WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2023 – 01:36 AM EDT

PDB ID	:	3EHZ
Title	:	X-ray structure of the pentameric ligand gated ion channel of Gloebacter violaceus (GLIC) in a presumptive open conformation
Authors	:	Hilf, R.J.C.; Dutzler, R.
Deposited on	:	2008-09-15
Resolution	:	3.10 Å(reported)

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

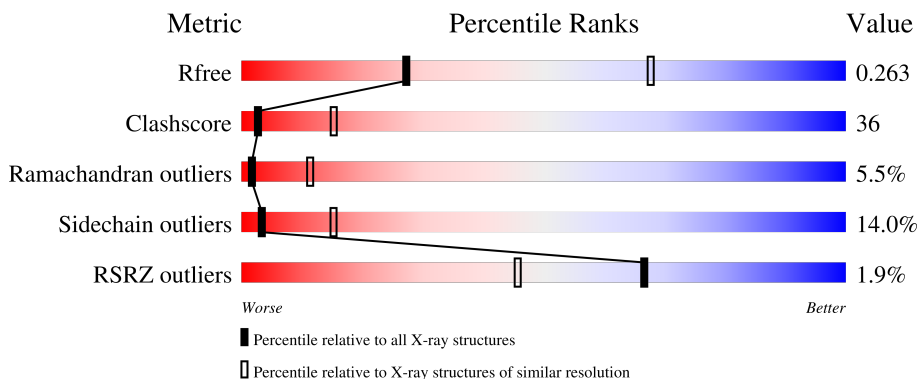|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance ⓘ

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	Percentile Ranks	Value
Rfree		0.263
Clashscore		36
Ramachandran outliers		5.5%
Sidechain outliers		14.0%
RSRZ outliers		1.9%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	317	.% — 41% / 46% / 11% ·
1	B	317	2% — 42% / 44% / 11% ··
1	C	317	2% — 44% / 42% / 11% ··
1	D	317	2% — 44% / 42% / 12% ·
1	E	317	2% — 43% / 44% / 11% ·

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.

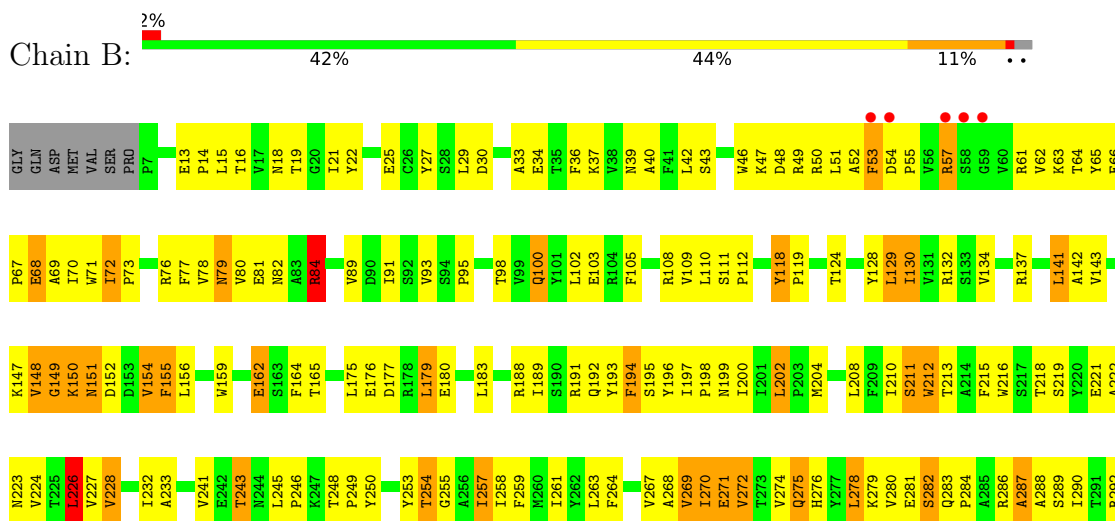| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	8	Total 8	O 8	0	0
2	B	9	Total 9	O 9	0	0
2	C	11	Total 11	O 11	0	0
2	D	10	Total 10	O 10	0	0
2	E	9	Total 9	O 9	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
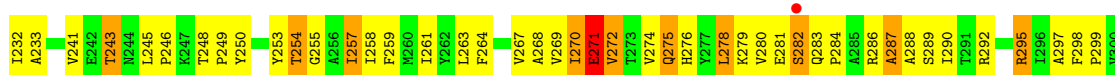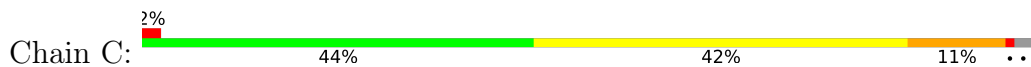
• Molecule 1: Glr4197 protein
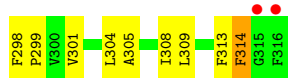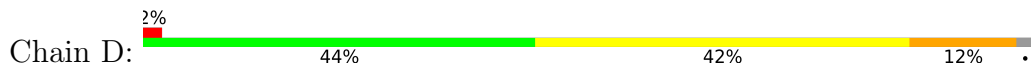

• Molecule 1: Glr4197 protein

R295 I296 A297 F298 P299 V300 V301 L304 A305 I308 L309 F313 F314 G315 F316

● Molecule 1: Glr4197 protein

Chain C:

2%
44% 42% 11%

GLY GLN ASP MET VAL SER PRO P7 E13 P14 L15 T16 V17 N18 T19 Y22 E25 C26 Y27 S28 L29 A33 E34 T35 F36 K37 V38 N39 A40 F41 L42 S43 W46 K47 D48 R49 R50 L51 A52 F53 D54 P55 V56 R57 S58 G59 V60 R61 V62 K63 T64 Y65 E66 P67 E68

A69 I70 W71 I72 P73 R76 F77 V78 N79 V80 E81 N82 A83 R84 V89 D90 I91 S92 V93 S94 P95 T98 V99 Q100 Y101 L102 E103 R104 F105 R108 V109 S111 P112 R116 R117 Y118 P119 T124 Y128 L129 I130 V134 R137 L141 A142 V143 K147 V148

G149 K150 N151 D152 D153 V154 F155 L156 W159 E162 S163 F164 T165 D177 R178 L179 L183 I189 S190 R191 Q192 Y193 F194 S195 Y196 I197 P198 N199 I200 I201 L202 P203 M204 L208 F209 I210 S211 W212 T213 W216 S217 T218 S219 Y220 E221 A222 N223 V224 T225 I226 V227 V228

I232 A233 V241 E242 T243 N244 L245 P246 K247 T248 P249 Y250 Y253 T254 G255 A256 I257 I258 F259 M260 I261 Y262 L263 F264 V267 A268 V269 I270 E271 V272 T273 V274 Q275 H276 Y277 L278 K279 V280 E281 S282 Q283 P284 A285 R286 A287 A288 S289 I290 T291 R292 R295 I296 A297 F298 P299 V300

