Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:37 AM GMT

PDB ID	:	2XQ5
Title	:	PENTAMERIC LIGAND GATED ION CHANNEL GLIC IN COMPLEX WITH TETRAETHYLARSONIUM (TEAS)
Authors	:	Hilf, R.J.C.; Bertozzi, C.; Zimmermann, I.; Reiter, A.; Trauner, D.; Dutzler, R.
Deposited on	:	2010-09-01
Resolution	:	3.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

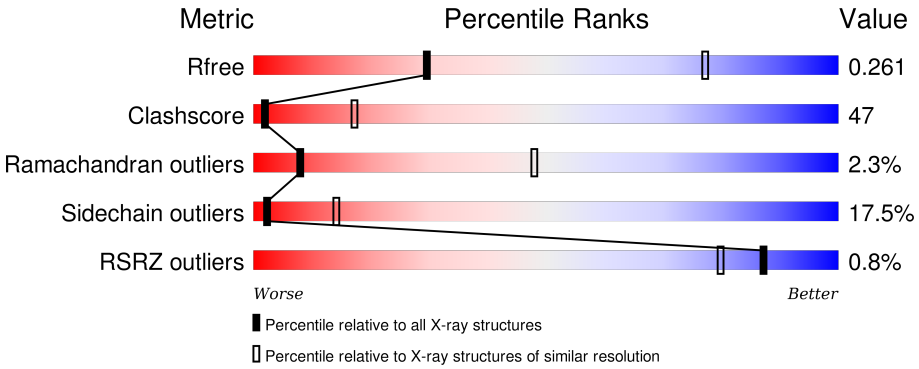
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 <=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	31% 54% 12%
1	B	317	32% 53% 12%
1	C	317	35% 51% 12%
1	D	317	32% 53% 13%
1	E	317	34% 52% 11%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12606 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			

- Molecule 2 is ARSENIC (three-letter code: ARS) (formula: As).

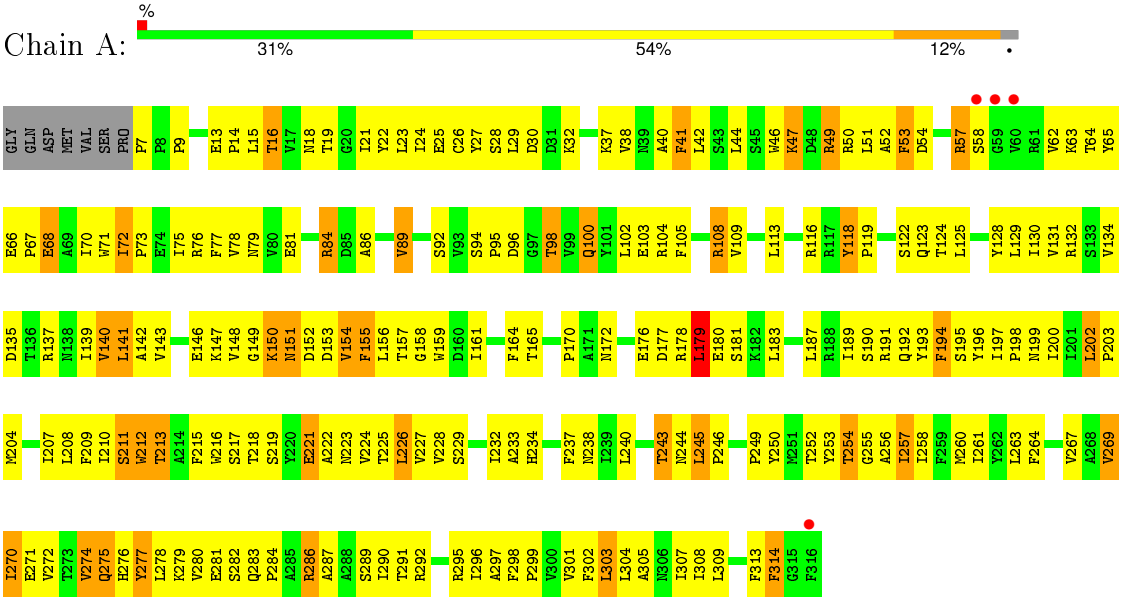
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total	As	0	0
			1	1		

3 Residue-property plots (i)

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.

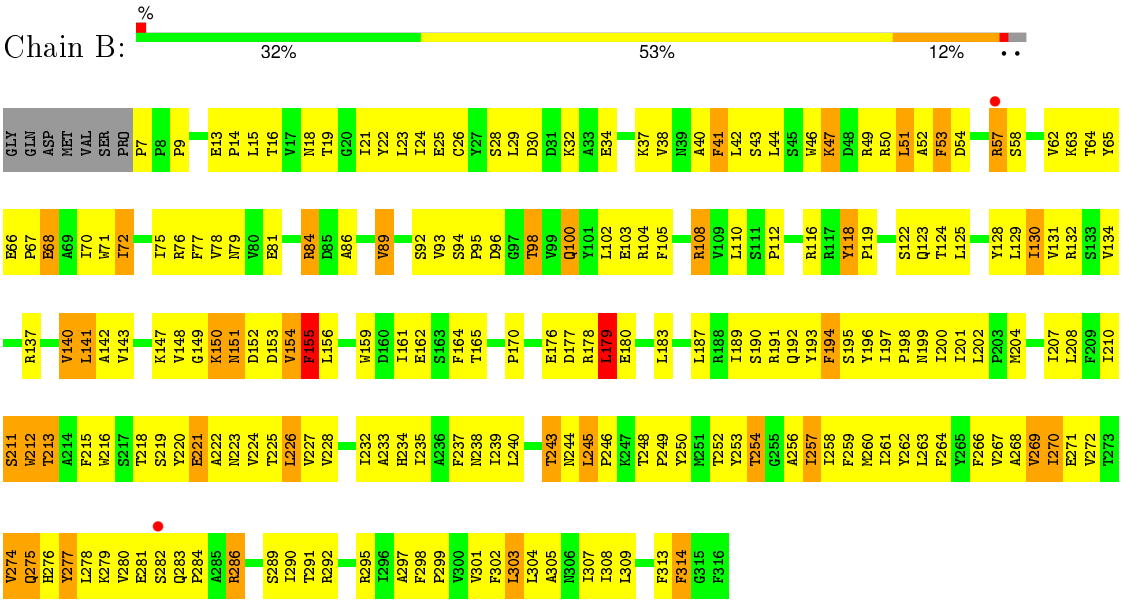
- Molecule 1: GLR4197 PROTEIN

Chain A:



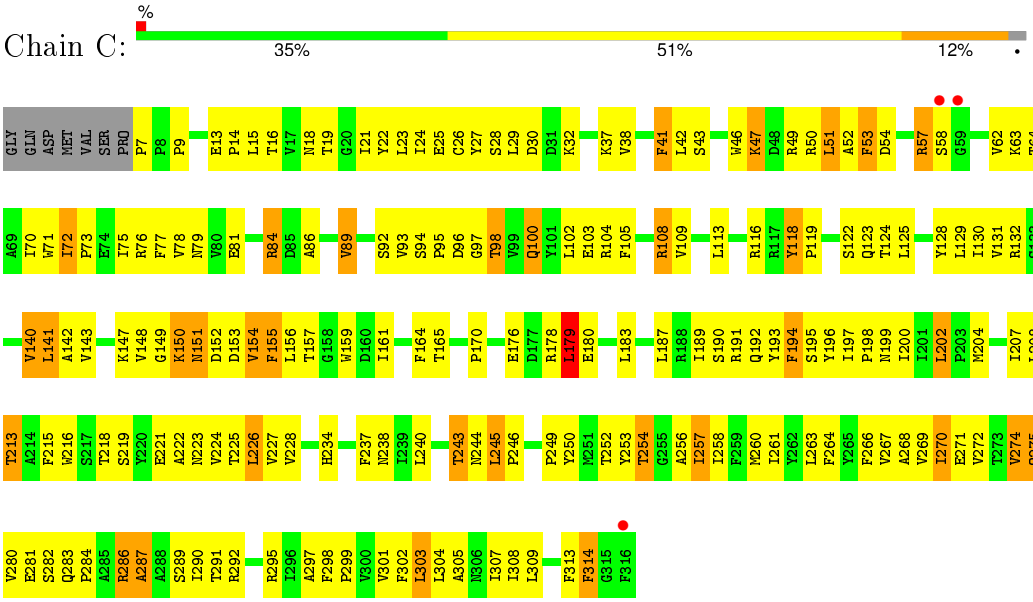
- Molecule 1: GLR4197 PROTEIN

Chain B:



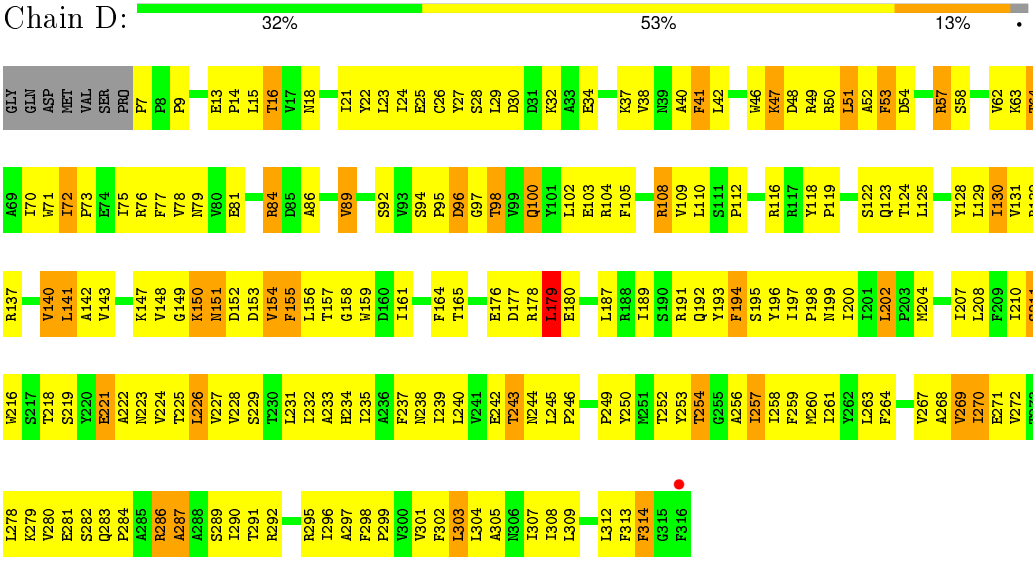
• Molecule 1: GLR4197 PROTEIN

Chain C:



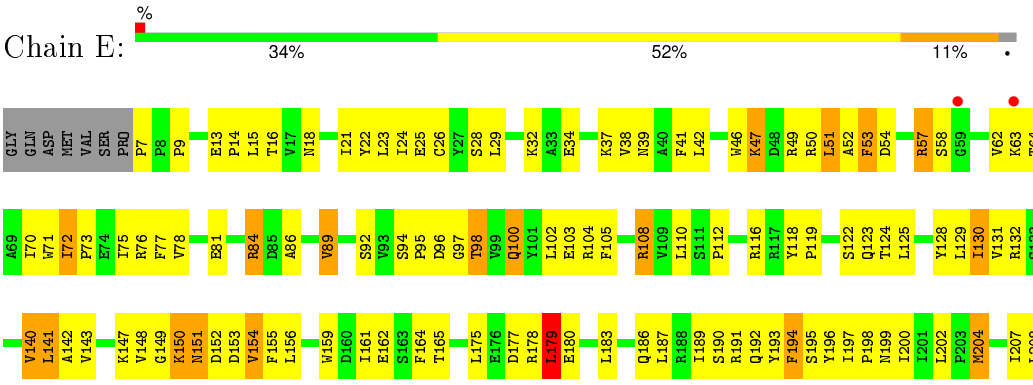
• Molecule 1: GLR4197 PROTEIN

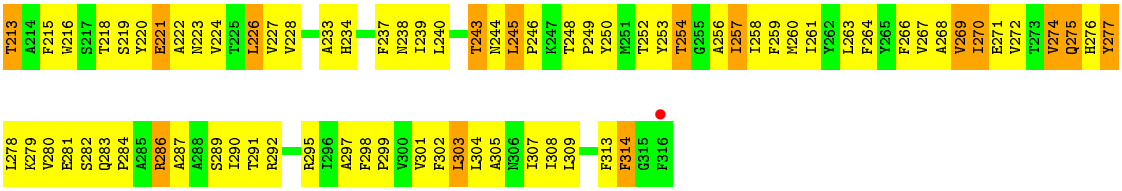
Chain D:



• Molecule 1: GLR4197 PROTEIN

Chain E:




T213 A214 F215 W216 S217 T218 S219 Y220 E221 A222 N223 V224 T225 L226 V227 V228 A233 H234 F237 N238 I239 L240 T243 N244 L245 P246 K247 T248 P249 Y250 N251 T252 Y253 T254 G255 A256 I257 I258 F259 N260 I261 Y262 L263 F264 Y265 F266 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 F302 L303 L304 A305 N306 I307 I308 L309 F313 F314 G315 F316

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	183.31Å 128.31Å 164.37Å 90.00° 104.04° 90.00°	Depositor
Resolution (Å)	40.20 – 3.50 40.20 – 3.38	Depositor EDS
% Data completeness (in resolution range)	97.7 (40.20-3.50) 95.6 (40.20-3.38)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.86 (at 3.40Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.249 , 0.266 0.243 , 0.261	Depositor DCC
R_{free} test set	2299 reflections (5.04%)	DCC
Wilson B-factor (Å^2)	98.3	Xtriage
Anisotropy	0.282	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 82.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Outliers	1 of 51417 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	12606	wwPDB-VP
Average B, all atoms (Å^2)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ARS

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	0.69	3/3535 (0.1%)
1	B	0.48	0/2589	0.70	2/3535 (0.1%)
1	C	0.48	0/2589	0.69	3/3535 (0.1%)
1	D	0.50	0/2589	0.70	3/3535 (0.1%)
1	E	0.49	0/2589	0.70	3/3535 (0.1%)
All	All	0.49	0/12945	0.70	14/17675 (0.1%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	179	LEU	CA-CB-CG	5.68	128.37	115.30
1	A	179	LEU	CA-CB-CG	5.68	128.36	115.30
1	D	179	LEU	CA-CB-CG	5.67	128.35	115.30
1	E	179	LEU	CA-CB-CG	5.67	128.34	115.30
1	B	179	LEU	CA-CB-CG	5.66	128.32	115.30
1	C	135	ASP	N-CA-CB	-5.43	100.82	110.60
1	E	134	VAL	CB-CA-C	5.31	121.49	111.40
1	D	134	VAL	CB-CA-C	5.29	121.46	111.40
1	B	134	VAL	CB-CA-C	5.29	121.45	111.40
1	A	134	VAL	CB-CA-C	5.27	121.42	111.40
1	C	134	VAL	CB-CA-C	5.17	121.23	111.40
1	E	135	ASP	N-CA-CB	-5.15	101.33	110.60
1	A	135	ASP	N-CA-CB	-5.10	101.42	110.60
1	D	135	ASP	N-CA-CB	-5.05	101.50	110.60

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	278	0
1	B	2521	0	2537	267	0
1	C	2521	0	2537	235	0
1	D	2521	0	2537	270	0
1	E	2521	0	2537	243	0
2	C	1	0	0	0	0
All	All	12606	0	12685	1177	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 47.

