



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:37 AM GMT

PDB ID : 2XQ4
Title : PENTAMERIC LIGAND GATED ION CHANNEL GLIC IN COMPLEX
WITH TETRAMETHYLARSONIUM (TMAS)
Authors : Hilf, R.J.C.; Bertozzi, C.; Zimmermann, I.; Reiter, A.; Trauner, D.; Dutzler,
R.
Deposited on : 2010-09-01
Resolution : 3.60 Å(reported)

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

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

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

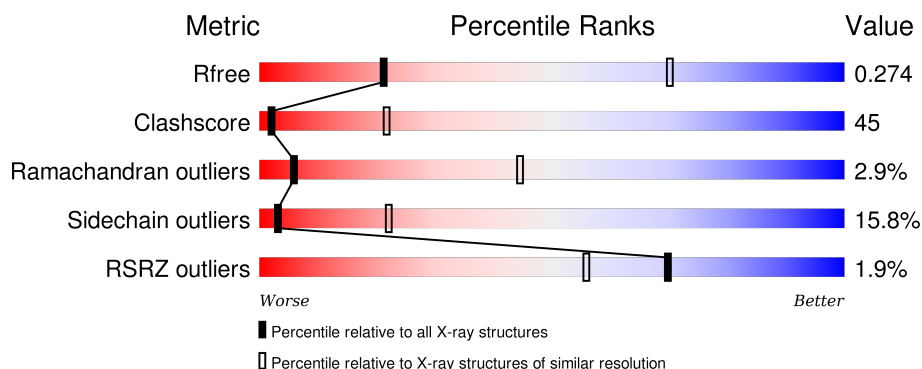
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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	1408 (3.80-3.40)
Clashscore	102246	1010 (3.74-3.46)
Ramachandran outliers	100387	1007 (3.76-3.44)
Sidechain outliers	100360	1007 (3.76-3.44)
RSRZ outliers	91569	1003 (3.78-3.42)

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

Mol	Chain	Length	Quality of chain
1	A	317	<div> <div>2%</div> <div>34%</div> <div>52%</div> <div>11%</div> <div>..</div> </div>
1	B	317	<div> <div>3%</div> <div>32%</div> <div>54%</div> <div>11%</div> <div>..</div> </div>
1	C	317	<div> <div>2%</div> <div>35%</div> <div>51%</div> <div>11%</div> <div>..</div> </div>
1	D	317	<div> <div>33%</div> <div>53%</div> <div>12%</div> <div>.</div> </div>
1	E	317	<div> <div>3%</div> <div>36%</div> <div>51%</div> <div>10%</div> <div>..</div> </div>

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			

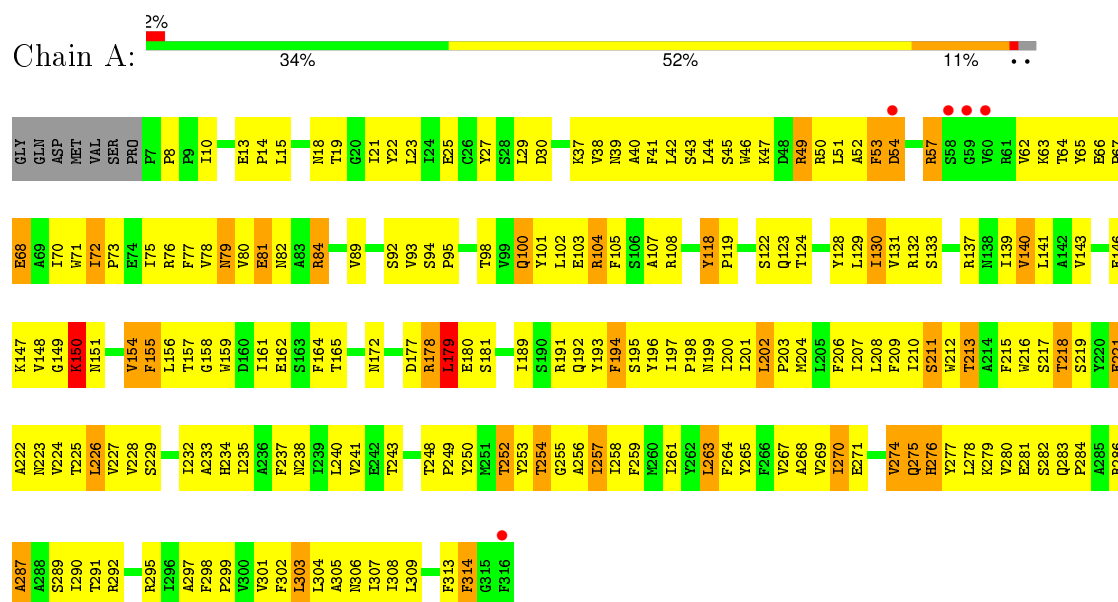
- Molecule 2 is ARSENIC (three-letter code: ARS) (formula: As).

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

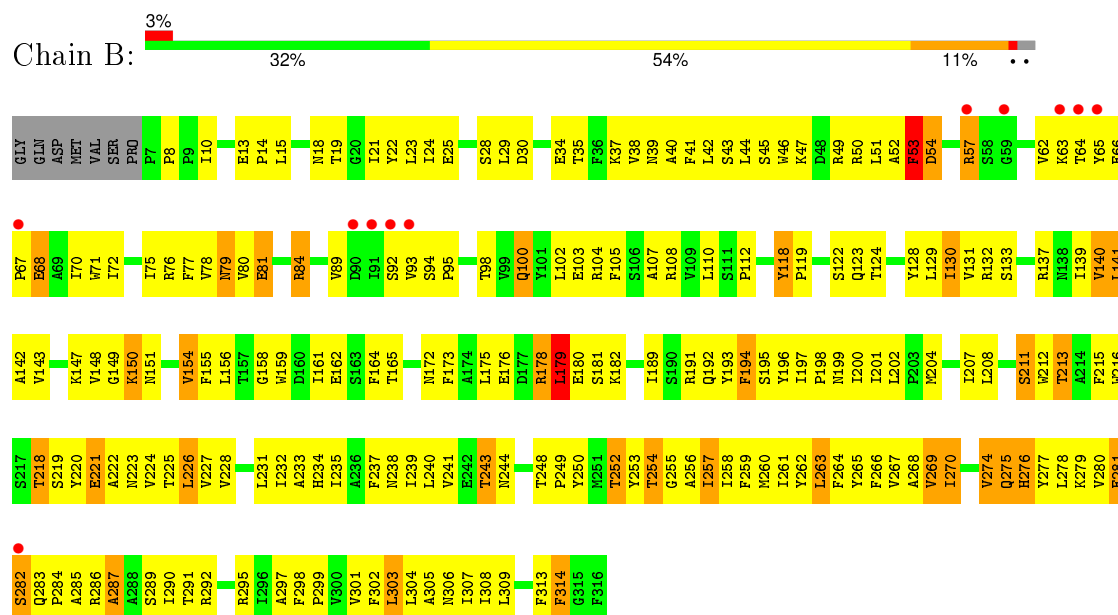
3 Residue-property plots

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

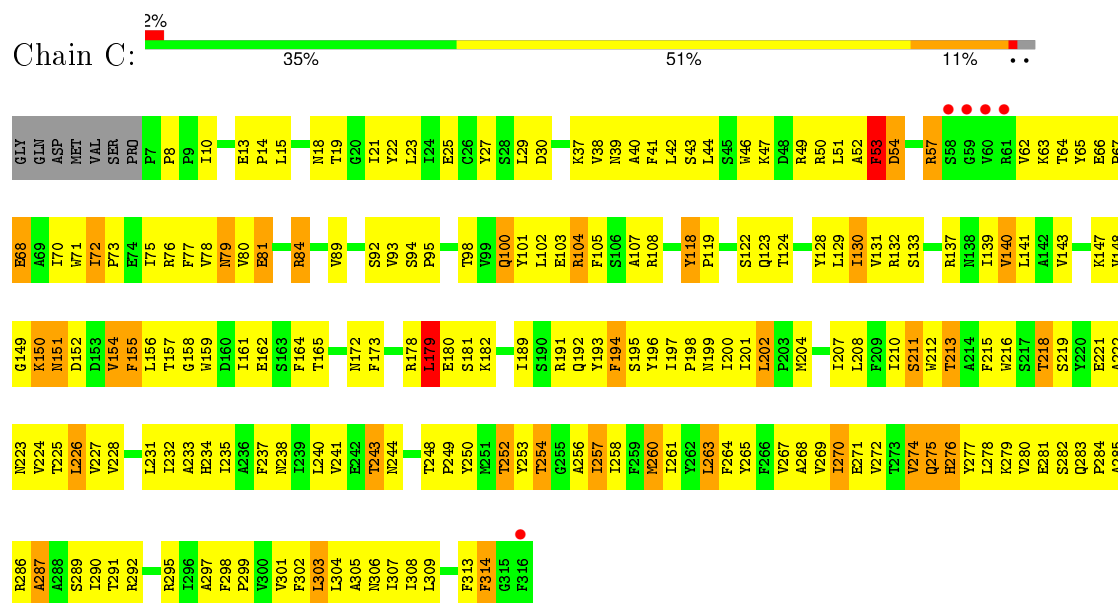
• Molecule 1: GLR4197 PROTEIN



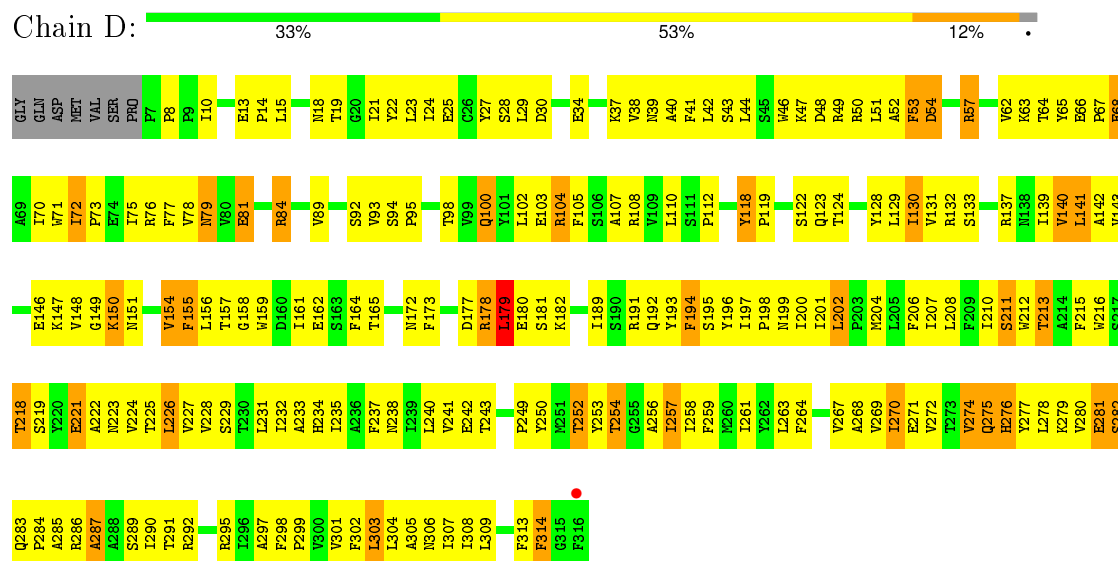
• Molecule 1: GLR4197 PROTEIN



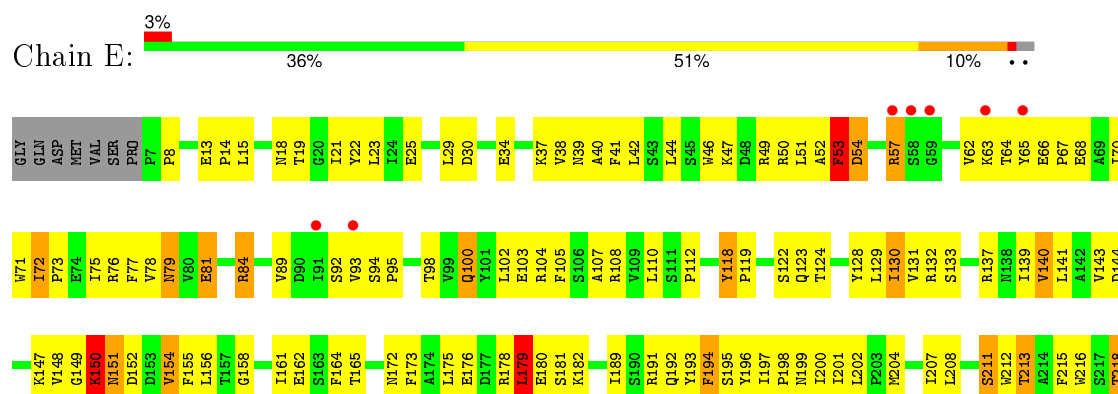
- Molecule 1: GLR4197 PROTEIN



- Molecule 1: GLR4197 PROTEIN



- Molecule 1: GLR4197 PROTEIN



R286	R287	R288	R289	T290	T291	R292	R295	T296	A297	F298	F299	V300	V301	F302	L303	L304	A305	N306	I307	I308	L309	F313	F314	G315	F316	S219	E220	E221	A222	N223	T224	T225	L226	L227	V228	I232	A233	H234	I235	A236	F237	N238	I239	L240	V241	E242	T243	N244	F249	Y250	T251	T252	Y253	T254	G255	A256	I257	L258	F259	M260	I261	Y262	L263	F264	Y265	F266	V267	A268	V269	I270	V274	Q275	H276	Y277	L278	V279	V280	E281	S282	Q283	P284	A285
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4 Data and refinement statistics

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 – 3.60 40.20 – 3.60	Depositor EDS
% Data completeness (in resolution range)	98.8 (40.20-3.60) 98.9 (40.20-3.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.05 (at 3.57Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.259 , 0.272 0.255 , 0.274	Depositor DCC
R_{free} test set	2143 reflections (5.05%)	DCC
Wilson B-factor (Å ²)	97.7	Xtriage
Anisotropy	0.376	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 88.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	1 of 43106 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)	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

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	0.68	3/3535 (0.1%)
1	B	0.49	0/2589	0.68	4/3535 (0.1%)
1	C	0.50	0/2589	0.69	3/3535 (0.1%)
1	D	0.51	0/2589	0.69	3/3535 (0.1%)
1	E	0.51	0/2589	0.69	4/3535 (0.1%)
All	All	0.50	0/12945	0.68	17/17675 (0.1%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	179	LEU	CA-CB-CG	5.56	128.08	115.30
1	B	281	GLU	N-CA-C	-5.55	96.02	111.00
1	C	179	LEU	CA-CB-CG	5.53	128.01	115.30
1	E	179	LEU	CA-CB-CG	5.52	128.00	115.30
1	D	276	HIS	N-CA-CB	-5.45	100.80	110.60
1	C	276	HIS	N-CA-CB	-5.38	100.91	110.60
1	D	281	GLU	N-CA-C	-5.38	96.47	111.00
1	A	276	HIS	N-CA-CB	-5.37	100.94	110.60
1	E	53	PHE	N-CA-C	5.34	125.42	111.00
1	E	150	LYS	N-CA-C	-5.26	96.80	111.00
1	A	150	LYS	N-CA-C	-5.25	96.83	111.00
1	B	53	PHE	N-CA-C	5.25	125.17	111.00
1	D	179	LEU	CA-CB-CG	5.23	127.33	115.30
1	B	276	HIS	N-CA-CB	-5.22	101.20	110.60
1	E	281	GLU	N-CA-C	-5.15	97.10	111.00
1	A	179	LEU	CA-CB-CG	5.15	127.14	115.30
1	C	53	PHE	N-CA-C	5.01	124.53	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2521	0	2537	278	0
1	B	2521	0	2537	274	0
1	C	2521	0	2537	232	0
1	D	2521	0	2537	272	0
1	E	2521	0	2537	241	0
2	C	1	0	0	0	0
All	All	12606	0	12685	1150	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 45.