V301 L304 A305 I308 L309 F313 F314 G315 F316

● Molecule 1: Glr4197 protein

Chain D:

2%
44% 42% 12%

GLY GLN ASP MET VAL SER PRO P7 E13 P14 L15 T16 V17 N18 T19 G20 I21 Y22 E25 C26 Y27 S28 L29 D30 A33 E34 T35 F36 K37 V38 N39 A40 F41 L42 S43 K47 D48 R49 R50 L51 A52 F53 D54 P55 V56 R57 R61 V62 K63 T64 Y65 E66 P67 E68 A69

I70 W71 I72 P73 R76 F77 V78 N79 V80 E81 N82 A83 R84 V89 D90 I91 S92 V93 S94 P95 T98 V99 Q100 Y101 L102 E103 R104 F105 R108 V109 L110 S111 P112 F115 Y118 P119 T124 Y128 L129 I130 V131 R132 S133 V134 R137 L141 A142 V143 K147

V148 G149 K150 N151 D152 D153 V154 F155 W159 E162 S163 F164 T165 D177 R178 L179 E180 L183 I189 S190 R191 Q192 Y193 F194 S195 Y196 I197 P198 N199 I200 I201 L202 P203 M204 L208 F209 I210 S211 W212 T213 A214 F215 W216 S217 T218 S219 Y220 E221 A222 N223 V224 T225 L226 V227

V228 I232 A233 V241 E242 T243 N244 L245 P246 K247 T248 P249 Y250 M251 T252 Y253 T254 G255 A256 I257 I258 F259 M260 I261 Y262 L263 F264 V267 A268 V269 I270 E271 V272 T273 V274 Q275 H276 Y277 L278 K279 V280 E281 S282 Q283 P284 A285 R286 A287 A288 S289 I290 T291 R292 R295 I296 A297

F298 P299 V300 V301 L304 A305 I308 L309 F313 F314 G315 F316

● Molecule 1: Glr4197 protein

Chain E:

2%
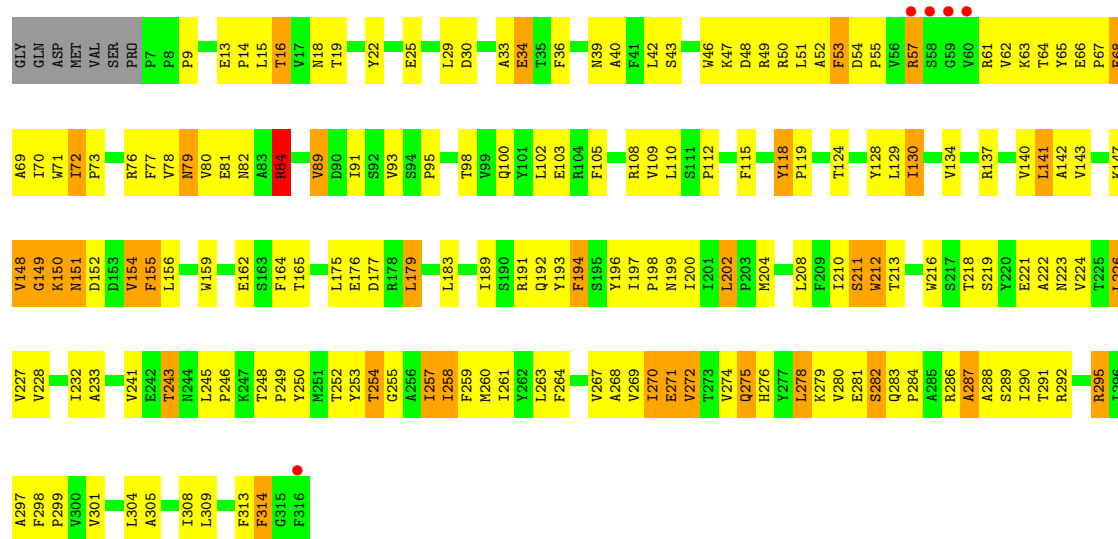43% 44% 11%

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	2.48 (at 3.11Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.238 , 0.266 0.237 , 0.263	Depositor DCC
R_{free} test set	3368 reflections (4.99%)	wwPDB-VP
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
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	0.90	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.*

