



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:40 AM UTC

PDB ID : 2XQ4 / pdb_00002xq4
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

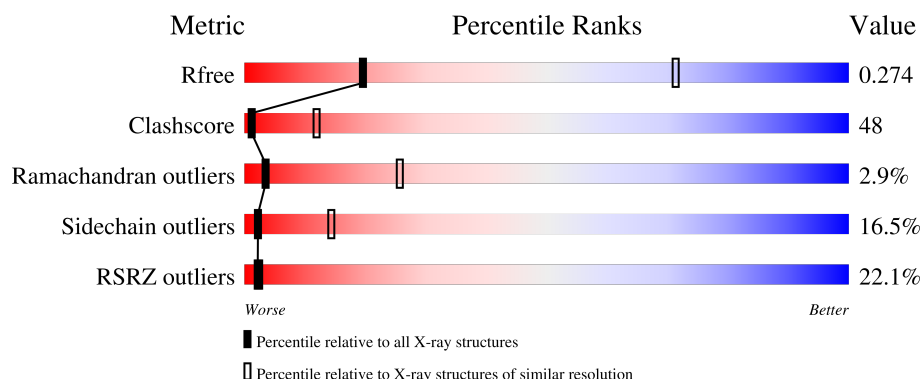
1 Overall quality at a glance

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}	180053	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	23% 31% 53% 13% ..
1	B	317	19% 30% 53% 13% ..
1	C	317	18% 34% 50% 13% ..
1	D	317	25% 32% 53% 12% ..
1	E	317	23% 34% 50% 13% ..

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			

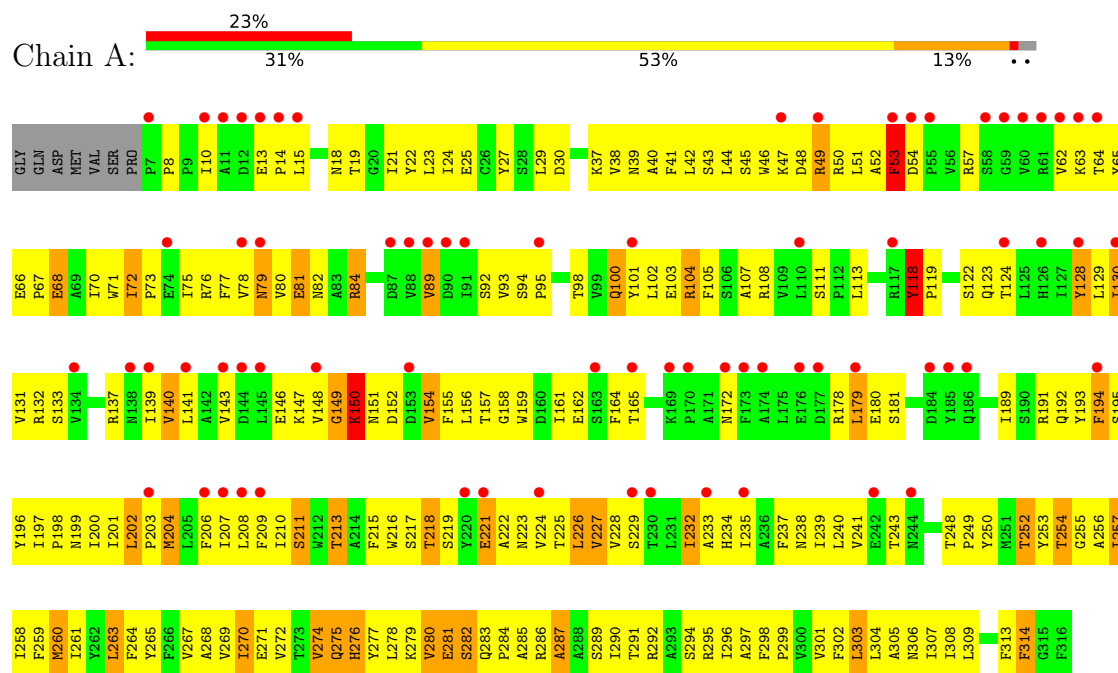
- Molecule 2 is ARSENIC (CCD ID: ARS) (formula: As).

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

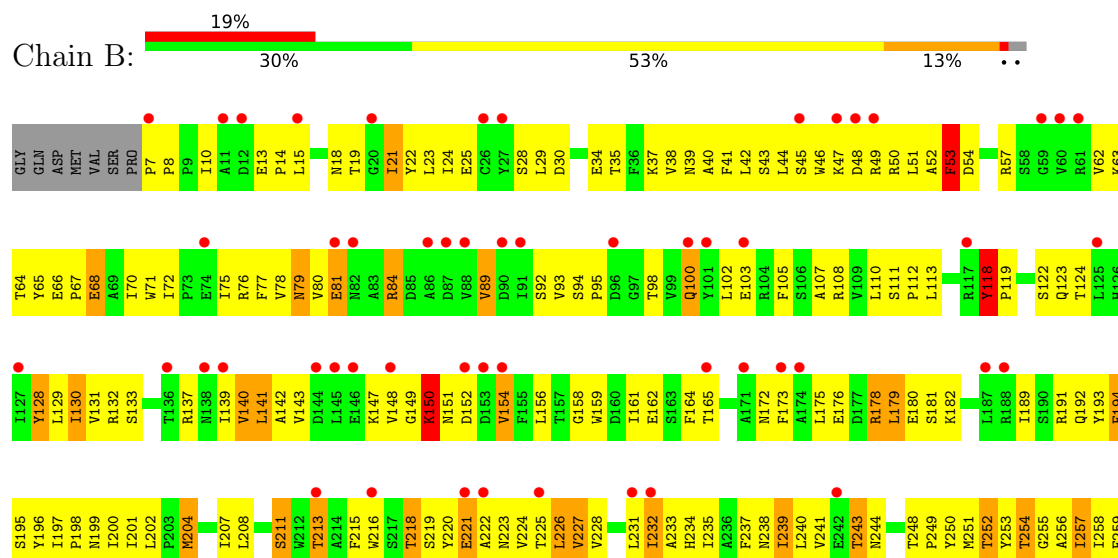
3 Residue-property plots

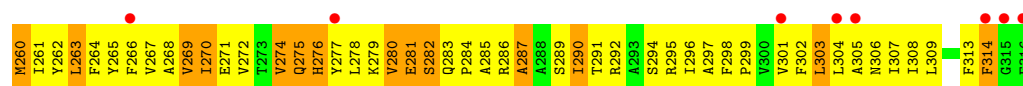
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: GLR4197 PROTEIN

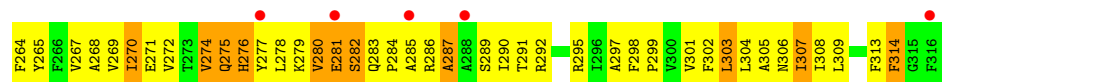
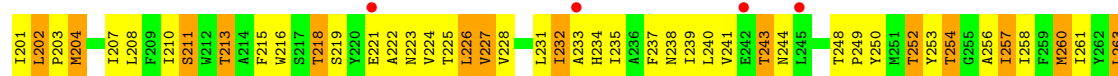
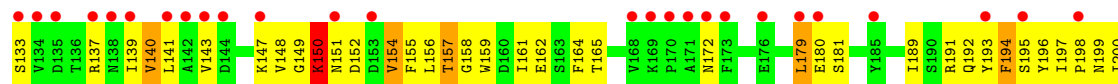
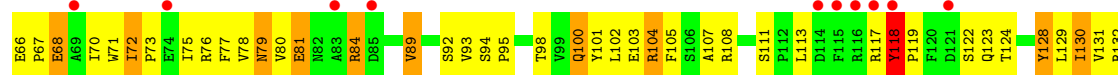


• Molecule 1: GLR4197 PROTEIN

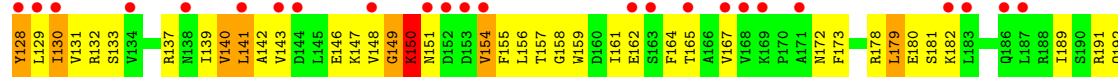
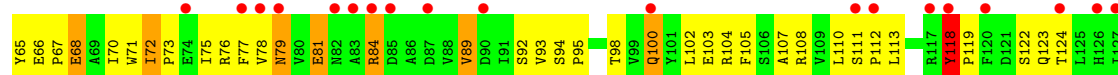
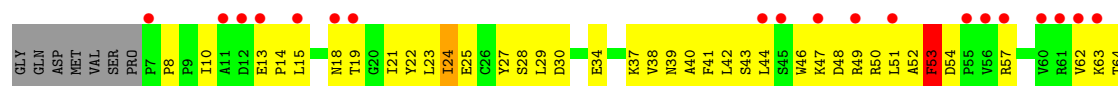




● Molecule 1: GLR4197 PROTEIN

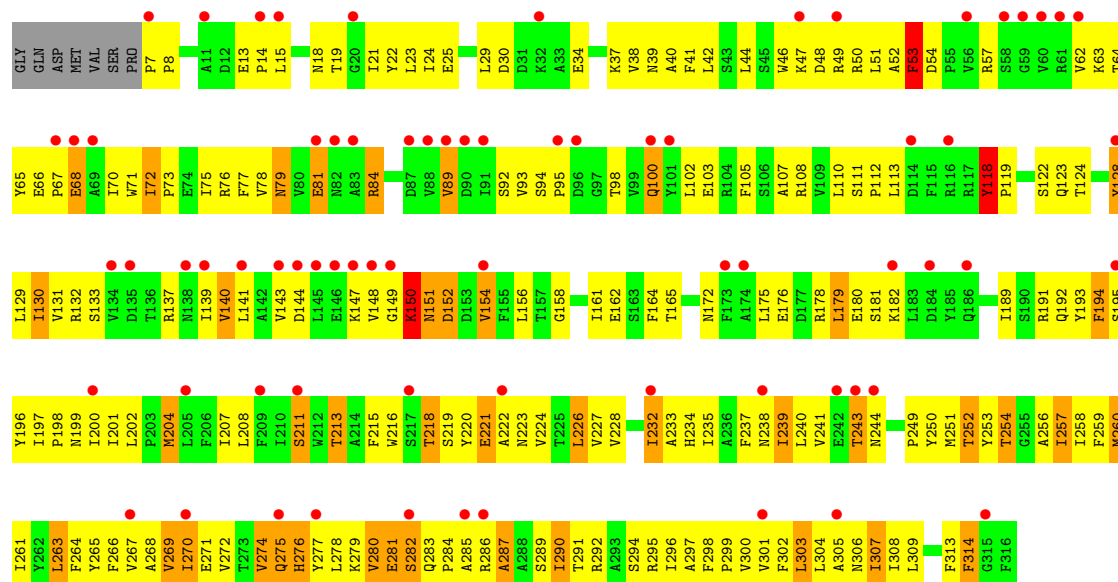


● Molecule 1: GLR4197 PROTEIN



● Molecule 1: GLR4197 PROTEIN





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) 98.8 (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 0.258 , 0.274	Depositor DCC
R_{free} test set	2172 reflections (5.04%)	wwPDB-VP
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 , 96.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.61	0/2589	1.01	13/3535 (0.4%)
1	B	0.61	0/2589	1.02	12/3535 (0.3%)
1	C	0.62	0/2589	1.02	12/3535 (0.3%)
1	D	0.63	0/2589	1.02	12/3535 (0.3%)
1	E	0.61	0/2589	1.02	13/3535 (0.4%)
All	All	0.62	0/12945	1.02	62/17675 (0.4%)

There are no bond length outliers.