All (1150) 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:155:PHE:CE1	1:B:112:PRO:HB3	1.77	1.18
1:A:27:TYR:HB3	1:B:110:LEU:HD11	1.22	1.15
1:D:155:PHE:CE1	1:E:112:PRO:HB3	1.84	1.11
1:A:222:ALA:HB2	1:B:221:GLU:HA	1.37	1.06
1:A:240:LEU:HD13	1:B:239:ILE:HG12	1.28	1.05
1:C:149:GLY:O	1:C:164:PHE:HD1	1.38	1.04
1:A:226:LEU:HD23	1:B:224:VAL:HB	1.33	1.04
1:A:149:GLY:O	1:A:164:PHE:HD1	1.41	1.02
1:E:149:GLY:O	1:E:164:PHE:HD1	1.42	1.01
1:D:149:GLY:O	1:D:164:PHE:HD1	1.41	1.01
1:B:149:GLY:O	1:B:164:PHE:HD1	1.42	0.99
1:A:226:LEU:CD2	1:B:224:VAL:HB	1.95	0.95
1:D:253:TYR:HA	1:D:313:PHE:HE2	1.33	0.94
1:D:253:TYR:HA	1:D:313:PHE:CE2	2.04	0.92
1:A:253:TYR:HA	1:A:313:PHE:HE2	1.34	0.92
1:B:76:ARG:HH22	1:B:130:ILE:HD12	1.34	0.92
1:C:253:TYR:HA	1:C:313:PHE:HE2	1.35	0.91
1:D:253:TYR:HD1	1:D:313:PHE:HD2	1.19	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:GLU:HB3	1:B:221:GLU:HG2	1.52	0.90
1:E:78:VAL:HG22	1:E:130:ILE:HG12	1.53	0.90
1:D:210:ILE:HG23	1:E:269:VAL:HG11	1.53	0.90
1:E:253:TYR:HA	1:E:313:PHE:CE2	2.07	0.90
1:D:225:THR:CG2	1:E:224:VAL:HG23	2.02	0.89
1:A:27:TYR:CB	1:B:110:LEU:HD11	2.03	0.89
1:D:225:THR:HG21	1:E:224:VAL:HG23	1.54	0.89
1:A:76:ARG:NH2	1:A:130:ILE:HD12	1.87	0.89
1:B:253:TYR:HA	1:B:313:PHE:HE2	1.37	0.89
1:A:155:PHE:CZ	1:B:112:PRO:HB3	2.06	0.89
1:B:76:ARG:NH2	1:B:130:ILE:HD12	1.87	0.88
1:A:253:TYR:HA	1:A:313:PHE:CE2	2.07	0.88
1:C:76:ARG:NH2	1:C:130:ILE:HD12	1.89	0.88
1:C:253:TYR:HA	1:C:313:PHE:CE2	2.08	0.87
1:E:253:TYR:HA	1:E:313:PHE:HE2	1.36	0.87
1:A:104:ARG:NH2	1:B:78:VAL:HA	1.89	0.87
1:B:147:LYS:C	1:B:149:GLY:H	1.76	0.87
1:C:147:LYS:C	1:C:149:GLY:H	1.77	0.87
1:E:147:LYS:C	1:E:149:GLY:H	1.75	0.86
1:B:253:TYR:HA	1:B:313:PHE:CE2	2.09	0.86
1:D:240:LEU:HD13	1:E:239:ILE:HG12	1.56	0.86
1:C:22:TYR:HA	1:C:149:GLY:HA3	1.58	0.86
1:A:253:TYR:HD1	1:A:313:PHE:HD2	1.23	0.86
1:D:76:ARG:NH2	1:D:130:ILE:HD12	1.91	0.86
1:D:155:PHE:HE1	1:E:112:PRO:HB3	1.38	0.85
1:C:76:ARG:HH22	1:C:130:ILE:HD12	1.39	0.85
1:B:78:VAL:HG22	1:B:130:ILE:HG12	1.56	0.85
1:E:76:ARG:HH22	1:E:130:ILE:HD12	1.42	0.85
1:A:76:ARG:HH22	1:A:130:ILE:HD12	1.40	0.85
1:C:22:TYR:HA	1:C:149:GLY:CA	2.07	0.85
1:D:76:ARG:HH22	1:D:130:ILE:HD12	1.40	0.85
1:D:147:LYS:C	1:D:149:GLY:H	1.79	0.85
1:A:104:ARG:HH22	1:B:78:VAL:HA	1.42	0.84
1:D:104:ARG:HH22	1:E:78:VAL:HA	1.41	0.84
1:D:210:ILE:HG13	1:E:266:PHE:CE1	2.12	0.84
1:D:78:VAL:HG22	1:D:130:ILE:HG12	1.57	0.84
1:A:202:LEU:HD12	1:B:259:PHE:CZ	2.13	0.84
1:C:78:VAL:HG22	1:C:130:ILE:HG12	1.58	0.83
1:A:147:LYS:C	1:A:149:GLY:H	1.79	0.83
1:E:76:ARG:NH2	1:E:130:ILE:HD12	1.92	0.83
1:A:22:TYR:HA	1:A:149:GLY:HA3	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:ILE:HD11	1:B:240:LEU:HD23	1.60	0.82
1:B:257:ILE:O	1:B:261:ILE:HG12	1.78	0.82
1:A:22:TYR:HA	1:A:149:GLY:CA	2.09	0.82
1:D:22:TYR:HA	1:D:149:GLY:HA3	1.62	0.82
1:E:200:ILE:HD11	1:E:240:LEU:HD23	1.59	0.82
1:B:22:TYR:HA	1:B:149:GLY:HA3	1.62	0.82
1:D:22:TYR:HA	1:D:149:GLY:CA	2.09	0.82
1:E:257:ILE:O	1:E:261:ILE:HG12	1.80	0.81
1:A:78:VAL:HG22	1:A:130:ILE:HG12	1.60	0.81
1:B:22:TYR:HA	1:B:149:GLY:CA	2.10	0.81
1:C:149:GLY:O	1:C:164:PHE:CD1	2.31	0.81
1:E:234:HIS:CE1	1:E:261:ILE:HG21	2.15	0.81
1:C:200:ILE:HD11	1:C:240:LEU:HD23	1.60	0.81
1:C:234:HIS:CE1	1:C:261:ILE:HG21	2.16	0.81
1:C:53:PHE:HE2	1:C:63:LYS:HB3	1.47	0.80
1:D:253:TYR:HD1	1:D:313:PHE:CD2	1.99	0.80
1:A:155:PHE:CE1	1:B:112:PRO:CB	2.63	0.80
1:E:89:VAL:HG11	1:E:102:LEU:HD23	1.64	0.80
1:D:257:ILE:O	1:D:261:ILE:HG12	1.82	0.80
1:E:79:ASN:HD22	1:E:79:ASN:H	1.29	0.80
1:A:200:ILE:HD11	1:A:240:LEU:HD23	1.63	0.79
1:D:200:ILE:HD11	1:D:240:LEU:HD23	1.64	0.79
1:B:238:ASN:HA	1:B:258:ILE:HD11	1.62	0.79
1:D:253:TYR:CD1	1:D:313:PHE:HD2	2.01	0.79
1:E:53:PHE:HE2	1:E:63:LYS:HB3	1.47	0.79
1:A:257:ILE:O	1:A:261:ILE:HG12	1.82	0.79
1:A:226:LEU:HD23	1:B:224:VAL:CB	2.11	0.79
1:E:238:ASN:HA	1:E:258:ILE:HD11	1.62	0.79
1:D:53:PHE:HE2	1:D:63:LYS:HB3	1.47	0.79
1:E:22:TYR:HA	1:E:149:GLY:CA	2.12	0.79
1:E:253:TYR:HD1	1:E:313:PHE:HD2	1.29	0.79
1:C:197:ILE:HB	1:C:198:PRO:HD3	1.63	0.79
1:B:253:TYR:HD1	1:B:313:PHE:HD2	1.29	0.78
1:A:297:ALA:O	1:A:301:VAL:HG23	1.83	0.78
1:A:149:GLY:O	1:A:164:PHE:CD1	2.32	0.78
1:C:27:TYR:HB3	1:D:110:LEU:HD11	1.66	0.78
1:B:79:ASN:H	1:B:79:ASN:HD22	1.31	0.78
1:A:197:ILE:HB	1:A:198:PRO:HD3	1.65	0.78
1:A:253:TYR:HD1	1:A:313:PHE:CD2	2.02	0.78
1:C:257:ILE:O	1:C:261:ILE:HG12	1.83	0.78
1:B:15:LEU:HD11	1:B:46:TRP:HB2	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:22:TYR:HA	1:E:149:GLY:HA3	1.65	0.78
1:D:149:GLY:O	1:D:164:PHE:CD1	2.33	0.78
1:A:283:GLN:N	1:A:284:PRO:HD3	1.98	0.78
1:A:53:PHE:HE2	1:A:63:LYS:HB3	1.47	0.78
1:C:297:ALA:O	1:C:301:VAL:HG23	1.84	0.78
1:C:283:GLN:N	1:C:284:PRO:HD3	2.00	0.76
1:B:53:PHE:HE2	1:B:63:LYS:HB3	1.48	0.76
1:C:253:TYR:HD1	1:C:313:PHE:HD2	1.32	0.76
1:E:15:LEU:HD11	1:E:46:TRP:HB2	1.67	0.76
1:E:197:ILE:HB	1:E:198:PRO:HD3	1.66	0.76
1:A:253:TYR:CD1	1:A:313:PHE:HD2	2.04	0.76
1:A:15:LEU:HD11	1:A:46:TRP:HB2	1.68	0.76
1:D:128:TYR:O	1:D:129:LEU:HB2	1.86	0.76
1:D:210:ILE:HG13	1:E:266:PHE:HE1	1.49	0.75
1:D:89:VAL:HG11	1:D:102:LEU:HD23	1.68	0.75
1:D:15:LEU:HD11	1:D:46:TRP:HB2	1.69	0.75
1:E:283:GLN:N	1:E:284:PRO:HD3	2.01	0.75
1:D:81:GLU:HG3	1:D:108:ARG:HG3	1.68	0.75
1:D:283:GLN:N	1:D:284:PRO:HD3	2.01	0.75
1:B:283:GLN:N	1:B:284:PRO:HD3	2.01	0.75
1:D:218:THR:HG22	1:D:279:LYS:HE2	1.69	0.75
1:D:238:ASN:HA	1:D:258:ILE:HD11	1.68	0.75
1:B:89:VAL:HG11	1:B:102:LEU:HD23	1.68	0.75
1:B:22:TYR:CD1	1:B:149:GLY:HA2	2.22	0.74
1:B:13:GLU:HB3	1:B:14:PRO:HD2	1.69	0.74
1:C:15:LEU:HD11	1:C:46:TRP:HB2	1.68	0.74
1:A:240:LEU:CD1	1:B:239:ILE:HG12	2.14	0.74
1:A:234:HIS:CE1	1:A:261:ILE:HG21	2.23	0.74
1:D:79:ASN:HD22	1:D:79:ASN:H	1.34	0.74
1:B:149:GLY:O	1:B:164:PHE:CD1	2.34	0.74
1:D:197:ILE:HB	1:D:198:PRO:HD3	1.69	0.74
1:D:21:ILE:O	1:D:149:GLY:HA3	1.87	0.74
1:B:234:HIS:CE1	1:B:261:ILE:HG21	2.23	0.74
1:E:238:ASN:HA	1:E:258:ILE:CD1	2.18	0.74
1:A:221:GLU:HB3	1:B:221:GLU:CG	2.16	0.74
1:A:89:VAL:HG11	1:A:102:LEU:HD23	1.70	0.74
1:D:22:TYR:CD1	1:D:149:GLY:HA2	2.23	0.73
1:C:13:GLU:HB3	1:C:14:PRO:HD2	1.70	0.73
1:E:253:TYR:HD1	1:E:313:PHE:CD2	2.07	0.73
1:C:238:ASN:HA	1:C:258:ILE:HD11	1.71	0.73
1:B:197:ILE:HB	1:B:198:PRO:HD3	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:ILE:O	1:A:149:GLY:HA3	1.89	0.73
1:E:128:TYR:O	1:E:129:LEU:HB2	1.87	0.73
1:D:94:SER:OG	1:D:95:PRO:HD2	1.89	0.73
1:C:199:ASN:HB3	1:D:242:GLU:CD	2.09	0.73
1:C:94:SER:OG	1:C:95:PRO:HD2	1.89	0.73
1:D:13:GLU:HB3	1:D:14:PRO:HD2	1.71	0.73
1:B:253:TYR:HD1	1:B:313:PHE:CD2	2.07	0.73
1:A:139:ILE:HG12	1:A:172:ASN:HD21	1.54	0.73
1:C:139:ILE:HG12	1:C:172:ASN:HD21	1.53	0.72
1:E:139:ILE:HG12	1:E:172:ASN:HD21	1.53	0.72
1:C:42:LEU:HB3	1:C:103:GLU:HG3	1.72	0.72
1:C:22:TYR:CD1	1:C:149:GLY:HA2	2.24	0.72
1:A:42:LEU:HB3	1:A:103:GLU:HG3	1.72	0.72
1:D:234:HIS:CE1	1:D:261:ILE:HG21	2.25	0.72
1:D:104:ARG:NH2	1:E:78:VAL:HA	2.03	0.72
1:C:128:TYR:O	1:C:129:LEU:HB2	1.88	0.72
1:C:21:ILE:O	1:C:149:GLY:HA3	1.90	0.72
1:A:27:TYR:HB3	1:B:110:LEU:CD1	2.13	0.72
1:C:215:PHE:O	1:C:291:THR:HG22	1.90	0.72
1:A:202:LEU:HD12	1:B:259:PHE:HZ	1.54	0.72
1:D:229:SER:CB	1:E:228:VAL:HG11	2.19	0.72
1:A:238:ASN:HA	1:A:258:ILE:HD11	1.72	0.72
1:A:79:ASN:HD22	1:A:79:ASN:H	1.35	0.72
1:C:202:LEU:HD12	1:D:259:PHE:CE1	2.25	0.71
1:D:276:HIS:C	1:D:278:LEU:H	1.94	0.71
1:A:222:ALA:O	1:A:226:LEU:HB2	1.90	0.71
1:A:22:TYR:CD1	1:A:149:GLY:HA2	2.25	0.71
1:C:253:TYR:HD1	1:C:313:PHE:CD2	2.09	0.71
1:E:150:LYS:CG	1:E:154:VAL:HG21	2.21	0.71
1:A:218:THR:HG22	1:A:279:LYS:HE2	1.71	0.71
1:E:13:GLU:HB3	1:E:14:PRO:HD2	1.71	0.71
1:B:81:GLU:HG3	1:B:108:ARG:HG3	1.71	0.71
1:A:13:GLU:HB3	1:A:14:PRO:HD2	1.71	0.71
1:E:218:THR:HG22	1:E:279:LYS:HE2	1.72	0.71
1:B:21:ILE:O	1:B:149:GLY:HA3	1.89	0.71
1:B:42:LEU:HB3	1:B:103:GLU:HG3	1.73	0.71
1:B:218:THR:HG22	1:B:279:LYS:HE2	1.73	0.71
1:D:27:TYR:HB3	1:E:110:LEU:HD11	1.73	0.71
1:B:297:ALA:O	1:B:301:VAL:HG23	1.91	0.71
1:B:29:LEU:HB2	1:B:156:LEU:HD11	1.73	0.70
1:E:253:TYR:CD1	1:E:313:PHE:HD2	2.08	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:PHE:O	1:A:291:THR:HG22	1.91	0.70
1:D:42:LEU:HB3	1:D:103:GLU:HG3	1.73	0.70
1:E:22:TYR:CD1	1:E:149:GLY:HA2	2.25	0.70
1:E:215:PHE:O	1:E:291:THR:HG22	1.92	0.70
1:A:128:TYR:O	1:A:129:LEU:HB2	1.91	0.70
1:E:21:ILE:O	1:E:149:GLY:HA3	1.91	0.70
1:E:47:LYS:HD2	1:E:49:ARG:HH21	1.55	0.70
1:E:147:LYS:C	1:E:149:GLY:N	2.44	0.70
1:C:79:ASN:HD22	1:C:79:ASN:H	1.39	0.70
1:A:157:THR:CG2	1:B:34:GLU:OE1	2.40	0.70
1:C:47:LYS:HD2	1:C:49:ARG:HH21	1.56	0.70
1:E:42:LEU:HB3	1:E:103:GLU:HG3	1.71	0.70
1:B:215:PHE:O	1:B:291:THR:HG22	1.92	0.70
1:B:253:TYR:CD1	1:B:313:PHE:HD2	2.09	0.69
1:B:238:ASN:HA	1:B:258:ILE:CD1	2.21	0.69
1:D:221:GLU:OE2	1:E:221:GLU:CD	2.31	0.69
1:C:29:LEU:HB2	1:C:156:LEU:HD11	1.74	0.69
1:E:149:GLY:O	1:E:164:PHE:CD1	2.35	0.69
1:C:253:TYR:CD1	1:C:313:PHE:HD2	2.11	0.69
1:C:218:THR:HG22	1:C:279:LYS:HE2	1.74	0.69
1:E:215:PHE:HZ	1:E:298:PHE:CE1	2.10	0.69
1:D:304:LEU:O	1:D:308:ILE:HG12	1.92	0.69
1:A:94:SER:OG	1:A:95:PRO:HD2	1.93	0.69
1:E:297:ALA:O	1:E:301:VAL:HG23	1.92	0.69
1:D:215:PHE:O	1:D:291:THR:HG22	1.92	0.69
1:B:276:HIS:C	1:B:278:LEU:H	1.95	0.69
1:A:77:PHE:CD1	1:A:84:ARG:HD2	2.28	0.69
1:C:89:VAL:HG11	1:C:102:LEU:HD23	1.74	0.69
1:D:257:ILE:HG22	1:D:309:LEU:HD23	1.75	0.69
1:E:222:ALA:O	1:E:226:LEU:HB2	1.93	0.69
1:D:47:LYS:HD2	1:D:49:ARG:HH21	1.58	0.69
1:A:77:PHE:H	1:A:84:ARG:HD3	1.58	0.69
1:B:200:ILE:O	1:B:204:MET:HB2	1.92	0.68
1:C:213:THR:HG22	1:C:226:LEU:HD11	1.73	0.68
1:D:222:ALA:O	1:D:226:LEU:HB2	1.93	0.68
1:E:81:GLU:HG3	1:E:108:ARG:HG3	1.73	0.68
1:E:276:HIS:C	1:E:278:LEU:H	1.96	0.68
1:B:47:LYS:HD2	1:B:49:ARG:HH21	1.58	0.68
1:E:29:LEU:HB2	1:E:156:LEU:HD11	1.76	0.68
1:E:150:LYS:HG3	1:E:154:VAL:HG21	1.75	0.68
1:A:257:ILE:HG22	1:A:309:LEU:HD23	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:100:GLN:HE21	1:D:100:GLN:HA	1.59	0.68
1:A:150:LYS:CG	1:A:154:VAL:HG21	2.24	0.68
1:A:219:SER:OG	1:A:222:ALA:HB3	1.94	0.68
1:D:238:ASN:HA	1:D:258:ILE:CD1	2.24	0.68
1:C:202:LEU:HD12	1:D:259:PHE:HE1	1.59	0.68
1:A:215:PHE:HZ	1:A:298:PHE:CE1	2.12	0.68
1:B:100:GLN:HA	1:B:100:GLN:HE21	1.59	0.68
1:B:131:VAL:HG11	1:B:140:VAL:HG13	1.74	0.68
1:A:147:LYS:C	1:A:149:GLY:N	2.48	0.67
1:D:147:LYS:C	1:D:149:GLY:N	2.47	0.67
1:E:66:GLU:HG3	1:E:67:PRO:HD2	1.77	0.67
1:A:238:ASN:HA	1:A:258:ILE:CD1	2.25	0.67
1:D:139:ILE:HG12	1:D:172:ASN:HD21	1.57	0.67
1:A:200:ILE:O	1:A:204:MET:HB2	1.94	0.67
1:C:150:LYS:CG	1:C:154:VAL:HG21	2.24	0.67
1:A:303:LEU:O	1:A:307:ILE:HD12	1.94	0.67
1:C:131:VAL:HG11	1:C:140:VAL:HG13	1.75	0.67
1:A:81:GLU:HG3	1:A:108:ARG:HG3	1.75	0.67
1:D:77:PHE:CD1	1:D:84:ARG:HD2	2.29	0.67
1:C:81:GLU:HG3	1:C:108:ARG:HG3	1.77	0.67
1:A:150:LYS:HG3	1:A:154:VAL:HG21	1.77	0.66
1:A:42:LEU:HD23	1:A:103:GLU:OE1	1.94	0.66
1:A:225:THR:HG22	1:B:224:VAL:HG23	1.76	0.66
1:C:226:LEU:HD21	1:D:224:VAL:HB	1.78	0.66
1:E:257:ILE:HG22	1:E:309:LEU:HD23	1.76	0.66
1:B:304:LEU:O	1:B:308:ILE:HG12	1.96	0.66
1:B:150:LYS:CG	1:B:154:VAL:HG21	2.26	0.66
1:C:147:LYS:C	1:C:149:GLY:N	2.46	0.66
1:C:213:THR:HG22	1:C:226:LEU:CD1	2.26	0.66
1:C:238:ASN:HA	1:C:258:ILE:CD1	2.25	0.66
1:A:47:LYS:HD2	1:A:49:ARG:HH21	1.61	0.66
1:A:217:SER:OG	1:B:220:TYR:CE2	2.45	0.66
1:C:200:ILE:O	1:C:204:MET:HB2	1.96	0.66
1:C:150:LYS:HG3	1:C:154:VAL:HG21	1.78	0.66
1:B:276:HIS:O	1:B:280:VAL:HG22	1.96	0.66
1:B:139:ILE:HG12	1:B:172:ASN:HD21	1.60	0.66
1:E:42:LEU:HD23	1:E:103:GLU:OE1	1.96	0.65
1:B:191:ARG:HG3	1:B:192:GLN:N	2.11	0.65
1:E:200:ILE:O	1:E:204:MET:HB2	1.97	0.65
1:C:42:LEU:HD23	1:C:103:GLU:OE1	1.95	0.65
1:A:157:THR:HG21	1:B:34:GLU:OE1	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:SER:OG	1:C:222:ALA:HB3	1.97	0.65
1:D:131:VAL:HG11	1:D:140:VAL:HG13	1.79	0.65
1:B:147:LYS:C	1:B:149:GLY:N	2.45	0.65
1:C:257:ILE:HG22	1:C:309:LEU:HD23	1.78	0.65
1:B:66:GLU:HG3	1:B:67:PRO:HD2	1.77	0.65
1:B:215:PHE:HZ	1:B:298:PHE:CE1	2.15	0.65
1:D:66:GLU:HG3	1:D:67:PRO:HD2	1.79	0.65
1:B:128:TYR:O	1:B:129:LEU:HB2	1.96	0.65
1:E:200:ILE:CD1	1:E:240:LEU:HD23	2.27	0.65
1:C:215:PHE:HZ	1:C:298:PHE:CE1	2.15	0.65
1:A:29:LEU:HB2	1:A:156:LEU:HD11	1.78	0.65
1:B:94:SER:OG	1:B:95:PRO:HD2	1.98	0.64
1:C:276:HIS:C	1:C:278:LEU:H	2.00	0.64
1:C:66:GLU:HG3	1:C:67:PRO:HD2	1.78	0.64
1:B:13:GLU:HB3	1:B:14:PRO:CD	2.27	0.64
1:A:276:HIS:C	1:A:278:LEU:H	2.00	0.64
1:C:77:PHE:CD1	1:C:84:ARG:HD2	2.32	0.64
1:E:94:SER:OG	1:E:95:PRO:HD2	1.97	0.64
1:D:297:ALA:O	1:D:301:VAL:HG23	1.97	0.64
1:E:89:VAL:CG1	1:E:102:LEU:HD23	2.27	0.64
1:A:283:GLN:N	1:A:284:PRO:CD	2.60	0.64
1:D:53:PHE:CE1	1:D:95:PRO:HA	2.33	0.64
