



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:02 PM UTC

PDB ID : 2XQ3 / pdb_00002xq3
Title : Pentameric ligand gated ion channel GLIC in complex with Br-lidocaine
Authors : Hilf, R.J.C.; Bertozzi, C.; Zimmermann, I.; Reiter, A.; Trauner, D.; Dutzler, R.
Deposited on : 2010-09-01
Resolution : 3.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<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

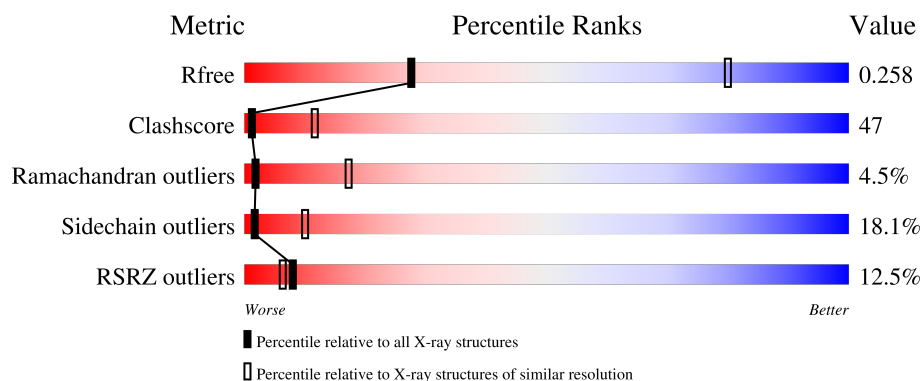
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	15% 32% 49% 15% ..
1	B	317	11% 32% 48% 16% ..
1	C	317	10% 36% 45% 16% ..
1	D	317	12% 34% 47% 16% ..
1	E	317	13% 32% 50% 15% ..

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			

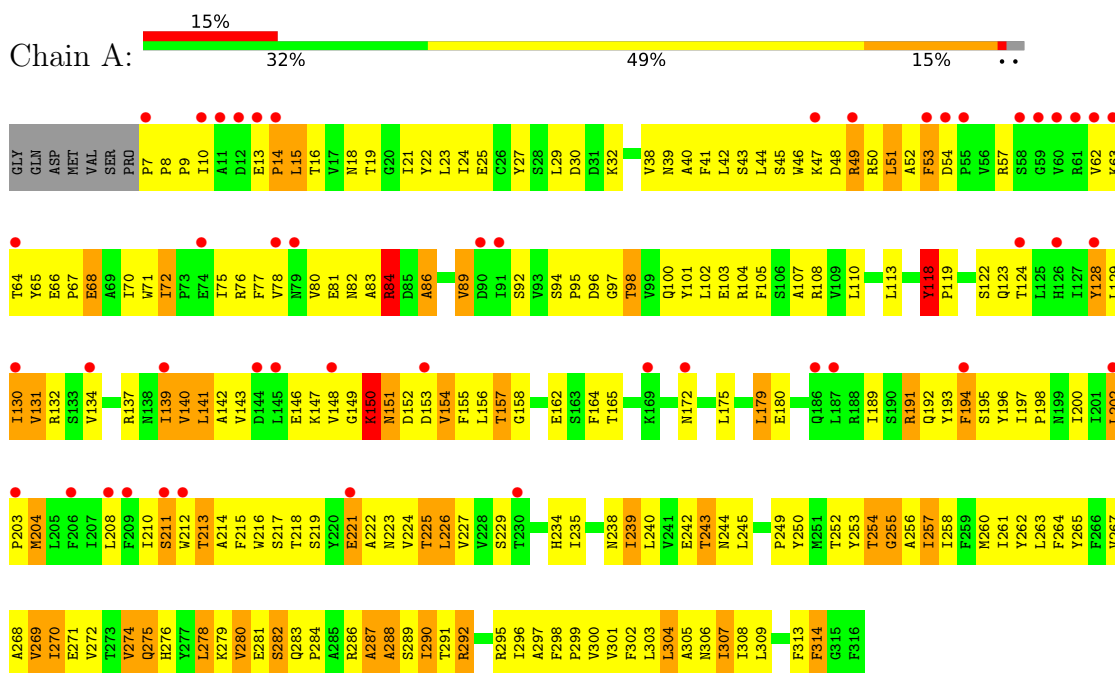
- Molecule 2 is BROMIDE ION (CCD ID: BR) (formula: Br).

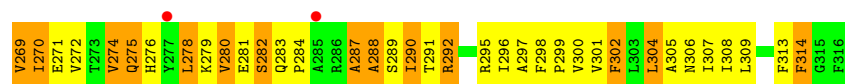
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total	Br	0	0
			1	1		

3 Residue-property plots

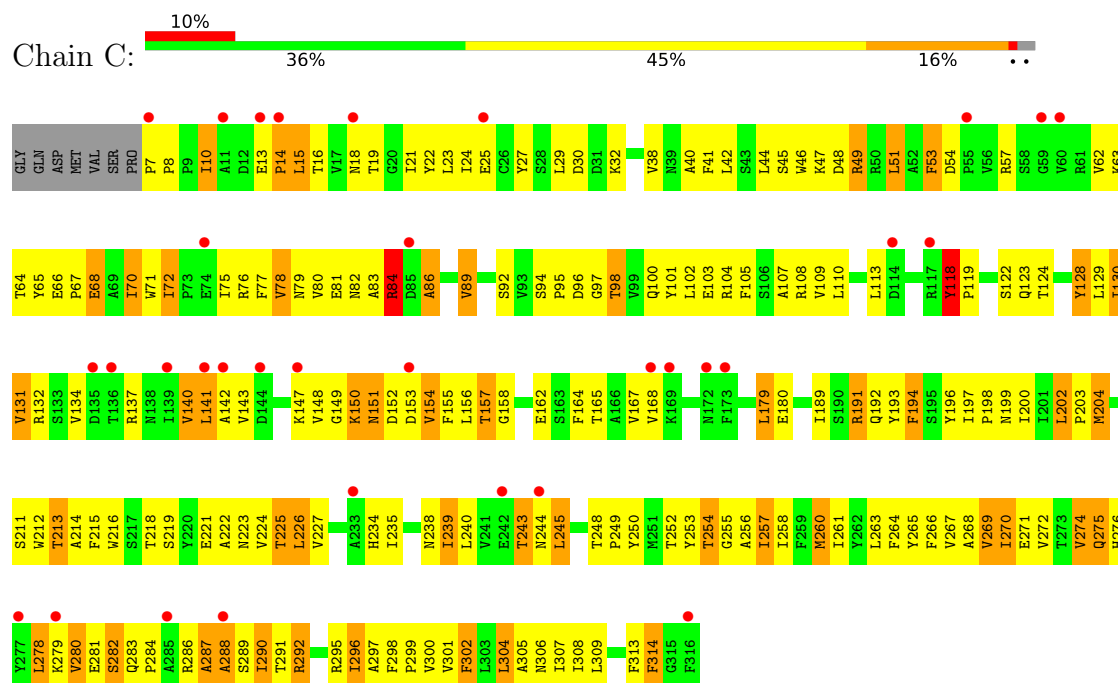
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