All (1177) 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:A:226:LEU:HD23	1:B:224:VAL:HB	1.33	1.06
1:D:155:PHE:CE1	1:E:112:PRO:HB3	1.92	1.03
1:A:155:PHE:CE1	1:B:112:PRO:HB3	1.94	1.01
1:A:222:ALA:HB2	1:B:221:GLU:HA	1.42	1.01
1:A:27:TYR:HB3	1:B:110:LEU:HD11	1.42	0.99
1:D:210:ILE:HG23	1:E:269:VAL:HG11	1.44	0.97
1:A:155:PHE:CZ	1:B:112:PRO:HB3	1.98	0.97
1:D:76:ARG:NH2	1:D:130:ILE:HD12	1.81	0.95
1:B:89:VAL:HG11	1:B:102:LEU:HD23	1.48	0.95
1:A:76:ARG:NH2	1:A:130:ILE:HD12	1.82	0.95
1:B:76:ARG:NH2	1:B:130:ILE:HD12	1.81	0.95
1:D:89:VAL:HG11	1:D:102:LEU:HD23	1.50	0.94
1:C:78:VAL:HG22	1:C:130:ILE:HG12	1.50	0.93
1:E:76:ARG:NH2	1:E:130:ILE:HD12	1.84	0.93
1:E:89:VAL:HG11	1:E:102:LEU:HD23	1.50	0.92
1:B:78:VAL:HG22	1:B:130:ILE:HG12	1.51	0.92
1:C:22:TYR:HA	1:C:149:GLY:HA3	1.51	0.92
1:A:27:TYR:CB	1:B:110:LEU:HD11	1.99	0.91
1:C:22:TYR:HA	1:C:149:GLY:CA	2.02	0.90
1:A:89:VAL:HG11	1:A:102:LEU:HD23	1.53	0.90
1:D:78:VAL:HG22	1:D:130:ILE:HG12	1.52	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:ARG:HH22	1:B:130:ILE:HD12	1.33	0.90
1:E:78:VAL:HG22	1:E:130:ILE:HG12	1.50	0.90
1:A:78:VAL:HG22	1:A:130:ILE:HG12	1.52	0.90
1:C:76:ARG:NH2	1:C:130:ILE:HD12	1.86	0.90
1:D:76:ARG:HH22	1:D:130:ILE:HD12	1.37	0.89
1:C:27:TYR:HB3	1:D:110:LEU:HD11	1.55	0.88
1:D:22:TYR:HA	1:D:149:GLY:HA3	1.56	0.88
1:E:76:ARG:HH22	1:E:130:ILE:HD12	1.38	0.88
1:D:22:TYR:HA	1:D:149:GLY:CA	2.04	0.87
1:B:147:LYS:C	1:B:149:GLY:H	1.77	0.87
1:B:22:TYR:HA	1:B:149:GLY:HA3	1.57	0.87
1:A:22:TYR:HA	1:A:149:GLY:CA	2.04	0.86
1:A:22:TYR:HA	1:A:149:GLY:HA3	1.56	0.86
1:B:22:TYR:HA	1:B:149:GLY:CA	2.06	0.85
1:A:104:ARG:HH22	1:B:78:VAL:HA	1.38	0.85
1:E:147:LYS:C	1:E:149:GLY:H	1.76	0.85
1:C:234:HIS:CE1	1:C:261:ILE:HG21	2.12	0.85
1:D:253:TYR:HA	1:D:313:PHE:CE2	2.11	0.84
1:C:89:VAL:HG11	1:C:102:LEU:HD23	1.58	0.84
1:A:226:LEU:CD2	1:B:224:VAL:HB	2.07	0.84
1:C:76:ARG:HH22	1:C:130:ILE:HD12	1.41	0.83
1:C:147:LYS:C	1:C:149:GLY:H	1.79	0.83
1:E:253:TYR:HA	1:E:313:PHE:CE2	2.13	0.83
1:D:253:TYR:HA	1:D:313:PHE:HE2	1.41	0.83
1:E:253:TYR:HA	1:E:313:PHE:HE2	1.43	0.83
1:C:253:TYR:HA	1:C:313:PHE:CE2	2.14	0.83
1:B:253:TYR:HA	1:B:313:PHE:CE2	2.14	0.83
1:A:76:ARG:HH22	1:A:130:ILE:HD12	1.40	0.82
1:D:147:LYS:C	1:D:149:GLY:H	1.80	0.82
1:A:253:TYR:HA	1:A:313:PHE:CE2	2.14	0.82
1:A:147:LYS:C	1:A:149:GLY:H	1.81	0.82
1:B:253:TYR:HA	1:B:313:PHE:HE2	1.44	0.82
1:E:22:TYR:HA	1:E:149:GLY:CA	2.09	0.81
1:C:253:TYR:HA	1:C:313:PHE:HE2	1.45	0.81
1:A:202:LEU:HD12	1:B:259:PHE:CZ	2.16	0.81
1:A:253:TYR:HA	1:A:313:PHE:HE2	1.45	0.80
1:E:22:TYR:HA	1:E:149:GLY:HA3	1.61	0.80
1:A:210:ILE:HG23	1:B:269:VAL:HG11	1.61	0.80
1:A:221:GLU:HB3	1:B:221:GLU:HG2	1.63	0.80
1:A:202:LEU:HD12	1:B:259:PHE:HZ	1.46	0.80
1:E:234:HIS:CE1	1:E:261:ILE:HG21	2.17	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:HIS:CE1	1:A:261:ILE:HG21	2.18	0.79
1:C:131:VAL:HG11	1:C:140:VAL:HG13	1.65	0.78
1:A:104:ARG:NH2	1:B:78:VAL:HA	1.98	0.78
1:D:155:PHE:CZ	1:E:112:PRO:HB3	2.18	0.77
1:A:219:SER:OG	1:A:222:ALA:HB3	1.85	0.77
1:B:22:TYR:CD1	1:B:149:GLY:HA2	2.20	0.77
1:B:131:VAL:HG11	1:B:140:VAL:HG13	1.66	0.76
1:A:77:PHE:H	1:A:84:ARG:HD3	1.48	0.76
1:B:234:HIS:CE1	1:B:261:ILE:HG21	2.21	0.76
1:D:77:PHE:H	1:D:84:ARG:HD3	1.50	0.76
1:A:132:ARG:HA	1:A:180:GLU:HG2	1.69	0.75
1:A:131:VAL:HG11	1:A:140:VAL:HG13	1.67	0.75
1:E:131:VAL:HG11	1:E:140:VAL:HG13	1.67	0.75
1:A:128:TYR:O	1:A:129:LEU:HB2	1.86	0.75
1:B:257:ILE:O	1:B:261:ILE:HG12	1.86	0.75
1:D:22:TYR:CD1	1:D:149:GLY:HA2	2.22	0.75
1:C:219:SER:OG	1:C:222:ALA:HB3	1.87	0.74
1:C:77:PHE:H	1:C:84:ARG:HD3	1.52	0.74
1:A:77:PHE:CD1	1:A:84:ARG:HD2	2.23	0.74
1:D:54:ASP:HB2	1:D:57:ARG:HG3	1.69	0.74
1:D:128:TYR:O	1:D:129:LEU:HB2	1.87	0.73
1:D:47:LYS:HD2	1:D:49:ARG:HH21	1.53	0.73
1:A:149:GLY:O	1:A:164:PHE:HD1	1.71	0.73
1:C:65:TYR:CG	1:C:70:ILE:HD11	2.24	0.73
1:C:22:TYR:CD1	1:C:149:GLY:HA2	2.23	0.73
1:C:149:GLY:O	1:C:164:PHE:HD1	1.72	0.73
1:D:234:HIS:CE1	1:D:261:ILE:HG21	2.24	0.73
1:B:54:ASP:HB2	1:B:57:ARG:HG3	1.70	0.73
1:C:94:SER:OG	1:C:95:PRO:HD2	1.89	0.73
1:D:131:VAL:HG11	1:D:140:VAL:HG13	1.71	0.73
1:C:157:THR:HG21	1:D:34:GLU:HG3	1.71	0.73
1:D:149:GLY:O	1:D:164:PHE:HD1	1.72	0.72
1:B:77:PHE:H	1:B:84:ARG:HD3	1.54	0.72
1:E:149:GLY:O	1:E:164:PHE:HD1	1.71	0.72
1:C:54:ASP:HB2	1:C:57:ARG:HG3	1.71	0.72
1:C:226:LEU:CD2	1:D:224:VAL:HB	2.19	0.72
1:D:77:PHE:CD1	1:D:84:ARG:HD2	2.25	0.72
1:E:54:ASP:HB2	1:E:57:ARG:HG3	1.71	0.72
1:B:47:LYS:HD2	1:B:49:ARG:HH21	1.55	0.72
1:C:222:ALA:HB2	1:D:221:GLU:HA	1.70	0.71
1:E:238:ASN:HA	1:E:258:ILE:HD11	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:229:SER:CB	1:E:228:VAL:HG11	2.20	0.71
1:E:22:TYR:CD1	1:E:149:GLY:HA2	2.25	0.71
1:E:147:LYS:C	1:E:149:GLY:N	2.43	0.71
1:C:128:TYR:O	1:C:129:LEU:HB2	1.90	0.71
1:D:141:LEU:HD23	1:D:142:ALA:H	1.55	0.71
1:A:283:GLN:N	1:A:284:PRO:HD3	2.05	0.71
1:A:54:ASP:HB2	1:A:57:ARG:HG3	1.72	0.71
1:B:149:GLY:O	1:B:164:PHE:HD1	1.73	0.70
1:A:21:ILE:O	1:A:149:GLY:HA3	1.92	0.70
1:B:238:ASN:HA	1:B:258:ILE:HD11	1.73	0.70
1:B:147:LYS:C	1:B:149:GLY:N	2.44	0.70
1:B:89:VAL:CG1	1:B:102:LEU:HD23	2.20	0.70
1:D:257:ILE:O	1:D:261:ILE:HG12	1.91	0.70
1:E:257:ILE:O	1:E:261:ILE:HG12	1.91	0.70
1:A:13:GLU:HB3	1:A:14:PRO:HD2	1.73	0.70
1:B:254:THR:O	1:B:258:ILE:HB	1.91	0.70
1:D:283:GLN:N	1:D:284:PRO:HD3	2.06	0.70
1:C:199:ASN:HB3	1:D:242:GLU:CD	2.11	0.70
1:C:21:ILE:O	1:C:149:GLY:HA3	1.92	0.69
1:C:213:THR:HG22	1:C:226:LEU:HD11	1.73	0.69
1:D:21:ILE:O	1:D:149:GLY:HA3	1.92	0.69
1:E:254:THR:O	1:E:258:ILE:HB	1.93	0.69
1:B:283:GLN:N	1:B:284:PRO:HD3	2.07	0.69
1:C:42:LEU:HB3	1:C:103:GLU:HG3	1.74	0.69
1:E:47:LYS:HD2	1:E:49:ARG:HH21	1.57	0.69
1:D:65:TYR:CG	1:D:70:ILE:HD11	2.27	0.69
1:E:42:LEU:HB3	1:E:103:GLU:HG3	1.75	0.69
1:B:77:PHE:CD1	1:B:84:ARG:HD2	2.27	0.69
1:E:65:TYR:CG	1:E:70:ILE:HD11	2.27	0.69
1:B:13:GLU:HB3	1:B:14:PRO:HD2	1.73	0.69
1:E:128:TYR:O	1:E:129:LEU:HB2	1.90	0.69
1:C:84:ARG:HB2	1:C:84:ARG:HH11	1.57	0.69
1:E:283:GLN:N	1:E:284:PRO:HD3	2.07	0.69
1:A:22:TYR:CD1	1:A:149:GLY:HA2	2.27	0.69
1:A:94:SER:OG	1:A:95:PRO:HD2	1.91	0.69
1:A:65:TYR:CG	1:A:70:ILE:HD11	2.27	0.69
1:E:77:PHE:CD1	1:E:84:ARG:HD2	2.27	0.69
1:E:13:GLU:HB3	1:E:14:PRO:HD2	1.74	0.69
1:D:276:HIS:O	1:D:280:VAL:HG22	1.93	0.69
1:B:65:TYR:CG	1:B:70:ILE:HD11	2.27	0.69
1:C:257:ILE:O	1:C:261:ILE:HG12	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:ILE:O	1:A:261:ILE:HG12	1.93	0.69
1:D:254:THR:O	1:D:258:ILE:HB	1.92	0.69
1:A:42:LEU:HB3	1:A:103:GLU:HG3	1.75	0.69
1:B:81:GLU:HG3	1:B:108:ARG:HG2	1.75	0.68
1:C:77:PHE:CD1	1:C:84:ARG:HD2	2.27	0.68
1:C:84:ARG:NH1	1:C:84:ARG:HB2	2.07	0.68
1:D:94:SER:OG	1:D:95:PRO:HD2	1.93	0.68
1:B:47:LYS:HD2	1:B:49:ARG:NH2	2.08	0.68
1:C:47:LYS:HD2	1:C:49:ARG:HH21	1.59	0.68
1:B:276:HIS:O	1:B:280:VAL:HG22	1.93	0.68
1:D:13:GLU:HB3	1:D:14:PRO:HD2	1.75	0.68
1:E:77:PHE:H	1:E:84:ARG:HD3	1.56	0.68
1:E:21:ILE:O	1:E:149:GLY:HA3	1.93	0.68
1:D:238:ASN:HA	1:D:258:ILE:HD11	1.74	0.68
1:C:132:ARG:HA	1:C:180:GLU:HG2	1.75	0.68
1:E:276:HIS:O	1:E:280:VAL:HG22	1.94	0.68
1:E:89:VAL:CG1	1:E:102:LEU:HD23	2.22	0.68
1:D:225:THR:HG21	1:E:224:VAL:HG23	1.76	0.68
1:C:13:GLU:HB3	1:C:14:PRO:HD2	1.74	0.68
1:A:240:LEU:HD13	1:B:239:ILE:HG12	1.76	0.68
1:C:283:GLN:N	1:C:284:PRO:HD3	2.09	0.68
1:D:225:THR:CG2	1:E:224:VAL:HG23	2.25	0.67
1:D:84:ARG:NH1	1:D:84:ARG:HB2	2.08	0.67
1:B:132:ARG:HA	1:B:180:GLU:HG2	1.75	0.67
1:C:84:ARG:CB	1:C:84:ARG:HH11	2.07	0.67
1:E:53:PHE:CE1	1:E:95:PRO:HA	2.29	0.67
1:D:81:GLU:HG3	1:D:108:ARG:HG2	1.76	0.67
1:E:94:SER:OG	1:E:95:PRO:HD2	1.94	0.67
1:B:141:LEU:HD23	1:B:142:ALA:H	1.59	0.67
1:A:226:LEU:HD22	1:B:228:VAL:HG21	1.77	0.67
1:A:147:LYS:C	1:A:149:GLY:N	2.48	0.67
1:E:84:ARG:HB2	1:E:84:ARG:NH1	2.09	0.67
1:A:229:SER:HB2	1:B:228:VAL:HG11	1.76	0.67
1:D:89:VAL:CG1	1:D:102:LEU:HD23	2.24	0.67
1:C:238:ASN:HA	1:C:258:ILE:HD11	1.76	0.67
1:D:132:ARG:HA	1:D:180:GLU:HG2	1.75	0.67
1:C:276:HIS:O	1:C:280:VAL:HG22	1.95	0.67
1:E:238:ASN:HA	1:E:258:ILE:CD1	2.24	0.67
1:B:53:PHE:CE1	1:B:95:PRO:HA	2.30	0.67
1:D:53:PHE:CE1	1:D:95:PRO:HA	2.29	0.67
1:E:84:ARG:HH11	1:E:84:ARG:HB2	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:47:LYS:HD2	1:D:49:ARG:NH2	2.10	0.67
1:A:254:THR:O	1:A:258:ILE:HB	1.94	0.67
1:B:21:ILE:O	1:B:149:GLY:HA3	1.94	0.66
1:A:276:HIS:O	1:A:280:VAL:HG22	1.95	0.66
1:A:81:GLU:HG3	1:A:108:ARG:HG2	1.76	0.66
1:B:100:GLN:HA	1:B:100:GLN:HE21	1.60	0.66
1:A:84:ARG:HB2	1:A:84:ARG:NH1	2.10	0.66
1:D:147:LYS:C	1:D:149:GLY:N	2.48	0.66
1:D:221:GLU:OE2	1:E:221:GLU:CD	2.34	0.66
1:D:42:LEU:HB3	1:D:103:GLU:HG3	1.77	0.66
1:C:226:LEU:HD23	1:D:224:VAL:HB	1.77	0.66
1:A:155:PHE:CE1	1:B:112:PRO:CB	2.75	0.66
1:B:42:LEU:HB3	1:B:103:GLU:HG3	1.78	0.66
1:B:128:TYR:O	1:B:129:LEU:HB2	1.95	0.66
1:B:84:ARG:CB	1:B:84:ARG:HH11	2.09	0.66
1:A:267:VAL:HG23	1:A:298:PHE:CZ	2.30	0.66
1:E:84:ARG:CB	1:E:84:ARG:HH11	2.07	0.66
1:C:200:ILE:HD11	1:C:240:LEU:HD23	1.78	0.66
1:C:197:ILE:HB	1:C:198:PRO:HD3	1.76	0.66
1:E:132:ARG:HA	1:E:180:GLU:HG2	1.76	0.66
1:A:238:ASN:HA	1:A:258:ILE:HD11	1.78	0.66
1:B:84:ARG:NH1	1:B:84:ARG:HB2	2.11	0.65
1:D:84:ARG:HB2	1:D:84:ARG:HH11	1.61	0.65
1:C:238:ASN:HA	1:C:258:ILE:CD1	2.26	0.65
1:D:304:LEU:O	1:D:308:ILE:HG12	1.97	0.65
1:B:94:SER:OG	1:B:95:PRO:HD2	1.97	0.65
1:A:213:THR:HG22	1:A:226:LEU:HD11	1.79	0.65
1:C:254:THR:O	1:C:258:ILE:HB	1.95	0.65
1:B:66:GLU:HG3	1:B:67:PRO:HD2	1.78	0.65
1:E:197:ILE:HB	1:E:198:PRO:HD3	1.79	0.65
1:C:53:PHE:CE1	1:C:95:PRO:HA	2.31	0.65
1:B:191:ARG:HG3	1:B:192:GLN:N	2.12	0.65
1:A:47:LYS:HD2	1:A:49:ARG:HH21	1.61	0.65
1:D:104:ARG:HH22	1:E:78:VAL:HA	1.61	0.64
1:C:147:LYS:C	1:C:149:GLY:N	2.46	0.64
1:A:22:TYR:HA	1:A:149:GLY:HA2	1.78	0.64
1:E:53:PHE:HE2	1:E:63:LYS:HB3	1.62	0.64
1:D:84:ARG:CB	1:D:84:ARG:HH11	2.09	0.64
1:B:249:PRO:HD2	1:B:250:TYR:CD1	2.31	0.64
1:D:22:TYR:HA	1:D:149:GLY:HA2	1.78	0.64
1:A:53:PHE:CE1	1:A:95:PRO:HA	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:81:GLU:HG3	1:E:108:ARG:HG2	1.79	0.64
1:A:226:LEU:HD23	1:B:224:VAL:CB	2.20	0.64
1:B:22:TYR:HA	1:B:149:GLY:HA2	1.80	0.64
1:D:54:ASP:HB2	1:D:57:ARG:CG	2.27	0.64
1:A:84:ARG:HB2	1:A:84:ARG:HH11	1.63	0.64
1:E:66:GLU:HG3	1:E:67:PRO:HD2	1.80	0.64
1:C:81:GLU:HG3	1:C:108:ARG:HG2	1.78	0.63
1:E:249:PRO:HD2	1:E:250:TYR:CD1	2.33	0.63
1:E:219:SER:OG	1:E:222:ALA:HB3	1.98	0.63
1:C:53:PHE:HE2	1:C:63:LYS:HB3	1.63	0.63
1:C:22:TYR:HA	1:C:149:GLY:HA2	1.78	0.63
1:E:22:TYR:HA	1:E:149:GLY:HA2	1.80	0.63
1:C:215:PHE:O	1:C:291:THR:HG22	1.98	0.63
1:E:267:VAL:HG23	1:E:298:PHE:CZ	2.34	0.63
1:B:53:PHE:HE2	1:B:63:LYS:HB3	1.64	0.63
1:B:123:GLN:HA	1:B:123:GLN:NE2	2.12	0.63
1:A:303:LEU:O	1:A:307:ILE:HD12	1.99	0.63
1:A:215:PHE:HZ	1:A:298:PHE:CE1	2.17	0.63
1:C:213:THR:HG22	1:C:226:LEU:CD1	2.27	0.63
1:A:84:ARG:CB	1:A:84:ARG:HH11	2.10	0.63
1:E:208:LEU:O	1:E:211:SER:HB3	1.99	0.63
1:E:100:GLN:HE21	1:E:100:GLN:HA	1.64	0.63
1:D:66:GLU:HG3	1:D:67:PRO:HD2	1.80	0.63
1:B:213:THR:HG22	1:B:226:LEU:HD11	1.81	0.62
1:B:54:ASP:HB2	1:B:57:ARG:CG	2.29	0.62
1:A:53:PHE:HE2	1:A:63:LYS:HB3	1.64	0.62
1:D:123:GLN:NE2	1:D:123:GLN:HA	2.14	0.62
1:C:267:VAL:HG23	1:C:298:PHE:CZ	2.34	0.62
1:E:303:LEU:O	1:E:307:ILE:HD12	2.00	0.62
1:D:219:SER:OG	1:D:222:ALA:HB3	2.00	0.62
1:A:197:ILE:HB	1:A:198:PRO:HD3	1.80	0.62
1:B:200:ILE:HD11	1:B:240:LEU:HD23	1.79	0.62
1:A:229:SER:HB3	1:B:228:VAL:CG1	2.29	0.62
1:B:238:ASN:HA	1:B:258:ILE:CD1	2.28	0.62
1:C:66:GLU:HG3	1:C:67:PRO:HD2	1.82	0.62
1:D:210:ILE:HG13	1:E:266:PHE:CE1	2.34	0.62
1:D:215:PHE:HZ	1:D:298:PHE:CE1	2.18	0.62
1:C:47:LYS:HD2	1:C:49:ARG:NH2	2.15	0.62
1:B:215:PHE:HZ	1:B:298:PHE:CE1	2.18	0.62
1:E:47:LYS:HD2	1:E:49:ARG:NH2	2.13	0.62
1:D:191:ARG:HG3	1:D:192:GLN:N	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:100:GLN:HE21	1:D:100:GLN:HA	1.64	0.62
1:A:229:SER:CB	1:B:228:VAL:HG11	2.29	0.62
1:C:89:VAL:CG1	1:C:102:LEU:HD23	2.28	0.62
1:E:200:ILE:HD11	1:E:240:LEU:HD23	1.81	0.62
1:B:208:LEU:O	1:B:211:SER:HB3	2.00	0.62
1:C:54:ASP:HB2	1:C:57:ARG:CG	2.29	0.62
1:A:89:VAL:CG1	1:A:102:LEU:HD23	2.27	0.61
1:E:215:PHE:O	1:E:291:THR:HG22	2.00	0.61
1:A:217:SER:OG	1:B:220:TYR:CE2	2.51	0.61
1:C:297:ALA:O	1:C:301:VAL:HG23	2.00	0.61
1:E:147:LYS:O	1:E:149:GLY:N	2.33	0.61
1:C:234:HIS:CE1	1:C:261:ILE:CG2	2.82	0.61
1:D:267:VAL:HG23	1:D:298:PHE:CZ	2.35	0.61
1:B:42:LEU:HB3	1:B:103:GLU:CG	2.30	0.61
1:A:213:THR:HG22	1:A:226:LEU:CD1	2.29	0.61
1:C:147:LYS:HE2	1:C:165:THR:HA	1.82	0.61
1:C:215:PHE:HZ	1:C:298:PHE:CE1	2.18	0.61
1:D:53:PHE:HE2	1:D:63:LYS:HB3	1.63	0.61
1:D:238:ASN:HA	1:D:258:ILE:CD1	2.30	0.61
1:B:84:ARG:HH11	1:B:84:ARG:HB2	1.64	0.61
1:D:197:ILE:HB	1:D:198:PRO:HD3	1.82	0.61
1:B:147:LYS:O	1:B:149:GLY:N	2.33	0.61
1:D:229:SER:HB3	1:E:228:VAL:CG1	2.31	0.61
1:A:238:ASN:HA	1:A:258:ILE:CD1	2.31	0.61
1:A:47:LYS:HD2	1:A:49:ARG:NH2	2.16	0.61
1:A:297:ALA:O	1:A:301:VAL:HG23	2.00	0.61
1:E:215:PHE:HZ	1:E:298:PHE:CE1	2.19	0.61