1:A:222:ALA:HA	1:B:221:GLU:OE1	1.98	0.64
1:D:215:PHE:HZ	1:D:298:PHE:CE1	2.16	0.64
1:A:131:VAL:HG11	1:A:140:VAL:HG13	1.79	0.64
1:B:77:PHE:CD1	1:B:84:ARG:HD2	2.33	0.63
1:C:222:ALA:O	1:C:226:LEU:HB2	1.97	0.63
1:D:77:PHE:H	1:D:84:ARG:HD3	1.62	0.63
1:B:42:LEU:HD23	1:B:103:GLU:OE1	1.98	0.63
1:D:42:LEU:HD23	1:D:103:GLU:OE1	1.97	0.63
1:C:23:LEU:HG	1:C:164:PHE:CE1	2.34	0.63
1:C:283:GLN:N	1:C:284:PRO:CD	2.61	0.63
1:E:147:LYS:HE2	1:E:165:THR:HA	1.80	0.63
1:D:283:GLN:N	1:D:284:PRO:CD	2.62	0.63
1:C:222:ALA:HB2	1:D:221:GLU:HA	1.79	0.63
1:C:195:SER:O	1:C:199:ASN:HB2	1.97	0.63
1:C:226:LEU:CD2	1:D:224:VAL:HB	2.29	0.63
1:E:304:LEU:O	1:E:308:ILE:HG12	1.97	0.63
1:A:66:GLU:HG3	1:A:67:PRO:HD2	1.80	0.63
1:A:281:GLU:O	1:A:283:GLN:N	2.32	0.63
1:E:215:PHE:CZ	1:E:298:PHE:CD1	2.86	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:LEU:O	1:B:307:ILE:HD12	1.98	0.63
1:D:150:LYS:CG	1:D:154:VAL:HG21	2.29	0.63
1:B:257:ILE:HG22	1:B:309:LEU:HD23	1.81	0.63
1:C:200:ILE:CD1	1:C:240:LEU:HD23	2.29	0.63
1:A:215:PHE:CZ	1:A:298:PHE:CD1	2.86	0.63
1:C:147:LYS:HE2	1:C:165:THR:HA	1.80	0.63
1:D:225:THR:HG22	1:E:224:VAL:HG23	1.78	0.63
1:C:13:GLU:HB3	1:C:14:PRO:CD	2.28	0.63
1:C:77:PHE:H	1:C:84:ARG:HD3	1.64	0.63
1:A:290:ILE:HG22	1:A:291:THR:N	2.14	0.62
1:C:208:LEU:O	1:C:211:SER:HB3	1.99	0.62
1:A:222:ALA:CB	1:B:221:GLU:HA	2.22	0.62
1:C:54:ASP:HB2	1:C:57:ARG:HG3	1.81	0.62
1:D:222:ALA:CB	1:E:220:TYR:CD2	2.83	0.62
1:A:276:HIS:O	1:A:280:VAL:HG22	2.00	0.62
1:D:191:ARG:HG3	1:D:192:GLN:N	2.14	0.62
1:D:29:LEU:HB2	1:D:156:LEU:HD11	1.79	0.62
1:A:229:SER:HB2	1:B:228:VAL:HG11	1.81	0.62
1:E:213:THR:HG22	1:E:226:LEU:CD1	2.30	0.62
1:D:13:GLU:HB3	1:D:14:PRO:CD	2.30	0.62
1:C:104:ARG:NH2	1:D:77:PHE:O	2.25	0.62
1:A:147:LYS:HE2	1:A:165:THR:HA	1.79	0.62
1:B:150:LYS:HG3	1:B:154:VAL:HG21	1.81	0.62
1:B:54:ASP:HB2	1:B:57:ARG:HG3	1.82	0.62
1:E:283:GLN:N	1:E:284:PRO:CD	2.63	0.62
1:A:23:LEU:HG	1:A:164:PHE:CE1	2.35	0.62
1:C:47:LYS:HD2	1:C:49:ARG:NH2	2.15	0.62
1:A:213:THR:HG22	1:A:226:LEU:HD11	1.82	0.62
1:E:23:LEU:HG	1:E:164:PHE:CE1	2.35	0.62
1:B:222:ALA:O	1:B:226:LEU:HB2	2.00	0.62
1:D:89:VAL:CG1	1:D:102:LEU:HD23	2.29	0.62
1:E:213:THR:HG22	1:E:226:LEU:HD11	1.82	0.61
1:A:54:ASP:HB2	1:A:57:ARG:HG3	1.82	0.61
1:C:276:HIS:O	1:C:280:VAL:HG22	1.99	0.61
1:B:77:PHE:H	1:B:84:ARG:HD3	1.65	0.61
1:E:47:LYS:HD2	1:E:49:ARG:NH2	2.16	0.61
1:E:131:VAL:HG11	1:E:140:VAL:HG13	1.80	0.61
1:E:100:GLN:HE21	1:E:100:GLN:HA	1.65	0.61
1:B:283:GLN:N	1:B:284:PRO:CD	2.63	0.61
1:B:47:LYS:HD2	1:B:49:ARG:NH2	2.15	0.61
1:E:208:LEU:O	1:E:211:SER:HB3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:GLN:HE21	1:A:100:GLN:HA	1.66	0.61
1:B:208:LEU:O	1:B:211:SER:HB3	1.99	0.61
1:D:41:PHE:HE2	1:E:175:LEU:HD23	1.65	0.61
1:A:13:GLU:HB3	1:A:14:PRO:CD	2.30	0.61
1:A:53:PHE:CE2	1:A:63:LYS:HB3	2.33	0.61
1:E:276:HIS:O	1:E:280:VAL:HG22	2.00	0.61
1:E:77:PHE:CD1	1:E:84:ARG:HD2	2.34	0.61
1:E:147:LYS:O	1:E:149:GLY:N	2.34	0.61
1:D:213:THR:HG22	1:D:226:LEU:CD1	2.31	0.61
1:E:215:PHE:HZ	1:E:298:PHE:CD1	2.19	0.61
1:B:147:LYS:O	1:B:149:GLY:N	2.34	0.61
1:C:215:PHE:CZ	1:C:298:PHE:CD1	2.89	0.61
1:A:208:LEU:O	1:A:211:SER:HB3	2.00	0.61
1:B:89:VAL:CG1	1:B:102:LEU:HD23	2.30	0.60
1:C:157:THR:HG21	1:D:34:GLU:HG3	1.83	0.60
1:D:23:LEU:HG	1:D:164:PHE:CE1	2.36	0.60
1:D:54:ASP:HB2	1:D:57:ARG:HG3	1.82	0.60
1:B:53:PHE:CE1	1:B:95:PRO:HA	2.37	0.60
1:E:275:GLN:HG3	1:E:291:THR:OG1	2.01	0.60
1:E:234:HIS:CE1	1:E:261:ILE:CG2	2.84	0.60
1:C:267:VAL:HA	1:C:270:ILE:HB	1.84	0.60
1:A:215:PHE:HZ	1:A:298:PHE:CD1	2.19	0.60
1:B:213:THR:HG22	1:B:226:LEU:HD11	1.84	0.60
1:E:53:PHE:CE2	1:E:63:LYS:HB3	2.34	0.60
1:D:303:LEU:O	1:D:307:ILE:HD12	2.01	0.60
1:E:22:TYR:HA	1:E:149:GLY:HA2	1.84	0.60
1:D:200:ILE:O	1:D:204:MET:HB2	2.01	0.60
1:A:202:LEU:HD12	1:B:259:PHE:CE1	2.37	0.60
1:E:54:ASP:HB2	1:E:57:ARG:HG3	1.83	0.60
1:D:276:HIS:O	1:D:280:VAL:HG22	2.00	0.60
1:A:210:ILE:HG23	1:B:269:VAL:HG11	1.84	0.60
1:B:254:THR:O	1:B:258:ILE:HB	2.02	0.60
1:D:47:LYS:HD2	1:D:49:ARG:NH2	2.17	0.60
1:C:234:HIS:CE1	1:C:261:ILE:CG2	2.83	0.60
1:D:157:THR:HG21	1:E:34:GLU:OE1	2.01	0.60
1:C:53:PHE:CE2	1:C:63:LYS:HB3	2.33	0.60
1:E:53:PHE:CE1	1:E:95:PRO:HA	2.37	0.60
1:B:53:PHE:CE2	1:B:63:LYS:HB3	2.35	0.60
1:C:275:GLN:HG3	1:C:291:THR:OG1	2.02	0.60
1:B:213:THR:HG22	1:B:226:LEU:CD1	2.32	0.60
1:C:193:TYR:O	1:C:194:PHE:HB2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:TYR:O	1:A:194:PHE:HB2	2.01	0.60
1:B:22:TYR:HA	1:B:149:GLY:HA2	1.84	0.59
1:A:25:GLU:HG3	1:B:79:ASN:HA	1.84	0.59
1:B:123:GLN:HA	1:B:123:GLN:NE2	2.17	0.59
1:A:213:THR:HG22	1:A:226:LEU:CD1	2.31	0.59
1:D:229:SER:HB3	1:E:228:VAL:HG11	1.84	0.59
1:E:264:PHE:CE2	1:E:302:PHE:HB2	2.37	0.59
1:E:267:VAL:HA	1:E:270:ILE:HB	1.82	0.59
1:D:215:PHE:CZ	1:D:298:PHE:CD1	2.91	0.59
1:B:23:LEU:HG	1:B:164:PHE:CE1	2.36	0.59
1:D:193:TYR:O	1:D:194:PHE:HB2	2.01	0.59
1:D:146:GLU:HG3	1:E:176:GLU:HG2	1.83	0.59
1:D:155:PHE:CZ	1:E:112:PRO:HB3	2.35	0.59
1:D:208:LEU:O	1:D:211:SER:HB3	2.02	0.59
1:C:281:GLU:O	1:C:283:GLN:N	2.33	0.59
1:A:146:GLU:HG3	1:B:176:GLU:HG2	1.84	0.59
1:D:81:GLU:HG3	1:D:108:ARG:CG	2.32	0.59
1:B:267:VAL:HA	1:B:270:ILE:HB	1.84	0.59
1:E:77:PHE:H	1:E:84:ARG:HD3	1.67	0.59
1:A:19:THR:HG22	1:A:44:LEU:CD2	2.33	0.59
1:A:223:ASN:O	1:A:227:VAL:HG23	2.02	0.59
1:D:22:TYR:HA	1:D:149:GLY:HA2	1.84	0.59
1:C:225:THR:HG21	1:D:225:THR:OG1	2.03	0.59
1:C:215:PHE:HZ	1:C:298:PHE:CD1	2.21	0.59
1:A:275:GLN:HG3	1:A:291:THR:OG1	2.03	0.59
1:A:147:LYS:O	1:A:149:GLY:N	2.35	0.59
1:E:223:ASN:O	1:E:227:VAL:HG23	2.03	0.59
1:D:41:PHE:HE2	1:E:175:LEU:CD2	2.16	0.58
1:C:147:LYS:O	1:C:149:GLY:N	2.36	0.58
1:D:210:ILE:HG13	1:E:266:PHE:CD1	2.38	0.58
1:D:150:LYS:HG3	1:D:154:VAL:HG21	1.84	0.58
1:A:254:THR:O	1:A:258:ILE:HB	2.03	0.58
1:D:213:THR:HG22	1:D:226:LEU:HD11	1.85	0.58
1:D:161:ILE:HA	1:D:189:ILE:HG22	1.85	0.58
1:A:104:ARG:NH2	1:B:77:PHE:O	2.36	0.58
1:B:200:ILE:CD1	1:B:240:LEU:HD23	2.32	0.58
1:C:223:ASN:O	1:C:227:VAL:HG23	2.02	0.58
1:A:229:SER:HB3	1:B:228:VAL:CG1	2.33	0.58
1:D:225:THR:CG2	1:E:224:VAL:CG2	2.79	0.58
1:B:215:PHE:CZ	1:B:298:PHE:CD1	2.90	0.58
1:D:195:SER:O	1:D:199:ASN:HB2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:ASN:O	1:B:227:VAL:HG23	2.04	0.58
1:A:53:PHE:CE1	1:A:95:PRO:HA	2.39	0.58
1:B:281:GLU:O	1:B:283:GLN:N	2.35	0.58
1:B:147:LYS:HE2	1:B:165:THR:HA	1.86	0.58
1:A:195:SER:O	1:A:199:ASN:HB2	2.03	0.58
1:B:137:ARG:HD2	1:B:179:LEU:HG	1.86	0.58
1:E:219:SER:OG	1:E:222:ALA:HB3	2.04	0.58
1:D:123:GLN:NE2	1:D:123:GLN:HA	2.19	0.58
1:C:62:VAL:HG13	1:C:93:VAL:O	2.04	0.58
1:B:81:GLU:HG3	1:B:108:ARG:CG	2.33	0.58
1:C:194:PHE:C	1:C:196:TYR:N	2.57	0.58
1:E:79:ASN:ND2	1:E:79:ASN:H	1.99	0.58
1:E:281:GLU:O	1:E:283:GLN:N	2.34	0.58
1:D:254:THR:O	1:D:258:ILE:HB	2.04	0.58
1:C:53:PHE:CE1	1:C:95:PRO:HA	2.39	0.57
1:A:222:ALA:HB2	1:B:221:GLU:CA	2.23	0.57
1:D:192:GLN:OE1	1:E:249:PRO:HB3	2.03	0.57
1:D:147:LYS:O	1:D:149:GLY:N	2.37	0.57
1:D:229:SER:HB3	1:E:228:VAL:CG1	2.34	0.57
1:B:264:PHE:CE2	1:B:302:PHE:HB2	2.39	0.57
1:A:47:LYS:HD2	1:A:49:ARG:NH2	2.19	0.57
1:B:161:ILE:HA	1:B:189:ILE:HG22	1.87	0.57
1:B:197:ILE:HA	1:B:201:ILE:HB	1.85	0.57
1:D:275:GLN:HG3	1:D:291:THR:OG1	2.04	0.57
1:C:100:GLN:HE21	1:C:100:GLN:HA	1.69	0.57
1:C:304:LEU:O	1:C:308:ILE:HG12	2.03	0.57
1:A:232:ILE:HG22	1:A:233:ALA:N	2.18	0.57
1:B:119:PRO:O	1:B:193:TYR:HB3	2.04	0.57
1:B:275:GLN:HG3	1:B:291:THR:OG1	2.03	0.57
1:A:304:LEU:O	1:A:308:ILE:HG12	2.03	0.57
1:E:161:ILE:HA	1:E:189:ILE:HG22	1.86	0.57
1:C:22:TYR:HA	1:C:149:GLY:HA2	1.83	0.57
1:C:119:PRO:O	1:C:193:TYR:HB3	2.05	0.57
1:B:194:PHE:C	1:B:196:TYR:N	2.58	0.57
1:C:274:VAL:C	1:C:276:HIS:H	2.08	0.57
1:A:274:VAL:C	1:A:276:HIS:H	2.08	0.57
1:A:240:LEU:HD13	1:B:239:ILE:CG1	2.19	0.57
1:A:119:PRO:O	1:A:193:TYR:HB3	2.04	0.57
1:C:264:PHE:CE2	1:C:302:PHE:HB2	2.40	0.57
1:D:215:PHE:HZ	1:D:298:PHE:CD1	2.22	0.57
1:A:229:SER:CB	1:B:228:VAL:HG11	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:254:THR:O	1:E:258:ILE:HB	2.04	0.57
1:B:275:GLN:HG2	1:B:275:GLN:O	2.05	0.57
1:A:22:TYR:HB3	1:A:41:PHE:HB2	1.87	0.56
1:E:13:GLU:HB3	1:E:14:PRO:CD	2.32	0.56
1:E:195:SER:O	1:E:199:ASN:HB2	2.05	0.56
1:A:89:VAL:CG1	1:A:102:LEU:HD23	2.34	0.56
1:D:267:VAL:HA	1:D:270:ILE:HB	1.86	0.56
1:E:81:GLU:HG3	1:E:108:ARG:CG	2.35	0.56
1:D:194:PHE:C	1:D:196:TYR:N	2.56	0.56
1:C:191:ARG:HG3	1:C:192:GLN:N	2.18	0.56
1:A:229:SER:CB	1:B:228:VAL:CG1	2.84	0.56
1:A:22:TYR:HA	1:A:149:GLY:HA2	1.84	0.56
1:B:305:ALA:O	1:B:309:LEU:HB2	2.05	0.56
1:C:254:THR:O	1:C:258:ILE:HB	2.06	0.56
1:B:215:PHE:HZ	1:B:298:PHE:CD1	2.23	0.56
1:D:221:GLU:OE2	1:E:221:GLU:OE2	2.22	0.56
1:A:137:ARG:HD2	1:A:179:LEU:HG	1.87	0.56
1:A:225:THR:CG2	1:B:224:VAL:HG23	2.35	0.56
1:D:79:ASN:ND2	1:D:79:ASN:H	2.03	0.56
1:E:305:ALA:O	1:E:309:LEU:HB2	2.05	0.56
1:D:53:PHE:CE2	1:D:63:LYS:HB3	2.34	0.56
1:A:191:ARG:HG3	1:A:192:GLN:N	2.21	0.56
1:D:197:ILE:HA	1:D:201:ILE:HB	1.86	0.56
1:B:232:ILE:HG22	1:B:233:ALA:N	2.20	0.56
1:E:303:LEU:O	1:E:307:ILE:HD12	2.06	0.56
1:B:79:ASN:H	1:B:79:ASN:ND2	2.00	0.56
1:D:275:GLN:O	1:D:275:GLN:HG2	2.06	0.56
1:E:119:PRO:O	1:E:193:TYR:HB3	2.06	0.56
1:C:215:PHE:HB2	1:C:216:TRP:CZ3	2.40	0.56
1:C:200:ILE:HD11	1:C:240:LEU:CD2	2.35	0.56
1:C:81:GLU:HG3	1:C:108:ARG:CG	2.36	0.56
1:D:119:PRO:O	1:D:193:TYR:HB3	2.05	0.56
1:B:193:TYR:O	1:B:194:PHE:HB2	2.06	0.56
1:A:146:GLU:HG3	1:B:176:GLU:CG	2.36	0.56
1:B:62:VAL:HG13	1:B:93:VAL:O	2.06	0.56
1:B:274:VAL:C	1:B:276:HIS:H	2.09	0.55
1:D:223:ASN:O	1:D:227:VAL:HG23	2.06	0.55
1:C:193:TYR:O	1:C:194:PHE:CB	2.54	0.55
1:B:215:PHE:HB2	1:B:216:TRP:CZ3	2.42	0.55
1:A:139:ILE:HG12	1:A:172:ASN:ND2	2.21	0.55
1:A:123:GLN:HA	1:A:123:GLN:NE2	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:226:LEU:HD23	1:D:224:VAL:CG2	2.37	0.55
1:A:81:GLU:HG3	1:A:108:ARG:CG	2.36	0.55
1:A:314:PHE:HD1	1:A:314:PHE:N	2.05	0.55
1:D:264:PHE:CE2	1:D:302:PHE:HB2	2.41	0.55
1:A:264:PHE:CE2	1:A:302:PHE:HB2	2.42	0.55
1:A:179:LEU:HD12	1:A:179:LEU:O	2.07	0.55
1:D:232:ILE:HG22	1:D:233:ALA:N	2.20	0.55
1:A:305:ALA:O	1:A:309:LEU:HB2	2.07	0.55
1:A:193:TYR:O	1:A:194:PHE:CB	2.54	0.55
1:D:290:ILE:HG22	1:D:291:THR:N	2.21	0.55
1:A:314:PHE:CD1	1:A:314:PHE:N	2.75	0.55
1:C:232:ILE:HG22	1:C:233:ALA:N	2.22	0.55
1:A:194:PHE:C	1:A:196:TYR:N	2.60	0.55
1:A:267:VAL:HA	1:A:270:ILE:HB	1.88	0.55
1:E:215:PHE:HB3	1:E:295:ARG:HG2	1.89	0.55
1:A:157:THR:HG22	1:B:34:GLU:OE1	2.06	0.55
1:D:219:SER:OG	1:D:222:ALA:HB3	2.07	0.55
1:D:215:PHE:HB2	1:D:216:TRP:CZ3	2.41	0.55
1:C:314:PHE:HD1	1:C:314:PHE:N	2.05	0.55
1:C:303:LEU:O	1:C:307:ILE:HD12	2.07	0.55
1:A:275:GLN:HG2	1:A:275:GLN:O	2.07	0.54
1:B:234:HIS:CE1	1:B:261:ILE:CG2	2.90	0.54
1:E:194:PHE:C	1:E:196:TYR:N	2.60	0.54
1:D:18:ASN:HB3	1:D:143:VAL:HG23	1.87	0.54
1:E:191:ARG:HG3	1:E:192:GLN:N	2.22	0.54
1:C:147:LYS:O	1:C:147:LYS:HG2	2.06	0.54
1:A:234:HIS:CE1	1:A:261:ILE:CG2	2.90	0.54
1:D:27:TYR:CB	1:E:110:LEU:HD11	2.37	0.54
1:A:200:ILE:CD1	1:A:240:LEU:HD23	2.33	0.54
1:E:193:TYR:O	1:E:194:PHE:HB2	2.06	0.54
1:D:193:TYR:O	1:D:194:PHE:CB	2.54	0.54
1:C:314:PHE:CD1	1:C:314:PHE:N	2.75	0.54
1:A:207:ILE:HG22	1:B:231:LEU:HD21	1.89	0.54
1:E:200:ILE:HD11	1:E:240:LEU:CD2	2.35	0.54
1:C:290:ILE:HG22	1:C:291:THR:N	2.22	0.54
1:A:233:ALA:HB1	1:B:235:ILE:HD13	1.90	0.54
1:D:155:PHE:HE1	1:E:112:PRO:CB	2.17	0.54
1:C:89:VAL:CG1	1:C:102:LEU:HD23	2.36	0.54
1:E:173:PHE:HZ	1:E:182:LYS:HZ1	1.56	0.54
1:C:194:PHE:C	1:C:196:TYR:H	2.10	0.54
1:E:298:PHE:HB2	1:E:299:PRO:HD3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:GLU:OE1	1:B:14:PRO:HD3	2.08	0.53
1:B:29:LEU:HD23	1:B:30:ASP:N	2.24	0.53
1:C:305:ALA:O	1:C:309:LEU:HB2	2.08	0.53
1:B:290:ILE:HG22	1:B:291:THR:N	2.24	0.53
1:B:179:LEU:O	1:B:179:LEU:HD12	2.07	0.53
1:D:210:ILE:CG1	1:E:266:PHE:CD1	2.91	0.53
1:C:215:PHE:HB3	1:C:295:ARG:HG2	1.90	0.53
1:B:314:PHE:N	1:B:314:PHE:HD1	2.07	0.53
1:D:147:LYS:HE2	1:D:165:THR:HA	1.90	0.53
1:D:234:HIS:CE1	1:D:261:ILE:CG2	2.91	0.53
1:D:305:ALA:O	1:D:309:LEU:HB2	2.08	0.53
1:D:210:ILE:HD11	1:E:266:PHE:HD1	1.73	0.53
1:C:75:ILE:HD13	1:C:131:VAL:HB	1.91	0.53
1:A:18:ASN:HB3	1:A:143:VAL:HG23	1.90	0.53
1:E:314:PHE:N	1:E:314:PHE:CD1	2.77	0.53
1:E:147:LYS:CE	1:E:165:THR:HA	2.38	0.53
1:B:249:PRO:HD2	1:B:250:TYR:CD1	2.44	0.53
1:B:215:PHE:HB3	1:B:295:ARG:HG2	1.90	0.53
1:C:137:ARG:HD2	1:C:179:LEU:HG	1.90	0.53
1:D:210:ILE:CG1	1:E:266:PHE:CE1	2.90	0.53
1:A:215:PHE:HB2	1:A:216:TRP:CZ3	2.42	0.53
1:E:275:GLN:O	1:E:275:GLN:HG2	2.09	0.53
1:A:217:SER:OG	1:B:220:TYR:HE2	1.90	0.53
1:D:194:PHE:C	1:D:196:TYR:H	2.12	0.53
1:E:232:ILE:HG22	1:E:233:ALA:N	2.22	0.53