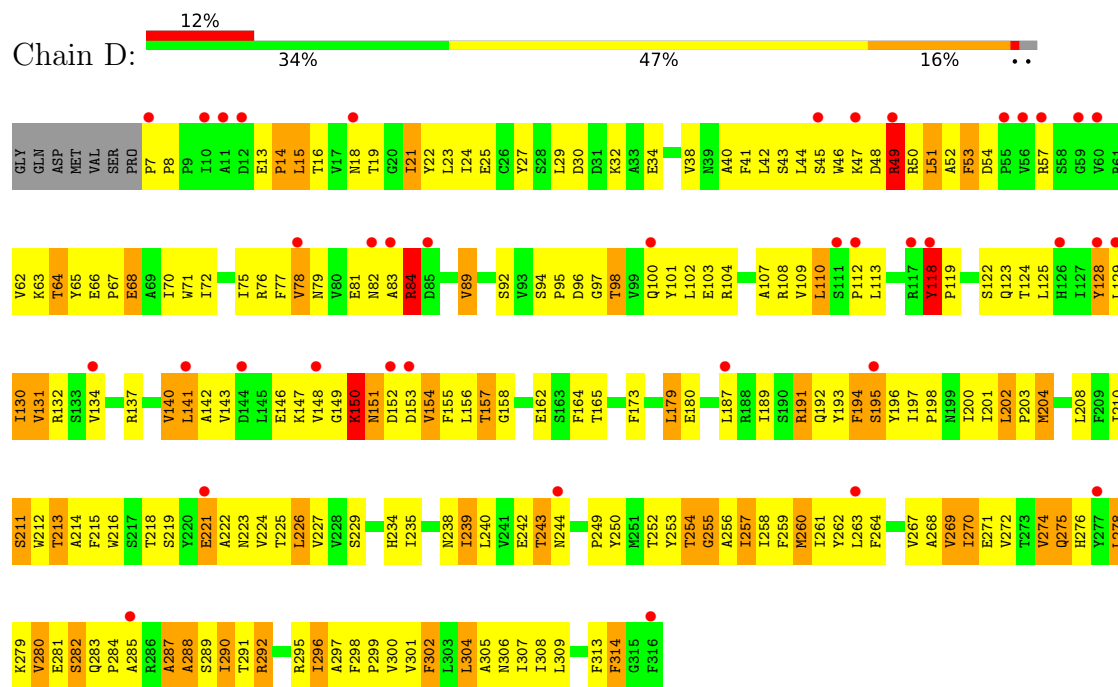




• Molecule 1: GLR4197 PROTEIN

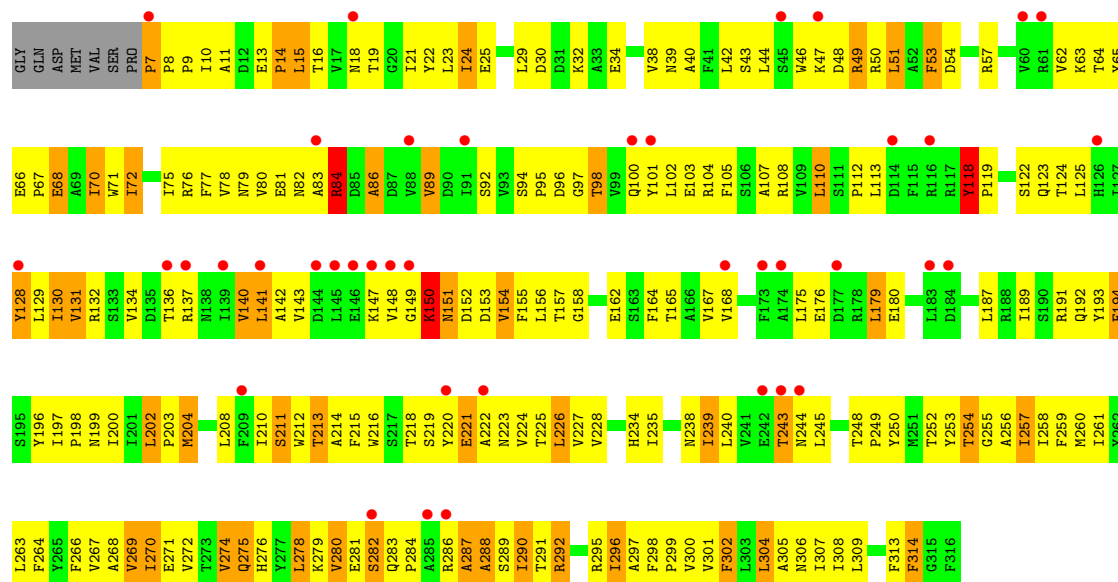


• Molecule 1: GLR4197 PROTEIN



• Molecule 1: GLR4197 PROTEIN





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 – 3.50 40.20 – 3.50	Depositor EDS
% Data completeness (in resolution range)	95.2 (40.20-3.50) 95.2 (40.20-3.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 3.48Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.248 , 0.257 0.250 , 0.258	Depositor DCC
R_{free} test set	2351 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	102.0	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 82.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	12606	wwPDB-VP
Average B, all atoms (Å ²)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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: BR

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	0.66	0/2589	1.03	12/3535 (0.3%)
1	B	0.63	0/2589	1.04	14/3535 (0.4%)
1	C	0.67	1/2589 (0.0%)	1.03	13/3535 (0.4%)
1	D	0.66	0/2589	1.03	14/3535 (0.4%)
1	E	0.66	1/2589 (0.0%)	1.03	11/3535 (0.3%)
All	All	0.66	2/12945 (0.0%)	1.03	64/17675 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	128	TYR	CA-C	5.39	1.56	1.52
1	E	128	TYR	CA-C	5.36	1.56	1.52