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	53	PHE	N-CA-C	9.89	125.17	109.83
1	C	53	PHE	N-CA-C	9.49	124.53	109.83
1	B	281	GLU	N-CA-C	-9.36	96.02	109.96
1	D	281	GLU	N-CA-C	-9.05	96.47	109.96
1	A	53	PHE	N-CA-C	8.96	123.72	109.83
1	E	281	GLU	N-CA-C	-8.50	97.10	109.59
1	C	281	GLU	N-CA-C	-8.09	97.91	109.96
1	A	281	GLU	N-CA-C	-7.79	98.35	109.96
1	E	53	PHE	N-CA-C	6.86	125.42	110.80
1	E	128	TYR	N-CA-C	6.71	121.12	112.12
1	C	128	TYR	N-CA-C	6.62	121.19	112.13
1	A	280	VAL	N-CA-C	-6.59	106.14	111.81
1	E	150	LYS	N-CA-C	-6.57	96.80	110.80
1	D	118	TYR	CA-C-N	-6.57	112.93	119.56
1	D	118	TYR	C-N-CA	-6.57	112.93	119.56
1	A	150	LYS	N-CA-C	-6.56	96.83	110.80
1	E	280	VAL	N-CA-C	-6.36	106.34	111.81
1	B	280	VAL	N-CA-C	-6.33	106.37	111.81
1	C	280	VAL	N-CA-C	-6.19	106.49	111.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	53	PHE	N-CA-C	6.15	123.90	110.80
1	C	150	LYS	N-CA-C	-6.14	97.72	110.80
1	C	307	ILE	N-CA-C	-6.14	104.52	110.72
1	D	150	LYS	N-CA-C	-6.12	97.77	110.80
1	E	111	SER	CA-C-N	6.09	126.06	120.03
1	E	111	SER	C-N-CA	6.09	126.06	120.03
1	B	150	LYS	N-CA-C	-6.09	97.83	110.80
1	D	111	SER	CA-C-N	6.08	126.27	120.31
1	D	111	SER	C-N-CA	6.08	126.27	120.31
1	B	128	TYR	N-CA-C	6.06	120.24	112.12
1	A	118	TYR	CA-C-N	-6.05	113.45	119.56
1	A	118	TYR	C-N-CA	-6.05	113.45	119.56
1	D	128	TYR	N-CA-C	6.04	120.21	112.12
1	B	118	TYR	CA-C-N	-6.00	113.44	119.56
1	B	118	TYR	C-N-CA	-6.00	113.44	119.56
1	C	24	ILE	N-CA-C	-5.95	106.70	111.81
1	C	118	TYR	CA-C-N	-5.90	113.60	119.56
1	C	118	TYR	C-N-CA	-5.90	113.60	119.56
1	A	24	ILE	N-CA-C	-5.83	106.79	111.81
1	E	118	TYR	CA-C-N	-5.81	113.70	119.56
1	E	118	TYR	C-N-CA	-5.81	113.70	119.56
1	D	276	HIS	N-CA-CB	-5.74	100.80	110.49
1	C	276	HIS	N-CA-CB	-5.67	100.91	110.49
1	A	276	HIS	N-CA-CB	-5.65	100.94	110.49
1	B	152	ASP	N-CA-C	-5.65	106.28	112.72
1	B	111	SER	CA-C-N	5.63	125.61	120.03
1	B	111	SER	C-N-CA	5.63	125.61	120.03
1	A	111	SER	CA-C-N	5.56	125.76	120.31
1	A	111	SER	C-N-CA	5.56	125.76	120.31
1	E	307	ILE	N-CA-C	-5.51	105.00	111.00
1	B	276	HIS	N-CA-CB	-5.50	101.20	110.49
1	D	167	VAL	CB-CA-C	-5.48	105.99	111.80
1	A	152	ASP	N-CA-C	-5.29	106.68	112.72
1	E	152	ASP	N-CA-C	-5.29	106.69	112.72
1	E	24	ILE	N-CA-C	-5.25	107.29	111.81
1	D	149	GLY	N-CA-C	5.17	125.42	113.18
1	A	128	TYR	N-CA-C	5.16	119.03	112.12
1	D	24	ILE	N-CA-C	-5.15	107.38	111.81
1	C	111	SER	CA-C-N	5.09	125.30	120.31
1	C	111	SER	C-N-CA	5.09	125.30	120.31
1	E	276	HIS	N-CA-CB	-5.06	101.94	110.49
1	A	149	GLY	N-CA-C	5.05	125.15	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	21	ILE	N-CA-C	5.03	115.22	107.77

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	292	0
1	B	2521	0	2537	289	0
1	C	2521	0	2537	242	0
1	D	2521	0	2537	281	0
1	E	2521	0	2537	255	0
2	C	1	0	0	0	0
All	All	12606	0	12685	1205	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 48.