1:E:137:ARG:HD2	1:E:179:LEU:HG	1.91	0.53
1:A:41:PHE:HE2	1:B:175:LEU:HD23	1.72	0.53
1:C:261:ILE:CD1	1:C:302:PHE:HE1	2.22	0.53
1:B:278:LEU:HD21	1:B:286:ARG:HB3	1.91	0.53
1:E:123:GLN:NE2	1:E:123:GLN:HA	2.23	0.53
1:E:215:PHE:HB2	1:E:216:TRP:CZ3	2.43	0.53
1:D:62:VAL:HG13	1:D:93:VAL:O	2.09	0.53
1:B:195:SER:O	1:B:199:ASN:HB2	2.09	0.53
1:D:200:ILE:CD1	1:D:240:LEU:HD23	2.37	0.53
1:E:139:ILE:HG12	1:E:172:ASN:ND2	2.21	0.53
1:E:29:LEU:HD23	1:E:30:ASP:N	2.23	0.53
1:A:75:ILE:HD13	1:A:131:VAL:HB	1.90	0.52
1:B:29:LEU:HD23	1:B:29:LEU:C	2.29	0.52
1:A:233:ALA:HB1	1:B:235:ILE:CD1	2.39	0.52
1:D:274:VAL:C	1:D:276:HIS:H	2.12	0.52
1:C:18:ASN:HB3	1:C:143:VAL:HG23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:54:ASP:HB2	1:D:57:ARG:HB2	1.90	0.52
1:E:274:VAL:C	1:E:276:HIS:H	2.12	0.52
1:D:158:GLY:HA2	1:D:192:GLN:OE1	2.10	0.52
1:E:314:PHE:N	1:E:314:PHE:HD1	2.07	0.52
1:C:179:LEU:O	1:C:179:LEU:HD12	2.09	0.52
1:C:161:ILE:HA	1:C:189:ILE:HG22	1.90	0.52
1:A:79:ASN:ND2	1:A:79:ASN:H	2.04	0.52
1:D:137:ARG:HD2	1:D:179:LEU:HG	1.91	0.52
1:A:155:PHE:HE1	1:B:112:PRO:CA	2.23	0.52
1:C:79:ASN:H	1:C:79:ASN:ND2	2.07	0.52
1:C:22:TYR:HB3	1:C:41:PHE:HB2	1.92	0.52
1:A:197:ILE:HA	1:A:201:ILE:HB	1.91	0.52
1:C:139:ILE:HG12	1:C:172:ASN:ND2	2.23	0.52
1:B:194:PHE:C	1:B:196:TYR:H	2.13	0.52
1:B:52:ALA:HA	1:B:95:PRO:O	2.10	0.52
1:D:179:LEU:O	1:D:179:LEU:HD12	2.10	0.52
1:C:65:TYR:CG	1:C:70:ILE:HD11	2.45	0.52
1:C:155:PHE:CE1	1:D:112:PRO:HB3	2.45	0.52
1:C:275:GLN:HG2	1:C:275:GLN:O	2.10	0.52
1:B:75:ILE:HD13	1:B:131:VAL:HB	1.91	0.52
1:E:249:PRO:HD2	1:E:250:TYR:CD1	2.45	0.52
1:B:18:ASN:HB3	1:B:143:VAL:HG23	1.92	0.52
1:C:197:ILE:HA	1:C:201:ILE:HB	1.92	0.52
1:A:298:PHE:HB2	1:A:299:PRO:HD3	1.92	0.52
1:C:29:LEU:C	1:C:29:LEU:HD23	2.29	0.52
1:E:75:ILE:HD13	1:E:131:VAL:HB	1.92	0.52
1:A:62:VAL:HG11	1:A:92:SER:HB3	1.92	0.52
1:C:123:GLN:NE2	1:C:123:GLN:HA	2.25	0.52
1:A:27:TYR:CB	1:B:110:LEU:CD1	2.83	0.51
1:B:193:TYR:O	1:B:194:PHE:CB	2.58	0.51
1:A:42:LEU:HB3	1:A:103:GLU:CG	2.41	0.51
1:C:298:PHE:HB2	1:C:299:PRO:HD3	1.91	0.51
1:C:29:LEU:HD23	1:C:30:ASP:N	2.25	0.51
1:A:104:ARG:NH1	1:B:76:ARG:HB3	2.25	0.51
1:D:222:ALA:HB3	1:E:220:TYR:CD2	2.44	0.51
1:B:286:ARG:O	1:B:289:SER:HB3	2.10	0.51
1:C:215:PHE:HB2	1:C:216:TRP:CE3	2.46	0.51
1:D:147:LYS:O	1:D:147:LYS:HG2	2.11	0.51
1:E:179:LEU:O	1:E:179:LEU:HD12	2.11	0.51
1:A:62:VAL:HG13	1:A:93:VAL:O	2.11	0.51
1:B:219:SER:OG	1:B:222:ALA:HB3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:224:VAL:C	1:E:226:LEU:N	2.64	0.51
1:E:193:TYR:O	1:E:194:PHE:CB	2.58	0.51
1:D:53:PHE:O	1:D:54:ASP:C	2.48	0.51
1:E:29:LEU:C	1:E:29:LEU:HD23	2.31	0.51
1:A:226:LEU:HD21	1:B:224:VAL:HB	1.90	0.51
1:E:147:LYS:O	1:E:147:LYS:HG2	2.10	0.51
1:B:54:ASP:HB2	1:B:57:ARG:CG	2.40	0.51
1:D:276:HIS:C	1:D:278:LEU:N	2.63	0.51
1:E:70:ILE:HG22	1:E:71:TRP:N	2.26	0.51
1:E:18:ASN:HB3	1:E:143:VAL:HG23	1.91	0.51
1:E:22:TYR:HB3	1:E:41:PHE:HB2	1.92	0.51
1:E:261:ILE:CD1	1:E:302:PHE:HE1	2.24	0.51
1:C:210:ILE:CD1	1:D:231:LEU:HD22	2.40	0.51
1:A:19:THR:HG22	1:A:44:LEU:HD23	1.93	0.51
1:A:161:ILE:HA	1:A:189:ILE:HG22	1.92	0.51
1:A:84:ARG:HA	1:A:107:ALA:HB2	1.93	0.51
1:D:157:THR:CG2	1:E:34:GLU:OE1	2.59	0.51
1:B:70:ILE:HG22	1:B:71:TRP:N	2.26	0.51
1:C:27:TYR:CE1	1:D:81:GLU:OE1	2.64	0.51
1:C:42:LEU:HB3	1:C:103:GLU:CG	2.40	0.51
1:A:179:LEU:HD12	1:A:179:LEU:C	2.32	0.51
1:E:62:VAL:HG13	1:E:93:VAL:O	2.10	0.51
1:B:173:PHE:HZ	1:B:182:LYS:HZ1	1.57	0.50
1:C:197:ILE:CB	1:C:198:PRO:HD3	2.37	0.50
1:B:54:ASP:HB2	1:B:57:ARG:HB2	1.93	0.50
1:D:118:TYR:HB2	1:D:252:THR:HG22	1.94	0.50
1:A:226:LEU:HD22	1:B:228:VAL:HG21	1.92	0.50
1:D:54:ASP:HB2	1:D:57:ARG:CG	2.40	0.50
1:C:62:VAL:HG11	1:C:92:SER:HB3	1.93	0.50
1:C:54:ASP:HB2	1:C:57:ARG:CG	2.41	0.50
1:E:52:ALA:HA	1:E:95:PRO:O	2.11	0.50
1:D:52:ALA:HA	1:D:95:PRO:O	2.12	0.50
1:A:215:PHE:HB2	1:A:216:TRP:CE3	2.46	0.50
1:E:216:TRP:CZ2	1:E:295:ARG:HB3	2.47	0.50
1:B:215:PHE:HB2	1:B:216:TRP:CE3	2.47	0.50
1:E:19:THR:HG22	1:E:44:LEU:CD2	2.41	0.50
1:E:197:ILE:HA	1:E:201:ILE:HB	1.92	0.50
1:A:267:VAL:HG23	1:A:298:PHE:CZ	2.47	0.50
1:E:298:PHE:CB	1:E:299:PRO:HD3	2.42	0.50
1:D:215:PHE:HB2	1:D:216:TRP:CE3	2.47	0.50
1:D:139:ILE:HG12	1:D:172:ASN:ND2	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:LEU:HD23	1:A:29:LEU:C	2.32	0.50
1:B:118:TYR:HB2	1:B:252:THR:HG22	1.93	0.50
1:A:118:TYR:HB2	1:A:252:THR:HG22	1.94	0.50
1:C:267:VAL:HG23	1:C:298:PHE:CZ	2.46	0.50
1:D:286:ARG:O	1:D:289:SER:HB3	2.11	0.50
1:D:75:ILE:HD13	1:D:131:VAL:HB	1.93	0.50
1:A:224:VAL:C	1:A:226:LEU:N	2.63	0.50
1:A:194:PHE:C	1:A:196:TYR:H	2.14	0.50
1:B:139:ILE:HG12	1:B:172:ASN:ND2	2.27	0.50
1:C:286:ARG:O	1:C:289:SER:HB3	2.11	0.50
1:A:225:THR:HG21	1:B:225:THR:OG1	2.11	0.50
1:D:65:TYR:CG	1:D:70:ILE:HD11	2.46	0.50
1:A:203:PRO:HB3	1:B:262:TYR:CZ	2.46	0.50
1:A:194:PHE:HE2	1:B:250:TYR:O	1.95	0.50
1:E:62:VAL:HG11	1:E:92:SER:HB3	1.92	0.50
1:C:13:GLU:OE1	1:C:14:PRO:HD3	2.12	0.50
1:B:314:PHE:N	1:B:314:PHE:CD1	2.76	0.50
1:D:42:LEU:HB3	1:D:103:GLU:CG	2.40	0.49
1:B:298:PHE:HB2	1:B:299:PRO:HD3	1.93	0.49
1:D:215:PHE:HB3	1:D:295:ARG:HG2	1.93	0.49
1:E:179:LEU:HD12	1:E:179:LEU:C	2.33	0.49
1:C:249:PRO:HD2	1:C:250:TYR:CD1	2.47	0.49
1:E:65:TYR:CG	1:E:70:ILE:HD11	2.48	0.49
1:D:281:GLU:O	1:D:283:GLN:N	2.38	0.49
1:D:216:TRP:CZ2	1:D:295:ARG:HB3	2.46	0.49
1:A:65:TYR:CG	1:A:70:ILE:HD11	2.48	0.49
1:A:27:TYR:CG	1:B:110:LEU:CD1	2.96	0.49
1:A:222:ALA:O	1:B:224:VAL:HG21	2.12	0.49
1:C:215:PHE:O	1:C:291:THR:CG2	2.59	0.49
1:E:84:ARG:CB	1:E:84:ARG:HH11	2.26	0.49
1:D:179:LEU:C	1:D:179:LEU:HD12	2.33	0.49
1:D:29:LEU:HD23	1:D:29:LEU:C	2.33	0.49
1:A:147:LYS:O	1:A:147:LYS:HG2	2.13	0.49
1:A:29:LEU:HD23	1:A:30:ASP:N	2.27	0.49
1:B:179:LEU:HD12	1:B:179:LEU:C	2.33	0.49
1:B:224:VAL:O	1:B:228:VAL:HB	2.12	0.49
1:C:52:ALA:HA	1:C:95:PRO:O	2.12	0.49
1:B:42:LEU:HB3	1:B:103:GLU:CG	2.39	0.49
1:A:216:TRP:CZ2	1:A:295:ARG:HB3	2.48	0.49
1:A:155:PHE:CZ	1:B:112:PRO:CB	2.89	0.49
1:A:155:PHE:HE1	1:B:112:PRO:CB	2.17	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:29:LEU:HD23	1:D:30:ASP:N	2.27	0.49
1:A:41:PHE:HZ	1:B:76:ARG:NH2	2.11	0.49
1:B:147:LYS:HG2	1:B:147:LYS:O	2.12	0.49
1:B:22:TYR:HB3	1:B:41:PHE:HB2	1.95	0.49
1:C:118:TYR:CD1	1:C:118:TYR:C	2.85	0.49
1:A:54:ASP:HB2	1:A:57:ARG:CG	2.42	0.49
1:E:276:HIS:C	1:E:278:LEU:N	2.65	0.49
1:D:84:ARG:CB	1:D:84:ARG:HH11	2.26	0.49
1:B:65:TYR:CG	1:B:70:ILE:HD11	2.48	0.49
1:D:70:ILE:HG22	1:D:71:TRP:N	2.27	0.49
1:C:23:LEU:HB2	1:C:150:LYS:HA	1.95	0.49
1:A:215:PHE:HB3	1:A:295:ARG:HG2	1.95	0.49
1:E:268:ALA:HA	1:E:298:PHE:HE1	1.78	0.49
1:E:278:LEU:HD21	1:E:286:ARG:HB3	1.94	0.49
1:A:18:ASN:HB2	1:A:45:SER:OG	2.12	0.49
1:B:118:TYR:C	1:B:118:TYR:CD1	2.86	0.49
1:A:52:ALA:HA	1:A:95:PRO:O	2.13	0.49
1:D:13:GLU:OE1	1:D:14:PRO:HD3	2.13	0.49
1:A:215:PHE:O	1:A:291:THR:CG2	2.61	0.49
1:B:233:ALA:O	1:B:237:PHE:HD1	1.95	0.49
1:D:19:THR:HG22	1:D:44:LEU:CD2	2.43	0.49
1:A:159:TRP:CE3	1:A:189:ILE:HD12	2.48	0.49
1:B:19:THR:HG22	1:B:44:LEU:CD2	2.43	0.49
1:C:25:GLU:HA	1:C:25:GLU:OE1	2.12	0.49
1:C:213:THR:CG2	1:C:226:LEU:HD11	2.43	0.49
1:D:298:PHE:HB2	1:D:299:PRO:HD3	1.95	0.48
1:E:54:ASP:HB2	1:E:57:ARG:HB2	1.95	0.48
1:D:192:GLN:CD	1:E:249:PRO:HB3	2.34	0.48
1:D:62:VAL:HG11	1:D:92:SER:HB3	1.94	0.48
1:B:261:ILE:CD1	1:B:302:PHE:HE1	2.25	0.48
1:C:54:ASP:HB2	1:C:57:ARG:HB2	1.96	0.48
1:D:68:GLU:H	1:D:68:GLU:CD	2.17	0.48
1:E:215:PHE:HB2	1:E:216:TRP:CE3	2.49	0.48
1:E:54:ASP:HB2	1:E:57:ARG:CG	2.42	0.48
1:A:140:VAL:HG22	1:A:181:SER:HB3	1.95	0.48
1:A:132:ARG:NH2	1:A:178:ARG:HB2	2.29	0.48
1:A:147:LYS:CE	1:A:165:THR:HA	2.44	0.48
1:A:38:VAL:HG22	1:A:39:ASN:N	2.27	0.48
1:A:261:ILE:CD1	1:A:302:PHE:HE1	2.26	0.48
1:E:118:TYR:HB2	1:E:252:THR:HG22	1.94	0.48
1:A:118:TYR:C	1:A:118:TYR:CD1	2.86	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:222:ALA:HB3	1:E:220:TYR:HD2	1.78	0.48
1:E:286:ARG:O	1:E:289:SER:HB3	2.14	0.48
1:E:194:PHE:C	1:E:196:TYR:H	2.16	0.48
1:D:53:PHE:CD1	1:D:95:PRO:HA	2.48	0.48
1:A:13:GLU:OE1	1:A:14:PRO:HD3	2.13	0.48
1:D:224:VAL:C	1:D:226:LEU:N	2.65	0.48
1:A:192:GLN:CD	1:B:249:PRO:HB3	2.34	0.48
1:D:278:LEU:HD21	1:D:286:ARG:HB3	1.94	0.48
1:C:222:ALA:HA	1:D:221:GLU:OE1	2.13	0.48
1:A:232:ILE:HA	1:A:235:ILE:HD12	1.96	0.48
1:D:51:LEU:CD1	1:D:70:ILE:HD12	2.44	0.48
1:A:249:PRO:HD2	1:A:250:TYR:CD1	2.49	0.48
1:C:19:THR:HG22	1:C:44:LEU:CD2	2.43	0.48
1:D:261:ILE:CD1	1:D:302:PHE:HE1	2.26	0.48
1:E:53:PHE:O	1:E:54:ASP:C	2.52	0.48
1:E:267:VAL:HG23	1:E:298:PHE:CZ	2.49	0.48
1:A:210:ILE:HG12	1:B:269:VAL:HG11	1.96	0.48
1:C:70:ILE:HG22	1:C:71:TRP:N	2.28	0.48
1:A:27:TYR:CG	1:B:110:LEU:HD12	2.49	0.47
1:E:238:ASN:CA	1:E:258:ILE:HD11	2.41	0.47
1:A:192:GLN:CG	1:B:249:PRO:HB3	2.44	0.47
1:E:13:GLU:OE1	1:E:14:PRO:HD3	2.13	0.47
1:E:215:PHE:O	1:E:291:THR:CG2	2.61	0.47
1:A:286:ARG:O	1:A:289:SER:HB3	2.13	0.47
1:A:206:PHE:CD1	1:B:262:TYR:HB3	2.49	0.47
1:E:118:TYR:C	1:E:118:TYR:CD1	2.83	0.47
1:C:194:PHE:HA	1:C:197:ILE:HD12	1.96	0.47
1:C:298:PHE:CB	1:C:299:PRO:HD3	2.44	0.47
1:A:54:ASP:HB2	1:A:57:ARG:HB2	1.96	0.47
1:A:298:PHE:CB	1:A:299:PRO:HD3	2.44	0.47
1:C:84:ARG:HA	1:C:107:ALA:HB2	1.96	0.47
1:C:157:THR:HG22	1:D:34:GLU:OE1	2.14	0.47
1:A:133:SER:HB2	1:A:137:ARG:HH11	1.79	0.47
1:D:314:PHE:N	1:D:314:PHE:HD1	2.12	0.47
1:A:196:TYR:CD1	1:A:196:TYR:N	2.82	0.47
1:E:47:LYS:CD	1:E:49:ARG:NH2	2.77	0.47
1:E:8:PRO:O	1:E:50:ARG:NH1	2.48	0.47
1:D:22:TYR:HB3	1:D:41:PHE:HB2	1.97	0.47
1:B:200:ILE:HD11	1:B:240:LEU:CD2	2.39	0.47
1:A:255:GLY:O	1:A:258:ILE:HG22	2.14	0.47
1:E:215:PHE:CE1	1:E:298:PHE:CD1	3.03	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:222:ALA:HB1	1:E:220:TYR:CD2	2.50	0.47
1:C:222:ALA:HB2	1:D:221:GLU:HG2	1.97	0.47
1:D:267:VAL:HG23	1:D:298:PHE:CZ	2.49	0.47
1:A:37:LYS:HG2	1:A:108:ARG:HB3	1.96	0.47
1:D:84:ARG:HB3	1:D:84:ARG:HH11	1.79	0.47
1:D:137:ARG:HA	1:D:137:ARG:HD3	1.62	0.47
1:B:51:LEU:CD1	1:B:70:ILE:HD12	2.44	0.47
1:D:314:PHE:N	1:D:314:PHE:CD1	2.82	0.47
1:D:249:PRO:HD2	1:D:250:TYR:CD1	2.49	0.47
1:C:147:LYS:CE	1:C:165:THR:HA	2.45	0.47
1:C:118:TYR:HB2	1:C:252:THR:HG22	1.96	0.47
1:E:290:ILE:HG22	1:E:291:THR:N	2.28	0.47
1:E:216:TRP:CH2	1:E:295:ARG:HB3	2.50	0.47
1:E:23:LEU:HB2	1:E:150:LYS:HA	1.96	0.47
1:B:24:ILE:HB	1:B:39:ASN:O	2.15	0.47
1:B:53:PHE:O	1:B:54:ASP:C	2.52	0.47
1:C:84:ARG:CB	1:C:84:ARG:HH11	2.28	0.47
1:C:41:PHE:HZ	1:D:76:ARG:NH2	2.13	0.47
1:B:23:LEU:HD22	1:B:38:VAL:HG21	1.96	0.47
1:B:216:TRP:CZ2	1:B:295:ARG:HB3	2.50	0.47
1:C:137:ARG:HA	1:C:137:ARG:HD3	1.60	0.47
1:C:38:VAL:HG22	1:C:39:ASN:N	2.30	0.47
1:A:84:ARG:CB	1:A:84:ARG:HH11	2.28	0.46
1:D:47:LYS:CD	1:D:49:ARG:NH2	2.78	0.46
1:C:140:VAL:HG22	1:C:181:SER:HB3	1.96	0.46
1:D:233:ALA:O	1:D:237:PHE:HD1	1.98	0.46
1:C:179:LEU:C	1:C:179:LEU:HD12	2.36	0.46
1:A:8:PRO:O	1:A:50:ARG:NH1	2.49	0.46
1:E:291:THR:O	1:E:295:ARG:HG3	2.14	0.46
1:C:133:SER:HB2	1:C:137:ARG:HH11	1.80	0.46
1:A:27:TYR:CD1	1:B:81:GLU:OE2	2.68	0.46
1:A:196:TYR:HD1	1:A:196:TYR:N	2.13	0.46
1:D:298:PHE:CB	1:D:299:PRO:HD3	2.45	0.46
1:A:51:LEU:CD1	1:A:70:ILE:HD12	2.45	0.46
1:B:253:TYR:O	1:B:256:ALA:HB3	2.15	0.46
1:C:276:HIS:C	1:C:278:LEU:N	2.68	0.46
1:C:40:ALA:HB3	1:C:105:PHE:CZ	2.51	0.46
1:C:263:LEU:C	1:C:265:TYR:H	2.18	0.46
1:A:104:ARG:HH22	1:B:78:VAL:CA	2.20	0.46
1:B:84:ARG:CB	1:B:84:ARG:HH11	2.28	0.46
1:E:197:ILE:CB	1:E:198:PRO:HD3	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:PHE:CD1	1:B:95:PRO:HA	2.50	0.46
1:E:233:ALA:O	1:E:237:PHE:HD1	1.98	0.46
1:A:132:ARG:HA	1:A:180:GLU:HG2	1.97	0.46
1:E:196:TYR:CD1	1:E:196:TYR:N	2.84	0.46
1:E:283:GLN:C	1:E:285:ALA:N	2.69	0.46
1:D:278:LEU:HD23	1:D:287:ALA:HA	1.97	0.46
1:C:226:LEU:HD23	1:D:224:VAL:HG21	1.97	0.46
1:B:62:VAL:HG11	1:B:92:SER:HB3	1.97	0.46
1:B:84:ARG:HA	1:B:107:ALA:HB2	1.98	0.46
1:E:264:PHE:HE2	1:E:302:PHE:HB2	1.79	0.46
1:C:118:TYR:HB3	1:C:119:PRO:HD3	1.97	0.46
1:A:233:ALA:O	1:A:237:PHE:HD1	1.98	0.46
1:E:253:TYR:HA	1:E:313:PHE:CD2	2.50	0.46
1:B:47:LYS:CD	1:B:49:ARG:NH2	2.79	0.46
1:A:70:ILE:HG22	1:A:71:TRP:N	2.30	0.46
1:B:224:VAL:C	1:B:226:LEU:N	2.65	0.46
1:A:118:TYR:CZ	1:A:196:TYR:HE2	2.34	0.46
1:A:270:ILE:HG22	1:A:271:GLU:N	2.31	0.46
1:C:224:VAL:C	1:C:226:LEU:N	2.68	0.46
1:D:23:LEU:HB2	1:D:150:LYS:HA	1.97	0.45
1:A:215:PHE:CE1	1:A:298:PHE:CD1	3.05	0.45
1:A:276:HIS:C	1:A:278:LEU:N	2.69	0.45
1:E:140:VAL:HG22	1:E:181:SER:HB3	1.98	0.45
1:E:84:ARG:HA	1:E:107:ALA:HB2	1.98	0.45
1:E:51:LEU:CD1	1:E:70:ILE:HD12	2.46	0.45
1:D:48:ASP:O	1:D:50:ARG:N	2.49	0.45
1:B:132:ARG:HA	1:B:180:GLU:HG2	1.99	0.45
1:B:84:ARG:HH11	1:B:84:ARG:HB3	1.81	0.45
1:C:222:ALA:CB	1:D:221:GLU:HA	2.44	0.45
1:D:141:LEU:HD23	1:D:142:ALA:H	1.81	0.45
