



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:24 AM GMT

PDB ID : 3EHZ
Title : X-ray structure of the pentameric ligand gated ion channel of *Gloeobacter violaceus* (GLIC) in a presumptive open conformation
Authors : Hilf, R.J.C.; Dutzler, R.
Deposited on : 2008-09-15
Resolution : 3.10 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

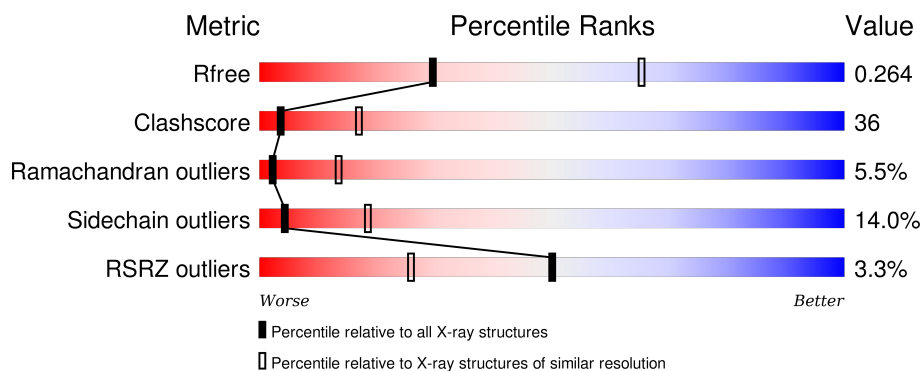
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	317	<div> <div>3%</div> <div>41%</div> <div>46%</div> <div>11%</div> <div>.</div> </div>
1	B	317	<div> <div>3%</div> <div>42%</div> <div>44%</div> <div>11%</div> <div>..</div> </div>
1	C	317	<div> <div>4%</div> <div>44%</div> <div>42%</div> <div>11%</div> <div>..</div> </div>
1	D	317	<div> <div>3%</div> <div>44%</div> <div>42%</div> <div>12%</div> <div>.</div> </div>
1	E	317	<div> <div>3%</div> <div>43%</div> <div>44%</div> <div>11%</div> <div>.</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12652 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 Glr4197 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2521	1662	403	452	4			
1	B	310	Total	C	N	O	S	0	0	0
			2521	1662	403	452	4			
1	C	310	Total	C	N	O	S	0	0	0
			2521	1662	403	452	4			
1	D	310	Total	C	N	O	S	0	0	0
			2521	1662	403	452	4			
1	E	310	Total	C	N	O	S	0	0	0
			2521	1662	403	452	4			

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	EXPRESSION TAG	UNP Q7NDN8
A	1	GLN	-	EXPRESSION TAG	UNP Q7NDN8
A	2	ASP	-	EXPRESSION TAG	UNP Q7NDN8
A	3	MET	-	EXPRESSION TAG	UNP Q7NDN8
A	4	VAL	-	EXPRESSION TAG	UNP Q7NDN8
A	5	SER	-	EXPRESSION TAG	UNP Q7NDN8
A	6	PRO	-	EXPRESSION TAG	UNP Q7NDN8
B	0	GLY	-	EXPRESSION TAG	UNP Q7NDN8
B	1	GLN	-	EXPRESSION TAG	UNP Q7NDN8
B	2	ASP	-	EXPRESSION TAG	UNP Q7NDN8
B	3	MET	-	EXPRESSION TAG	UNP Q7NDN8
B	4	VAL	-	EXPRESSION TAG	UNP Q7NDN8
B	5	SER	-	EXPRESSION TAG	UNP Q7NDN8
B	6	PRO	-	EXPRESSION TAG	UNP Q7NDN8
C	0	GLY	-	EXPRESSION TAG	UNP Q7NDN8
C	1	GLN	-	EXPRESSION TAG	UNP Q7NDN8
C	2	ASP	-	EXPRESSION TAG	UNP Q7NDN8
C	3	MET	-	EXPRESSION TAG	UNP Q7NDN8
C	4	VAL	-	EXPRESSION TAG	UNP Q7NDN8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	5	SER	-	EXPRESSION TAG	UNP Q7NDN8
C	6	PRO	-	EXPRESSION TAG	UNP Q7NDN8
D	0	GLY	-	EXPRESSION TAG	UNP Q7NDN8
D	1	GLN	-	EXPRESSION TAG	UNP Q7NDN8
D	2	ASP	-	EXPRESSION TAG	UNP Q7NDN8
D	3	MET	-	EXPRESSION TAG	UNP Q7NDN8
D	4	VAL	-	EXPRESSION TAG	UNP Q7NDN8
D	5	SER	-	EXPRESSION TAG	UNP Q7NDN8
D	6	PRO	-	EXPRESSION TAG	UNP Q7NDN8
E	0	GLY	-	EXPRESSION TAG	UNP Q7NDN8
E	1	GLN	-	EXPRESSION TAG	UNP Q7NDN8
E	2	ASP	-	EXPRESSION TAG	UNP Q7NDN8
E	3	MET	-	EXPRESSION TAG	UNP Q7NDN8
E	4	VAL	-	EXPRESSION TAG	UNP Q7NDN8
E	5	SER	-	EXPRESSION TAG	UNP Q7NDN8
E	6	PRO	-	EXPRESSION TAG	UNP Q7NDN8

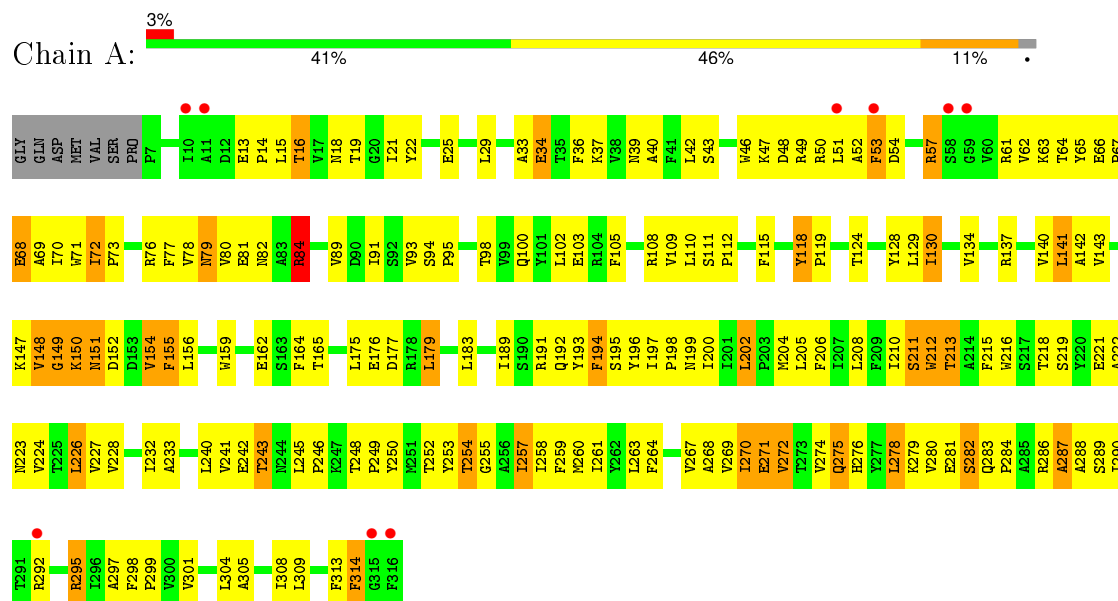
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	8	Total O 8 8	0	0
2	B	9	Total O 9 9	0	0
2	C	11	Total O 11 11	0	0
2	D	10	Total O 10 10	0	0
2	E	9	Total O 9 9	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

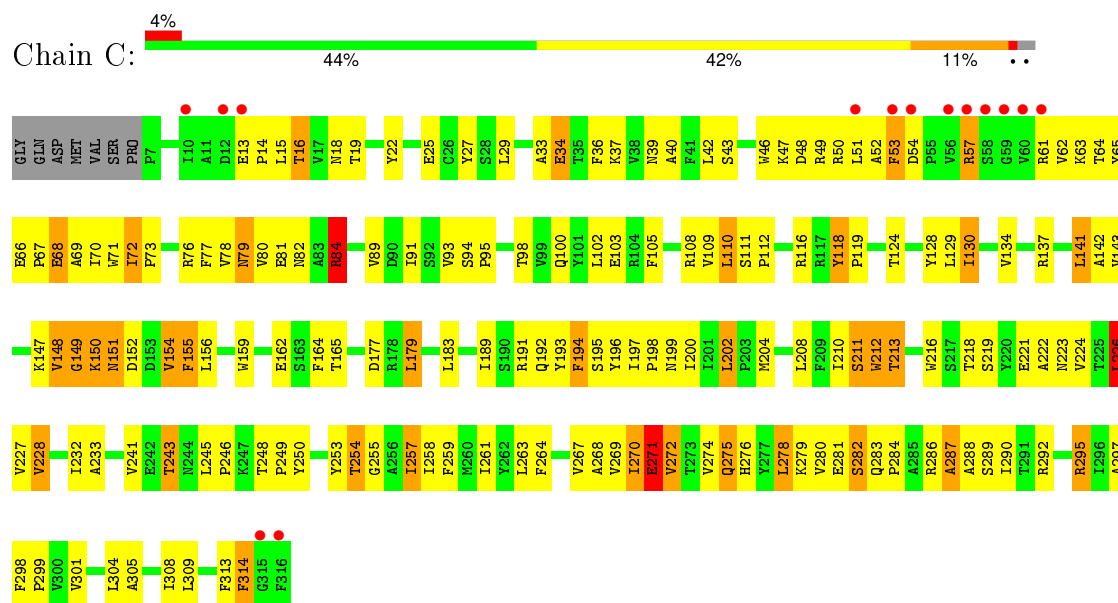
• Molecule 1: Glr4197 protein



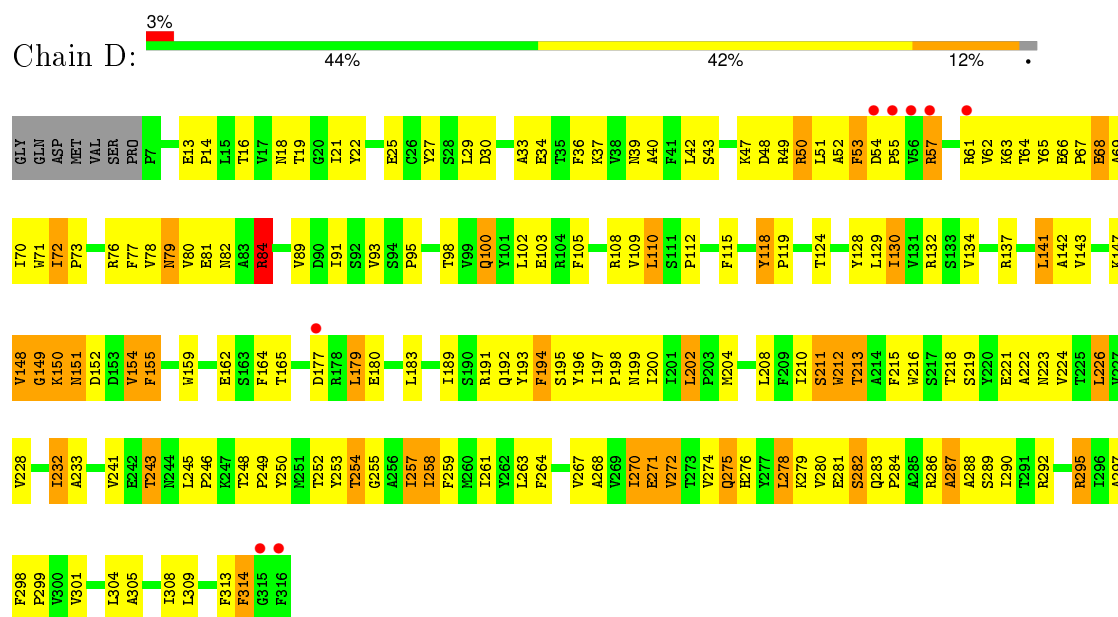
• Molecule 1: Glr4197 protein



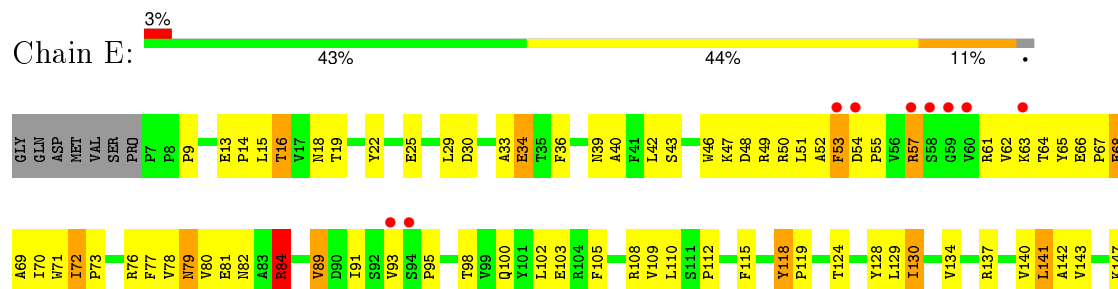
- Molecule 1: Glr4197 protein



- Molecule 1: Glr4197 protein



- Molecule 1: Glr4197 protein



A297	V227	V148
F298	V228	K149
P299		K150
V300	T232	N151
V301	A233	D152
		D153
L304	V241	F154
A305	E242	F155
	T243	L156
I308	N244	
L309	L245	W159
	T246	
F313	T247	E162
F314	T248	S163
	P249	F164
G315	V250	T165
F316	N251	
	T252	L175
	T253	E176
	T254	D177
	G255	R178
	A256	L179
	T257	
	L258	L183
	F259	
	M260	I189
	T261	S190
	V262	R191
	L263	Q192
	F264	Y193
		F194
	V267	S195
	A268	Y196
	V269	I197
	T270	P198
	E271	N199
	V272	I200
	T273	I201
	V274	L202
	Q275	P203
	T276	M204
	V277	
	L278	L208
	T279	F209
	V280	I210
	E281	S211
	S282	W212
	Q283	T213
	F284	
	A285	W216
	T286	S217
	A287	T218
	A288	S219
	S289	Y220
	T290	E221
	T291	A222
	R292	N223
		V224
	R295	T225
		T226