1:C:42:LEU:HB3	1:C:103:GLU:CG	2.31	0.60
1:E:24:ILE:HD13	1:E:104:ARG:HE	1.67	0.60
1:D:229:SER:HB3	1:E:228:VAL:HG11	1.83	0.60
1:D:202:LEU:HD12	1:E:259:PHE:HZ	1.66	0.60
1:E:150:LYS:CG	1:E:154:VAL:HG21	2.31	0.60
1:E:54:ASP:HB2	1:E:57:ARG:CG	2.30	0.60
1:C:15:LEU:HD11	1:C:46:TRP:HB2	1.83	0.60
1:E:213:THR:HG22	1:E:226:LEU:HD11	1.84	0.60
1:B:245:LEU:HD12	1:B:246:PRO:HD2	1.83	0.60
1:B:223:ASN:O	1:B:227:VAL:HG23	2.01	0.60
1:A:157:THR:CG2	1:B:34:GLU:OE1	2.50	0.60
1:A:277:TYR:O	1:A:281:GLU:CG	2.50	0.60
1:A:54:ASP:HB2	1:A:57:ARG:CG	2.31	0.60
1:D:277:TYR:O	1:D:281:GLU:CG	2.50	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:LEU:HD11	1:B:46:TRP:HB2	1.82	0.60
1:A:141:LEU:HD23	1:A:142:ALA:H	1.67	0.60
1:A:229:SER:CB	1:B:228:VAL:CG1	2.80	0.60
1:C:249:PRO:HD2	1:C:250:TYR:CD1	2.37	0.60
1:E:304:LEU:O	1:E:308:ILE:HG12	2.01	0.60
1:B:303:LEU:O	1:B:307:ILE:HD12	2.02	0.60
1:B:213:THR:HG22	1:B:226:LEU:CD1	2.32	0.60
1:D:223:ASN:O	1:D:227:VAL:HG23	2.02	0.60
1:E:277:TYR:O	1:E:281:GLU:CG	2.50	0.60
1:E:151:ASN:HD22	1:E:152:ASP:H	1.49	0.60
1:A:233:ALA:HB1	1:B:235:ILE:CD1	2.31	0.60
1:A:147:LYS:HE2	1:A:165:THR:HA	1.83	0.59
1:B:13:GLU:HB3	1:B:14:PRO:CD	2.32	0.59
1:A:223:ASN:O	1:A:227:VAL:HG23	2.01	0.59
1:B:219:SER:OG	1:B:222:ALA:HB3	2.03	0.59
1:C:29:LEU:HB2	1:C:156:LEU:HD11	1.83	0.59
1:A:221:GLU:OE2	1:B:221:GLU:OE2	2.21	0.59
1:A:27:TYR:HB3	1:B:110:LEU:CD1	2.24	0.59
1:E:15:LEU:HD11	1:E:46:TRP:HB2	1.83	0.59
1:B:267:VAL:HG23	1:B:298:PHE:CZ	2.37	0.59
1:C:25:GLU:HA	1:C:25:GLU:OE1	2.01	0.59
1:C:147:LYS:HG2	1:C:147:LYS:O	2.01	0.59
1:C:65:TYR:CD2	1:C:70:ILE:HD11	2.37	0.59
1:E:213:THR:HG22	1:E:226:LEU:CD1	2.33	0.59
1:A:208:LEU:O	1:A:211:SER:HB3	2.02	0.59
1:A:249:PRO:HD2	1:A:250:TYR:CD1	2.38	0.59
1:E:218:THR:HG22	1:E:279:LYS:HE2	1.84	0.59
1:C:303:LEU:O	1:C:307:ILE:HD12	2.02	0.59
1:B:29:LEU:HB2	1:B:156:LEU:HD11	1.84	0.59
1:E:141:LEU:HD23	1:E:142:ALA:H	1.68	0.59
1:D:15:LEU:HD11	1:D:46:TRP:HB2	1.85	0.59
1:B:297:ALA:O	1:B:301:VAL:HG23	2.03	0.59
1:D:212:TRP:HZ3	1:D:264:PHE:HD2	1.50	0.59
1:B:277:TYR:O	1:B:281:GLU:CG	2.50	0.59
1:C:151:ASN:HD22	1:C:152:ASP:H	1.49	0.59
1:C:245:LEU:HD12	1:C:246:PRO:HD2	1.85	0.59
1:A:191:ARG:HG3	1:A:192:GLN:N	2.18	0.59
1:C:223:ASN:O	1:C:227:VAL:HG23	2.02	0.59
1:E:245:LEU:HD12	1:E:246:PRO:HD2	1.85	0.59
1:C:225:THR:HG21	1:D:225:THR:OG1	2.03	0.58
1:A:215:PHE:O	1:A:291:THR:HG22	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:260:MET:HE2	1:E:309:LEU:HD22	1.85	0.58
1:A:100:GLN:HE21	1:A:100:GLN:HA	1.69	0.58
1:C:150:LYS:CG	1:C:154:VAL:HG21	2.33	0.58
1:A:22:TYR:HB3	1:A:41:PHE:HB2	1.86	0.58
1:E:42:LEU:HB3	1:E:103:GLU:CG	2.32	0.58
1:D:42:LEU:HB3	1:D:103:GLU:CG	2.33	0.58
1:C:200:ILE:CD1	1:C:240:LEU:HD23	2.33	0.58
1:D:200:ILE:HD11	1:D:240:LEU:HD23	1.85	0.58
1:A:245:LEU:HD12	1:A:246:PRO:HD2	1.84	0.58
1:D:253:TYR:HD1	1:D:313:PHE:CD2	2.21	0.58
1:B:215:PHE:O	1:B:291:THR:HG22	2.02	0.58
1:C:277:TYR:O	1:C:281:GLU:CG	2.50	0.58
1:C:100:GLN:HE21	1:C:100:GLN:HA	1.69	0.58
1:D:24:ILE:HD13	1:D:104:ARG:HE	1.69	0.58
1:C:13:GLU:HB3	1:C:14:PRO:CD	2.34	0.58
1:E:223:ASN:O	1:E:227:VAL:HG23	2.03	0.58
1:C:314:PHE:CD1	1:C:314:PHE:N	2.71	0.58
1:A:13:GLU:HB3	1:A:14:PRO:CD	2.33	0.58
1:D:276:HIS:C	1:D:278:LEU:H	2.07	0.58
1:A:276:HIS:C	1:A:278:LEU:H	2.07	0.58
1:E:297:ALA:O	1:E:301:VAL:HG23	2.04	0.58
1:C:191:ARG:HG3	1:C:192:GLN:N	2.17	0.58
1:B:304:LEU:O	1:B:308:ILE:HG12	2.04	0.58
1:D:215:PHE:O	1:D:291:THR:HG22	2.03	0.58
1:A:218:THR:HG22	1:A:279:LYS:HE2	1.86	0.58
1:A:66:GLU:HG3	1:A:67:PRO:HD2	1.85	0.58
1:D:155:PHE:HE1	1:E:112:PRO:HB3	1.59	0.58
1:A:24:ILE:HD13	1:A:104:ARG:HE	1.69	0.58
1:E:276:HIS:C	1:E:278:LEU:H	2.07	0.58
1:A:15:LEU:HD11	1:A:46:TRP:HB2	1.86	0.58
1:A:222:ALA:O	1:A:226:LEU:HB2	2.03	0.58
1:D:147:LYS:O	1:D:149:GLY:N	2.37	0.57
1:A:212:TRP:HZ3	1:A:264:PHE:HD2	1.52	0.57
1:A:42:LEU:HB3	1:A:103:GLU:CG	2.33	0.57
1:C:276:HIS:C	1:C:278:LEU:H	2.07	0.57
1:A:314:PHE:CD1	1:A:314:PHE:N	2.71	0.57
1:A:151:ASN:HD22	1:A:152:ASP:H	1.51	0.57
1:D:215:PHE:CZ	1:D:298:PHE:CD1	2.92	0.57
1:A:298:PHE:HB2	1:A:299:PRO:HD3	1.87	0.57
1:D:13:GLU:HB3	1:D:14:PRO:CD	2.35	0.57
1:A:157:THR:HG21	1:B:34:GLU:OE1	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:297:ALA:O	1:D:301:VAL:HG23	2.04	0.57
1:E:29:LEU:HB2	1:E:156:LEU:HD11	1.85	0.57
1:A:215:PHE:CZ	1:A:298:PHE:CD1	2.91	0.57
1:B:281:GLU:O	1:B:283:GLN:N	2.36	0.57
1:E:123:GLN:NE2	1:E:123:GLN:HA	2.19	0.57
1:D:194:PHE:C	1:D:196:TYR:N	2.57	0.57
1:A:314:PHE:HD1	1:A:314:PHE:N	2.03	0.57
1:C:147:LYS:O	1:C:149:GLY:N	2.37	0.57
1:E:234:HIS:CE1	1:E:261:ILE:CG2	2.87	0.57
1:D:249:PRO:HD2	1:D:250:TYR:CD1	2.40	0.57
1:D:18:ASN:HB3	1:D:143:VAL:HG23	1.85	0.57
1:A:281:GLU:O	1:A:283:GLN:N	2.36	0.57
1:A:200:ILE:HD11	1:A:240:LEU:HD23	1.86	0.57
1:B:218:THR:HG22	1:B:279:LYS:HE2	1.86	0.57
1:C:212:TRP:HZ3	1:C:264:PHE:HD2	1.52	0.57
1:B:200:ILE:O	1:B:204:MET:HB2	2.05	0.57
1:C:202:LEU:HD12	1:D:259:PHE:CE1	2.40	0.57
1:D:218:THR:HG22	1:D:279:LYS:HE2	1.86	0.57
1:A:150:LYS:CG	1:A:154:VAL:HG21	2.35	0.57
1:E:212:TRP:HZ3	1:E:264:PHE:HD2	1.52	0.57
1:B:151:ASN:HD22	1:B:152:ASP:H	1.52	0.57
1:C:226:LEU:HD21	1:D:224:VAL:HB	1.86	0.57
1:C:24:ILE:HD13	1:C:104:ARG:HE	1.69	0.57
1:A:65:TYR:CD2	1:A:70:ILE:HD11	2.40	0.56
1:B:159:TRP:CE3	1:B:189:ILE:HD12	2.39	0.56
1:C:215:PHE:CZ	1:C:298:PHE:CD1	2.93	0.56
1:E:298:PHE:HB2	1:E:299:PRO:HD3	1.87	0.56
1:A:234:HIS:CE1	1:A:261:ILE:CG2	2.89	0.56
1:A:290:ILE:HG22	1:A:291:THR:N	2.19	0.56
1:A:277:TYR:O	1:A:281:GLU:HG3	2.05	0.56
1:C:29:LEU:C	1:C:29:LEU:HD23	2.25	0.56
1:D:245:LEU:HD12	1:D:246:PRO:HD2	1.87	0.56
1:C:208:LEU:O	1:C:211:SER:HB3	2.05	0.56
1:D:213:THR:HG22	1:D:226:LEU:CD1	2.35	0.56
1:D:208:LEU:O	1:D:211:SER:HB3	2.05	0.56
1:D:298:PHE:HB2	1:D:299:PRO:HD3	1.87	0.56
1:D:277:TYR:O	1:D:281:GLU:HG3	2.05	0.56
1:B:277:TYR:O	1:B:281:GLU:HG3	2.06	0.56
1:A:159:TRP:CE3	1:A:189:ILE:HD12	2.40	0.56
1:E:147:LYS:HE2	1:E:165:THR:HA	1.87	0.56
1:C:253:TYR:O	1:C:256:ALA:HB3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:298:PHE:HB2	1:C:299:PRO:HD3	1.87	0.56
1:E:65:TYR:CD2	1:E:70:ILE:HD11	2.40	0.56
1:E:13:GLU:HB3	1:E:14:PRO:CD	2.35	0.56
1:B:197:ILE:HB	1:B:198:PRO:HD3	1.87	0.56
1:B:260:MET:HE2	1:B:309:LEU:HD22	1.87	0.56
1:D:54:ASP:HB2	1:D:57:ARG:HB2	1.88	0.56
1:B:276:HIS:C	1:B:278:LEU:H	2.07	0.56
1:A:147:LYS:O	1:A:149:GLY:N	2.38	0.56
1:D:52:ALA:HA	1:D:95:PRO:O	2.06	0.56
1:E:137:ARG:HD2	1:E:179:LEU:HG	1.88	0.56
1:B:150:LYS:CG	1:B:154:VAL:HG21	2.36	0.56
1:D:290:ILE:HG22	1:D:291:THR:N	2.21	0.56
1:B:212:TRP:HZ3	1:B:264:PHE:HD2	1.51	0.56
1:C:277:TYR:O	1:C:281:GLU:HG3	2.06	0.56
1:C:314:PHE:HD1	1:C:314:PHE:N	2.04	0.56
1:D:303:LEU:O	1:D:307:ILE:HD12	2.06	0.56
1:A:222:ALA:HA	1:B:221:GLU:OE1	2.06	0.56
1:D:213:THR:HG22	1:D:226:LEU:HD11	1.87	0.56
1:C:150:LYS:HG3	1:C:154:VAL:HG21	1.88	0.56
1:B:24:ILE:HD13	1:B:104:ARG:HE	1.69	0.56
1:C:218:THR:HG22	1:C:279:LYS:HE2	1.87	0.56
1:E:147:LYS:O	1:E:147:LYS:HG2	2.06	0.56
1:B:215:PHE:CZ	1:B:298:PHE:CD1	2.93	0.56
1:B:298:PHE:HB2	1:B:299:PRO:HD3	1.87	0.56
1:D:29:LEU:HB2	1:D:156:LEU:HD11	1.88	0.56
1:E:275:GLN:HG3	1:E:291:THR:OG1	2.06	0.55
1:B:253:TYR:O	1:B:256:ALA:HB3	2.07	0.55
1:B:54:ASP:HB2	1:B:57:ARG:HB2	1.88	0.55
1:D:147:LYS:O	1:D:147:LYS:HG2	2.07	0.55
1:D:192:GLN:CD	1:E:249:PRO:HB3	2.27	0.55
1:D:260:MET:HE2	1:D:309:LEU:HD22	1.87	0.55
1:E:277:TYR:O	1:E:281:GLU:HG3	2.06	0.55
1:D:29:LEU:HD23	1:D:29:LEU:C	2.27	0.55
1:C:260:MET:HE2	1:C:309:LEU:HD22	1.88	0.55
1:C:46:TRP:HH2	1:C:72:ILE:HG23	1.69	0.55
1:D:194:PHE:C	1:D:196:TYR:H	2.09	0.55
1:B:29:LEU:HD23	1:B:29:LEU:C	2.27	0.55
1:E:25:GLU:HA	1:E:25:GLU:OE1	2.04	0.55
1:A:275:GLN:HG3	1:A:291:THR:OG1	2.07	0.55
1:E:191:ARG:HG3	1:E:192:GLN:N	2.21	0.55
1:A:193:TYR:O	1:A:194:PHE:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:LEU:C	1:A:29:LEU:HD23	2.26	0.55
1:C:290:ILE:HG22	1:C:291:THR:N	2.22	0.55
1:C:195:SER:O	1:C:199:ASN:HB2	2.07	0.55
1:C:194:PHE:C	1:C:196:TYR:N	2.59	0.55
1:B:234:HIS:CE1	1:B:261:ILE:CG2	2.90	0.55
1:D:283:GLN:N	1:D:284:PRO:CD	2.70	0.55
1:A:123:GLN:HA	1:A:123:GLN:NE2	2.22	0.55
1:A:18:ASN:HB3	1:A:143:VAL:HG23	1.89	0.55
1:D:275:GLN:HG3	1:D:291:THR:OG1	2.06	0.55
1:A:75:ILE:HD13	1:A:131:VAL:HB	1.88	0.55
1:A:51:LEU:CD1	1:A:70:ILE:HD12	2.37	0.55
1:B:314:PHE:N	1:B:314:PHE:CD1	2.75	0.55
1:A:147:LYS:O	1:A:147:LYS:HG2	2.07	0.54
1:A:215:PHE:HZ	1:A:298:PHE:CD1	2.25	0.54
1:C:281:GLU:O	1:C:283:GLN:N	2.38	0.54
1:A:192:GLN:CD	1:B:249:PRO:HB3	2.27	0.54
1:D:159:TRP:CE3	1:D:189:ILE:HD12	2.43	0.54
1:C:123:GLN:NE2	1:C:123:GLN:HA	2.22	0.54
1:E:314:PHE:N	1:E:314:PHE:CD1	2.74	0.54
1:D:253:TYR:O	1:D:256:ALA:HB3	2.06	0.54
1:B:290:ILE:HG22	1:B:291:THR:N	2.22	0.54
1:A:253:TYR:O	1:A:256:ALA:HB3	2.07	0.54
1:B:65:TYR:CD2	1:B:70:ILE:HD11	2.42	0.54
1:C:141:LEU:HD23	1:C:142:ALA:H	1.71	0.54
1:E:194:PHE:C	1:E:196:TYR:H	2.11	0.54
1:D:149:GLY:O	1:D:150:LYS:HB2	2.07	0.54
1:B:275:GLN:HG3	1:B:291:THR:OG1	2.08	0.54
1:E:75:ILE:HD13	1:E:131:VAL:HB	1.88	0.54
1:B:51:LEU:CD1	1:B:70:ILE:HD12	2.38	0.54
1:C:256:ALA:HB1	1:C:309:LEU:HD21	1.90	0.54
1:C:194:PHE:C	1:C:196:TYR:H	2.09	0.54
1:A:304:LEU:O	1:A:308:ILE:HG12	2.06	0.54
1:C:54:ASP:HB2	1:C:57:ARG:HB2	1.90	0.54
1:A:29:LEU:HB2	1:A:156:LEU:HD11	1.90	0.54
1:D:275:GLN:O	1:D:275:GLN:HG2	2.08	0.54
1:D:215:PHE:HZ	1:D:298:PHE:CD1	2.26	0.54
1:B:267:VAL:HA	1:B:270:ILE:HB	1.90	0.54
1:E:194:PHE:C	1:E:196:TYR:N	2.60	0.54
1:E:275:GLN:O	1:E:275:GLN:HG2	2.08	0.54
1:A:283:GLN:N	1:A:284:PRO:CD	2.70	0.54
1:B:283:GLN:N	1:B:284:PRO:CD	2.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:193:TYR:O	1:D:194:PHE:HB2	2.06	0.54
1:E:267:VAL:HA	1:E:270:ILE:HB	1.88	0.54
1:E:215:PHE:CZ	1:E:298:PHE:CD1	2.95	0.54
1:D:51:LEU:CD1	1:D:70:ILE:HD12	2.38	0.54
1:D:192:GLN:OE1	1:E:249:PRO:HB3	2.07	0.54
1:D:222:ALA:O	1:D:226:LEU:HB2	2.07	0.54
1:C:275:GLN:HG2	1:C:275:GLN:O	2.08	0.54
1:D:53:PHE:CD1	1:D:95:PRO:HA	2.43	0.54
1:B:25:GLU:OE1	1:B:25:GLU:HA	2.07	0.54
1:E:150:LYS:HG3	1:E:154:VAL:HG21	1.89	0.53
1:C:275:GLN:HG3	1:C:291:THR:OG1	2.08	0.53
1:B:147:LYS:HE2	1:B:165:THR:HA	1.90	0.53
1:C:215:PHE:HZ	1:C:298:PHE:CD1	2.26	0.53
1:B:305:ALA:O	1:B:309:LEU:HB2	2.08	0.53
1:A:275:GLN:HG2	1:A:275:GLN:O	2.08	0.53
1:C:18:ASN:HB3	1:C:143:VAL:HG23	1.90	0.53
1:A:209:PHE:HB2	1:B:266:PHE:CE1	2.43	0.53
1:A:150:LYS:HG3	1:A:154:VAL:HG21	1.89	0.53
1:B:275:GLN:HG2	1:B:275:GLN:O	2.08	0.53
1:B:194:PHE:C	1:B:196:TYR:N	2.61	0.53
1:E:222:ALA:O	1:E:226:LEU:HB2	2.09	0.53
1:E:54:ASP:HB2	1:E:57:ARG:HB2	1.90	0.53
1:E:53:PHE:CD1	1:E:95:PRO:HA	2.44	0.53
1:D:65:TYR:CD2	1:D:70:ILE:HD11	2.43	0.53
1:B:147:LYS:HG2	1:B:147:LYS:O	2.08	0.53
1:E:22:TYR:HB3	1:E:41:PHE:HB2	1.90	0.53
1:E:290:ILE:HG22	1:E:291:THR:N	2.22	0.53
1:C:199:ASN:HB3	1:D:242:GLU:OE2	2.08	0.53
1:A:46:TRP:HH2	1:A:72:ILE:HG23	1.72	0.53
1:A:225:THR:HG21	1:B:225:THR:OG1	2.09	0.53
1:B:215:PHE:HZ	1:B:298:PHE:CD1	2.27	0.53
1:C:283:GLN:N	1:C:284:PRO:CD	2.71	0.53
1:C:193:TYR:O	1:C:194:PHE:HB2	2.08	0.53
1:E:281:GLU:O	1:E:283:GLN:N	2.39	0.53
1:E:147:LYS:CE	1:E:165:THR:HA	2.39	0.53
1:C:215:PHE:HB2	1:C:216:TRP:CZ3	2.43	0.53
1:C:267:VAL:HA	1:C:270:ILE:HB	1.91	0.53
1:B:298:PHE:CB	1:B:299:PRO:HD3	2.39	0.53
1:A:298:PHE:CB	1:A:299:PRO:HD3	2.39	0.53
1:B:200:ILE:CD1	1:B:240:LEU:HD23	2.39	0.53
1:B:125:LEU:HB2	1:B:187:LEU:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:298:PHE:CB	1:E:299:PRO:HD3	2.39	0.52
1:D:281:GLU:O	1:D:283:GLN:N	2.36	0.52
1:E:51:LEU:CD1	1:E:70:ILE:HD12	2.38	0.52
1:C:237:PHE:HE1	1:D:235:ILE:HD13	1.74	0.52
1:D:221:GLU:OE2	1:E:221:GLU:OE2	2.27	0.52
1:E:305:ALA:O	1:E:309:LEU:HB2	2.08	0.52
1:C:51:LEU:CD1	1:C:70:ILE:HD12	2.40	0.52
1:D:314:PHE:N	1:D:314:PHE:CD1	2.76	0.52
1:C:22:TYR:HB3	1:C:41:PHE:HB2	1.91	0.52
1:D:298:PHE:CB	1:D:299:PRO:HD3	2.39	0.52
1:D:157:THR:HG21	1:E:34:GLU:OE1	2.10	0.52
1:C:304:LEU:O	1:C:308:ILE:HG12	2.08	0.52
1:E:200:ILE:O	1:E:204:MET:HB2	2.08	0.52
1:B:18:ASN:HB3	1:B:143:VAL:HG23	1.91	0.52
1:D:25:GLU:HA	1:D:25:GLU:OE1	2.08	0.52
1:E:253:TYR:HD1	1:E:313:PHE:CD2	2.27	0.52
1:E:200:ILE:CD1	1:E:240:LEU:HD23	2.38	0.52
1:E:18:ASN:HB3	1:E:143:VAL:HG23	1.90	0.52
1:B:7:PRO:O	1:B:50:ARG:NH2	2.43	0.52
1:A:221:GLU:HB3	1:B:221:GLU:CG	2.37	0.52
1:A:260:MET:HE2	1:A:309:LEU:HD22	1.90	0.52
1:D:53:PHE:O	1:D:53:PHE:CD1	2.63	0.52
1:B:53:PHE:CD1	1:B:53:PHE:O	2.63	0.52
1:B:53:PHE:CD1	1:B:95:PRO:HA	2.44	0.52
1:A:53:PHE:CD1	1:A:53:PHE:O	2.63	0.52
1:D:193:TYR:O	1:D:194:PHE:CB	2.56	0.52
1:C:222:ALA:HA	1:D:221:GLU:OE1	2.10	0.52
1:A:194:PHE:C	1:A:196:TYR:N	2.62	0.52
1:E:314:PHE:N	1:E:314:PHE:HD1	2.07	0.52
1:A:25:GLU:HA	1:A:25:GLU:OE1	2.09	0.52
1:A:7:PRO:O	1:A:50:ARG:NH2	2.42	0.52
1:A:27:TYR:CG	1:B:110:LEU:CD1	2.92	0.52
1:D:267:VAL:HA	1:D:270:ILE:HB	1.90	0.52
1:B:123:GLN:HB2	1:B:189:ILE:HG13	1.92	0.52
1:E:29:LEU:C	1:E:29:LEU:HD23	2.30	0.52
1:D:68:GLU:H	1:D:68:GLU:CD	2.11	0.52