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[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 (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(^{o})	Ideal(^{o})
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:B:13:GLU:HB3	1:B:14:PRO:HD2	1.47	0.97
1:C:22:TYR:HA	1:C:149:GLY:HA2	1.46	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:C:54:ASP:HB2	1:C:57:ARG:HB2	1.56	0.87
1:E:84:ARG:HH11	1:E:84:ARG:HB2	1.40	0.87
1:E:22:TYR:HA	1:E:149:GLY:CA	2.04	0.87
1:B:77:PHE:CD1	1:B:84:ARG:HD2	2.09	0.87
1:E:54:ASP:HB2	1:E:57:ARG:HB2	1.57	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:C:147:LYS:C	1:C:149:GLY:H	1.77	0.85
1:D:151:ASN:HD22	1:D:152:ASP:H	1.21	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:HB2	1:D:84:ARG:NH1	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:B:197:ILE:HB	1:B:198:PRO:HD3	1.59	0.83
1:C:84:ARG:HB2	1:C:84:ARG:HH11	1.44	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:H	1:D:79:ASN:HD22	1.26	0.82
1:A:84:ARG:HH11	1:A:84:ARG:HB2	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:A:79:ASN:HD22	1:A:79:ASN:H	1.25	0.81
1:D:84:ARG:HH11	1:D:84:ARG:CB	1.94	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:HB2	1:C:84:ARG:NH1	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:HH11	1:A:84:ARG:CB	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:B:77:PHE:HD1	1:B:84:ARG:HD2	1.44	0.79
1:E:149:GLY:O	1:E:150:LYS:HB2	1.81	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:HB2	1:B:84:ARG:NH1	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:48:ASP:O	1:D:51:LEU:HD23	1.82	0.78
1:D:76:ARG:NH2	1:D:130:ILE:HD12	1.99	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:A:80:VAL:HG12	1:A:82:ASN:O	1.85	0.77
1:E:13:GLU:HB3	1:E:14:PRO:CD	2.14	0.77
1:D:13:GLU:HB3	1:D:14:PRO:CD	2.14	0.76
1:C:84:ARG:HH11	1:C:84:ARG:CB	1.97	0.76
1:E:128:TYR:O	1:E:129:LEU:HB2	1.84	0.76
1:B:84:ARG:HH11	1:B:84:ARG:CB	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:D:208:LEU:O	1:D:211:SER:HB3	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:249:PRO:HD2	1:E:250:TYR:HD1	1.53	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:B:128:TYR:O	1:B:129:LEU:HB2	1.90	0.72
1:E:147:LYS:HE2	1:E:165:THR:HA	1.72	0.72
1:A:249:PRO:HD2	1:A:250:TYR:HD1	1.54	0.71
1:A:147:LYS:HE2	1:A:165:THR:HA	1.72	0.71
1:E:151:ASN:HD22	1:E:152:ASP:N	1.87	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:D:42:LEU:HB3	1:D:103:GLU:HG2	1.72	0.70
1:E:282:SER:C	1:E:284:PRO:HD3	2.12	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:B:48:ASP:O	1:B:51:LEU:HD23	1.90	0.69
1:C:282:SER:C	1:C:284:PRO:HD3	2.11	0.69
1:E:275:GLN:O	1:E:275:GLN:HG2	1.91	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:D:151:ASN:HD22	1:D:152:ASP:N	1.90	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:202:LEU:HD12	1:C:259:PHE:CZ	2.28	0.69
1:B:282:SER:C	1:B:284:PRO:HD3	2.13	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:B:253:TYR:HA	1:B:313:PHE:CE2	2.27	0.68
1:C:147:LYS:C	1:C:149:GLY:N	2.47	0.68
1:C:275:GLN:O	1:C:275:GLN:HG2	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:A:282:SER:C	1:A:284:PRO:HD3	2.14	0.67
1:E:76:ARG:HH22	1:E:130:ILE:HD12	1.57	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:D:276:HIS:O	1:D:280:VAL:HG22	1.95	0.67
1:E:80:VAL:CG1	1:E:82:ASN:O	2.42	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:A:80:VAL:CG1	1:A:82:ASN:O	2.43	0.67
1:E:77:PHE:H	1:E:84:ARG:HD3	1.60	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:A:267:VAL:HA	1:A:270:ILE:HB	1.77	0.66
1:A:276:HIS:O	1:A:280:VAL:HG22	1.95	0.66
1:B:276:HIS:O	1:B:280:VAL:HG22	1.96	0.66
1:C:42:LEU:HB3	1:C:103:GLU:HG2	1.76	0.66
1:D:275:GLN:O	1:D:275:GLN:HG2	1.95	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:C:80:VAL:CG1	1:C:82:ASN:O	2.44	0.66
1:E:53:PHE:O	1:E:53:PHE:CD1	2.49	0.66
1:B:42:LEU:HB3	1:B:103:GLU:HG2	1.76	0.66
1:B:53:PHE:O	1:B:53:PHE:CD1	2.48	0.66
1:D:76:ARG:HH22	1:D:130:ILE:HD12	1.59	0.66
1:A:297:ALA:O	1:A:301:VAL:HG23	1.95	0.65
1:C:54:ASP:HB2	1:C:57:ARG:CB	2.26	0.65
1:C:267:VAL:HA	1:C:270:ILE:HB	1.78	0.65
1:D:65:TYR:CG	1:D:70:ILE:HD11	2.31	0.65
1:A:275:GLN:O	1:A:275:GLN:HG2	1.94	0.65
1:C:65:TYR:CG	1:C:70:ILE:HD11	2.31	0.65
1:D:80:VAL:CG1	1:D:82:ASN:O	2.43	0.65
1:A:53:PHE:O	1:A:53:PHE:CD1	2.49	0.65
1:D:147:LYS:C	1:D:149:GLY:N	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:B:267:VAL:HA	1:B:270:ILE:HB	1.77	0.65
1:D:202:LEU:HD12	1:E:259:PHE:CZ	2.31	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:O	1:C:53:PHE:CD1	2.51	0.64
1:C:276:HIS:O	1:C:280:VAL:HG22	1.96	0.64
1:E:54:ASP:HB2	1:E:57:ARG:CB	2.27	0.64
1:B:159:TRP:CE3	1:B:189:ILE:HD12	2.32	0.64
1:C:76:ARG:HH22	1:C:130:ILE:HD12	1.61	0.64
1:A:54:ASP:HB2	1:A:57:ARG:CB	2.28	0.64
1:E:147:LYS:C	1:E:149:GLY:N	2.47	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:CD1	1:D:53:PHE:O	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:A:65:TYR:CG	1:A:70:ILE:HD11	2.34	0.62
1:E:281:GLU:O	1:E:283:GLN:N	2.31	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:O	1:B:53:PHE:HD1	1.83	0.61
1:A:53:PHE:O	1:A:53:PHE:HD1	1.84	0.61
1:A:159:TRP:CE3	1:A:189:ILE:HD12	2.35	0.61
1:E:53:PHE:O	1:E:53:PHE:HD1	1.84	0.61
1:B:89:VAL:HG11	1:B:102:LEU:HD23	1.82	0.60