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	179.22Å 132.86Å 161.42Å 90.00° 102.19° 90.00°	Depositor
Resolution (Å)	19.97 – 3.10 29.86 – 3.09	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.97-3.10) 99.5 (29.86-3.09)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 3.11Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.238 , 0.266 0.234 , 0.264	Depositor DCC
R_{free} test set	3356 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	77.1	Xtriage
Anisotropy	0.296	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 63.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 67466 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	12652	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.49	0/2589	0.67	0/3535
1	B	0.49	0/2589	0.68	1/3535 (0.0%)
1	C	0.49	0/2589	0.67	0/3535
1	D	0.51	0/2589	0.67	0/3535
1	E	0.50	0/2589	0.67	0/3535
All	All	0.49	0/12945	0.67	1/17675 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	84	ARG	NE-CZ-NH1	5.62	123.11	120.30

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	2521	0	2537	190	0
1	B	2521	0	2537	190	0
1	C	2521	0	2537	185	0
1	D	2521	0	2537	189	0
1	E	2521	0	2537	182	0
2	A	8	0	0	0	0
2	B	9	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	11	0	0	0	0
2	D	10	0	0	0	0
2	E	9	0	0	0	0
All	All	12652	0	12685	906	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 36.

All (906) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:22:TYR:HA	1:D:149:GLY:HA2	1.43	0.99
1:C:22:TYR:HA	1:C:149:GLY:HA2	1.46	0.97
1:B:13:GLU:HB3	1:B:14:PRO:HD2	1.47	0.97
1:B:22:TYR:HA	1:B:149:GLY:HA2	1.43	0.96
1:C:13:GLU:HB3	1:C:14:PRO:HD2	1.48	0.96
1:E:22:TYR:HA	1:E:149:GLY:HA2	1.47	0.95
1:E:13:GLU:HB3	1:E:14:PRO:HD2	1.47	0.95
1:D:13:GLU:HB3	1:D:14:PRO:HD2	1.47	0.93
1:A:22:TYR:HA	1:A:149:GLY:HA2	1.47	0.93
1:A:13:GLU:HB3	1:A:14:PRO:HD2	1.48	0.92
1:E:151:ASN:HD22	1:E:152:ASP:H	1.17	0.92
1:A:151:ASN:HD22	1:A:152:ASP:H	1.18	0.91
1:D:22:TYR:HA	1:D:149:GLY:CA	2.00	0.91
1:A:77:PHE:CD1	1:A:84:ARG:HD2	2.05	0.91
1:E:77:PHE:CD1	1:E:84:ARG:HD2	2.08	0.89
1:B:22:TYR:HA	1:B:149:GLY:CA	2.01	0.89
1:C:77:PHE:CD1	1:C:84:ARG:HD2	2.07	0.89
1:D:54:ASP:HB2	1:D:57:ARG:HB2	1.52	0.89
1:B:147:LYS:C	1:B:149:GLY:H	1.76	0.89
1:B:78:VAL:HG22	1:B:130:ILE:HG12	1.55	0.88
1:D:77:PHE:CD1	1:D:84:ARG:HD2	2.07	0.88
1:C:151:ASN:HD22	1:C:152:ASP:H	1.20	0.88
1:E:147:LYS:C	1:E:149:GLY:H	1.76	0.88
1:D:84:ARG:HB2	1:D:84:ARG:HH11	1.39	0.88
1:E:141:LEU:HD23	1:E:142:ALA:H	1.40	0.88
1:E:84:ARG:HH11	1:E:84:ARG:HB2	1.40	0.87
1:C:54:ASP:HB2	1:C:57:ARG:HB2	1.56	0.87
1:E:22:TYR:HA	1:E:149:GLY:CA	2.04	0.87
1:E:54:ASP:HB2	1:E:57:ARG:HB2	1.57	0.87
1:B:77:PHE:CD1	1:B:84:ARG:HD2	2.09	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:LYS:C	1:A:149:GLY:H	1.78	0.87
1:B:249:PRO:HD2	1:B:250:TYR:CD1	2.10	0.86
1:E:197:ILE:HB	1:E:198:PRO:HD3	1.58	0.86
1:D:197:ILE:HB	1:D:198:PRO:HD3	1.57	0.86
1:B:151:ASN:HD22	1:B:152:ASP:H	1.21	0.86
1:E:249:PRO:HD2	1:E:250:TYR:CD1	2.11	0.86
1:D:77:PHE:HD1	1:D:84:ARG:HD2	1.41	0.86
1:A:249:PRO:HD2	1:A:250:TYR:CD1	2.11	0.86
1:B:54:ASP:HB2	1:B:57:ARG:HB2	1.57	0.85
1:A:22:TYR:HA	1:A:149:GLY:CA	2.05	0.85
1:C:249:PRO:HD2	1:C:250:TYR:CD1	2.12	0.85
1:D:151:ASN:HD22	1:D:152:ASP:H	1.21	0.85
1:C:147:LYS:C	1:C:149:GLY:H	1.77	0.85
1:C:22:TYR:HA	1:C:149:GLY:CA	2.05	0.85
1:B:141:LEU:HD23	1:B:142:ALA:H	1.42	0.84
1:C:197:ILE:HB	1:C:198:PRO:HD3	1.58	0.84
1:D:249:PRO:HD2	1:D:250:TYR:CD1	2.13	0.84
1:D:84:ARG:NH1	1:D:84:ARG:HB2	1.93	0.84
1:C:79:ASN:HD22	1:C:79:ASN:H	1.26	0.83
1:D:141:LEU:HD23	1:D:142:ALA:H	1.41	0.83
1:D:78:VAL:HG22	1:D:130:ILE:HG12	1.60	0.83
1:C:84:ARG:HB2	1:C:84:ARG:HH11	1.44	0.83
1:B:197:ILE:HB	1:B:198:PRO:HD3	1.59	0.83
1:A:78:VAL:HG22	1:A:130:ILE:HG12	1.61	0.83
1:A:54:ASP:HB2	1:A:57:ARG:HB2	1.59	0.82
1:E:84:ARG:HB2	1:E:84:ARG:NH1	1.95	0.82
1:D:79:ASN:HD22	1:D:79:ASN:H	1.26	0.82
1:A:84:ARG:HB2	1:A:84:ARG:HH11	1.43	0.82
1:E:78:VAL:HG22	1:E:130:ILE:HG12	1.60	0.82
1:C:77:PHE:HD1	1:C:84:ARG:HD2	1.45	0.82
1:A:84:ARG:HB2	1:A:84:ARG:NH1	1.95	0.82
1:D:147:LYS:C	1:D:149:GLY:H	1.79	0.81
1:A:77:PHE:HD1	1:A:84:ARG:HD2	1.42	0.81
1:D:84:ARG:CB	1:D:84:ARG:HH11	1.94	0.81
1:A:79:ASN:HD22	1:A:79:ASN:H	1.25	0.81
1:D:149:GLY:O	1:D:150:LYS:HB2	1.81	0.81
1:E:84:ARG:HH11	1:E:84:ARG:CB	1.93	0.81
1:B:79:ASN:H	1:B:79:ASN:HD22	1.25	0.81
1:C:78:VAL:HG22	1:C:130:ILE:HG12	1.63	0.81
1:B:80:VAL:HG12	1:B:82:ASN:O	1.80	0.81
1:A:197:ILE:HB	1:A:198:PRO:HD3	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:ARG:NH2	1:A:130:ILE:HD12	1.96	0.80
1:B:149:GLY:O	1:B:150:LYS:HB2	1.79	0.80
1:A:141:LEU:HD23	1:A:142:ALA:H	1.46	0.79
1:C:84:ARG:NH1	1:C:84:ARG:HB2	1.97	0.79
1:B:84:ARG:HH11	1:B:84:ARG:HB2	1.45	0.79
1:D:128:TYR:O	1:D:129:LEU:HB2	1.83	0.79
1:A:84:ARG:CB	1:A:84:ARG:HH11	1.95	0.79
1:E:80:VAL:HG12	1:E:82:ASN:O	1.83	0.79
1:C:149:GLY:O	1:C:150:LYS:HB2	1.81	0.79
1:E:149:GLY:O	1:E:150:LYS:HB2	1.81	0.79
1:B:77:PHE:HD1	1:B:84:ARG:HD2	1.44	0.79
1:E:76:ARG:NH2	1:E:130:ILE:HD12	1.98	0.79
1:E:79:ASN:HD22	1:E:79:ASN:H	1.30	0.79
1:B:84:ARG:NH1	1:B:84:ARG:HB2	1.98	0.78
1:D:80:VAL:HG12	1:D:82:ASN:O	1.82	0.78
1:E:77:PHE:HD1	1:E:84:ARG:HD2	1.45	0.78
1:D:76:ARG:NH2	1:D:130:ILE:HD12	1.99	0.78
1:D:48:ASP:O	1:D:51:LEU:HD23	1.82	0.78
1:A:149:GLY:O	1:A:150:LYS:HB2	1.81	0.78
1:B:13:GLU:HB3	1:B:14:PRO:CD	2.13	0.78
1:A:128:TYR:O	1:A:129:LEU:HB2	1.84	0.77
1:C:76:ARG:NH2	1:C:130:ILE:HD12	1.99	0.77
1:B:76:ARG:NH2	1:B:130:ILE:HD12	1.98	0.77
1:C:80:VAL:HG12	1:C:82:ASN:O	1.84	0.77
1:C:141:LEU:HD23	1:C:142:ALA:H	1.47	0.77
1:C:13:GLU:HB3	1:C:14:PRO:CD	2.14	0.77
1:A:13:GLU:HB3	1:A:14:PRO:CD	2.14	0.77
1:E:13:GLU:HB3	1:E:14:PRO:CD	2.14	0.77
1:A:80:VAL:HG12	1:A:82:ASN:O	1.85	0.77
1:D:13:GLU:HB3	1:D:14:PRO:CD	2.14	0.76
1:C:84:ARG:CB	1:C:84:ARG:HH11	1.97	0.76
1:E:128:TYR:O	1:E:129:LEU:HB2	1.84	0.76
1:B:84:ARG:CB	1:B:84:ARG:HH11	1.99	0.76
1:A:208:LEU:O	1:A:211:SER:HB3	1.87	0.75
1:C:48:ASP:O	1:C:51:LEU:HD23	1.87	0.74
1:C:128:TYR:O	1:C:129:LEU:HB2	1.87	0.74
1:E:208:LEU:O	1:E:211:SER:HB3	1.88	0.74
1:B:208:LEU:O	1:B:211:SER:HB3	1.87	0.73
1:E:48:ASP:O	1:E:51:LEU:HD23	1.88	0.72
1:D:253:TYR:HA	1:D:313:PHE:CE2	2.24	0.72
1:E:249:PRO:HD2	1:E:250:TYR:HD1	1.53	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:208:LEU:O	1:D:211:SER:HB3	1.89	0.72
1:D:77:PHE:H	1:D:84:ARG:HD3	1.55	0.72
1:A:151:ASN:HD22	1:A:152:ASP:N	1.87	0.72
1:D:249:PRO:HD2	1:D:250:TYR:HD1	1.54	0.72
1:E:147:LYS:HE2	1:E:165:THR:HA	1.72	0.72
1:B:128:TYR:O	1:B:129:LEU:HB2	1.90	0.72
1:A:249:PRO:HD2	1:A:250:TYR:HD1	1.54	0.71
1:E:151:ASN:HD22	1:E:152:ASP:N	1.87	0.71
1:A:147:LYS:HE2	1:A:165:THR:HA	1.72	0.71
1:E:66:GLU:HG3	1:E:67:PRO:HD2	1.72	0.71
1:B:66:GLU:HG3	1:B:67:PRO:HD2	1.73	0.70
1:B:249:PRO:HD2	1:B:250:TYR:HD1	1.53	0.70
1:A:48:ASP:O	1:A:51:LEU:HD23	1.91	0.70
1:A:253:TYR:HA	1:A:313:PHE:CE2	2.26	0.70
1:C:208:LEU:O	1:C:211:SER:HB3	1.92	0.70
1:E:253:TYR:HA	1:E:313:PHE:CE2	2.25	0.70
1:E:151:ASN:ND2	1:E:152:ASP:H	1.89	0.70
1:A:77:PHE:H	1:A:84:ARG:HD3	1.56	0.70
1:E:282:SER:C	1:E:284:PRO:HD3	2.12	0.70
1:D:42:LEU:HB3	1:D:103:GLU:HG2	1.72	0.70
1:A:151:ASN:ND2	1:A:152:ASP:H	1.90	0.70
1:B:76:ARG:HH22	1:B:130:ILE:HD12	1.57	0.70
1:C:253:TYR:HA	1:C:313:PHE:CE2	2.26	0.69
1:E:275:GLN:O	1:E:275:GLN:HG2	1.91	0.69
1:C:282:SER:C	1:C:284:PRO:HD3	2.11	0.69
1:B:48:ASP:O	1:B:51:LEU:HD23	1.90	0.69
1:D:151:ASN:HD22	1:D:152:ASP:N	1.90	0.69
1:B:147:LYS:C	1:B:149:GLY:N	2.46	0.69
1:C:77:PHE:H	1:C:84:ARG:HD3	1.57	0.69
1:C:151:ASN:HD22	1:C:152:ASP:N	1.90	0.69
1:B:80:VAL:CG1	1:B:82:ASN:O	2.40	0.69
1:B:282:SER:C	1:B:284:PRO:HD3	2.13	0.69
1:B:202:LEU:HD12	1:C:259:PHE:CZ	2.28	0.69
1:E:42:LEU:HB3	1:E:103:GLU:HG2	1.75	0.69
1:A:76:ARG:HH22	1:A:130:ILE:HD12	1.57	0.69
1:C:151:ASN:ND2	1:C:152:ASP:H	1.91	0.68
1:B:275:GLN:HG2	1:B:275:GLN:O	1.93	0.68
1:C:147:LYS:C	1:C:149:GLY:N	2.47	0.68
1:B:253:TYR:HA	1:B:313:PHE:CE2	2.27	0.68
1:C:275:GLN:HG2	1:C:275:GLN:O	1.93	0.68
1:B:77:PHE:H	1:B:84:ARG:HD3	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:249:PRO:HD2	1:C:250:TYR:HD1	1.55	0.68
1:C:147:LYS:HE2	1:C:165:THR:HA	1.74	0.68
1:D:282:SER:C	1:D:284:PRO:HD3	2.14	0.68
1:A:42:LEU:HB3	1:A:103:GLU:HG2	1.77	0.67
1:E:76:ARG:HH22	1:E:130:ILE:HD12	1.57	0.67
1:A:282:SER:C	1:A:284:PRO:HD3	2.14	0.67
1:B:151:ASN:HD22	1:B:152:ASP:N	1.90	0.67
1:D:147:LYS:HE2	1:D:165:THR:HA	1.76	0.67
1:E:80:VAL:CG1	1:E:82:ASN:O	2.42	0.67
1:D:276:HIS:O	1:D:280:VAL:HG22	1.95	0.67
1:B:151:ASN:ND2	1:B:152:ASP:H	1.92	0.67
1:B:147:LYS:HE2	1:B:165:THR:HA	1.75	0.67
1:E:77:PHE:H	1:E:84:ARG:HD3	1.60	0.67
1:A:80:VAL:CG1	1:A:82:ASN:O	2.43	0.67
1:D:66:GLU:HG3	1:D:67:PRO:HD2	1.77	0.67
1:C:66:GLU:HG3	1:C:67:PRO:HD2	1.76	0.66
1:B:276:HIS:O	1:B:280:VAL:HG22	1.96	0.66
1:D:275:GLN:O	1:D:275:GLN:HG2	1.95	0.66
1:A:276:HIS:O	1:A:280:VAL:HG22	1.95	0.66
1:A:267:VAL:HA	1:A:270:ILE:HB	1.77	0.66
1:C:42:LEU:HB3	1:C:103:GLU:HG2	1.76	0.66
1:E:276:HIS:O	1:E:280:VAL:HG22	1.95	0.66
1:D:54:ASP:HB2	1:D:57:ARG:CB	2.24	0.66
1:D:202:LEU:HD12	1:E:259:PHE:HZ	1.61	0.66
1:B:202:LEU:HD12	1:C:259:PHE:HZ	1.59	0.66
1:E:53:PHE:O	1:E:53:PHE:CD1	2.49	0.66
1:C:80:VAL:CG1	1:C:82:ASN:O	2.44	0.66
1:B:53:PHE:CD1	1:B:53:PHE:O	2.48	0.66
1:D:76:ARG:HH22	1:D:130:ILE:HD12	1.59	0.66
1:B:42:LEU:HB3	1:B:103:GLU:HG2	1.76	0.66
1:C:54:ASP:HB2	1:C:57:ARG:CB	2.26	0.65
1:D:65:TYR:CG	1:D:70:ILE:HD11	2.31	0.65
1:A:297:ALA:O	1:A:301:VAL:HG23	1.95	0.65
1:C:267:VAL:HA	1:C:270:ILE:HB	1.78	0.65
1:A:275:GLN:O	1:A:275:GLN:HG2	1.94	0.65
1:D:80:VAL:CG1	1:D:82:ASN:O	2.43	0.65
1:C:65:TYR:CG	1:C:70:ILE:HD11	2.31	0.65
1:D:147:LYS:C	1:D:149:GLY:N	2.49	0.65
1:A:53:PHE:CD1	1:A:53:PHE:O	2.49	0.65
1:A:66:GLU:HG3	1:A:67:PRO:HD2	1.78	0.65
1:D:267:VAL:HA	1:D:270:ILE:HB	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:151:ASN:ND2	1:D:152:ASP:H	1.92	0.65
1:D:202:LEU:HD12	1:E:259:PHE:CZ	2.31	0.65
1:B:267:VAL:HA	1:B:270:ILE:HB	1.77	0.65
1:B:54:ASP:HB2	1:B:57:ARG:CB	2.27	0.64
1:B:65:TYR:CG	1:B:70:ILE:HD11	2.31	0.64
1:C:53:PHE:CD1	1:C:53:PHE:O	2.51	0.64
1:E:54:ASP:HB2	1:E:57:ARG:CB	2.27	0.64
1:C:276:HIS:O	1:C:280:VAL:HG22	1.96	0.64
