	1.66	0.77
1:G:294:LEU:HA	1:G:297:GLN:NE2	1.99	0.77
1:B:198:ARG:O	1:B:200:PRO:HD3	1.84	0.77
1:D:145:ILE:H	1:D:145:ILE:HD12	1.49	0.77
1:I:140:LEU:HD13	1:I:190:ILE:HG13	1.67	0.77
1:E:293:ASP:HB2	1:E:296:ILE:HG22	1.66	0.77
1:J:28:THR:HB	1:J:255:LEU:HD21	1.68	0.77
1:C:256:PRO:HG2	1:C:257:TYR:CD1	2.20	0.76
1:F:162:ILE:HG22	1:F:163:ARG:H	1.50	0.76
1:I:209:LEU:HB3	1:I:210:PRO:CD	2.13	0.76
1:J:123:ARG:HD2	1:J:197:VAL:HG22	1.67	0.76
1:J:256:PRO:HG2	1:J:257:TYR:HD1	1.50	0.76
1:C:28:THR:HB	1:C:255:LEU:HD21	1.67	0.76
1:F:293:ASP:HB2	1:F:296:ILE:HG22	1.66	0.76
1:I:119:PHE:HB3	1:I:120:PRO:HD3	1.67	0.76
1:B:293:ASP:HB2	1:B:296:ILE:HG22	1.67	0.76
1:D:293:ASP:HB2	1:D:296:ILE:HG22	1.68	0.76
1:I:44:THR:HA	1:I:99:ARG:HA	1.67	0.76
1:I:223:TRP:NE1	1:I:300:ARG:HB3	2.00	0.76
1:A:44:THR:HA	1:A:99:ARG:HA	1.67	0.76
1:C:140:LEU:HD13	1:C:190:ILE:HG13	1.66	0.76
1:A:224:LEU:HD21	1:B:231:LEU:HD22	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:256:PRO:HG2	1:D:257:TYR:CD1	2.20	0.76
1:E:227:PHE:HA	1:E:230:ARG:HH11	1.49	0.76
1:E:256:PRO:HG2	1:E:257:TYR:CD1	2.21	0.76
1:J:164:LYS:HZ2	1:J:165:ALA:N	1.83	0.76
1:E:223:TRP:NE1	1:E:300:ARG:HB3	1.99	0.76
1:G:28:THR:HB	1:G:255:LEU:HD21	1.68	0.76
1:J:227:PHE:HA	1:J:230:ARG:HH11	1.51	0.76
1:G:91:ARG:HB2	1:H:133:PHE:HE2	1.51	0.76
1:A:198:ARG:O	1:A:200:PRO:HD3	1.86	0.75
1:G:293:ASP:HB2	1:G:296:ILE:HG22	1.66	0.75
1:A:119:PHE:HB3	1:A:120:PRO:HD3	1.67	0.75
1:I:162:ILE:HG22	1:I:163:ARG:H	1.49	0.75
1:A:148:TYR:OH	1:B:176:HIS:CE1	2.39	0.75
1:E:119:PHE:HB3	1:E:120:PRO:HD3	1.68	0.75
1:E:198:ARG:O	1:E:200:PRO:HD3	1.86	0.75
1:C:227:PHE:HA	1:C:230:ARG:HH11	1.51	0.75
1:H:293:ASP:HB2	1:H:296:ILE:HG22	1.68	0.75
1:E:72:TRP:CZ2	1:E:74:PRO:HG3	2.22	0.75
1:C:72:TRP:CZ2	1:C:74:PRO:HG3	2.22	0.75
1:C:215:ILE:O	1:C:218:SER:HB3	1.87	0.75
1:A:294:LEU:HA	1:A:297:GLN:NE2	2.02	0.74
1:G:44:THR:HA	1:G:99:ARG:HA	1.67	0.74
1:H:28:THR:HB	1:H:255:LEU:HD21	1.70	0.74
1:J:218:SER:HA	1:J:237:LEU:HD21	1.68	0.74
1:C:294:LEU:HA	1:C:297:GLN:HE21	1.51	0.74
1:E:215:ILE:O	1:E:218:SER:HB3	1.87	0.74
1:J:44:THR:HA	1:J:99:ARG:HA	1.67	0.74
1:J:256:PRO:HG2	1:J:257:TYR:CD1	2.22	0.74
1:H:72:TRP:CZ2	1:H:74:PRO:HG3	2.23	0.74
1:A:148:TYR:OH	1:B:176:HIS:NE2	2.20	0.74
1:H:215:ILE:O	1:H:218:SER:HB3	1.87	0.74
1:E:294:LEU:HA	1:E:297:GLN:NE2	2.02	0.74
1:J:294:LEU:HA	1:J:297:GLN:NE2	2.03	0.74
1:B:294:LEU:HA	1:B:297:GLN:HE21	1.52	0.74
1:D:218:SER:HA	1:D:237:LEU:HD21	1.69	0.74
1:B:223:TRP:NE1	1:B:300:ARG:HB3	2.03	0.74
1:D:294:LEU:HA	1:D:297:GLN:NE2	2.02	0.74
1:G:237:LEU:HD13	1:H:235:PHE:CD2	2.23	0.74
1:F:223:TRP:NE1	1:F:300:ARG:HB3	2.02	0.73
1:G:72:TRP:CZ2	1:G:74:PRO:HG3	2.22	0.73
1:A:256:PRO:HG2	1:A:257:TYR:CD1	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:123:ARG:HD2	1:E:197:VAL:HG22	1.70	0.73
1:F:218:SER:HA	1:F:237:LEU:HD21	1.68	0.73
1:G:198:ARG:O	1:G:200:PRO:HD3	1.87	0.73
1:I:148:TYR:OH	1:J:176:HIS:CE1	2.41	0.73
1:B:227:PHE:HA	1:B:230:ARG:HH11	1.52	0.73
1:D:28:THR:HB	1:D:255:LEU:HD21	1.70	0.73
1:A:39:ILE:HD11	1:A:78:PHE:CZ	2.23	0.73
1:A:227:PHE:HA	1:A:230:ARG:HH11	1.52	0.73
1:E:44:THR:HA	1:E:99:ARG:HA	1.70	0.73
1:F:44:THR:HA	1:F:99:ARG:HA	1.68	0.73
1:F:239:LEU:HD23	1:J:240:THR:HA	1.71	0.73
1:C:44:THR:HA	1:C:99:ARG:HA	1.71	0.73
1:D:164:LYS:HZ2	1:D:164:LYS:HA	1.54	0.73
1:G:91:ARG:HD2	1:H:134:SER:HB3	1.69	0.73
1:G:218:SER:HA	1:G:237:LEU:HD21	1.70	0.73
1:F:220:SER:HB2	1:G:280:ILE:HD13	1.71	0.73
1:D:223:TRP:NE1	1:D:300:ARG:HB3	2.02	0.72
1:D:227:PHE:HA	1:D:230:ARG:HH11	1.52	0.72
1:G:251:ILE:HG13	1:H:249:SER:HB3	1.71	0.72
1:B:173:ARG:NH2	1:I:139:GLN:HE22	1.87	0.72
1:F:237:LEU:HD13	1:G:235:PHE:CE2	2.24	0.72
1:H:164:LYS:HZ2	1:H:165:ALA:N	1.87	0.72
1:F:28:THR:HB	1:F:255:LEU:HD21	1.72	0.72
1:I:164:LYS:NZ	1:I:165:ALA:N	2.34	0.72
1:J:209:LEU:HB3	1:J:210:PRO:CD	2.20	0.72
1:D:119:PHE:HB3	1:D:120:PRO:HD3	1.72	0.72
1:G:227:PHE:HA	1:G:230:ARG:HH11	1.55	0.72
1:A:293:ASP:HB2	1:A:296:ILE:CG2	2.19	0.71
1:E:209:LEU:HB3	1:E:210:PRO:CD	2.20	0.71
1:F:294:LEU:HA	1:F:297:GLN:NE2	2.04	0.71
1:A:215:ILE:O	1:A:218:SER:HB3	1.90	0.71
1:C:123:ARG:HD2	1:C:197:VAL:HG22	1.73	0.71
1:I:227:PHE:HA	1:I:230:ARG:HH11	1.55	0.71
1:E:28:THR:HB	1:E:255:LEU:HD21	1.71	0.71
1:B:44:THR:HA	1:B:99:ARG:HA	1.72	0.71
1:E:39:ILE:HD11	1:E:78:PHE:CZ	2.25	0.71
1:J:162:ILE:HG22	1:J:163:ARG:H	1.54	0.71
1:A:78:PHE:HB3	1:A:81:VAL:HG23	1.71	0.71
1:D:91:ARG:HB2	1:E:133:PHE:CE2	2.26	0.71
1:F:227:PHE:HA	1:F:230:ARG:HH11	1.55	0.71
1:B:148:TYR:OH	1:C:176:HIS:NE2	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:226:SER:O	1:E:230:ARG:HD3	1.91	0.71
1:A:28:THR:HB	1:A:255:LEU:HD21	1.72	0.71
1:B:224:LEU:O	1:B:230:ARG:HD2	1.90	0.71
1:C:39:ILE:HD11	1:C:78:PHE:CZ	2.25	0.71
1:E:150:GLU:HB3	1:E:153:ASP:HB2	1.73	0.71
1:F:78:PHE:HB3	1:F:81:VAL:HG23	1.73	0.71
1:I:294:LEU:HA	1:I:297:GLN:NE2	2.06	0.71
1:E:78:PHE:HB3	1:E:81:VAL:HG23	1.73	0.70
1:H:209:LEU:HB3	1:H:210:PRO:CD	2.21	0.70
1:F:150:GLU:HB3	1:F:153:ASP:HB2	1.74	0.70
1:J:293:ASP:HB2	1:J:296:ILE:CG2	2.21	0.70
1:D:301:LEU:HD23	1:D:301:LEU:O	1.91	0.70
1:G:164:LYS:HA	1:G:164:LYS:HZ2	1.55	0.70
1:H:227:PHE:HA	1:H:230:ARG:HH11	1.57	0.70
1:I:28:THR:HB	1:I:255:LEU:HD21	1.72	0.70
1:H:52:GLY:O	1:H:53:ASP:HB2	1.91	0.70
1:H:294:LEU:HA	1:H:297:GLN:NE2	2.05	0.70
1:I:78:PHE:HB3	1:I:81:VAL:HG23	1.73	0.70
1:I:293:ASP:HB2	1:I:296:ILE:CG2	2.21	0.70
1:D:91:ARG:HD2	1:E:134:SER:HB3	1.74	0.70
1:E:301:LEU:O	1:E:301:LEU:HD23	1.91	0.70
1:F:254:ARG:O	1:F:255:LEU:HD23	1.91	0.70
1:A:162:ILE:HD12	1:A:162:ILE:N	2.07	0.70
1:I:148:TYR:CE2	1:J:176:HIS:NE2	2.60	0.69
1:D:224:LEU:O	1:D:230:ARG:HD2	1.92	0.69
1:H:226:SER:O	1:H:230:ARG:HD3	1.91	0.69
1:I:202:TYR:HB2	1:J:256:PRO:O	1.93	0.69
1:J:211:LEU:O	1:J:215:ILE:HG12	1.91	0.69
1:C:293:ASP:HB2	1:C:296:ILE:CG2	2.22	0.69
1:D:52:GLY:O	1:D:53:ASP:HB2	1.93	0.69
1:G:150:GLU:HB3	1:G:153:ASP:HB2	1.73	0.69
1:H:39:ILE:HD11	1:H:78:PHE:CZ	2.26	0.69
1:H:254:ARG:O	1:H:255:LEU:HD23	1.92	0.69
1:H:150:GLU:HB3	1:H:153:ASP:HB2	1.74	0.69
1:D:78:PHE:HB3	1:D:81:VAL:HG23	1.72	0.69
1:G:162:ILE:HD12	1:G:162:ILE:N	2.07	0.69
1:C:301:LEU:O	1:C:301:LEU:HD23	1.93	0.69
1:D:209:LEU:HB3	1:D:210:PRO:CD	2.23	0.69
1:I:148:TYR:HE2	1:J:176:HIS:HE2	1.38	0.69
1:E:52:GLY:O	1:E:53:ASP:HB2	1.92	0.69
1:F:301:LEU:O	1:F:301:LEU:HD23	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:39:ILE:HD11	1:J:78:PHE:CZ	2.28	0.69
1:D:150:GLU:HB3	1:D:153:ASP:HB2	1.75	0.69
1:B:215:ILE:O	1:B:218:SER:HB3	1.93	0.69
1:D:226:SER:O	1:D:230:ARG:HD3	1.93	0.69
1:A:150:GLU:HB3	1:A:153:ASP:HB2	1.74	0.68
1:C:150:GLU:HB3	1:C:153:ASP:HB2	1.73	0.68
1:E:293:ASP:HB2	1:E:296:ILE:CG2	2.23	0.68
1:G:215:ILE:O	1:G:218:SER:HB3	1.93	0.68
1:J:150:GLU:HB3	1:J:153:ASP:HB2	1.73	0.68
1:B:209:LEU:HB3	1:B:210:PRO:CD	2.24	0.68
1:I:218:SER:HA	1:I:237:LEU:HD21	1.74	0.68
1:B:218:SER:HA	1:B:237:LEU:HD21	1.73	0.68
1:H:167:THR:HG22	1:H:168:HIS:N	2.07	0.68
1:J:162:ILE:N	1:J:162:ILE:HD12	2.08	0.68
1:B:72:TRP:CZ2	1:B:74:PRO:HG3	2.28	0.68
1:B:167:THR:HG22	1:B:168:HIS:N	2.08	0.68
1:D:72:TRP:O	1:D:72:TRP:CD1	2.47	0.68
1:E:227:PHE:HA	1:E:230:ARG:NH1	2.08	0.68
1:G:240:THR:HA	1:H:239:LEU:HD23	1.75	0.68
1:I:167:THR:HG22	1:I:168:HIS:N	2.08	0.68
1:G:78:PHE:HB3	1:G:81:VAL:HG23	1.76	0.68
1:E:164:LYS:HZ3	1:E:164:LYS:HA	1.59	0.68
1:I:164:LYS:HZ2	1:I:165:ALA:H	1.42	0.68
1:A:123:ARG:HD2	1:A:197:VAL:HG22	1.74	0.68
1:B:39:ILE:HD11	1:B:78:PHE:CZ	2.29	0.68
1:A:52:GLY:O	1:A:53:ASP:HB2	1.94	0.68
1:A:301:LEU:HD23	1:A:301:LEU:O	1.94	0.68
1:B:167:THR:O	1:B:168:HIS:HB2	1.94	0.68
1:E:218:SER:HA	1:E:237:LEU:HD21	1.74	0.68
1:G:167:THR:O	1:G:168:HIS:HB2	1.93	0.68
1:A:202:TYR:HB2	1:B:256:PRO:O	1.94	0.67
1:A:226:SER:O	1:A:230:ARG:HD3	1.94	0.67
1:B:150:GLU:HB3	1:B:153:ASP:HB2	1.75	0.67
1:C:226:SER:O	1:C:230:ARG:HD3	1.93	0.67
1:C:294:LEU:HA	1:C:297:GLN:NE2	2.08	0.67
1:G:293:ASP:HB2	1:G:296:ILE:CG2	2.23	0.67
1:B:28:THR:HB	1:B:255:LEU:HD21	1.76	0.67
1:C:209:LEU:HB3	1:C:210:PRO:CD	2.24	0.67
1:D:164:LYS:NZ	1:D:165:ALA:N	2.36	0.67
1:G:127:VAL:O	1:G:128:LEU:HD12	1.93	0.67
1:H:78:PHE:HB3	1:H:81:VAL:HG23	1.74	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:PRO:HG2	1:B:257:TYR:CD1	2.29	0.67
1:B:294:LEU:HA	1:B:297:GLN:NE2	2.09	0.67
1:C:91:ARG:CD	1:D:134:SER:HB3	2.25	0.67
1:D:293:ASP:HB2	1:D:296:ILE:CG2	2.24	0.67
1:F:123:ARG:HD2	1:F:197:VAL:HG22	1.77	0.67
1:G:72:TRP:HZ3	1:G:135:TYR:CZ	2.11	0.67
1:F:157:ILE:HD11	1:G:115:ASP:OD2	1.94	0.67
1:F:293:ASP:HB2	1:F:296:ILE:CG2	2.24	0.67
1:A:148:TYR:CE2	1:B:176:HIS:NE2	2.62	0.67
1:D:211:LEU:O	1:D:215:ILE:HG12	1.95	0.67
1:B:256:PRO:HG2	1:B:257:TYR:HD1	1.59	0.67
1:I:150:GLU:HB3	1:I:153:ASP:HB2	1.75	0.67
1:J:259:THR:O	1:J:263:GLN:HG3	1.95	0.67
1:A:218:SER:HA	1:A:237:LEU:HD21	1.77	0.66
1:E:72:TRP:HZ3	1:E:135:TYR:CZ	2.12	0.66
1:B:226:SER:O	1:B:230:ARG:HD3	1.95	0.66
1:G:52:GLY:O	1:G:53:ASP:HB2	1.96	0.66
1:F:211:LEU:O	1:F:215:ILE:HG12	1.96	0.66
1:J:78:PHE:HB3	1:J:81:VAL:HG23	1.77	0.66
1:B:293:ASP:HB2	1:B:296:ILE:CG2	2.24	0.66
1:H:293:ASP:HB2	1:H:296:ILE:CG2	2.25	0.66
1:B:123:ARG:HD2	1:B:197:VAL:HG22	1.76	0.66
1:H:301:LEU:O	1:H:301:LEU:HD23	1.96	0.66
1:A:115:ASP:OD2	1:E:157:ILE:HD11	1.95	0.66
1:A:254:ARG:O	1:A:255:LEU:HD23	1.96	0.66
1:D:127:VAL:O	1:D:128:LEU:HD12	1.96	0.66
1:D:220:SER:HB2	1:E:280:ILE:HD13	1.76	0.66
1:F:247:TYR:CE1	1:G:245:ALA:HB1	2.30	0.66
1:I:301:LEU:HD23	1:I:301:LEU:O	1.95	0.66
1:D:155:GLU:HB3	1:D:161:TRP:CD1	2.31	0.66
1:J:301:LEU:HD23	1:J:301:LEU:O	1.95	0.66
1:B:301:LEU:HD23	1:B:301:LEU:O	1.96	0.65
1:J:72:TRP:HZ3	1:J:135:TYR:CZ	2.14	0.65
1:B:226:SER:HB3	1:B:229:GLU:HG3	1.77	0.65
1:B:247:TYR:HE1	1:C:249:SER:HG	1.42	0.65
1:H:239:LEU:CD1	1:I:239:LEU:HD21	2.26	0.65
1:H:72:TRP:HZ3	1:H:135:TYR:CZ	2.14	0.65
1:I:226:SER:HB3	1:I:229:GLU:HG3	1.78	0.65
1:A:209:LEU:HB3	1:A:210:PRO:CD	2.26	0.65
1:B:169:ILE:HB	1:I:168:HIS:ND1	2.12	0.65
1:J:226:SER:O	1:J:230:ARG:HD3	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:TYR:CZ	1:B:176:HIS:NE2	2.65	0.65
1:A:204:LEU:HD23	1:A:208:ILE:HG13	1.78	0.65
1:B:162:ILE:N	1:B:162:ILE:HD12	2.10	0.65
1:E:167:THR:HG22	1:E:168:HIS:N	2.08	0.65
1:A:259:THR:O	1:A:263:GLN:HG3	1.97	0.65
1:J:78:PHE:HB3	1:J:81:VAL:CG2	2.27	0.65
1:A:162:ILE:HD12	1:A:162:ILE:H	1.61	0.65
1:E:254:ARG:O	1:E:255:LEU:HD23	1.96	0.65
1:G:254:ARG:O	1:G:255:LEU:HD23	1.96	0.65
1:H:204:LEU:HD23	1:H:208:ILE:HG13	1.79	0.65
1:H:226:SER:HB3	1:H:229:GLU:HG3	1.79	0.64
1:H:239:LEU:HD13	1:I:239:LEU:HD21	1.79	0.64
1:D:237:LEU:HD13	1:E:235:PHE:CE2	2.31	0.64
1:G:204:LEU:HD23	1:G:208:ILE:HG13	1.79	0.64
1:G:226:SER:HB3	1:G:229:GLU:HG3	1.78	0.64
1:G:301:LEU:HD23	1:G:301:LEU:O	1.97	0.64
1:A:78:PHE:HB3	1:A:81:VAL:CG2	2.27	0.64
1:D:254:ARG:O	1:D:255:LEU:HD23	1.97	0.64
1:F:209:LEU:HB3	1:F:210:PRO:CD	2.28	0.64
1:F:91:ARG:HB2	1:G:133:PHE:HE2	1.60	0.64
1:D:78:PHE:HB3	1:D:81:VAL:CG2	2.28	0.64
1:D:247:TYR:CE1	1:E:245:ALA:HB1	2.33	0.64
1:G:209:LEU:HB3	1:G:210:PRO:CD	2.26	0.64
1:H:211:LEU:O	1:H:215:ILE:HG12	1.96	0.64
1:I:52:GLY:O	1:I:53:ASP:HB2	1.97	0.64
1:E:204:LEU:HD23	1:E:208:ILE:HG13	1.80	0.64
1:I:72:TRP:HZ3	1:I:135:TYR:CZ	2.15	0.64
1:A:247:TYR:HE1	1:B:249:SER:HG	1.46	0.64
1:F:134:SER:HB3	1:J:91:ARG:CD	2.28	0.64
1:H:112:ASN:OD1	1:H:113:ASP:N	2.30	0.64
1:J:227:PHE:HA	1:J:230:ARG:NH1	2.13	0.64
1:J:254:ARG:O	1:J:255:LEU:HD23	1.98	0.64
1:C:72:TRP:HZ3	1:C:135:TYR:CZ	2.16	0.64
1:C:254:ARG:O	1:C:255:LEU:HD23	1.96	0.64
1:E:226:SER:HB3	1:E:229:GLU:HG3	1.80	0.64
1:H:224:LEU:O	1:H:230:ARG:HD2	1.97	0.64
1:I:254:ARG:O	1:I:255:LEU:HD23	1.98	0.64
1:A:167:THR:HG22	1:A:168:HIS:N	2.10	0.64
1:E:78:PHE:HB3	1:E:81:VAL:CG2	2.28	0.64
1:F:162:ILE:HD12	1:F:162:ILE:N	2.12	0.64
1:D:226:SER:HB3	1:D:229:GLU:HG3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:237:LEU:HD13	1:D:235:PHE:CD2	2.33	0.63
1:H:78:PHE:HB3	1:H:81:VAL:CG2	2.29	0.63
1:D:227:PHE:HA	1:D:230:ARG:NH1	2.14	0.63
1:D:39:ILE:HD11	1:D:78:PHE:CZ	2.32	0.63
1:F:78:PHE:HB3	1:F:81:VAL:CG2	2.28	0.63
1:F:164:LYS:HZ2	1:F:165:ALA:H	0.80	0.63
1:G:123:ARG:HD2	1:G:197:VAL:HG22	1.78	0.63
1:I:164:LYS:HZ2	1:I:164:LYS:CA	2.12	0.63
1:B:227:PHE:HA	1:B:230:ARG:NH1	2.13	0.63
1:C:226:SER:HB3	1:C:229:GLU:HG3	1.81	0.63
1:B:224:LEU:HB2	1:B:230:ARG:HG3	1.79	0.63
1:G:91:ARG:HB2	1:H:133:PHE:CE2	2.34	0.63
1:I:39:ILE:HD11	1:I:78:PHE:CZ	2.32	0.63
1:D:123:ARG:HD2	1:D:197:VAL:HG22	1.80	0.63
1:B:204:LEU:HD23	1:B:208:ILE:HG13	1.79	0.63
1:E:162:ILE:N	1:E:162:ILE:HD12	2.14	0.63
1:G:226:SER:O	1:G:230:ARG:HD3	1.98	0.63
1:A:231:LEU:HD23	1:A:231:LEU:C	2.19	0.62
1:A:288:ASN:CG	1:A:289:GLY:N	2.52	0.62
1:F:231:LEU:HD23	1:F:231:LEU:C	2.20	0.62
1:G:91:ARG:CD	1:H:134:SER:HB3	2.28	0.62
1:B:223:TRP:CE3	1:C:280:ILE:HG22	2.34	0.62
1:G:162:ILE:HD12	1:G:162:ILE:H	1.61	0.62
1:B:148:TYR:OH	1:C:176:HIS:CE1	2.52	0.62
1:C:52:GLY:O	1:C:53:ASP:HB2	1.97	0.62
1:G:127:VAL:C	1:G:128:LEU:HD12	2.19	0.62
1:C:78:PHE:HB3	1:C:81:VAL:HG23	1.80	0.62
1:D:59:GLU:O	1:D:63:ILE:HG13	1.99	0.62
1:F:72:TRP:CH2	1:F:74:PRO:HG3	2.34	0.62
1:F:220:SER:HB2	1:G:280:ILE:CD1	2.30	0.62
1:I:169:ILE:HD12	1:I:190:ILE:HG12	1.82	0.62
1:A:134:SER:HB3	1:E:91:ARG:CD	2.29	0.62
1:D:251:ILE:HG13	1:E:249:SER:HB3	1.80	0.62
1:F:52:GLY:O	1:F:53:ASP:HB2	1.99	0.62
1:G:224:LEU:O	1:G:230:ARG:HD2	1.98	0.62
1:J:162:ILE:HD12	1:J:162:ILE:H	1.63	0.62
1:A:249:SER:HB3	1:E:251:ILE:CG1	2.29	0.62
1:F:167:THR:HG22	1:F:168:HIS:N	2.14	0.62
1:G:169:ILE:HD12	1:G:190:ILE:HG12	1.82	0.62
1:A:226:SER:HB3	1:A:229:GLU:HG3	1.82	0.62
1:A:280:ILE:CD1	1:E:220:SER:HB2	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:56:LEU:HD13	1:D:57:ILE:N	2.15	0.62
1:F:162:ILE:HD12	1:F:162:ILE:H	1.65	0.62
1:B:127:VAL:O	1:B:128:LEU:HD12	2.00	0.62
1:F:226:SER:HB3	1:F:229:GLU:HG3	1.80	0.62
1:G:167:THR:O	1:G:168:HIS:CB	2.48	0.62
1:A:72:TRP:CH2	1:A:74:PRO:HG3	2.35	0.61
1:A:227:PHE:HA	1:A:230:ARG:NH1	2.15	0.61
1:C:162:ILE:HD12	1:C:162:ILE:N	2.15	0.61
1:C:211:LEU:O	1:C:215:ILE:HG12	2.00	0.61
1:F:239:LEU:CD2	1:J:240:THR:HA	2.31	0.61
1:I:224:LEU:O	1:I:230:ARG:HD2	2.00	0.61
1:D:162:ILE:HD12	1:D:162:ILE:N	2.14	0.61
1:E:224:LEU:O	1:E:230:ARG:HD2	2.01	0.61
1:G:227:PHE:HA	1:G:230:ARG:NH1	2.15	0.61
1:C:227:PHE:HA	1:C:230:ARG:NH1	2.14	0.61
1:F:224:LEU:O	1:F:230:ARG:HD2	2.00	0.61
1:I:231:LEU:HD23	1:I:231:LEU:C	2.20	0.61
1:I:288:ASN:CG	1:I:289:GLY:N	2.54	0.61
1:J:204:LEU:HD23	1:J:208:ILE:HG13	1.83	0.61
1:J:288:ASN:CG	1:J:289:GLY:N	2.54	0.61
1:I:226:SER:O	1:I:230:ARG:HD3	2.01	0.61
1:J:167:THR:HG22	1:J:168:HIS:N	2.13	0.61
1:C:78:PHE:HB3	1:C:81:VAL:CG2	2.30	0.61
1:G:219:TRP:C	1:G:221:VAL:H	2.04	0.61
1:A:112:ASN:OD1	1:A:113:ASP:N	2.34	0.61
1:C:204:LEU:HD23	1:C:208:ILE:HG13	1.82	0.61
1:I:148:TYR:OH	1:J:176:HIS:NE2	2.33	0.61
1:B:52:GLY:O	1:B:53:ASP:HB2	1.99	0.61
1:B:202:TYR:HB2	1:C:256:PRO:O	2.00	0.61
1:C:224:LEU:O	1:C:230:ARG:HD2	2.00	0.61
1:F:39:ILE:HD11	1:F:78:PHE:CZ	2.36	0.61
1:B:251:ILE:HG13	1:C:249:SER:HB3	1.82	0.61
1:E:211:LEU:O	1:E:215:ILE:HG12	2.01	0.61
1:H:288:ASN:CG	1:H:289:GLY:N	2.54	0.61
1:B:288:ASN:CG	1:B:289:GLY:N	2.54	0.60
1:D:288:ASN:CG	1:D:289:GLY:N	2.55	0.60
1:E:155:GLU:HB3	1:E:161:TRP:CD1	2.34	0.60
1:F:240:THR:HA	1:G:239:LEU:HD23	1.83	0.60
1:F:288:ASN:CG	1:F:289:GLY:N	2.54	0.60
1:J:155:GLU:HB3	1:J:161:TRP:CD1	2.36	0.60
1:C:155:GLU:HB3	1:C:161:TRP:CD1	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:162:ILE:HD12	1:I:162:ILE:N	2.16	0.60
1:D:162:ILE:HD12	1:D:162:ILE:H	1.66	0.60
1:D:224:LEU:HB2	1:D:230:ARG:HG3	1.84	0.60
1:J:210:PRO:O	1:J:214:ILE:HG12	2.00	0.60
1:D:259:THR:O	1:D:263:GLN:HG3	2.02	0.60
1:E:288:ASN:CG	1:E:289:GLY:N	2.54	0.60
1:F:169:ILE:HD12	1:F:190:ILE:HG12	1.84	0.60
1:F:255:LEU:HB3	1:F:256:PRO:HD2	1.83	0.60
1:G:72:TRP:CD1	1:G:72:TRP:O	2.55	0.60
1:H:72:TRP:O	1:H:72:TRP:CD1	2.55	0.60
1:A:210:PRO:O	1:A:214:ILE:HG12	2.01	0.60
1:B:72:TRP:HZ3	1:B:135:TYR:CZ	2.19	0.60
1:B:162:ILE:HD12	1:B:162:ILE:H	1.66	0.60
1:F:91:ARG:HB2	1:G:133:PHE:CE2	2.35	0.60
1:F:239:LEU:HD23	1:J:240:THR:OG1	2.01	0.60
1:G:39:ILE:HD11	1:G:78:PHE:CZ	2.35	0.60
1:J:226:SER:HB3	1:J:229:GLU:HG3	1.83	0.60
1:A:211:LEU:O	1:A:215:ILE:HG12	2.01	0.60
1:C:288:ASN:CG	1:C:289:GLY:N	2.54	0.60
1:I:211:LEU:O	1:I:215:ILE:HG12	2.01	0.60
1:J:51:PRO:HD2	1:J:56:LEU:HD23	1.83	0.60
1:D:72:TRP:HZ3	1:D:135:TYR:CZ	2.20	0.60
1:D:112:ASN:OD1	1:D:113:ASP:N	2.35	0.60
1:F:226:SER:O	1:F:230:ARG:HD3	2.02	0.60
1:J:231:LEU:C	1:J:231:LEU:HD23	2.22	0.60
1:B:65:ARG:HD2	1:C:68:ASN:ND2	2.16	0.60
1:B:164:LYS:HZ2	1:B:164:LYS:HA	1.67	0.60
1:D:72:TRP:CH2	1:D:74:PRO:HG3	2.37	0.60
1:A:269:TYR:CD2	1:E:210:PRO:HB3	2.36	0.59
1:F:251:ILE:HG13	1:G:249:SER:HB3	1.81	0.59
1:G:91:ARG:HD2	1:H:134:SER:CB	2.31	0.59
1:H:155:GLU:HB3	1:H:161:TRP:CD1	2.37	0.59
1:I:78:PHE:HB3	1:I:81:VAL:CG2	2.33	0.59
1:J:127:VAL:O	1:J:128:LEU:HD12	2.02	0.59
1:A:148:TYR:HE2	1:B:176:HIS:HE2	1.49	0.59
1:D:255:LEU:HB3	1:D:256:PRO:HD2	1.84	0.59
1:G:211:LEU:O	1:G:215:ILE:HG12	2.02	0.59
1:A:280:ILE:HG22	1:E:223:TRP:CE3	2.37	0.59
1:A:240:THR:OG1	1:B:239:LEU:HD23	2.03	0.59
1:C:240:THR:HA	1:D:239:LEU:HD23	1.83	0.59
1:D:185:ASN:N	1:D:185:ASN:HD22	2.00	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:72:TRP:HZ3	1:F:135:TYR:CZ	2.20	0.59
1:F:259:THR:O	1:F:263:GLN:HG3	2.03	0.59
1:I:290:VAL:O	1:I:290:VAL:HG12	2.02	0.59
1:A:155:GLU:HB3	1:A:161:TRP:CD1	2.37	0.59
1:B:112:ASN:OD1	1:B:113:ASP:N	2.36	0.59
1:G:288:ASN:CG	1:G:289:GLY:N	2.52	0.59
1:I:123:ARG:HD2	1:I:197:VAL:HG22	1.85	0.59
1:I:224:LEU:HB2	1:I:230:ARG:HG3	1.84	0.59
1:B:127:VAL:C	1:B:128:LEU:HD12	2.23	0.59
1:C:51:PRO:HD2	1:C:56:LEU:HD23	1.85	0.59
1:F:134:SER:CB	1:J:91:ARG:HD2	2.32	0.59
1:H:145:ILE:HD12	1:H:145:ILE:N	2.17	0.59
1:F:134:SER:HB3	1:J:91:ARG:HD2	1.84	0.58
1:A:235:PHE:HD2	1:E:237:LEU:HD13	1.65	0.58
1:D:231:LEU:HD23	1:D:231:LEU:C	2.24	0.58
1:G:210:PRO:HB3	1:H:269:TYR:CD2	2.37	0.58