1:B:267:VAL:HG23	1:B:298:PHE:CZ	2.36	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:89:VAL:HG11	1:E:102:LEU:HD23	1.83	0.60
1:E:283:GLN:HE21	1:E:286:ARG:HB2	1.66	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:A:40:ALA:HB3	1:A:105:PHE:CZ	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:LEU:HD12	1:B:259:PHE:HZ	1.66	0.60
1:B:147:LYS:O	1:B:149:GLY:N	2.34	0.60
1:B:281:GLU:O	1:B:283:GLN:N	2.30	0.60
1:A:281:GLU:O	1:A:283:GLN:N	2.32	0.59
1:B:100:GLN:HE21	1:B:100:GLN:HA	1.66	0.59
1:D:267:VAL:HG23	1:D:298:PHE:CZ	2.37	0.59
1:D:278:LEU:HD21	1:D:286:ARG:HB3	1.84	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:A:255:GLY:O	1:A:258:ILE:HG22	2.02	0.59
1:C:278:LEU:HD21	1:C:286:ARG:HB3	1.85	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:B:283:GLN:HE21	1:B:286:ARG:HB2	1.66	0.59
1:E:283:GLN:N	1:E:284:PRO:HD3	2.18	0.59
1:A:202:LEU:HD12	1:B:259:PHE:CZ	2.37	0.59
1:A:212:TRP:HZ3	1:A:264:PHE:HD2	1.51	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:210:ILE:HG23	1:C:269:VAL:HG11	1.85	0.59
1:B:254:THR:O	1:B:258:ILE:HB	2.02	0.59
1:C:53:PHE:O	1:C:53:PHE:HD1	1.86	0.58
1:C:283:GLN:N	1:C:284:PRO:HD3	2.17	0.58
1:D:212:TRP:HZ3	1:D:264:PHE:HD2	1.50	0.58
1:D:274:VAL:C	1:D:276:HIS:H	2.06	0.58
1:C:255:GLY:O	1:C:258:ILE:HG22	2.03	0.58
1:E:147:LYS:O	1:E:149:GLY:N	2.36	0.58
1:C:274:VAL:C	1:C:276:HIS:H	2.05	0.58
1:A:283:GLN:N	1:A:284:PRO:HD3	2.19	0.58
1:C:276:HIS:C	1:C:278:LEU:H	2.07	0.58
1:C:151:ASN:O	1:C:154:VAL:HG22	2.04	0.58
1:A:274:VAL:C	1:A:276:HIS:H	2.06	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:E:100:GLN:HA	1:E:100:GLN:HE21	1.68	0.58
1:A:267:VAL:HG23	1:A:298:PHE:CZ	2.39	0.57
1:A:278:LEU:HD21	1:A:286:ARG:HB3	1.85	0.57
1:B:276:HIS:C	1:B:278:LEU:H	2.07	0.57
1:C:254:THR:O	1:C:258:ILE:HB	2.03	0.57
1:D:276:HIS:C	1:D:278:LEU:H	2.07	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:283:GLN:N	1:D:284:PRO:HD3	2.18	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:D:100:GLN:HE21	1:D:100:GLN:HA	1.69	0.57
1:E:274:VAL:C	1:E:276:HIS:H	2.08	0.57
1:A:259:PHE:HZ	1:E:202:LEU:HD12	1.69	0.57
1:D:53:PHE:O	1:D:53:PHE:HD1	1.87	0.57
1:A:100:GLN:HE21	1:A:100:GLN:HA	1.69	0.57
1:A:254:THR:O	1:A:258:ILE:HB	2.04	0.57
1:A:276:HIS:C	1:A:278:LEU:H	2.08	0.57
1:D:255:GLY:O	1:D:258:ILE:HG22	2.05	0.57
1:B:255:GLY:O	1:B:258:ILE:HG22	2.05	0.57
1:E:267:VAL:HG23	1:E:298:PHE:CZ	2.39	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:C:202:LEU:HD12	1:D:259:PHE:CZ	2.41	0.56
1:E:70:ILE:HG22	1:E:71:TRP:O	2.05	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:B:89:VAL:CG1	1:B:102:LEU:HD23	2.36	0.56
1:C:271:GLU:OE2	1:C:272:VAL:N	2.39	0.56
1:D:200:ILE:O	1:D:204:MET:HB2	2.06	0.56
1:A:147:LYS:O	1:A:149:GLY:N	2.38	0.56
1:D:147:LYS:O	1:D:149:GLY:N	2.39	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:89:VAL:HG11	1:C:102:LEU:HD23	1.88	0.55
1:C:281:GLU:O	1:C:283:GLN:N	2.32	0.55
1:D:216:TRP:CE2	1:D:295:ARG:HD3	2.42	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:E:151:ASN:O	1:E:154:VAL:HG22	2.05	0.55
1:A:79:ASN:H	1:A:79:ASN:ND2	2.02	0.55
1:C:54:ASP:HB2	1:C:57:ARG:CG	2.36	0.55
1:D:254:THR:O	1:D:258:ILE:HB	2.06	0.55
1:E:208:LEU:HD13	1:E:261:ILE:HG23	1.89	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:A:200:ILE:O	1:A:204:MET:HB2	2.07	0.55
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:E:54:ASP:HB2	1:E:57:ARG:CG	2.37	0.55
1:A:216:TRP:CE2	1:A:295:ARG:HD3	2.42	0.55
1:D:54:ASP:HB2	1:D:57:ARG:CG	2.37	0.55
1:C:216:TRP:CE2	1:C:295:ARG:HD3	2.42	0.55
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:B:79:ASN:H	1:B:79:ASN:ND2	2.01	0.54
1:C:224:VAL:O	1:C:228:VAL:HB	2.07	0.54
1:E:286:ARG:O	1:E:289:SER:HB3	2.06	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:248:THR:HB	1:E:250:TYR:CE1	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:E:216:TRP:CE2	1:E:295:ARG:HD3	2.42	0.54
1:B:248:THR:HB	1:B:250:TYR:CE1	2.43	0.54
1:D:77:PHE:HD1	1:D:84:ARG:CD	2.16	0.54
1:E:89:VAL:CG1	1:E:102:LEU:HD23	2.37	0.54
1:D:314:PHE:CD1	1:D:314:PHE:N	2.76	0.54
1:E:314:PHE:CD1	1:E:314:PHE:N	2.76	0.54
1:A:18:ASN:HB3	1:A:143:VAL:HG23	1.89	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:D:210:ILE:HG23	1:E:269:VAL:HG11	1.89	0.54
1:B:216:TRP:CE2	1:B:295:ARG:HD3	2.42	0.54
1:E:53:PHE:HD1	1:E:53:PHE:C	2.11	0.54
1:D:298:PHE:HB2	1:D:299:PRO:HD3	1.91	0.53
1:E:271:GLU:OE2	1:E:272:VAL:N	2.41	0.53
1:B:271:GLU:OE2	1:B:272:VAL:N	2.40	0.53
1:D:248:THR:HB	1:D:250:TYR:CE1	2.43	0.53
1:E:33:ALA:O	1:E:34:GLU:HB2	2.08	0.53
1:E:298:PHE:HB2	1:E:299:PRO:HD3	1.90	0.53
1:A:155:PHE:CE1	1:B:112:PRO:HB3	2.43	0.53
1:D:89:VAL:HG11	1:D:102:LEU:HD23	1.90	0.53
1:A:22:TYR:HA	1:A:149:GLY:HA3	1.87	0.53
1:B:40:ALA:HB3	1:B:105:PHE:CZ	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:151:ASN:O	1:D:154:VAL:HG22	2.08	0.53
1:A:25:GLU:HB2	1:A:39:ASN:HB3	1.91	0.53
1:E:77:PHE:HD1	1:E:84:ARG:CD	2.17	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: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:C:287:ALA:O	1:C:289:SER:N	2.42	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:A:89:VAL:HG11	1:A:102:LEU:HD23	1.91	0.53
1:D:278:LEU:HD23	1:D:287:ALA:HB2	1.91	0.53
1:E:278:LEU:HD23	1:E:287:ALA:HB2	1.91	0.53