1:C:76:ARG:HH22	1:C:130:ILE:HD12	1.61	0.64
1:B:159:TRP:CE3	1:B:189:ILE:HD12	2.32	0.64
1:E:147:LYS:C	1:E:149:GLY:N	2.47	0.64
1:A:54:ASP:HB2	1:A:57:ARG:CB	2.28	0.64
1:C:297:ALA:O	1:C:301:VAL:HG23	1.98	0.64
1:E:65:TYR:CG	1:E:70:ILE:HD11	2.31	0.64
1:E:297:ALA:O	1:E:301:VAL:HG23	1.99	0.63
1:B:297:ALA:O	1:B:301:VAL:HG23	1.98	0.63
1:D:53:PHE:O	1:D:53:PHE:CD1	2.52	0.63
1:C:283:GLN:HE21	1:C:286:ARG:HB2	1.65	0.62
1:D:22:TYR:HA	1:D:149:GLY:HA3	1.82	0.62
1:E:267:VAL:HA	1:E:270:ILE:HB	1.79	0.62
1:E:281:GLU:O	1:E:283:GLN:N	2.31	0.62
1:A:65:TYR:CG	1:A:70:ILE:HD11	2.34	0.62
1:C:159:TRP:CE3	1:C:189:ILE:HD12	2.35	0.61
1:E:40:ALA:HB3	1:E:105:PHE:CZ	2.35	0.61
1:A:147:LYS:C	1:A:149:GLY:N	2.48	0.61
1:B:53:PHE:HD1	1:B:53:PHE:O	1.83	0.61
1:A:53:PHE:HD1	1:A:53:PHE:O	1.84	0.61
1:A:159:TRP:CE3	1:A:189:ILE:HD12	2.35	0.61
1:E:53:PHE:HD1	1:E:53:PHE:O	1.84	0.61
1:B:267:VAL:HG23	1:B:298:PHE:CZ	2.36	0.60
1:B:89:VAL:HG11	1:B:102:LEU:HD23	1.82	0.60
1:B:212:TRP:HZ3	1:B:264:PHE:HD2	1.49	0.60
1:D:283:GLN:HE21	1:D:286:ARG:HB2	1.65	0.60
1:D:297:ALA:O	1:D:301:VAL:HG23	1.99	0.60
1:D:281:GLU:O	1:D:283:GLN:N	2.31	0.60
1:E:283:GLN:HE21	1:E:286:ARG:HB2	1.66	0.60
1:E:89:VAL:HG11	1:E:102:LEU:HD23	1.83	0.60
1:C:40:ALA:HB3	1:C:105:PHE:CZ	2.37	0.60
1:D:159:TRP:CE3	1:D:189:ILE:HD12	2.36	0.60
1:E:212:TRP:HZ3	1:E:264:PHE:HD2	1.49	0.60
1:B:147:LYS:O	1:B:149:GLY:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:GLU:O	1:B:283:GLN:N	2.30	0.60
1:A:40:ALA:HB3	1:A:105:PHE:CZ	2.37	0.60
1:A:202:LEU:HD12	1:B:259:PHE:HZ	1.66	0.60
1:A:281:GLU:O	1:A:283:GLN:N	2.32	0.59
1:B:100:GLN:HA	1:B:100:GLN:HE21	1.66	0.59
1:D:278:LEU:HD21	1:D:286:ARG:HB3	1.84	0.59
1:D:267:VAL:HG23	1:D:298:PHE:CZ	2.37	0.59
1:E:276:HIS:C	1:E:278:LEU:H	2.05	0.59
1:A:283:GLN:HE21	1:A:286:ARG:HB2	1.68	0.59
1:C:267:VAL:HG23	1:C:298:PHE:CZ	2.38	0.59
1:C:278:LEU:HD21	1:C:286:ARG:HB3	1.85	0.59
1:A:255:GLY:O	1:A:258:ILE:HG22	2.02	0.59
1:E:278:LEU:HD21	1:E:286:ARG:HB3	1.84	0.59
1:A:259:PHE:CZ	1:E:202:LEU:HD12	2.38	0.59
1:E:283:GLN:N	1:E:284:PRO:HD3	2.18	0.59
1:B:283:GLN:HE21	1:B:286:ARG:HB2	1.66	0.59
1:A:212:TRP:HZ3	1:A:264:PHE:HD2	1.51	0.59
1:A:202:LEU:HD12	1:B:259:PHE:CZ	2.37	0.59
1:E:254:THR:O	1:E:258:ILE:HB	2.03	0.59
1:E:255:GLY:O	1:E:258:ILE:HG22	2.03	0.59
1:B:254:THR:O	1:B:258:ILE:HB	2.02	0.59
1:B:210:ILE:HG23	1:C:269:VAL:HG11	1.85	0.59
1:C:53:PHE:HD1	1:C:53:PHE:O	1.86	0.58
1:C:283:GLN:N	1:C:284:PRO:HD3	2.17	0.58
1:D:274:VAL:C	1:D:276:HIS:H	2.06	0.58
1:D:212:TRP:HZ3	1:D:264:PHE:HD2	1.50	0.58
1:E:147:LYS:O	1:E:149:GLY:N	2.36	0.58
1:C:255:GLY:O	1:C:258:ILE:HG22	2.03	0.58
1:C:274:VAL:C	1:C:276:HIS:H	2.05	0.58
1:C:276:HIS:C	1:C:278:LEU:H	2.07	0.58
1:A:283:GLN:N	1:A:284:PRO:HD3	2.19	0.58
1:C:151:ASN:O	1:C:154:VAL:HG22	2.04	0.58
1:B:274:VAL:C	1:B:276:HIS:H	2.05	0.58
1:B:283:GLN:N	1:B:284:PRO:HD3	2.19	0.58
1:A:274:VAL:C	1:A:276:HIS:H	2.06	0.58
1:E:100:GLN:HE21	1:E:100:GLN:HA	1.68	0.58
1:B:276:HIS:C	1:B:278:LEU:H	2.07	0.57
1:D:276:HIS:C	1:D:278:LEU:H	2.07	0.57
1:D:283:GLN:N	1:D:284:PRO:HD3	2.18	0.57
1:A:278:LEU:HD21	1:A:286:ARG:HB3	1.85	0.57
1:A:267:VAL:HG23	1:A:298:PHE:CZ	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:254:THR:O	1:C:258:ILE:HB	2.03	0.57
1:C:212:TRP:HZ3	1:C:264:PHE:HD2	1.50	0.57
1:E:159:TRP:CE3	1:E:189:ILE:HD12	2.39	0.57
1:A:77:PHE:HD1	1:A:84:ARG:CD	2.16	0.57
1:E:274:VAL:C	1:E:276:HIS:H	2.08	0.57
1:D:100:GLN:HE21	1:D:100:GLN:HA	1.69	0.57
1:D:53:PHE:O	1:D:53:PHE:HD1	1.87	0.57
1:A:259:PHE:HZ	1:E:202:LEU:HD12	1.69	0.57
1:A:100:GLN:HE21	1:A:100:GLN:HA	1.69	0.57
1:A:276:HIS:C	1:A:278:LEU:H	2.08	0.57
1:A:254:THR:O	1:A:258:ILE:HB	2.04	0.57
1:D:255:GLY:O	1:D:258:ILE:HG22	2.05	0.57
1:E:267:VAL:HG23	1:E:298:PHE:CZ	2.39	0.57
1:B:255:GLY:O	1:B:258:ILE:HG22	2.05	0.57
1:D:271:GLU:OE2	1:D:272:VAL:N	2.38	0.56
1:B:151:ASN:O	1:B:154:VAL:HG22	2.06	0.56
1:E:70:ILE:HG22	1:E:71:TRP:O	2.05	0.56
1:C:202:LEU:HD12	1:D:259:PHE:CZ	2.41	0.56
1:D:286:ARG:O	1:D:289:SER:HB3	2.06	0.56
1:C:147:LYS:O	1:C:149:GLY:N	2.37	0.56
1:E:22:TYR:HA	1:E:149:GLY:HA3	1.86	0.56
1:B:286:ARG:O	1:B:289:SER:HB3	2.04	0.56
1:C:271:GLU:OE2	1:C:272:VAL:N	2.39	0.56
1:B:89:VAL:CG1	1:B:102:LEU:HD23	2.36	0.56
1:D:200:ILE:O	1:D:204:MET:HB2	2.06	0.56
1:D:147:LYS:O	1:D:149:GLY:N	2.39	0.56
1:A:147:LYS:O	1:A:149:GLY:N	2.38	0.56
1:C:155:PHE:CE1	1:D:112:PRO:HB3	2.41	0.56
1:A:33:ALA:O	1:A:34:GLU:HB2	2.06	0.55
1:D:40:ALA:HB3	1:D:105:PHE:CZ	2.41	0.55
1:C:281:GLU:O	1:C:283:GLN:N	2.32	0.55
1:C:89:VAL:HG11	1:C:102:LEU:HD23	1.88	0.55
1:D:216:TRP:CE2	1:D:295:ARG:HD3	2.42	0.55
1:E:151:ASN:O	1:E:154:VAL:HG22	2.05	0.55
1:A:54:ASP:HB2	1:A:57:ARG:CG	2.36	0.55
1:B:200:ILE:O	1:B:204:MET:HB2	2.06	0.55
1:A:79:ASN:ND2	1:A:79:ASN:H	2.02	0.55
1:C:54:ASP:HB2	1:C:57:ARG:CG	2.36	0.55
1:E:208:LEU:HD13	1:E:261:ILE:HG23	1.89	0.55
1:D:254:THR:O	1:D:258:ILE:HB	2.06	0.55
1:A:151:ASN:O	1:A:154:VAL:HG22	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:ASP:HB2	1:B:57:ARG:CG	2.36	0.55
1:B:70:ILE:HG22	1:B:71:TRP:O	2.06	0.55
1:E:200:ILE:O	1:E:204:MET:HB2	2.06	0.55
1:A:200:ILE:O	1:A:204:MET:HB2	2.07	0.55
1:E:54:ASP:HB2	1:E:57:ARG:CG	2.37	0.55
1:D:54:ASP:HB2	1:D:57:ARG:CG	2.37	0.55
1:A:216:TRP:CE2	1:A:295:ARG:HD3	2.42	0.55
1:C:216:TRP:CE2	1:C:295:ARG:HD3	2.42	0.55
1:B:79:ASN:H	1:B:79:ASN:ND2	2.01	0.54
1:E:286:ARG:O	1:E:289:SER:HB3	2.06	0.54
1:A:271:GLU:OE2	1:A:272:VAL:N	2.40	0.54
1:A:286:ARG:O	1:A:289:SER:HB3	2.07	0.54
1:C:224:VAL:O	1:C:228:VAL:HB	2.07	0.54
1:E:248:THR:HB	1:E:250:TYR:CE1	2.42	0.54
1:B:53:PHE:HD1	1:B:53:PHE:C	2.11	0.54
1:B:278:LEU:HD21	1:B:286:ARG:HB3	1.90	0.54
1:D:18:ASN:HB3	1:D:143:VAL:HG23	1.89	0.54
1:E:216:TRP:CE2	1:E:295:ARG:HD3	2.42	0.54
1:A:36:PHE:CE1	1:A:109:VAL:HB	2.43	0.54
1:C:200:ILE:O	1:C:204:MET:HB2	2.07	0.54
1:D:77:PHE:HD1	1:D:84:ARG:CD	2.16	0.54
1:B:248:THR:HB	1:B:250:TYR:CE1	2.43	0.54
1:E:89:VAL:CG1	1:E:102:LEU:HD23	2.37	0.54
1:D:314:PHE:N	1:D:314:PHE:CD1	2.76	0.54
1:E:314:PHE:N	1:E:314:PHE:CD1	2.76	0.54
1:A:257:ILE:O	1:A:261:ILE:HG12	2.07	0.54
1:C:202:LEU:HD12	1:D:259:PHE:HZ	1.73	0.54
1:A:18:ASN:HB3	1:A:143:VAL:HG23	1.89	0.54
1:D:210:ILE:HG23	1:E:269:VAL:HG11	1.89	0.54
1:E:53:PHE:HD1	1:E:53:PHE:C	2.11	0.54
1:B:216:TRP:CE2	1:B:295:ARG:HD3	2.42	0.54
1:E:271:GLU:OE2	1:E:272:VAL:N	2.41	0.53
1:D:298:PHE:HB2	1:D:299:PRO:HD3	1.91	0.53
1:D:248:THR:HB	1:D:250:TYR:CE1	2.43	0.53
1:B:271:GLU:OE2	1:B:272:VAL:N	2.40	0.53
1:E:298:PHE:HB2	1:E:299:PRO:HD3	1.90	0.53
1:E:33:ALA:O	1:E:34:GLU:HB2	2.08	0.53
1:D:89:VAL:HG11	1:D:102:LEU:HD23	1.90	0.53
1:A:155:PHE:CE1	1:B:112:PRO:HB3	2.43	0.53
1:D:151:ASN:O	1:D:154:VAL:HG22	2.08	0.53
1:A:22:TYR:HA	1:A:149:GLY:HA3	1.87	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:ALA:HB3	1:B:105:PHE:CZ	2.43	0.53
1:E:77:PHE:HD1	1:E:84:ARG:CD	2.17	0.53
1:A:25:GLU:HB2	1:A:39:ASN:HB3	1.91	0.53
1:C:18:ASN:HB3	1:C:143:VAL:HG23	1.89	0.53
1:D:25:GLU:HB2	1:D:39:ASN:HB3	1.91	0.53
1:A:248:THR:HB	1:A:250:TYR:CE1	2.43	0.53
1:C:287:ALA:O	1:C:289:SER:N	2.42	0.53
1:A:314:PHE:CD1	1:A:314:PHE:N	2.77	0.53
1:C:100:GLN:HE21	1:C:100:GLN:HA	1.73	0.53
1:D:70:ILE:HG22	1:D:71:TRP:O	2.09	0.53
1:A:53:PHE:HD1	1:A:53:PHE:C	2.12	0.53
1:C:286:ARG:O	1:C:289:SER:HB3	2.08	0.53
1:E:219:SER:OG	1:E:222:ALA:HB3	2.09	0.53
1:E:278:LEU:HD23	1:E:287:ALA:HB2	1.91	0.53
1:D:278:LEU:HD23	1:D:287:ALA:HB2	1.91	0.53
1:A:89:VAL:HG11	1:A:102:LEU:HD23	1.91	0.53
1:E:79:ASN:ND2	1:E:79:ASN:H	2.05	0.52
1:E:287:ALA:O	1:E:289:SER:N	2.42	0.52
1:C:278:LEU:HD23	1:C:287:ALA:HB2	1.90	0.52
1:C:314:PHE:CD1	1:C:314:PHE:N	2.77	0.52
1:C:79:ASN:ND2	1:C:79:ASN:H	2.02	0.52
1:B:53:PHE:CD1	1:B:53:PHE:C	2.82	0.52
1:C:248:THR:HB	1:C:250:TYR:CE1	2.45	0.52
1:D:54:ASP:CB	1:D:57:ARG:HB2	2.33	0.52
1:C:53:PHE:CD1	1:C:53:PHE:C	2.83	0.52
1:A:271:GLU:O	1:A:272:VAL:C	2.48	0.52
1:B:22:TYR:HA	1:B:149:GLY:HA3	1.85	0.52
1:C:53:PHE:HD1	1:C:53:PHE:C	2.13	0.52
1:A:193:TYR:O	1:A:194:PHE:HB2	2.09	0.52
1:C:77:PHE:HD1	1:C:84:ARG:CD	2.19	0.52
1:C:70:ILE:HG22	1:C:71:TRP:O	2.10	0.52
1:C:241:VAL:C	1:C:243:THR:H	2.12	0.52
1:D:29:LEU:HD23	1:D:29:LEU:C	2.29	0.52
1:C:257:ILE:O	1:C:261:ILE:HG12	2.10	0.52
1:A:298:PHE:HB2	1:A:299:PRO:HD3	1.92	0.52
1:C:245:LEU:HD12	1:C:246:PRO:HD2	1.92	0.52
1:A:76:ARG:O	1:A:129:LEU:HA	2.09	0.52
1:A:287:ALA:O	1:A:289:SER:N	2.43	0.52
1:A:149:GLY:O	1:A:150:LYS:CB	2.57	0.51
1:E:18:ASN:HB3	1:E:143:VAL:HG23	1.91	0.51
1:E:25:GLU:HB2	1:E:39:ASN:HB3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:GLU:O	1:B:272:VAL:C	2.49	0.51
1:C:298:PHE:HB2	1:C:299:PRO:HD3	1.91	0.51
1:A:70:ILE:HG22	1:A:71:TRP:O	2.09	0.51
1:B:29:LEU:HD23	1:B:29:LEU:C	2.31	0.51
1:E:147:LYS:O	1:E:147:LYS:HG2	2.11	0.51
1:A:278:LEU:HD23	1:A:287:ALA:HB2	1.93	0.51
1:B:298:PHE:HB2	1:B:299:PRO:HD3	1.92	0.51
1:D:89:VAL:CG1	1:D:102:LEU:HD23	2.41	0.51
1:A:274:VAL:O	1:A:276:HIS:N	2.42	0.51
1:C:147:LYS:O	1:C:147:LYS:HG2	2.11	0.51
1:D:53:PHE:C	1:D:53:PHE:CD1	2.84	0.51
1:E:53:PHE:C	1:E:53:PHE:CD1	2.82	0.51
1:A:13:GLU:CB	1:A:14:PRO:CD	2.87	0.51
1:D:53:PHE:C	1:D:53:PHE:HD1	2.14	0.51
1:D:33:ALA:O	1:D:34:GLU:HB2	2.11	0.51
1:E:151:ASN:ND2	1:E:152:ASP:N	2.55	0.51
1:A:53:PHE:CD1	1:A:53:PHE:C	2.83	0.51
1:E:13:GLU:CB	1:E:14:PRO:CD	2.86	0.51
1:A:150:LYS:CG	1:A:154:VAL:HG21	2.41	0.51
1:A:208:LEU:HD13	1:A:261:ILE:HG23	1.92	0.51
1:B:278:LEU:HD23	1:B:287:ALA:HB2	1.92	0.51
1:B:314:PHE:N	1:B:314:PHE:CD1	2.77	0.51
1:C:22:TYR:HA	1:C:149:GLY:HA3	1.89	0.50
1:B:22:TYR:CA	1:B:149:GLY:HA2	2.29	0.50
1:B:77:PHE:HD1	1:B:84:ARG:CD	2.19	0.50
1:B:208:LEU:HD13	1:B:261:ILE:HG23	1.93	0.50
1:D:208:LEU:HD13	1:D:261:ILE:HG23	1.92	0.50
1:D:241:VAL:C	1:D:243:THR:H	2.13	0.50
1:B:193:TYR:O	1:B:194:PHE:HB2	2.10	0.50
1:A:224:VAL:O	1:A:228:VAL:HB	2.10	0.50
1:B:179:LEU:HD12	1:B:179:LEU:C	2.32	0.50
1:E:34:GLU:OE2	1:E:112:PRO:HA	2.10	0.50
1:C:25:GLU:HB2	1:C:39:ASN:HB3	1.92	0.50
1:D:193:TYR:O	1:D:194:PHE:HB2	2.10	0.50
1:C:193:TYR:O	1:C:194:PHE:HB2	2.10	0.50
1:A:245:LEU:HD12	1:A:246:PRO:HD2	1.93	0.50
1:C:76:ARG:O	1:C:129:LEU:HA	2.12	0.50
1:A:29:LEU:C	1:A:29:LEU:HD23	2.32	0.50
1:C:34:GLU:OE2	1:C:112:PRO:HA	2.11	0.50
1:E:70:ILE:HD13	1:E:70:ILE:N	2.26	0.50