1:I:185:ASN:N	1:I:185:ASN:HD22	2.00	0.58
1:B:155:GLU:HB3	1:B:161:TRP:CD1	2.38	0.58
1:F:155:GLU:HB3	1:F:161:TRP:CD1	2.38	0.58
1:A:285:ARG:HA	1:A:285:ARG:NE	2.18	0.58
1:A:290:VAL:O	1:A:290:VAL:HG12	2.04	0.58
1:B:107:LEU:HD23	1:C:83:GLY:HA2	1.85	0.58
1:D:72:TRP:CD1	1:D:72:TRP:C	2.76	0.58
1:F:227:PHE:HA	1:F:230:ARG:NH1	2.19	0.58
1:G:155:GLU:HB3	1:G:161:TRP:CD1	2.38	0.58
1:A:127:VAL:O	1:A:128:LEU:HD12	2.04	0.58
1:B:78:PHE:HB3	1:B:81:VAL:HG23	1.86	0.58
1:C:72:TRP:O	1:C:72:TRP:CD1	2.55	0.58
1:E:162:ILE:HD12	1:E:162:ILE:H	1.67	0.58
1:G:285:ARG:NE	1:G:285:ARG:HA	2.17	0.58
1:H:162:ILE:N	1:H:162:ILE:HD12	2.18	0.58
1:I:72:TRP:O	1:I:72:TRP:CD1	2.57	0.58
1:I:227:PHE:HA	1:I:230:ARG:NH1	2.17	0.58
1:J:52:GLY:O	1:J:53:ASP:HB2	2.02	0.58
1:E:185:ASN:HD22	1:E:185:ASN:N	1.99	0.58
1:D:91:ARG:CD	1:E:134:SER:HB3	2.34	0.58
1:F:224:LEU:HB2	1:F:230:ARG:HG3	1.86	0.58
1:I:285:ARG:HA	1:I:285:ARG:NE	2.19	0.58
1:J:224:LEU:HB2	1:J:230:ARG:HG3	1.86	0.58
1:A:231:LEU:HD22	1:E:224:LEU:HD21	1.86	0.58
1:F:112:ASN:OD1	1:F:113:ASP:N	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:174:TYR:O	1:H:177:LEU:HD11	2.04	0.58
1:C:162:ILE:HD12	1:C:162:ILE:H	1.68	0.58
1:H:148:TYR:OH	1:I:176:HIS:NE2	2.36	0.58
1:I:204:LEU:HD23	1:I:208:ILE:HG13	1.86	0.58
1:A:140:LEU:HD22	1:A:190:ILE:HD11	1.86	0.58
1:A:299:CYS:HB2	1:A:302:ALA:CB	2.34	0.58
1:C:91:ARG:HD2	1:D:134:SER:HB3	1.85	0.58
1:C:251:ILE:HG13	1:D:249:SER:HB3	1.84	0.58
1:E:290:VAL:O	1:E:290:VAL:HG12	2.04	0.58
1:C:285:ARG:NE	1:C:285:ARG:HA	2.18	0.57
1:H:290:VAL:O	1:H:290:VAL:HG12	2.04	0.57
1:F:64:GLU:HG3	1:J:61:THR:HG21	1.84	0.57
1:G:299:CYS:HB2	1:G:302:ALA:CB	2.34	0.57
1:A:224:LEU:O	1:A:230:ARG:HD2	2.05	0.57
1:C:185:ASN:HD22	1:C:185:ASN:N	2.03	0.57
1:C:231:LEU:HD23	1:C:231:LEU:C	2.24	0.57
1:D:290:VAL:O	1:D:290:VAL:HG12	2.04	0.57
1:E:127:VAL:O	1:E:128:LEU:HD12	2.04	0.57
1:F:51:PRO:HD2	1:F:56:LEU:HD23	1.85	0.57
1:G:290:VAL:O	1:G:290:VAL:HG12	2.04	0.57
1:H:164:LYS:HZ2	1:H:164:LYS:HA	1.70	0.57
1:B:169:ILE:HD12	1:B:190:ILE:HG12	1.86	0.57
1:E:231:LEU:C	1:E:231:LEU:HD23	2.25	0.57
1:F:204:LEU:HD23	1:F:208:ILE:HG13	1.87	0.57
1:A:133:PHE:HE2	1:E:91:ARG:HB2	1.69	0.57
1:C:224:LEU:HB2	1:C:230:ARG:HG3	1.87	0.57
1:H:91:ARG:CD	1:I:134:SER:HB3	2.35	0.57
1:B:173:ARG:NH2	1:I:139:GLN:NE2	2.43	0.57
1:C:112:ASN:OD1	1:C:113:ASP:N	2.37	0.57
1:F:305:LEU:C	1:F:305:LEU:HD12	2.25	0.57
1:J:145:ILE:HD12	1:J:145:ILE:N	2.13	0.57
1:B:240:THR:HA	1:C:239:LEU:HD23	1.85	0.57
1:D:240:THR:HA	1:E:239:LEU:HD23	1.86	0.57
1:F:290:VAL:O	1:F:290:VAL:HG12	2.04	0.57
1:H:251:ILE:HG13	1:I:249:SER:HB3	1.87	0.57
1:C:91:ARG:HD2	1:D:134:SER:CB	2.35	0.57
1:C:223:TRP:CE2	1:C:300:ARG:HD3	2.40	0.57
1:H:227:PHE:HA	1:H:230:ARG:NH1	2.18	0.57
1:A:59:GLU:O	1:A:63:ILE:HG13	2.05	0.57
1:B:23:ILE:HG21	1:B:126:PHE:CD2	2.41	0.56
1:C:255:LEU:HB3	1:C:256:PRO:HD2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:290:VAL:HG12	1:C:290:VAL:O	2.04	0.56
1:F:72:TRP:O	1:F:72:TRP:CD1	2.58	0.56
1:J:255:LEU:HB3	1:J:256:PRO:HD2	1.86	0.56
1:J:290:VAL:O	1:J:290:VAL:HG12	2.04	0.56
1:A:56:LEU:HD13	1:A:57:ILE:N	2.20	0.56
1:A:65:ARG:HD2	1:B:68:ASN:ND2	2.20	0.56
1:B:167:THR:O	1:B:168:HIS:CB	2.51	0.56
1:D:167:THR:HG22	1:D:168:HIS:N	2.19	0.56
1:G:167:THR:HG22	1:G:168:HIS:N	2.17	0.56
1:G:259:THR:O	1:G:263:GLN:HG3	2.05	0.56
1:I:59:GLU:O	1:I:63:ILE:HG13	2.05	0.56
1:B:115:ASP:H	1:B:124:GLN:HE22	1.53	0.56
1:B:290:VAL:O	1:B:290:VAL:HG12	2.04	0.56
1:E:112:ASN:OD1	1:E:113:ASP:N	2.38	0.56
1:G:112:ASN:OD1	1:G:113:ASP:N	2.38	0.56
1:G:224:LEU:HB2	1:G:230:ARG:HG3	1.85	0.56
1:B:211:LEU:O	1:B:215:ILE:HG12	2.05	0.56
1:B:223:TRP:CE3	1:C:280:ILE:CG2	2.88	0.56
1:G:185:ASN:HD22	1:G:185:ASN:N	2.02	0.56
1:B:305:LEU:C	1:B:305:LEU:HD12	2.26	0.56
1:D:305:LEU:C	1:D:305:LEU:HD12	2.26	0.56
1:E:305:LEU:HD12	1:E:305:LEU:C	2.26	0.56
1:F:285:ARG:NE	1:F:285:ARG:HA	2.21	0.56
1:H:231:LEU:HD23	1:H:231:LEU:C	2.26	0.56
1:H:252:LEU:HG	1:H:253:PRO:HD2	1.87	0.56
1:A:167:THR:O	1:A:168:HIS:HB2	2.05	0.56
1:E:224:LEU:HB2	1:E:230:ARG:HG3	1.88	0.56
1:E:262:ASP:O	1:E:266:ILE:HG12	2.06	0.56
1:F:299:CYS:HB2	1:F:302:ALA:CB	2.36	0.56
1:H:145:ILE:HG21	1:H:192:VAL:HG11	1.88	0.56
1:I:127:VAL:O	1:I:128:LEU:HD12	2.05	0.56
1:A:262:ASP:O	1:A:266:ILE:HG12	2.06	0.56
1:G:294:LEU:CA	1:G:297:GLN:HE21	2.18	0.56
1:I:174:TYR:O	1:I:177:LEU:HD11	2.06	0.56
1:J:112:ASN:OD1	1:J:113:ASP:N	2.39	0.56
1:J:285:ARG:NE	1:J:285:ARG:HA	2.20	0.56
1:D:204:LEU:HD23	1:D:208:ILE:HG13	1.86	0.56
1:G:237:LEU:HD13	1:H:235:PHE:HD2	1.68	0.56
1:I:148:TYR:CZ	1:J:176:HIS:NE2	2.73	0.56
1:J:223:TRP:CE2	1:J:300:ARG:HD3	2.41	0.56
1:B:226:SER:HB3	1:B:229:GLU:CG	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:LEU:C	1:A:305:LEU:HD12	2.27	0.55
1:B:164:LYS:HZ2	1:B:164:LYS:CA	2.18	0.55
1:C:259:THR:O	1:C:263:GLN:HG3	2.06	0.55
1:E:285:ARG:NE	1:E:285:ARG:HA	2.21	0.55
1:B:173:ARG:HH22	1:I:139:GLN:CD	2.09	0.55
1:I:209:LEU:HB3	1:I:210:PRO:HD3	1.85	0.55
1:D:285:ARG:HA	1:D:285:ARG:NE	2.21	0.55
1:G:199:ASN:HD22	1:G:199:ASN:C	2.10	0.55
1:H:56:LEU:HD13	1:H:57:ILE:N	2.21	0.55
1:H:202:TYR:HB2	1:I:256:PRO:O	2.05	0.55
1:H:255:LEU:HB3	1:H:256:PRO:HD2	1.88	0.55
1:J:231:LEU:HD23	1:J:232:GLN:N	2.21	0.55
1:F:303:PHE:N	1:F:304:PRO:CD	2.70	0.55
1:I:162:ILE:HD12	1:I:162:ILE:H	1.69	0.55
1:G:78:PHE:HB3	1:G:81:VAL:CG2	2.36	0.55
1:B:259:THR:O	1:B:263:GLN:HG3	2.07	0.55
1:D:127:VAL:C	1:D:128:LEU:HD12	2.26	0.55
1:G:164:LYS:NZ	1:G:165:ALA:N	2.41	0.55
1:I:299:CYS:HB2	1:I:302:ALA:CB	2.37	0.55
1:J:164:LYS:HZ2	1:J:164:LYS:HA	1.71	0.55
1:A:185:ASN:N	1:A:185:ASN:HD22	2.05	0.55
1:D:51:PRO:HD2	1:D:56:LEU:HD23	1.89	0.55
1:D:57:ILE:HD13	1:E:134:SER:O	2.06	0.55
1:H:59:GLU:O	1:H:63:ILE:HG13	2.07	0.55
1:H:210:PRO:O	1:H:214:ILE:HG12	2.06	0.55
1:H:224:LEU:HB2	1:H:230:ARG:HG3	1.89	0.55
1:B:78:PHE:HB3	1:B:81:VAL:CG2	2.37	0.55
1:F:185:ASN:HD22	1:F:185:ASN:N	2.04	0.55
1:H:223:TRP:CE2	1:H:300:ARG:HD3	2.42	0.55
1:J:224:LEU:O	1:J:230:ARG:HD2	2.07	0.55
1:B:72:TRP:CD1	1:B:72:TRP:O	2.60	0.54
1:E:72:TRP:CD1	1:E:72:TRP:O	2.59	0.54
1:G:65:ARG:HD2	1:H:68:ASN:ND2	2.22	0.54
1:H:162:ILE:HG22	1:H:163:ARG:N	2.16	0.54
1:H:299:CYS:HB2	1:H:302:ALA:CB	2.37	0.54
1:I:210:PRO:O	1:I:214:ILE:HG12	2.06	0.54
1:I:280:ILE:O	1:I:280:ILE:HG22	2.07	0.54
1:D:299:CYS:HB2	1:D:302:ALA:CB	2.38	0.54
1:H:162:ILE:HD12	1:H:162:ILE:H	1.71	0.54
1:H:259:THR:O	1:H:263:GLN:HG3	2.08	0.54
1:I:259:THR:O	1:I:263:GLN:HG3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:167:THR:O	1:J:168:HIS:HB2	2.08	0.54
1:J:280:ILE:HG22	1:J:280:ILE:O	2.08	0.54
1:B:51:PRO:HD2	1:B:56:LEU:HD23	1.87	0.54
1:B:174:TYR:O	1:B:177:LEU:HD11	2.07	0.54
1:C:167:THR:HG22	1:C:168:HIS:N	2.19	0.54
1:F:231:LEU:HD23	1:F:232:GLN:N	2.21	0.54
1:F:262:ASP:O	1:F:266:ILE:HG12	2.07	0.54
1:G:23:ILE:HG21	1:G:126:PHE:CD2	2.43	0.54
1:G:147:VAL:CG2	1:G:165:ALA:HB2	2.37	0.54
1:G:231:LEU:HD23	1:G:231:LEU:C	2.27	0.54
1:A:239:LEU:HD13	1:B:239:LEU:HD21	1.89	0.54
1:E:56:LEU:HD13	1:E:57:ILE:N	2.21	0.54
1:E:210:PRO:O	1:E:214:ILE:HG12	2.08	0.54
1:F:219:TRP:C	1:F:221:VAL:H	2.11	0.54
1:E:299:CYS:HB2	1:E:302:ALA:CB	2.37	0.54
1:B:185:ASN:HD22	1:B:185:ASN:N	2.05	0.54
1:B:285:ARG:NE	1:B:285:ARG:HA	2.22	0.54
1:G:255:LEU:HB3	1:G:256:PRO:HD2	1.90	0.54
1:A:72:TRP:HZ3	1:A:135:TYR:CZ	2.25	0.54
1:F:91:ARG:HD2	1:G:134:SER:HB3	1.89	0.54
1:H:285:ARG:NE	1:H:285:ARG:HA	2.23	0.54
1:I:226:SER:HB3	1:I:229:GLU:CG	2.38	0.54
1:I:155:GLU:HB3	1:I:161:TRP:CD1	2.43	0.54
1:A:134:SER:HB3	1:E:91:ARG:HD2	1.89	0.54
1:B:145:ILE:HD12	1:B:145:ILE:N	2.16	0.54
1:E:145:ILE:HD12	1:E:145:ILE:N	2.19	0.54
1:G:48:ARG:HB2	1:G:48:ARG:CZ	2.38	0.54
1:H:296:ILE:HG23	1:H:297:GLN:N	2.23	0.54
1:A:72:TRP:O	1:A:72:TRP:CD1	2.61	0.53
1:C:305:LEU:C	1:C:305:LEU:HD12	2.29	0.53
1:I:164:LYS:HZ2	1:I:165:ALA:N	2.02	0.53
1:J:72:TRP:CH2	1:J:74:PRO:HG3	2.42	0.53
1:B:240:THR:OG1	1:C:239:LEU:HD23	2.08	0.53
1:B:254:ARG:O	1:B:255:LEU:HD23	2.09	0.53
1:E:305:LEU:HD12	1:E:306:GLY:N	2.24	0.53
1:H:185:ASN:HD22	1:H:185:ASN:N	2.05	0.53
1:H:305:LEU:C	1:H:305:LEU:HD12	2.28	0.53
1:I:145:ILE:H	1:I:145:ILE:CD1	2.13	0.53
1:A:134:SER:CB	1:E:91:ARG:HD2	2.38	0.53
1:F:91:ARG:CD	1:G:134:SER:HB3	2.37	0.53
1:H:148:TYR:OH	1:I:176:HIS:CE1	2.61	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:97:ASP:OD1	1:J:99:ARG:HG2	2.09	0.53
1:A:239:LEU:CD1	1:B:239:LEU:HD21	2.37	0.53
1:A:245:ALA:HB1	1:E:247:TYR:CE1	2.43	0.53
1:C:72:TRP:CH2	1:C:74:PRO:HG3	2.43	0.53
1:C:219:TRP:C	1:C:221:VAL:H	2.12	0.53
1:D:251:ILE:CD1	1:E:249:SER:HB3	2.39	0.53
1:J:174:TYR:O	1:J:177:LEU:HD11	2.08	0.53
1:J:185:ASN:HD22	1:J:185:ASN:N	2.06	0.53
1:A:174:TYR:O	1:A:177:LEU:HD11	2.09	0.53
1:B:81:VAL:HG11	1:B:85:PRO:HD3	1.91	0.53
1:C:127:VAL:C	1:C:128:LEU:HD12	2.28	0.53
1:D:231:LEU:HD23	1:D:232:GLN:N	2.24	0.53
1:E:219:TRP:C	1:E:221:VAL:H	2.11	0.53
1:B:210:PRO:O	1:B:214:ILE:HG12	2.09	0.53
1:C:239:LEU:HD13	1:D:239:LEU:HD21	1.89	0.53
1:F:305:LEU:HD12	1:F:306:GLY:N	2.24	0.53
1:G:305:LEU:C	1:G:305:LEU:HD12	2.29	0.53
1:I:72:TRP:CD1	1:I:72:TRP:C	2.82	0.53
1:J:299:CYS:HB2	1:J:302:ALA:CB	2.39	0.53
1:D:251:ILE:CG1	1:E:249:SER:HB3	2.38	0.53
1:A:169:ILE:HD12	1:A:190:ILE:HG12	1.90	0.53
1:B:303:PHE:N	1:B:304:PRO:CD	2.72	0.53
1:D:81:VAL:HG11	1:D:85:PRO:HD3	1.91	0.53
1:G:267:ALA:HB1	1:G:307:PHE:HZ	1.74	0.53
1:I:303:PHE:N	1:I:304:PRO:CD	2.72	0.53
1:I:305:LEU:C	1:I:305:LEU:HD12	2.30	0.53
1:F:59:GLU:O	1:F:63:ILE:HG13	2.09	0.53
1:F:118:LEU:N	1:F:118:LEU:HD23	2.23	0.53
1:F:280:ILE:O	1:F:280:ILE:HG22	2.09	0.53
1:G:210:PRO:O	1:G:214:ILE:HG12	2.09	0.53
1:H:303:PHE:N	1:H:304:PRO:CD	2.73	0.53
1:A:294:LEU:CA	1:A:297:GLN:HE21	2.21	0.52
1:F:210:PRO:O	1:F:214:ILE:HG12	2.08	0.52
1:H:123:ARG:HD2	1:H:197:VAL:HG22	1.90	0.52
1:A:172:ILE:HD13	1:A:189:ARG:HB3	1.91	0.52
1:A:255:LEU:HB3	1:A:256:PRO:HD2	1.90	0.52
1:C:127:VAL:HG22	1:C:193:ARG:HG2	1.92	0.52
1:E:51:PRO:HD2	1:E:56:LEU:HD23	1.90	0.52
1:E:181:GLN:H	1:E:182:PRO:CD	2.22	0.52
1:D:162:ILE:HG22	1:D:163:ARG:N	2.21	0.52
1:J:127:VAL:HG22	1:J:193:ARG:HG2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:ILE:HD13	1:E:220:SER:HB2	1.91	0.52
1:I:172:ILE:HD13	1:I:189:ARG:HB3	1.90	0.52
1:I:231:LEU:HD23	1:I:232:GLN:N	2.24	0.52
1:A:81:VAL:HG11	1:A:85:PRO:HD3	1.91	0.52
1:A:202:TYR:HB2	1:B:256:PRO:C	2.30	0.52
1:A:239:LEU:CD2	1:E:240:THR:HA	2.38	0.52
1:A:299:CYS:HB2	1:A:302:ALA:HB3	1.92	0.52
1:B:255:LEU:HB3	1:B:256:PRO:HD2	1.90	0.52
1:B:280:ILE:HG22	1:B:280:ILE:O	2.09	0.52
1:C:91:ARG:HB2	1:D:133:PHE:HE2	1.74	0.52
1:C:315:VAL:O	1:C:315:VAL:HG12	2.10	0.52
1:D:169:ILE:HD12	1:D:190:ILE:HG12	1.91	0.52
1:D:203:TYR:O	1:D:208:ILE:HG12	2.09	0.52
1:H:51:PRO:HD2	1:H:56:LEU:HD23	1.91	0.52
1:H:91:ARG:HD3	1:I:134:SER:HB3	1.90	0.52
1:H:276:ILE:O	1:H:280:ILE:HG13	2.09	0.52
1:I:72:TRP:CH2	1:I:74:PRO:HG3	2.44	0.52
1:A:162:ILE:HG22	1:A:163:ARG:N	2.21	0.52
1:D:199:ASN:HD22	1:D:199:ASN:C	2.12	0.52
1:E:62:GLN:HE22	1:E:65:ARG:HH11	1.58	0.52
1:C:231:LEU:HD23	1:C:232:GLN:N	2.25	0.52
1:D:294:LEU:CA	1:D:297:GLN:HE21	2.21	0.52
1:I:247:TYR:HE1	1:J:249:SER:HG	1.58	0.52
1:I:262:ASP:O	1:I:266:ILE:HG12	2.08	0.52
1:F:181:GLN:H	1:F:182:PRO:CD	2.22	0.52
1:I:167:THR:CG2	1:I:168:HIS:H	2.14	0.52
1:D:293:ASP:O	1:D:296:ILE:HG22	2.10	0.52
1:E:72:TRP:CH2	1:E:74:PRO:HG3	2.44	0.52
1:G:220:SER:HB2	1:H:280:ILE:HD13	1.91	0.52
1:H:91:ARG:HD2	1:I:134:SER:HB2	1.91	0.52
1:D:91:ARG:HD2	1:E:134:SER:CB	2.40	0.52
1:D:219:TRP:C	1:D:221:VAL:H	2.13	0.52
1:E:23:ILE:HG21	1:E:126:PHE:CD2	2.45	0.52
1:J:181:GLN:H	1:J:182:PRO:CD	2.23	0.52
1:J:219:TRP:C	1:J:221:VAL:H	2.14	0.52
1:A:181:GLN:H	1:A:182:PRO:CD	2.23	0.51
1:A:305:LEU:HD12	1:A:306:GLY:N	2.25	0.51
1:C:220:SER:HB2	1:D:280:ILE:CD1	2.39	0.51
1:D:303:PHE:N	1:D:304:PRO:CD	2.72	0.51
1:D:305:LEU:HD12	1:D:306:GLY:N	2.26	0.51
1:G:72:TRP:CH2	1:G:74:PRO:HG3	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:174:TYR:O	1:C:177:LEU:HD11	2.09	0.51
1:D:167:THR:O	1:D:168:HIS:HB2	2.11	0.51
1:F:57:ILE:HD13	1:G:134:SER:O	2.09	0.51
1:G:51:PRO:HD2	1:G:56:LEU:HD23	1.93	0.51
1:H:199:ASN:C	1:H:199:ASN:HD22	2.11	0.51
1:I:72:TRP:CZ3	1:I:135:TYR:CZ	2.98	0.51
1:A:231:LEU:HD23	1:A:232:GLN:N	2.25	0.51
1:D:223:TRP:CE2	1:D:300:ARG:HD3	2.45	0.51
1:J:305:LEU:C	1:J:305:LEU:HD12	2.31	0.51
1:B:203:TYR:O	1:B:208:ILE:HG12	2.10	0.51
1:I:112:ASN:OD1	1:I:113:ASP:N	2.43	0.51
1:J:127:VAL:C	1:J:128:LEU:HD12	2.31	0.51
1:A:252:LEU:HG	1:A:253:PRO:HD2	1.92	0.51
1:B:114:MET:HE2	1:B:124:GLN:HG2	1.91	0.51
1:C:172:ILE:HD13	1:C:189:ARG:HB3	1.93	0.51
1:F:276:ILE:O	1:F:280:ILE:HG13	2.11	0.51
1:J:140:LEU:HD22	1:J:190:ILE:HD11	1.93	0.51
1:J:169:ILE:HD12	1:J:190:ILE:HG12	1.92	0.51
1:B:305:LEU:HD12	1:B:306:GLY:N	2.25	0.51
1:D:181:GLN:H	1:D:182:PRO:CD	2.23	0.51
1:F:56:LEU:HD13	1:F:57:ILE:N	2.26	0.51
1:G:303:PHE:N	1:G:304:PRO:CD	2.74	0.51
1:H:91:ARG:HD2	1:I:134:SER:CB	2.40	0.51
1:J:180:VAL:HG21	1:J:184:GLN:HB2	1.93	0.51
1:B:299:CYS:HB2	1:B:302:ALA:CB	2.40	0.51
1:C:157:ILE:HD11	1:D:115:ASP:OD2	2.09	0.51
1:C:210:PRO:O	1:C:214:ILE:HG12	2.10	0.51
1:C:276:ILE:O	1:C:280:ILE:HG13	2.11	0.51
1:D:118:LEU:N	1:D:118:LEU:HD23	2.26	0.51
1:E:276:ILE:O	1:E:280:ILE:HG13	2.10	0.51
1:H:167:THR:O	1:H:168:HIS:HB2	2.10	0.51
1:H:223:TRP:CE3	1:I:280:ILE:HG22	2.45	0.51
1:I:267:ALA:HB1	1:I:307:PHE:HZ	1.75	0.51
1:J:81:VAL:HG11	1:J:85:PRO:HD3	1.93	0.51
1:J:119:PHE:CB	1:J:120:PRO:HD3	2.37	0.51
1:B:56:LEU:HD13	1:B:57:ILE:N	2.26	0.51
1:B:223:TRP:CE2	1:B:300:ARG:HD3	2.46	0.51
1:D:115:ASP:H	1:D:124:GLN:HE22	1.59	0.51
1:D:209:LEU:HB3	1:D:210:PRO:HD3	1.93	0.51
1:E:223:TRP:CE2	1:E:300:ARG:HD3	2.46	0.51
1:F:226:SER:HB3	1:F:229:GLU:CG	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:303:PHE:N	1:C:304:PRO:CD	2.73	0.51
1:E:72:TRP:CZ3	1:E:135:TYR:CZ	2.96	0.51
1:F:239:LEU:HD23	1:J:240:THR:CA	2.39	0.51
1:G:28:THR:HB	1:G:255:LEU:CD2	2.39	0.51
1:G:226:SER:HB3	1:G:229:GLU:CG	2.41	0.51
1:G:299:CYS:HB2	1:G:302:ALA:HB3	1.93	0.51
1:G:305:LEU:HD12	1:G:306:GLY:N	2.25	0.51
1:H:219:TRP:C	1:H:221:VAL:H	2.14	0.51
1:A:72:TRP:CZ2	1:A:74:PRO:CG	2.90	0.50
1:C:305:LEU:HD12	1:C:306:GLY:N	2.27	0.50
1:D:252:LEU:HG	1:D:253:PRO:HD2	1.93	0.50
1:D:315:VAL:O	1:D:315:VAL:HG12	2.11	0.50
1:E:294:LEU:CA	1:E:297:GLN:HE21	2.21	0.50
1:G:248:THR:HG23	1:G:252:LEU:HD22	1.92	0.50
1:G:315:VAL:O	1:G:315:VAL:HG12	2.12	0.50
1:H:181:GLN:H	1:H:182:PRO:CD	2.23	0.50
1:A:117:ARG:HG2	1:A:117:ARG:HH11	1.76	0.50
1:B:219:TRP:C	1:B:221:VAL:H	2.14	0.50
1:B:231:LEU:C	1:B:231:LEU:HD23	2.31	0.50
1:C:62:GLN:HE22	1:C:65:ARG:HH11	1.58	0.50
1:C:164:LYS:HA	1:C:164:LYS:HZ3	1.76	0.50
1:D:157:ILE:HD11	1:E:115:ASP:OD2	2.11	0.50
1:E:248:THR:HG23	1:E:252:LEU:HD22	1.93	0.50
1:H:237:LEU:HD13	1:I:235:PHE:CD2	2.45	0.50
1:B:209:LEU:HB3	1:B:210:PRO:HD3	1.94	0.50
1:B:263:GLN:HA	1:B:266:ILE:HG12	1.93	0.50
1:C:167:THR:O	1:C:168:HIS:HB2	2.11	0.50
1:G:181:GLN:H	1:G:182:PRO:CD	2.25	0.50
1:I:81:VAL:HG11	1:I:85:PRO:HD3	1.93	0.50
1:J:172:ILE:HD13	1:J:189:ARG:HB3	1.93	0.50
1:A:224:LEU:HB2	1:A:230:ARG:HG3	1.92	0.50
1:B:181:GLN:H	1:B:182:PRO:CD	2.24	0.50
1:D:27:ASN:HB3	1:D:32:THR:HB	1.93	0.50
1:F:200:PRO:O	1:F:201:SER:C	2.50	0.50
1:G:223:TRP:CE2	1:G:300:ARG:HD3	2.46	0.50
1:G:247:TYR:CE1	1:H:245:ALA:HB1	2.47	0.50
1:H:172:ILE:HD13	1:H:189:ARG:HB3	1.93	0.50
1:H:226:SER:HB3	1:H:229:GLU:CG	2.40	0.50
1:I:255:LEU:HB3	1:I:256:PRO:HD2	1.93	0.50
1:B:164:LYS:HZ1	1:B:165:ALA:H	1.49	0.50
1:C:293:ASP:O	1:C:296:ILE:HG22	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:19:PHE:CE2	1:I:146:GLN:HG3	2.46	0.50
1:I:293:ASP:O	1:I:296:ILE:HG22	2.11	0.50
1:A:51:PRO:HD2	1:A:56:LEU:HD23	1.92	0.50
1:C:248:THR:HG23	1:C:252:LEU:HD22	1.94	0.50
1:F:237:LEU:HD13	1:G:235:PHE:HD2	1.72	0.50
1:F:237:LEU:CD1	1:G:235:PHE:CE2	2.93	0.50
1:G:240:THR:OG1	1:H:239:LEU:HD23	2.12	0.50
1:H:293:ASP:O	1:H:296:ILE:HG22	2.12	0.50
1:J:23:ILE:HG21	1:J:126:PHE:CD2	2.47	0.50
1:J:315:VAL:O	1:J:315:VAL:HG12	2.12	0.50
1:A:145:ILE:HG21	1:A:192:VAL:HG11	1.92	0.50
1:A:219:TRP:C	1:A:221:VAL:H	2.15	0.50
1:D:220:SER:HB2	1:E:280:ILE:CD1	2.41	0.50
1:J:263:GLN:HA	1:J:266:ILE:HG12	1.94	0.50
1:A:199:ASN:C	1:A:199:ASN:HD22	2.14	0.50
1:B:59:GLU:O	1:B:63:ILE:HG13	2.11	0.50
1:C:181:GLN:H	1:C:182:PRO:CD	2.24	0.50
1:E:209:LEU:HB3	1:E:210:PRO:HD3	1.92	0.50
1:G:114:MET:CE	1:G:124:GLN:HG2	2.42	0.50
1:H:72:TRP:CH2	1:H:74:PRO:HG3	2.47	0.50
1:I:181:GLN:H	1:I:182:PRO:CD	2.25	0.50
1:A:303:PHE:N	1:A:304:PRO:CD	2.74	0.50
1:C:59:GLU:O	1:C:63:ILE:HG13	2.11	0.50
1:C:127:VAL:O	1:C:128:LEU:HD12	2.12	0.50
1:D:120:PRO:HD2	1:D:260:VAL:HG23	1.94	0.50
1:D:180:VAL:HG21	1:D:184:GLN:HB2	1.93	0.50
1:E:231:LEU:HD23	1:E:232:GLN:N	2.26	0.50
1:H:65:ARG:HD2	1:I:68:ASN:ND2	2.26	0.50
1:B:91:ARG:CD	1:C:134:SER:HB3	2.42	0.49
1:C:119:PHE:CB	1:C:120:PRO:HD3	2.40	0.49
1:C:220:SER:HB2	1:D:280:ILE:HD13	1.94	0.49
1:C:223:TRP:NE1	1:C:300:ARG:HD3	2.27	0.49
1:D:89:ASN:O	1:D:104:ALA:HA	2.12	0.49
1:D:239:LEU:HD13	1:E:239:LEU:HD21	1.94	0.49
1:G:114:MET:HE2	1:G:124:GLN:HG2	1.93	0.49
1:H:315:VAL:O	1:H:315:VAL:HG12	2.12	0.49
1:A:167:THR:O	1:A:168:HIS:CB	2.60	0.49
1:F:77:GLU:O	1:F:130:LEU:HD23	2.11	0.49
1:G:72:TRP:CD1	1:G:72:TRP:C	2.83	0.49
1:I:145:ILE:HG21	1:I:192:VAL:HG11	1.93	0.49
1:B:148:TYR:CZ	1:C:176:HIS:NE2	2.80	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:ASP:O	1:B:266:ILE:HG12	2.12	0.49
1:D:296:ILE:HG23	1:D:297:GLN:N	2.27	0.49
1:E:303:PHE:N	1:E:304:PRO:CD	2.75	0.49
1:H:72:TRP:CZ3	1:H:135:TYR:CZ	2.96	0.49
1:H:209:LEU:HB3	1:H:210:PRO:HD3	1.93	0.49
1:A:72:TRP:CD1	1:A:72:TRP:C	2.85	0.49
1:B:199:ASN:HD22	1:B:199:ASN:C	2.14	0.49
1:B:202:TYR:HB2	1:C:256:PRO:C	2.32	0.49
1:F:127:VAL:C	1:F:128:LEU:HD12	2.33	0.49
1:I:219:TRP:C	1:I:221:VAL:H	2.14	0.49
1:A:280:ILE:CG2	1:E:223:TRP:CE3	2.96	0.49
1:F:81:VAL:HG11	1:F:85:PRO:HD3	1.94	0.49
1:F:263:GLN:HA	1:F:266:ILE:HG12	1.94	0.49