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	7	PRO	CA-C-N	9.10	126.21	119.66
1	E	7	PRO	C-N-CA	9.10	126.21	119.66
1	B	7	PRO	CA-C-N	8.91	126.07	119.66
1	B	7	PRO	C-N-CA	8.91	126.07	119.66
1	D	7	PRO	CA-C-N	8.29	125.63	119.66
1	D	7	PRO	C-N-CA	8.29	125.63	119.66
1	A	280	VAL	N-CA-C	-8.14	105.55	113.53
1	D	118	TYR	CA-C-N	-8.09	111.39	119.56
1	D	118	TYR	C-N-CA	-8.09	111.39	119.56
1	C	7	PRO	CA-C-N	8.08	125.48	119.66
1	C	7	PRO	C-N-CA	8.08	125.48	119.66
1	A	118	TYR	CA-C-N	-7.67	111.81	119.56
1	A	118	TYR	C-N-CA	-7.67	111.81	119.56
1	C	128	TYR	N-CA-C	7.65	122.64	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	128	TYR	N-CA-C	7.64	122.59	112.13
1	E	128	TYR	N-CA-C	7.63	122.62	111.02
1	A	7	PRO	CA-C-N	7.58	125.12	119.66
1	A	7	PRO	C-N-CA	7.58	125.12	119.66
1	B	280	VAL	N-CA-C	-7.51	106.17	113.53
1	C	118	TYR	CA-C-N	-7.37	112.04	119.56
1	C	118	TYR	C-N-CA	-7.37	112.04	119.56
1	B	118	TYR	CA-C-N	-7.35	112.06	119.56
1	B	118	TYR	C-N-CA	-7.35	112.06	119.56
1	D	280	VAL	N-CA-C	-7.23	106.45	113.53
1	E	118	TYR	CA-C-N	-7.01	112.41	119.56
1	E	118	TYR	C-N-CA	-7.01	112.41	119.56
1	A	128	TYR	N-CA-C	6.98	121.63	111.02
1	D	128	TYR	N-CA-C	6.97	121.61	111.02
1	A	265	TYR	N-CA-C	-6.79	105.53	113.88
1	E	280	VAL	N-CA-C	-6.49	105.83	113.42
1	C	8	PRO	N-CA-C	6.12	117.13	110.58
1	C	280	VAL	N-CA-C	-6.06	106.33	113.42
1	B	78	VAL	N-CA-C	5.90	116.11	110.74
1	A	255	GLY	N-CA-C	-5.87	105.05	113.86
1	A	8	PRO	N-CA-C	5.73	116.71	110.58
1	D	255	GLY	N-CA-C	-5.73	105.26	113.86
1	C	86	ALA	N-CA-C	5.66	118.70	109.59
1	B	220	TYR	N-CA-C	-5.64	105.05	111.14
1	C	78	VAL	N-CA-C	5.63	115.86	110.74
1	E	8	PRO	CA-C-N	5.61	126.86	119.84
1	E	8	PRO	C-N-CA	5.61	126.86	119.84
1	C	265	TYR	N-CA-C	-5.55	106.64	113.41
1	B	260	MET	N-CA-C	-5.46	105.33	111.28
1	D	45	SER	N-CA-C	5.45	116.69	108.46
1	C	260	MET	N-CA-C	-5.45	105.34	111.28
1	D	78	VAL	N-CA-C	5.38	115.64	110.74
1	D	8	PRO	N-CA-C	5.38	116.33	110.58
1	E	24	ILE	N-CA-C	-5.38	107.19	111.81
1	E	8	PRO	N-CA-C	5.35	116.31	110.58
1	C	255	GLY	N-CA-C	-5.34	105.85	113.86
1	B	8	PRO	N-CA-C	5.32	116.27	110.58
1	B	255	GLY	N-CA-C	-5.29	105.93	113.86
1	D	195	SER	N-CA-C	-5.28	106.53	112.87
1	E	86	ALA	N-CA-C	5.27	118.08	109.59
1	A	139	ILE	N-CA-C	-5.23	100.85	108.17
1	A	45	SER	N-CA-C	5.19	116.30	108.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	8	PRO	O-C-N	5.12	123.56	121.15
1	D	21	ILE	N-CA-C	5.07	115.28	107.77
1	D	285	ALA	N-CA-C	-5.06	104.84	111.02
1	C	45	SER	N-CA-C	5.06	116.09	108.46
1	D	260	MET	N-CA-C	-5.05	105.77	111.28
1	B	265	TYR	N-CA-C	-5.05	107.25	113.41
1	B	86	ALA	N-CA-C	5.05	117.71	109.59
1	A	86	ALA	N-CA-C	5.03	117.69	109.59

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	271	0
1	B	2521	0	2537	264	0
1	C	2521	0	2537	240	0
1	D	2521	0	2537	275	0
1	E	2521	0	2537	254	0
2	C	1	0	0	0	0
All	All	12606	0	12685	1200	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 47.