1:B:219:SER:OG	1:B:222:ALA:HB3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:LYS:CG	1:C:154:VAL:HG21	2.42	0.50
1:E:271:GLU:O	1:E:272:VAL:C	2.50	0.50
1:D:155:PHE:CE1	1:E:112:PRO:HB3	2.47	0.50
1:C:54:ASP:CB	1:C:57:ARG:HB2	2.36	0.50
1:D:257:ILE:O	1:D:261:ILE:HG12	2.10	0.50
1:D:281:GLU:C	1:D:283:GLN:H	2.15	0.50
1:D:155:PHE:CZ	1:E:112:PRO:HB3	2.46	0.50
1:A:219:SER:OG	1:A:222:ALA:HB3	2.11	0.50
1:E:29:LEU:C	1:E:29:LEU:HD23	2.32	0.50
1:C:271:GLU:O	1:C:272:VAL:C	2.49	0.50
1:C:33:ALA:O	1:C:34:GLU:HB2	2.12	0.50
1:D:179:LEU:C	1:D:179:LEU:HD12	2.32	0.50
1:C:72:ILE:HG22	1:C:73:PRO:HD2	1.94	0.50
1:B:150:LYS:HG2	1:B:154:VAL:HG21	1.94	0.50
1:B:281:GLU:C	1:B:283:GLN:H	2.14	0.50
1:A:269:VAL:HG11	1:E:210:ILE:HG23	1.94	0.50
1:D:219:SER:OG	1:D:222:ALA:HB3	2.12	0.50
1:B:224:VAL:O	1:B:228:VAL:HB	2.12	0.50
1:B:54:ASP:HB2	1:B:57:ARG:HG3	1.94	0.49
1:D:76:ARG:O	1:D:129:LEU:HA	2.12	0.49
1:B:274:VAL:O	1:B:276:HIS:N	2.41	0.49
1:E:241:VAL:C	1:E:243:THR:H	2.13	0.49
1:A:54:ASP:CB	1:A:57:ARG:HB2	2.39	0.49
1:A:54:ASP:HB2	1:A:57:ARG:HG3	1.93	0.49
1:A:268:ALA:O	1:A:272:VAL:HG22	2.11	0.49
1:A:15:LEU:HD11	1:A:46:TRP:HB2	1.94	0.49
1:D:147:LYS:O	1:D:147:LYS:HG2	2.12	0.49
1:B:287:ALA:O	1:B:289:SER:N	2.46	0.49
1:C:219:SER:OG	1:C:222:ALA:HB3	2.13	0.49
1:E:245:LEU:HD12	1:E:246:PRO:HD2	1.95	0.49
1:A:241:VAL:C	1:A:243:THR:H	2.15	0.49
1:D:53:PHE:O	1:D:54:ASP:C	2.50	0.49
1:D:79:ASN:ND2	1:D:79:ASN:H	2.03	0.49
1:B:257:ILE:O	1:B:261:ILE:HG12	2.11	0.49
1:C:281:GLU:C	1:C:283:GLN:H	2.16	0.49
1:B:48:ASP:HB3	1:B:51:LEU:HD21	1.95	0.49
1:D:287:ALA:O	1:D:289:SER:N	2.46	0.49
1:B:245:LEU:HD12	1:B:246:PRO:HD2	1.93	0.49
1:A:179:LEU:HD12	1:A:179:LEU:C	2.33	0.49
1:D:271:GLU:O	1:D:272:VAL:C	2.52	0.49
1:C:36:PHE:CE1	1:C:109:VAL:HB	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:274:VAL:O	1:E:276:HIS:N	2.45	0.49
1:A:89:VAL:CG1	1:A:102:LEU:HD23	2.43	0.49
1:D:224:VAL:O	1:D:228:VAL:HB	2.13	0.49
1:D:245:LEU:HD12	1:D:246:PRO:HD2	1.95	0.49
1:B:147:LYS:HG2	1:B:147:LYS:O	2.13	0.48
1:C:54:ASP:HB2	1:C:57:ARG:HG3	1.94	0.48
1:E:76:ARG:O	1:E:129:LEU:HA	2.12	0.48
1:E:40:ALA:HB3	1:E:105:PHE:CE1	2.48	0.48
1:A:40:ALA:HB3	1:A:105:PHE:CE1	2.48	0.48
1:B:268:ALA:O	1:B:272:VAL:HG22	2.14	0.48
1:E:118:TYR:C	1:E:118:TYR:CD1	2.84	0.48
1:E:224:VAL:O	1:E:228:VAL:HB	2.13	0.48
1:E:281:GLU:C	1:E:283:GLN:H	2.15	0.48
1:B:25:GLU:HB2	1:B:39:ASN:HB3	1.94	0.48
1:E:54:ASP:HB2	1:E:57:ARG:HG3	1.94	0.48
1:A:57:ARG:HA	1:A:57:ARG:HE	1.79	0.48
1:B:34:GLU:OE2	1:B:112:PRO:HA	2.14	0.48
1:C:150:LYS:HG2	1:C:154:VAL:HG21	1.96	0.48
1:A:151:ASN:ND2	1:A:152:ASP:N	2.56	0.48
1:E:54:ASP:CB	1:E:57:ARG:HB2	2.37	0.48
1:C:49:ARG:C	1:C:51:LEU:H	2.17	0.48
1:C:89:VAL:CG1	1:C:102:LEU:HD23	2.42	0.48
1:B:33:ALA:O	1:B:34:GLU:HB2	2.12	0.48
1:C:193:TYR:O	1:C:194:PHE:CB	2.61	0.48
1:B:155:PHE:CZ	1:C:112:PRO:HB3	2.48	0.48
1:B:18:ASN:HB3	1:B:143:VAL:HG23	1.96	0.48
1:E:141:LEU:HD23	1:E:142:ALA:N	2.19	0.48
1:C:29:LEU:C	1:C:29:LEU:HD23	2.33	0.48
1:E:193:TYR:O	1:E:194:PHE:HB2	2.12	0.48
1:B:151:ASN:ND2	1:B:152:ASP:N	2.58	0.48
1:E:150:LYS:CG	1:E:154:VAL:HG21	2.43	0.48
1:B:141:LEU:HD23	1:B:142:ALA:N	2.20	0.48
1:E:257:ILE:O	1:E:261:ILE:HG12	2.14	0.48
1:E:49:ARG:C	1:E:51:LEU:H	2.17	0.48
1:E:36:PHE:CE1	1:E:109:VAL:HB	2.49	0.48
1:A:72:ILE:HG22	1:A:73:PRO:HD2	1.95	0.48
1:D:137:ARG:HA	1:D:137:ARG:HD3	1.75	0.48
1:B:19:THR:HA	1:B:43:SER:O	2.13	0.48
1:A:147:LYS:O	1:A:147:LYS:HG2	2.13	0.48
1:B:76:ARG:O	1:B:129:LEU:HA	2.14	0.48
1:E:193:TYR:O	1:E:194:PHE:CB	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:THR:HA	1:A:43:SER:O	2.13	0.48
1:C:19:THR:HA	1:C:43:SER:O	2.14	0.48
1:D:22:TYR:CA	1:D:149:GLY:HA2	2.29	0.48
1:D:149:GLY:O	1:D:150:LYS:CB	2.59	0.48
1:B:13:GLU:CB	1:B:14:PRO:CD	2.85	0.48
1:B:150:LYS:CG	1:B:154:VAL:HG21	2.44	0.48
1:E:150:LYS:HG2	1:E:154:VAL:HG21	1.96	0.48
1:D:274:VAL:O	1:D:276:HIS:N	2.44	0.48
1:A:281:GLU:C	1:A:283:GLN:H	2.15	0.48
1:D:193:TYR:O	1:D:194:PHE:CB	2.62	0.48
1:C:179:LEU:C	1:C:179:LEU:HD12	2.34	0.48
1:E:19:THR:HA	1:E:43:SER:O	2.14	0.48
1:D:54:ASP:HB2	1:D:57:ARG:HG3	1.96	0.47
1:A:193:TYR:O	1:A:194:PHE:CB	2.62	0.47
1:B:270:ILE:HD13	1:B:270:ILE:HA	1.71	0.47
1:E:179:LEU:HD12	1:E:179:LEU:C	2.34	0.47
1:C:208:LEU:HD13	1:C:261:ILE:HG23	1.97	0.47
1:C:268:ALA:O	1:C:272:VAL:HG22	2.15	0.47
1:D:212:TRP:CE3	1:D:298:PHE:HD1	2.32	0.47
1:B:241:VAL:C	1:B:243:THR:H	2.16	0.47
1:D:19:THR:HA	1:D:43:SER:O	2.14	0.47
1:E:84:ARG:CB	1:E:84:ARG:NH1	2.66	0.47
1:B:53:PHE:O	1:B:54:ASP:C	2.53	0.47
1:B:70:ILE:HD13	1:B:70:ILE:N	2.29	0.47
1:C:155:PHE:CZ	1:D:112:PRO:HB3	2.49	0.47
1:A:196:TYR:CD1	1:A:196:TYR:N	2.83	0.47
1:D:61:ARG:HG2	1:D:62:VAL:HG23	1.96	0.47
1:D:36:PHE:CE1	1:D:109:VAL:HB	2.50	0.47
1:C:49:ARG:O	1:C:51:LEU:N	2.48	0.47
1:A:112:PRO:HB3	1:E:155:PHE:CE1	2.49	0.47
1:B:137:ARG:HD2	1:B:179:LEU:HG	1.96	0.47
1:D:118:TYR:CD1	1:D:118:TYR:C	2.87	0.47
1:C:48:ASP:HB3	1:C:51:LEU:HD21	1.97	0.47
1:A:48:ASP:HB3	1:A:51:LEU:HD21	1.97	0.47
1:E:268:ALA:O	1:E:272:VAL:HG22	2.14	0.47
1:C:274:VAL:O	1:C:276:HIS:N	2.43	0.47
1:B:49:ARG:C	1:B:51:LEU:H	2.18	0.47
1:D:150:LYS:CG	1:D:154:VAL:HG21	2.45	0.47
1:E:147:LYS:CG	1:E:147:LYS:O	2.63	0.47
1:E:270:ILE:HA	1:E:270:ILE:HD13	1.68	0.47
1:C:196:TYR:N	1:C:196:TYR:CD1	2.83	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:LEU:HD23	1:A:142:ALA:N	2.24	0.47
1:E:49:ARG:O	1:E:51:LEU:N	2.48	0.47
1:A:70:ILE:N	1:A:70:ILE:HD13	2.29	0.47
1:E:118:TYR:HB3	1:E:119:PRO:HD3	1.96	0.47
1:B:62:VAL:HG13	1:B:93:VAL:O	2.15	0.47
1:D:81:GLU:HG3	1:D:108:ARG:HG3	1.96	0.47
1:A:232:ILE:HG22	1:A:233:ALA:N	2.29	0.47
1:C:61:ARG:HG2	1:C:62:VAL:HG23	1.97	0.47
1:C:226:LEU:HA	1:C:226:LEU:HD22	1.71	0.47
1:D:72:ILE:HG22	1:D:73:PRO:HD2	1.96	0.47
1:A:210:ILE:HG23	1:B:269:VAL:HG11	1.97	0.47
1:A:118:TYR:C	1:A:118:TYR:CD1	2.87	0.47
1:C:147:LYS:O	1:C:147:LYS:CG	2.63	0.46
1:B:271:GLU:O	1:B:274:VAL:N	2.48	0.46
1:D:34:GLU:OE2	1:D:112:PRO:HA	2.14	0.46
1:A:137:ARG:HD3	1:A:137:ARG:HA	1.72	0.46
1:E:15:LEU:HD11	1:E:46:TRP:HB2	1.97	0.46
1:D:147:LYS:CG	1:D:147:LYS:O	2.63	0.46
1:D:141:LEU:HD23	1:D:142:ALA:N	2.20	0.46
1:C:212:TRP:CE3	1:C:298:PHE:HD1	2.33	0.46
1:B:196:TYR:N	1:B:196:TYR:CD1	2.84	0.46
1:E:48:ASP:HB3	1:E:51:LEU:HD21	1.96	0.46
1:E:212:TRP:CE3	1:E:298:PHE:HD1	2.32	0.46
1:A:193:TYR:C	1:A:193:TYR:CD2	2.89	0.46
1:A:305:ALA:O	1:A:309:LEU:HB2	2.15	0.46
1:D:151:ASN:ND2	1:D:152:ASP:N	2.58	0.46
1:B:257:ILE:O	1:B:261:ILE:CG1	2.64	0.46
1:D:118:TYR:HB3	1:D:119:PRO:HD3	1.98	0.46
1:E:62:VAL:HG13	1:E:93:VAL:O	2.16	0.46
1:B:150:LYS:HB3	1:B:150:LYS:HE2	1.70	0.46
1:E:274:VAL:HG12	1:E:275:GLN:N	2.30	0.46
1:A:42:LEU:HB3	1:A:103:GLU:CG	2.45	0.46
1:D:65:TYR:CD1	1:D:70:ILE:HD11	2.51	0.46
1:C:111:SER:HA	1:C:112:PRO:HD2	1.78	0.46
1:A:137:ARG:HD2	1:A:179:LEU:HG	1.96	0.46
1:C:118:TYR:HB3	1:C:119:PRO:HD3	1.95	0.46
1:B:49:ARG:O	1:B:51:LEU:N	2.49	0.46
1:D:70:ILE:N	1:D:70:ILE:HD13	2.30	0.46
1:C:40:ALA:HB3	1:C:105:PHE:CE1	2.50	0.46
1:A:218:THR:HG22	1:A:279:LYS:HE2	1.98	0.46
1:C:15:LEU:HD11	1:C:46:TRP:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:305:ALA:O	1:B:309:LEU:HB2	2.16	0.46
1:C:57:ARG:HA	1:C:57:ARG:HE	1.80	0.46
1:D:48:ASP:HB3	1:D:51:LEU:HD21	1.97	0.46
1:E:276:HIS:C	1:E:278:LEU:N	2.69	0.46
1:C:155:PHE:HB3	1:C:156:LEU:H	1.58	0.46
1:B:199:ASN:O	1:B:200:ILE:HD13	2.16	0.46
1:B:304:LEU:O	1:B:308:ILE:HG12	2.16	0.46
1:E:196:TYR:CD1	1:E:196:TYR:N	2.84	0.46
1:E:72:ILE:HG22	1:E:73:PRO:HD2	1.98	0.46
1:D:68:GLU:N	1:D:68:GLU:CD	2.68	0.46
1:A:61:ARG:HG2	1:A:62:VAL:HG23	1.98	0.46
1:D:150:LYS:HB3	1:D:150:LYS:HE2	1.73	0.46
1:D:241:VAL:C	1:D:243:THR:N	2.70	0.46
1:C:81:GLU:HG3	1:C:108:ARG:HG3	1.98	0.46
1:D:150:LYS:HG2	1:D:154:VAL:HG21	1.97	0.46
1:A:147:LYS:O	1:A:147:LYS:CG	2.64	0.46
1:E:57:ARG:HE	1:E:57:ARG:HA	1.81	0.46
1:D:49:ARG:C	1:D:51:LEU:H	2.19	0.46
1:C:241:VAL:C	1:C:243:THR:N	2.69	0.46
1:B:193:TYR:O	1:B:194:PHE:CB	2.62	0.46
1:C:191:ARG:HG3	1:C:192:GLN:N	2.31	0.46
1:C:53:PHE:O	1:C:54:ASP:C	2.55	0.45
1:B:54:ASP:CB	1:B:57:ARG:HB2	2.37	0.45
1:A:94:SER:OG	1:A:95:PRO:HD2	2.16	0.45
1:B:274:VAL:HG12	1:B:275:GLN:N	2.31	0.45
1:D:270:ILE:HA	1:D:270:ILE:HD13	1.68	0.45
1:E:53:PHE:O	1:E:54:ASP:C	2.53	0.45
1:A:49:ARG:C	1:A:51:LEU:H	2.19	0.45
1:B:65:TYR:CD1	1:B:70:ILE:HD11	2.50	0.45
1:B:36:PHE:CE1	1:B:109:VAL:HB	2.51	0.45
1:C:149:GLY:O	1:C:150:LYS:CB	2.58	0.45
1:A:53:PHE:O	1:A:54:ASP:C	2.55	0.45
1:E:65:TYR:CD1	1:E:70:ILE:HD11	2.52	0.45
1:B:309:LEU:HD12	1:B:309:LEU:HA	1.75	0.45
1:A:257:ILE:O	1:A:261:ILE:CG1	2.64	0.45
1:A:271:GLU:O	1:A:274:VAL:N	2.49	0.45
1:A:212:TRP:CE3	1:A:298:PHE:HD1	2.34	0.45
1:D:304:LEU:O	1:D:308:ILE:HG12	2.17	0.45
1:A:191:ARG:HG3	1:A:192:GLN:N	2.32	0.45
1:B:15:LEU:HD11	1:B:46:TRP:HB2	1.99	0.45
1:D:53:PHE:CE1	1:D:95:PRO:HA	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:223:ASN:HB3	1:D:272:VAL:HG11	1.99	0.45
1:B:155:PHE:CE1	1:C:112:PRO:HB3	2.51	0.45
1:D:268:ALA:O	1:D:272:VAL:HG22	2.16	0.45
1:A:34:GLU:OE2	1:A:112:PRO:HA	2.15	0.45
1:A:155:PHE:CZ	1:B:112:PRO:HB3	2.51	0.45
1:D:193:TYR:CD2	1:D:193:TYR:C	2.90	0.45
1:C:118:TYR:CD1	1:C:118:TYR:C	2.88	0.45
1:E:149:GLY:O	1:E:164:PHE:HD1	2.00	0.45
1:C:70:ILE:N	1:C:70:ILE:HD13	2.31	0.45
1:E:241:VAL:C	1:E:243:THR:N	2.69	0.45
1:E:305:ALA:O	1:E:309:LEU:HB2	2.17	0.45
1:B:81:GLU:HG3	1:B:108:ARG:HG3	1.99	0.45
1:C:22:TYR:CA	1:C:149:GLY:HA2	2.32	0.45
1:A:150:LYS:HG2	1:A:154:VAL:HG21	1.97	0.45
1:B:57:ARG:HA	1:B:57:ARG:HE	1.81	0.45
1:B:118:TYR:C	1:B:118:TYR:CD1	2.86	0.45
1:B:72:ILE:HG22	1:B:73:PRO:HD2	1.98	0.45
1:B:274:VAL:C	1:B:276:HIS:N	2.70	0.45
1:B:232:ILE:HG22	1:B:233:ALA:N	2.32	0.45
1:E:218:THR:HG22	1:E:279:LYS:HE2	1.99	0.45
1:C:304:LEU:O	1:C:308:ILE:HG12	2.16	0.45
1:C:128:TYR:O	1:C:183:LEU:O	2.35	0.45
1:A:49:ARG:O	1:A:51:LEU:N	2.50	0.45
1:B:226:LEU:HA	1:B:226:LEU:HD22	1.68	0.45
1:D:194:PHE:C	1:D:196:TYR:N	2.70	0.45
1:C:137:ARG:HD2	1:C:179:LEU:HG	1.99	0.45
1:E:304:LEU:O	1:E:308:ILE:HG12	2.17	0.45
1:B:47:LYS:HD2	1:B:49:ARG:HH21	1.81	0.44
1:A:274:VAL:HG12	1:A:275:GLN:N	2.32	0.44
1:E:155:PHE:HB3	1:E:156:LEU:H	1.60	0.44
1:A:150:LYS:HB3	1:A:150:LYS:HE2	1.73	0.44
1:D:57:ARG:HE	1:D:57:ARG:HA	1.81	0.44