1:E:79:ASN:H	1:E:79:ASN:ND2	2.05	0.52
1:C:278:LEU:HD23	1:C:287:ALA:HB2	1.90	0.52
1:E:287:ALA:O	1:E:289:SER:N	2.42	0.52
1:C:314:PHE:CD1	1:C:314:PHE:N	2.77	0.52
1:C:79:ASN:H	1:C:79:ASN:ND2	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:A:271:GLU:O	1:A:272:VAL:C	2.48	0.52
1:C:53:PHE:CD1	1:C:53:PHE:C	2.83	0.52
1:D:54:ASP:CB	1:D:57:ARG:HB2	2.33	0.52
1:A:193:TYR:O	1:A:194:PHE:HB2	2.09	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:C:70:ILE:HG22	1:C:71:TRP:O	2.10	0.52
1:C:77:PHE:HD1	1:C:84:ARG:CD	2.19	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: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:C:257:ILE:O	1:C:261:ILE:HG12	2.10	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:A:70:ILE:HG22	1:A:71:TRP:O	2.09	0.51
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:B:29:LEU:HD23	1:B:29:LEU:C	2.31	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:E:147:LYS:O	1:E:147:LYS:HG2	2.11	0.51
1:A:274:VAL:O	1:A:276:HIS:N	2.42	0.51
1:D:89:VAL:CG1	1:D:102:LEU:HD23	2.41	0.51
1:C:147:LYS:O	1:C:147:LYS:HG2	2.11	0.51
1:D:53:PHE:CD1	1:D:53:PHE:C	2.84	0.51
1:E:53:PHE:CD1	1:E:53:PHE:C	2.82	0.51
1:A:13:GLU:CB	1:A:14:PRO:CD	2.87	0.51
1:D:33:ALA:O	1:D:34:GLU:HB2	2.11	0.51
1:D:53:PHE:HD1	1:D:53:PHE:C	2.14	0.51
1:A:53:PHE:CD1	1:A:53:PHE:C	2.83	0.51
1:E:151:ASN:ND2	1:E:152:ASP:N	2.55	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:E:13:GLU:CB	1:E:14:PRO:CD	2.86	0.51
1:B:314:PHE:N	1:B:314:PHE:CD1	2.77	0.51
1:A:224:VAL:O	1:A:228:VAL:HB	2.10	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:179:LEU:HD12	1:B:179:LEU:C	2.32	0.50
1:B:193:TYR:O	1:B:194:PHE:HB2	2.10	0.50
1:B:208:LEU:HD13	1:B:261:ILE:HG23	1.93	0.50
1:C:22:TYR:HA	1:C:149:GLY:HA3	1.89	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:A:245:LEU:HD12	1:A:246:PRO:HD2	1.93	0.50
1:C:25:GLU:HB2	1:C:39:ASN:HB3	1.92	0.50
1:C:193:TYR:O	1:C:194:PHE:HB2	2.10	0.50
1:D:193:TYR:O	1:D:194:PHE:HB2	2.10	0.50
1:E:34:GLU:OE2	1:E:112:PRO:HA	2.10	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:C:76:ARG:O	1:C:129:LEU:HA	2.12	0.50
1:B:219:SER:OG	1:B:222:ALA:HB3	2.11	0.50
1:E:70:ILE:HD13	1:E:70:ILE:N	2.26	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:D:155:PHE:CE1	1:E:112:PRO:HB3	2.47	0.50
1:E:271:GLU:O	1:E:272:VAL:C	2.50	0.50
1:A:219:SER:OG	1:A:222:ALA:HB3	2.11	0.50
1:C:54:ASP:CB	1:C:57:ARG:HB2	2.36	0.50
1:D:155:PHE:CZ	1:E:112:PRO:HB3	2.46	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:E:29:LEU:C	1:E:29:LEU:HD23	2.32	0.50
1:C:33:ALA:O	1:C:34:GLU:HB2	2.12	0.50
1:C:72:ILE:HG22	1:C:73:PRO:HD2	1.94	0.50
1:C:271:GLU:O	1:C:272:VAL:C	2.49	0.50
1:D:179:LEU:HD12	1:D:179:LEU:C	2.32	0.50
1:A:269:VAL:HG11	1:E:210:ILE:HG23	1.94	0.50
1:B:150:LYS:HG2	1:B:154:VAL:HG21	1.94	0.50
1:B:224:VAL:O	1:B:228:VAL:HB	2.12	0.50
1:B:281:GLU:C	1:B:283:GLN:H	2.14	0.50
1:D:219:SER:OG	1:D:222:ALA:HB3	2.12	0.50
1:B:54:ASP:HB2	1:B:57:ARG:HG3	1.94	0.49
1:B:274:VAL:O	1:B:276:HIS:N	2.41	0.49
1:D:76:ARG:O	1:D:129:LEU:HA	2.12	0.49
1:E:241:VAL:C	1:E:243:THR:H	2.13	0.49
1:A:15:LEU:HD11	1:A:46:TRP:HB2	1.94	0.49
1:A:54:ASP:HB2	1:A:57:ARG:HG3	1.93	0.49
1:A:54:ASP:CB	1:A:57:ARG:HB2	2.39	0.49
1:A:268:ALA:O	1:A:272:VAL:HG22	2.11	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:A:241:VAL:C	1:A:243:THR:H	2.15	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:179:LEU:C	1:A:179:LEU:HD12	2.33	0.49
1:B:48:ASP:HB3	1:B:51:LEU:HD21	1.95	0.49
1:B:245:LEU:HD12	1:B:246:PRO:HD2	1.93	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:D:53:PHE:O	1:D:54:ASP:C	2.50	0.49
1:D:79:ASN:H	1:D:79:ASN:ND2	2.03	0.49
1:D:287:ALA:O	1:D:289:SER:N	2.46	0.49
1:C:36:PHE:CE1	1:C:109:VAL:HB	2.47	0.49
1:D:271:GLU:O	1:D:272:VAL:C	2.52	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:A:40:ALA:HB3	1:A:105:PHE:CE1	2.48	0.48
1:B:147:LYS:O	1:B:147:LYS:HG2	2.13	0.48
1:C:54:ASP:HB2	1:C:57:ARG:HG3	1.94	0.48
1:E:40:ALA:HB3	1:E:105:PHE:CE1	2.48	0.48
1:E:76:ARG:O	1:E:129:LEU:HA	2.12	0.48
1:B:268:ALA:O	1:B:272:VAL:HG22	2.14	0.48
1:E:118:TYR:CD1	1:E:118:TYR:C	2.84	0.48
1:E:224:VAL:O	1:E:228:VAL:HB	2.13	0.48
1:B:25:GLU:HB2	1:B:39:ASN:HB3	1.94	0.48
1:E:281:GLU:C	1:E:283:GLN:H	2.15	0.48
1:A:57:ARG:HE	1:A:57:ARG:HA	1.79	0.48
1:B:34:GLU:OE2	1:B:112:PRO:HA	2.14	0.48
1:E:54:ASP:HB2	1:E:57:ARG:HG3	1.94	0.48
1:A:151:ASN:ND2	1:A:152:ASP:N	2.56	0.48
1:B:18:ASN:HB3	1:B:143:VAL:HG23	1.96	0.48
1:B:33:ALA:O	1:B:34:GLU:HB2	2.12	0.48
1:B:155:PHE:CZ	1:C:112:PRO:HB3	2.48	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:C:150:LYS:HG2	1:C:154:VAL:HG21	1.96	0.48
1:C:193:TYR:O	1:C:194:PHE:CB	2.61	0.48
1:E:54:ASP:CB	1:E:57:ARG:HB2	2.37	0.48
1:C:29:LEU:C	1:C:29:LEU:HD23	2.33	0.48
1:E:141:LEU:HD23	1:E:142:ALA:N	2.19	0.48
1:E:193:TYR:O	1:E:194:PHE:HB2	2.12	0.48
1:A:72:ILE:HG22	1:A:73:PRO:HD2	1.95	0.48
1:B:141:LEU:HD23	1:B:142:ALA:N	2.20	0.48
1:B:151:ASN:ND2	1:B:152:ASP:N	2.58	0.48
1:E:36:PHE:CE1	1:E:109:VAL:HB	2.49	0.48
1:E:49:ARG:C	1:E:51:LEU:H	2.17	0.48
1:E:150:LYS:CG	1:E:154:VAL:HG21	2.43	0.48
1:E:257:ILE:O	1:E:261:ILE:HG12	2.14	0.48
1:B:19:THR:HA	1:B:43:SER:O	2.13	0.48
1:D:137:ARG:HA	1:D:137:ARG:HD3	1.75	0.48
1:A:19:THR:HA	1:A: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