All (1200) 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:B:53:PHE:HE2	1:B:63:LYS:HB3	1.18	1.08
1:D:53:PHE:HE2	1:D:63:LYS:HB3	1.13	1.06
1:A:53:PHE:HE2	1:A:63:LYS:HB3	1.19	1.03
1:C:53:PHE:HE2	1:C:63:LYS:HB3	1.22	1.02
1:E:53:PHE:HE2	1:E:63:LYS:HB3	1.24	1.01
1:B:76:ARG:HH22	1:B:130:ILE:HD12	1.28	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:ARG:NH2	1:B:130:ILE:HD12	1.79	0.97
1:A:155:PHE:CE1	1:B:112:PRO:HB3	1.99	0.96
1:B:22:TYR:HA	1:B:149:GLY:HA3	1.45	0.95
1:D:210:ILE:HG23	1:E:269:VAL:HG11	1.47	0.95
1:D:53:PHE:CE2	1:D:63:LYS:HB3	2.00	0.95
1:C:22:TYR:HA	1:C:149:GLY:HA3	1.48	0.94
1:D:53:PHE:HE2	1:D:63:LYS:CB	1.81	0.93
1:D:22:TYR:HA	1:D:149:GLY:HA3	1.49	0.92
1:E:22:TYR:HA	1:E:149:GLY:HA3	1.50	0.91
1:B:254:THR:O	1:B:258:ILE:HB	1.72	0.90
1:D:76:ARG:NH2	1:D:130:ILE:HD12	1.86	0.89
1:E:76:ARG:NH2	1:E:130:ILE:HD12	1.87	0.89
1:D:155:PHE:CE1	1:E:112:PRO:HB3	2.06	0.89
1:E:76:ARG:HH22	1:E:130:ILE:HD12	1.35	0.89
1:E:149:GLY:O	1:E:164:PHE:HD1	1.56	0.88
1:A:22:TYR:HA	1:A:149:GLY:HA3	1.54	0.88
1:A:89:VAL:HG11	1:A:102:LEU:HD23	1.56	0.88
1:D:76:ARG:HH22	1:D:130:ILE:HD12	1.38	0.88
1:E:150:LYS:HG3	1:E:154:VAL:HG21	1.54	0.87
1:A:221:GLU:HB3	1:B:221:GLU:HG2	1.57	0.87
1:A:149:GLY:O	1:A:164:PHE:HD1	1.57	0.87
1:C:200:ILE:HD11	1:C:240:LEU:HD23	1.56	0.86
1:A:240:LEU:HD13	1:B:239:ILE:HG12	1.56	0.86
1:A:53:PHE:HE2	1:A:63:LYS:CB	1.87	0.86
1:C:234:HIS:CE1	1:C:261:ILE:HG21	2.10	0.86
1:A:53:PHE:CE2	1:A:63:LYS:HB3	2.10	0.86
1:B:150:LYS:HG3	1:B:154:VAL:HG21	1.57	0.86
1:B:53:PHE:CE2	1:B:63:LYS:HB3	2.10	0.86
1:C:199:ASN:HB3	1:D:242:GLU:CD	2.00	0.85
1:A:150:LYS:HG3	1:A:154:VAL:HG21	1.56	0.85
1:C:76:ARG:NH2	1:C:130:ILE:HD12	1.91	0.85
1:C:254:THR:O	1:C:258:ILE:HB	1.77	0.85
1:D:149:GLY:O	1:D:164:PHE:HD1	1.59	0.84
1:D:89:VAL:HG11	1:D:102:LEU:HD23	1.56	0.84
1:B:22:TYR:CD1	1:B:149:GLY:HA2	2.12	0.84
1:C:53:PHE:HE2	1:C:63:LYS:CB	1.91	0.84
1:E:254:THR:O	1:E:258:ILE:HB	1.78	0.84
1:E:89:VAL:HG11	1:E:102:LEU:HD23	1.58	0.84
1:B:53:PHE:HE2	1:B:63:LYS:CB	1.90	0.83
1:A:76:ARG:NH2	1:A:130:ILE:HD12	1.93	0.83
1:E:147:LYS:C	1:E:149:GLY:H	1.85	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:PHE:CE2	1:C:63:LYS:HB3	2.12	0.83
1:D:150:LYS:HG3	1:D:154:VAL:HG21	1.59	0.83
1:C:147:LYS:C	1:C:149:GLY:H	1.85	0.83
1:C:149:GLY:O	1:C:164:PHE:HD1	1.62	0.83
1:C:76:ARG:HH22	1:C:130:ILE:HD12	1.44	0.83
1:D:234:HIS:CE1	1:D:261:ILE:HG21	2.13	0.83
1:A:222:ALA:HB2	1:B:221:GLU:HA	1.59	0.83
1:C:22:TYR:CD1	1:C:149:GLY:HA2	2.13	0.83
1:C:89:VAL:HG11	1:C:102:LEU:HD23	1.61	0.83
1:B:149:GLY:O	1:B:164:PHE:HD1	1.60	0.82
1:B:89:VAL:HG11	1:B:102:LEU:HD23	1.59	0.82
1:E:22:TYR:CD1	1:E:149:GLY:HA2	2.14	0.82
1:E:234:HIS:CE1	1:E:261:ILE:HG21	2.14	0.82
1:A:234:HIS:CE1	1:A:261:ILE:HG21	2.14	0.82
1:A:226:LEU:HD23	1:B:224:VAL:HB	1.59	0.82
1:D:254:THR:O	1:D:258:ILE:HB	1.79	0.82
1:A:254:THR:O	1:A:258:ILE:HB	1.79	0.81
1:B:147:LYS:C	1:B:149:GLY:H	1.86	0.81
1:E:200:ILE:HD11	1:E:240:LEU:HD23	1.61	0.81
1:A:147:LYS:C	1:A:149:GLY:H	1.87	0.81
1:A:202:LEU:HD12	1:B:259:PHE:CZ	2.15	0.81
1:C:131:VAL:HG11	1:C:140:VAL:HG13	1.63	0.80
1:A:42:LEU:HB3	1:A:103:GLU:HG3	1.63	0.80
1:D:22:TYR:CD1	1:D:149:GLY:HA2	2.16	0.80
1:D:42:LEU:HB3	1:D:103:GLU:HG3	1.64	0.80
1:C:27:TYR:HB3	1:D:110:LEU:HD11	1.64	0.80
1:D:147:LYS:C	1:D:149:GLY:H	1.90	0.80
1:E:53:PHE:HE2	1:E:63:LYS:CB	1.94	0.79
1:A:76:ARG:HH22	1:A:130:ILE:HD12	1.44	0.79
1:B:257:ILE:O	1:B:261:ILE:HG12	1.81	0.79
1:E:42:LEU:HB3	1:E:103:GLU:HG3	1.65	0.79
1:B:42:LEU:HB3	1:B:103:GLU:HG3	1.65	0.79
1:D:131:VAL:HG11	1:D:140:VAL:HG13	1.65	0.79
1:A:200:ILE:HD11	1:A:240:LEU:HD23	1.65	0.78
1:C:225:THR:HG21	1:D:225:THR:OG1	1.82	0.78
1:A:27:TYR:CB	1:B:110:LEU:HD11	2.13	0.78
1:A:22:TYR:CD1	1:A:149:GLY:HA2	2.19	0.78