1:C:274:VAL:HG12	1:C:275:GLN:N	2.32	0.44
1:B:155:PHE:HB3	1:B:156:LEU:H	1.58	0.44
1:A:81:GLU:HG3	1:A:108:ARG:HG3	1.99	0.44
1:B:42:LEU:HB3	1:B:103:GLU:CG	2.45	0.44
1:A:304:LEU:O	1:A:308:ILE:HG12	2.16	0.44
1:D:305:ALA:O	1:D:309:LEU:HB2	2.16	0.44
1:E:53:PHE:CE2	1:E:63:LYS:HB3	2.53	0.44
1:B:197:ILE:HB	1:B:198:PRO:CD	2.41	0.44
1:D:62:VAL:HG13	1:D:93:VAL:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:VAL:C	1:A:276:HIS:N	2.71	0.44
1:B:212:TRP:CE3	1:B:298:PHE:HD1	2.36	0.44
1:A:68:GLU:CD	1:A:68:GLU:N	2.71	0.44
1:D:22:TYR:CD1	1:D:149:GLY:HA2	2.52	0.44
1:D:274:VAL:C	1:D:276:HIS:N	2.71	0.44
1:A:223:ASN:HB3	1:A:272:VAL:HG11	2.00	0.44
1:A:241:VAL:C	1:A:243:THR:N	2.71	0.44
1:C:287:ALA:C	1:C:289:SER:N	2.71	0.44
1:D:212:TRP:HB2	1:D:215:PHE:CE1	2.53	0.44
1:A:118:TYR:HB3	1:A:119:PRO:HD3	1.99	0.44
1:C:68:GLU:N	1:C:68:GLU:CD	2.71	0.44
1:E:22:TYR:CD1	1:E:149:GLY:HA2	2.53	0.44
1:B:53:PHE:CE1	1:B:95:PRO:HA	2.53	0.44
1:C:274:VAL:C	1:C:276:HIS:N	2.71	0.44
1:B:212:TRP:CZ3	1:B:264:PHE:HD2	2.33	0.44
1:A:65:TYR:CD1	1:A:70:ILE:HD11	2.52	0.44
1:D:210:ILE:O	1:D:213:THR:HB	2.17	0.44
1:A:155:PHE:HB3	1:A:156:LEU:H	1.59	0.44
1:B:194:PHE:C	1:B:196:TYR:N	2.71	0.44
1:E:137:ARG:HA	1:E:137:ARG:HD3	1.77	0.44
1:E:232:ILE:HG22	1:E:233:ALA:N	2.32	0.44
1:B:147:LYS:CG	1:B:147:LYS:O	2.66	0.44
1:C:62:VAL:HG13	1:C:93:VAL:O	2.18	0.44
1:C:218:THR:HG22	1:C:279:LYS:HE2	2.00	0.43
1:B:53:PHE:CE2	1:B:63:LYS:HB3	2.53	0.43
1:A:53:PHE:CE1	1:A:95:PRO:HA	2.53	0.43
1:E:271:GLU:O	1:E:274:VAL:N	2.51	0.43
1:D:276:HIS:C	1:D:278:LEU:N	2.71	0.43
1:A:287:ALA:C	1:A:289:SER:N	2.72	0.43
1:D:27:TYR:HB3	1:E:110:LEU:HD11	2.00	0.43
1:C:149:GLY:O	1:C:164:PHE:HD1	2.01	0.43
1:E:47:LYS:HD2	1:E:49:ARG:HH21	1.82	0.43
1:D:253:TYR:CA	1:D:313:PHE:CE2	3.00	0.43
1:C:65:TYR:CD1	1:C:70:ILE:HD11	2.52	0.43
1:E:226:LEU:HD22	1:E:226:LEU:HA	1.67	0.43
1:B:137:ARG:HA	1:B:137:ARG:HD3	1.78	0.43
1:C:37:LYS:HG2	1:C:108:ARG:HB3	1.99	0.43
1:A:175:LEU:O	1:A:176:GLU:HB2	2.17	0.43
1:B:68:GLU:CD	1:B:68:GLU:N	2.70	0.43
1:D:13:GLU:CB	1:D:14:PRO:CD	2.87	0.43
1:A:52:ALA:HA	1:A:95:PRO:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:271:GLU:O	1:C:274:VAL:N	2.51	0.43
1:D:314:PHE:N	1:D:314:PHE:HD1	2.16	0.43
1:B:61:ARG:HG2	1:B:62:VAL:HG23	2.01	0.43
1:A:309:LEU:HD12	1:A:309:LEU:HA	1.79	0.43
1:A:22:TYR:CD1	1:A:149:GLY:HA2	2.53	0.43
1:E:287:ALA:C	1:E:289:SER:N	2.71	0.43
1:D:212:TRP:HB2	1:D:215:PHE:CD1	2.53	0.43
1:D:216:TRP:CH2	1:D:295:ARG:HB3	2.53	0.43
1:E:199:ASN:O	1:E:200:ILE:HD13	2.19	0.43
1:E:216:TRP:CH2	1:E:295:ARG:HB3	2.54	0.43
1:E:194:PHE:C	1:E:196:TYR:N	2.70	0.43
1:E:137:ARG:HD2	1:E:179:LEU:HG	1.99	0.43
1:B:241:VAL:C	1:B:243:THR:N	2.71	0.43
1:E:223:ASN:O	1:E:227:VAL:HG23	2.19	0.43
1:A:298:PHE:CB	1:A:299:PRO:HD3	2.49	0.43
1:C:212:TRP:CZ3	1:C:264:PHE:HD2	2.35	0.43
1:B:118:TYR:HB3	1:B:119:PRO:HD3	2.00	0.43
1:C:53:PHE:CE2	1:C:63:LYS:HB3	2.54	0.43
1:E:128:TYR:O	1:E:183:LEU:O	2.37	0.43
1:D:274:VAL:HG12	1:D:275:GLN:N	2.33	0.43
1:D:30:ASP:HB3	1:D:33:ALA:HB3	2.00	0.43
1:C:199:ASN:O	1:C:200:ILE:HD13	2.19	0.43
1:C:194:PHE:C	1:C:196:TYR:N	2.70	0.43
1:D:132:ARG:HA	1:D:180:GLU:HG2	2.01	0.43
1:C:305:ALA:O	1:C:309:LEU:HB2	2.17	0.43
1:B:22:TYR:CD1	1:B:149:GLY:HA2	2.54	0.43
1:B:149:GLY:O	1:B:150:LYS:CB	2.57	0.43
1:C:52:ALA:HA	1:C:95:PRO:O	2.18	0.43
1:D:49:ARG:O	1:D:51:LEU:N	2.51	0.43
1:E:9:PRO:HB3	1:E:48:ASP:OD1	2.18	0.43
1:D:40:ALA:HB3	1:D:105:PHE:CE1	2.53	0.43
1:A:37:LYS:HG2	1:A:108:ARG:HB3	2.01	0.43
1:D:218:THR:HG22	1:D:279:LYS:HE2	2.01	0.43
1:E:53:PHE:CE1	1:E:95:PRO:HA	2.54	0.43
1:E:257:ILE:O	1:E:261:ILE:CG1	2.67	0.43
1:C:53:PHE:CE1	1:C:95:PRO:HA	2.54	0.43
1:C:94:SER:OG	1:C:95:PRO:HD2	2.19	0.43
1:E:298:PHE:CB	1:E:299:PRO:HD3	2.49	0.43
1:A:111:SER:HA	1:A:112:PRO:HD2	1.78	0.43
1:B:193:TYR:CD2	1:B:193:TYR:C	2.92	0.43
1:E:61:ARG:HG2	1:E:62:VAL:HG23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:PHE:O	1:A:252:THR:HG22	2.19	0.43
1:C:151:ASN:ND2	1:C:152:ASP:N	2.57	0.42
1:D:128:TYR:O	1:D:183:LEU:O	2.37	0.42
1:A:140:VAL:CG2	1:A:183:LEU:HG	2.49	0.42
1:B:30:ASP:HB3	1:B:33:ALA:HB3	2.00	0.42
1:A:62:VAL:HG13	1:A:93:VAL:O	2.18	0.42
1:D:191:ARG:HG3	1:D:192:GLN:N	2.33	0.42
1:D:257:ILE:O	1:D:261:ILE:CG1	2.67	0.42
1:C:257:ILE:O	1:C:261:ILE:CG1	2.67	0.42
1:B:287:ALA:C	1:B:289:SER:N	2.73	0.42
1:E:42:LEU:HB3	1:E:103:GLU:CG	2.48	0.42
1:D:202:LEU:HD22	1:D:202:LEU:HA	1.94	0.42
1:D:199:ASN:O	1:D:200:ILE:HD13	2.19	0.42
1:B:191:ARG:HG3	1:B:192:GLN:N	2.34	0.42
1:B:52:ALA:HA	1:B:95:PRO:O	2.19	0.42
1:E:42:LEU:O	1:E:102:LEU:HD12	2.19	0.42
1:A:276:HIS:C	1:A:278:LEU:N	2.72	0.42
1:C:232:ILE:HG22	1:C:233:ALA:N	2.34	0.42
1:E:115:PHE:O	1:E:252:THR:HG22	2.19	0.42
1:B:218:THR:HG22	1:B:279:LYS:HE2	2.01	0.42
1:C:27:TYR:HB3	1:D:110:LEU:HD11	2.01	0.42
1:E:191:ARG:HG3	1:E:192:GLN:N	2.34	0.42
1:C:79:ASN:HD22	1:C:79:ASN:N	2.05	0.42
1:A:128:TYR:O	1:A:183:LEU:O	2.37	0.42
1:D:196:TYR:N	1:D:196:TYR:CD1	2.85	0.42
1:B:27:TYR:HB3	1:C:110:LEU:HD11	2.02	0.42
1:A:53:PHE:CE2	1:A:63:LYS:HB3	2.54	0.42
1:C:223:ASN:HB3	1:C:272:VAL:HG11	2.00	0.42
1:C:298:PHE:CB	1:C:299:PRO:HD3	2.48	0.42
1:C:65:TYR:CD2	1:C:70:ILE:HD11	2.54	0.42
1:C:193:TYR:CD2	1:C:193:TYR:C	2.92	0.42
1:A:226:LEU:HD23	1:B:224:VAL:HB	2.01	0.42
1:E:193:TYR:C	1:E:193:TYR:CD2	2.92	0.42
1:E:260:MET:HE3	1:E:309:LEU:HD22	2.00	0.42
1:D:232:ILE:HG22	1:D:233:ALA:N	2.35	0.42
1:B:21:ILE:O	1:B:149:GLY:HA3	2.19	0.42
1:E:52:ALA:HA	1:E:95:PRO:O	2.20	0.42
1:D:47:LYS:HD2	1:D:49:ARG:HH21	1.85	0.42
1:D:42:LEU:O	1:D:102:LEU:HD12	2.19	0.42
1:D:271:GLU:O	1:D:274:VAL:N	2.52	0.42
1:E:65:TYR:CD2	1:E:70:ILE:HD11	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:137:ARG:HD2	1:D:179:LEU:HG	2.02	0.42
1:C:25:GLU:HA	1:C:25:GLU:OE1	2.20	0.42
1:E:81:GLU:HG3	1:E:108:ARG:HG3	2.00	0.42
1:E:175:LEU:O	1:E:176:GLU:HB2	2.20	0.42
1:D:21:ILE:O	1:D:149:GLY:HA3	2.19	0.42
1:B:283:GLN:N	1:B:284:PRO:CD	2.83	0.42
1:D:70:ILE:HG22	1:D:71:TRP:N	2.34	0.42
1:D:298:PHE:CB	1:D:299:PRO:HD3	2.48	0.42
1:A:194:PHE:C	1:A:196:TYR:N	2.71	0.42
1:C:47:LYS:HD2	1:C:49:ARG:HH21	1.85	0.42
1:D:212:TRP:CZ3	1:D:264:PHE:HD2	2.34	0.42
1:B:195:SER:O	1:B:199:ASN:HB2	2.20	0.42
1:A:210:ILE:O	1:A:213:THR:HB	2.19	0.42
1:B:77:PHE:H	1:B:84:ARG:CD	2.29	0.42
1:B:223:ASN:HB3	1:B:272:VAL:HG11	2.00	0.42
1:B:276:HIS:C	1:B:278:LEU:N	2.71	0.42
1:C:226:LEU:HD23	1:D:224:VAL:HB	2.01	0.42
1:C:210:ILE:O	1:C:213:THR:HB	2.20	0.42
1:A:22:TYR:CA	1:A:149:GLY:HA2	2.34	0.41
1:C:141:LEU:HD23	1:C:142:ALA:N	2.26	0.41
1:A:47:LYS:HD2	1:A:49:ARG:HH21	1.84	0.41
1:C:283:GLN:N	1:C:284:PRO:CD	2.82	0.41
1:B:275:GLN:O	1:B:275:GLN:CG	2.67	0.41
1:E:314:PHE:N	1:E:314:PHE:HD1	2.17	0.41
1:B:37:LYS:HE3	1:B:108:ARG:HD2	2.02	0.41
1:A:202:LEU:HD22	1:A:202:LEU:HA	1.87	0.41
1:A:224:VAL:HB	1:E:226:LEU:HD23	2.02	0.41
1:A:205:LEU:O	1:A:206:PHE:C	2.58	0.41
1:A:242:GLU:O	1:A:242:GLU:HG2	2.20	0.41
1:A:77:PHE:H	1:A:84:ARG:CD	2.29	0.41
1:A:270:ILE:HA	1:A:270:ILE:HD13	1.67	0.41
1:D:195:SER:O	1:D:199:ASN:HB2	2.20	0.41
1:D:149:GLY:O	1:D:164:PHE:HD1	2.02	0.41
1:B:128:TYR:O	1:B:183:LEU:O	2.38	0.41
1:B:298:PHE:CB	1:B:299:PRO:HD3	2.50	0.41
1:D:50:ARG:HG2	1:D:50:ARG:O	2.20	0.41
1:E:68:GLU:N	1:E:68:GLU:CD	2.73	0.41
1:A:149:GLY:O	1:A:164:PHE:HD1	2.03	0.41
1:D:52:ALA:HB1	1:D:95:PRO:O	2.21	0.41
1:E:54:ASP:HA	1:E:55:PRO:HD2	1.89	0.41
1:E:253:TYR:HB2	1:E:313:PHE:HD2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:283:GLN:N	1:D:284:PRO:CD	2.83	0.41
1:D:287:ALA:C	1:D:289:SER:N	2.73	0.41
1:A:212:TRP:HB2	1:A:215:PHE:CD1	2.56	0.41
1:D:68:GLU:H	1:D:68:GLU:CD	2.23	0.41
1:B:149:GLY:O	1:B:164:PHE:HD1	2.03	0.41
1:D:84:ARG:NH1	1:D:84:ARG:CB	2.66	0.41
1:C:270:ILE:HA	1:C:270:ILE:HD13	1.70	0.41
1:D:25:GLU:HA	1:D:25:GLU:OE1	2.21	0.41
1:C:137:ARG:HA	1:C:137:ARG:HD3	1.74	0.41
1:A:21:ILE:O	1:A:149:GLY:HA3	2.20	0.41
1:D:197:ILE:HB	1:D:198:PRO:CD	2.40	0.41
1:A:195:SER:O	1:A:199:ASN:HB2	2.20	0.41
1:B:132:ARG:HA	1:B:180:GLU:HG2	2.02	0.41
1:A:84:ARG:NH1	1:A:84:ARG:CB	2.66	0.41
1:C:77:PHE:H	1:C:84:ARG:CD	2.30	0.41
1:C:195:SER:O	1:C:199:ASN:HB2	2.21	0.41
1:B:216:TRP:CH2	1:B:295:ARG:HB3	2.55	0.41
1:B:111:SER:HA	1:B:112:PRO:HD2	1.80	0.41
1:C:196:TYR:HD1	1:C:196:TYR:N	2.18	0.41
1:A:226:LEU:HA	1:A:226:LEU:HD22	1.73	0.41
1:D:53:PHE:CE2	1:D:63:LYS:HB3	2.55	0.41
1:D:77:PHE:H	1:D:84:ARG:CD	2.27	0.41
1:B:54:ASP:HA	1:B:55:PRO:HD2	1.88	0.41
1:A:253:TYR:CA	1:A:313:PHE:CE2	3.01	0.41
1:B:223:ASN:O	1:B:227:VAL:HG23	2.20	0.41
1:A:314:PHE:HD1	1:A:314:PHE:N	2.19	0.41
1:A:15:LEU:HD12	1:A:16:THR:N	2.36	0.41
1:E:196:TYR:N	1:E:196:TYR:HD1	2.19	0.41
1:A:260:MET:HE3	1:A:309:LEU:HD22	2.03	0.41
1:D:309:LEU:HA	1:D:309:LEU:HD12	1.75	0.41
1:B:175:LEU:O	1:B:176:GLU:HB2	2.20	0.41
1:B:226:LEU:HD23	1:C:224:VAL:HB	2.03	0.41
1:E:30:ASP:HB3	1:E:33:ALA:HB3	2.02	0.41
1:B:196:TYR:HD1	1:B:196:TYR:N	2.18	0.41
1:A:223:ASN:O	1:A:227:VAL:HG23	2.21	0.40
1:B:212:TRP:HB2	1:B:215:PHE:CD1	2.56	0.40
1:B:40:ALA:HB3	1:B:105:PHE:CE1	2.56	0.40
1:B:25:GLU:OE1	1:B:25:GLU:HA	2.22	0.40
1:D:37:LYS:HG2	1:D:108:ARG:HB3	2.02	0.40
1:C:276:HIS:C	1:C:278:LEU:N	2.71	0.40
1:A:212:TRP:HB2	1:A:215:PHE:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:LEU:HD12	1:C:16:THR:N	2.36	0.40
1:D:115:PHE:O	1:D:252:THR:HG22	2.22	0.40
1:C:116:ARG:HG3	1:C:250:TYR:CD2	2.57	0.40
1:E:76:ARG:HH12	1:E:130:ILE:HD11	1.86	0.40
1:E:282:SER:C	1:E:284:PRO:CD	2.86	0.40
1:A:283:GLN:N	1:A:284:PRO:CD	2.83	0.40
1:E:15:LEU:HD12	1:E:16:THR:N	2.37	0.40
1:C:253:TYR:CA	1:C:313:PHE:CE2	3.01	0.40
1:C:223:ASN:O	1:C:227:VAL:HG23	2.21	0.40
1:C:275:GLN:CG	1:C:275:GLN:O	2.67	0.40
1:C:42:LEU:O	1:C:102:LEU:HD12	2.22	0.40
1:B:162:GLU:HB2	1:B:188:ARG:O	2.21	0.40
1:E:253:TYR:CA	1:E:313:PHE:CE2	3.01	0.40
1:E:283:GLN:N	1:E:284:PRO:CD	2.82	0.40
1:C:253:TYR:HB2	1:C:313:PHE:HD2	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	308/317 (97%)	239 (78%)	52 (17%)	17 (6%)	2	13
1	B	308/317 (97%)	243 (79%)	49 (16%)	16 (5%)	2	15
1	C	308/317 (97%)	242 (79%)	48 (16%)	18 (6%)	2	12
1	D	308/317 (97%)	244 (79%)	47 (15%)	17 (6%)	2	13
1	E	308/317 (97%)	243 (79%)	48 (16%)	17 (6%)	2	13
All	All	1540/1585 (97%)	1211 (79%)	244 (16%)	85 (6%)	2	13