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:70:ILE:N	1:D:70:ILE:HD13	2.30	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:C:57:ARG:HE	1:C:57:ARG:HA	1.80	0.46
1:C:155:PHE:HB3	1:C:156:LEU:H	1.58	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:A:61:ARG:HG2	1:A:62:VAL:HG23	1.98	0.46
1:D:68:GLU:CD	1:D:68:GLU:N	2.68	0.46
1:E:72:ILE:HG22	1:E:73:PRO:HD2	1.98	0.46
1:E:196:TYR:N	1:E:196:TYR:CD1	2.84	0.46
1:C:81:GLU:HG3	1:C:108:ARG:HG3	1.98	0.46
1:D:150:LYS:HE2	1:D:150:LYS:HB3	1.73	0.46
1:D:241:VAL:C	1:D:243:THR:N	2.70	0.46
1:A:147:LYS:O	1:A:147:LYS:CG	2.64	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:241:VAL:C	1:C:243:THR:N	2.69	0.46
1:D:49:ARG:C	1:D:51:LEU:H	2.19	0.46
1:D:150:LYS:HG2	1:D:154:VAL:HG21	1.97	0.46
1:E:57:ARG:HE	1:E:57:ARG:HA	1.81	0.46
1:A:94:SER:OG	1:A:95:PRO:HD2	2.16	0.45
1:B:54:ASP:CB	1:B:57:ARG:HB2	2.37	0.45
1:B:274:VAL:HG12	1:B:275:GLN:N	2.31	0.45
1:C:53:PHE:O	1:C:54:ASP:C	2.55	0.45
1:D:270:ILE:HD13	1:D:270:ILE:HA	1.68	0.45
1:A:49:ARG:C	1:A:51:LEU:H	2.19	0.45
1:B:36:PHE:CE1	1:B:109:VAL:HB	2.51	0.45
1:B:65:TYR:CD1	1:B:70:ILE:HD11	2.50	0.45
1:E:53:PHE:O	1:E:54:ASP:C	2.53	0.45
1:A:53:PHE:O	1:A:54:ASP:C	2.55	0.45
1:B:309:LEU:HD12	1:B:309:LEU:HA	1.75	0.45
1:C:149:GLY:O	1:C:150:LYS:CB	2.58	0.45
1:E:65:TYR:CD1	1:E:70:ILE:HD11	2.52	0.45
1:A:191:ARG:HG3	1:A:192:GLN:N	2.32	0.45
1:A:212:TRP:CE3	1:A:298:PHE:HD1	2.34	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:B:15:LEU:HD11	1:B:46:TRP:HB2	1.99	0.45
1:D:304:LEU:O	1:D:308:ILE:HG12	2.17	0.45
1:B:155:PHE:CE1	1:C:112:PRO:HB3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:53:PHE:CE1	1:D:95:PRO:HA	2.52	0.45
1:D:223:ASN:HB3	1:D:272:VAL:HG11	1.99	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:C:118:TYR:CD1	1:C:118:TYR:C	2.88	0.45
1:D:193:TYR:CD2	1:D:193:TYR:C	2.90	0.45
1:D:268:ALA:O	1:D:272:VAL:HG22	2.16	0.45
1:B:81:GLU:HG3	1:B:108:ARG:HG3	1.99	0.45
1:C:70:ILE:HD13	1:C:70:ILE:N	2.31	0.45
1:E:149:GLY:O	1:E:164:PHE:HD1	2.00	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:A:150:LYS:HG2	1:A:154:VAL:HG21	1.97	0.45
1:B:57:ARG:HE	1:B:57:ARG:HA	1.81	0.45
1:B:72:ILE:HG22	1:B:73:PRO:HD2	1.98	0.45
1:B:118:TYR:CD1	1:B:118:TYR:C	2.86	0.45
1:C:22:TYR:CA	1:C:149:GLY:HA2	2.32	0.45
1:B:232:ILE:HG22	1:B:233:ALA:N	2.32	0.45
1:B:274:VAL:C	1:B:276:HIS:N	2.70	0.45
1:C:304:LEU:O	1:C:308:ILE:HG12	2.16	0.45
1:E:218:THR:HG22	1:E:279:LYS:HE2	1.99	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:C:128:TYR:O	1:C:183:LEU:O	2.35	0.45
1:C:137:ARG:HD2	1:C:179:LEU:HG	1.99	0.45
1:D:194:PHE:C	1:D:196:TYR:N	2.70	0.45
1:E:304:LEU:O	1:E:308:ILE:HG12	2.17	0.45
1:A:274:VAL:HG12	1:A:275:GLN:N	2.32	0.44
1:B:47:LYS:HD2	1:B:49:ARG:HH21	1.81	0.44
1:E:155:PHE:HB3	1:E:156:LEU:H	1.60	0.44
1:A:81:GLU:HG3	1:A:108:ARG:HG3	1.99	0.44
1:A:150:LYS:HB3	1:A:150:LYS:HE2	1.73	0.44
1:B:155:PHE:HB3	1:B:156:LEU:H	1.58	0.44
1:C:274:VAL:HG12	1:C:275:GLN:N	2.32	0.44
1:D:57:ARG:HE	1:D:57:ARG:HA	1.81	0.44
1:A:304:LEU:O	1:A:308:ILE:HG12	2.16	0.44
1:B:42:LEU:HB3	1:B:103:GLU:CG	2.45	0.44
1:D:305:ALA:O	1:D:309:LEU:HB2	2.16	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
1:E:53:PHE:CE2	1:E:63:LYS:HB3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:GLU:N	1:A:68:GLU:CD	2.71	0.44
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: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: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:118:TYR:HB3	1:A:119:PRO:HD3	1.99	0.44
1:C:68:GLU:CD	1:C:68:GLU: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:65:TYR:CD1	1:A:70:ILE:HD11	2.52	0.44
1:A:155:PHE:HB3	1:A:156:LEU:H	1.59	0.44
1:B:53:PHE:CE1	1:B:95:PRO:HA	2.53	0.44
1:B:194:PHE:C	1:B:196:TYR:N	2.71	0.44
1:B:212:TRP:CZ3	1:B:264:PHE:HD2	2.33	0.44
1:C:274:VAL:C	1:C:276:HIS:N	2.71	0.44
1:D:210:ILE:O	1:D:213:THR:HB	2.17	0.44
1:E:22:TYR:CD1	1:E:149:GLY:HA2	2.53	0.44
1:E:137:ARG:HD3	1:E:137:ARG:HA	1.77	0.44
1:E:232:ILE:HG22	1:E:233:ALA:N	2.32	0.44
1:B:147:LYS:O	1:B:147:LYS:CG	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:A:53:PHE:CE1	1:A:95:PRO:HA	2.53	0.43
1:A:287:ALA:C	1:A:289:SER:N	2.72	0.43
1:B:53:PHE:CE2	1:B:63:LYS:HB3	2.53	0.43
1:D:27:TYR:HB3	1:E:110:LEU:HD11	2.00	0.43
1:D:276:HIS:C	1:D:278:LEU:N	2.71	0.43
1:E:271:GLU:O	1:E:274:VAL:N	2.51	0.43
1:A:175:LEU:O	1:A:176:GLU:HB2	2.17	0.43
1:B:68:GLU:N	1:B:68:GLU:CD	2.70	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:C:65:TYR:CD1	1:C:70:ILE:HD11	2.52	0.43
1:C:149:GLY:O	1:C:164:PHE:HD1	2.01	0.43
1:D:253:TYR:CA	1:D:313:PHE:CE2	3.00	0.43
1:E:47:LYS:HD2	1:E:49:ARG:HH21	1.82	0.43
1:E:226:LEU:HA	1:E:226:LEU:HD22	1.67	0.43
1:A:52:ALA:HA	1:A:95:PRO:O	2.18	0.43
1:A:309:LEU:HD12	1:A:309:LEU:HA	1.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:ARG:HG2	1:B:62:VAL:HG23	2.01	0.43
1:C:271:GLU:O	1:C:274:VAL:N	2.51	0.43
1:D:13:GLU:CB	1:D:14:PRO:CD	2.87	0.43
1:D:314:PHE:N	1:D:314:PHE:HD1	2.16	0.43
1:A:22:TYR:CD1	1:A:149:GLY:HA2	2.53	0.43
1:B:241:VAL:C	1:B:243:THR: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:137:ARG:HD2	1:E:179:LEU:HG	1.99	0.43
1:E:194:PHE:C	1:E:196:TYR:N	2.70	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:223:ASN:O	1:E:227:VAL:HG23	2.19	0.43
1:E:287:ALA:C	1:E:289:SER:N	2.71	0.43
1:A:298:PHE:CB	1:A:299:PRO:HD3	2.49	0.43
1:B:118:TYR:HB3	1:B:119:PRO:HD3	2.00	0.43
1:C:212:TRP:CZ3	1:C:264:PHE:HD2	2.35	0.43
1:C:53:PHE:CE2	1:C:63:LYS:HB3	2.54	0.43
1:C:194:PHE:C	1:C:196:TYR:N	2.70	0.43
1:C:199:ASN:O	1:C:200:ILE:HD13	2.19	0.43
1:C:305:ALA:O	1:C:309:LEU:HB2	2.17	0.43
1:D:30:ASP:HB3	1:D:33:ALA:HB3	2.00	0.43
1:D:132:ARG:HA	1:D:180:GLU:HG2	2.01	0.43
1:D:274:VAL:HG12	1:D:275:GLN:N	2.33	0.43