All (1205) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:LYS:C	1:C:149:GLY:H	1.77	0.92
1:A:253:TYR:HA	1:A:313:PHE:HE2	1.34	0.92
1:D:253:TYR:HA	1:D:313:PHE:CE2	2.04	0.92
1:B:76:ARG:HH22	1:B:130:ILE:HD12	1.34	0.92
1:B:147:LYS:C	1:B:149:GLY:H	1.76	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
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:E:147:LYS:C	1:E:149:GLY:H	1.75	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:A:76:ARG:NH2	1:A:130:ILE:HD12	1.87	0.89
1:D:225:THR:HG21	1:E:224:VAL:HG23	1.54	0.89
1:B:253:TYR:HA	1:B:313:PHE:HE2	1.37	0.89
1:D:147:LYS:C	1:D:149:GLY:H	1.79	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:147:LYS:C	1:A:149:GLY:H	1.79	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: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:C:76:ARG:HH22	1:C:130:ILE:HD12	1.39	0.85
1:D:155:PHE:HE1	1:E:112:PRO:HB3	1.38	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:LEU:HD12	1:B:259:PHE:CZ	2.13	0.84
1:D:78:VAL:HG22	1:D:130:ILE:HG12	1.57	0.84
1:C:78:VAL:HG22	1:C:130:ILE:HG12	1.58	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
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:C:200:ILE:HD11	1:C:240:LEU:HD23	1.60	0.81
1:E:234:HIS:CE1	1:E:261:ILE:HG21	2.15	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:B:238:ASN:HA	1:B:258:ILE:HD11	1.62	0.79
1:D:200:ILE:HD11	1:D:240:LEU:HD23	1.64	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:D:53:PHE:HE2	1:D:63:LYS:HB3	1.47	0.79
1:E:238:ASN:HA	1:E:258:ILE:HD11	1.62	0.79
1:C:197:ILE:HB	1:C:198:PRO:HD3	1.63	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:ILE:HB	1:A:198:PRO:HD3	1.65	0.78
1:B:79:ASN:H	1:B:79:ASN:HD22	1.31	0.78
1:A:253:TYR:HD1	1:A:313:PHE:CD2	2.02	0.78
1:B:15:LEU:HD11	1:B:46:TRP:HB2	1.66	0.78
1:C:257:ILE:O	1:C:261:ILE:HG12	1.83	0.78
1:C:199:ASN:HB3	1:D:242:GLU:CD	2.09	0.78
1:A:53:PHE:HE2	1:A:63:LYS:HB3	1.47	0.78
1:A:283:GLN:N	1:A:284:PRO:HD3	1.98	0.78
1:C:297:ALA:O	1:C:301:VAL:HG23	1.84	0.78
1:D:149:GLY:O	1:D:164:PHE:CD1	2.33	0.78
1:E:22:TYR:HA	1:E:149:GLY:HA3	1.65	0.78
1:B:53:PHE:HE2	1:B:63:LYS:HB3	1.48	0.76
1:C:283:GLN:N	1:C:284:PRO:HD3	2.00	0.76
1:C:253:TYR:HD1	1:C:313:PHE:HD2	1.32	0.76
1:D:276:HIS:C	1:D:278:LEU:H	1.94	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:15:LEU:HD11	1:A:46:TRP:HB2	1.68	0.76
1:A:253:TYR:CD1	1:A:313:PHE:HD2	2.04	0.76
1:D:128:TYR:O	1:D:129:LEU:HB2	1.86	0.76
1:D:89:VAL:HG11	1:D:102:LEU:HD23	1.68	0.75
1:D:210:ILE:HG13	1:E:266:PHE:HE1	1.49	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:B:89:VAL:HG11	1:B:102:LEU:HD23	1.68	0.75
1:D:238:ASN:HA	1:D:258:ILE:HD11	1.68	0.75
1:B:13:GLU:HB3	1:B:14:PRO:HD2	1.69	0.74
1:B:22:TYR:CD1	1:B:149:GLY:HA2	2.22	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:H	1:D:79:ASN:HD22	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:221:GLU:OE2	1:E:221:GLU:CD	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:238:ASN:HA	1:E:258:ILE:CD1	2.18	0.74
1:A:89:VAL:HG11	1:A:102:LEU:HD23	1.70	0.74
1:A:221:GLU:HB3	1:B:221:GLU:CG	2.16	0.74
1:B:276:HIS:C	1:B:278:LEU:H	1.95	0.73
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:A:260:MET:HE3	1:A:309:LEU:HD22	1.68	0.73
1:C:238:ASN:HA	1:C:258:ILE:HD11	1.71	0.73
1:E:253:TYR:HD1	1:E:313:PHE:CD2	2.07	0.73
1:B:197:ILE:HB	1:B:198:PRO:HD3	1.70	0.73
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:E:276:HIS:C	1:E:278:LEU:H	1.96	0.73
1:B:260:MET:HE3	1:B:309:LEU:HD22	1.68	0.73
1:D:94:SER:OG	1:D:95:PRO:HD2	1.89	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:A:139:ILE:HG12	1:A:172:ASN:HD21	1.54	0.73
1:B:253:TYR:HD1	1:B:313:PHE:CD2	2.07	0.73
1:C:42:LEU:HB3	1:C:103:GLU:HG3	1.72	0.72
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: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:C:128:TYR:O	1:C:129:LEU:HB2	1.88	0.72
1:D:104:ARG:NH2	1:E:78:VAL:HA	2.03	0.72
1:D:234:HIS:CE1	1:D:261:ILE:HG21	2.25	0.72
1:E:147:LYS:C	1:E:149:GLY:N	2.44	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:A:79:ASN:HD22	1:A:79:ASN:H	1.35	0.72
1:A:238:ASN:HA	1:A:258:ILE:HD11	1.72	0.72
1:D:229:SER:CB	1:E:228:VAL:HG11	2.19	0.72
1:C:202:LEU:HD12	1:D:259:PHE:CE1	2.25	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:150:LYS:CG	1:E:154:VAL:HG21	2.21	0.71
1:A:13:GLU:HB3	1:A:14:PRO:HD2	1.71	0.71
1:B:81:GLU:HG3	1:B:108:ARG:HG3	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:E:260:MET:HE3	1:E:309:LEU:HD22	1.73	0.71
1:B:29:LEU:HB2	1:B:156:LEU:HD11	1.73	0.70
1:D:260:MET:HE3	1:D:309:LEU:HD22	1.71	0.70
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:253:TYR:CD1	1:E:313:PHE:HD2	2.08	0.70
1:A:128:TYR:O	1:A:129:LEU:HB2	1.91	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: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: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:147:LYS:C	1:B:149:GLY:N	2.45	0.69
1:B:238:ASN:HA	1:B:258:ILE:CD1	2.21	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:276:HIS:C	1:C:278:LEU:H	2.00	0.69
1:C:218:THR:HG22	1:C:279:LYS:HE2	1.74	0.69
1:C:253:TYR:CD1	1:C:313:PHE:HD2	2.11	0.69
1:D:304:LEU:O	1:D:308:ILE:HG12	1.92	0.69
1:E:215:PHE:HZ	1:E:298:PHE:CE1	2.10	0.69
1:A:276:HIS:C	1:A:278:LEU:H	2.00	0.69
1:A:77:PHE:CD1	1:A:84:ARG:HD2	2.28	0.69
1:A:94:SER:OG	1:A:95:PRO:HD2	1.93	0.69
1:A:147:LYS:C	1:A:149:GLY:N	2.48	0.69
1:D:215:PHE:O	1:D:291:THR:HG22	1.92	0.69
1:E:297:ALA:O	1:E:301:VAL:HG23	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:VAL:HG11	1:C:102:LEU:HD23	1.74	0.69
1:D:47:LYS:HD2	1:D:49:ARG:HH21	1.58	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: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: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:A:257:ILE:HG22	1:A:309:LEU:HD23	1.75	0.68
1:D:100:GLN:HE21	1:D:100:GLN:HA	1.59	0.68
1:E:150:LYS:HG3	1:E:154:VAL:HG21	1.75	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:C:202:LEU:HD12	1:D:259:PHE:HE1	1.59	0.68
1:D:238:ASN:HA	1:D:258:ILE:CD1	2.24	0.68
1:A:215:PHE:HZ	1:A:298:PHE:CE1	2.12	0.68
1:B:100:GLN:HE21	1:B:100:GLN:HA	1.59	0.68
1:B:131:VAL:HG11	1:B:140:VAL:HG13	1.74	0.68
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:81:GLU:HG3	1:A:108:ARG:HG3	1.75	0.67
1:A:200:ILE:O	1:A:204:MET:HB2	1.94	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:C:150:LYS:CG	1:C:154:VAL:HG21	2.24	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:B:304:LEU:O	1:B:308:ILE:HG12	1.96	0.66
1:E:257:ILE:HG22	1:E:309:LEU:HD23	1.76	0.66
1:B:150:LYS:CG	1:B:154:VAL:HG21	2.26	0.66
1:C:213:THR:HG22	1:C:226:LEU:CD1	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:238:ASN:HA	1:C:258:ILE:CD1	2.25	0.66
1:C:200:ILE:O	1:C:204:MET:HB2	1.96	0.66
1:B:139:ILE:HG12	1:B:172:ASN:HD21	1.60	0.66
1:B:276:HIS:O	1:B:280:VAL:HG22	1.96	0.66
1:C:150:LYS:HG3	1:C:154:VAL:HG21	1.78	0.66
1:C:260:MET:HE3	1:C:309:LEU:HD22	1.75	0.66
1:E:42:LEU:HD23	1:E:103:GLU:OE1	1.96	0.65
1:A:157:THR:HG21	1:B:34:GLU:OE1	1.96	0.65
1:C:42:LEU:HD23	1:C:103:GLU:OE1	1.95	0.65
1:E:200:ILE:O	1:E:204:MET:HB2	1.97	0.65
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: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:128:TYR:O	1:B:129:LEU:HB2	1.96	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:A:29:LEU:HB2	1:A:156:LEU:HD11	1.78	0.65
1:C:215:PHE:HZ	1:C:298:PHE:CE1	2.15	0.65
1:E:200:ILE:CD1	1:E:240:LEU:HD23	2.27	0.65
1:B:94:SER:OG	1:B:95:PRO:HD2	1.98	0.64
1:B:191:ARG:HG3	1:B:192:GLN:N	2.11	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:C:77:PHE:CD1	1:C:84:ARG:HD2	2.32	0.64
1:D:297:ALA:O	1:D:301:VAL:HG23	1.97	0.64
1:E:94:SER:OG	1:E:95:PRO:HD2	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:131:VAL:HG11	1:A:140:VAL:HG13	1.79	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: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:C:222:ALA:HB2	1:D:221:GLU:HA	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:283:GLN:N	1:D:284:PRO:CD	2.62	0.63
1:E:147:LYS:HE2	1:E:165:THR:HA	1.80	0.63
1:A:66:GLU:HG3	1:A:67:PRO:HD2	1.80	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:281:GLU:O	1:A:283:GLN:N	2.32	0.63
1:B:303:LEU:O	1:B:307:ILE:HD12	1.98	0.63
1:E:215:PHE:CZ	1:E:298:PHE:CD1	2.86	0.63
1:A:215:PHE:CZ	1:A:298:PHE:CD1	2.86	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:D:150:LYS:CG	1:D:154:VAL:HG21	2.29	0.63
1:D:198:PRO:CG	1:E:251:MET:HE1	2.29	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: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: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:A:276:HIS:O	1:A:280:VAL:HG22	2.00	0.62
1:C:54:ASP:HB2	1:C:57:ARG:HG3	1.81	0.62
1:D:191:ARG:HG3	1:D:192:GLN:N	2.14	0.62
1:D:222:ALA:CB	1:E:220:TYR:CD2	2.83	0.62
1:A:229:SER:HB2	1:B:228:VAL:HG11	1.81	0.62
1:D:13:GLU:HB3	1:D:14:PRO:CD	2.30	0.62
1:D:29:LEU:HB2	1:D:156:LEU:HD11	1.79	0.62
1:E:213:THR:HG22	1:E:226:LEU:CD1	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:54:ASP:HB2	1:B:57:ARG:HG3	1.82	0.62
1:B:150:LYS:HG3	1:B:154:VAL:HG21	1.81	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:A:274:VAL:C	1:A:276:HIS:H	2.08	0.62
1:C:274:VAL:C	1:C:276:HIS:H	2.08	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:89:VAL:CG1	1:D:102:LEU:HD23	2.29	0.62
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:E:213:THR:HG22	1:E:226:LEU:HD11	1.82	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:100:GLN:HA	1:E:100:GLN:HE21	1.65	0.61
1:E:131:VAL:HG11	1:E:140:VAL:HG13	1.80	0.61
1:A:198:PRO:CG	1:B:251:MET:HE1	2.30	0.61
1:B:47:LYS:HD2	1:B:49:ARG:NH2	2.15	0.61
1:B:283:GLN:N	1:B:284:PRO:CD	2.63	0.61
1:E:208:LEU:O	1:E:211:SER:HB3	2.00	0.61
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:A:13:GLU:HB3	1:A:14:PRO:CD	2.30	0.61
1:D:41:PHE:HE2	1:E:175:LEU:HD23	1.65	0.61
1:A:53:PHE:CE2	1:A:63:LYS:HB3	2.33	0.61
1:E:77:PHE:CD1	1:E:84:ARG:HD2	2.34	0.61
1:E:276:HIS:O	1:E:280:VAL:HG22	2.00	0.61
1:C:147:LYS:C	1:C:149:GLY:N	2.46	0.61
1:D:213:THR:HG22	1:D:226:LEU:CD1	2.31	0.61
1:E:147:LYS:O	1:E:149:GLY:N	2.34	0.61
1:E:215:PHE:HZ	1:E:298:PHE:CD1	2.19	0.61
1:A:208:LEU:O	1:A:211:SER:HB3	2.00	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: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:B:53:PHE:CE1	1:B:95:PRO:HA	2.37	0.60
1:C:194:PHE:C	1:C:196:TYR:N	2.57	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:E:275:GLN:HG3	1:E:291:THR:OG1	2.01	0.60
1:A:215:PHE:HZ	1:A:298:PHE:CD1	2.19	0.60
1:C:267:VAL:HA	1:C:270:ILE:HB	1.84	0.60
1:E:234:HIS:CE1	1:E:261:ILE:CG2	2.84	0.60
1:B:213:THR:HG22	1:B:226:LEU:HD11	1.84	0.60
1:B:274:VAL:C	1:B:276:HIS:H	2.09	0.60
1:D:303:LEU:O	1:D:307:ILE:HD12	2.01	0.60
1:E:53:PHE:CE2	1:E:63:LYS:HB3	2.34	0.60