1:C:298:PHE:CB	1:C:299:PRO:HD3	2.39	0.52
1:E:53:PHE:O	1:E:53:PHE:CD1	2.63	0.52
1:E:52:ALA:HA	1:E:95:PRO:O	2.09	0.52
1:A:193:TYR:O	1:A:194:PHE:CB	2.57	0.52
1:B:161:ILE:HA	1:B:189:ILE:HG22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:THR:HG22	1:B:244:ASN:ND2	2.25	0.52
1:A:27:TYR:CB	1:B:110:LEU:CD1	2.82	0.52
1:D:210:ILE:CG2	1:E:269:VAL:HG11	2.29	0.52
1:B:215:PHE:HB2	1:B:216:TRP:CZ3	2.45	0.52
1:C:53:PHE:CD1	1:C:53:PHE:O	2.63	0.52
1:D:150:LYS:CG	1:D:154:VAL:HG21	2.40	0.51
1:A:222:ALA:CB	1:B:221:GLU:HA	2.27	0.51
1:D:75:ILE:HD13	1:D:131:VAL:HB	1.93	0.51
1:A:137:ARG:HD2	1:A:179:LEU:HG	1.92	0.51
1:C:222:ALA:O	1:C:226:LEU:HB2	2.11	0.51
1:E:283:GLN:N	1:E:284:PRO:CD	2.71	0.51
1:B:194:PHE:C	1:B:196:TYR:H	2.13	0.51
1:C:222:ALA:CB	1:D:221:GLU:HA	2.40	0.51
1:D:305:ALA:O	1:D:309:LEU:HB2	2.10	0.51
1:C:193:TYR:O	1:C:194:PHE:CB	2.58	0.51
1:D:240:LEU:HD13	1:E:239:ILE:HG12	1.92	0.51
1:C:210:ILE:CD1	1:D:231:LEU:HD22	2.41	0.51
1:A:195:SER:O	1:A:199:ASN:HB2	2.10	0.51
1:A:53:PHE:HE2	1:A:63:LYS:CB	2.24	0.51
1:C:159:TRP:CE3	1:C:189:ILE:HD12	2.45	0.51
1:E:216:TRP:CZ2	1:E:295:ARG:HB3	2.46	0.51
1:E:161:ILE:HA	1:E:189:ILE:HG22	1.93	0.51
1:C:68:GLU:CD	1:C:68:GLU:H	2.14	0.51
1:A:104:ARG:HH22	1:B:78:VAL:CA	2.17	0.51
1:A:277:TYR:O	1:A:281:GLU:HG2	2.11	0.51
1:D:277:TYR:O	1:D:281:GLU:HG2	2.11	0.51
1:B:46:TRP:HH2	1:B:72:ILE:HG23	1.75	0.51
1:D:147:LYS:HE2	1:D:165:THR:HA	1.92	0.51
1:A:305:ALA:O	1:A:309:LEU:HB2	2.11	0.51
1:C:75:ILE:HD13	1:C:131:VAL:HB	1.92	0.51
1:A:54:ASP:HB2	1:A:57:ARG:HB2	1.93	0.51
1:B:193:TYR:O	1:B:194:PHE:HB2	2.10	0.51
1:D:151:ASN:HD22	1:D:152:ASP:H	1.56	0.51
1:A:253:TYR:HD1	1:A:313:PHE:CD2	2.29	0.51
1:E:125:LEU:HB2	1:E:187:LEU:HB3	1.93	0.51
1:D:225:THR:O	1:D:225:THR:HG22	2.11	0.51
1:D:210:ILE:HG13	1:E:266:PHE:HE1	1.76	0.51
1:D:53:PHE:HE2	1:D:63:LYS:CB	2.24	0.51
1:C:53:PHE:HE2	1:C:63:LYS:CB	2.24	0.51
1:B:277:TYR:O	1:B:281:GLU:HG2	2.11	0.51
1:A:194:PHE:C	1:A:196:TYR:H	2.13	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:PHE:N	1:B:314:PHE:HD1	2.07	0.51
1:D:22:TYR:HB3	1:D:41:PHE:HB2	1.93	0.50
1:D:257:ILE:HG22	1:D:309:LEU:HD23	1.94	0.50
1:A:51:LEU:HD13	1:A:70:ILE:HD12	1.93	0.50
1:A:37:LYS:CG	1:A:108:ARG:HB2	2.40	0.50
1:E:7:PRO:O	1:E:50:ARG:NH2	2.44	0.50
1:D:96:ASP:OD1	1:D:98:THR:HB	2.12	0.50
1:C:271:GLU:OE2	1:C:272:VAL:N	2.44	0.50
1:E:243:THR:HG22	1:E:244:ASN:ND2	2.26	0.50
1:A:216:TRP:CZ2	1:A:295:ARG:HB3	2.46	0.50
1:C:53:PHE:CD1	1:C:53:PHE:C	2.85	0.50
1:D:274:VAL:C	1:D:276:HIS:H	2.15	0.50
1:C:274:VAL:C	1:C:276:HIS:H	2.15	0.50
1:A:53:PHE:CD1	1:A:95:PRO:HA	2.47	0.50
1:C:204:MET:O	1:C:207:ILE:HG12	2.12	0.50
1:E:37:LYS:HG3	1:E:108:ARG:HB2	1.94	0.50
1:D:123:GLN:HB2	1:D:189:ILE:HG13	1.93	0.50
1:C:123:GLN:HB2	1:C:189:ILE:HG13	1.94	0.50
1:E:193:TYR:O	1:E:194:PHE:HB2	2.10	0.50
1:A:78:VAL:HB	1:A:128:TYR:HB2	1.93	0.50
1:B:22:TYR:HB3	1:B:41:PHE:HB2	1.94	0.50
1:C:264:PHE:CE2	1:C:302:PHE:HB2	2.47	0.50
1:E:215:PHE:HB2	1:E:216:TRP:CZ3	2.46	0.50
1:A:53:PHE:CE2	1:A:63:LYS:HB3	2.47	0.50
1:E:277:TYR:O	1:E:281:GLU:HG2	2.11	0.50
1:B:274:VAL:C	1:B:276:HIS:H	2.15	0.50
1:A:68:GLU:H	1:A:68:GLU:CD	2.15	0.50
1:D:215:PHE:HB2	1:D:216:TRP:CZ3	2.45	0.50
1:E:215:PHE:HZ	1:E:298:PHE:CD1	2.30	0.50
1:B:53:PHE:C	1:B:53:PHE:CD1	2.85	0.50
1:A:53:PHE:CD1	1:A:53:PHE:C	2.85	0.50
1:E:46:TRP:HH2	1:E:72:ILE:HG23	1.76	0.50
1:D:104:ARG:NH2	1:E:78:VAL:HA	2.26	0.50
1:D:53:PHE:C	1:D:53:PHE:CD1	2.85	0.50
1:A:274:VAL:C	1:A:276:HIS:H	2.15	0.50
1:D:81:GLU:HG3	1:D:108:ARG:CG	2.42	0.50
1:C:51:LEU:HD13	1:C:70:ILE:HD12	1.94	0.50
1:B:52:ALA:HA	1:B:95:PRO:O	2.12	0.50
1:C:15:LEU:O	1:C:15:LEU:HG	2.10	0.50
1:C:46:TRP:CH2	1:C:72:ILE:HG23	2.47	0.50
1:B:222:ALA:O	1:B:226:LEU:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:155:PHE:CZ	1:D:112:PRO:HB3	2.47	0.50
1:B:23:LEU:HD22	1:B:38:VAL:HG21	1.93	0.50
1:E:204:MET:O	1:E:207:ILE:HG12	2.11	0.50
1:B:224:VAL:O	1:B:228:VAL:HB	2.12	0.49
1:A:23:LEU:HG	1:A:164:PHE:CE1	2.47	0.49
1:C:53:PHE:CE2	1:C:63:LYS:HB3	2.46	0.49
1:A:151:ASN:HB3	1:A:153:ASP:H	1.77	0.49
1:D:314:PHE:N	1:D:314:PHE:HD1	2.10	0.49
1:D:234:HIS:CE1	1:D:261:ILE:CG2	2.94	0.49
1:D:264:PHE:CE2	1:D:302:PHE:HB2	2.47	0.49
1:C:52:ALA:HA	1:C:95:PRO:O	2.12	0.49
1:C:42:LEU:HD23	1:C:103:GLU:OE1	2.11	0.49
1:E:159:TRP:CE3	1:E:189:ILE:HD12	2.47	0.49
1:C:271:GLU:O	1:C:272:VAL:C	2.50	0.49
1:E:53:PHE:HE2	1:E:63:LYS:CB	2.25	0.49
1:E:53:PHE:C	1:E:53:PHE:CD1	2.85	0.49
1:A:204:MET:O	1:A:207:ILE:HG12	2.12	0.49
1:D:216:TRP:CZ2	1:D:295:ARG:HB3	2.47	0.49
1:B:75:ILE:HD13	1:B:131:VAL:HB	1.93	0.49
1:C:119:PRO:O	1:C:193:TYR:HB3	2.13	0.49
1:D:195:SER:O	1:D:199:ASN:HB2	2.13	0.49
1:C:23:LEU:HB2	1:C:150:LYS:HA	1.95	0.49
1:D:23:LEU:HB2	1:D:150:LYS:HA	1.95	0.49
1:A:37:LYS:HG2	1:A:108:ARG:HB2	1.95	0.49
1:D:27:TYR:CB	1:E:110:LEU:HD11	2.43	0.49
1:C:213:THR:CG2	1:C:226:LEU:HD11	2.42	0.49
1:A:147:LYS:CE	1:A:165:THR:HA	2.42	0.49
1:A:149:GLY:O	1:A:150:LYS:HB2	2.13	0.49
1:A:215:PHE:HB2	1:A:216:TRP:CZ3	2.47	0.49
1:A:267:VAL:HA	1:A:270:ILE:HB	1.93	0.49
1:B:81:GLU:HG3	1:B:108:ARG:CG	2.42	0.49
1:C:277:TYR:O	1:C:281:GLU:HG2	2.11	0.49
1:C:243:THR:HG22	1:C:244:ASN:ND2	2.28	0.49
1:E:149:GLY:O	1:E:150:LYS:HB2	2.13	0.49
1:A:200:ILE:CD1	1:A:240:LEU:HD23	2.43	0.49
1:A:200:ILE:O	1:A:204:MET:HB2	2.12	0.49
1:D:161:ILE:HA	1:D:189:ILE:HG22	1.94	0.49
1:D:200:ILE:O	1:D:204:MET:HB2	2.13	0.49
1:D:27:TYR:HB3	1:E:110:LEU:HD11	1.94	0.49
1:D:7:PRO:O	1:D:50:ARG:NH2	2.43	0.49
1:B:76:ARG:HH12	1:B:130:ILE:HD11	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:GLY:O	1:B:150:LYS:HB2	2.12	0.49
1:C:253:TYR:HD1	1:C:313:PHE:CD2	2.30	0.49
1:B:264:PHE:CE2	1:B:302:PHE:HB2	2.47	0.49
1:B:119:PRO:O	1:B:193:TYR:HB3	2.12	0.49
1:A:271:GLU:OE2	1:A:272:VAL:N	2.46	0.49
1:D:222:ALA:CB	1:E:220:TYR:CD2	2.96	0.49
1:C:23:LEU:HG	1:C:164:PHE:CE1	2.48	0.49
1:D:37:LYS:CG	1:D:108:ARG:HB2	2.43	0.49
1:E:23:LEU:HD22	1:E:38:VAL:HG21	1.94	0.49
1:A:264:PHE:CE2	1:A:302:PHE:HB2	2.48	0.49
1:A:119:PRO:O	1:A:193:TYR:HB3	2.12	0.49
1:C:202:LEU:HD12	1:D:259:PHE:CZ	2.48	0.49
1:C:155:PHE:CE1	1:D:112:PRO:HB3	2.48	0.48
1:C:305:ALA:O	1:C:309:LEU:HB2	2.13	0.48
1:E:264:PHE:CE2	1:E:302:PHE:HB2	2.48	0.48
1:B:216:TRP:CZ2	1:B:295:ARG:HB3	2.48	0.48
1:E:193:TYR:O	1:E:194:PHE:CB	2.60	0.48
1:D:243:THR:HG22	1:D:244:ASN:ND2	2.28	0.48
1:E:76:ARG:HH12	1:E:130:ILE:HD11	1.78	0.48
1:E:264:PHE:O	1:E:268:ALA:HB2	2.13	0.48
1:B:53:PHE:HE2	1:B:63:LYS:CB	2.25	0.48
1:C:53:PHE:CD1	1:C:95:PRO:HA	2.48	0.48
1:A:157:THR:HG21	1:B:34:GLU:HG3	1.94	0.48
1:A:72:ILE:HG22	1:A:73:PRO:HD2	1.95	0.48
1:B:271:GLU:OE2	1:B:272:VAL:N	2.46	0.48
1:C:200:ILE:O	1:C:204:MET:HB2	2.12	0.48
1:E:81:GLU:HG3	1:E:108:ARG:CG	2.44	0.48
1:B:193:TYR:O	1:B:194:PHE:CB	2.59	0.48
1:E:215:PHE:HB3	1:E:295:ARG:HG2	1.95	0.48
1:A:9:PRO:HD3	1:A:71:TRP:CE3	2.49	0.48
1:A:253:TYR:CA	1:A:313:PHE:HE2	2.22	0.48
1:C:65:TYR:CD1	1:C:70:ILE:HD11	2.48	0.48
1:D:65:TYR:CD1	1:D:70:ILE:HD11	2.48	0.48
1:C:7:PRO:O	1:C:50:ARG:NH2	2.45	0.48
1:E:274:VAL:C	1:E:276:HIS:H	2.15	0.48
1:A:123:GLN:HB2	1:A:189:ILE:HG13	1.94	0.48
1:B:68:GLU:CD	1:B:68:GLU:H	2.16	0.48
1:A:243:THR:HG22	1:A:244:ASN:ND2	2.29	0.48
1:A:23:LEU:HD22	1:A:38:VAL:HG21	1.94	0.48
1:A:52:ALA:HA	1:A:95:PRO:O	2.13	0.48
1:E:70:ILE:HD13	1:E:70:ILE:N	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:202:LEU:HD12	1:E:259:PHE:CZ	2.47	0.48
1:D:137:ARG:HD2	1:D:179:LEU:HG	1.94	0.48
1:E:68:GLU:H	1:E:68:GLU:CD	2.17	0.48
1:A:96:ASP:OD1	1:A:98:THR:HB	2.12	0.48
1:D:210:ILE:HG13	1:E:266:PHE:CD1	2.48	0.48
1:B:9:PRO:HD3	1:B:71:TRP:CE3	2.49	0.48
1:C:125:LEU:HB2	1:C:187:LEU:HB3	1.96	0.48
1:D:41:PHE:HE2	1:E:175:LEU:CD2	2.27	0.48
1:C:215:PHE:HB2	1:C:216:TRP:CE3	2.49	0.48
1:C:215:PHE:HB3	1:C:295:ARG:HG2	1.95	0.48
1:A:192:GLN:CG	1:B:249:PRO:HB3	2.44	0.48
1:C:81:GLU:HG3	1:C:108:ARG:CG	2.44	0.48
1:A:137:ARG:HD3	1:A:137:ARG:HA	1.57	0.48
1:D:271:GLU:OE2	1:D:272:VAL:N	2.46	0.48
1:E:70:ILE:HG22	1:E:71:TRP:N	2.29	0.47
1:D:158:GLY:HA2	1:D:192:GLN:OE1	2.14	0.47
1:A:25:GLU:HG3	1:B:79:ASN:HA	1.95	0.47
1:B:179:LEU:O	1:B:179:LEU:HD12	2.14	0.47
1:A:104:ARG:NH1	1:B:77:PHE:O	2.44	0.47
1:C:257:ILE:HG22	1:C:309:LEU:HD23	1.96	0.47
1:B:215:PHE:HB3	1:B:295:ARG:HG2	1.95	0.47
1:B:253:TYR:CA	1:B:313:PHE:HE2	2.22	0.47
1:E:53:PHE:CE2	1:E:63:LYS:HB3	2.45	0.47
1:A:232:ILE:HG22	1:A:233:ALA:N	2.30	0.47
1:E:86:ALA:HB2	1:E:105:PHE:HB3	1.96	0.47
1:C:147:LYS:CE	1:C:165:THR:HA	2.43	0.47
1:B:261:ILE:HD13	1:B:302:PHE:HE1	1.80	0.47
1:C:179:LEU:O	1:C:179:LEU:HD12	2.14	0.47
1:D:210:ILE:CG1	1:E:266:PHE:CD1	2.97	0.47
1:D:256:ALA:HB1	1:D:309:LEU:HD21	1.97	0.47
1:E:151:ASN:HB3	1:E:153:ASP:H	1.78	0.47
1:C:78:VAL:HB	1:C:128:TYR:HB2	1.97	0.47
1:C:23:LEU:HD22	1:C:38:VAL:HG21	1.97	0.47
1:B:253:TYR:HD1	1:B:313:PHE:CD2	2.32	0.47
1:D:179:LEU:O	1:D:179:LEU:HD12	2.14	0.47
1:C:137:ARG:HD2	1:C:179:LEU:HG	1.95	0.47
1:E:23:LEU:HG	1:E:164:PHE:CE1	2.49	0.47
1:B:233:ALA:O	1:B:237:PHE:HD1	1.97	0.47
1:D:78:VAL:HB	1:D:128:TYR:HB2	1.95	0.47
1:D:23:LEU:HD22	1:D:38:VAL:HG21	1.97	0.47
1:B:150:LYS:HG3	1:B:154:VAL:HG21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:ARG:HH22	1:A:176:GLU:HB2	1.80	0.47
1:B:151:ASN:HB3	1:B:153:ASP:H	1.79	0.47
1:E:137:ARG:HA	1:E:137:ARG:HD3	1.60	0.47
1:E:179:LEU:O	1:E:179:LEU:HD12	2.14	0.47
1:E:195:SER:O	1:E:199:ASN:HB2	2.15	0.47
1:E:62:VAL:HG11	1:E:92:SER:HB3	1.97	0.47
1:A:212:TRP:HB2	1:A:215:PHE:CE1	2.50	0.47
1:A:125:LEU:HB2	1:A:187:LEU:HB3	1.96	0.47
1:D:70:ILE:HG22	1:D:71:TRP:N	2.29	0.47
1:C:132:ARG:HH22	1:C:176:GLU:HB2	1.80	0.47
1:C:151:ASN:HB3	1:C:153:ASP:H	1.80	0.47
1:D:151:ASN:HB3	1:D:153:ASP:H	1.80	0.47
1:E:76:ARG:CZ	1:E:130:ILE:HD12	2.44	0.47
1:D:150:LYS:HG3	1:D:154:VAL:HG21	1.98	0.47
1:E:253:TYR:O	1:E:256:ALA:HB3	2.14	0.47
1:A:132:ARG:CA	1:A:180:GLU:HG2	2.43	0.47
1:E:37:LYS:CG	1:E:108:ARG:HB2	2.45	0.47
1:C:149:GLY:O	1:C:150:LYS:HB2	2.15	0.46
1:D:215:PHE:HB3	1:D:295:ARG:HG2	1.97	0.46
1:E:233:ALA:O	1:E:237:PHE:HD1	1.98	0.46
1:B:65:TYR:CD1	1:B:70:ILE:HD11	2.50	0.46
1:A:179:LEU:HD12	1:A:179:LEU:O	2.14	0.46
1:B:232:ILE:HG22	1:B:233:ALA:N	2.30	0.46
1:D:232:ILE:HG22	1:D:233:ALA:N	2.30	0.46
1:E:96:ASP:OD1	1:E:98:THR:HB	2.15	0.46
1:A:225:THR:CG2	1:B:224:VAL:HG23	2.46	0.46
1:A:27:TYR:CG	1:B:110:LEU:HD11	2.50	0.46
1:E:23:LEU:HB2	1:E:150:LYS:HA	1.96	0.46
1:A:256:ALA:HB1	1:A:309:LEU:HD21	1.97	0.46
1:A:196:TYR:HD1	1:A:196:TYR:N	2.13	0.46
1:A:221:GLU:HA	1:A:221:GLU:OE1	2.14	0.46
1:E:9:PRO:HD3	1:E:71:TRP:CE3	2.50	0.46
1:A:157:THR:HG22	1:B:34:GLU:OE1	2.15	0.46
1:A:15:LEU:HD12	1:A:16:THR:N	2.30	0.46
1:A:46:TRP:CH2	1:A:72:ILE:HG23	2.49	0.46
1:A:23:LEU:HB2	1:A:150:LYS:HA	1.97	0.46
1:D:270:ILE:HA	1:D:270:ILE:HD13	1.62	0.46
1:B:215:PHE:HB2	1:B:216:TRP:CE3	2.50	0.46
1:B:204:MET:O	1:B:207:ILE:HG12	2.16	0.46
1:E:151:ASN:ND2	1:E:152:ASP:H	2.13	0.46
1:A:19:THR:HG22	1:A:44:LEU:CD2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:LEU:HA	1:B:226:LEU:HD22	1.71	0.46
1:D:41:PHE:HE2	1:E:175:LEU:HD23	1.80	0.46
1:D:23:LEU:HG	1:D:164:PHE:CE1	2.50	0.46
1:B:23:LEU:HB2	1:B:150:LYS:HA	1.97	0.46
1:D:215:PHE:HB2	1:D:216:TRP:CE3	2.51	0.46
1:D:131:VAL:CG1	1:D:140:VAL:HG13	2.44	0.46
1:E:51:LEU:HD13	1:E:70:ILE:HD12	1.97	0.46
1:D:119:PRO:O	1:D:193:TYR:HB3	2.15	0.46
1:B:195:SER:O	1:B:199:ASN:HB2	2.16	0.46
1:A:224:VAL:C	1:A:226:LEU:N	2.69	0.46
1:C:72:ILE:HG22	1:C:73:PRO:HD2	1.97	0.46
1:C:151:ASN:ND2	1:C:152:ASP:H	2.14	0.46
1:E:123:GLN:HB2	1:E:189:ILE:HG13	1.96	0.46
1:D:54:ASP:HB2	1:D:57:ARG:CB	2.44	0.46
1:A:271:GLU:O	1:A:272:VAL:C	2.53	0.46
1:D:253:TYR:CA	1:D:313:PHE:HE2	2.20	0.46
1:A:215:PHE:HB2	1:A:216:TRP:CE3	2.51	0.46
1:D:53:PHE:CE2	1:D:63:LYS:HB3	2.47	0.46
1:A:196:TYR:CD1	1:A:196:TYR:N	2.84	0.46
1:D:200:ILE:CD1	1:D:240:LEU:HD23	2.46	0.46
1:E:224:VAL:C	1:E:226:LEU:H	2.19	0.45
1:C:29:LEU:HD23	1:C:30:ASP:N	2.31	0.45
1:D:196:TYR:N	1:D:196:TYR:HD1	2.14	0.45
1:E:119:PRO:O	1:E:193:TYR:HB3	2.16	0.45
1:B:264:PHE:O	1:B:268:ALA:HB2	2.16	0.45
1:A:257:ILE:HG22	1:A:309:LEU:HD23	1.97	0.45
1:B:54:ASP:HB2	1:B:57:ARG:CB	2.46	0.45
1:B:53:PHE:CE2	1:B:63:LYS:HB3	2.48	0.45
1:C:224:VAL:O	1:C:228:VAL:HB	2.15	0.45
1:A:65:TYR:CD1	1:A:70:ILE:HD11	2.50	0.45
1:B:86:ALA:HB2	1:B:105:PHE:HB3	1.98	0.45
1:D:79:ASN:OD1	1:D:109:VAL:HG12	2.16	0.45
1:D:76:ARG:HH12	1:D:130:ILE:HD11	1.82	0.45
1:C:216:TRP:CZ2	1:C:295:ARG:HB3	2.51	0.45
1:E:256:ALA:HB1	1:E:309:LEU:HD21	1.97	0.45
1:A:131:VAL:CG1	1:A:140:VAL:HG13	2.41	0.45
1:A:161:ILE:HA	1:A:189:ILE:HG22	1.99	0.45
1:C:96:ASP:OD1	1:C:98:THR:HB	2.17	0.45
1:D:224:VAL:O	1:D:228:VAL:HB	2.16	0.45
1:A:215:PHE:HB3	1:A:295:ARG:HG2	1.98	0.45
1:D:29:LEU:HD23	1:D:30:ASP:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:ARG:HD2	1:B:179:LEU:HG	1.98	0.45
1:A:225:THR:HG22	1:A:225:THR:O	2.17	0.45
1:D:76:ARG:CZ	1:D:130:ILE:HD12	2.44	0.45
1:C:76:ARG:HH12	1:C:130:ILE:HD11	1.82	0.45
1:B:53:PHE:O	1:B:54:ASP:C	2.55	0.45