1:E:128:TYR:O	1:E:183:LEU:O	2.37	0.43
1:A:37:LYS:HG2	1:A:108:ARG:HB3	2.01	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:40:ALA:HB3	1:D:105:PHE:CE1	2.53	0.43
1:D:49:ARG:O	1:D:51:LEU:N	2.51	0.43
1:D:218:THR:HG22	1:D:279:LYS:HE2	2.01	0.43
1:E:9:PRO:HB3	1:E:48:ASP:OD1	2.18	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:A:111:SER:HA	1:A:112:PRO:HD2	1.78	0.43
1:A:115:PHE:O	1:A:252:THR:HG22	2.19	0.43
1:B:193:TYR:CD2	1:B:193:TYR:C	2.92	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: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:E:298:PHE:CB	1:E:299:PRO:HD3	2.49	0.43
1:A:62:VAL:HG13	1:A:93:VAL:O	2.18	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: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:D:191:ARG:HG3	1:D:192:GLN:N	2.33	0.42
1:B:191:ARG:HG3	1:B:192:GLN:N	2.34	0.42
1:B:287:ALA:C	1:B:289:SER:N	2.73	0.42
1:C:257:ILE:O	1:C:261:ILE:CG1	2.67	0.42
1:D:199:ASN:O	1:D:200:ILE:HD13	2.19	0.42
1:D:202:LEU:HD22	1:D:202:LEU:HA	1.94	0.42
1:D:257:ILE:O	1:D:261:ILE:CG1	2.67	0.42
1:E:42:LEU:HB3	1:E:103:GLU:CG	2.48	0.42
1:A:276:HIS:C	1:A:278:LEU:N	2.72	0.42
1:B:52:ALA:HA	1:B:95:PRO:O	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:C:232:ILE:HG22	1:C:233:ALA:N	2.34	0.42
1:E:42:LEU:O	1:E:102:LEU:HD12	2.19	0.42
1:E:115:PHE:O	1:E:252:THR:HG22	2.19	0.42
1:E:191:ARG:HG3	1:E:192:GLN:N	2.34	0.42
1:A:128:TYR:O	1:A:183:LEU:O	2.37	0.42
1:B:27:TYR:HB3	1:C:110:LEU:HD11	2.02	0.42
1:C:79:ASN:HD22	1:C:79:ASN:N	2.05	0.42
1:D:196:TYR:N	1:D:196:TYR:CD1	2.85	0.42
1:A:53:PHE:CE2	1:A:63:LYS:HB3	2.54	0.42
1:A:226:LEU:HD23	1:B:224:VAL:HB	2.01	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: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:D:232:ILE:HG22	1:D:233:ALA:N	2.35	0.42
1:E:193:TYR:CD2	1:E:193:TYR:C	2.92	0.42
1:E:260:MET:HE3	1:E:309:LEU:HD22	2.00	0.42
1:B:21:ILE:O	1:B:149:GLY:HA3	2.19	0.42
1:D:42:LEU:O	1:D:102:LEU:HD12	2.19	0.42
1:D:47:LYS:HD2	1:D:49:ARG:HH21	1.85	0.42
1:D:137:ARG:HD2	1:D:179:LEU:HG	2.02	0.42
1:D:271:GLU:O	1:D:274:VAL:N	2.52	0.42
1:E:52:ALA:HA	1:E:95:PRO:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:65:TYR:CD2	1:E:70:ILE:HD11	2.54	0.42
1:C:25:GLU:OE1	1:C:25:GLU:HA	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:A:194:PHE:C	1:A:196:TYR:N	2.71	0.42
1:B:283:GLN:N	1:B:284:PRO:CD	2.83	0.42
1:D:21:ILE:O	1:D:149:GLY:HA3	2.19	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:210:ILE:O	1:A:213:THR:HB	2.19	0.42
1:B:195:SER:O	1:B:199:ASN:HB2	2.20	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: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:210:ILE:O	1:C:213:THR:HB	2.20	0.42
1:C:226:LEU:HD23	1:D:224:VAL:HB	2.01	0.42
1:A:22:TYR:CA	1:A:149:GLY:HA2	2.34	0.41
1:A:47:LYS:HD2	1:A:49:ARG:HH21	1.84	0.41
1:B:37:LYS:HE3	1:B:108:ARG:HD2	2.02	0.41
1:B:275:GLN:O	1:B:275:GLN:CG	2.67	0.41
1:C:141:LEU:HD23	1:C:142:ALA:N	2.26	0.41
1:C:283:GLN:N	1:C:284:PRO:CD	2.82	0.41
1:E:314:PHE:N	1:E:314:PHE:HD1	2.17	0.41
1:A:202:LEU:HD22	1:A:202:LEU:HA	1.87	0.41
1:A:205:LEU:O	1:A:206:PHE:C	2.58	0.41
1:A:224:VAL:HB	1:E:226:LEU:HD23	2.02	0.41
1:A:242:GLU:HG2	1:A:242:GLU:O	2.20	0.41
1:A:77:PHE:H	1:A:84:ARG:CD	2.29	0.41
1:A:270:ILE:HD13	1:A:270:ILE:HA	1.67	0.41
1:D:195:SER:O	1:D:199:ASN:HB2	2.20	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:O	1:D:50:ARG:HG2	2.20	0.41
1:D:149:GLY:O	1:D:164:PHE:HD1	2.02	0.41
1:E:68:GLU:CD	1:E:68:GLU:N	2.73	0.41
1:A:149:GLY:O	1:A:164:PHE:HD1	2.03	0.41
1:A:212:TRP:HB2	1:A:215:PHE:CD1	2.56	0.41
1:D:52:ALA:HB1	1:D:95:PRO:O	2.21	0.41
1:D:68:GLU:CD	1:D:68:GLU:H	2.23	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: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
1:B:149:GLY:O	1:B:164:PHE:HD1	2.03	0.41
1:C:137:ARG:HA	1:C:137:ARG:HD3	1.74	0.41
1:C:270:ILE:HD13	1:C:270:ILE:HA	1.70	0.41
1:D:25:GLU:OE1	1:D:25:GLU:HA	2.21	0.41
1:D:84:ARG:NH1	1:D:84:ARG:CB	2.66	0.41
1:A:21:ILE:O	1:A:149:GLY:HA3	2.20	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:D:197:ILE:HB	1:D:198:PRO:CD	2.40	0.41
1:A:84:ARG:NH1	1:A:84:ARG:CB	2.66	0.41
1:A:226:LEU:HA	1:A:226:LEU:HD22	1.73	0.41
1:B:111:SER:HA	1:B:112:PRO:HD2	1.80	0.41
1:B:216:TRP:CH2	1:B:295:ARG:HB3	2.55	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:C:196:TYR:N	1:C:196:TYR:HD1	2.18	0.41
1:A:15:LEU:HD12	1:A:16:THR:N	2.36	0.41
1:A:253:TYR:CA	1:A:313:PHE:CE2	3.01	0.41
1:A:260:MET:HE3	1:A:309:LEU:HD22	2.03	0.41
1:A:314:PHE:N	1:A:314:PHE:HD1	2.19	0.41
1:B:54:ASP:HA	1:B:55:PRO:HD2	1.88	0.41
1:B:175:LEU:O	1:B:176:GLU:HB2	2.20	0.41
1:B:223:ASN:O	1:B:227:VAL:HG23	2.20	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:D:309:LEU:HA	1:D:309:LEU:HD12	1.75	0.41
1:E:196:TYR:N	1:E:196:TYR:HD1	2.19	0.41
1:B:196:TYR:N	1:B:196:TYR:HD1	2.18	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:A:223:ASN:O	1:A:227:VAL:HG23	2.21	0.40
1:B:25:GLU:OE1	1:B:25:GLU:HA	2.22	0.40
1:B:40:ALA:HB3	1:B:105:PHE:CE1	2.56	0.40
1:B:212:TRP:HB2	1:B:215:PHE:CD1	2.56	0.40
1:D:37:LYS:HG2	1:D:108:ARG:HB3	2.02	0.40
1:A:212:TRP:HB2	1:A:215:PHE:CE1	2.56	0.40
1:C:15:LEU:HD12	1:C:16:THR:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:276:HIS:C	1:C:278:LEU:N	2.71	0.40
1:D:115:PHE:O	1:D:252:THR:HG22	2.22	0.40
1:A:283:GLN:N	1:A:284:PRO:CD	2.83	0.40
1:C:116:ARG:HG3	1:C:250:TYR:CD2	2.57	0.40
1:E:15:LEU:HD12	1:E:16:THR:N	2.37	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:B:162:GLU:HB2	1:B:188:ARG:O	2.21	0.40
1:C:42:LEU:O	1:C:102:LEU:HD12	2.22	0.40
1:C:223:ASN:O	1:C:227:VAL:HG23	2.21	0.40
1:C:253:TYR:CA	1:C:313:PHE:CE2	3.01	0.40
1:C:275:GLN:O	1:C:275:GLN:CG	2.67	0.40
1:C:253:TYR:HB2	1:C:313:PHE:HD2	1.86	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