1:A:202:LEU:HD12	1:B:259:PHE:CE1	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:ILE:HG23	1:B:269:VAL:HG11	1.84	0.60
1:D:200:ILE:O	1:D:204:MET:HB2	2.01	0.60
1:D:276:HIS:O	1:D:280:VAL:HG22	2.00	0.60
1:E:22:TYR:HA	1:E:149:GLY:HA2	1.84	0.60
1:E:54:ASP:HB2	1:E:57:ARG:HG3	1.83	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:B:53:PHE:CE2	1:B:63:LYS:HB3	2.35	0.60
1:C:53:PHE:CE2	1:C:63:LYS:HB3	2.33	0.60
1:C:275:GLN:HG3	1:C:291:THR:OG1	2.02	0.60
1:E:53:PHE:CE1	1:E:95:PRO:HA	2.37	0.60
1:A:193:TYR:O	1:A:194:PHE:HB2	2.01	0.60
1:A:194:PHE:C	1:A:196:TYR:N	2.60	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
1:A:25:GLU:HG3	1:B:79:ASN:HA	1.84	0.59
1:B:22:TYR:HA	1:B:149:GLY:HA2	1.84	0.59
1:B:123:GLN:HA	1:B:123:GLN:NE2	2.17	0.59
1:D:194:PHE:C	1:D:196:TYR:N	2.56	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:146:GLU:HG3	1:E:176:GLU:HG2	1.83	0.59
1:D:193:TYR:O	1:D:194:PHE:HB2	2.01	0.59
1:B:194:PHE:C	1:B:196:TYR:N	2.58	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:A:146:GLU:HG3	1:B:176:GLU:HG2	1.84	0.59
1:C:281:GLU:O	1:C:283:GLN:N	2.33	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:B:267:VAL:HA	1:B:270:ILE:HB	1.84	0.59
1:D:81:GLU:HG3	1:D:108:ARG:CG	2.32	0.59
1:E:77:PHE:H	1:E:84:ARG:HD3	1.67	0.59
1:A:275:GLN:HG3	1:A:291:THR:OG1	2.03	0.59
1:C:215:PHE:HZ	1:C:298:PHE:CD1	2.21	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:225:THR:HG21	1:D:225:THR:OG1	2.03	0.59
1:D:22:TYR:HA	1:D:149:GLY:HA2	1.84	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:E:194:PHE:C	1:E:196:TYR:N	2.60	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:A:254:THR:O	1:A:258:ILE:HB	2.03	0.58
1:D:150:LYS:HG3	1:D:154:VAL:HG21	1.84	0.58
1:D:161:ILE:HA	1:D:189:ILE:HG22	1.85	0.58
1:D:213:THR:HG22	1:D:226:LEU:HD11	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:B:215:PHE:CZ	1:B:298:PHE:CD1	2.90	0.58
1:B:223:ASN:O	1:B:227:VAL:HG23	2.04	0.58
1:C:194:PHE:C	1:C:196:TYR:H	2.10	0.58
1:D:195:SER:O	1:D:199:ASN:HB2	2.03	0.58
1:D:225:THR:CG2	1:E:224:VAL:CG2	2.79	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: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:B:147:LYS:HE2	1:B:165:THR:HA	1.86	0.58
1:C:62:VAL:HG13	1:C:93:VAL:O	2.04	0.58
1:D:123:GLN:HA	1:D:123:GLN:NE2	2.19	0.58
1:E:219:SER:OG	1:E:222:ALA:HB3	2.04	0.58
1:B:81:GLU:HG3	1:B:108:ARG:CG	2.33	0.58
1:D:254:THR:O	1:D:258:ILE:HB	2.04	0.58
1:E:281:GLU:O	1:E:283:GLN:N	2.34	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:A:47:LYS:HD2	1:A:49:ARG:NH2	2.19	0.57
1:B:29:LEU:HD23	1:B:29:LEU:C	2.29	0.57
1:B:161:ILE:HA	1:B:189:ILE:HG22	1.87	0.57
1:B:264:PHE:CE2	1:B:302:PHE:HB2	2.39	0.57
1:D:229:SER:HB3	1:E:228:VAL:CG1	2.34	0.57
1:A:232:ILE:HG22	1:A:233:ALA:N	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:ILE:HA	1:B:201:ILE:HB	1.85	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:D:275:GLN:HG3	1:D:291:THR:OG1	2.04	0.57
1:A:304:LEU:O	1:A:308:ILE:HG12	2.03	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:D:147:LYS:O	1:D:149:GLY:N	2.37	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:A:119:PRO:O	1:A:193:TYR:HB3	2.04	0.57
1:A:240:LEU:HD13	1:B:239:ILE:CG1	2.19	0.57
1:D:274:VAL:C	1:D:276:HIS:H	2.12	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:E:274:VAL:C	1:E:276:HIS:H	2.12	0.57
1:A:229:SER:CB	1:B:228:VAL:HG11	2.35	0.57
1:B:275:GLN:HG2	1:B:275:GLN:O	2.05	0.57
1:E:254:THR:O	1:E:258:ILE:HB	2.04	0.57
1:A:22:TYR:HB3	1:A:41:PHE:HB2	1.87	0.56
1:C:29:LEU:C	1:C:29:LEU:HD23	2.29	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:B:194:PHE:C	1:B:196:TYR:H	2.13	0.56
1:C:191:ARG:HG3	1:C:192:GLN:N	2.18	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:A:22:TYR:HA	1:A:149:GLY:HA2	1.84	0.56
1:A:137:ARG:HD2	1:A:179:LEU:HG	1.87	0.56
1:A:229:SER:CB	1:B:228:VAL:CG1	2.84	0.56
1:B:215:PHE:HZ	1:B:298:PHE:CD1	2.23	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:D:221:GLU:OE2	1:E:221:GLU:OE2	2.22	0.56
1:A:225:THR:CG2	1:B:224:VAL:HG23	2.35	0.56
1:D:79:ASN:H	1:D:79:ASN:ND2	2.03	0.56
1:A:191:ARG:HG3	1:A:192:GLN:N	2.21	0.56
1:D:53:PHE:CE2	1:D:63:LYS:HB3	2.34	0.56
1:D:194:PHE:C	1:D:196:TYR:H	2.12	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:305:ALA:O	1:E:309:LEU:HB2	2.05	0.56
1:B:232:ILE:HG22	1:B:233:ALA:N	2.20	0.56
1:D:197:ILE:HA	1:D:201:ILE:HB	1.86	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:C:215:PHE:HB2	1:C:216:TRP:CZ3	2.40	0.56
1:D:53:PHE:O	1:D:54:ASP:C	2.48	0.56
1:E:29:LEU:C	1:E:29:LEU:HD23	2.31	0.56
1:E:119:PRO:O	1:E:193:TYR:HB3	2.06	0.56
1:C:81:GLU:HG3	1:C:108:ARG:CG	2.36	0.56
1:C:200:ILE:HD11	1:C:240:LEU:CD2	2.35	0.56
1:D:119:PRO:O	1:D:193:TYR:HB3	2.05	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:193:TYR:O	1:B:194:PHE:HB2	2.06	0.56
1:D:223:ASN:O	1:D:227:VAL:HG23	2.06	0.55
1:A:179:LEU:C	1:A:179:LEU:HD12	2.32	0.55
1:B:215:PHE:HB2	1:B:216:TRP:CZ3	2.42	0.55
1:C:193:TYR:O	1:C:194:PHE:CB	2.54	0.55
1:A:123:GLN:HA	1:A:123:GLN:NE2	2.21	0.55
1:A:139:ILE:HG12	1:A:172:ASN:ND2	2.21	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:C:226:LEU:HD23	1:D:224:VAL:CG2	2.37	0.55
1:A:179:LEU:HD12	1:A:179:LEU:O	2.07	0.55
1:A:264:PHE:CE2	1:A:302:PHE:HB2	2.42	0.55
1:D:232:ILE:HG22	1:D:233:ALA:N	2.20	0.55
1:D:264:PHE:CE2	1:D:302:PHE:HB2	2.41	0.55
1:A:29:LEU:C	1:A:29:LEU:HD23	2.32	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:A:224:VAL:C	1:A:226:LEU:N	2.63	0.55
1:A:314:PHE:N	1:A:314:PHE:CD1	2.75	0.55
1:C:232:ILE:HG22	1:C:233:ALA:N	2.22	0.55
1:D:290:ILE:HG22	1:D:291:THR:N	2.21	0.55
1:A:157:THR:HG22	1:B:34:GLU:OE1	2.06	0.55
1:A:194:PHE:C	1:A:196:TYR:H	2.14	0.55
1:A:267:VAL:HA	1:A:270:ILE:HB	1.88	0.55
1:C:303:LEU:O	1:C:307:ILE:HD12	2.07	0.55
1:C:314:PHE:HD1	1:C:314:PHE:N	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:215:PHE:HB2	1:D:216:TRP:CZ3	2.41	0.55
1:D:219:SER:OG	1:D:222:ALA:HB3	2.07	0.55
1:E:215:PHE:HB3	1:E:295:ARG:HG2	1.89	0.55
1:B:234:HIS:CE1	1:B:261:ILE:CG2	2.90	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:A:234:HIS:CE1	1:A:261:ILE:CG2	2.90	0.54
1:C:147:LYS:O	1:C:147:LYS:HG2	2.06	0.54
1:D:27:TYR:CB	1:E:110:LEU:HD11	2.37	0.54
1:E:224:VAL:C	1:E:226:LEU:N	2.64	0.54
1:A:200:ILE:CD1	1:A:240:LEU:HD23	2.33	0.54
1:C:314:PHE:N	1:C:314:PHE:CD1	2.75	0.54
1:D:193:TYR:O	1:D:194:PHE:CB	2.54	0.54
1:E:193:TYR:O	1:E:194:PHE:HB2	2.06	0.54
1:A:207:ILE:HG22	1:B:231:LEU:HD21	1.89	0.54
1:C:290:ILE:HG22	1:C:291:THR:N	2.22	0.54
1:E:200:ILE:HD11	1:E:240:LEU:CD2	2.35	0.54
1:B:179:LEU:HD12	1:B:179:LEU:C	2.33	0.54
1:D:29:LEU:HD23	1:D:29:LEU:C	2.33	0.54
1:A:233:ALA:HB1	1:B:235:ILE:HD13	1.90	0.54
1:C:118:TYR:CD1	1:C:118:TYR:C	2.85	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:D:179:LEU:HD12	1:D:179:LEU:C	2.33	0.54
1:E:298:PHE:HB2	1:E:299:PRO:HD3	1.89	0.54
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:B:118:TYR:CD1	1:B:118:TYR:C	2.86	0.53
1:B:179:LEU:HD12	1:B:179:LEU:O	2.07	0.53
1:B:290:ILE:HG22	1:B:291:THR:N	2.24	0.53
1:C:305:ALA:O	1:C:309:LEU:HB2	2.08	0.53
1:E:179:LEU:C	1:E:179:LEU:HD12	2.33	0.53
1:B:314:PHE:N	1:B:314:PHE:HD1	2.07	0.53
1:C:215:PHE:HB3	1:C:295:ARG:HG2	1.90	0.53
1:D:210:ILE:CG1	1:E:266:PHE:CD1	2.91	0.53
1:A:18:ASN:HB3	1:A:143:VAL:HG23	1.90	0.53
1:C:75:ILE:HD13	1:C:131:VAL:HB	1.91	0.53
1:D:147:LYS:HE2	1:D:165:THR:HA	1.90	0.53
1:D:210:ILE:HD11	1:E:266:PHE:HD1	1.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:314:PHE:CD1	1:E:314:PHE:N	2.77	0.53
1:B:215:PHE:HB3	1:B:295:ARG:HG2	1.90	0.53
1:B:249:PRO:HD2	1:B:250:TYR:CD1	2.44	0.53
1:C:137:ARG:HD2	1:C:179:LEU:HG	1.90	0.53
1:E:147:LYS:CE	1:E:165:THR:HA	2.38	0.53
1:A:215:PHE:HB2	1:A:216:TRP:CZ3	2.42	0.53
1:A:217:SER:OG	1:B:220:TYR:HE2	1.90	0.53
1:D:68:GLU:CD	1:D:68:GLU:H	2.17	0.53
1:D:210:ILE:CG1	1:E:266:PHE:CE1	2.90	0.53
1:E:137:ARG:HD2	1:E:179:LEU:HG	1.91	0.53
1:E:232:ILE:HG22	1:E:233:ALA:N	2.22	0.53
1:E:275:GLN:O	1:E:275:GLN:HG2	2.09	0.53
1:A:41:PHE:HE2	1:B:175:LEU:HD23	1.72	0.53
1:B:278:LEU:HD21	1:B:286:ARG:HB3	1.91	0.53
1:C:261:ILE:CD1	1:C:302:PHE:HE1	2.22	0.53
1:E:123:GLN:NE2	1:E:123:GLN:HA	2.23	0.53
1:A:118:TYR:CD1	1:A:118:TYR:C	2.86	0.53
1:B:195:SER:O	1:B:199:ASN:HB2	2.09	0.53
1:D:62:VAL:HG13	1:D:93:VAL:O	2.09	0.53
1:E:215:PHE:HB2	1:E:216:TRP:CZ3	2.43	0.53
1:D:200:ILE:CD1	1:D:240:LEU:HD23	2.37	0.53
1:E:29:LEU:HD23	1:E:30:ASP:N	2.23	0.53
1:E:139:ILE:HG12	1:E:172:ASN:ND2	2.21	0.53
1:A:75:ILE:HD13	1:A:131:VAL:HB	1.90	0.52
1:A:192:GLN:CD	1:B:249:PRO:HB3	2.34	0.52
1:A:275:GLN:O	1:A:275:GLN:HG2	2.07	0.52
1:E:53:PHE:O	1:E:54:ASP:C	2.52	0.52
1:E:194:PHE:C	1:E:196:TYR:H	2.16	0.52
1:A:233:ALA:HB1	1:B:235:ILE:CD1	2.39	0.52
1:A:198:PRO:HG3	1:B:251:MET:HE1	1.90	0.52
1:C:18:ASN:HB3	1:C:143:VAL:HG23	1.92	0.52
1:C:161:ILE:HA	1:C:189:ILE:HG22	1.90	0.52
1:C:179:LEU:O	1:C:179:LEU:HD12	2.09	0.52
1:D:54:ASP:HB2	1:D:57:ARG:HB2	1.90	0.52
1:D:158:GLY:HA2	1:D:192:GLN:OE1	2.10	0.52
1:E:118:TYR:CD1	1:E:118:TYR:C	2.83	0.52
1:E:314:PHE:N	1:E:314:PHE:HD1	2.07	0.52
1:A:79:ASN:H	1:A:79:ASN:ND2	2.04	0.52
1:D:137:ARG:HD2	1:D:179:LEU:HG	1.91	0.52
1:D:192:GLN:CD	1:E:249:PRO:HB3	2.34	0.52
1:D:224:VAL:C	1:D:226:LEU:N	2.65	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:197:ILE:HA	1:A:201:ILE:HB	1.91	0.52
1:C:22:TYR:HB3	1:C:41:PHE:HB2	1.92	0.52
1:C:139:ILE:HG12	1:C:172:ASN:ND2	2.23	0.52
1:B:52:ALA:HA	1:B:95:PRO:O	2.10	0.52
1:C:65:TYR:CG	1:C:70:ILE:HD11	2.45	0.52
1:D:179:LEU:HD12	1:D:179:LEU:O	2.10	0.52
1:B:18:ASN:HB3	1:B:143:VAL:HG23	1.92	0.52
1:B:75:ILE:HD13	1:B:131:VAL:HB	1.91	0.52
1:C:155:PHE:CE1	1:D:112:PRO:HB3	2.45	0.52
1:C:275:GLN:O	1:C:275:GLN:HG2	2.10	0.52
1:E:249:PRO:HD2	1:E:250:TYR:CD1	2.45	0.52
1:A:62:VAL:HG11	1:A:92:SER:HB3	1.92	0.52
1:A:298:PHE:HB2	1:A:299:PRO:HD3	1.92	0.52
1:C:123:GLN:HA	1:C:123:GLN:NE2	2.25	0.52
1:C:197:ILE:HA	1:C:201:ILE:HB	1.92	0.52
1:C:263:LEU:C	1:C:265:TYR:H	2.18	0.52
1:E:75:ILE:HD13	1:E:131:VAL:HB	1.92	0.52
1:A:27:TYR:CB	1:B:110:LEU:CD1	2.83	0.51
1:A:42:LEU:HB3	1:A:103:GLU:CG	2.41	0.51
1:B:193:TYR:O	1:B:194:PHE:CB	2.58	0.51
1:C:29:LEU:HD23	1:C:30:ASP:N	2.25	0.51
1:C:298:PHE:HB2	1:C:299:PRO:HD3	1.91	0.51
1:E:79:ASN:H	1:E:79:ASN:ND2	1.99	0.51
1:A:104:ARG:NH1	1:B:76:ARG:HB3	2.25	0.51
1:B:53:PHE:O	1:B:54:ASP:C	2.52	0.51
1:B:286:ARG:O	1:B:289:SER:HB3	2.10	0.51
1:D:222:ALA:HB3	1:E:220:TYR:CD2	2.44	0.51
1:B:224:VAL:C	1:B:226:LEU:N	2.65	0.51
1:C:179:LEU:HD12	1:C:179:LEU:C	2.36	0.51
1:C:215:PHE:HB2	1:C:216:TRP:CE3	2.46	0.51
1:A:62:VAL:HG13	1:A:93:VAL:O	2.11	0.51
1:D:147:LYS:O	1:D:147:LYS:HG2	2.11	0.51
1:E:179:LEU:HD12	1:E:179:LEU:O	2.11	0.51
1:B:219:SER:OG	1:B:222:ALA:HB3	2.11	0.51
1:B:276:HIS:C	1:B:278:LEU:N	2.64	0.51
1:E:193:TYR:O	1:E:194:PHE:CB	2.58	0.51