1:C:37:LYS:CG	1:C:108:ARG:HB2	2.46	0.45
1:B:137:ARG:HD3	1:B:137:ARG:HA	1.58	0.45
1:C:253:TYR:HB2	1:C:313:PHE:HD2	1.82	0.45
1:E:215:PHE:HB2	1:E:216:TRP:CE3	2.52	0.45
1:E:257:ILE:HG22	1:E:309:LEU:HD23	1.98	0.45
1:B:270:ILE:HD13	1:B:270:ILE:HA	1.64	0.45
1:C:53:PHE:O	1:C:54:ASP:C	2.55	0.45
1:E:65:TYR:CD1	1:E:70:ILE:HD11	2.51	0.45
1:D:196:TYR:N	1:D:196:TYR:CD1	2.84	0.45
1:A:224:VAL:O	1:A:228:VAL:HB	2.16	0.45
1:E:78:VAL:HB	1:E:128:TYR:HB2	1.97	0.45
1:C:21:ILE:HA	1:C:41:PHE:O	2.17	0.45
1:A:47:LYS:HE2	1:A:47:LYS:HB3	1.75	0.45
1:B:271:GLU:O	1:B:272:VAL:C	2.53	0.45
1:C:226:LEU:HA	1:C:226:LEU:HD22	1.66	0.45
1:C:54:ASP:HB2	1:C:57:ARG:CB	2.47	0.45
1:A:255:GLY:O	1:A:258:ILE:HG22	2.17	0.45
1:D:195:SER:HB3	1:E:248:THR:O	2.17	0.45
1:A:213:THR:CG2	1:A:226:LEU:HD11	2.46	0.45
1:E:224:VAL:C	1:E:226:LEU:N	2.69	0.45
1:E:54:ASP:HB2	1:E:57:ARG:CB	2.47	0.45
1:D:51:LEU:HD13	1:D:70:ILE:HD12	1.99	0.45
1:E:276:HIS:C	1:E:278:LEU:N	2.71	0.45
1:C:28:SER:HB2	1:C:37:LYS:HD2	1.99	0.45
1:C:86:ALA:HB2	1:C:105:PHE:HB3	1.97	0.45
1:B:78:VAL:HB	1:B:128:TYR:HB2	1.97	0.44
1:A:270:ILE:HA	1:A:270:ILE:HD13	1.63	0.44
1:B:70:ILE:HG22	1:B:71:TRP:N	2.32	0.44
1:D:204:MET:O	1:D:207:ILE:HG12	2.17	0.44
1:E:119:PRO:HB3	1:E:196:TYR:HD2	1.82	0.44
1:A:76:ARG:CZ	1:A:130:ILE:HD12	2.45	0.44
1:D:37:LYS:HG3	1:D:108:ARG:HB2	1.99	0.44
1:A:253:TYR:HB2	1:A:313:PHE:HD2	1.81	0.44
1:A:62:VAL:HG11	1:A:92:SER:HB3	1.98	0.44
1:E:271:GLU:O	1:E:272:VAL:C	2.54	0.44
1:A:53:PHE:O	1:A:54:ASP:C	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:132:ARG:CA	1:D:180:GLU:HG2	2.47	0.44
1:A:276:HIS:C	1:A:278:LEU:N	2.71	0.44
1:B:86:ALA:HA	1:B:105:PHE:HA	1.98	0.44
1:E:271:GLU:OE2	1:E:272:VAL:N	2.50	0.44
1:B:76:ARG:CZ	1:B:130:ILE:HD12	2.45	0.44
1:D:95:PRO:C	1:D:97:GLY:H	2.20	0.44
1:A:282:SER:C	1:A:284:PRO:HD3	2.38	0.44
1:B:276:HIS:C	1:B:278:LEU:N	2.71	0.44
1:D:46:TRP:HH2	1:D:72:ILE:HG23	1.82	0.44
1:B:224:VAL:C	1:B:226:LEU:N	2.69	0.44
1:B:147:LYS:CE	1:B:165:THR:HA	2.47	0.44
1:D:212:TRP:HB2	1:D:215:PHE:CE1	2.52	0.44
1:D:125:LEU:HB2	1:D:187:LEU:HB3	1.99	0.44
1:A:79:ASN:OD1	1:A:109:VAL:HG12	2.18	0.44
1:D:64:THR:O	1:D:64:THR:HG22	2.17	0.44
1:D:226:LEU:HD23	1:E:224:VAL:HB	1.99	0.44
1:C:89:VAL:CG2	1:D:76:ARG:HD3	2.48	0.44
1:D:261:ILE:HD13	1:D:302:PHE:HE1	1.82	0.44
1:E:53:PHE:O	1:E:54:ASP:C	2.55	0.44
1:D:132:ARG:HH22	1:D:176:GLU:HB2	1.83	0.44
1:D:276:HIS:C	1:D:278:LEU:N	2.71	0.44
1:C:118:TYR:HB3	1:C:119:PRO:HD3	1.99	0.44
1:C:240:LEU:HD22	1:D:239:ILE:HG12	1.99	0.44
1:A:151:ASN:ND2	1:A:152:ASP:H	2.15	0.44
1:D:226:LEU:HD22	1:D:226:LEU:HA	1.67	0.44
1:C:155:PHE:HD1	1:D:110:LEU:HD22	1.83	0.44
1:B:256:ALA:HB1	1:B:309:LEU:HD21	1.99	0.44
1:A:202:LEU:HD12	1:B:259:PHE:CE1	2.53	0.44
1:A:42:LEU:HD23	1:A:103:GLU:OE1	2.17	0.44
1:D:48:ASP:O	1:D:50:ARG:N	2.51	0.44
1:C:105:PHE:HD1	1:C:105:PHE:H	1.64	0.44
1:B:224:VAL:C	1:B:226:LEU:H	2.21	0.44
1:D:149:GLY:O	1:D:150:LYS:CB	2.66	0.44
1:C:70:ILE:HG22	1:C:71:TRP:N	2.33	0.44
1:B:37:LYS:CG	1:B:108:ARG:HB2	2.48	0.44
1:C:161:ILE:HA	1:C:189:ILE:HG22	1.99	0.44
1:B:257:ILE:HG22	1:B:309:LEU:HD23	2.00	0.43
1:B:131:VAL:CG1	1:B:140:VAL:HG13	2.41	0.43
1:D:53:PHE:O	1:D:54:ASP:C	2.55	0.43
1:C:86:ALA:HA	1:C:105:PHE:HA	2.00	0.43
1:A:222:ALA:HB2	1:B:221:GLU:CA	2.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:TYR:CE1	1:D:81:GLU:OE1	2.72	0.43
1:E:291:THR:O	1:E:295:ARG:HG3	2.18	0.43
1:A:215:PHE:CE1	1:A:298:PHE:CD1	3.07	0.43
1:C:276:HIS:C	1:C:278:LEU:N	2.71	0.43
1:A:81:GLU:HG3	1:A:108:ARG:CG	2.45	0.43
1:A:118:TYR:HB3	1:A:119:PRO:HD3	1.99	0.43
1:A:29:LEU:HD23	1:A:30:ASP:N	2.33	0.43
1:B:196:TYR:HD1	1:B:196:TYR:N	2.16	0.43
1:B:19:THR:HA	1:B:43:SER:O	2.17	0.43
1:B:282:SER:C	1:B:284:PRO:HD3	2.39	0.43
1:E:46:TRP:CH2	1:E:72:ILE:HG23	2.53	0.43
1:D:79:ASN:OD1	1:D:109:VAL:CG1	2.66	0.43
1:A:170:PRO:HB3	1:A:183:LEU:CD2	2.48	0.43
1:B:96:ASP:OD1	1:B:98:THR:HB	2.17	0.43
1:B:47:LYS:HB3	1:B:47:LYS:HE2	1.73	0.43
1:B:249:PRO:HD2	1:B:250:TYR:CE1	2.53	0.43
1:E:72:ILE:HG22	1:E:73:PRO:HD2	2.00	0.43
1:E:196:TYR:N	1:E:196:TYR:HD1	2.17	0.43
1:D:86:ALA:HA	1:D:105:PHE:HA	2.00	0.43
1:D:86:ALA:HB2	1:D:105:PHE:HB3	2.00	0.43
1:A:86:ALA:HA	1:A:105:PHE:HA	2.00	0.43
1:A:226:LEU:CD2	1:B:228:VAL:HG21	2.47	0.43
1:D:155:PHE:CE1	1:E:112:PRO:CB	2.83	0.43
1:B:23:LEU:HA	1:B:40:ALA:HB2	2.00	0.43
1:C:264:PHE:O	1:C:268:ALA:HB2	2.18	0.43
1:D:77:PHE:HB2	1:D:84:ARG:HD2	2.00	0.43
1:B:28:SER:HB2	1:B:37:LYS:HD2	2.00	0.43
1:E:86:ALA:HA	1:E:105:PHE:HA	2.00	0.43
1:C:131:VAL:CG1	1:C:140:VAL:HG13	2.43	0.43
1:A:70:ILE:HG22	1:A:71:TRP:N	2.33	0.43
1:C:37:LYS:HG2	1:C:108:ARG:HB2	1.99	0.43
1:A:86:ALA:HB2	1:A:105:PHE:HB3	2.00	0.43
1:A:78:VAL:CG2	1:A:130:ILE:HG12	2.37	0.43
1:E:212:TRP:HB2	1:E:215:PHE:CE1	2.53	0.43
1:C:157:THR:HG22	1:D:34:GLU:OE1	2.19	0.43
1:A:194:PHE:HE2	1:B:250:TYR:O	2.01	0.43
1:D:271:GLU:O	1:D:272:VAL:C	2.56	0.43
1:D:233:ALA:O	1:D:237:PHE:HD1	2.02	0.43
1:A:139:ILE:HG12	1:A:172:ASN:HD21	1.84	0.43
1:D:286:ARG:O	1:D:289:SER:HB3	2.18	0.43
1:B:76:ARG:NH1	1:B:130:ILE:HD11	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:131:VAL:CG1	1:E:140:VAL:HG13	2.42	0.43
1:E:283:GLN:O	1:E:283:GLN:HG2	2.19	0.43
1:E:53:PHE:HD1	1:E:53:PHE:C	2.22	0.43
1:E:70:ILE:HG22	1:E:71:TRP:O	2.18	0.43
1:A:28:SER:HB2	1:A:37:LYS:HD2	2.01	0.43
1:E:28:SER:HB2	1:E:37:LYS:HD2	2.01	0.43
1:D:157:THR:CG2	1:E:34:GLU:OE1	2.66	0.43
1:A:76:ARG:HH12	1:A:130:ILE:HD11	1.83	0.42
1:D:28:SER:HB2	1:D:37:LYS:HD2	2.01	0.42
1:A:261:ILE:HD13	1:A:302:PHE:HE1	1.84	0.42
1:E:238:ASN:HA	1:E:258:ILE:HD13	2.01	0.42
1:C:238:ASN:HA	1:C:258:ILE:HD13	2.00	0.42
1:A:155:PHE:CZ	1:B:112:PRO:CB	2.87	0.42
1:C:291:THR:O	1:C:295:ARG:HG3	2.19	0.42
1:D:215:PHE:CE1	1:D:298:PHE:CD1	3.08	0.42
1:E:268:ALA:HA	1:E:298:PHE:HE1	1.85	0.42
1:E:95:PRO:C	1:E:97:GLY:H	2.23	0.42
1:E:282:SER:C	1:E:284:PRO:HD3	2.38	0.42
1:B:51:LEU:HD13	1:B:70:ILE:HD12	2.00	0.42
1:C:132:ARG:CA	1:C:180:GLU:HG2	2.45	0.42
1:B:29:LEU:HD23	1:B:30:ASP:N	2.34	0.42
1:E:25:GLU:HB2	1:E:39:ASN:HB3	2.01	0.42
1:C:224:VAL:C	1:C:226:LEU:N	2.71	0.42
1:D:224:VAL:C	1:D:226:LEU:N	2.73	0.42
1:B:23:LEU:HG	1:B:164:PHE:CE1	2.55	0.42
1:A:21:ILE:HA	1:A:41:PHE:O	2.19	0.42
1:A:146:GLU:HG3	1:B:176:GLU:CD	2.39	0.42
1:A:286:ARG:O	1:A:289:SER:HB3	2.19	0.42
1:E:224:VAL:O	1:E:228:VAL:HB	2.19	0.42
1:D:210:ILE:O	1:D:211:SER:C	2.58	0.42
1:E:150:LYS:HG2	1:E:154:VAL:HG21	2.01	0.42
1:A:146:GLU:HG3	1:B:176:GLU:CG	2.50	0.42
1:C:119:PRO:HB3	1:C:196:TYR:HD2	1.84	0.42
1:A:179:LEU:HD12	1:A:179:LEU:C	2.40	0.42
1:C:78:VAL:CG2	1:C:130:ILE:HG12	2.36	0.42
1:D:291:THR:O	1:D:295:ARG:HG3	2.19	0.42
1:B:291:THR:O	1:B:295:ARG:HG3	2.20	0.42
1:D:54:ASP:CB	1:D:57:ARG:HG3	2.44	0.42
1:B:42:LEU:HD23	1:B:103:GLU:OE1	2.19	0.42
1:C:179:LEU:C	1:C:179:LEU:HD12	2.40	0.42
1:B:170:PRO:HB3	1:B:183:LEU:CD2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:LEU:O	1:A:15:LEU:HG	2.20	0.42
1:B:196:TYR:N	1:B:196:TYR:CD1	2.87	0.42
1:D:105:PHE:H	1:D:105:PHE:HD1	1.66	0.42
1:C:79:ASN:OD1	1:C:109:VAL:HG12	2.19	0.42
1:B:213:THR:CG2	1:B:226:LEU:HD11	2.48	0.42
1:C:261:ILE:HD13	1:C:302:PHE:HE1	1.84	0.42
1:E:215:PHE:CE1	1:E:298:PHE:CD1	3.07	0.42
1:A:291:THR:O	1:A:295:ARG:HG3	2.20	0.42
1:E:47:LYS:HB3	1:E:47:LYS:HE2	1.71	0.42
1:B:13:GLU:OE1	1:B:14:PRO:HD3	2.19	0.42
1:B:179:LEU:HD12	1:B:179:LEU:C	2.40	0.42
1:C:62:VAL:HG13	1:C:93:VAL:O	2.20	0.42
1:E:76:ARG:NH1	1:E:130:ILE:HD11	2.34	0.42
1:E:261:ILE:HD13	1:E:302:PHE:HE1	1.84	0.42
1:B:253:TYR:HB2	1:B:313:PHE:HD2	1.85	0.42
1:D:95:PRO:O	1:D:97:GLY:N	2.53	0.42
1:C:202:LEU:HD22	1:C:202:LEU:HA	1.86	0.42
1:A:203:PRO:HB3	1:B:262:TYR:CZ	2.55	0.42
1:D:62:VAL:HG11	1:D:92:SER:HB3	2.01	0.42
1:B:286:ARG:O	1:B:289:SER:HB3	2.20	0.42
1:A:53:PHE:HD1	1:A:53:PHE:C	2.23	0.42
1:B:62:VAL:HG11	1:B:92:SER:HB3	2.02	0.42
1:B:225:THR:HG21	1:C:224:VAL:HG23	2.02	0.41
1:E:270:ILE:HA	1:E:270:ILE:HD13	1.60	0.41
1:C:9:PRO:HD3	1:C:71:TRP:CE3	2.54	0.41
1:B:155:PHE:HB3	1:B:156:LEU:H	1.68	0.41
1:E:196:TYR:CD1	1:E:196:TYR:N	2.87	0.41
1:A:105:PHE:HD1	1:A:105:PHE:H	1.67	0.41
1:D:312:LEU:HA	1:D:312:LEU:HD12	1.86	0.41
1:E:226:LEU:HD22	1:E:226:LEU:HA	1.67	0.41
1:C:155:PHE:CD1	1:D:110:LEU:CD2	3.02	0.41
1:B:53:PHE:C	1:B:53:PHE:HD1	2.23	0.41
1:D:278:LEU:HD23	1:D:287:ALA:HA	2.02	0.41
1:B:132:ARG:HH22	1:B:176:GLU:HB2	1.85	0.41
1:E:179:LEU:HD12	1:E:179:LEU:C	2.40	0.41
1:D:156:LEU:HA	1:D:156:LEU:HD12	1.87	0.41
1:B:23:LEU:HD22	1:B:38:VAL:CG2	2.49	0.41
1:E:164:PHE:HD2	1:E:186:GLN:O	2.02	0.41
1:C:278:LEU:HD23	1:C:287:ALA:HA	2.02	0.41
1:D:42:LEU:HD23	1:D:103:GLU:OE1	2.20	0.41
1:C:196:TYR:O	1:C:200:ILE:HB	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:TYR:HB3	1:B:119:PRO:HD3	2.01	0.41
1:D:23:LEU:HD22	1:D:38:VAL:CG2	2.51	0.41
1:E:21:ILE:HA	1:E:41:PHE:O	2.20	0.41
1:E:253:TYR:CA	1:E:313:PHE:HE2	2.22	0.41
1:C:70:ILE:N	1:C:70:ILE:HD13	2.35	0.41
1:B:37:LYS:HG3	1:B:108:ARG:HB2	2.02	0.41
1:A:240:LEU:HD22	1:B:239:ILE:HG12	2.02	0.41
1:D:72:ILE:HG22	1:D:73:PRO:HD2	2.02	0.41
1:B:151:ASN:ND2	1:B:152:ASP:H	2.16	0.41
1:C:19:THR:HA	1:C:43:SER:O	2.20	0.41
1:A:224:VAL:C	1:A:226:LEU:H	2.23	0.41
1:A:210:ILE:O	1:A:211:SER:C	2.59	0.41
1:A:77:PHE:CG	1:A:84:ARG:HD2	2.54	0.41
1:D:53:PHE:C	1:D:53:PHE:HD1	2.22	0.41
1:D:48:ASP:C	1:D:50:ARG:N	2.74	0.41
1:C:170:PRO:HB3	1:C:183:LEU:CD2	2.50	0.41
1:E:128:TYR:O	1:E:183:LEU:O	2.39	0.41
1:A:54:ASP:HB2	1:A:57:ARG:CB	2.50	0.41
1:D:282:SER:C	1:D:284:PRO:HD3	2.40	0.41
1:A:278:LEU:HD23	1:A:287:ALA:HA	2.02	0.41
1:B:46:TRP:CH2	1:B:72:ILE:HG23	2.54	0.41
1:A:269:VAL:HA	1:A:272:VAL:HG22	2.02	0.41
1:D:179:LEU:C	1:D:179:LEU:HD12	2.40	0.41
1:C:224:VAL:C	1:C:226:LEU:H	2.23	0.41
1:A:23:LEU:HD22	1:A:38:VAL:CG2	2.51	0.41
1:C:212:TRP:HB2	1:C:215:PHE:CE1	2.55	0.41
1:E:42:LEU:HD23	1:E:103:GLU:OE1	2.21	0.41
1:A:158:GLY:HA2	1:A:192:GLN:OE1	2.21	0.41
1:C:62:VAL:HG11	1:C:92:SER:HB3	2.03	0.41
1:C:286:ARG:O	1:C:289:SER:HB3	2.21	0.41
1:A:149:GLY:O	1:A:150:LYS:CB	2.68	0.41
1:D:9:PRO:HD3	1:D:71:TRP:CE3	2.55	0.41
1:E:286:ARG:O	1:E:289:SER:HB3	2.21	0.41
1:A:76:ARG:NH1	1:A:130:ILE:HD11	2.36	0.41
1:A:23:LEU:HA	1:A:40:ALA:HB2	2.03	0.41
1:E:23:LEU:HD22	1:E:38:VAL:CG2	2.51	0.41
1:C:270:ILE:HA	1:C:270:ILE:HD13	1.66	0.41
1:C:215:PHE:CE1	1:C:298:PHE:CD1	3.09	0.41
1:B:215:PHE:CE1	1:B:298:PHE:CD1	3.08	0.41
1:B:70:ILE:HG22	1:B:71:TRP:O	2.21	0.41
1:B:132:ARG:CA	1:B:180:GLU:HG2	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:249:PRO:HD2	1:E:250:TYR:CE1	2.56	0.41
1:B:196:TYR:O	1:B:201:ILE:HG12	2.19	0.41
1:D:269:VAL:HA	1:D:272:VAL:HG22	2.02	0.41
1:A:225:THR:HG22	1:B:224:VAL:HG23	2.03	0.41
1:D:23:LEU:HA	1:D:40:ALA:HB2	2.02	0.41
1:C:282:SER:C	1:C:284:PRO:HD3	2.41	0.41
1:A:119:PRO:HB3	1:A:196:TYR:HD2	1.86	0.41
1:A:195:SER:HB3	1:B:248:THR:O	2.20	0.41
1:C:137:ARG:HA	1:C:137:ARG:HD3	1.55	0.41
1:C:23:LEU:HD22	1:C:38:VAL:CG2	2.51	0.40
1:A:140:VAL:HG22	1:A:181:SER:CB	2.51	0.40
1:D:94:SER:OG	1:D:95:PRO:CD	2.67	0.40
1:C:95:PRO:C	1:C:97:GLY:H	2.25	0.40
1:C:197:ILE:CB	1:C:198:PRO:HD3	2.49	0.40
1:B:19:THR:HG22	1:B:44:LEU:CD2	2.51	0.40
1:B:210:ILE:HG13	1:C:266:PHE:HE1	1.85	0.40
1:D:296:ILE:HA	1:D:296:ILE:HD13	1.93	0.40
1:B:149:GLY:O	1:B:150:LYS:CB	2.70	0.40
1:D:264:PHE:O	1:D:268:ALA:HB2	2.22	0.40
1:D:47:LYS:HE2	1:D:47:LYS:HB3	1.70	0.40
1:E:278:LEU:HD23	1:E:287:ALA:HA	2.02	0.40
1:E:132:ARG:CA	1:E:180:GLU:HG2	2.46	0.40
1:D:15:LEU:HD12	1:D:16:THR:N	2.36	0.40
1:B:212:TRP:HB2	1:B:215:PHE:CE1	2.56	0.40
1:A:140:VAL:HG22	1:A:181:SER:HB3	2.03	0.40
1:C:118:TYR:CZ	1:C:196:TYR:HE2	2.40	0.40
1:A:118:TYR:CZ	1:A:196:TYR:HE2	2.40	0.40
1:A:233:ALA:O	1:A:237:PHE:HD1	2.04	0.40
1:D:224:VAL:C	1:D:226:LEU:H	2.24	0.40
1:A:155:PHE:HE1	1:B:112:PRO:CA	2.34	0.40
1:E:269:VAL:HA	1:E:272:VAL:HG22	2.03	0.40
1:D:76:ARG:NH1	1:D:130:ILE:HD11	2.37	0.40
1:C:253:TYR:CA	1:C:313:PHE:HE2	2.23	0.40
1:A:140:VAL:HG22	1:A:181:SER:OG	2.21	0.40
1:A:70:ILE:HG22	1:A:71:TRP:O	2.21	0.40
1:C:47:LYS:HB3	1:C:47:LYS:HE2	1.72	0.40
1:E:210:ILE:O	1:E:211:SER:C	2.60	0.40
1:A:217:SER:OG	1:B:220:TYR:HE2	1.96	0.40
1:E:15:LEU:HG	1:E:15:LEU:O	2.16	0.40
1:C:210:ILE:HD12	1:D:231:LEU:CD2	2.51	0.40
1:E:105:PHE:HD1	1:E:105:PHE:H	1.67	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:PRO:HB3	1:C:183:LEU:HD23	2.03	0.40
1:A:296:ILE:HD13	1:A:296:ILE:HA	1.95	0.40
1:D:222:ALA:HB3	1:E:220:TYR:CD2	2.56	0.40
1:B:150:LYS:HG2	1:B:154:VAL:HG21	2.03	0.40
1:B:70:ILE:N	1:B:70:ILE:HD13	2.35	0.40
1:A:37:LYS:HG3	1:A:108:ARG:HB2	2.02	0.40
1:C:151:ASN:HD22	1:C:152:ASP:N	2.18	0.40
1:B:62:VAL:HG13	1:B:93:VAL:O	2.22	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%)	245 (80%)	56 (18%)	7 (2%)	8	48
1	B	308/317 (97%)	250 (81%)	51 (17%)	7 (2%)	8	48
1	C	308/317 (97%)	249 (81%)	52 (17%)	7 (2%)	8	48
1	D	308/317 (97%)	253 (82%)	47 (15%)	8 (3%)	7	45
1	E	308/317 (97%)	250 (81%)	52 (17%)	6 (2%)	10	51
All	All	1540/1585 (97%)	1247 (81%)	258 (17%)	35 (2%)	8	48