1:E:38:VAL:HG22	1:E:39:ASN:N	2.31	0.45
1:E:204:MET:O	1:E:207:ILE:HG12	2.15	0.45
1:A:194:PHE:CE2	1:B:250:TYR:O	2.70	0.45
1:C:47:LYS:CD	1:C:49:ARG:NH2	2.78	0.45
1:B:278:LEU:HD23	1:B:287:ALA:HA	1.98	0.45
1:D:118:TYR:CD1	1:D:118:TYR:C	2.88	0.45
1:A:206:PHE:HD1	1:B:262:TYR:HB3	1.80	0.45
1:C:204:MET:O	1:C:207:ILE:HG12	2.17	0.45
1:D:196:TYR:N	1:D:196:TYR:HD1	2.15	0.45
1:A:44:LEU:HD12	1:A:101:TYR:CD2	2.52	0.45
1:D:159:TRP:CE3	1:D:189:ILE:HD12	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:ILE:CB	1:A:198:PRO:HD3	2.41	0.45
1:A:270:ILE:HA	1:A:270:ILE:HD13	1.57	0.45
1:D:215:PHE:O	1:D:291:THR:CG2	2.62	0.45
1:A:137:ARG:HD3	1:A:137:ARG:HA	1.60	0.45
1:A:268:ALA:HA	1:A:298:PHE:HE1	1.81	0.45
1:C:77:PHE:HB3	1:C:80:VAL:CG2	2.47	0.45
1:E:133:SER:HB2	1:E:137:ARG:HH11	1.81	0.45
1:C:53:PHE:HE2	1:C:63:LYS:CB	2.24	0.45
1:D:216:TRP:CE2	1:D:295:ARG:HD3	2.52	0.45
1:C:51:LEU:CD1	1:C:70:ILE:HD12	2.46	0.45
1:A:209:PHE:HB2	1:B:266:PHE:CE1	2.52	0.45
1:D:132:ARG:HA	1:D:180:GLU:HG2	1.98	0.45
1:B:38:VAL:HG22	1:B:39:ASN:N	2.32	0.45
1:A:158:GLY:HA2	1:A:192:GLN:OE1	2.17	0.45
1:E:42:LEU:HB3	1:E:103:GLU:CG	2.42	0.45
1:C:210:ILE:HD12	1:D:231:LEU:HD22	1.98	0.45
1:D:226:LEU:HD22	1:D:226:LEU:HA	1.57	0.45
1:D:84:ARG:HA	1:D:107:ALA:HB2	1.98	0.45
1:D:196:TYR:N	1:D:196:TYR:CD1	2.84	0.45
1:B:8:PRO:O	1:B:50:ARG:NH1	2.50	0.45
1:C:68:GLU:H	1:C:68:GLU:CD	2.20	0.45
1:D:173:PHE:HZ	1:D:182:LYS:HZ1	1.63	0.45
1:A:200:ILE:HD11	1:A:240:LEU:CD2	2.39	0.45
1:C:210:ILE:HG21	1:D:228:VAL:HG22	1.99	0.45
1:D:77:PHE:CD1	1:D:84:ARG:CD	3.00	0.45
1:D:206:PHE:CE1	1:E:263:LEU:CD1	3.00	0.45
1:E:224:VAL:C	1:E:226:LEU:H	2.19	0.45
1:D:38:VAL:HG22	1:D:39:ASN:N	2.31	0.44
1:B:196:TYR:N	1:B:196:TYR:CD1	2.85	0.44
1:E:53:PHE:CD1	1:E:95:PRO:HA	2.51	0.44
1:B:291:THR:O	1:B:295:ARG:HG3	2.16	0.44
1:D:146:GLU:HG3	1:E:176:GLU:CG	2.47	0.44
1:C:201:ILE:HA	1:C:201:ILE:HD13	1.83	0.44
1:C:53:PHE:O	1:C:54:ASP:C	2.54	0.44
1:D:37:LYS:HG2	1:D:108:ARG:HB3	1.99	0.44
1:B:283:GLN:C	1:B:285:ALA:N	2.70	0.44
1:A:77:PHE:CD1	1:A:84:ARG:CD	2.99	0.44
1:A:278:LEU:HD23	1:A:287:ALA:HA	1.98	0.44
1:B:159:TRP:CE3	1:B:189:ILE:HD12	2.52	0.44
1:C:159:TRP:CE3	1:C:189:ILE:HD12	2.52	0.44
1:C:72:ILE:HG22	1:C:73:PRO:HD2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:LEU:HD23	1:B:224:VAL:CG2	2.46	0.44
1:C:291:THR:O	1:C:295:ARG:HG3	2.17	0.44
1:C:89:VAL:CG2	1:D:76:ARG:HD3	2.47	0.44
1:D:210:ILE:CG2	1:E:269:VAL:HG11	2.36	0.44
1:C:8:PRO:O	1:C:50:ARG:NH1	2.50	0.44
1:D:253:TYR:O	1:D:256:ALA:HB3	2.17	0.44
1:C:155:PHE:HD1	1:D:110:LEU:HD22	1.82	0.44
1:B:267:VAL:HG23	1:B:298:PHE:CZ	2.52	0.44
1:C:278:LEU:HD23	1:C:287:ALA:HA	1.99	0.44
1:E:196:TYR:N	1:E:196:TYR:HD1	2.15	0.44
1:C:118:TYR:CZ	1:C:196:TYR:HE2	2.36	0.44
1:E:23:LEU:HG	1:E:164:PHE:CD1	2.52	0.44
1:D:225:THR:HG21	1:E:224:VAL:CG2	2.37	0.44
1:A:201:ILE:HA	1:A:201:ILE:HD13	1.86	0.44
1:C:268:ALA:HA	1:C:298:PHE:HE1	1.82	0.44
1:C:278:LEU:HD21	1:C:286:ARG:HB3	1.98	0.44
1:A:18:ASN:O	1:A:44:LEU:HA	2.18	0.44
1:B:141:LEU:HD23	1:B:142:ALA:H	1.82	0.44
1:E:72:ILE:HG22	1:E:73:PRO:HD2	1.99	0.44
1:A:53:PHE:O	1:A:54:ASP:C	2.56	0.44
1:C:216:TRP:CZ2	1:C:295:ARG:HB3	2.52	0.44
1:C:270:ILE:HA	1:C:270:ILE:HD13	1.61	0.44
1:E:300:VAL:O	1:E:304:LEU:HB2	2.18	0.44
1:D:118:TYR:CZ	1:D:196:TYR:HE2	2.36	0.44
1:B:232:ILE:HA	1:B:235:ILE:HD12	2.00	0.44
1:A:23:LEU:HB2	1:A:150:LYS:HA	1.99	0.44
1:E:23:LEU:HD22	1:E:38:VAL:HG21	1.99	0.44
1:D:225:THR:HG22	1:E:224:VAL:CG2	2.44	0.44
1:A:202:LEU:CB	1:B:259:PHE:HE1	2.31	0.44
1:C:283:GLN:C	1:C:285:ALA:N	2.71	0.44
1:C:202:LEU:HD12	1:D:259:PHE:CZ	2.53	0.44
1:B:298:PHE:CB	1:B:299:PRO:HD3	2.47	0.44
1:B:140:VAL:HG22	1:B:181:SER:HB3	2.00	0.44
1:D:202:LEU:HD12	1:E:259:PHE:HZ	1.82	0.44
1:C:264:PHE:HE2	1:C:302:PHE:HB2	1.82	0.43
1:C:196:TYR:O	1:C:200:ILE:HB	2.17	0.43
1:B:268:ALA:HA	1:B:298:PHE:HE1	1.82	0.43
1:D:224:VAL:O	1:D:228:VAL:HB	2.17	0.43
1:C:232:ILE:HA	1:C:235:ILE:HD12	1.99	0.43
1:C:23:LEU:CD1	1:C:164:PHE:CD1	3.01	0.43
1:B:23:LEU:HB2	1:B:150:LYS:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:118:TYR:CZ	1:E:196:TYR:HE2	2.36	0.43
1:B:119:PRO:HD3	1:B:254:THR:OG1	2.18	0.43
1:E:263:LEU:C	1:E:265:TYR:H	2.21	0.43
1:A:253:TYR:O	1:A:256:ALA:HB3	2.18	0.43
1:B:215:PHE:O	1:B:291:THR:CG2	2.62	0.43
1:C:27:TYR:HB3	1:D:110:LEU:CD1	2.44	0.43
1:B:216:TRP:CH2	1:B:295:ARG:HB3	2.53	0.43
1:D:216:TRP:CH2	1:D:295:ARG:HB3	2.53	0.43
1:A:224:VAL:C	1:A:226:LEU:H	2.22	0.43
1:A:204:MET:O	1:A:207:ILE:HG12	2.19	0.43
1:C:37:LYS:HG2	1:C:108:ARG:HB3	1.99	0.43
1:D:72:ILE:HG22	1:D:73:PRO:HD2	2.00	0.43
1:C:173:PHE:HZ	1:C:182:LYS:HZ1	1.65	0.43
1:B:147:LYS:CE	1:B:165:THR:HA	2.49	0.43
1:C:199:ASN:HB3	1:D:242:GLU:OE1	2.18	0.43
1:C:222:ALA:HB2	1:D:221:GLU:CG	2.47	0.43
1:D:8:PRO:O	1:D:50:ARG:NH1	2.52	0.43
1:E:40:ALA:HB3	1:E:105:PHE:CZ	2.54	0.43
1:C:256:ALA:HB1	1:C:309:LEU:HD21	2.00	0.43
1:C:226:LEU:HA	1:C:226:LEU:HD22	1.58	0.43
1:A:224:VAL:O	1:A:228:VAL:HB	2.18	0.43
1:C:260:MET:HE3	1:C:309:LEU:HD22	2.01	0.43
1:E:118:TYR:HB3	1:E:119:PRO:HD3	2.00	0.43
1:E:270:ILE:HA	1:E:270:ILE:HD13	1.59	0.43
1:D:268:ALA:HA	1:D:298:PHE:HE1	1.84	0.43
1:D:140:VAL:HG22	1:D:181:SER:HB3	1.99	0.43
1:C:231:LEU:HD13	1:C:265:TYR:HB3	2.00	0.43
1:B:40:ALA:HB3	1:B:105:PHE:CZ	2.54	0.43
1:D:256:ALA:HB1	1:D:309:LEU:HD21	2.01	0.43
1:E:196:TYR:O	1:E:200:ILE:HB	2.18	0.43
1:B:249:PRO:HD2	1:B:250:TYR:CE1	2.54	0.43
1:D:283:GLN:C	1:D:285:ALA:N	2.71	0.43
1:A:217:SER:CB	1:B:220:TYR:CE2	3.02	0.43
1:A:140:VAL:HG22	1:A:181:SER:CB	2.49	0.43
1:B:123:GLN:HA	1:B:123:GLN:HE21	1.83	0.43
1:E:232:ILE:HA	1:E:235:ILE:HD12	2.01	0.43
1:E:25:GLU:HA	1:E:25:GLU:OE1	2.19	0.43
1:B:196:TYR:HD1	1:B:196:TYR:N	2.16	0.43
1:A:253:TYR:HA	1:A:313:PHE:CD2	2.52	0.42
1:B:204:MET:O	1:B:207:ILE:HG12	2.19	0.42
1:E:256:ALA:HB1	1:E:309:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:TRP:CH2	1:A:295:ARG:HB3	2.54	0.42
1:D:291:THR:O	1:D:295:ARG:HG3	2.18	0.42
1:B:158:GLY:HA2	1:B:192:GLN:OE1	2.19	0.42
1:E:137:ARG:HA	1:E:137:ARG:HD3	1.66	0.42
1:A:118:TYR:HB3	1:A:119:PRO:HD3	2.01	0.42
1:C:51:LEU:HD13	1:C:70:ILE:HD12	2.01	0.42
1:A:23:LEU:HD22	1:A:38:VAL:HG21	2.00	0.42
1:C:53:PHE:CD1	1:C:95:PRO:HA	2.54	0.42
1:C:215:PHE:CE1	1:C:298:PHE:CD1	3.07	0.42
1:B:226:LEU:HA	1:B:226:LEU:HD22	1.61	0.42
1:E:119:PRO:HD3	1:E:254:THR:OG1	2.19	0.42
1:E:278:LEU:HD23	1:E:287:ALA:HA	2.00	0.42
1:C:65:TYR:CD2	1:C:70:ILE:HD11	2.54	0.42
1:D:132:ARG:NH2	1:D:178:ARG:HB2	2.35	0.42
1:D:286:ARG:O	1:D:287:ALA:C	2.58	0.42
1:D:213:THR:CG2	1:D:226:LEU:HD11	2.48	0.42
1:A:47:LYS:CD	1:A:49:ARG:NH2	2.81	0.42
1:B:25:GLU:OE1	1:B:25:GLU:HA	2.19	0.42
1:E:76:ARG:CZ	1:E:130:ILE:HD12	2.48	0.42
1:B:118:TYR:HB3	1:B:119:PRO:HD3	2.00	0.42
1:A:53:PHE:CD1	1:A:95:PRO:HA	2.53	0.42
1:B:18:ASN:HB2	1:B:45:SER:OG	2.20	0.42
1:A:213:THR:CG2	1:A:226:LEU:HD11	2.48	0.42
1:C:197:ILE:HB	1:C:198:PRO:CD	2.43	0.42
1:B:118:TYR:CZ	1:B:196:TYR:HE2	2.37	0.42
1:B:53:PHE:HE2	1:B:63:LYS:CB	2.26	0.42
1:C:77:PHE:HB3	1:C:80:VAL:HG23	2.01	0.42
1:C:151:ASN:ND2	1:C:152:ASP:H	2.17	0.42
1:D:25:GLU:HA	1:D:25:GLU:OE1	2.19	0.42
1:E:132:ARG:HA	1:E:180:GLU:HG2	2.01	0.42
1:D:278:LEU:HD23	1:D:287:ALA:CA	2.50	0.42
1:A:77:PHE:HB3	1:A:80:VAL:CG2	2.49	0.42
1:D:133:SER:HB2	1:D:137:ARG:HH11	1.84	0.42
1:A:68:GLU:CD	1:A:68:GLU:H	2.23	0.42
1:E:130:ILE:HG23	1:E:182:LYS:HB2	2.01	0.42
1:B:282:SER:C	1:B:284:PRO:HD3	2.39	0.42
1:A:291:THR:O	1:A:295:ARG:HG3	2.20	0.42
1:B:133:SER:HB2	1:B:137:ARG:HH11	1.84	0.42
1:A:278:LEU:HD21	1:A:286:ARG:HB3	2.01	0.42
1:A:286:ARG:O	1:A:287:ALA:C	2.58	0.42
1:A:248:THR:HB	1:A:250:TYR:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:THR:HG22	1:B:244:ASN:ND2	2.34	0.42
1:E:243:THR:HG22	1:E:244:ASN:ND2	2.35	0.42
1:E:260:MET:HE1	1:E:305:ALA:C	2.41	0.41
1:B:238:ASN:CA	1:B:258:ILE:HD11	2.43	0.41
1:A:25:GLU:HA	1:A:25:GLU:OE1	2.20	0.41
1:B:248:THR:HB	1:B:250:TYR:CE1	2.55	0.41
1:D:201:ILE:HA	1:D:201:ILE:HD13	1.81	0.41
1:C:132:ARG:HA	1:C:180:GLU:HG2	2.01	0.41
1:A:216:TRP:CE2	1:A:295:ARG:HD3	2.55	0.41
1:B:215:PHE:CE1	1:B:298:PHE:CD1	3.07	0.41
1:D:224:VAL:C	1:D:226:LEU:H	2.22	0.41
1:C:140:VAL:HG22	1:C:181:SER:CB	2.50	0.41
1:D:84:ARG:NH1	1:D:84:ARG:CB	2.84	0.41
1:E:140:VAL:HG22	1:E:181:SER:CB	2.50	0.41
1:A:19:THR:HA	1:A:43:SER:O	2.20	0.41
1:C:233:ALA:O	1:C:237:PHE:HD1	2.02	0.41
1:D:18:ASN:O	1:D:44:LEU:HA	2.20	0.41
1:C:44:LEU:HD12	1:C:101:TYR:CD2	2.55	0.41
1:D:28:SER:HB2	1:D:37:LYS:HD2	2.02	0.41
1:A:53:PHE:HE2	1:A:63:LYS:CB	2.25	0.41
1:C:224:VAL:O	1:C:228:VAL:HB	2.19	0.41
1:D:215:PHE:CE1	1:D:298:PHE:CD1	3.09	0.41
1:C:158:GLY:HA2	1:C:192:GLN:OE1	2.20	0.41
1:E:158:GLY:HA2	1:E:192:GLN:OE1	2.19	0.41
1:B:132:ARG:NH2	1:B:178:ARG:HB2	2.35	0.41
1:D:40:ALA:HB3	1:D:105:PHE:CZ	2.55	0.41
1:A:104:ARG:NH1	1:B:77:PHE:O	2.53	0.41
1:E:224:VAL:O	1:E:228:VAL:HB	2.21	0.41
1:A:264:PHE:HE2	1:A:302:PHE:HB2	1.84	0.41
1:A:194:PHE:HA	1:A:197:ILE:HD12	2.03	0.41
1:C:274:VAL:C	1:C:276:HIS:N	2.72	0.41
1:D:50:ARG:HB3	1:D:50:ARG:HE	1.69	0.41
1:B:224:VAL:C	1:B:226:LEU:H	2.22	0.41
1:D:24:ILE:HB	1:D:39:ASN:O	2.20	0.41
1:C:196:TYR:N	1:C:196:TYR:CD1	2.88	0.41
1:E:37:LYS:HG2	1:E:108:ARG:HB3	2.02	0.41
1:A:274:VAL:C	1:A:276:HIS:N	2.72	0.41
1:B:68:GLU:H	1:B:68:GLU:CD	2.23	0.41
1:E:213:THR:HG22	1:E:226:LEU:HD12	2.01	0.41
1:E:213:THR:CG2	1:E:226:LEU:HD11	2.48	0.41
1:B:194:PHE:HA	1:B:197:ILE:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:218:THR:HA	1:C:275:GLN:HE22	1.86	0.41
1:C:77:PHE:CD1	1:C:84:ARG:CD	3.03	0.41
1:A:18:ASN:HB3	1:A:143:VAL:CG2	2.50	0.41
1:D:48:ASP:C	1:D:50:ARG:N	2.73	0.41
1:A:263:LEU:C	1:A:265:TYR:H	2.24	0.41
1:D:200:ILE:HD11	1:D:240:LEU:CD2	2.43	0.41
1:D:259:PHE:C	1:D:259:PHE:CD2	2.94	0.41
1:E:84:ARG:HB3	1:E:84:ARG:HH11	1.83	0.41
1:C:271:GLU:O	1:C:272:VAL:C	2.58	0.41
1:B:37:LYS:HG2	1:B:108:ARG:HB3	2.03	0.41
1:D:155:PHE:HB3	1:D:156:LEU:H	1.73	0.41
1:E:150:LYS:HG2	1:E:154:VAL:HG21	2.01	0.41
1:D:23:LEU:CD2	1:D:38:VAL:HG21	2.51	0.41
1:A:192:GLN:HB3	1:B:249:PRO:HB3	2.02	0.41
1:D:123:GLN:HB2	1:D:189:ILE:HG13	2.03	0.41
1:A:51:LEU:HD13	1:A:70:ILE:HD12	2.02	0.41
1:C:19:THR:HA	1:C:43:SER:O	2.20	0.41
1:B:28:SER:HB2	1:B:37:LYS:HD2	2.03	0.41
1:B:213:THR:CG2	1:B:226:LEU:HD11	2.49	0.41
1:B:23:LEU:HG	1:B:164:PHE:CD1	2.55	0.41
1:D:204:MET:O	1:D:207:ILE:HG12	2.21	0.41
1:E:194:PHE:O	1:E:198:PRO:HD2	2.20	0.41
1:A:194:PHE:CE2	1:B:250:TYR:C	2.95	0.41
1:D:213:THR:HG22	1:D:226:LEU:HD12	2.01	0.41
1:A:80:VAL:HG12	1:A:82:ASN:O	2.21	0.41
1:E:286:ARG:O	1:E:287:ALA:C	2.59	0.41
1:C:286:ARG:O	1:C:287:ALA:C	2.59	0.41
1:D:18:ASN:HB3	1:D:143:VAL:CG2	2.51	0.41
1:E:65:TYR:CD2	1:E:70:ILE:HD11	2.56	0.41
1:B:263:LEU:C	1:B:265:TYR:H	2.23	0.41
1:B:35:THR:OG1	1:B:108:ARG:NH2	2.54	0.41
1:D:41:PHE:CE2	1:E:175:LEU:CD2	3.01	0.41
1:D:253:TYR:HA	1:D:313:PHE:CD2	2.49	0.41
1:E:282:SER:C	1:E:284:PRO:HD3	2.41	0.41
1:A:84:ARG:HB3	1:A:84:ARG:HH11	1.86	0.41
1:C:237:PHE:CE1	1:D:235:ILE:HG21	2.56	0.41
1:D:282:SER:C	1:D:284:PRO:HD3	2.40	0.40
1:D:197:ILE:CB	1:D:198:PRO:HD3	2.45	0.40
1:A:157:THR:HG21	1:B:34:GLU:HG3	2.03	0.40
1:B:278:LEU:HD23	1:B:287:ALA:CA	2.51	0.40
1:C:248:THR:HB	1:C:250:TYR:CE1	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:ALA:HB3	1:A:105:PHE:CZ	2.56	0.40
1:A:259:PHE:C	1:A:259:PHE:CD2	2.94	0.40
1:A:155:PHE:CE1	1:B:112:PRO:CA	3.03	0.40
1:C:194:PHE:O	1:C:198:PRO:HD2	2.21	0.40
1:D:232:ILE:HA	1:D:235:ILE:HD12	2.02	0.40
1:E:51:LEU:HD13	1:E:70:ILE:HD12	2.03	0.40
1:A:65:TYR:CD2	1:A:70:ILE:HD11	2.56	0.40
1:A:8:PRO:HA	1:A:71:TRP:CG	2.57	0.40
1:C:243:THR:HG22	1:C:244:ASN:ND2	2.37	0.40
1:E:151:ASN:ND2	1:E:152:ASP:H	2.19	0.40
1:D:271:GLU:OE2	1:D:272:VAL:N	2.54	0.40
1:B:77:PHE:HB3	1:B:80:VAL:CG2	2.51	0.40
1:C:253:TYR:HA	1:C:313:PHE:CD2	2.51	0.40
1:B:19:THR:HA	1:B:43:SER:O	2.22	0.40
1:A:27:TYR:CE1	1:B:81:GLU:CD	2.94	0.40
1:E:144:ASP:HA	1:E:147:LYS:HB3	2.04	0.40
1:C:23:LEU:HG	1:C:164:PHE:CD1	2.56	0.40
1:B:130:ILE:HG23	1:B:182:LYS:HB2	2.03	0.40
1:B:23:LEU:CD2	1:B:38:VAL:HG21	2.51	0.40
1:C:253:TYR:O	1:C:256:ALA:HB3	2.21	0.40
1:B:255:GLY:O	1:B:258:ILE:HG22	2.21	0.40
1:B:274:VAL:C	1:B:276:HIS:N	2.74	0.40
1:B:137:ARG:HD3	1:B:137:ARG:HA	1.65	0.40
1:D:19:THR:HA	1:D:43:SER:O	2.22	0.40
1:A:72:ILE:HG22	1:A:73:PRO:HD2	2.04	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%)	59 (19%)	10 (3%)	5	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	308/317 (97%)	238 (77%)	61 (20%)	9 (3%)	6	44
1	C	308/317 (97%)	235 (76%)	64 (21%)	9 (3%)	6	44
1	D	308/317 (97%)	238 (77%)	61 (20%)	9 (3%)	6	44
1	E	308/317 (97%)	239 (78%)	61 (20%)	8 (3%)	7	46
All	All	1540/1585 (97%)	1189 (77%)	306 (20%)	45 (3%)	6	44