1:A:226:LEU:HD21	1:B:224:VAL:HB	1.90	0.51
1:B:54:ASP:HB2	1:B:57:ARG:CG	2.40	0.51
1:E:18:ASN:HB3	1:E:143:VAL:HG23	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:70:ILE:HG22	1:E:71:TRP:N	2.26	0.51
1:E:147:LYS:O	1:E:147:LYS:HG2	2.10	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:C:210:ILE:CD1	1:D:231:LEU:HD22	2.40	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:A:84:ARG:HA	1:A:107:ALA:HB2	1.93	0.51
1:B:70:ILE:HG22	1:B:71:TRP:N	2.26	0.51
1:D:157:THR:CG2	1:E:34:GLU:OE1	2.59	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:D:276:HIS:C	1:D:278:LEU:N	2.63	0.51
1:E:62:VAL:HG13	1:E:93:VAL:O	2.10	0.51
1:B:54:ASP:HB2	1:B:57:ARG:HB2	1.93	0.50
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: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:C:62:VAL:HG11	1:C:92:SER:HB3	1.93	0.50
1:D:54:ASP:HB2	1:D:57:ARG:CG	2.40	0.50
1:A:215:PHE:HB2	1:A:216:TRP:CE3	2.46	0.50
1:B:215:PHE:HB2	1:B:216:TRP:CE3	2.47	0.50
1:C:54:ASP:HB2	1:C:57:ARG:CG	2.41	0.50
1:D:52:ALA:HA	1:D:95:PRO:O	2.12	0.50
1:E:19:THR:HG22	1:E:44:LEU:CD2	2.41	0.50
1:E:52:ALA:HA	1:E:95:PRO:O	2.11	0.50
1:E:216:TRP:CZ2	1:E:295:ARG:HB3	2.47	0.50
1:A:267:VAL:HG23	1:A:298:PHE:CZ	2.47	0.50
1:C:224:VAL:C	1:C:226:LEU:N	2.68	0.50
1:D:139:ILE:HG12	1:D:172:ASN:ND2	2.25	0.50
1:D:215:PHE:HB2	1:D:216:TRP:CE3	2.47	0.50
1:E:197:ILE:HA	1:E:201:ILE:HB	1.92	0.50
1:E:298:PHE:CB	1:E:299:PRO:HD3	2.42	0.50
1:A:118:TYR:HB2	1:A:252:THR:HG22	1.94	0.50
1:B:118:TYR:HB2	1:B:252:THR:HG22	1.93	0.50
1:C:267:VAL:HG23	1:C:298:PHE:CZ	2.46	0.50
1:D:75:ILE:HD13	1:D:131:VAL:HB	1.93	0.50
1:D:286:ARG:O	1:D:289:SER:HB3	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:PRO:HB3	1:B:262:TYR:CZ	2.46	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:D:118:TYR:CD1	1:D:118:TYR:C	2.88	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:B:314:PHE:N	1:B:314:PHE:CD1	2.76	0.50
1:C:13:GLU:OE1	1:C:14:PRO:HD3	2.12	0.50
1:B:298:PHE:HB2	1:B:299:PRO:HD3	1.93	0.49
1:C:68:GLU:H	1:C:68:GLU:CD	2.20	0.49
1:C:249:PRO:HD2	1:C:250:TYR:CD1	2.47	0.49
1:D:42:LEU:HB3	1:D:103:GLU:CG	2.40	0.49
1:D:215:PHE:HB3	1:D:295:ARG:HG2	1.93	0.49
1:E:65:TYR:CG	1:E:70:ILE:HD11	2.48	0.49
1:A:65:TYR:CG	1:A:70:ILE:HD11	2.48	0.49
1:D:216:TRP:CZ2	1:D:295:ARG:HB3	2.46	0.49
1:D:281:GLU:O	1:D:283:GLN:N	2.38	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:A:29:LEU:HD23	1:A:30:ASP:N	2.27	0.49
1:A:147:LYS:O	1:A:147:LYS:HG2	2.13	0.49
1:A:216:TRP:CZ2	1:A:295:ARG:HB3	2.48	0.49
1:B:42:LEU:HB3	1:B:103:GLU:CG	2.39	0.49
1:B:224:VAL:O	1:B:228:VAL:HB	2.12	0.49
1:B:283:GLN:C	1:B:285:ALA:N	2.70	0.49
1:C:52:ALA:HA	1:C:95:PRO:O	2.12	0.49
1:C:53:PHE:O	1:C:54:ASP:C	2.54	0.49
1:A:41:PHE:HZ	1:B:76:ARG:NH2	2.11	0.49
1:A:54:ASP:HB2	1:A:57:ARG:CG	2.42	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
1:B:22:TYR:HB3	1:B:41:PHE:HB2	1.95	0.49
1:B:65:TYR:CG	1:B:70:ILE:HD11	2.48	0.49
1:B:147:LYS:O	1:B:147:LYS:HG2	2.12	0.49
1:C:276:HIS:C	1:C:278:LEU:N	2.68	0.49
1:D:29:LEU:HD23	1:D:30:ASP:N	2.27	0.49
1:D:70:ILE:HG22	1:D:71:TRP:N	2.27	0.49
1:D:84:ARG:CB	1:D:84:ARG:HH11	2.26	0.49
1:A:18:ASN:HB2	1:A:45:SER:OG	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:PHE:HB3	1:A:295:ARG:HG2	1.95	0.49
1:C:23:LEU:HB2	1:C:150:LYS:HA	1.95	0.49
1:E:224:VAL:C	1:E:226:LEU:H	2.19	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:52:ALA:HA	1:A:95:PRO:O	2.13	0.49
1:A:159:TRP:CE3	1:A:189:ILE:HD12	2.48	0.49
1:A:215:PHE:O	1:A:291:THR:CG2	2.61	0.49
1:B:19:THR:HG22	1:B:44:LEU:CD2	2.43	0.49
1:B:233:ALA:O	1:B:237:PHE:HD1	1.95	0.49
1:C:25:GLU:OE1	1:C:25:GLU:HA	2.12	0.49
1:D:13:GLU:OE1	1:D:14:PRO:HD3	2.13	0.49
1:D:19:THR:HG22	1:D:44:LEU:CD2	2.43	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:A:53:PHE:O	1:A:54:ASP:C	2.56	0.48
1:C:283:GLN:C	1:C:285:ALA:N	2.71	0.48
1:D:62:VAL:HG11	1:D:92:SER:HB3	1.94	0.48
1:E:54:ASP:HB2	1:E:57:ARG:HB2	1.95	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:E:215:PHE:HB2	1:E:216:TRP:CE3	2.49	0.48
1:A:132:ARG:NH2	1:A:178:ARG:HB2	2.29	0.48
1:A:140:VAL:HG22	1:A:181:SER:HB3	1.95	0.48
1:E:54:ASP:HB2	1:E:57:ARG:CG	2.42	0.48
1:A:38:VAL:HG22	1:A:39:ASN:N	2.27	0.48
1:A:147:LYS:CE	1:A:165:THR:HA	2.44	0.48
1:A:261:ILE:CD1	1:A:302:PHE:HE1	2.26	0.48
1:A:276:HIS:C	1:A:278:LEU:N	2.69	0.48
1:D:222:ALA:HB3	1:E:220:TYR:HD2	1.78	0.48
1:E:118:TYR:HB2	1:E:252:THR:HG22	1.94	0.48
1:E:286:ARG:O	1:E:289:SER:HB3	2.14	0.48
1:A:13:GLU:OE1	1:A:14:PRO:HD3	2.13	0.48
1:D:53:PHE:CD1	1:D:95:PRO:HA	2.48	0.48
1:E:283:GLN:C	1:E:285:ALA:N	2.69	0.48
1:A:232:ILE:HA	1:A:235:ILE:HD12	1.96	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:C:222:ALA:HA	1:D:221:GLU:OE1	2.13	0.48
1:D:51:LEU:CD1	1:D:70:ILE:HD12	2.44	0.48
1:D:278:LEU:HD21	1:D:286:ARG:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:ILE:HG12	1:B:269:VAL:HG11	1.96	0.48
1:D:261:ILE:CD1	1:D:302:PHE:HE1	2.26	0.48
1:E:267:VAL:HG23	1:E:298:PHE:CZ	2.49	0.48
1:A:27:TYR:CG	1:B:110:LEU:HD12	2.49	0.47
1:A:192:GLN:CG	1:B:249:PRO:HB3	2.44	0.47
1:A:206:PHE:CD1	1:B:262:TYR:HB3	2.49	0.47
1:A:286:ARG:O	1:A:289:SER:HB3	2.13	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:E:238:ASN:CA	1:E:258:ILE:HD11	2.41	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:C:70:ILE:HG22	1:C:71:TRP:N	2.28	0.47
1:E:263:LEU:C	1:E:265:TYR:H	2.21	0.47
1:A:54:ASP:HB2	1:A:57:ARG:HB2	1.96	0.47
1:A:133:SER:HB2	1:A:137:ARG:HH11	1.79	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:D:283:GLN:C	1:D:285:ALA:N	2.71	0.47
1:D:314:PHE:HD1	1:D:314:PHE:N	2.12	0.47
1:A:196:TYR:N	1:A:196:TYR:CD1	2.82	0.47
1:E:8:PRO:O	1:E:50:ARG:NH1	2.48	0.47
1:E:47:LYS:CD	1:E:49:ARG:NH2	2.77	0.47
1:A:37:LYS:HG2	1:A:108:ARG:HB3	1.96	0.47
1:A:255:GLY:O	1:A:258:ILE:HG22	2.14	0.47
1:B:51:LEU:CD1	1:B:70:ILE:HD12	2.44	0.47
1:B:200:ILE:HD11	1:B:240:LEU:CD2	2.39	0.47
1:C:222:ALA:HB2	1:D:221:GLU:HG2	1.97	0.47
1:D:22:TYR:HB3	1:D:41:PHE:HB2	1.97	0.47
1:D:84:ARG:HH11	1:D:84:ARG:HB3	1.79	0.47
1:D:137:ARG:HA	1:D:137:ARG:HD3	1.62	0.47
1:D:222:ALA:HB1	1:E:220:TYR:CD2	2.50	0.47
1:D:249:PRO:HD2	1:D:250:TYR:CD1	2.49	0.47
1:D:267:VAL:HG23	1:D:298:PHE:CZ	2.49	0.47
1:D:286:ARG:O	1:D:287:ALA:C	2.58	0.47
1:D:314:PHE:N	1:D:314:PHE:CD1	2.82	0.47
1:E:215:PHE:CE1	1:E:298:PHE:CD1	3.03	0.47
1:C:118:TYR:HB2	1:C:252:THR:HG22	1.96	0.47
1:C:147:LYS:CE	1:C:165:THR:HA	2.45	0.47
1:E:216:TRP:CH2	1:E:295:ARG:HB3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:290:ILE:HG22	1:E:291:THR:N	2.28	0.47
1:B:24:ILE:HB	1:B:39:ASN:O	2.15	0.47
1:C:84:ARG:HH11	1:C:84:ARG:CB	2.28	0.47
1:E:23:LEU:HB2	1:E:150:LYS:HA	1.96	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:38:VAL:HG22	1:C:39:ASN:N	2.30	0.47
1:C:41:PHE:HZ	1:D:76:ARG:NH2	2.13	0.47
1:C:137:ARG:HA	1:C:137:ARG:HD3	1.60	0.47
1:A:8:PRO:O	1:A:50:ARG:NH1	2.49	0.46
1:A:84:ARG:CB	1:A:84:ARG:HH11	2.28	0.46
1:B:282:SER:C	1:B:284:PRO:HD3	2.39	0.46
1:C:140:VAL:HG22	1:C:181:SER:HB3	1.96	0.46
1:D:47:LYS:CD	1:D:49:ARG:NH2	2.78	0.46
1:D:233:ALA:O	1:D:237:PHE:HD1	1.98	0.46
1:A:286:ARG:O	1:A:287:ALA:C	2.58	0.46
1:C:133:SER:HB2	1:C:137:ARG:HH11	1.80	0.46
1:E:291:THR:O	1:E:295:ARG:HG3	2.14	0.46
1:A:27:TYR:CD1	1:B:81:GLU:OE2	2.68	0.46
1:A:51:LEU:CD1	1:A:70:ILE:HD12	2.45	0.46
1:A:196:TYR:N	1:A:196:TYR:HD1	2.13	0.46
1:D:298:PHE:CB	1:D:299:PRO:HD3	2.45	0.46
1:A:224:VAL:C	1:A:226:LEU:H	2.22	0.46
1:B:253:TYR:O	1:B:256:ALA:HB3	2.15	0.46
1:C:40:ALA:HB3	1:C:105:PHE:CZ	2.51	0.46
1:A:104:ARG:HH22	1:B:78:VAL:CA	2.20	0.46
1:A:132:ARG:HA	1:A:180:GLU:HG2	1.97	0.46
1:B:53:PHE:CD1	1:B:95:PRO:HA	2.50	0.46
1:B:84:ARG:CB	1:B:84:ARG:HH11	2.28	0.46
1:D:282:SER:C	1:D:284:PRO:HD3	2.40	0.46
1:E:197:ILE:CB	1:E:198:PRO:HD3	2.41	0.46
1:E:233:ALA:O	1:E:237:PHE:HD1	1.98	0.46
1:A:282:SER:C	1:A:284:PRO:HD3	2.40	0.46
1:B:62:VAL:HG11	1:B:92:SER:HB3	1.97	0.46
1:B:224:VAL:C	1:B:226:LEU:H	2.22	0.46
1:C:226:LEU:HD23	1:D:224:VAL:HG21	1.97	0.46
1:D:224:VAL:C	1:D:226:LEU:H	2.22	0.46
1:D:278:LEU:HD23	1:D:287:ALA:HA	1.97	0.46
1:E:196:TYR:N	1:E:196:TYR:CD1	2.84	0.46
1:A:233:ALA:O	1:A:237:PHE:HD1	1.98	0.46
1:B:84:ARG:HA	1:B:107:ALA:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:TYR:HB3	1:C:119:PRO:HD3	1.97	0.46
1:D:259:PHE:CD2	1:D:259:PHE:C	2.94	0.46
1:E:264:PHE:HE2	1:E:302:PHE:HB2	1.79	0.46
1:A:70:ILE:HG22	1:A:71:TRP:N	2.30	0.46
1:A:263:LEU:C	1:A:265:TYR:H	2.24	0.46
1:B:47:LYS:CD	1:B:49:ARG:NH2	2.79	0.46
1:C:271:GLU:O	1:C:272:VAL:C	2.58	0.46
1:E:253:TYR:HA	1:E:313:PHE:CD2	2.50	0.46
1:A:27:TYR:CE1	1:B:81:GLU:CD	2.94	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:B:263:LEU:C	1:B:265:TYR:H	2.23	0.46
1:A:215:PHE:CE1	1:A:298:PHE:CD1	3.05	0.45
1:B:132:ARG:HA	1:B:180:GLU:HG2	1.99	0.45
1:C:286:ARG:O	1:C:287:ALA:C	2.59	0.45
1:D:23:LEU:HB2	1:D:150:LYS:HA	1.97	0.45
1:D:48:ASP:O	1:D:50:ARG:N	2.49	0.45
1:E:51:LEU:CD1	1:E:70:ILE:HD12	2.46	0.45
1:E:84:ARG:HA	1:E:107:ALA:HB2	1.98	0.45
1:E:140:VAL:HG22	1:E:181:SER:HB3	1.98	0.45
1:E:286:ARG:O	1:E:287:ALA:C	2.59	0.45
1:A:194:PHE:CE2	1:B:250:TYR:C	2.95	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:C:274:VAL:C	1:C:276:HIS:N	2.72	0.45
1:D:141:LEU:HD23	1:D:142:ALA:H	1.81	0.45
1:A:194:PHE:CE2	1:B:250:TYR:O	2.70	0.45
1:A:206:PHE:HD1	1:B:262:TYR:HB3	1.80	0.45
1:B:278:LEU:HD23	1:B:287:ALA:HA	1.98	0.45
1:C:47:LYS:CD	1:C:49:ARG:NH2	2.78	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:E:282:SER:C	1:E:284:PRO:HD3	2.41	0.45
1:A:44:LEU:HD12	1:A:101:TYR:CD2	2.52	0.45
1:A:68:GLU:H	1:A:68:GLU:CD	2.23	0.45
1:A:259:PHE:CD2	1:A:259:PHE:C	2.94	0.45
1:C:204:MET:O	1:C:207:ILE:HG12	2.17	0.45
1:D:159:TRP:CE3	1:D:189:ILE:HD12	2.51	0.45
1:D:196:TYR:N	1:D:196:TYR:HD1	2.15	0.45
1:A:137:ARG:HA	1:A:137:ARG:HD3	1.60	0.45
1:A:197:ILE:CB	1:A:198:PRO:HD3	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:ILE:HD13	1:A:270:ILE:HA	1.57	0.45
1:B:68:GLU:CD	1:B:68:GLU:H	2.23	0.45
1:D:198:PRO:HG2	1:E:251:MET:HE1	1.98	0.45
1:D:215:PHE:O	1:D:291:THR:CG2	2.62	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:A:209:PHE:HB2	1:B:266:PHE:CE1	2.52	0.45
1:C:51:LEU:CD1	1:C:70:ILE:HD12	2.46	0.45
1:C:53:PHE:HE2	1:C:63:LYS:CB	2.24	0.45
1:D:132:ARG:HA	1:D:180:GLU:HG2	1.98	0.45
1:D:216:TRP:CE2	1:D:295:ARG:HD3	2.52	0.45
1:A:158:GLY:HA2	1:A:192:GLN:OE1	2.17	0.45
1:B:8:PRO:O	1:B:50:ARG:NH1	2.50	0.45
1:B:38:VAL:HG22	1:B:39:ASN:N	2.32	0.45
1:B:274:VAL:C	1:B:276:HIS:N	2.74	0.45
1:C:210:ILE:HD12	1:D:231:LEU:HD22	1.98	0.45
1:D:84:ARG:HA	1:D:107:ALA:HB2	1.98	0.45
1:D:173:PHE:HZ	1:D:182:LYS:HZ1	1.63	0.45
1:D:196:TYR:N	1:D:196:TYR:CD1	2.84	0.45
1:D:226:LEU:HD22	1:D:226:LEU:HA	1.57	0.45
1:E:42:LEU:HB3	1:E:103:GLU:CG	2.42	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:147:LYS:C	1:D:149:GLY:N	2.47	0.45