1:G:120:PRO:HD2	1:G:260:VAL:HG23	1.93	0.49
1:H:296:ILE:CG2	1:H:297:GLN:N	2.75	0.49
1:A:223:TRP:CE2	1:A:300:ARG:HD3	2.48	0.49
1:A:315:VAL:O	1:A:315:VAL:HG12	2.13	0.49
1:B:172:ILE:HD13	1:B:189:ARG:HB3	1.94	0.49
1:C:27:ASN:HB3	1:C:32:THR:HB	1.95	0.49
1:E:226:SER:HB3	1:E:229:GLU:CG	2.42	0.49
1:E:280:ILE:HG22	1:E:280:ILE:O	2.13	0.49
1:F:251:ILE:CG1	1:G:249:SER:HB3	2.41	0.49
1:G:15:SER:HG	1:G:142:PHE:HD1	1.60	0.49
1:G:203:TYR:O	1:G:208:ILE:HG12	2.12	0.49
1:H:169:ILE:HD12	1:H:190:ILE:HG12	1.93	0.49
1:I:164:LYS:HZ1	1:I:165:ALA:N	1.94	0.49
1:J:62:GLN:HE22	1:J:65:ARG:HH11	1.60	0.49
1:J:203:TYR:O	1:J:208:ILE:HG12	2.12	0.49
1:A:167:THR:CG2	1:A:168:HIS:H	2.19	0.49
1:C:72:TRP:CZ3	1:C:135:TYR:CZ	2.99	0.49
1:C:226:SER:HB3	1:C:229:GLU:CG	2.43	0.49
1:D:172:ILE:HD13	1:D:189:ARG:HB3	1.95	0.49
1:E:114:MET:HE2	1:E:124:GLN:HG2	1.93	0.49
1:H:305:LEU:HD12	1:H:306:GLY:N	2.27	0.49
1:D:143:SER:HB3	1:D:167:THR:HG21	1.93	0.49
1:E:114:MET:CE	1:E:124:GLN:HG2	2.42	0.49
1:E:167:THR:O	1:E:168:HIS:HB2	2.13	0.49
1:G:199:ASN:C	1:G:199:ASN:ND2	2.66	0.49
1:A:133:PHE:CE2	1:E:91:ARG:HB2	2.48	0.49
1:B:72:TRP:CZ3	1:B:135:TYR:CZ	3.01	0.49
1:C:81:VAL:HG11	1:C:85:PRO:HD3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:180:VAL:HG21	1:G:184:GLN:HB2	1.94	0.49
1:B:140:LEU:HD22	1:B:190:ILE:HD11	1.95	0.49
1:B:180:VAL:HG21	1:B:184:GLN:HB2	1.94	0.49
1:C:267:ALA:HB1	1:C:307:PHE:HZ	1.78	0.49
1:D:226:SER:HB3	1:D:229:GLU:CG	2.42	0.49
1:E:127:VAL:C	1:E:128:LEU:HD12	2.33	0.49
1:G:231:LEU:HD23	1:G:232:GLN:N	2.28	0.49
1:G:247:TYR:HD1	1:H:246:ALA:HA	1.76	0.49
1:D:299:CYS:HB2	1:D:302:ALA:HB3	1.95	0.48
1:G:262:ASP:O	1:G:266:ILE:HG12	2.13	0.48
1:J:72:TRP:CD1	1:J:72:TRP:O	2.66	0.48
1:B:293:ASP:O	1:B:296:ILE:HG22	2.13	0.48
1:D:210:PRO:O	1:D:214:ILE:HG12	2.13	0.48
1:F:72:TRP:CZ2	1:F:74:PRO:CG	2.92	0.48
1:F:239:LEU:HD21	1:J:239:LEU:HD13	1.95	0.48
1:H:81:VAL:HG11	1:H:85:PRO:HD3	1.95	0.48
1:I:296:ILE:HG23	1:I:297:GLN:N	2.28	0.48
1:C:72:TRP:CD1	1:C:72:TRP:C	2.85	0.48
1:C:114:MET:CE	1:C:124:GLN:HG2	2.43	0.48
1:C:263:GLN:HA	1:C:266:ILE:HG12	1.94	0.48
1:D:200:PRO:O	1:D:201:SER:C	2.52	0.48
1:E:59:GLU:O	1:E:63:ILE:HG13	2.13	0.48
1:F:174:TYR:O	1:F:177:LEU:HD11	2.12	0.48
1:G:56:LEU:HD13	1:G:57:ILE:N	2.28	0.48
1:G:72:TRP:CZ3	1:G:135:TYR:CZ	2.97	0.48
1:J:223:TRP:NE1	1:J:300:ARG:HD3	2.28	0.48
1:A:180:VAL:HG21	1:A:184:GLN:HB2	1.95	0.48
1:A:222:PHE:CE2	1:A:299:CYS:SG	3.06	0.48
1:C:56:LEU:HD13	1:C:57:ILE:N	2.28	0.48
1:C:280:ILE:HG22	1:C:280:ILE:O	2.13	0.48
1:E:167:THR:CG2	1:E:168:HIS:H	2.18	0.48
1:G:119:PHE:CB	1:G:120:PRO:HD3	2.38	0.48
1:J:145:ILE:HG21	1:J:192:VAL:HG11	1.95	0.48
1:A:23:ILE:HG21	1:A:126:PHE:CD2	2.48	0.48
1:A:66:TRP:HB3	1:A:71:LEU:HD12	1.95	0.48
1:C:199:ASN:C	1:C:199:ASN:HD22	2.16	0.48
1:E:97:ASP:OD1	1:E:99:ARG:HG2	2.13	0.48
1:E:255:LEU:HB3	1:E:256:PRO:HD2	1.94	0.48
1:F:117:ARG:HG2	1:F:117:ARG:HH11	1.79	0.48
1:F:252:LEU:HG	1:F:253:PRO:HD2	1.95	0.48
1:G:181:GLN:CG	1:G:182:PRO:HD3	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:72:TRP:CZ3	1:J:135:TYR:CZ	2.99	0.48
1:A:303:PHE:C	1:A:303:PHE:HD1	2.17	0.48
1:C:117:ARG:HG2	1:C:117:ARG:HH11	1.79	0.48
1:C:299:CYS:HB2	1:C:302:ALA:CB	2.42	0.48
1:E:162:ILE:HG22	1:E:163:ARG:N	2.22	0.48
1:E:293:ASP:O	1:E:296:ILE:HG22	2.13	0.48
1:G:204:LEU:HA	1:G:208:ILE:CG1	2.44	0.48
1:I:145:ILE:HD12	1:I:145:ILE:N	2.13	0.48
1:I:203:TYR:O	1:I:208:ILE:HG12	2.14	0.48
1:I:315:VAL:HG12	1:I:315:VAL:O	2.14	0.48
1:J:222:PHE:CE2	1:J:299:CYS:SG	3.06	0.48
1:J:288:ASN:OD1	1:J:291:GLU:HB3	2.14	0.48
1:J:303:PHE:N	1:J:304:PRO:CD	2.77	0.48
1:F:62:GLN:HE22	1:F:65:ARG:HH11	1.61	0.48
1:F:267:ALA:HB1	1:F:307:PHE:HZ	1.78	0.48
1:I:173:ARG:HA	1:I:185:ASN:O	2.13	0.48
1:I:223:TRP:CE2	1:I:300:ARG:HD3	2.49	0.48
1:I:299:CYS:HB2	1:I:302:ALA:HB3	1.95	0.48
1:J:294:LEU:CA	1:J:297:GLN:HE21	2.22	0.48
1:A:127:VAL:C	1:A:128:LEU:HD12	2.34	0.48
1:B:147:VAL:CG2	1:B:165:ALA:HB2	2.44	0.48
1:C:65:ARG:HD2	1:D:68:ASN:ND2	2.29	0.48
1:F:223:TRP:CE2	1:F:300:ARG:HD3	2.49	0.48
1:H:200:PRO:O	1:H:201:SER:C	2.51	0.48
1:I:181:GLN:CG	1:I:182:PRO:HD3	2.38	0.48
1:A:114:MET:CE	1:A:124:GLN:HG2	2.44	0.48
1:A:226:SER:HB3	1:A:229:GLU:CG	2.42	0.48
1:A:247:TYR:HE1	1:B:249:SER:OG	1.96	0.48
1:A:286:GLN:HB2	1:A:288:ASN:OD1	2.13	0.48
1:E:315:VAL:O	1:E:315:VAL:HG12	2.14	0.48
1:F:296:ILE:HG23	1:F:297:GLN:N	2.29	0.48
1:G:263:GLN:HA	1:G:266:ILE:HG12	1.96	0.48
1:G:293:ASP:O	1:G:296:ILE:HG22	2.14	0.48
1:H:299:CYS:HB2	1:H:302:ALA:HB3	1.96	0.48
1:J:209:LEU:HB3	1:J:210:PRO:HD3	1.93	0.48
1:J:303:PHE:HD1	1:J:303:PHE:C	2.16	0.48
1:B:303:PHE:O	1:B:307:PHE:HB2	2.14	0.48
1:C:91:ARG:HD3	1:D:134:SER:HB3	1.96	0.48
1:D:59:GLU:OE2	1:E:75:ALA:HB3	2.14	0.48
1:D:262:ASP:O	1:D:266:ILE:HG12	2.13	0.48
1:E:81:VAL:HG11	1:E:85:PRO:HD3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:172:ILE:HD13	1:E:189:ARG:HB3	1.96	0.48
1:E:200:PRO:O	1:E:201:SER:C	2.51	0.48
1:F:172:ILE:HD13	1:F:189:ARG:HB3	1.95	0.48
1:F:286:GLN:HB2	1:F:288:ASN:OD1	2.14	0.48
1:G:157:ILE:HD11	1:H:115:ASP:CG	2.34	0.48
1:I:119:PHE:CB	1:I:120:PRO:HD3	2.43	0.48
1:I:252:LEU:HG	1:I:253:PRO:HD2	1.95	0.48
1:J:286:GLN:HB2	1:J:288:ASN:OD1	2.14	0.48
1:E:72:TRP:HZ3	1:E:135:TYR:CE1	2.32	0.47
1:F:27:ASN:HB3	1:F:32:THR:HB	1.95	0.47
1:G:220:SER:HB2	1:H:280:ILE:CD1	2.43	0.47
1:I:127:VAL:C	1:I:128:LEU:HD12	2.34	0.47
1:J:303:PHE:O	1:J:307:PHE:HB2	2.14	0.47
1:B:19:PHE:CE2	1:B:146:GLN:HG3	2.49	0.47
1:B:62:GLN:HE22	1:B:65:ARG:HH11	1.62	0.47
1:E:27:ASN:HB3	1:E:32:THR:HB	1.96	0.47
1:G:303:PHE:C	1:G:303:PHE:HD1	2.16	0.47
1:I:89:ASN:HB3	1:J:133:PHE:CE2	2.49	0.47
1:D:303:PHE:C	1:D:303:PHE:HD1	2.17	0.47
1:E:252:LEU:HG	1:E:253:PRO:HD2	1.96	0.47
1:G:288:ASN:OD1	1:G:291:GLU:HB3	2.14	0.47
1:G:296:ILE:HG23	1:G:297:GLN:N	2.30	0.47
1:J:303:PHE:C	1:J:303:PHE:CD1	2.88	0.47
1:A:119:PHE:CB	1:A:120:PRO:HD3	2.42	0.47
1:B:72:TRP:CD1	1:B:72:TRP:C	2.86	0.47
1:C:115:ASP:H	1:C:124:GLN:HE22	1.61	0.47
1:C:303:PHE:O	1:C:307:PHE:HB2	2.14	0.47
1:D:62:GLN:HE22	1:D:65:ARG:HH11	1.63	0.47
1:E:299:CYS:HB2	1:E:302:ALA:HB3	1.95	0.47
1:F:72:TRP:CD1	1:F:72:TRP:C	2.88	0.47
1:F:288:ASN:OD1	1:F:291:GLU:HB3	2.15	0.47
1:H:199:ASN:C	1:H:199:ASN:ND2	2.68	0.47
1:B:147:VAL:O	1:B:147:VAL:HG12	2.14	0.47
1:E:145:ILE:HG21	1:E:192:VAL:HG11	1.96	0.47
1:F:89:ASN:O	1:F:104:ALA:HA	2.15	0.47
1:F:299:CYS:HB2	1:F:302:ALA:HB3	1.95	0.47
1:H:72:TRP:CD1	1:H:72:TRP:C	2.85	0.47
1:J:262:ASP:O	1:J:266:ILE:HG12	2.13	0.47
1:A:140:LEU:HD13	1:A:190:ILE:CG1	2.37	0.47
1:C:91:ARG:HB2	1:D:133:PHE:CE2	2.49	0.47
1:C:120:PRO:HD2	1:C:260:VAL:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:303:PHE:HD1	1:C:303:PHE:C	2.18	0.47
1:D:72:TRP:CZ2	1:D:74:PRO:CG	2.90	0.47
1:E:267:ALA:HB1	1:E:307:PHE:HZ	1.80	0.47
1:E:303:PHE:O	1:E:307:PHE:HB2	2.14	0.47
1:G:303:PHE:C	1:G:303:PHE:CD1	2.88	0.47
1:H:119:PHE:O	1:H:120:PRO:C	2.52	0.47
1:I:301:LEU:C	1:I:304:PRO:HD2	2.35	0.47
1:A:200:PRO:O	1:A:201:SER:C	2.52	0.47
1:A:293:ASP:O	1:A:296:ILE:HG22	2.14	0.47
1:C:203:TYR:O	1:C:208:ILE:HG12	2.14	0.47
1:C:209:LEU:HB3	1:C:210:PRO:HD3	1.97	0.47
1:C:296:ILE:HG23	1:C:297:GLN:N	2.29	0.47
1:F:180:VAL:HG21	1:F:184:GLN:HB2	1.96	0.47
1:G:61:THR:HG21	1:H:64:GLU:HG3	1.95	0.47
1:G:81:VAL:HG11	1:G:85:PRO:HD3	1.96	0.47
1:G:117:ARG:HG2	1:G:117:ARG:HH11	1.80	0.47
1:G:119:PHE:O	1:G:120:PRO:C	2.53	0.47
1:G:276:ILE:O	1:G:280:ILE:HG13	2.14	0.47
1:J:187:PHE:CD1	1:J:187:PHE:N	2.83	0.47
1:B:288:ASN:OD1	1:B:291:GLU:HB3	2.15	0.47
1:F:58:VAL:HB	1:F:92:LEU:HB2	1.95	0.47
1:F:114:MET:CE	1:F:124:GLN:HG2	2.45	0.47
1:G:252:LEU:HG	1:G:253:PRO:HD2	1.96	0.47
1:I:294:LEU:CA	1:I:297:GLN:HE21	2.25	0.47
1:I:305:LEU:HD12	1:I:306:GLY:N	2.29	0.47
1:J:299:CYS:HB2	1:J:302:ALA:HB3	1.96	0.47
1:A:303:PHE:O	1:A:307:PHE:HB2	2.14	0.47
1:D:120:PRO:HD2	1:D:260:VAL:CG2	2.44	0.47
1:D:303:PHE:O	1:D:307:PHE:HB2	2.14	0.47
1:E:172:ILE:N	1:E:172:ILE:HD12	2.30	0.47
1:E:199:ASN:C	1:E:199:ASN:HD22	2.17	0.47
1:F:127:VAL:O	1:F:128:LEU:HD12	2.15	0.47
1:F:172:ILE:HD12	1:F:172:ILE:N	2.30	0.47
1:J:252:LEU:HG	1:J:253:PRO:HD2	1.97	0.47
1:J:305:LEU:HD12	1:J:306:GLY:N	2.29	0.47
1:D:251:ILE:HD11	1:E:249:SER:HB3	1.97	0.47
1:E:259:THR:O	1:E:263:GLN:HG3	2.15	0.47
1:F:303:PHE:O	1:F:307:PHE:HB2	2.14	0.47
1:F:315:VAL:HG12	1:F:315:VAL:O	2.14	0.47
1:G:219:TRP:C	1:G:221:VAL:N	2.68	0.47
1:G:240:THR:HA	1:H:239:LEU:CD2	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:288:ASN:OD1	1:H:291:GLU:HB3	2.15	0.47
1:A:107:LEU:HD23	1:B:83:GLY:HA2	1.97	0.46
1:B:147:VAL:O	1:B:149:THR:N	2.45	0.46
1:C:118:LEU:N	1:C:118:LEU:HD23	2.30	0.46
1:D:92:LEU:HD23	1:D:92:LEU:HA	1.79	0.46
1:D:303:PHE:C	1:D:303:PHE:CD1	2.89	0.46
1:E:296:ILE:HG23	1:E:297:GLN:N	2.30	0.46
1:H:148:TYR:CZ	1:I:176:HIS:NE2	2.82	0.46
1:J:167:THR:CG2	1:J:168:HIS:H	2.22	0.46
1:J:257:TYR:CD1	1:J:257:TYR:N	2.83	0.46
1:A:115:ASP:CG	1:E:157:ILE:HD11	2.34	0.46
1:A:303:PHE:C	1:A:303:PHE:CD1	2.88	0.46
1:B:248:THR:HG23	1:B:252:LEU:HD22	1.96	0.46
1:C:309:ALA:O	1:C:313:VAL:HG23	2.16	0.46
1:F:303:PHE:N	1:F:304:PRO:HD3	2.30	0.46
1:H:280:ILE:HG22	1:H:280:ILE:O	2.15	0.46
1:I:223:TRP:CE3	1:J:280:ILE:HG22	2.50	0.46
1:J:119:PHE:HB3	1:J:259:THR:HB	1.97	0.46
1:A:58:VAL:HB	1:A:92:LEU:HB2	1.97	0.46
1:A:97:ASP:OD1	1:A:99:ARG:HG2	2.15	0.46
1:D:117:ARG:HG2	1:D:117:ARG:HH11	1.80	0.46
1:F:231:LEU:HD22	1:J:224:LEU:HD21	1.97	0.46
1:F:235:PHE:CD2	1:J:237:LEU:HD13	2.49	0.46
1:G:147:VAL:HG21	1:G:165:ALA:HB2	1.96	0.46
1:G:280:ILE:O	1:G:280:ILE:HG22	2.15	0.46
1:H:27:ASN:HB3	1:H:32:THR:HB	1.97	0.46
1:H:286:GLN:HB2	1:H:288:ASN:OD1	2.14	0.46
1:H:303:PHE:HD1	1:H:303:PHE:C	2.18	0.46
1:H:309:ALA:O	1:H:313:VAL:HG23	2.16	0.46
1:J:293:ASP:O	1:J:296:ILE:HG22	2.15	0.46
1:C:204:LEU:HA	1:C:208:ILE:CG1	2.45	0.46
1:D:288:ASN:OD1	1:D:291:GLU:HB3	2.16	0.46
1:E:288:ASN:OD1	1:E:291:GLU:HB3	2.16	0.46
1:G:89:ASN:O	1:G:104:ALA:HA	2.15	0.46
1:H:97:ASP:OD1	1:H:99:ARG:HG2	2.14	0.46
1:H:115:ASP:H	1:H:124:GLN:HE22	1.62	0.46
1:I:286:GLN:HB2	1:I:288:ASN:OD1	2.15	0.46
1:A:296:ILE:HG23	1:A:297:GLN:N	2.30	0.46
1:B:91:ARG:HD2	1:C:134:SER:CB	2.46	0.46
1:B:247:TYR:HE1	1:C:249:SER:OG	1.98	0.46
1:F:209:LEU:HB3	1:F:210:PRO:HD3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:250:ASN:HD22	1:J:250:ASN:ND2	2.13	0.46
1:G:97:ASP:OD1	1:G:99:ARG:HG2	2.16	0.46
1:J:120:PRO:HD2	1:J:260:VAL:HG23	1.98	0.46
1:A:27:ASN:HB3	1:A:32:THR:HB	1.96	0.46
1:F:199:ASN:C	1:F:199:ASN:HD22	2.19	0.46
1:H:301:LEU:C	1:H:304:PRO:HD2	2.36	0.46
1:I:51:PRO:HD2	1:I:56:LEU:HD23	1.96	0.46
1:I:222:PHE:CE2	1:I:299:CYS:SG	3.08	0.46
1:J:172:ILE:N	1:J:172:ILE:HD12	2.30	0.46
1:B:309:ALA:O	1:B:313:VAL:HG23	2.16	0.46
1:D:181:GLN:CG	1:D:182:PRO:HD3	2.40	0.46
1:D:223:TRP:NE1	1:D:300:ARG:HD3	2.31	0.46
1:E:72:TRP:CD1	1:E:72:TRP:C	2.88	0.46
1:E:112:ASN:ND2	1:E:127:VAL:CG2	2.79	0.46
1:F:246:ALA:HA	1:J:247:TYR:HD1	1.80	0.46
1:F:293:ASP:O	1:F:296:ILE:HG22	2.16	0.46
1:G:219:TRP:O	1:G:221:VAL:N	2.49	0.46
1:H:231:LEU:HD23	1:H:232:GLN:N	2.30	0.46
1:H:262:ASP:O	1:H:266:ILE:HG12	2.16	0.46
1:I:56:LEU:HD13	1:I:57:ILE:N	2.30	0.46
1:I:185:ASN:N	1:I:185:ASN:ND2	2.63	0.46
1:I:288:ASN:OD1	1:I:291:GLU:HB3	2.16	0.46
1:J:167:THR:O	1:J:168:HIS:CB	2.64	0.46
1:B:92:LEU:HA	1:B:92:LEU:HD23	1.76	0.46
1:B:119:PHE:O	1:B:120:PRO:C	2.54	0.46
1:B:267:ALA:HB1	1:B:307:PHE:HZ	1.81	0.46
1:E:119:PHE:HB3	1:E:259:THR:HB	1.96	0.46
1:F:203:TYR:O	1:F:208:ILE:HG12	2.16	0.46
1:I:27:ASN:HB3	1:I:32:THR:HB	1.96	0.46
1:I:147:VAL:O	1:I:147:VAL:HG12	2.16	0.46
1:J:199:ASN:HD22	1:J:199:ASN:C	2.17	0.46
1:A:120:PRO:HD2	1:A:260:VAL:HG23	1.98	0.46
1:A:209:LEU:HB3	1:A:210:PRO:HD3	1.97	0.46
1:A:239:LEU:HD21	1:E:239:LEU:HD13	1.98	0.46
1:B:72:TRP:CH2	1:B:74:PRO:HG3	2.51	0.46
1:E:303:PHE:HD1	1:E:303:PHE:C	2.19	0.46
1:F:23:ILE:HG21	1:F:126:PHE:CD2	2.51	0.46
1:H:247:TYR:HE1	1:I:249:SER:HG	1.62	0.46
1:I:169:ILE:CD1	1:I:190:ILE:HG12	2.46	0.46
1:A:239:LEU:HD23	1:E:240:THR:CA	2.43	0.46
1:A:276:ILE:O	1:A:280:ILE:HG13	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:ILE:HD12	1:C:172:ILE:N	2.31	0.46
1:E:119:PHE:O	1:E:120:PRO:C	2.54	0.46
1:E:120:PRO:HD2	1:E:260:VAL:HG23	1.98	0.46
1:F:134:SER:HB3	1:J:91:ARG:HD3	1.98	0.46
1:F:167:THR:O	1:F:168:HIS:HB2	2.16	0.46
1:G:112:ASN:ND2	1:G:127:VAL:CG2	2.79	0.46
1:H:223:TRP:NE1	1:H:300:ARG:HD3	2.31	0.46
1:J:56:LEU:HD13	1:J:57:ILE:N	2.31	0.46
1:J:58:VAL:HB	1:J:92:LEU:HB2	1.98	0.46
1:B:303:PHE:HD1	1:B:303:PHE:C	2.20	0.45
1:C:303:PHE:C	1:C:303:PHE:CD1	2.89	0.45
1:D:174:TYR:O	1:D:177:LEU:HD11	2.15	0.45
1:E:185:ASN:N	1:E:185:ASN:ND2	2.64	0.45
1:F:219:TRP:O	1:F:221:VAL:N	2.49	0.45
1:F:249:SER:HG	1:J:247:TYR:HE1	1.64	0.45
1:G:169:ILE:CD1	1:G:190:ILE:HG12	2.46	0.45
1:G:174:TYR:O	1:G:177:LEU:HD11	2.15	0.45
1:H:167:THR:O	1:H:168:HIS:CB	2.64	0.45
1:H:173:ARG:HA	1:H:185:ASN:O	2.16	0.45
1:H:240:THR:OG1	1:I:239:LEU:HD23	2.15	0.45
1:H:303:PHE:O	1:H:307:PHE:HB2	2.16	0.45
1:J:89:ASN:O	1:J:104:ALA:HA	2.16	0.45
1:J:200:PRO:O	1:J:201:SER:C	2.54	0.45
1:J:267:ALA:HB1	1:J:307:PHE:HZ	1.80	0.45
1:J:309:ALA:O	1:J:313:VAL:HG23	2.16	0.45
1:A:280:ILE:HG22	1:A:280:ILE:O	2.16	0.45
1:C:39:ILE:HD13	1:C:39:ILE:HG21	1.60	0.45
1:D:280:ILE:O	1:D:280:ILE:HG22	2.16	0.45
1:F:91:ARG:HD2	1:G:134:SER:CB	2.47	0.45
1:G:303:PHE:O	1:G:307:PHE:HB2	2.16	0.45
1:I:62:GLN:HE22	1:I:65:ARG:HH11	1.63	0.45
1:I:209:LEU:HD23	1:I:209:LEU:C	2.36	0.45
1:A:162:ILE:N	1:A:162:ILE:CD1	2.76	0.45
1:A:181:GLN:CG	1:A:182:PRO:HD3	2.39	0.45
1:C:77:GLU:O	1:C:130:LEU:HD23	2.16	0.45
1:C:145:ILE:HD12	1:C:145:ILE:N	2.15	0.45
1:D:72:TRP:CZ3	1:D:135:TYR:CZ	3.02	0.45
1:D:296:ILE:CG2	1:D:297:GLN:N	2.79	0.45
1:E:180:VAL:HG21	1:E:184:GLN:HB2	1.97	0.45
1:F:251:ILE:HG22	1:F:251:ILE:O	2.16	0.45
1:G:128:LEU:HD12	1:G:128:LEU:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:200:PRO:O	1:I:201:SER:C	2.54	0.45
1:A:173:ARG:HA	1:A:185:ASN:O	2.16	0.45
1:A:286:GLN:HA	1:A:291:GLU:OE1	2.17	0.45
1:B:296:ILE:HG23	1:B:297:GLN:N	2.31	0.45
1:E:110:PHE:CD1	1:E:110:PHE:N	2.84	0.45
1:E:119:PHE:CB	1:E:120:PRO:HD3	2.43	0.45
1:H:127:VAL:HG22	1:H:193:ARG:HG2	1.96	0.45
1:H:267:ALA:HB1	1:H:307:PHE:HZ	1.80	0.45
1:J:226:SER:HB3	1:J:229:GLU:CG	2.47	0.45
1:B:247:TYR:HD1	1:C:246:ALA:HA	1.82	0.45
1:C:114:MET:HE2	1:C:124:GLN:HG2	1.98	0.45
1:D:122:ASP:OD2	1:D:198:ARG:NE	2.36	0.45
1:D:286:GLN:HB2	1:D:288:ASN:OD1	2.16	0.45
1:F:15:SER:HG	1:F:142:PHE:HD1	1.64	0.45
1:G:157:ILE:HD11	1:H:115:ASP:OD2	2.16	0.45
1:I:119:PHE:O	1:I:120:PRO:C	2.55	0.45
1:I:257:TYR:CD1	1:I:257:TYR:N	2.85	0.45
1:C:181:GLN:CG	1:C:182:PRO:HD3	2.40	0.45
1:C:209:LEU:HD23	1:C:209:LEU:C	2.37	0.45
1:E:231:LEU:HD12	1:E:280:ILE:HG12	1.98	0.45
1:E:237:LEU:HD12	1:E:237:LEU:HA	1.85	0.45
1:F:134:SER:HB2	1:J:91:ARG:HD2	1.99	0.45
1:F:249:SER:HB3	1:J:251:ILE:CG1	2.43	0.45
1:G:62:GLN:HE22	1:G:65:ARG:HH11	1.64	0.45
1:H:89:ASN:HB3	1:I:133:PHE:CD2	2.52	0.45
1:H:92:LEU:HA	1:H:92:LEU:HD23	1.75	0.45
1:H:127:VAL:O	1:H:128:LEU:HD12	2.16	0.45
1:I:199:ASN:C	1:I:199:ASN:HD22	2.19	0.45
1:J:276:ILE:O	1:J:280:ILE:HG13	2.17	0.45
1:B:119:PHE:CB	1:B:120:PRO:HD3	2.38	0.45
1:B:204:LEU:HA	1:B:208:ILE:CG1	2.47	0.45
1:D:185:ASN:N	1:D:185:ASN:ND2	2.65	0.45
1:H:303:PHE:C	1:H:303:PHE:CD1	2.89	0.45
1:I:130:LEU:HD23	1:I:130:LEU:HA	1.71	0.45
1:I:296:ILE:CG2	1:I:297:GLN:N	2.79	0.45
1:A:267:ALA:HB1	1:A:307:PHE:HZ	1.82	0.45
1:B:169:ILE:HG22	1:B:170:SER:N	2.32	0.45
1:B:286:GLN:HB2	1:B:288:ASN:OD1	2.16	0.45
1:C:180:VAL:HG21	1:C:184:GLN:HB2	1.99	0.45
1:C:288:ASN:OD1	1:C:291:GLU:HB3	2.16	0.45
1:D:19:PHE:CE2	1:D:146:GLN:HG3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:181:GLN:N	1:F:182:PRO:CD	2.80	0.45
1:G:110:PHE:N	1:G:110:PHE:CD1	2.84	0.45
1:G:223:TRP:NE1	1:G:300:ARG:HD3	2.32	0.45
1:H:110:PHE:CD1	1:H:110:PHE:N	2.85	0.45
1:I:187:PHE:N	1:I:187:PHE:CD1	2.85	0.45
1:J:143:SER:HB3	1:J:167:THR:HG21	1.99	0.45
1:B:91:ARG:HD3	1:C:134:SER:HB3	1.99	0.45
1:B:117:ARG:HH11	1:B:117:ARG:HG2	1.81	0.45
1:B:127:VAL:HG22	1:B:193:ARG:HG2	1.99	0.45
1:C:299:CYS:HB2	1:C:302:ALA:HB3	1.99	0.45
1:E:286:GLN:HB2	1:E:288:ASN:OD1	2.17	0.45
1:F:110:PHE:N	1:F:110:PHE:CD1	2.84	0.45
1:G:140:LEU:HD13	1:G:190:ILE:CG1	2.43	0.45
1:I:263:GLN:HA	1:I:266:ILE:HG12	1.99	0.45
1:J:118:LEU:N	1:J:118:LEU:HD23	2.32	0.45
1:B:147:VAL:C	1:B:149:THR:H	2.21	0.45
1:E:174:TYR:O	1:E:177:LEU:HD11	2.17	0.45
1:F:176:HIS:NE2	1:J:148:TYR:OH	2.50	0.45
1:G:167:THR:CG2	1:G:168:HIS:H	2.25	0.45
1:G:231:LEU:HD12	1:G:280:ILE:HG12	1.97	0.45
1:H:119:PHE:CB	1:H:120:PRO:HD3	2.41	0.45
1:I:112:ASN:ND2	1:I:127:VAL:CG2	2.79	0.45
1:I:303:PHE:CD1	1:I:303:PHE:C	2.91	0.45
1:D:199:ASN:C	1:D:199:ASN:ND2	2.70	0.44
1:E:115:ASP:H	1:E:124:GLN:HE22	1.65	0.44
1:E:263:GLN:HA	1:E:266:ILE:HG12	1.98	0.44
1:G:162:ILE:HG22	1:G:163:ARG:N	2.22	0.44
1:I:303:PHE:N	1:I:304:PRO:HD3	2.32	0.44
1:D:263:GLN:HA	1:D:266:ILE:HG12	2.00	0.44
1:E:19:PHE:CE2	1:E:146:GLN:HG3	2.52	0.44
1:F:157:ILE:HD11	1:G:115:ASP:CG	2.38	0.44
1:F:303:PHE:C	1:F:303:PHE:HD1	2.20	0.44
1:G:119:PHE:HB3	1:G:259:THR:HB	1.99	0.44
1:H:117:ARG:HG2	1:H:117:ARG:HH11	1.81	0.44
1:I:140:LEU:HD13	1:I:190:ILE:CG1	2.43	0.44
1:I:303:PHE:C	1:I:303:PHE:HD1	2.20	0.44
1:A:248:THR:HG23	1:A:252:LEU:HD22	1.99	0.44
1:G:172:ILE:N	1:G:172:ILE:HD12	2.32	0.44
1:H:62:GLN:HE22	1:H:65:ARG:HH11	1.64	0.44
1:H:66:TRP:HB3	1:H:71:LEU:HD12	1.98	0.44
1:H:72:TRP:HZ3	1:H:135:TYR:CE1	2.34	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:167:THR:CG2	1:H:168:HIS:H	2.19	0.44
1:H:180:VAL:HG21	1:H:184:GLN:HB2	1.99	0.44
1:I:303:PHE:O	1:I:307:PHE:HB2	2.17	0.44
1:J:296:ILE:HG23	1:J:297:GLN:N	2.31	0.44
1:A:134:SER:HB3	1:E:91:ARG:HD3	1.98	0.44
1:B:315:VAL:O	1:B:315:VAL:HG12	2.16	0.44
1:C:120:PRO:HD2	1:C:260:VAL:CG2	2.46	0.44
1:D:110:PHE:N	1:D:110:PHE:CD1	2.85	0.44
1:F:187:PHE:N	1:F:187:PHE:CD1	2.85	0.44
1:F:296:ILE:CG2	1:F:297:GLN:N	2.80	0.44