There are no symmetry-related clashes.

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	308/317 (97%)	239 (78%)	52 (17%)	17 (6%)	2	11
1	B	308/317 (97%)	243 (79%)	49 (16%)	16 (5%)	2	12
1	C	308/317 (97%)	242 (79%)	48 (16%)	18 (6%)	1	10
1	D	308/317 (97%)	244 (79%)	47 (15%)	17 (6%)	2	11
1	E	308/317 (97%)	243 (79%)	48 (16%)	17 (6%)	2	11
All	All	1540/1585 (97%)	1211 (79%)	244 (16%)	85 (6%)	2	11

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%)	4	16
1	B	278/284 (98%)	238 (86%)	40 (14%)	3	14
1	C	278/284 (98%)	240 (86%)	38 (14%)	3	16
1	D	278/284 (98%)	238 (86%)	40 (14%)	3	14
1	E	278/284 (98%)	239 (86%)	39 (14%)	3	15
All	All	1390/1420 (98%)	1196 (86%)	194 (14%)	3	15

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

Sometimes 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 (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	-0.37	4 (1%)	77	59	56, 83, 126, 163	0
1	B	310/317 (97%)	-0.44	7 (2%)	60	39	57, 83, 125, 163	0
1	C	310/317 (97%)	-0.41	7 (2%)	60	39	58, 82, 126, 164	0
1	D	310/317 (97%)	-0.43	6 (1%)	66	46	57, 83, 124, 163	0
1	E	310/317 (97%)	-0.38	5 (1%)	72	51	57, 82, 125, 164	0
All	All	1550/1585 (97%)	-0.41	29 (1%)	66	46	56, 83, 126, 164	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	316	PHE	4.3
1	D	55	PRO	4.3
1	E	59	GLY	4.0
1	E	58	SER	3.8
1	E	316	PHE	3.7
1	A	316	PHE	3.6
1	B	316	PHE	3.5
1	D	56	VAL	3.5
1	B	57	ARG	3.2
1	E	60	VAL	3.2
1	D	316	PHE	3.1
1	C	58	SER	3.1
1	B	58	SER	2.9
1	A	58	SER	2.9
1	E	57	ARG	2.8
1	A	59	GLY	2.8
1	B	59	GLY	2.8
1	D	57	ARG	2.7
1	D	177	ASP	2.6
1	B	315	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	59	GLY	2.6
1	C	56	VAL	2.5
1	B	54	ASP	2.5
1	A	315	GLY	2.4
1	B	53	PHE	2.3
1	C	54	ASP	2.3
1	C	57	ARG	2.1
1	C	282	SER	2.1
1	D	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 monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.