1:A:155:PHE:CZ	1:B:112:PRO:HB3	2.19	0.78
1:A:131:VAL:HG11	1:A:140:VAL:HG13	1.66	0.78
1:C:42:LEU:HB3	1:C:103:GLU:HG3	1.64	0.78
1:E:253:TYR:HA	1:E:313:PHE:CE2	2.19	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:53:PHE:CE2	1:E:63:LYS:HB3	2.15	0.77
1:D:221:GLU:OE2	1:E:221:GLU:CD	2.28	0.77
1:C:22:TYR:HA	1:C:149:GLY:CA	2.15	0.77
1:B:131:VAL:HG11	1:B:140:VAL:HG13	1.65	0.77
1:D:81:GLU:HG3	1:D:108:ARG:HG3	1.67	0.77
1:B:22:TYR:HA	1:B:149:GLY:CA	2.15	0.76
1:D:257:ILE:O	1:D:261:ILE:HG12	1.85	0.76
1:A:253:TYR:HA	1:A:313:PHE:CE2	2.21	0.76
1:C:65:TYR:CG	1:C:70:ILE:HD11	2.21	0.76
1:D:253:TYR:HA	1:D:313:PHE:CE2	2.21	0.76
1:E:131:VAL:HG11	1:E:140:VAL:HG13	1.66	0.75
1:D:77:PHE:H	1:D:84:ARG:HD3	1.52	0.75
1:C:253:TYR:HA	1:C:313:PHE:CE2	2.22	0.75
1:A:77:PHE:H	1:A:84:ARG:HD3	1.50	0.75
1:B:200:ILE:HD11	1:B:240:LEU:HD23	1.67	0.75
1:E:253:TYR:HA	1:E:313:PHE:HE2	1.51	0.75
1:E:257:ILE:O	1:E:261:ILE:HG12	1.87	0.74
1:D:200:ILE:HD11	1:D:240:LEU:HD23	1.68	0.74
1:D:22:TYR:HA	1:D:149:GLY:CA	2.18	0.74
1:B:66:GLU:HG3	1:B:67:PRO:HD2	1.69	0.74
1:D:65:TYR:CG	1:D:70:ILE:HD11	2.23	0.74
1:A:22:TYR:HA	1:A:149:GLY:CA	2.16	0.74
1:A:65:TYR:CG	1:A:70:ILE:HD11	2.23	0.74
1:B:234:HIS:CE1	1:B:261:ILE:HG21	2.22	0.74
1:B:65:TYR:CG	1:B:70:ILE:HD11	2.24	0.73
1:E:128:TYR:O	1:E:129:LEU:HB2	1.88	0.73
1:C:257:ILE:O	1:C:261:ILE:HG12	1.88	0.73
1:A:24:ILE:HD13	1:A:104:ARG:HE	1.54	0.73
1:B:253:TYR:HA	1:B:313:PHE:CE2	2.23	0.73
1:E:65:TYR:CG	1:E:70:ILE:HD11	2.23	0.73
1:A:257:ILE:O	1:A:261:ILE:HG12	1.88	0.73
1:B:81:GLU:HG3	1:B:108:ARG:HG3	1.68	0.73
1:C:77:PHE:H	1:C:84:ARG:HD3	1.54	0.73
1:E:22:TYR:HA	1:E:149:GLY:CA	2.19	0.73
1:C:222:ALA:HB2	1:D:221:GLU:HA	1.71	0.72
1:E:66:GLU:HG3	1:E:67:PRO:HD2	1.71	0.72
1:E:81:GLU:HG3	1:E:108:ARG:HG3	1.68	0.72
1:E:53:PHE:O	1:E:53:PHE:CD1	2.41	0.72
1:C:66:GLU:HG3	1:C:67:PRO:HD2	1.72	0.72
1:D:66:GLU:HG3	1:D:67:PRO:HD2	1.70	0.72
1:B:281:GLU:O	1:B:283:GLN:N	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:ASN:O	1:B:154:VAL:HG22	1.89	0.72
1:A:150:LYS:O	1:A:150:LYS:HG2	1.90	0.72
1:E:77:PHE:H	1:E:84:ARG:HD3	1.55	0.71
1:B:151:ASN:C	1:B:153:ASP:H	1.96	0.71
1:C:274:VAL:C	1:C:276:HIS:H	1.97	0.71
1:A:226:LEU:CD2	1:B:224:VAL:HB	2.20	0.71
1:C:202:LEU:HD12	1:D:259:PHE:CE1	2.26	0.71
1:E:147:LYS:O	1:E:149:GLY:N	2.23	0.71
1:E:151:ASN:C	1:E:153:ASP:H	1.98	0.71
1:B:76:ARG:HH22	1:B:130:ILE:CD1	2.02	0.71
1:B:200:ILE:O	1:B:204:MET:HB2	1.90	0.71
1:A:151:ASN:C	1:A:153:ASP:H	1.99	0.71
1:C:81:GLU:HG3	1:C:108:ARG:HG3	1.72	0.71
1:A:274:VAL:C	1:A:276:HIS:H	1.98	0.71
1:B:274:VAL:C	1:B:276:HIS:H	1.99	0.70
1:D:257:ILE:HG22	1:D:309:LEU:HD23	1.73	0.70
1:B:77:PHE:H	1:B:84:ARG:HD3	1.56	0.70
1:C:53:PHE:O	1:C:53:PHE:CD1	2.45	0.70
1:A:128:TYR:O	1:A:129:LEU:HB2	1.90	0.70
1:C:151:ASN:C	1:C:153:ASP:H	1.99	0.70
1:B:53:PHE:O	1:B:53:PHE:CD1	2.44	0.70
1:C:281:GLU:O	1:C:283:GLN:N	2.25	0.70
1:D:274:VAL:C	1:D:276:HIS:H	1.99	0.70
1:A:53:PHE:O	1:A:53:PHE:CD1	2.45	0.70
1:C:54:ASP:HB2	1:C:57:ARG:HG3	1.74	0.70
1:B:147:LYS:O	1:B:149:GLY:N	2.23	0.70
1:E:238:ASN:HA	1:E:258:ILE:HD11	1.74	0.70
1:A:151:ASN:O	1:A:154:VAL:HG22	1.91	0.70
1:A:210:ILE:HG23	1:B:269:VAL:HG11	1.73	0.70
1:E:150:LYS:O	1:E:150:LYS:HG2	1.90	0.70
1:E:151:ASN:O	1:E:154:VAL:HG22	1.92	0.70
1:D:304:LEU:O	1:D:308:ILE:HG12	1.92	0.69
1:A:81:GLU:HG3	1:A:108:ARG:HG3	1.73	0.69
1:E:304:LEU:O	1:E:308:ILE:HG12	1.92	0.69
1:D:24:ILE:HD13	1:D:104:ARG:HE	1.56	0.69
1:A:253:TYR:HA	1:A:313:PHE:HE2	1.56	0.69
1:D:238:ASN:HA	1:D:258:ILE:HD11	1.75	0.69
1:E:197:ILE:HB	1:E:198:PRO:HD3	1.74	0.69
1:E:281:GLU:O	1:E:283:GLN:N	2.26	0.68
1:A:54:ASP:HB2	1:A:57:ARG:HG3	1.74	0.68
1:A:62:VAL:HG11	1:A:92:SER:HB3	1.73	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:ARG:NH2	1:B:78:VAL:HA	2.08	0.68