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	118	TYR
1	A	148	VAL
1	A	150	LYS
1	A	194	PHE
1	B	118	TYR
1	B	148	VAL
1	B	150	LYS
1	B	194	PHE
1	C	118	TYR
1	C	148	VAL
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	277	TYR
1	B	275	GLN
1	B	277	TYR
1	C	277	TYR
1	D	277	TYR
1	E	275	GLN
1	E	277	TYR
1	A	275	GLN
1	B	81	GLU
1	C	275	GLN
1	D	275	GLN
1	D	287	ALA

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Mol	Chain	Res	Type
1	E	287	ALA
1	A	81	GLU
1	A	287	ALA
1	B	287	ALA
1	C	81	GLU
1	C	287	ALA
1	E	81	GLU
1	D	81	GLU
1	A	49	ARG
1	B	10	ILE
1	C	10	ILE
1	A	10	ILE
1	D	10	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%)	234 (84%)	44 (16%)	3	22
1	B	278/284 (98%)	234 (84%)	44 (16%)	3	22
1	C	278/284 (98%)	234 (84%)	44 (16%)	3	22
1	D	278/284 (98%)	234 (84%)	44 (16%)	3	22
1	E	278/284 (98%)	235 (84%)	43 (16%)	3	23
All	All	1390/1420 (98%)	1171 (84%)	219 (16%)	3	22