1:D:206:PHE:CE1	1:E:263:LEU:CD1	3.00	0.45
1:A:179:LEU:C	1:A:179:LEU:CD1	2.90	0.45
1:B:196:TYR:N	1:B:196:TYR:CD1	2.85	0.44
1:B:291:THR:O	1:B:295:ARG:HG3	2.16	0.44
1:D:38:VAL:HG22	1:D:39:ASN:N	2.31	0.44
1:D:146:GLU:HG3	1:E:176:GLU:CG	2.47	0.44
1:E:53:PHE:CD1	1:E:95:PRO:HA	2.51	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:72:ILE:HG22	1:C:73:PRO:HD2	1.99	0.44
1:C:159:TRP:CE3	1:C:189:ILE:HD12	2.52	0.44
1:C:201:ILE:HD13	1:C:201:ILE:HA	1.83	0.44
1:C:224:VAL:C	1:C:226:LEU:H	2.25	0.44
1:D:37:LYS:HG2	1:D:108:ARG:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:48:ASP:C	1:D:50:ARG:N	2.73	0.44
1:D:179:LEU:C	1:D:179:LEU:CD1	2.90	0.44
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:8:PRO:O	1:C:50:ARG:NH1	2.50	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:E:276:HIS:C	1:E:278:LEU:N	2.65	0.44
1:B:267:VAL:HG23	1:B:298:PHE:CZ	2.52	0.44
1:C:155:PHE:HD1	1:D:110:LEU:HD22	1.82	0.44
1:C:278:LEU:HD23	1:C:287:ALA:HA	1.99	0.44
1:D:253:TYR:O	1:D:256:ALA:HB3	2.17	0.44
1:A:104:ARG:HH22	1:B:77:PHE:C	2.24	0.44
1:C:118:TYR:CZ	1:C:196:TYR:HE2	2.36	0.44
1:E:196:TYR:N	1:E:196:TYR:HD1	2.15	0.44
1:A:18:ASN:O	1:A:44:LEU:HA	2.18	0.44
1:A:201:ILE:HD13	1:A:201:ILE:HA	1.86	0.44
1:A:283:GLN:C	1:A:285:ALA:N	2.75	0.44
1:B:141:LEU:HD23	1:B:142:ALA:H	1.82	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:D:225:THR:HG21	1:E:224:VAL:CG2	2.37	0.44
1:E:23:LEU:HG	1:E:164:PHE:CD1	2.52	0.44
1:E:72:ILE:HG22	1:E:73:PRO:HD2	1.99	0.44
1:B:232:ILE:HA	1:B:235:ILE:HD12	2.00	0.44
1:C:216:TRP:CZ2	1:C:295:ARG:HB3	2.52	0.44
1:C:270:ILE:HD13	1:C:270:ILE:HA	1.61	0.44
1:D:118:TYR:CZ	1:D:196:TYR:HE2	2.36	0.44
1:E:300:VAL:O	1:E:304:LEU:HB2	2.18	0.44
1:A:23:LEU:HB2	1:A:150:LYS:HA	1.99	0.44
1:A:202:LEU:CB	1:B:259:PHE:HE1	2.31	0.44
1:B:140:VAL:HG22	1:B:181:SER:HB3	2.00	0.44
1:B:298:PHE:CB	1:B:299:PRO:HD3	2.47	0.44
1:C:202:LEU:HD12	1:D:259:PHE:CZ	2.53	0.44
1:D:202:LEU:HD12	1:E:259:PHE:HZ	1.82	0.44
1:D:225:THR:HG22	1:E:224:VAL:CG2	2.44	0.44
1:E:23:LEU:HD22	1:E:38:VAL:HG21	1.99	0.44
1:B:268:ALA:HA	1:B:298:PHE:HE1	1.82	0.43
1:C:196:TYR:O	1:C:200:ILE:HB	2.17	0.43
1:C:232:ILE:HA	1:C:235:ILE:HD12	1.99	0.43
1:C:264:PHE:HE2	1:C:302:PHE:HB2	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:224:VAL:O	1:D:228:VAL:HB	2.17	0.43
1:D:283:GLN:C	1:D:285:ALA:H	2.26	0.43
1:B:23:LEU:HB2	1:B:150:LYS:HA	2.00	0.43
1:B:119:PRO:HD3	1:B:254:THR:OG1	2.18	0.43
1:C:23:LEU:CD1	1:C:164:PHE:CD1	3.01	0.43
1:E:68:GLU:CD	1:E:68:GLU:H	2.25	0.43
1:E:118:TYR:CZ	1:E:196:TYR:HE2	2.36	0.43
1:E:274:VAL:C	1:E:276:HIS:N	2.77	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:B:216:TRP:CH2	1:B:295:ARG:HB3	2.53	0.43
1:C:27:TYR:HB3	1:D:110:LEU:CD1	2.44	0.43
1:D:216:TRP:CH2	1:D:295:ARG:HB3	2.53	0.43
1:E:179:LEU:C	1:E:179:LEU:CD1	2.91	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: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:226:LEU:HD22	1:C:226:LEU:HA	1.58	0.43
1:C:256:ALA:HB1	1:C:309:LEU:HD21	2.00	0.43
1:D:263:LEU:C	1:D:265:TYR:H	2.26	0.43
1:A:224:VAL:O	1:A:228:VAL:HB	2.18	0.43
1:B:40:ALA:HB3	1:B:105:PHE:CZ	2.54	0.43
1:B:179:LEU:C	1:B:179:LEU:CD1	2.92	0.43
1:C:231:LEU:HD13	1:C:265:TYR:HB3	2.00	0.43
1:D:140:VAL:HG22	1:D:181:SER:HB3	1.99	0.43
1:D:268:ALA:HA	1:D:298:PHE:HE1	1.84	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:A:140:VAL:HG22	1:A:181:SER:CB	2.49	0.43
1:A:217:SER:CB	1:B:220:TYR:CE2	3.02	0.43
1:B:123:GLN:HA	1:B:123:GLN:HE21	1.83	0.43
1:B:249:PRO:HD2	1:B:250:TYR:CE1	2.54	0.43
1:C:263:LEU:C	1:C:265:TYR:N	2.77	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:E:232:ILE:HA	1:E:235:ILE:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:TYR:N	1:B:196:TYR:HD1	2.16	0.43
1:A:216:TRP:CH2	1:A:295:ARG:HB3	2.54	0.42
1:A:253:TYR:HA	1:A:313:PHE:CD2	2.52	0.42
1:B:158:GLY:HA2	1:B:192:GLN:OE1	2.19	0.42
1:B:204:MET:O	1:B:207:ILE:HG12	2.19	0.42
1:D:291:THR:O	1:D:295:ARG:HG3	2.18	0.42
1:E:137:ARG:HD3	1:E:137:ARG:HA	1.66	0.42
1:E:256:ALA:HB1	1:E:309:LEU:HD21	2.01	0.42
1:E:271:GLU:O	1:E:272:VAL:C	2.60	0.42
1:A:118:TYR:HB3	1:A:119:PRO:HD3	2.01	0.42
1:A:157:THR:HG21	1:B:34:GLU:CD	2.44	0.42
1:A:294:SER:C	1:A:296:ILE:H	2.27	0.42
1:C:51:LEU:HD13	1:C:70:ILE:HD12	2.01	0.42
1:E:259:PHE:CD2	1:E:259:PHE:C	2.96	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:A:271:GLU:O	1:A:272:VAL:C	2.62	0.42
1:B:226:LEU:HD22	1:B:226:LEU:HA	1.61	0.42
1:B:259:PHE:CD2	1:B:259:PHE:C	2.97	0.42
1:C:65:TYR:CD2	1:C:70:ILE:HD11	2.54	0.42
1:C:179:LEU:C	1:C:179:LEU:CD1	2.92	0.42
1:D:132:ARG:NH2	1:D:178:ARG:HB2	2.35	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:A:47:LYS:CD	1:A:49:ARG:NH2	2.81	0.42
1:B:25:GLU:HA	1:B:25:GLU:OE1	2.19	0.42
1:D:213:THR:CG2	1:D:226:LEU:HD11	2.48	0.42
1:E:283:GLN:C	1:E:285:ALA:H	2.26	0.42
1:A:48:ASP:C	1:A:50:ARG:N	2.78	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:B:118:TYR:HB3	1:B:119:PRO:HD3	2.00	0.42
1:B:271:GLU:O	1:B:272:VAL:C	2.61	0.42
1:B:294:SER:C	1:B:296:ILE:N	2.76	0.42
1:E:76:ARG:CZ	1:E:130:ILE:HD12	2.48	0.42
1:A:202:LEU:O	1:A:203:PRO:C	2.63	0.42
1:A:213:THR:CG2	1:A:226:LEU:HD11	2.48	0.42
1:B:53:PHE:HE2	1:B:63:LYS:CB	2.26	0.42
1:B:118:TYR:CZ	1:B:196:TYR:HE2	2.37	0.42
1:C:77:PHE:HB3	1:C:80:VAL:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:ASN:ND2	1:C:152:ASP:H	2.17	0.42
1:C:197:ILE:HB	1:C:198:PRO:CD	2.43	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:A:77:PHE:HB3	1:A:80:VAL:CG2	2.49	0.42
1:B:294:SER:C	1:B:296:ILE:H	2.26	0.42
1:D:133:SER:HB2	1:D:137:ARG:HH11	1.84	0.42
1:D:278:LEU:HD23	1:D:287:ALA:CA	2.50	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:D:287:ALA:C	1:D:289:SER:H	2.27	0.42
1:E:130:ILE:HG23	1:E:182:LYS:HB2	2.01	0.42
1:A:248:THR:HB	1:A:250:TYR:CE1	2.55	0.42
1:A:278:LEU:HD21	1:A:286:ARG:HB3	2.01	0.42
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:B:238:ASN:CA	1:B:258:ILE:HD11	2.43	0.41
1:B:248:THR:HB	1:B:250:TYR:CE1	2.55	0.41
1:B:286:ARG:O	1:B:287:ALA:C	2.61	0.41
1:C:132:ARG:HA	1:C:180:GLU:HG2	2.01	0.41
1:D:201:ILE:HD13	1:D:201:ILE:HA	1.81	0.41
1:E:7:PRO:C	1:E:50:ARG:HH12	2.27	0.41
1:E:294:SER:C	1:E:296:ILE:H	2.28	0.41
1:A:19:THR:HA	1:A:43:SER:O	2.20	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:C:44:LEU:HD12	1:C:101:TYR:CD2	2.55	0.41
1:C:140:VAL:HG22	1:C:181:SER:CB	2.50	0.41
1:C:233:ALA:O	1:C:237:PHE:HD1	2.02	0.41
1:C:282:SER:C	1:C:284:PRO:HD3	2.44	0.41
1:D:18:ASN:O	1:D:44:LEU:HA	2.20	0.41
1:D:84:ARG:CB	1:D:84:ARG:NH1	2.84	0.41
1:E:140:VAL:HG22	1:E:181:SER:CB	2.50	0.41
1:A:53:PHE:HE2	1:A:63:LYS:CB	2.25	0.41
1:B:132:ARG:NH2	1:B:178:ARG:HB2	2.35	0.41
1:C:158:GLY:HA2	1:C:192:GLN:OE1	2.20	0.41
1:C:224:VAL:O	1:C:228:VAL:HB	2.19	0.41
1:C:287:ALA:C	1:C:289:SER:H	2.28	0.41
1:D:28:SER:HB2	1:D:37:LYS:HD2	2.02	0.41
1:D:40:ALA:HB3	1:D:105:PHE:CZ	2.55	0.41
1:D:215:PHE:CE1	1:D:298:PHE:CD1	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:158:GLY:HA2	1:E:192:GLN:OE1	2.19	0.41
1:A:104:ARG:NH1	1:B:77:PHE:O	2.53	0.41
1:A:194:PHE:HA	1:A:197:ILE:HD12	2.03	0.41
1:A:264:PHE:HE2	1:A:302:PHE:HB2	1.84	0.41
1:D:50:ARG:HE	1:D:50:ARG:HB3	1.69	0.41
1:E:224:VAL:O	1:E:228:VAL:HB	2.21	0.41
1:E:287:ALA:C	1:E:289:SER:H	2.26	0.41
1:C:196:TYR:N	1:C:196:TYR:CD1	2.88	0.41
1:D:24:ILE:HB	1:D:39:ASN:O	2.20	0.41
1:E:37:LYS:HG2	1:E:108:ARG:HB3	2.02	0.41
1:A:18:ASN:HB3	1:A:143:VAL:CG2	2.50	0.41
1:B:194:PHE:HA	1:B:197:ILE:HD12	2.03	0.41
1:C:77:PHE:CD1	1:C:84:ARG:CD	3.03	0.41
1:C:218:THR:HA	1:C:275:GLN:HE22	1.86	0.41
1:D:68:GLU:CD	1:D:68:GLU:N	2.77	0.41
1:E:25:GLU:OE1	1:E:25:GLU:HA	2.19	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:D:200:ILE:HD11	1:D:240:LEU:CD2	2.43	0.41
1:E:48:ASP:C	1:E:50:ARG:N	2.78	0.41
1:E:84:ARG:HH11	1:E:84:ARG:HB3	1.83	0.41
1:E:263:LEU:C	1:E:265:TYR:N	2.79	0.41
1:A:51:LEU:HD13	1:A:70:ILE:HD12	2.02	0.41
1:A:192:GLN:HB3	1:B:249:PRO:HB3	2.02	0.41
1:B:37:LYS:HG2	1:B:108:ARG:HB3	2.03	0.41
1:C:19:THR:HA	1:C:43:SER:O	2.20	0.41
1:D:23:LEU:CD2	1:D:38:VAL:HG21	2.51	0.41
1:D:123:GLN:HB2	1:D:189:ILE:HG13	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:E:294:SER:C	1:E:296:ILE:N	2.79	0.41
1:A:80:VAL:HG12	1:A:82:ASN:O	2.21	0.41
1:B:7:PRO:C	1:B:50:ARG:HH12	2.28	0.41
1:B:23:LEU:HG	1:B:164:PHE:CD1	2.55	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:283:GLN:C	1:B:285:ALA:H	2.28	0.41
1:C:202:LEU:O	1:C:203:PRO:C	2.63	0.41
1:D:18:ASN:HB3	1:D:143:VAL:CG2	2.51	0.41
1:D:204:MET:O	1:D:207:ILE:HG12	2.21	0.41
1:D:213:THR:HG22	1:D:226:LEU:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:65:TYR:CD2	1:E:70:ILE:HD11	2.56	0.41
1:E:194:PHE:O	1:E:198:PRO:HD2	2.20	0.41
1:A:84:ARG:HH11	1:A:84:ARG:HB3	1.86	0.41
1:B:35:THR:OG1	1:B:108:ARG:NH2	2.54	0.41
1:C:237:PHE:CE1	1:D:235:ILE:HG21	2.56	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:A:40:ALA:HB3	1:A:105:PHE:CZ	2.56	0.40
1:A:157:THR:HG21	1:B:34:GLU:HG3	2.03	0.40
1:B:48:ASP:C	1:B:50:ARG:N	2.77	0.40
1:B:278:LEU:HD23	1:B:287:ALA:CA	2.51	0.40
1:C:7:PRO:C	1:C:50:ARG:HH12	2.29	0.40
1:C:248:THR:HB	1:C:250:TYR:CE1	2.55	0.40
1:D:197:ILE:CB	1:D:198:PRO:HD3	2.45	0.40
1:A:8:PRO:HA	1:A:71:TRP:CG	2.57	0.40
1:A:65:TYR:CD2	1:A:70:ILE:HD11	2.56	0.40
1:A:155:PHE:CE1	1:B:112:PRO:CA	3.03	0.40
1:A:287:ALA:C	1:A:289:SER:H	2.29	0.40
1:C:194:PHE:O	1:C:198:PRO:HD2	2.21	0.40
1:C:243:THR:HG22	1:C:244:ASN:ND2	2.37	0.40
1:D:232:ILE:HA	1:D:235:ILE:HD12	2.02	0.40
1:D:271:GLU:OE2	1:D:272:VAL:N	2.54	0.40
1:E:51:LEU:HD13	1:E:70:ILE:HD12	2.03	0.40
1:E:151:ASN:ND2	1:E:152:ASP:H	2.19	0.40
1:A:204:MET:HE2	1:A:204:MET:HB3	1.91	0.40
1:B:19:THR:HA	1:B:43:SER:O	2.22	0.40
1:B:77:PHE:HB3	1:B:80:VAL:CG2	2.51	0.40
1:C:53:PHE:CD1	1:C:53:PHE:C	3.00	0.40
1:C:253:TYR:HA	1:C:313:PHE:CD2	2.51	0.40
1:A:193:TYR:CD2	1:A:193:TYR:C	3.00	0.40
1:A:274:VAL:C	1:A:276:HIS:N	2.72	0.40
1:C:117:ARG:O	1:C:118:TYR:C	2.65	0.40
1:E:144:ASP:HA	1:E:147:LYS:HB3	2.04	0.40
1:E:302:PHE:C	1:E:304:LEU:N	2.78	0.40
1:A:72:ILE:HG22	1:A:73:PRO:HD2	2.04	0.40
1:B:23:LEU:CD2	1:B:38:VAL:HG21	2.51	0.40
1:B:130:ILE:HG23	1:B:182:LYS:HB2	2.03	0.40
1:B:137:ARG:HA	1:B:137:ARG:HD3	1.65	0.40
1:B:255:GLY:O	1:B:258:ILE:HG22	2.21	0.40
1:C:23:LEU:HG	1:C:164:PHE:CD1	2.56	0.40
1:C:27:TYR:CD1	1:D:81:GLU:CD	3.00	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:TYR:CD2	1:C:193:TYR:C	3.00	0.40
1:C:253:TYR:O	1:C:256:ALA:HB3	2.21	0.40
1:D:19:THR:HA	1:D:43:SER: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%)	239 (78%)	59 (19%)	10 (3%)	3	24
1	B	308/317 (97%)	238 (77%)	61 (20%)	9 (3%)	3	26
1	C	308/317 (97%)	235 (76%)	64 (21%)	9 (3%)	3	26
1	D	308/317 (97%)	238 (77%)	61 (20%)	9 (3%)	3	26
1	E	308/317 (97%)	239 (78%)	61 (20%)	8 (3%)	4	27
All	All	1540/1585 (97%)	1189 (77%)	306 (20%)	45 (3%)	3	26