1:B:47:LYS:HD2	1:B:49:ARG:HH21	1.59	0.68
1:C:197:ILE:HB	1:C:198:PRO:HD3	1.75	0.68
1:A:66:GLU:HG3	1:A:67:PRO:HD2	1.75	0.68
1:B:253:TYR:HA	1:B:313:PHE:HE2	1.57	0.68
1:E:274:VAL:C	1:E:276:HIS:H	2.00	0.68
1:C:151:ASN:O	1:C:154:VAL:HG22	1.94	0.68
1:E:54:ASP:HB2	1:E:57:ARG:HG3	1.75	0.68
1:B:54:ASP:HB2	1:B:57:ARG:HG3	1.76	0.68
1:D:281:GLU:O	1:D:283:GLN:N	2.25	0.68
1:D:253:TYR:HA	1:D:313:PHE:HE2	1.56	0.68
1:B:24:ILE:HD13	1:B:104:ARG:HE	1.57	0.68
1:C:128:TYR:O	1:C:129:LEU:HB2	1.94	0.68
1:D:150:LYS:HG2	1:D:150:LYS:O	1.93	0.68
1:C:147:LYS:O	1:C:149:GLY:N	2.26	0.67
1:B:13:GLU:HB3	1:B:14:PRO:HD2	1.76	0.67
1:A:157:THR:CG2	1:B:34:GLU:OE1	2.42	0.67
1:D:151:ASN:C	1:D:153:ASP:H	2.00	0.67
1:E:62:VAL:HG11	1:E:92:SER:HB3	1.76	0.67
1:D:54:ASP:HB2	1:D:57:ARG:HG3	1.76	0.67
1:D:89:VAL:CG1	1:D:102:LEU:HD23	2.25	0.67
1:D:240:LEU:HD13	1:E:239:ILE:HG12	1.76	0.67
1:A:147:LYS:O	1:A:149:GLY:N	2.26	0.67
1:E:24:ILE:HD13	1:E:104:ARG:HE	1.60	0.67
1:E:200:ILE:O	1:E:204:MET:HB2	1.95	0.67
1:A:304:LEU:O	1:A:308:ILE:HG12	1.94	0.67
1:B:128:TYR:O	1:B:129:LEU:HB2	1.94	0.67
1:B:238:ASN:HA	1:B:258:ILE:HD11	1.77	0.67
1:B:257:ILE:HG22	1:B:309:LEU:HD23	1.76	0.66
1:C:253:TYR:HA	1:C:313:PHE:HE2	1.59	0.66
1:C:257:ILE:HG22	1:C:309:LEU:HD23	1.76	0.66
1:D:47:LYS:HD2	1:D:49:ARG:HH21	1.60	0.66
1:D:225:THR:CG2	1:E:224:VAL:HG23	2.25	0.66
1:A:281:GLU:O	1:A:283:GLN:N	2.28	0.66
1:B:23:LEU:HA	1:B:40:ALA:HB2	1.78	0.66
1:C:147:LYS:O	1:C:147:LYS:HG2	1.96	0.66
1:D:147:LYS:O	1:D:147:LYS:HG2	1.96	0.66
1:D:151:ASN:O	1:D:154:VAL:HG22	1.96	0.66
1:E:257:ILE:HG22	1:E:309:LEU:HD23	1.77	0.66
1:C:200:ILE:O	1:C:204:MET:HB2	1.96	0.66
1:B:42:LEU:HB3	1:B:103:GLU:CG	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:LYS:O	1:B:150:LYS:HG2	1.96	0.65
1:D:42:LEU:HB3	1:D:103:GLU:CG	2.26	0.65
1:D:76:ARG:HH22	1:D:130:ILE:CD1	2.09	0.65
1:D:202:LEU:HD12	1:E:259:PHE:CZ	2.31	0.65
1:B:89:VAL:CG1	1:B:102:LEU:HD23	2.26	0.65
1:A:197:ILE:HB	1:A:198:PRO:HD3	1.79	0.65
1:A:257:ILE:HG22	1:A:309:LEU:HD23	1.77	0.65
1:A:200:ILE:O	1:A:204:MET:HB2	1.96	0.65
1:A:13:GLU:HB3	1:A:14:PRO:HD2	1.78	0.65
1:B:304:LEU:O	1:B:308:ILE:HG12	1.97	0.65
1:A:225:THR:HG21	1:B:225:THR:OG1	1.97	0.65
1:D:13:GLU:HB3	1:D:14:PRO:HD2	1.79	0.65
1:B:76:ARG:NH2	1:B:130:ILE:CD1	2.55	0.65
1:E:13:GLU:HB3	1:E:14:PRO:HD2	1.78	0.65
1:A:77:PHE:CD1	1:A:84:ARG:HD2	2.31	0.64
1:B:62:VAL:HG11	1:B:92:SER:HB3	1.78	0.64
1:C:213:THR:HG22	1:C:226:LEU:HD11	1.78	0.64
1:E:89:VAL:CG1	1:E:102:LEU:HD23	2.27	0.64
1:E:224:VAL:C	1:E:226:LEU:H	2.03	0.64
1:C:24:ILE:HD13	1:C:104:ARG:HE	1.61	0.64
1:A:89:VAL:CG1	1:A:102:LEU:HD23	2.27	0.64
1:A:202:LEU:HD12	1:B:259:PHE:HZ	1.58	0.64
1:E:238:ASN:HA	1:E:258:ILE:CD1	2.28	0.64
1:C:62:VAL:HG11	1:C:92:SER:HB3	1.78	0.64
1:E:76:ARG:HH22	1:E:130:ILE:CD1	2.07	0.64
1:D:62:VAL:HG11	1:D:92:SER:HB3	1.79	0.64
1:D:283:GLN:N	1:D:284:PRO:HD3	2.12	0.64
1:D:47:LYS:CD	1:D:49:ARG:HH21	2.10	0.64
1:A:27:TYR:HB3	1:B:110:LEU:HD11	1.78	0.64
1:A:47:LYS:HD2	1:A:49:ARG:HH21	1.62	0.64
1:D:200:ILE:O	1:D:204:MET:HB2	1.98	0.64
1:E:42:LEU:HB3	1:E:103:GLU:CG	2.27	0.64
1:D:202:LEU:HD12	1:E:259:PHE:HZ	1.63	0.63
1:C:304:LEU:O	1:C:308:ILE:HG12	1.98	0.63
1:D:18:ASN:HB3	1:D:143:VAL:HG23	1.79	0.63
1:D:197:ILE:HB	1:D:198:PRO:HD3	1.80	0.63
1:A:222:ALA:O	1:A:226:LEU:HB2	1.99	0.63
1:C:47:LYS:HD2	1:C:49:ARG:HH21	1.63	0.63
1:C:179:LEU:O	1:C:179:LEU:HD12	1.99	0.63
1:B:283:GLN:N	1:B:284:PRO:HD3	2.14	0.63
1:A:19:THR:HG22	1:A:44:LEU:CD2	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:THR:HG22	1:B:34:GLU:OE1	1.99	0.63
1:A:283:GLN:N	1:A:284:PRO:HD3	2.13	0.63
1:D:77:PHE:CD1	1:D:84:ARG:HD2	2.33	0.63
1:E:149:GLY:O	1:E:164:PHE:CD1	2.47	0.63