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	118	TYR
1	A	150	LYS
1	A	194	PHE
1	B	118	TYR
1	B	150	LYS
1	B	194	PHE

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Mol	Chain	Res	Type
1	C	118	TYR
1	C	150	LYS
1	C	194	PHE
1	D	118	TYR
1	D	148	VAL
1	D	150	LYS
1	D	194	PHE
1	E	118	TYR
1	E	148	VAL
1	E	150	LYS
1	E	194	PHE
1	A	148	VAL
1	A	277	TYR
1	B	148	VAL
1	B	277	TYR
1	C	148	VAL
1	C	277	TYR
1	D	277	TYR
1	E	277	TYR
1	A	275	GLN
1	B	275	GLN
1	C	275	GLN
1	D	96	ASP
1	D	275	GLN
1	E	275	GLN
1	A	49	ARG
1	B	155	PHE
1	C	287	ALA
1	D	287	ALA

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	278/284 (98%)	230 (83%)	48 (17%)	2 14
1	B	278/284 (98%)	228 (82%)	50 (18%)	2 12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	278/284 (98%)	230 (83%)	48 (17%)	2 14
1	D	278/284 (98%)	231 (83%)	47 (17%)	2 15
1	E	278/284 (98%)	228 (82%)	50 (18%)	2 12
All	All	1390/1420 (98%)	1147 (82%)	243 (18%)	2 14