1:I:145:ILE:CD1	1:I:145:ILE:N	2.77	0.44
1:I:147:VAL:O	1:I:149:THR:N	2.44	0.44
1:A:199:ASN:C	1:A:199:ASN:ND2	2.71	0.44
1:B:204:LEU:HA	1:B:208:ILE:HG12	1.99	0.44
1:B:240:THR:HA	1:C:239:LEU:CD2	2.48	0.44
1:E:181:GLN:N	1:E:182:PRO:CD	2.81	0.44
1:E:303:PHE:C	1:E:303:PHE:CD1	2.91	0.44
1:G:172:ILE:HD13	1:G:189:ARG:HB3	1.99	0.44
1:G:286:GLN:HB2	1:G:288:ASN:OD1	2.17	0.44
1:I:110:PHE:CD1	1:I:110:PHE:N	2.86	0.44
1:J:140:LEU:HD13	1:J:190:ILE:CG1	2.41	0.44
1:B:145:ILE:N	1:B:145:ILE:CD1	2.79	0.44
1:B:181:GLN:CG	1:B:182:PRO:HD3	2.38	0.44
1:B:237:LEU:HD12	1:B:237:LEU:HA	1.87	0.44
1:B:303:PHE:C	1:B:303:PHE:CD1	2.91	0.44
1:C:286:GLN:HB2	1:C:288:ASN:OD1	2.17	0.44
1:D:172:ILE:HD12	1:D:172:ILE:N	2.32	0.44
1:D:309:ALA:O	1:D:313:VAL:HG23	2.18	0.44
1:F:169:ILE:CD1	1:F:190:ILE:HG12	2.48	0.44
1:F:237:LEU:CD1	1:G:235:PHE:CD2	2.93	0.44
1:I:300:ARG:O	1:I:304:PRO:HG2	2.17	0.44
1:A:181:GLN:N	1:A:182:PRO:CD	2.81	0.44
1:B:187:PHE:CD1	1:B:187:PHE:N	2.85	0.44
1:C:169:ILE:HD12	1:C:190:ILE:HG12	2.00	0.44
1:C:252:LEU:HG	1:C:253:PRO:HD2	1.99	0.44
1:D:39:ILE:HD13	1:D:39:ILE:HG21	1.61	0.44
1:E:169:ILE:HD12	1:E:190:ILE:HG12	2.00	0.44
1:H:118:LEU:HD23	1:H:118:LEU:N	2.32	0.44
1:H:248:THR:HG23	1:H:252:LEU:HD22	2.00	0.44
1:I:239:LEU:CD1	1:J:239:LEU:HD21	2.48	0.44
1:J:223:TRP:CD1	1:J:300:ARG:HD3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:LEU:HA	1:A:208:ILE:CG1	2.48	0.44
1:B:128:LEU:HD12	1:B:128:LEU:N	2.29	0.44
1:C:296:ILE:CG2	1:C:297:GLN:N	2.81	0.44
1:D:119:PHE:O	1:D:120:PRO:C	2.57	0.44
1:E:48:ARG:CZ	1:E:48:ARG:HB2	2.47	0.44
1:F:178:SER:C	1:F:180:VAL:H	2.21	0.44
1:F:301:LEU:C	1:F:304:PRO:HD2	2.38	0.44
1:H:240:THR:HA	1:I:239:LEU:HD23	2.00	0.44
1:B:181:GLN:N	1:B:182:PRO:CD	2.81	0.44
1:D:119:PHE:CB	1:D:120:PRO:HD3	2.46	0.44
1:E:40:VAL:HA	1:E:102:TYR:O	2.17	0.44
1:E:292:ASP:O	1:E:297:GLN:NE2	2.51	0.44
1:F:303:PHE:C	1:F:303:PHE:CD1	2.91	0.44
1:J:92:LEU:HD23	1:J:92:LEU:HA	1.75	0.44
1:J:181:GLN:CG	1:J:182:PRO:HD3	2.40	0.44
1:J:248:THR:HG23	1:J:252:LEU:HD22	2.00	0.44
1:A:187:PHE:N	1:A:187:PHE:CD1	2.86	0.43
1:B:167:THR:CG2	1:B:168:HIS:H	2.20	0.43
1:B:169:ILE:CD1	1:B:190:ILE:HG12	2.48	0.43
1:D:147:VAL:O	1:D:149:THR:N	2.46	0.43
1:D:237:LEU:CD1	1:E:235:PHE:CE2	2.99	0.43
1:E:296:ILE:CG2	1:E:297:GLN:N	2.81	0.43
1:I:118:LEU:N	1:I:118:LEU:HD23	2.33	0.43
1:I:167:THR:O	1:I:168:HIS:HB2	2.17	0.43
1:J:145:ILE:H	1:J:145:ILE:CD1	2.14	0.43
1:J:181:GLN:N	1:J:182:PRO:CD	2.81	0.43
1:F:150:GLU:HB3	1:F:153:ASP:CB	2.47	0.43
1:G:127:VAL:HG22	1:G:193:ARG:HG2	1.98	0.43
1:G:185:ASN:N	1:G:185:ASN:ND2	2.67	0.43
1:A:309:ALA:O	1:A:313:VAL:HG23	2.18	0.43
1:F:119:PHE:CB	1:F:120:PRO:HD3	2.41	0.43
1:F:237:LEU:HD12	1:F:237:LEU:HA	1.91	0.43
1:F:251:ILE:CD1	1:G:249:SER:HB3	2.48	0.43
1:G:223:TRP:CD1	1:G:300:ARG:HD3	2.53	0.43
1:A:110:PHE:N	1:A:110:PHE:CD1	2.86	0.43
1:A:164:LYS:HZ3	1:A:164:LYS:HA	1.83	0.43
1:A:178:SER:C	1:A:180:VAL:H	2.22	0.43
1:B:303:PHE:N	1:B:304:PRO:HD3	2.33	0.43
1:F:133:PHE:HE2	1:J:91:ARG:HB2	1.84	0.43
1:G:285:ARG:NE	1:G:285:ARG:CA	2.82	0.43
1:B:173:ARG:HA	1:B:185:ASN:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:TRP:HB3	1:C:71:LEU:HD12	1.99	0.43
1:C:167:THR:O	1:C:168:HIS:CB	2.67	0.43
1:G:140:LEU:HD22	1:G:190:ILE:HD11	2.00	0.43
1:H:223:TRP:CD1	1:H:300:ARG:HD3	2.54	0.43
1:I:147:VAL:C	1:I:149:THR:H	2.20	0.43
1:J:149:THR:HG22	1:J:150:GLU:N	2.33	0.43
1:A:145:ILE:H	1:A:145:ILE:CD1	2.19	0.43
1:B:234:SER:HA	1:B:237:LEU:HB2	2.01	0.43
1:B:299:CYS:HB2	1:B:302:ALA:HB3	1.99	0.43
1:D:147:VAL:C	1:D:149:THR:H	2.21	0.43
1:E:149:THR:HG22	1:E:150:GLU:N	2.34	0.43
1:J:72:TRP:CD1	1:J:72:TRP:C	2.91	0.43
1:B:199:ASN:C	1:B:199:ASN:ND2	2.71	0.43
1:C:19:PHE:CE2	1:C:146:GLN:HG3	2.54	0.43
1:C:218:SER:CA	1:C:237:LEU:HD21	2.42	0.43
1:C:223:TRP:CD1	1:C:300:ARG:HD3	2.53	0.43
1:D:276:ILE:O	1:D:280:ILE:HG13	2.18	0.43
1:F:59:GLU:OE2	1:G:134:SER:OG	2.37	0.43
1:G:296:ILE:CG2	1:G:297:GLN:N	2.81	0.43
1:H:40:VAL:HA	1:H:102:TYR:O	2.19	0.43
1:H:149:THR:HG22	1:H:150:GLU:N	2.33	0.43
1:I:72:TRP:CZ2	1:I:74:PRO:CG	2.98	0.43
1:I:180:VAL:HG21	1:I:184:GLN:HB2	2.00	0.43
1:A:204:LEU:HA	1:A:208:ILE:HG12	2.00	0.43
1:C:119:PHE:HB3	1:C:259:THR:HB	2.01	0.43
1:C:150:GLU:CB	1:C:153:ASP:HB2	2.47	0.43
1:C:181:GLN:N	1:C:182:PRO:CD	2.81	0.43
1:D:119:PHE:HB3	1:D:259:THR:HB	2.00	0.43
1:D:178:SER:C	1:D:180:VAL:H	2.22	0.43
1:D:292:ASP:O	1:D:297:GLN:NE2	2.52	0.43
1:F:72:TRP:CZ3	1:F:135:TYR:CZ	3.05	0.43
1:F:147:VAL:C	1:F:149:THR:H	2.22	0.43
1:G:115:ASP:H	1:G:124:GLN:HE22	1.66	0.43
1:H:181:GLN:N	1:H:182:PRO:CD	2.81	0.43
1:I:16:VAL:HG12	1:I:17:SER:N	2.34	0.43
1:A:296:ILE:CG2	1:A:297:GLN:N	2.82	0.43
1:B:114:MET:CE	1:B:124:GLN:HG2	2.49	0.43
1:B:119:PHE:HB3	1:B:120:PRO:CD	2.42	0.43
1:C:79:ILE:HD13	1:C:79:ILE:HA	1.87	0.43
1:C:262:ASP:O	1:C:266:ILE:HG12	2.18	0.43
1:D:223:TRP:CD1	1:D:300:ARG:HD3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:309:ALA:O	1:E:313:VAL:HG23	2.18	0.43
1:F:176:HIS:CE1	1:J:148:TYR:OH	2.72	0.43
1:F:294:LEU:CA	1:F:297:GLN:HE21	2.22	0.43
1:G:145:ILE:H	1:G:145:ILE:CD1	2.17	0.43
1:G:204:LEU:HA	1:G:208:ILE:HG12	1.99	0.43
1:H:303:PHE:N	1:H:304:PRO:HD3	2.34	0.43
1:I:58:VAL:HB	1:I:92:LEU:HB2	2.01	0.43
1:J:150:GLU:HB3	1:J:153:ASP:CB	2.46	0.43
1:A:120:PRO:HD2	1:A:260:VAL:CG2	2.49	0.43
1:B:48:ARG:CZ	1:B:48:ARG:HB2	2.49	0.43
1:B:178:SER:C	1:B:180:VAL:H	2.23	0.43
1:C:200:PRO:O	1:C:201:SER:C	2.57	0.43
1:E:178:SER:C	1:E:180:VAL:H	2.21	0.43
1:F:248:THR:HG23	1:F:252:LEU:HD22	2.00	0.43
1:J:39:ILE:HG21	1:J:39:ILE:HD13	1.62	0.43
1:A:40:VAL:HA	1:A:102:TYR:O	2.19	0.42
1:A:92:LEU:HD23	1:A:92:LEU:HA	1.73	0.42
1:C:187:PHE:CD1	1:C:187:PHE:N	2.86	0.42
1:D:303:PHE:N	1:D:304:PRO:HD3	2.33	0.42
1:E:150:GLU:CB	1:E:153:ASP:HB2	2.46	0.42
1:F:239:LEU:HD13	1:G:239:LEU:HD21	2.00	0.42
1:G:145:ILE:HD12	1:G:145:ILE:N	2.21	0.42
1:G:157:ILE:HD12	1:H:115:ASP:HA	2.00	0.42
1:G:178:SER:C	1:G:180:VAL:H	2.21	0.42
1:I:140:LEU:HD22	1:I:190:ILE:HD11	2.01	0.42
1:I:181:GLN:N	1:I:182:PRO:CD	2.82	0.42
1:J:40:VAL:HA	1:J:102:TYR:O	2.19	0.42
1:J:300:ARG:O	1:J:304:PRO:HG2	2.19	0.42
1:D:112:ASN:ND2	1:D:127:VAL:CG2	2.82	0.42
1:D:127:VAL:HG22	1:D:193:ARG:HG2	2.01	0.42
1:D:167:THR:O	1:D:168:HIS:CB	2.66	0.42
1:E:204:LEU:HA	1:E:208:ILE:CG1	2.49	0.42
1:F:127:VAL:HG22	1:F:193:ARG:HG2	2.01	0.42
1:F:140:LEU:HD22	1:F:190:ILE:HD11	2.01	0.42
1:F:162:ILE:N	1:F:162:ILE:CD1	2.80	0.42
1:F:309:ALA:O	1:F:313:VAL:HG23	2.19	0.42
1:H:48:ARG:CZ	1:H:48:ARG:HB2	2.48	0.42
1:H:119:PHE:HB3	1:H:259:THR:HB	2.01	0.42
1:H:164:LYS:HZ2	1:H:164:LYS:CA	2.31	0.42
1:I:46:LYS:HA	1:I:47:PRO:HD2	1.78	0.42
1:I:89:ASN:O	1:I:104:ALA:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:143:SER:HB3	1:I:167:THR:HG21	2.01	0.42
1:A:231:LEU:HD12	1:A:280:ILE:HG12	2.01	0.42
1:A:250:ASN:HD22	1:E:250:ASN:ND2	2.18	0.42
1:B:97:ASP:OD1	1:B:99:ARG:HG2	2.19	0.42
1:B:301:LEU:C	1:B:304:PRO:HD2	2.39	0.42
1:C:167:THR:CG2	1:C:168:HIS:H	2.26	0.42
1:F:68:ASN:HA	1:J:65:ARG:NH1	2.34	0.42
1:F:147:VAL:CG2	1:F:165:ALA:HB2	2.49	0.42
1:G:301:LEU:C	1:G:304:PRO:HD2	2.39	0.42
1:A:223:TRP:NE1	1:A:300:ARG:HD3	2.34	0.42
1:A:234:SER:HA	1:A:237:LEU:HB2	2.02	0.42
1:A:301:LEU:C	1:A:304:PRO:HD2	2.39	0.42
1:B:200:PRO:O	1:B:201:SER:C	2.58	0.42
1:C:300:ARG:O	1:C:304:PRO:HG2	2.18	0.42
1:E:301:LEU:C	1:E:304:PRO:HD2	2.40	0.42
1:F:114:MET:HE3	1:F:124:GLN:HG2	2.01	0.42
1:F:251:ILE:O	1:F:251:ILE:CG2	2.67	0.42
1:G:118:LEU:N	1:G:118:LEU:HD23	2.35	0.42
1:I:292:ASP:O	1:I:297:GLN:NE2	2.53	0.42
1:J:27:ASN:HB3	1:J:32:THR:HB	2.01	0.42
1:J:59:GLU:O	1:J:63:ILE:HG13	2.19	0.42
1:A:147:VAL:C	1:A:149:THR:H	2.21	0.42
1:B:252:LEU:HG	1:B:253:PRO:HD2	2.01	0.42
1:C:251:ILE:O	1:C:251:ILE:CG2	2.68	0.42
1:E:120:PRO:HD2	1:E:260:VAL:CG2	2.50	0.42
1:F:83:GLY:HA2	1:J:107:LEU:HD23	2.02	0.42
1:F:164:LYS:HA	1:F:164:LYS:HZ3	1.85	0.42
1:G:309:ALA:O	1:G:313:VAL:HG23	2.19	0.42
1:I:23:ILE:HG21	1:I:126:PHE:CD2	2.55	0.42
1:A:48:ARG:HB2	1:A:48:ARG:CZ	2.49	0.42
1:A:136:ASN:ND2	1:A:184:GLN:HG3	2.34	0.42
1:B:162:ILE:HG22	1:B:163:ARG:N	2.26	0.42
1:C:92:LEU:HD23	1:C:92:LEU:HA	1.76	0.42
1:C:185:ASN:N	1:C:185:ASN:ND2	2.67	0.42
1:C:301:LEU:C	1:C:304:PRO:HD2	2.40	0.42
1:D:65:ARG:HD2	1:E:68:ASN:ND2	2.33	0.42
1:D:181:GLN:N	1:D:182:PRO:CD	2.81	0.42
1:E:150:GLU:HB3	1:E:153:ASP:CB	2.46	0.42
1:F:281:PHE:CZ	1:F:285:ARG:HG2	2.55	0.42
1:G:119:PHE:CB	1:G:120:PRO:CD	2.98	0.42
1:G:149:THR:HG22	1:G:150:GLU:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:ASN:HB3	1:B:32:THR:HB	2.00	0.42
1:B:89:ASN:O	1:B:104:ALA:HA	2.19	0.42
1:B:226:SER:HB3	1:B:229:GLU:OE1	2.19	0.42
1:B:296:ILE:CG2	1:B:297:GLN:N	2.82	0.42
1:C:303:PHE:N	1:C:304:PRO:HD3	2.34	0.42
1:D:130:LEU:HA	1:D:130:LEU:HD23	1.87	0.42
1:G:150:GLU:CB	1:G:153:ASP:HB2	2.46	0.42
1:G:187:PHE:CD1	1:G:187:PHE:N	2.88	0.42
1:H:140:LEU:HD22	1:H:190:ILE:HD11	2.01	0.42
1:I:48:ARG:HB2	1:I:48:ARG:CZ	2.50	0.42
1:I:162:ILE:HG22	1:I:163:ARG:N	2.26	0.42
1:J:48:ARG:CZ	1:J:48:ARG:HB2	2.49	0.42
1:J:296:ILE:CG2	1:J:297:GLN:N	2.83	0.42
1:A:15:SER:HG	1:A:142:PHE:HD1	1.65	0.42
1:A:145:ILE:HD12	1:A:145:ILE:N	2.19	0.42
1:A:300:ARG:O	1:A:304:PRO:HG2	2.19	0.42
1:C:28:THR:HB	1:C:255:LEU:CD2	2.41	0.42
1:C:97:ASP:OD1	1:C:99:ARG:HG2	2.20	0.42
1:D:48:ARG:HB2	1:D:48:ARG:CZ	2.50	0.42
1:D:204:LEU:HA	1:D:208:ILE:CG1	2.49	0.42
1:D:237:LEU:HD13	1:E:235:PHE:HD2	1.74	0.42
1:F:18:ILE:HB	1:F:145:ILE:HG22	2.02	0.42
1:F:119:PHE:O	1:F:120:PRO:C	2.58	0.42
1:G:285:ARG:C	1:G:285:ARG:HD3	2.40	0.42
1:I:120:PRO:HD2	1:I:260:VAL:CG2	2.50	0.42
1:J:216:ALA:C	1:J:218:SER:N	2.73	0.42
1:A:79:ILE:HD13	1:A:79:ILE:HA	1.83	0.42
1:A:223:TRP:CE3	1:B:280:ILE:HG22	2.55	0.42
1:C:181:GLN:O	1:C:182:PRO:C	2.58	0.42
1:C:224:LEU:HD21	1:D:231:LEU:HD22	2.00	0.42
1:G:72:TRP:HZ3	1:G:135:TYR:CE1	2.38	0.42
1:G:181:GLN:N	1:G:182:PRO:CD	2.82	0.42
1:G:200:PRO:O	1:G:201:SER:C	2.58	0.42
1:G:237:LEU:CD1	1:H:235:PHE:CD2	3.00	0.42
1:H:178:SER:C	1:H:180:VAL:H	2.22	0.42
1:H:218:SER:CA	1:H:237:LEU:HD21	2.43	0.42
1:I:120:PRO:HD2	1:I:260:VAL:HG23	2.01	0.42
1:I:208:ILE:HG23	1:I:264:MET:SD	2.59	0.42
1:A:288:ASN:OD1	1:A:291:GLU:HB3	2.19	0.42
1:D:46:LYS:HA	1:D:47:PRO:HD2	1.81	0.42
1:G:79:ILE:HD13	1:G:79:ILE:HA	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:234:SER:HA	1:G:237:LEU:HB2	2.01	0.42
1:I:178:SER:C	1:I:180:VAL:H	2.21	0.42
1:B:164:LYS:CD	1:I:163:ARG:HD2	2.41	0.41
1:C:119:PHE:O	1:C:120:PRO:C	2.58	0.41
1:C:204:LEU:HA	1:C:208:ILE:HG12	2.02	0.41
1:D:149:THR:HG22	1:D:150:GLU:N	2.35	0.41
1:E:167:THR:O	1:E:168:HIS:CB	2.68	0.41
1:I:209:LEU:C	1:I:209:LEU:CD2	2.89	0.41
1:J:119:PHE:CB	1:J:120:PRO:CD	2.98	0.41
1:J:178:SER:C	1:J:180:VAL:H	2.22	0.41
1:J:301:LEU:C	1:J:304:PRO:HD2	2.40	0.41
1:A:130:LEU:HD23	1:A:130:LEU:HA	1.84	0.41
1:A:140:LEU:HD12	1:A:188:SER:O	2.21	0.41
1:B:164:LYS:HG2	1:I:163:ARG:CB	2.21	0.41
1:C:157:ILE:HD11	1:D:115:ASP:CG	2.41	0.41
1:C:178:SER:C	1:C:180:VAL:H	2.23	0.41
1:C:231:LEU:HD12	1:C:280:ILE:HG12	2.02	0.41
1:C:251:ILE:O	1:C:251:ILE:HG22	2.18	0.41
1:F:119:PHE:HB3	1:F:259:THR:HB	2.02	0.41
1:F:149:THR:HG22	1:F:150:GLU:N	2.35	0.41
1:H:157:ILE:HD11	1:I:115:ASP:OD2	2.19	0.41
1:J:79:ILE:HD13	1:J:79:ILE:HA	1.83	0.41
1:J:115:ASP:H	1:J:124:GLN:HE22	1.68	0.41
1:A:303:PHE:N	1:A:304:PRO:HD3	2.35	0.41
1:B:140:LEU:HD13	1:B:190:ILE:CG1	2.41	0.41
1:D:15:SER:HG	1:D:142:PHE:HD1	1.66	0.41
1:F:216:ALA:C	1:F:218:SER:N	2.73	0.41
1:G:39:ILE:HD13	1:G:39:ILE:HG21	1.73	0.41
1:G:120:PRO:HB2	1:G:121:PHE:CE2	2.56	0.41
1:G:285:ARG:HD3	1:G:285:ARG:O	2.20	0.41
1:H:62:GLN:O	1:H:65:ARG:HB2	2.19	0.41
1:J:130:LEU:HD23	1:J:130:LEU:HA	1.82	0.41
1:A:122:ASP:HB2	1:A:198:ARG:HB2	2.03	0.41
1:A:149:THR:HG22	1:A:150:GLU:N	2.35	0.41
1:A:223:TRP:CD1	1:A:300:ARG:HD3	2.55	0.41
1:A:292:ASP:O	1:A:297:GLN:NE2	2.54	0.41
1:B:150:GLU:HB3	1:B:153:ASP:CB	2.48	0.41
1:C:147:VAL:C	1:C:149:THR:H	2.23	0.41
1:C:149:THR:HG22	1:C:150:GLU:N	2.35	0.41
1:F:92:LEU:HD23	1:F:92:LEU:HA	1.65	0.41
1:H:150:GLU:CB	1:H:153:ASP:HB2	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:114:MET:CE	1:I:124:GLN:HG2	2.51	0.41
1:I:172:ILE:CD1	1:I:189:ARG:HB3	2.49	0.41
1:A:28:THR:HB	1:A:255:LEU:CD2	2.47	0.41
1:A:249:SER:HG	1:E:247:TYR:HE1	1.63	0.41
1:B:223:TRP:NE1	1:B:300:ARG:HD3	2.35	0.41
1:C:125:GLN:OE1	1:C:193:ARG:HD3	2.21	0.41
1:D:59:GLU:OE1	1:E:75:ALA:HB2	2.21	0.41
1:D:187:PHE:CD1	1:D:187:PHE:N	2.88	0.41
1:F:141:ARG:HD3	1:F:142:PHE:CZ	2.55	0.41
1:I:149:THR:HG22	1:I:150:GLU:N	2.34	0.41
1:I:239:LEU:HD13	1:J:239:LEU:HD21	2.02	0.41
1:J:110:PHE:N	1:J:110:PHE:CD1	2.89	0.41
1:B:231:LEU:HD23	1:B:232:GLN:N	2.35	0.41
1:C:58:VAL:HB	1:C:92:LEU:HB2	2.03	0.41
1:E:66:TRP:HB3	1:E:71:LEU:HD12	2.03	0.41
1:F:136:ASN:ND2	1:F:184:GLN:HG3	2.36	0.41
1:G:147:VAL:HG23	1:G:165:ALA:HB2	2.02	0.41
1:G:303:PHE:N	1:G:304:PRO:HD3	2.35	0.41
1:H:136:ASN:ND2	1:H:184:GLN:HG3	2.36	0.41
1:H:231:LEU:HD12	1:H:280:ILE:HG12	2.02	0.41
1:H:300:ARG:O	1:H:304:PRO:HG2	2.21	0.41
1:I:172:ILE:HD12	1:I:172:ILE:N	2.35	0.41
1:A:39:ILE:HG21	1:A:39:ILE:HD13	1.63	0.41
1:A:119:PHE:O	1:A:120:PRO:C	2.57	0.41
1:C:23:ILE:HG21	1:C:126:PHE:CD2	2.56	0.41
1:C:46:LYS:HA	1:C:47:PRO:HD2	1.86	0.41
1:C:91:ARG:HD2	1:D:134:SER:HB2	2.02	0.41
1:D:66:TRP:HB3	1:D:71:LEU:HD12	2.03	0.41
1:E:300:ARG:O	1:E:304:PRO:HG2	2.20	0.41
1:F:39:ILE:HG13	1:F:106:PHE:CE2	2.56	0.41
1:F:185:ASN:N	1:F:185:ASN:ND2	2.68	0.41
1:H:23:ILE:HG21	1:H:126:PHE:CD2	2.56	0.41
1:H:187:PHE:CD1	1:H:187:PHE:N	2.88	0.41
1:A:237:LEU:HD12	1:A:237:LEU:HA	1.97	0.41
1:C:48:ARG:HB2	1:C:48:ARG:CZ	2.51	0.41
1:C:199:ASN:C	1:C:199:ASN:ND2	2.73	0.41
1:C:211:LEU:HD23	1:C:244:TYR:CE2	2.55	0.41
1:E:147:VAL:CG2	1:E:165:ALA:HB2	2.51	0.41
1:H:223:TRP:CE3	1:I:280:ILE:CG2	3.04	0.41
1:I:115:ASP:H	1:I:124:GLN:HE22	1.67	0.41
1:I:309:ALA:O	1:I:313:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:209:LEU:C	1:J:209:LEU:HD23	2.41	0.41
1:A:119:PHE:HB3	1:A:259:THR:HB	2.01	0.41
1:A:211:LEU:HD23	1:A:244:TYR:CE2	2.56	0.41
1:B:62:GLN:O	1:B:65:ARG:HB2	2.21	0.41
1:B:145:ILE:HG21	1:B:192:VAL:HG11	2.03	0.41
1:C:70:GLY:O	1:C:71:LEU:C	2.58	0.41
1:C:147:VAL:CG2	1:C:165:ALA:HB2	2.51	0.41
1:C:237:LEU:HD12	1:C:237:LEU:HA	1.84	0.41
1:D:28:THR:HB	1:D:255:LEU:CD2	2.45	0.41
1:D:114:MET:CE	1:D:124:GLN:HG2	2.50	0.41
1:D:301:LEU:C	1:D:304:PRO:HD2	2.42	0.41
1:E:89:ASN:O	1:E:104:ALA:HA	2.20	0.41
1:E:181:GLN:O	1:E:182:PRO:C	2.59	0.41
1:G:120:PRO:HD2	1:G:260:VAL:CG2	2.51	0.41
1:G:209:LEU:HB3	1:G:210:PRO:HD3	2.00	0.41
1:H:44:THR:HG23	1:H:99:ARG:H	1.86	0.41
1:I:40:VAL:HA	1:I:102:TYR:O	2.21	0.41
1:I:79:ILE:HD13	1:I:79:ILE:HA	1.86	0.41
1:I:97:ASP:OD1	1:I:99:ARG:HG2	2.20	0.41
1:I:248:THR:HG23	1:I:252:LEU:HD22	2.02	0.41
1:J:114:MET:HE2	1:J:124:GLN:HG2	2.02	0.41
1:J:208:ILE:HG12	1:J:208:ILE:H	1.67	0.41
1:A:285:ARG:NE	1:A:285:ARG:CA	2.83	0.41
1:B:70:GLY:O	1:B:71:LEU:C	2.59	0.41
1:B:164:LYS:HZ2	1:B:164:LYS:C	2.23	0.41
1:C:257:TYR:CD1	1:C:257:TYR:N	2.88	0.41
1:D:125:GLN:OE1	1:D:193:ARG:HD3	2.21	0.41
1:D:164:LYS:HZ2	1:D:164:LYS:CA	2.30	0.41
1:D:197:VAL:HG12	1:D:198:ARG:N	2.35	0.41
1:H:79:ILE:HD13	1:H:79:ILE:HA	1.81	0.41
1:H:209:LEU:C	1:H:209:LEU:HD23	2.41	0.41
1:I:285:ARG:NE	1:I:285:ARG:CA	2.84	0.41
1:J:119:PHE:O	1:J:120:PRO:C	2.58	0.41
1:J:237:LEU:HD12	1:J:237:LEU:HA	1.89	0.41
1:A:68:ASN:ND2	1:E:65:ARG:HD2	2.36	0.40
1:B:147:VAL:HG21	1:B:165:ALA:HB2	2.02	0.40
1:C:136:ASN:ND2	1:C:184:GLN:HG3	2.36	0.40
1:D:251:ILE:O	1:D:251:ILE:HG22	2.20	0.40
1:E:162:ILE:N	1:E:162:ILE:CD1	2.81	0.40
1:E:223:TRP:NE1	1:E:300:ARG:HD3	2.36	0.40
1:F:120:PRO:HD2	1:F:260:VAL:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:181:GLN:O	1:F:182:PRO:C	2.60	0.40
1:F:219:TRP:C	1:F:221:VAL:N	2.74	0.40
1:J:199:ASN:C	1:J:199:ASN:ND2	2.74	0.40
1:A:127:VAL:HG22	1:A:193:ARG:HG2	2.02	0.40
1:A:203:TYR:O	1:A:208:ILE:HG12	2.22	0.40
1:A:266:ILE:HD12	1:E:205:TRP:O	2.21	0.40
1:B:181:GLN:O	1:B:182:PRO:C	2.60	0.40
1:D:266:ILE:O	1:D:269:TYR:HB2	2.22	0.40
1:D:286:GLN:HA	1:D:291:GLU:OE1	2.22	0.40
1:G:19:PHE:CE2	1:G:146:GLN:HG3	2.55	0.40
1:H:136:ASN:ND2	1:H:184:GLN:HA	2.36	0.40
1:H:292:ASP:O	1:H:297:GLN:NE2	2.54	0.40
1:I:46:LYS:HD3	1:I:46:LYS:N	2.36	0.40
1:I:148:TYR:HE2	1:J:176:HIS:NE2	2.09	0.40
1:I:286:GLN:HA	1:I:291:GLU:OE1	2.21	0.40
1:A:114:MET:HE2	1:A:124:GLN:HG2	2.04	0.40
1:A:147:VAL:O	1:A:149:THR:N	2.47	0.40
1:D:181:GLN:O	1:D:182:PRO:C	2.59	0.40
1:F:286:GLN:HA	1:F:291:GLU:OE1	2.21	0.40
1:H:39:ILE:HD13	1:H:39:ILE:HG21	1.78	0.40
1:J:17:SER:O	1:J:40:VAL:HG23	2.20	0.40
1:J:114:MET:CE	1:J:124:GLN:HG2	2.52	0.40
1:J:147:VAL:CG2	1:J:165:ALA:HB2	2.51	0.40
1:J:147:VAL:C	1:J:149:THR:H	2.24	0.40
1:B:110:PHE:CD1	1:B:110:PHE:N	2.88	0.40
1:B:149:THR:HG22	1:B:150:GLU:N	2.36	0.40
1:C:294:LEU:CA	1:C:297:GLN:HE21	2.27	0.40
1:D:216:ALA:C	1:D:218:SER:N	2.74	0.40
1:E:73:VAL:HA	1:E:74:PRO:HD3	1.90	0.40
1:E:79:ILE:HD13	1:E:79:ILE:HA	1.84	0.40
1:F:46:LYS:HA	1:F:47:PRO:HD2	1.85	0.40
1:F:251:ILE:HD11	1:G:249:SER:HB3	2.03	0.40
1:G:77:GLU:CG	1:G:78:PHE:N	2.84	0.40
1:H:16:VAL:HA	1:H:40:VAL:O	2.22	0.40
1:H:148:TYR:HD1	1:H:148:TYR:HA	1.72	0.40
1:H:211:LEU:HD23	1:H:244:TYR:CE2	2.56	0.40
1:J:292:ASP:O	1:J:297:GLN:NE2	2.54	0.40
1:B:148:TYR:CE2	1:C:176:HIS:NE2	2.85	0.40
1:C:110:PHE:CD1	1:C:110:PHE:N	2.88	0.40
1:D:147:VAL:O	1:D:147:VAL:HG12	2.22	0.40
1:E:203:TYR:O	1:E:208:ILE:HG12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:199:ASN:C	1:F:199:ASN:ND2	2.75	0.40
1:H:19:PHE:CE2	1:H:146:GLN:HG3	2.56	0.40
1:H:181:GLN:O	1:H:182:PRO:C	2.60	0.40
1:J:16:VAL:HA	1:J:40:VAL:O	2.22	0.40
1:J:66:TRP:HB3	1:J:71:LEU:HD12	2.04	0.40
1:J:77:GLU:O	1:J:130:LEU:HD23	2.21	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:288:ASN:O	1:J:49:LYS:O[1_655]	1.93	0.27
1:D:139:GLN:NE2	1:G:173:ARG:NH2[2_354]	2.01	0.19
1:E:287:ALA:O	1:F:142:PHE:CD2[2_355]	2.12	0.08
1:A:291:GLU:OE1	1:D:49:LYS:NZ[1_556]	2.17	0.03