1:E:283:GLN:N	1:E:284:PRO:HD3	2.14	0.63
1:B:47:LYS:CD	1:B:49:ARG:HH21	2.12	0.63
1:A:42:LEU:HB3	1:A:103:GLU:CG	2.29	0.62
1:A:51:LEU:CD1	1:A:70:ILE:HD12	2.29	0.62
1:B:15:LEU:HD11	1:B:46:TRP:HB2	1.81	0.62
1:C:215:PHE:HZ	1:C:298:PHE:CE1	2.17	0.62
1:A:147:LYS:C	1:A:149:GLY:N	2.58	0.62
1:C:13:GLU:HB3	1:C:14:PRO:HD2	1.80	0.62
1:E:84:ARG:CB	1:E:84:ARG:HH11	2.12	0.62
1:A:267:VAL:HG23	1:A:298:PHE:CZ	2.35	0.62
1:A:276:HIS:O	1:A:280:VAL:HG22	2.00	0.62
1:E:70:ILE:HD13	1:E:70:ILE:N	2.14	0.62
1:A:147:LYS:O	1:A:147:LYS:HG2	1.99	0.62
1:D:147:LYS:O	1:D:149:GLY:N	2.29	0.62
1:D:276:HIS:O	1:D:280:VAL:HG22	2.00	0.62
1:E:243:THR:HG22	1:E:244:ASN:HD22	1.64	0.62
1:C:89:VAL:CG1	1:C:102:LEU:HD23	2.29	0.62
1:C:27:TYR:CB	1:D:110:LEU:HD11	2.30	0.62
1:D:229:SER:HB3	1:E:228:VAL:HG11	1.82	0.62
1:E:215:PHE:HZ	1:E:298:PHE:CE1	2.18	0.62
1:D:149:GLY:O	1:D:164:PHE:CD1	2.49	0.62
1:E:151:ASN:HD22	1:E:152:ASP:H	1.48	0.62
1:E:224:VAL:C	1:E:226:LEU:N	2.55	0.62
1:B:224:VAL:C	1:B:226:LEU:H	2.06	0.61
1:C:213:THR:HG22	1:C:226:LEU:CD1	2.29	0.61
1:D:54:ASP:HB2	1:D:57:ARG:CG	2.30	0.61
1:D:132:ARG:HA	1:D:180:GLU:HG2	1.82	0.61
1:A:238:ASN:HA	1:A:258:ILE:HD11	1.80	0.61
1:B:243:THR:HG22	1:B:244:ASN:HD22	1.65	0.61
1:C:78:VAL:HG22	1:C:130:ILE:HG12	1.80	0.61
1:E:47:LYS:HD2	1:E:49:ARG:HH21	1.63	0.61
1:E:276:HIS:O	1:E:280:VAL:HG22	2.00	0.61
1:C:29:LEU:C	1:C:29:LEU:HD23	2.24	0.61
1:B:18:ASN:HB3	1:B:143:VAL:HG23	1.82	0.61
1:A:221:GLU:OE1	1:A:221:GLU:HA	1.99	0.61
1:A:224:VAL:C	1:A:226:LEU:N	2.57	0.61
1:B:78:VAL:HG22	1:B:130:ILE:HG12	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51:LEU:CD1	1:C:70:ILE:HD12	2.30	0.61
1:A:29:LEU:C	1:A:29:LEU:HD23	2.26	0.61
1:B:224:VAL:C	1:B:226:LEU:N	2.55	0.61
1:C:18:ASN:HB3	1:C:143:VAL:HG23	1.83	0.61
1:C:283:GLN:N	1:C:284:PRO:HD3	2.16	0.61
1:B:77:PHE:CD1	1:B:84:ARG:HD2	2.36	0.61
1:D:215:PHE:HZ	1:D:298:PHE:CE1	2.19	0.61
1:A:27:TYR:CG	1:B:110:LEU:HD11	2.36	0.61
1:B:249:PRO:HD2	1:B:250:TYR:CD1	2.35	0.61
1:D:84:ARG:CB	1:D:84:ARG:HH11	2.14	0.61
1:E:15:LEU:HD11	1:E:46:TRP:HB2	1.82	0.61
1:A:18:ASN:HB3	1:A:143:VAL:HG23	1.83	0.61
1:B:151:ASN:HD22	1:B:152:ASP:H	1.48	0.61
1:C:54:ASP:HB2	1:C:57:ARG:CG	2.30	0.61
1:C:238:ASN:HA	1:C:258:ILE:HD11	1.82	0.61
1:D:53:PHE:CE2	1:D:63:LYS:CB	2.70	0.61
1:C:151:ASN:HD22	1:C:152:ASP:H	1.47	0.60
1:D:224:VAL:C	1:D:226:LEU:H	2.09	0.60
1:B:147:LYS:O	1:B:147:LYS:HG2	2.01	0.60
1:C:276:HIS:O	1:C:280:VAL:HG22	2.01	0.60
1:E:218:THR:HG22	1:E:279:LYS:HE2	1.82	0.60
1:B:54:ASP:HB2	1:B:57:ARG:CG	2.31	0.60
1:E:77:PHE:CD1	1:E:84:ARG:HD2	2.36	0.60
1:A:249:PRO:HD2	1:A:250:TYR:CD1	2.36	0.60
1:C:267:VAL:HG23	1:C:298:PHE:CZ	2.37	0.60
1:E:179:LEU:HD12	1:E:179:LEU:O	2.00	0.60
1:A:54:ASP:HB2	1:A:57:ARG:CG	2.31	0.60
1:E:76:ARG:NH2	1:E:130:ILE:CD1	2.61	0.60
1:C:77:PHE:CD1	1:C:84:ARG:HD2	2.36	0.60
1:D:53:PHE:CD1	1:D:53:PHE:O	2.54	0.60
1:E:47:LYS:CD	1:E:49:ARG:HH21	2.15	0.60
1:A:213:THR:HG22	1:A:226:LEU:CD1	2.32	0.60
1:E:249:PRO:HD2	1:E:250:TYR:CD1	2.37	0.60
1:C:150:LYS:HG3	1:C:154:VAL:HG21	1.82	0.59
1:D:179:LEU:HD12	1:D:179:LEU:O	2.02	0.59
1:A:132:ARG:HA	1:A:180:GLU:HG2	1.82	0.59
1:B:267:VAL:HG23	1:B:298:PHE:CZ	2.37	0.59
1:A:84:ARG:HA	1:A:107:ALA:HB2	1.84	0.59
1:C:194:PHE:C	1:C:196:TYR:N	2.59	0.59
1:D:238:ASN:HA	1:D:258:ILE:CD1	2.32	0.59
1:A:219:SER:OG	1:A:222:ALA:HB3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:76:ARG:NH2	1:D:130:ILE:CD1	2.61	0.59
1:E:147:LYS:O	1:E:147:LYS:HG2	2.01	0.59
1:A:218:THR:HG22	1:A:279:LYS:HE2	1.84	0.59
1:D:29:LEU:HD23	1:D:29:LEU:C	2.27	0.59
1:B:81:GLU:HG3	1:B:108:ARG:CG	2.33	0.59
1:B:215:PHE:HZ	1:B:298:PHE:CE1	2.21	0.59
1:B:238:ASN:HA	1:B:258:ILE:CD1	2.32	0.59
1:D:51:LEU:CD1	1:D:70:ILE:HD12	2.32	0.59
1:D:194:PHE:C	1:D:196:TYR:N	2.59	0.59