All (85) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	ARG
1	A	118	TYR
1	A	148	VAL
1	A	150	LYS
1	A	194	PHE
1	A	275	GLN
1	B	50	ARG
1	B	118	TYR
1	B	148	VAL
1	B	150	LYS
1	B	194	PHE
1	B	275	GLN
1	C	50	ARG
1	C	118	TYR
1	C	148	VAL
1	C	150	LYS
1	C	194	PHE
1	C	275	GLN
1	D	50	ARG
1	D	118	TYR
1	D	148	VAL
1	D	150	LYS
1	D	194	PHE
1	D	275	GLN
1	E	50	ARG
1	E	118	TYR
1	E	148	VAL
1	E	150	LYS
1	E	194	PHE
1	E	275	GLN
1	A	69	ALA
1	A	287	ALA
1	B	69	ALA
1	B	287	ALA
1	C	69	ALA
1	C	287	ALA
1	D	69	ALA
1	D	287	ALA
1	E	69	ALA
1	E	287	ALA
1	A	84	ARG
1	A	240	LEU
1	A	288	ALA

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Mol	Chain	Res	Type
1	A	295	ARG
1	B	84	ARG
1	C	84	ARG
1	D	84	ARG
1	E	84	ARG
1	E	288	ALA
1	B	226	LEU
1	B	282	SER
1	B	288	ALA
1	C	149	GLY
1	C	282	SER
1	C	288	ALA
1	D	282	SER
1	D	288	ALA
1	E	282	SER
1	E	295	ARG
1	A	34	GLU
1	A	278	LEU
1	B	149	GLY
1	B	278	LEU
1	C	226	LEU
1	C	271	GLU
1	C	278	LEU
1	C	295	ARG
1	D	226	LEU
1	D	278	LEU
1	E	34	GLU
1	E	149	GLY
1	E	278	LEU
1	A	149	GLY
1	A	282	SER
1	B	129	LEU
1	C	34	GLU
1	D	149	GLY
1	D	295	ARG
1	E	291	THR
1	B	290	ILE
1	D	55	PRO
1	D	290	ILE
1	E	290	ILE
1	C	290	ILE
1	A	290	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	278/284 (98%)	241 (87%)	37 (13%)	5	20
1	B	278/284 (98%)	238 (86%)	40 (14%)	4	17
1	C	278/284 (98%)	240 (86%)	38 (14%)	4	19
1	D	278/284 (98%)	238 (86%)	40 (14%)	4	17
1	E	278/284 (98%)	239 (86%)	39 (14%)	4	18
All	All	1390/1420 (98%)	1196 (86%)	194 (14%)	4	18