All (243) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	THR
1	A	26	CYS
1	A	32	LYS
1	A	41	PHE
1	A	47	LYS
1	A	53	PHE
1	A	57	ARG
1	A	58	SER
1	A	64	THR
1	A	68	GLU
1	A	72	ILE
1	A	84	ARG
1	A	89	VAL
1	A	98	THR
1	A	100	GLN
1	A	108	ARG
1	A	113	LEU
1	A	116	ARG
1	A	122	SER
1	A	124	THR
1	A	140	VAL
1	A	141	LEU
1	A	151	ASN
1	A	154	VAL
1	A	155	PHE
1	A	177	ASP
1	A	178	ARG
1	A	179	LEU
1	A	190	SER
1	A	202	LEU
1	A	211	SER
1	A	212	TRP
1	A	213	THR

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Mol	Chain	Res	Type
1	A	221	GLU
1	A	226	LEU
1	A	243	THR
1	A	245	LEU
1	A	252	THR
1	A	254	THR
1	A	257	ILE
1	A	263	LEU
1	A	269	VAL
1	A	270	ILE
1	A	274	VAL
1	A	286	ARG
1	A	292	ARG
1	A	303	LEU
1	A	314	PHE
1	B	16	THR
1	B	26	CYS
1	B	32	LYS
1	B	41	PHE
1	B	47	LYS
1	B	51	LEU
1	B	53	PHE
1	B	57	ARG
1	B	58	SER
1	B	64	THR
1	B	68	GLU
1	B	72	ILE
1	B	84	ARG
1	B	89	VAL
1	B	98	THR
1	B	100	GLN
1	B	108	ARG
1	B	116	ARG
1	B	122	SER
1	B	124	THR
1	B	130	ILE
1	B	140	VAL
1	B	141	LEU
1	B	151	ASN
1	B	154	VAL
1	B	155	PHE
1	B	162	GLU