All (219) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	PHE
1	A	54	ASP
1	A	57	ARG
1	A	64	THR
1	A	68	GLU
1	A	72	ILE

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Mol	Chain	Res	Type
1	A	79	ASN
1	A	84	ARG
1	A	98	THR
1	A	100	GLN
1	A	104	ARG
1	A	122	SER
1	A	124	THR
1	A	130	ILE
1	A	140	VAL
1	A	141	LEU
1	A	151	ASN
1	A	154	VAL
1	A	155	PHE
1	A	162	GLU
1	A	177	ASP
1	A	178	ARG
1	A	179	LEU
1	A	202	LEU
1	A	211	SER
1	A	212	TRP
1	A	213	THR
1	A	218	THR
1	A	221	GLU
1	A	226	LEU
1	A	241	VAL
1	A	243	THR
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	282	SER
1	A	292	ARG
1	A	303	LEU
1	A	306	ASN
1	A	314	PHE
1	B	53	PHE
1	B	54	ASP
1	B	57	ARG
1	B	64	THR

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Mol	Chain	Res	Type
1	B	68	GLU
1	B	72	ILE
1	B	79	ASN
1	B	84	ARG
1	B	98	THR
1	B	100	GLN
1	B	104	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
1	B	178	ARG
1	B	179	LEU
1	B	202	LEU
1	B	211	SER
1	B	212	TRP
1	B	213	THR
1	B	218	THR
1	B	221	GLU
1	B	226	LEU
1	B	241	VAL
1	B	243	THR
1	B	252	THR
1	B	254	THR
1	B	257	ILE
1	B	260	MET
1	B	263	LEU
1	B	269	VAL
1	B	270	ILE
1	B	274	VAL
1	B	282	SER
1	B	292	ARG
1	B	303	LEU
1	B	306	ASN
1	B	314	PHE
1	C	53	PHE
1	C	54	ASP