All (194) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	THR
1	A	53	PHE
1	A	57	ARG
1	A	64	THR
1	A	68	GLU
1	A	72	ILE
1	A	79	ASN
1	A	84	ARG
1	A	91	ILE
1	A	98	THR
1	A	110	LEU
1	A	124	THR
1	A	130	ILE
1	A	134	VAL
1	A	141	LEU
1	A	148	VAL
1	A	151	ASN
1	A	154	VAL
1	A	155	PHE
1	A	162	GLU
1	A	177	ASP
1	A	179	LEU
1	A	202	LEU

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Mol	Chain	Res	Type
1	A	211	SER
1	A	212	TRP
1	A	213	THR
1	A	221	GLU
1	A	226	LEU
1	A	243	THR
1	A	254	THR
1	A	257	ILE
1	A	263	LEU
1	A	270	ILE
1	A	271	GLU
1	A	272	VAL
1	A	292	ARG
1	A	314	PHE
1	B	16	THR
1	B	53	PHE
1	B	57	ARG
1	B	64	THR
1	B	68	GLU
1	B	72	ILE
1	B	79	ASN
1	B	84	ARG
1	B	91	ILE
1	B	98	THR
1	B	100	GLN
1	B	110	LEU
1	B	124	THR
1	B	130	ILE
1	B	134	VAL
1	B	141	LEU
1	B	148	VAL
1	B	151	ASN
1	B	154	VAL
1	B	155	PHE
1	B	162	GLU
1	B	177	ASP
1	B	179	LEU
1	B	202	LEU
1	B	211	SER
1	B	212	TRP
1	B	213	THR
1	B	221	GLU