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	304/321 (95%)	237 (78%)	44 (14%)	23 (8%)	1	6
1	B	304/321 (95%)	238 (78%)	43 (14%)	23 (8%)	1	6
1	C	304/321 (95%)	237 (78%)	44 (14%)	23 (8%)	1	6
1	D	304/321 (95%)	238 (78%)	43 (14%)	23 (8%)	1	6
1	E	304/321 (95%)	237 (78%)	44 (14%)	23 (8%)	1	6
1	F	304/321 (95%)	236 (78%)	45 (15%)	23 (8%)	1	6
1	G	304/321 (95%)	236 (78%)	45 (15%)	23 (8%)	1	6
1	H	304/321 (95%)	237 (78%)	44 (14%)	23 (8%)	1	6
1	I	304/321 (95%)	238 (78%)	43 (14%)	23 (8%)	1	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	J	304/321 (95%)	237 (78%)	44 (14%)	23 (8%)	1 6
All	All	3040/3210 (95%)	2371 (78%)	439 (14%)	230 (8%)	1 6

All (230) 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	119	PHE
1	B	141	ARG
1	B	151	ASN
1	B	168	HIS
1	B	201	SER
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	D	53	ASP
1	D	141	ARG
1	D	151	ASN
1	D	168	HIS
1	D	201	SER
1	E	53	ASP
1	E	119	PHE
1	E	141	ARG
1	E	151	ASN
1	E	168	HIS
1	E	201	SER
1	F	53	ASP
1	F	119	PHE
1	F	141	ARG
1	F	151	ASN
1	F	168	HIS
1	F	201	SER
1	G	53	ASP