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

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Mol	Chain	Res	Type
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
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%)	232 (84%)	46 (16%)	2	14
1	B	278/284 (98%)	231 (83%)	47 (17%)	2	13
1	C	278/284 (98%)	232 (84%)	46 (16%)	2	14
1	D	278/284 (98%)	234 (84%)	44 (16%)	2	15
1	E	278/284 (98%)	232 (84%)	46 (16%)	2	14
All	All	1390/1420 (98%)	1161 (84%)	229 (16%)	2	14

All (229) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	PHE
1	A	64	THR
1	A	68	GLU
1	A	72	ILE
1	A	79	ASN
1	A	84	ARG
1	A	89	VAL
1	A	98	THR
1	A	100	GLN
1	A	104	ARG
1	A	113	LEU
1	A	122	SER
1	A	124	THR
1	A	130	ILE
1	A	140	VAL
1	A	141	LEU
1	A	150	LYS
1	A	151	ASN
1	A	154	VAL
1	A	162	GLU
1	A	179	LEU
1	A	202	LEU
1	A	204	MET
1	A	211	SER
1	A	213	THR
1	A	218	THR
1	A	221	GLU
1	A	226	LEU
1	A	227	VAL
1	A	232	ILE
1	A	239	ILE

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Mol	Chain	Res	Type
1	A	241	VAL
1	A	243	THR
1	A	252	THR
1	A	254	THR
1	A	257	ILE
1	A	260	MET
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	64	THR
1	B	68	GLU
1	B	72	ILE
1	B	79	ASN
1	B	84	ARG
1	B	89	VAL
1	B	98	THR
1	B	100	GLN
1	B	113	LEU
1	B	122	SER
1	B	124	THR
1	B	130	ILE
1	B	140	VAL
1	B	141	LEU
1	B	150	LYS
1	B	151	ASN
1	B	154	VAL
1	B	162	GLU
1	B	178	ARG
1	B	179	LEU
1	B	202	LEU
1	B	204	MET
1	B	211	SER
1	B	213	THR
1	B	218	THR
1	B	221	GLU

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Mol	Chain	Res	Type
1	B	226	LEU
1	B	227	VAL
1	B	232	ILE
1	B	239	ILE
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	290	ILE
1	B	292	ARG
1	B	303	LEU
1	B	306	ASN
1	B	314	PHE
1	C	53	PHE
1	C	64	THR
1	C	68	GLU
1	C	72	ILE
1	C	79	ASN
1	C	84	ARG
1	C	89	VAL
1	C	98	THR
1	C	100	GLN
1	C	104	ARG
1	C	113	LEU
1	C	122	SER
1	C	124	THR
1	C	130	ILE
1	C	140	VAL
1	C	141	LEU
1	C	150	LYS
1	C	154	VAL
1	C	157	THR
1	C	162	GLU
1	C	179	LEU
1	C	202	LEU

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Mol	Chain	Res	Type
1	C	204	MET
1	C	211	SER
1	C	213	THR
1	C	218	THR
1	C	221	GLU
1	C	226	LEU
1	C	227	VAL
1	C	232	ILE
1	C	239	ILE
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
1	D	53	PHE
1	D	64	THR
1	D	68	GLU
1	D	72	ILE
1	D	79	ASN
1	D	84	ARG
1	D	89	VAL
1	D	98	THR
1	D	100	GLN
1	D	113	LEU
1	D	122	SER
1	D	124	THR
1	D	130	ILE
1	D	140	VAL
1	D	141	LEU
1	D	150	LYS
1	D	151	ASN
1	D	154	VAL

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Mol	Chain	Res	Type
1	D	162	GLU
1	D	179	LEU
1	D	202	LEU
1	D	204	MET
1	D	211	SER
1	D	213	THR
1	D	218	THR
1	D	221	GLU
1	D	226	LEU
1	D	227	VAL
1	D	232	ILE
1	D	239	ILE
1	D	241	VAL
1	D	243	THR
1	D	252	THR
1	D	254	THR
1	D	257	ILE
1	D	260	MET
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
1	D	306	ASN
1	E	53	PHE
1	E	64	THR
1	E	68	GLU
1	E	72	ILE
1	E	79	ASN
1	E	84	ARG
1	E	89	VAL
1	E	98	THR
1	E	100	GLN
1	E	113	LEU
1	E	122	SER
1	E	124	THR
1	E	130	ILE
1	E	140	VAL
1	E	141	LEU
1	E	150	LYS

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Mol	Chain	Res	Type
1	E	151	ASN
1	E	154	VAL
1	E	162	GLU
1	E	178	ARG
1	E	179	LEU
1	E	202	LEU
1	E	204	MET
1	E	211	SER
1	E	213	THR
1	E	218	THR
1	E	221	GLU
1	E	226	LEU
1	E	232	ILE
1	E	239	ILE
1	E	241	VAL
1	E	243	THR
1	E	252	THR
1	E	254	THR
1	E	257	ILE
1	E	260	MET
1	E	263	LEU
1	E	269	VAL
1	E	270	ILE
1	E	274	VAL
1	E	282	SER
1	E	290	ILE
1	E	292	ARG
1	E	303	LEU
1	E	306	ASN
1	E	314	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	ASN
1	A	100	GLN
1	A	151	ASN
1	A	172	ASN
1	A	234	HIS
1	A	238	ASN
1	A	244	ASN
1	A	275	GLN