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Mol	Chain	Res	Type
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	98	THR
1	C	100	GLN
1	C	104	ARG
1	C	122	SER
1	C	124	THR
1	C	130	ILE
1	C	140	VAL
1	C	141	LEU
1	C	151	ASN
1	C	154	VAL
1	C	155	PHE
1	C	162	GLU
1	C	178	ARG
1	C	179	LEU
1	C	202	LEU
1	C	211	SER
1	C	212	TRP
1	C	213	THR
1	C	218	THR
1	C	221	GLU
1	C	226	LEU
1	C	241	VAL
1	C	243	THR
1	C	252	THR
1	C	254	THR
1	C	257	ILE
1	C	260	MET
1	C	263	LEU
1	C	269	VAL
1	C	270	ILE
1	C	274	VAL
1	C	282	SER
1	C	292	ARG
1	C	303	LEU
1	C	306	ASN
1	C	314	PHE

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Mol	Chain	Res	Type
1	D	53	PHE
1	D	54	ASP
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	98	THR
1	D	100	GLN
1	D	104	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	162	GLU
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	218	THR
1	D	221	GLU
1	D	226	LEU
1	D	241	VAL
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	282	SER
1	D	292	ARG
1	D	303	LEU

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Mol	Chain	Res	Type
1	D	306	ASN
1	D	314	PHE
1	E	53	PHE
1	E	54	ASP
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	98	THR
1	E	100	GLN
1	E	104	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	178	ARG
1	E	179	LEU
1	E	202	LEU
1	E	211	SER
1	E	212	TRP
1	E	213	THR
1	E	218	THR
1	E	221	GLU
1	E	226	LEU
1	E	241	VAL
1	E	243	THR
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	282	SER
1	E	292	ARG

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Mol	Chain	Res	Type
1	E	303	LEU
1	E	306	ASN
1	E	314	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	ASN
1	A	100	GLN
1	A	151	ASN
1	A	244	ASN
1	A	275	GLN
1	B	79	ASN
1	B	100	GLN
1	B	151	ASN
1	B	244	ASN
1	B	275	GLN
1	C	79	ASN
1	C	100	GLN
1	C	151	ASN
1	C	234	HIS
1	C	244	ASN
1	C	275	GLN
1	D	79	ASN
1	D	100	GLN
1	D	123	GLN
1	D	151	ASN
1	D	244	ASN
1	D	275	GLN
1	E	79	ASN
1	E	100	GLN
1	E	151	ASN
1	E	244	ASN
1	E	275	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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, 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%)	-0.08	5 (1%) 74 61	77, 116, 170, 252	0
1	B	310/317 (97%)	-0.07	11 (3%) 48 34	77, 116, 170, 251	0
1	C	310/317 (97%)	-0.13	5 (1%) 74 61	77, 115, 169, 250	0
1	D	310/317 (97%)	-0.09	1 (0%) 94 90	75, 115, 169, 252	0
1	E	310/317 (97%)	-0.11	8 (2%) 59 44	79, 115, 170, 251	0
All	All	1550/1585 (97%)	-0.10	30 (1%) 70 56	75, 116, 170, 252	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	59	GLY	5.4
1	C	59	GLY	4.3
1	A	59	GLY	4.3
1	B	91	ILE	3.9
1	C	61	ARG	3.8
1	C	316	PHE	3.5
1	B	65	TYR	3.3
1	E	58	SER	3.3
1	A	60	VAL	2.9
1	B	63	LYS	2.9
1	C	60	VAL	2.9
1	B	90	ASP	2.9
1	A	316	PHE	2.9
1	E	65	TYR	2.8
1	E	315	GLY	2.8
1	B	64	THR	2.6
1	E	57	ARG	2.5
1	B	92	SER	2.5
1	B	67	PRO	2.4
1	B	57	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	93	VAL	2.2
1	A	54	ASP	2.2
1	A	58	SER	2.2
1	E	63	LYS	2.1
1	D	316	PHE	2.1
1	B	282	SER	2.1
1	E	91	ILE	2.1
1	C	58	SER	2.1
1	B	59	GLY	2.0
1	B	93	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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, 95th 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(\AA^2)	Q<0.9
2	ARS	C	1317	1/1	0.70	1.16	-	206,206,206,206	0

6.5 Other polymers [i](#)

There are no such residues in this entry.