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Mol	Chain	Res	Type
1	G	119	PHE
1	G	141	ARG
1	G	151	ASN
1	G	168	HIS
1	G	201	SER
1	H	53	ASP
1	H	119	PHE
1	H	141	ARG
1	H	151	ASN
1	H	168	HIS
1	H	201	SER
1	I	53	ASP
1	I	119	PHE
1	I	141	ARG
1	I	151	ASN
1	I	168	HIS
1	I	201	SER
1	J	53	ASP
1	J	119	PHE
1	J	141	ARG
1	J	151	ASN
1	J	168	HIS
1	J	201	SER
1	A	99	ARG
1	A	165	ALA
1	A	183	ASN
1	B	99	ARG
1	B	183	ASN
1	B	288	ASN
1	C	99	ARG
1	C	165	ALA
1	C	183	ASN
1	C	288	ASN
1	D	99	ARG
1	D	119	PHE
1	D	183	ASN
1	D	288	ASN
1	E	99	ARG
1	E	165	ALA
1	E	183	ASN
1	E	288	ASN
1	F	99	ARG

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Mol	Chain	Res	Type
1	F	165	ALA
1	F	183	ASN
1	F	288	ASN
1	G	99	ARG
1	G	165	ALA
1	G	183	ASN
1	G	220	SER
1	G	288	ASN
1	H	99	ARG
1	H	165	ALA
1	H	183	ASN
1	I	99	ARG
1	I	183	ASN
1	I	288	ASN
1	J	99	ARG
1	J	165	ALA
1	J	183	ASN
1	J	288	ASN
1	J	293	ASP
1	A	79	ILE
1	A	185	ASN
1	A	220	SER
1	A	226	SER
1	A	288	ASN
1	A	293	ASP
1	B	165	ALA
1	B	185	ASN
1	B	220	SER
1	B	226	SER
1	B	293	ASP
1	C	185	ASN
1	C	220	SER
1	C	226	SER
1	C	293	ASP
1	D	79	ILE
1	D	165	ALA
1	D	185	ASN
1	D	220	SER
1	D	226	SER
1	D	293	ASP
1	E	185	ASN
1	E	220	SER