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Mol	Chain	Res	Type
1	B	226	LEU
1	B	228	VAL
1	B	243	THR
1	B	254	THR
1	B	257	ILE
1	B	263	LEU
1	B	269	VAL
1	B	270	ILE
1	B	271	GLU
1	B	272	VAL
1	B	292	ARG
1	B	314	PHE
1	C	16	THR
1	C	53	PHE
1	C	57	ARG
1	C	64	THR
1	C	68	GLU
1	C	72	ILE
1	C	79	ASN
1	C	84	ARG
1	C	91	ILE
1	C	98	THR
1	C	110	LEU
1	C	124	THR
1	C	130	ILE
1	C	134	VAL
1	C	141	LEU
1	C	148	VAL
1	C	151	ASN
1	C	154	VAL
1	C	155	PHE
1	C	162	GLU
1	C	177	ASP
1	C	179	LEU
1	C	202	LEU
1	C	211	SER
1	C	212	TRP
1	C	213	THR
1	C	221	GLU
1	C	226	LEU
1	C	228	VAL
1	C	243	THR

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Mol	Chain	Res	Type
1	C	254	THR
1	C	257	ILE
1	C	263	LEU
1	C	270	ILE
1	C	271	GLU
1	C	272	VAL
1	C	292	ARG
1	C	314	PHE
1	D	16	THR
1	D	53	PHE
1	D	57	ARG
1	D	64	THR
1	D	68	GLU
1	D	72	ILE
1	D	79	ASN
1	D	84	ARG
1	D	91	ILE
1	D	98	THR
1	D	100	GLN
1	D	110	LEU
1	D	124	THR
1	D	130	ILE
1	D	134	VAL
1	D	141	LEU
1	D	148	VAL
1	D	151	ASN
1	D	154	VAL
1	D	155	PHE
1	D	162	GLU
1	D	177	ASP
1	D	179	LEU
1	D	202	LEU
1	D	211	SER
1	D	212	TRP
1	D	213	THR
1	D	221	GLU
1	D	226	LEU
1	D	232	ILE
1	D	243	THR
1	D	254	THR
1	D	257	ILE
1	D	258	ILE

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Mol	Chain	Res	Type
1	D	263	LEU
1	D	270	ILE
1	D	271	GLU
1	D	272	VAL
1	D	292	ARG
1	D	314	PHE
1	E	16	THR
1	E	53	PHE
1	E	57	ARG
1	E	64	THR
1	E	68	GLU
1	E	72	ILE
1	E	79	ASN
1	E	84	ARG
1	E	89	VAL
1	E	91	ILE
1	E	98	THR
1	E	124	THR
1	E	130	ILE
1	E	134	VAL
1	E	140	VAL
1	E	141	LEU
1	E	148	VAL
1	E	151	ASN
1	E	154	VAL
1	E	155	PHE
1	E	162	GLU
1	E	177	ASP
1	E	179	LEU
1	E	202	LEU
1	E	211	SER
1	E	212	TRP
1	E	213	THR
1	E	221	GLU
1	E	226	LEU
1	E	243	THR
1	E	254	THR
1	E	257	ILE
1	E	258	ILE
1	E	263	LEU
1	E	270	ILE
1	E	271	GLU

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Mol	Chain	Res	Type
1	E	272	VAL
1	E	292	ARG
1	E	314	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	ASN
1	A	100	GLN
1	A	123	GLN
1	A	151	ASN
1	A	283	GLN
1	B	79	ASN
1	B	100	GLN
1	B	123	GLN
1	B	151	ASN
1	B	283	GLN
1	C	79	ASN
1	C	100	GLN
1	C	151	ASN
1	C	283	GLN
1	D	79	ASN
1	D	100	GLN
1	D	151	ASN
1	D	283	GLN
1	E	79	ASN
1	E	100	GLN
1	E	123	GLN
1	E	151	ASN
1	E	283	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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	310/317 (97%)	-0.23	9 (2%)	55	31	56, 83, 126, 163	0
1	B	310/317 (97%)	-0.31	9 (2%)	55	31	57, 83, 125, 163	0
1	C	310/317 (97%)	-0.28	14 (4%)	37	17	58, 82, 126, 164	0
1	D	310/317 (97%)	-0.29	8 (2%)	59	35	57, 83, 124, 163	0
1	E	310/317 (97%)	-0.27	11 (3%)	48	23	57, 82, 125, 164	0
All	All	1550/1585 (97%)	-0.27	51 (3%)	50	26	56, 83, 126, 164	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	55	PRO	6.4
1	C	316	PHE	6.3
1	D	316	PHE	5.3
1	E	316	PHE	4.9
1	D	56	VAL	4.4
1	E	59	GLY	3.5
1	E	58	SER	3.5
1	C	58	SER	3.5
1	D	315	GLY	3.5
1	C	56	VAL	3.5
1	C	59	GLY	3.4
1	B	316	PHE	3.3
1	A	58	SER	3.2
1	B	59	GLY	3.1
1	D	57	ARG	3.0
1	E	60	VAL	3.0
1	A	59	GLY	3.0
1	B	57	ARG	2.9
1	E	53	PHE	2.9
1	B	58	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	316	PHE	2.8
1	A	53	PHE	2.8
1	C	61	ARG	2.8
1	E	57	ARG	2.7
1	C	54	ASP	2.7
1	D	54	ASP	2.7
1	C	53	PHE	2.6
1	C	315	GLY	2.6
1	C	12	ASP	2.6
1	A	11	ALA	2.5
1	B	315	GLY	2.5
1	B	53	PHE	2.5
1	C	10	ILE	2.4
1	B	54	ASP	2.4
1	D	177	ASP	2.3
1	C	51	LEU	2.3
1	B	10	ILE	2.3
1	A	10	ILE	2.2
1	C	57	ARG	2.2
1	E	54	ASP	2.2
1	E	63	LYS	2.2
1	A	51	LEU	2.2
1	C	60	VAL	2.2
1	E	315	GLY	2.1
1	C	13	GLU	2.1
1	B	60	VAL	2.1
1	D	61	ARG	2.0
1	E	93	VAL	2.0
1	E	94	SER	2.0
1	A	292	ARG	2.0
1	A	315	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates 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.