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Mol	Chain	Res	Type
1	B	39	ASN
1	B	79	ASN
1	B	100	GLN
1	B	151	ASN
1	B	172	ASN
1	B	238	ASN
1	B	244	ASN
1	B	275	GLN
1	C	39	ASN
1	C	79	ASN
1	C	100	GLN
1	C	151	ASN
1	C	172	ASN
1	C	234	HIS
1	C	238	ASN
1	C	244	ASN
1	C	275	GLN
1	D	39	ASN
1	D	79	ASN
1	D	100	GLN
1	D	123	GLN
1	D	151	ASN
1	D	234	HIS
1	D	238	ASN
1	D	244	ASN
1	D	275	GLN
1	E	39	ASN
1	E	79	ASN
1	E	100	GLN
1	E	151	ASN
1	E	172	ASN
1	E	238	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 ⓘ

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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%)	1.34	72 (23%) 2 2	77, 116, 170, 252	0
1	B	310/317 (97%)	1.26	61 (19%) 3 3	77, 116, 170, 251	0
1	C	310/317 (97%)	1.18	58 (18%) 3 4	77, 115, 169, 250	0
1	D	310/317 (97%)	1.43	79 (25%) 1 2	75, 115, 169, 252	0
1	E	310/317 (97%)	1.34	72 (23%) 2 2	79, 115, 170, 251	0
All	All	1550/1585 (97%)	1.31	342 (22%) 2 2	75, 116, 170, 252	0

All (342) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	153	ASP	11.2
1	A	60	VAL	8.0
1	E	144	ASP	7.8
1	C	60	VAL	7.3
1	E	147	LYS	6.9
1	C	144	ASP	6.8
1	E	88	VAL	6.0
1	B	152	ASP	5.9
1	D	83	ALA	5.9
1	B	88	VAL	5.9
1	A	59	GLY	5.8
1	A	62	VAL	5.7
1	A	74	GLU	5.7
1	B	153	ASP	5.7
1	B	47	LYS	5.6
1	A	153	ASP	5.3
1	C	59	GLY	5.2
1	D	85	ASP	5.1
1	E	47	LYS	5.0
1	B	144	ASP	5.0

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Mol	Chain	Res	Type	RSRZ
1	C	11	ALA	5.0
1	E	148	VAL	5.0
1	B	216	TRP	4.9
1	D	128	TYR	4.9
1	A	126	HIS	4.9
1	A	128	TYR	4.7
1	B	148	VAL	4.7
1	C	277	TYR	4.7
1	A	88	VAL	4.6
1	A	221	GLU	4.5
1	D	152	ASP	4.5
1	A	206	PHE	4.5
1	E	83	ALA	4.5
1	B	100	GLN	4.4
1	E	59	GLY	4.4
1	C	13	GLU	4.4
1	B	174	ALA	4.3
1	A	58	SER	4.3
1	C	139	ILE	4.2
1	A	11	ALA	4.2
1	D	82	ASN	4.2
1	B	101	TYR	4.2
1	E	146	GLU	4.2
1	C	153	ASP	4.2
1	B	91	ILE	4.2
1	A	13	GLU	4.2
1	A	139	ILE	4.1
1	B	90	ASP	4.1
1	A	144	ASP	4.0
1	D	11	ALA	3.9
1	D	78	VAL	3.9
1	B	49	ARG	3.9
1	A	79	ASN	3.9
1	C	147	LYS	3.9
1	B	60	VAL	3.9
1	C	133	SER	3.9
1	E	139	ILE	3.8
1	C	85	ASP	3.8
1	C	151	ASN	3.8
1	B	11	ALA	3.8
1	A	148	VAL	3.8
1	A	203	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	117	ARG	3.8
1	C	114	ASP	3.7
1	E	101	TYR	3.7
1	D	304	LEU	3.7
1	C	285	ALA	3.7
1	E	91	ILE	3.6
1	E	60	VAL	3.6
1	D	18	ASN	3.6
1	A	145	LEU	3.6
1	D	56	VAL	3.6
1	D	148	VAL	3.6
1	D	182	LYS	3.5
1	E	209	PHE	3.5
1	A	143	VAL	3.5
1	D	112	PRO	3.5
1	C	168	VAL	3.5
1	D	100	GLN	3.5
1	A	14	PRO	3.4
1	D	169	LYS	3.4
1	E	11	ALA	3.4
1	E	173	PHE	3.4
1	D	57	ARG	3.4
1	E	149	GLY	3.4
1	E	114	ASP	3.4
1	D	138	ASN	3.4
1	D	195	SER	3.4
1	C	116	ARG	3.4
1	D	117	ARG	3.4
1	A	12	ASP	3.4
1	B	222	ALA	3.4
1	E	138	ASN	3.4
1	B	231	LEU	3.3
1	A	61	ARG	3.3
1	E	90	ASP	3.3
1	A	224	VAL	3.3
1	C	138	ASN	3.3
1	E	128	TYR	3.3
1	D	168	VAL	3.3
1	E	277	TYR	3.3
1	E	100	GLN	3.3
1	A	172	ASN	3.2
1	D	151	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	222	ALA	3.2
1	A	78	VAL	3.2
1	E	242	GLU	3.2
1	C	83	ALA	3.2
1	D	187	LEU	3.2
1	C	176	GLU	3.2
1	A	7	PRO	3.2
1	D	12	ASP	3.2
1	C	221	GLU	3.2
1	D	7	PRO	3.2
1	C	172	ASN	3.2
1	C	142	ALA	3.2
1	D	183	LEU	3.2
1	A	165	THR	3.1
1	B	61	ARG	3.1
1	D	154	VAL	3.1
1	E	82	ASN	3.1
1	A	230	THR	3.1
1	B	138	ASN	3.1
1	E	68	GLU	3.1
1	B	136	THR	3.1
1	D	63	LYS	3.1
1	A	134	VAL	3.0
1	D	167	VAL	3.0
1	D	130	ILE	3.0
1	C	233	ALA	3.0
1	B	213	THR	3.0
1	E	174	ALA	3.0
1	E	116	ARG	3.0
1	D	200	ILE	3.0
1	A	89	VAL	3.0
1	B	188	ARG	3.0
1	D	126	HIS	3.0
1	C	143	VAL	3.0
1	A	10	ILE	3.0
1	A	64	THR	3.0
1	B	7	PRO	2.9
1	D	45	SER	2.9
1	E	186	GLN	2.9
1	A	91	ILE	2.9
1	E	232	ILE	2.9
1	C	18	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	221	GLU	2.9
1	B	187	LEU	2.9
1	B	165	THR	2.9
1	E	69	ALA	2.9
1	A	110	LEU	2.9
1	D	118	TYR	2.9
1	D	49	ARG	2.9
1	C	245	LEU	2.9
1	C	141	LEU	2.9
1	E	286	ARG	2.8
1	E	89	VAL	2.8
1	B	59	GLY	2.8
1	D	127	ILE	2.8
1	D	263	LEU	2.8
1	E	243	THR	2.8
1	D	55	PRO	2.8
1	C	134	VAL	2.8
1	E	305	ALA	2.8
1	A	233	ALA	2.8
1	A	47	LYS	2.8
1	A	170	PRO	2.8
1	A	124	THR	2.8
1	A	177	ASP	2.7
1	B	154	VAL	2.7
1	A	53	PHE	2.7
1	E	32	LYS	2.7
1	B	315	GLY	2.7
1	B	96	ASP	2.7
1	D	111	SER	2.7
1	A	209	PHE	2.7
1	B	173	PHE	2.7
1	D	241	VAL	2.7
1	B	171	ALA	2.7
1	B	15	LEU	2.7
1	E	282	SER	2.7
1	B	127	ILE	2.6
1	C	14	PRO	2.6
1	B	232	ILE	2.6
1	D	231	LEU	2.6
1	C	170	PRO	2.6
1	E	315	GLY	2.6
1	A	101	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	13	GLU	2.6
1	B	74	GLU	2.6
1	B	81	GLU	2.6
1	C	74	GLU	2.6
1	D	143	VAL	2.6
1	D	47	LYS	2.6
1	B	86	ALA	2.6
1	D	234	HIS	2.6
1	C	173	PHE	2.6
1	A	130	ILE	2.6
1	B	139	ILE	2.6
1	C	117	ARG	2.6
1	D	90	ASP	2.6
1	D	134	VAL	2.6
1	C	288	ALA	2.6
1	B	12	ASP	2.5
1	A	208	LEU	2.5
1	A	55	PRO	2.5
1	B	314	PHE	2.5
1	E	195	SER	2.5
1	D	74	GLU	2.5
1	D	162	GLU	2.5
1	A	63	LYS	2.5
1	A	169	LYS	2.5
1	B	48	ASP	2.5
1	C	169	LYS	2.5
1	D	171	ALA	2.5
1	C	61	ARG	2.5
1	C	58	SER	2.5
1	C	115	PHE	2.5
1	C	69	ALA	2.5
1	C	179	LEU	2.5
1	D	51	LEU	2.5
1	D	144	ASP	2.5
1	E	301	VAL	2.5
1	D	60	VAL	2.4
1	E	145	LEU	2.4
1	E	67	PRO	2.4
1	B	87	ASP	2.4
1	C	135	ASP	2.4
1	D	124	THR	2.4
1	B	125	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	242	GLU	2.4
1	B	304	LEU	2.4
1	D	19	THR	2.4
1	A	194	PHE	2.4
1	B	266	PHE	2.4
1	D	186	GLN	2.4
1	A	90	ASP	2.4
1	E	184	ASP	2.4
1	C	242	GLU	2.4
1	C	55	PRO	2.4
1	A	207	ILE	2.4
1	D	165	THR	2.4
1	E	62	VAL	2.4
1	C	193	TYR	2.3
1	C	281	GLU	2.3
1	C	316	PHE	2.3
1	E	211	SER	2.3
1	C	171	ALA	2.3
1	D	120	PHE	2.3
1	A	95	PRO	2.3
1	D	163	SER	2.3
1	E	217	SER	2.3
1	B	277	TYR	2.3
1	D	310	ALA	2.3
1	D	221	GLU	2.3
1	A	179	LEU	2.3
1	D	15	LEU	2.2
1	E	134	VAL	2.2
1	E	200	ILE	2.2
1	A	229	SER	2.2
1	B	301	VAL	2.2
1	E	141	LEU	2.2
1	B	225	THR	2.2
1	A	87	ASP	2.2
1	C	121	ASP	2.2
1	D	87	ASP	2.2
1	D	308	ILE	2.2
1	E	96	ASP	2.2
1	E	285	ALA	2.2
1	E	275	GLN	2.2
1	A	220	TYR	2.2
1	C	185	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	56	VAL	2.2
1	E	61	ARG	2.2
1	B	146	GLU	2.2
1	E	267	VAL	2.2
1	A	163	SER	2.2
1	C	137	ARG	2.2
1	D	62	VAL	2.2
1	B	20	GLY	2.2
1	A	235	ILE	2.2
1	C	7	PRO	2.2
1	E	7	PRO	2.2
1	E	270	ILE	2.2
1	A	184	ASP	2.2
1	A	186	GLN	2.2
1	E	95	PRO	2.2
1	D	79	ASN	2.2
1	A	174	ALA	2.1
1	B	145	LEU	2.2
1	A	49	ARG	2.1
1	A	185	TYR	2.1
1	E	154	VAL	2.1
1	B	316	PHE	2.1
1	A	15	LEU	2.1
1	A	138	ASN	2.1
1	D	199	ASN	2.1
1	D	61	ARG	2.1
1	A	54	ASP	2.1
1	D	313	PHE	2.1
1	C	180	GLU	2.1
1	E	14	PRO	2.1
1	E	81	GLU	2.1
1	D	141	LEU	2.1
1	E	15	LEU	2.1
1	B	82	ASN	2.1
1	E	58	SER	2.1
1	C	10	ILE	2.1
1	E	143	VAL	2.1
1	C	198	PRO	2.1
1	C	25	GLU	2.1
1	D	230	THR	2.1
1	E	49	ARG	2.1
1	C	195	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	12	ASP	2.1
1	D	129	LEU	2.1
1	B	26	CYS	2.1
1	D	77	PHE	2.1
1	D	44	LEU	2.1
1	B	27	TYR	2.1
1	D	262	TYR	2.1
1	D	249	PRO	2.1
1	B	45	SER	2.1
1	A	173	PHE	2.1
1	A	244	ASN	2.1
1	C	118	TYR	2.0
1	A	117	ARG	2.0
1	A	242	GLU	2.0
1	D	84	ARG	2.0
1	B	305	ALA	2.0
1	D	300	VAL	2.0
1	E	238	ASN	2.0
1	E	20	GLY	2.0
1	E	182	LYS	2.0
1	B	103	GLU	2.0
1	E	87	ASP	2.0
1	E	135	ASP	2.0
1	D	316	PHE	2.0
1	E	205	LEU	2.0
1	E	244	ASN	2.0
1	A	141	LEU	2.0
1	A	176	GLU	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 oligosaccharides 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. 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	B-factors($\text{\AA}^2$)	Q<0.9
2	ARS	C	1317	1/1	0.78	0.24	206,206,206,206	0

6.5 Other polymers [i](#)

There are no such residues in this entry.