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Mol	Chain	Res	Type
1	E	226	SER
1	E	293	ASP
1	F	185	ASN
1	F	220	SER
1	F	226	SER
1	F	293	ASP
1	G	185	ASN
1	G	226	SER
1	G	293	ASP
1	H	79	ILE
1	H	185	ASN
1	H	220	SER
1	H	226	SER
1	H	288	ASN
1	H	293	ASP
1	I	165	ALA
1	I	185	ASN
1	I	220	SER
1	I	226	SER
1	I	293	ASP
1	J	185	ASN
1	J	220	SER
1	J	226	SER
1	A	148	TYR
1	B	47	PRO
1	B	60	ASN
1	B	79	ILE
1	B	148	TYR
1	C	148	TYR
1	D	47	PRO
1	D	148	TYR
1	E	79	ILE
1	E	148	TYR
1	F	47	PRO
1	F	79	ILE
1	F	148	TYR
1	G	47	PRO
1	G	79	ILE
1	G	148	TYR
1	H	148	TYR
1	I	79	ILE
1	I	148	TYR

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Mol	Chain	Res	Type
1	J	47	PRO
1	J	60	ASN
1	J	79	ILE
1	J	148	TYR
1	A	47	PRO
1	A	60	ASN
1	A	181	GLN
1	A	289	GLY
1	B	181	GLN
1	B	289	GLY
1	C	47	PRO
1	C	60	ASN
1	C	79	ILE
1	C	181	GLN
1	C	289	GLY
1	D	55	PRO
1	D	60	ASN
1	D	181	GLN
1	D	289	GLY
1	E	47	PRO
1	E	55	PRO
1	E	60	ASN
1	E	181	GLN
1	E	289	GLY
1	F	60	ASN
1	F	181	GLN
1	F	289	GLY
1	G	55	PRO
1	G	60	ASN
1	G	181	GLN
1	G	289	GLY
1	H	47	PRO
1	H	60	ASN
1	H	181	GLN
1	H	289	GLY
1	I	47	PRO
1	I	60	ASN
1	I	181	GLN
1	I	289	GLY
1	J	181	GLN
1	J	289	GLY
1	A	55	PRO