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Mol	Chain	Res	Type
1	B	177	ASP
1	B	178	ARG
1	B	179	LEU
1	B	190	SER
1	B	202	LEU
1	B	211	SER
1	B	212	TRP
1	B	213	THR
1	B	221	GLU
1	B	226	LEU
1	B	243	THR
1	B	245	LEU
1	B	252	THR
1	B	254	THR
1	B	257	ILE
1	B	263	LEU
1	B	269	VAL
1	B	270	ILE
1	B	274	VAL
1	B	286	ARG
1	B	292	ARG
1	B	303	LEU
1	B	314	PHE
1	C	16	THR
1	C	26	CYS
1	C	32	LYS
1	C	41	PHE
1	C	47	LYS
1	C	51	LEU
1	C	53	PHE
1	C	57	ARG
1	C	58	SER
1	C	64	THR
1	C	68	GLU
1	C	72	ILE
1	C	84	ARG
1	C	89	VAL
1	C	98	THR
1	C	100	GLN
1	C	108	ARG
1	C	113	LEU
1	C	116	ARG

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Mol	Chain	Res	Type
1	C	122	SER
1	C	124	THR
1	C	140	VAL
1	C	141	LEU
1	C	151	ASN
1	C	154	VAL
1	C	155	PHE
1	C	178	ARG
1	C	179	LEU
1	C	190	SER
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	243	THR
1	C	245	LEU
1	C	252	THR
1	C	254	THR
1	C	257	ILE
1	C	263	LEU
1	C	269	VAL
1	C	270	ILE
1	C	274	VAL
1	C	286	ARG
1	C	292	ARG
1	C	303	LEU
1	C	314	PHE
1	D	16	THR
1	D	26	CYS
1	D	32	LYS
1	D	41	PHE
1	D	47	LYS
1	D	51	LEU
1	D	53	PHE
1	D	57	ARG
1	D	58	SER
1	D	64	THR
1	D	68	GLU
1	D	72	ILE
1	D	84	ARG

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Mol	Chain	Res	Type
1	D	89	VAL
1	D	98	THR
1	D	100	GLN
1	D	108	ARG
1	D	116	ARG
1	D	122	SER
1	D	124	THR
1	D	130	ILE
1	D	140	VAL
1	D	141	LEU
1	D	151	ASN
1	D	154	VAL
1	D	155	PHE
1	D	177	ASP
1	D	178	ARG
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	243	THR
1	D	252	THR
1	D	254	THR
1	D	257	ILE
1	D	263	LEU
1	D	269	VAL
1	D	270	ILE
1	D	274	VAL
1	D	286	ARG
1	D	292	ARG
1	D	303	LEU
1	D	314	PHE
1	E	16	THR
1	E	26	CYS
1	E	32	LYS
1	E	47	LYS
1	E	51	LEU
1	E	53	PHE
1	E	57	ARG
1	E	58	SER

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Mol	Chain	Res	Type
1	E	64	THR
1	E	68	GLU
1	E	72	ILE
1	E	84	ARG
1	E	89	VAL
1	E	98	THR
1	E	100	GLN
1	E	108	ARG
1	E	116	ARG
1	E	122	SER
1	E	124	THR
1	E	130	ILE
1	E	140	VAL
1	E	141	LEU
1	E	151	ASN
1	E	154	VAL
1	E	155	PHE
1	E	162	GLU
1	E	177	ASP
1	E	178	ARG
1	E	179	LEU
1	E	190	SER
1	E	202	LEU
1	E	204	MET
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	245	LEU
1	E	252	THR
1	E	254	THR
1	E	257	ILE
1	E	263	LEU
1	E	269	VAL
1	E	270	ILE
1	E	274	VAL
1	E	286	ARG
1	E	292	ARG
1	E	303	LEU
1	E	314	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	GLN
1	A	151	ASN
1	A	244	ASN
1	B	100	GLN
1	B	151	ASN
1	B	244	ASN
1	C	100	GLN
1	C	151	ASN
1	C	244	ASN
1	D	100	GLN
1	D	151	ASN
1	D	244	ASN
1	E	100	GLN
1	E	151	ASN
1	E	244	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	310/317 (97%)	-0.25	4 (1%)	79	70	64, 106, 164, 215	0
1	B	310/317 (97%)	-0.28	2 (0%)	90	85	69, 106, 164, 215	0
1	C	310/317 (97%)	-0.28	3 (0%)	84	76	66, 106, 163, 215	0
1	D	310/317 (97%)	-0.29	1 (0%)	94	91	66, 105, 164, 215	0
1	E	310/317 (97%)	-0.30	3 (0%)	84	76	70, 106, 164, 215	0
All	All	1550/1585 (97%)	-0.28	13 (0%)	87	80	64, 106, 164, 215	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	59	GLY	4.7
1	A	316	PHE	3.8
1	A	58	SER	3.2
1	E	59	GLY	3.1
1	D	316	PHE	3.0
1	A	60	VAL	3.0
1	B	57	ARG	2.8
1	E	316	PHE	2.6
1	E	63	LYS	2.4
1	C	59	GLY	2.3
1	B	282	SER	2.1
1	C	316	PHE	2.1
1	C	58	SER	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 (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	ARS	C	1317	1/1	0.88	0.49	-	144,144,144,144	0

6.5 Other polymers (i)

There are no such residues in this entry.