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Mol	Chain	Res	Type
1	A	182	PRO
1	B	55	PRO
1	B	182	PRO
1	C	55	PRO
1	C	182	PRO
1	D	182	PRO
1	E	182	PRO
1	F	55	PRO
1	F	182	PRO
1	G	182	PRO
1	H	55	PRO
1	H	182	PRO
1	I	182	PRO
1	J	182	PRO
1	I	55	PRO
1	J	55	PRO
1	A	303	PHE
1	B	303	PHE
1	C	303	PHE
1	D	303	PHE
1	E	303	PHE
1	F	303	PHE
1	G	303	PHE
1	H	303	PHE
1	I	303	PHE
1	J	303	PHE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	274/283 (97%)	249 (91%)	25 (9%)	9 31
1	B	274/283 (97%)	249 (91%)	25 (9%)	9 31
1	C	274/283 (97%)	250 (91%)	24 (9%)	10 33
1	D	274/283 (97%)	250 (91%)	24 (9%)	10 33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	274/283 (97%)	250 (91%)	24 (9%)	10 33
1	F	274/283 (97%)	250 (91%)	24 (9%)	10 33
1	G	274/283 (97%)	251 (92%)	23 (8%)	11 35
1	H	274/283 (97%)	250 (91%)	24 (9%)	10 33
1	I	274/283 (97%)	251 (92%)	23 (8%)	11 35
1	J	274/283 (97%)	250 (91%)	24 (9%)	10 33
All	All	2740/2830 (97%)	2500 (91%)	240 (9%)	10 33

All (240) 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	56	LEU
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	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
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

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Mol	Chain	Res	Type
1	B	56	LEU
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	154	ASN
1	B	162	ILE
1	B	171	ASP
1	B	176	HIS
1	B	177	LEU
1	B	181	GLN
1	B	184	GLN
1	B	185	ASN
1	B	199	ASN
1	B	252	LEU
1	B	285	ARG
1	B	286	GLN
1	B	303	PHE
1	C	29	LEU
1	C	40	VAL
1	C	43	TRP
1	C	50	THR
1	C	56	LEU
1	C	71	LEU
1	C	72	TRP
1	C	78	PHE
1	C	118	LEU
1	C	142	PHE
1	C	145	ILE
1	C	154	ASN
1	C	162	ILE
1	C	171	ASP
1	C	176	HIS
1	C	177	LEU
1	C	181	GLN
1	C	184	GLN
1	C	185	ASN
1	C	199	ASN
1	C	252	LEU

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Mol	Chain	Res	Type
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	138	GLN
1	D	142	PHE
1	D	145	ILE
1	D	154	ASN
1	D	162	ILE
1	D	171	ASP
1	D	176	HIS
1	D	177	LEU
1	D	181	GLN
1	D	184	GLN
1	D	185	ASN
1	D	199	ASN
1	D	252	LEU
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	138	GLN
1	E	142	PHE
1	E	145	ILE
1	E	154	ASN
1	E	162	ILE
1	E	171	ASP
1	E	176	HIS

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Mol	Chain	Res	Type
1	E	177	LEU
1	E	181	GLN
1	E	184	GLN
1	E	185	ASN
1	E	199	ASN
1	E	252	LEU
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	142	PHE
1	F	145	ILE
1	F	154	ASN
1	F	162	ILE
1	F	171	ASP
1	F	176	HIS
1	F	177	LEU
1	F	181	GLN
1	F	184	GLN
1	F	185	ASN
1	F	199	ASN
1	F	209	LEU
1	F	252	LEU
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
1	G	72	TRP
1	G	78	PHE
1	G	118	LEU
1	G	142	PHE

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Mol	Chain	Res	Type
1	G	145	ILE
1	G	154	ASN
1	G	162	ILE
1	G	171	ASP
1	G	176	HIS
1	G	177	LEU
1	G	181	GLN
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	154	ASN
1	H	162	ILE
1	H	171	ASP
1	H	176	HIS
1	H	177	LEU
1	H	181	GLN
1	H	184	GLN
1	H	185	ASN
1	H	199	ASN
1	H	252	LEU
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

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Mol	Chain	Res	Type
1	I	71	LEU
1	I	72	TRP
1	I	78	PHE
1	I	118	LEU
1	I	138	GLN
1	I	142	PHE
1	I	145	ILE
1	I	154	ASN
1	I	162	ILE
1	I	171	ASP
1	I	176	HIS
1	I	177	LEU
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	154	ASN
1	J	162	ILE
1	J	171	ASP
1	J	176	HIS
1	J	177	LEU
1	J	181	GLN
1	J	184	GLN
1	J	185	ASN
1	J	199	ASN
1	J	252	LEU
1	J	285	ARG
1	J	286	GLN

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Mol	Chain	Res	Type
1	J	303	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (103) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	124	GLN
1	A	136	ASN
1	A	151	ASN
1	A	154	ASN
1	A	185	ASN
1	A	199	ASN
1	A	232	GLN
1	A	250	ASN
1	A	297	GLN
1	B	42	GLN
1	B	62	GLN
1	B	68	ASN
1	B	124	GLN
1	B	136	ASN
1	B	151	ASN
1	B	154	ASN
1	B	185	ASN
1	B	199	ASN
1	B	263	GLN
1	B	297	GLN
1	C	42	GLN
1	C	62	GLN
1	C	124	GLN
1	C	136	ASN
1	C	151	ASN
1	C	154	ASN
1	C	185	ASN
1	C	199	ASN
1	C	232	GLN
1	C	250	ASN
1	C	263	GLN
1	C	297	GLN
1	D	42	GLN
1	D	62	GLN
1	D	124	GLN
1	D	136	ASN

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Mol	Chain	Res	Type
1	D	151	ASN
1	D	154	ASN
1	D	185	ASN
1	D	199	ASN
1	D	250	ASN
1	D	297	GLN
1	E	42	GLN
1	E	62	GLN
1	E	124	GLN
1	E	136	ASN
1	E	151	ASN
1	E	154	ASN
1	E	185	ASN
1	E	199	ASN
1	E	284	HIS
1	E	297	GLN
1	F	42	GLN
1	F	68	ASN
1	F	124	GLN
1	F	136	ASN
1	F	151	ASN
1	F	154	ASN
1	F	185	ASN
1	F	199	ASN
1	F	232	GLN
1	F	250	ASN
1	F	297	GLN
1	G	42	GLN
1	G	124	GLN
1	G	136	ASN
1	G	151	ASN
1	G	154	ASN
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	136	ASN
1	H	151	ASN
1	H	154	ASN
1	H	185	ASN

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Mol	Chain	Res	Type
1	H	199	ASN
1	H	250	ASN
1	H	263	GLN
1	H	297	GLN
1	I	42	GLN
1	I	62	GLN
1	I	124	GLN
1	I	136	ASN
1	I	139	GLN
1	I	151	ASN
1	I	154	ASN
1	I	185	ASN
1	I	199	ASN
1	I	263	GLN
1	I	297	GLN
1	J	42	GLN
1	J	124	GLN
1	J	136	ASN
1	J	151	ASN
1	J	154	ASN
1	J	185	ASN
1	J	199	ASN
1	J	263	GLN
1	J	297	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

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, 95^{th} 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%)	0.16	27 (8%)	10 10	64, 105, 278, 412	0
1	B	306/321 (95%)	0.15	22 (7%)	15 15	60, 103, 278, 412	0
1	C	306/321 (95%)	0.19	20 (6%)	18 18	60, 104, 278, 412	0
1	D	306/321 (95%)	0.28	21 (6%)	16 16	59, 103, 277, 401	0
1	E	306/321 (95%)	0.15	18 (5%)	22 22	62, 105, 278, 413	0
1	F	306/321 (95%)	0.09	21 (6%)	16 16	62, 105, 277, 412	0
1	G	306/321 (95%)	0.21	18 (5%)	22 22	59, 104, 277, 412	0
1	H	306/321 (95%)	0.37	29 (9%)	8 8	63, 104, 278, 413	0
1	I	306/321 (95%)	0.20	20 (6%)	18 18	56, 102, 278, 407	0
1	J	306/321 (95%)	0.14	32 (10%)	6 6	62, 105, 278, 412	0
All	All	3060/3210 (95%)	0.20	228 (7%)	14 13	56, 104, 287, 413	0

All (228) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	179	SER	18.6
1	E	289	GLY	16.4
1	H	290	VAL	14.6
1	H	289	GLY	11.4
1	C	152	ILE	11.0
1	H	178	SER	10.9
1	H	152	ILE	10.8
1	C	288	ASN	10.0
1	E	290	VAL	8.5
1	D	178	SER	8.4
1	A	152	ILE	7.9
1	B	290	VAL	7.8
1	I	181	GLN	7.7

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Mol	Chain	Res	Type	RSRZ
1	B	152	ILE	7.6
1	E	179	SER	7.6
1	D	153	ASP	7.4
1	B	289	GLY	7.0
1	C	289	GLY	6.8
1	B	288	ASN	6.5
1	F	181	GLN	6.4
1	E	152	ILE	6.3
1	A	316	ILE	6.3
1	I	178	SER	6.3
1	D	290	VAL	6.2
1	H	151	ASN	6.1
1	B	316	ILE	6.1
1	G	152	ILE	6.0
1	C	151	ASN	5.9
1	C	316	ILE	5.9
1	G	314	LEU	5.9
1	D	289	GLY	5.9
1	H	181	GLN	5.8
1	H	180	VAL	5.7
1	C	290	VAL	5.6
1	G	313	VAL	5.6
1	J	287	ALA	5.5
1	F	152	ILE	5.5
1	F	316	ILE	5.4
1	E	286	GLN	5.2
1	D	179	SER	5.2
1	D	177	LEU	5.1
1	H	288	ASN	5.1
1	G	151	ASN	5.1
1	G	156	GLU	5.1
1	I	289	GLY	5.1
1	A	291	GLU	5.1
1	A	185	ASN	4.9
1	I	180	VAL	4.9
1	E	178	SER	4.8
1	J	288	ASN	4.8
1	J	305	LEU	4.7
1	H	148	TYR	4.7
1	D	49	LYS	4.7
1	D	157	ILE	4.6
1	F	177	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	305	LEU	4.5
1	B	151	ASN	4.5
1	A	313	VAL	4.4
1	F	289	GLY	4.4
1	J	152	ILE	4.4
1	C	287	ALA	4.4
1	G	179	SER	4.3
1	G	312	CYS	4.3
1	A	174	TYR	4.3
1	B	179	SER	4.3
1	D	182	PRO	4.2
1	F	285	ARG	4.2
1	H	287	ALA	4.1
1	D	287	ALA	4.1
1	A	314	LEU	4.0
1	E	153	ASP	4.0
1	F	176	HIS	4.0
1	F	286	GLN	4.0
1	F	175	ASP	4.0
1	J	303	PHE	3.9
1	I	287	ALA	3.9
1	A	312	CYS	3.9
1	I	294	LEU	3.8
1	E	288	ASN	3.8
1	I	179	SER	3.8
1	H	314	LEU	3.7
1	H	291	GLU	3.7
1	I	290	VAL	3.7
1	F	173	ARG	3.6
1	B	295	LEU	3.6
1	J	304	PRO	3.6
1	H	305	LEU	3.6
1	A	305	LEU	3.6
1	I	177	LEU	3.6
1	D	154	ASN	3.6
1	E	177	LEU	3.6
1	E	182	PRO	3.6
1	J	286	GLN	3.6
1	B	178	SER	3.5
1	D	176	HIS	3.5
1	E	157	ILE	3.5
1	H	163	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	315	VAL	3.4
1	H	138	GLN	3.3
1	F	174	TYR	3.3
1	B	177	LEU	3.3
1	H	313	VAL	3.3
1	C	179	SER	3.2
1	J	289	GLY	3.2
1	A	309	ALA	3.2
1	A	176	HIS	3.2
1	B	297	GLN	3.2
1	D	150	GLU	3.1
1	F	151	ASN	3.1
1	H	292	ASP	3.1
1	A	286	GLN	3.1
1	F	141	ARG	3.1
1	A	151	ASN	3.1
1	D	288	ASN	3.1
1	A	285	ARG	3.1
1	J	179	SER	3.0
1	C	182	PRO	3.0
1	J	156	GLU	3.0
1	C	161	TRP	3.0
1	B	296	ILE	3.0
1	C	294	LEU	3.0
1	C	313	VAL	3.0
1	H	182	PRO	3.0
1	J	236	THR	2.9
1	C	302	ALA	2.9
1	H	177	LEU	2.9
1	D	286	GLN	2.9
1	I	284	HIS	2.9
1	H	153	ASP	2.9
1	D	181	GLN	2.9
1	H	184	GLN	2.9
1	A	175	ASP	2.8
1	J	307	PHE	2.8
1	G	288	ASN	2.8
1	B	236	THR	2.8
1	F	290	VAL	2.8
1	C	181	GLN	2.8
1	F	287	ALA	2.8
1	A	172	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	187	PHE	2.8
1	I	236	THR	2.8
1	J	302	ALA	2.8
1	B	138	GLN	2.7
1	B	291	GLU	2.7
1	F	157	ILE	2.7
1	C	171	ASP	2.7
1	B	157	ILE	2.7
1	F	178	SER	2.7
1	D	305	LEU	2.7
1	I	295	LEU	2.7
1	G	309	ALA	2.7
1	A	177	LEU	2.7
1	C	306	GLY	2.7
1	A	289	GLY	2.7
1	B	148	TYR	2.6
1	J	290	VAL	2.6
1	I	176	HIS	2.6
1	G	289	GLY	2.6
1	G	301	LEU	2.6
1	A	296	ILE	2.6
1	B	287	ALA	2.6
1	J	285	ARG	2.5
1	J	151	ASN	2.5
1	A	173	ARG	2.5
1	H	310	ILE	2.5
1	J	291	GLU	2.5
1	J	314	LEU	2.5
1	C	183	ASN	2.5
1	H	161	TRP	2.5
1	H	316	ILE	2.5
1	A	184	GLN	2.5
1	A	236	THR	2.5
1	I	153	ASP	2.5
1	I	157	ILE	2.5
1	I	185	ASN	2.4
1	H	173	ARG	2.4
1	E	154	ASN	2.4
1	J	281	PHE	2.4
1	F	49	LYS	2.4
1	J	313	VAL	2.4
1	B	294	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	J	301	LEU	2.4
1	I	286	GLN	2.4
1	J	316	ILE	2.4
1	G	286	GLN	2.4
1	F	182	PRO	2.4
1	A	294	LEU	2.3
1	J	280	ILE	2.3
1	D	296	ILE	2.3
1	J	157	ILE	2.3
1	G	181	GLN	2.3
1	A	281	PHE	2.3
1	G	139	GLN	2.3
1	D	158	ASP	2.3
1	I	283	HIS	2.3
1	J	292	ASP	2.3
1	F	142	PHE	2.3
1	G	296	ILE	2.3
1	E	148	TYR	2.3
1	J	52	GLY	2.2
1	E	302	ALA	2.2
1	J	257	TYR	2.2
1	J	49	LYS	2.2
1	G	294	LEU	2.2
1	F	156	GLU	2.2
1	C	314	LEU	2.2
1	E	287	ALA	2.2
1	A	315	VAL	2.2
1	J	172	ILE	2.1
1	J	308	LEU	2.1
1	B	292	ASP	2.1
1	D	205	TRP	2.1
1	E	236	THR	2.1
1	H	240	THR	2.1
1	D	285	ARG	2.1
1	J	173	ARG	2.1
1	A	178	SER	2.0
1	G	303	PHE	2.0
1	H	156	GLU	2.0
1	I	148	TYR	2.0
1	G	311	GLY	2.0
1	B	303	PHE	2.0
1	B	302	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	H	164	LYS	2.0
1	J	158	ASP	2.0
1	E	151	ASN	2.0
1	I	240	THR	2.0
1	E	285	ARG	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.