1:A:194:PHE:C	1:A:196:TYR:N	2.59	0.59
1:D:224:VAL:C	1:D:226:LEU:N	2.58	0.59
1:E:18:ASN:HB3	1:E:143:VAL:HG23	1.83	0.59
1:A:179:LEU:O	1:A:179:LEU:HD12	2.03	0.59
1:A:202:LEU:HD12	1:B:259:PHE:CE1	2.37	0.59
1:B:84:ARG:CB	1:B:84:ARG:HH11	2.16	0.59
1:C:215:PHE:CZ	1:C:298:PHE:CD1	2.91	0.59
1:C:253:TYR:HB2	1:C:313:PHE:HD2	1.68	0.59
1:B:29:LEU:HD23	1:B:29:LEU:C	2.27	0.59
1:B:149:GLY:O	1:B:164:PHE:CD1	2.50	0.59
1:C:224:VAL:C	1:C:226:LEU:N	2.59	0.59
1:A:221:GLU:OE1	1:A:221:GLU:O	2.21	0.58
1:B:197:ILE:HB	1:B:198:PRO:HD3	1.85	0.58
1:B:179:LEU:HD12	1:B:179:LEU:O	2.02	0.58
1:B:276:HIS:O	1:B:280:VAL:HG22	2.03	0.58
1:D:222:ALA:O	1:D:226:LEU:HB2	2.03	0.58
1:E:147:LYS:C	1:E:149:GLY:N	2.56	0.58
1:D:54:ASP:HB2	1:D:57:ARG:HB2	1.85	0.58
1:D:78:VAL:HB	1:D:128:TYR:HB2	1.85	0.58
1:E:51:LEU:CD1	1:E:70:ILE:HD12	2.32	0.58
1:C:42:LEU:HB3	1:C:103:GLU:CG	2.31	0.58
1:C:132:ARG:HA	1:C:180:GLU:HG2	1.84	0.58
1:B:51:LEU:CD1	1:B:70:ILE:HD12	2.33	0.58
1:A:27:TYR:CG	1:B:110:LEU:CD1	2.86	0.58
1:C:238:ASN:HA	1:C:258:ILE:CD1	2.34	0.58
1:D:218:THR:HG22	1:D:279:LYS:HE2	1.84	0.58
1:C:200:ILE:CD1	1:C:240:LEU:HD23	2.30	0.58
1:D:147:LYS:C	1:D:149:GLY:N	2.60	0.58
1:A:23:LEU:HA	1:A:40:ALA:HB2	1.86	0.58
1:A:47:LYS:CD	1:A:49:ARG:HH21	2.16	0.58
1:B:147:LYS:C	1:B:149:GLY:N	2.56	0.58
1:D:81:GLU:HG3	1:D:108:ARG:CG	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:155:PHE:CZ	1:E:112:PRO:HB3	2.38	0.58
1:C:202:LEU:HD12	1:D:259:PHE:HE1	1.69	0.58
1:D:141:LEU:HD23	1:D:142:ALA:H	1.68	0.58
1:E:54:ASP:HB2	1:E:57:ARG:CG	2.32	0.58
1:B:70:ILE:N	1:B:70:ILE:HD13	2.19	0.57
1:C:249:PRO:HD2	1:C:250:TYR:CD1	2.39	0.57
1:C:264:PHE:HZ	1:C:301:VAL:HG12	1.69	0.57
1:D:15:LEU:HD11	1:D:46:TRP:HB2	1.86	0.57
1:E:29:LEU:C	1:E:29:LEU:HD23	2.29	0.57
1:E:194:PHE:C	1:E:196:TYR:N	2.60	0.57
1:A:78:VAL:HB	1:A:128:TYR:HB2	1.86	0.57
1:C:234:HIS:CE1	1:C:261:ILE:CG2	2.84	0.57
1:D:276:HIS:C	1:D:278:LEU:H	2.12	0.57
1:E:276:HIS:C	1:E:278:LEU:H	2.12	0.57
1:A:215:PHE:HZ	1:A:298:PHE:CE1	2.23	0.57
1:C:215:PHE:HZ	1:C:298:PHE:CD1	2.22	0.57
1:D:23:LEU:HA	1:D:40:ALA:HB2	1.85	0.57
1:D:84:ARG:HA	1:D:107:ALA:HB2	1.87	0.57
1:D:210:ILE:HD11	1:E:266:PHE:HD1	1.69	0.57
1:A:75:ILE:HD13	1:A:131:VAL:HB	1.87	0.57
1:A:213:THR:HG22	1:A:226:LEU:HD11	1.85	0.57
1:C:226:LEU:CD2	1:D:224:VAL:HB	2.34	0.57
1:E:222:ALA:O	1:E:226:LEU:HB2	2.05	0.57
1:B:222:ALA:O	1:B:226:LEU:HB2	2.04	0.57
1:C:47:LYS:CD	1:C:49:ARG:HH21	2.17	0.57
1:C:274:VAL:O	1:C:276:HIS:N	2.37	0.57
1:D:78:VAL:HG22	1:D:130:ILE:HG12	1.86	0.57
1:E:19:THR:HG22	1:E:44:LEU:CD2	2.35	0.57
1:E:264:PHE:HE2	1:E:302:PHE:HB2	1.68	0.57
1:E:264:PHE:CE2	1:E:302:PHE:HB2	2.38	0.57
1:B:264:PHE:CE2	1:B:302:PHE:HB2	2.39	0.57
1:C:218:THR:HG22	1:C:279:LYS:HE2	1.87	0.57
1:E:81:GLU:HG3	1:E:108:ARG:CG	2.35	0.57
1:C:224:VAL:C	1:C:226:LEU:H	2.10	0.57
1:A:15:LEU:HD11	1:A:46:TRP:HB2	1.87	0.57
1:A:224:VAL:C	1:A:226:LEU:H	2.10	0.57
1:E:23:LEU:HD22	1:E:38:VAL:HG21	1.87	0.57
1:E:215:PHE:O	1:E:291:THR:HG22	2.05	0.57
1:C:78:VAL:HB	1:C:128:TYR:HB2	1.87	0.56
1:C:81:GLU:HG3	1:C:108:ARG:CG	2.35	0.56
1:D:179:LEU:HD12	1:D:179:LEU:C	2.30	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:215:PHE:CZ	1:D:298:PHE:CD1	2.92	0.56
1:E:78:VAL:HG22	1:E:130:ILE:HG12	1.85	0.56
1:E:75:ILE:HD13	1:E:131:VAL:HB	1.87	0.56
1:C:15:LEU:HD11	1:C:46:TRP:HB2	1.87	0.56
1:C:70:ILE:HD13	1:C:70:ILE:N	2.20	0.56
1:C:84:ARG:HA	1:C:107:ALA:HB2	1.87	0.56
1:C:104:ARG:NH2	1:D:77:PHE:O	2.38	0.56
1:D:151:ASN:HD22	1:D:152:ASP:H	1.53	0.56
1:D:243:THR:HG22	1:D:244:ASN:HD22	1.70	0.56
1:E:215:PHE:CZ	1:E:298:PHE:CD1	2.93	0.56
1:E:264:PHE:HZ	1:E:301:VAL:HG12	1.70	0.56
1:A:151:ASN:HD22	1:A:152:ASP:H	1.52	0.56
1:A:194:PHE:C	1:A:196:TYR:H	2.12	0.56
1:B:19:THR:HG22	1:B:44:LEU:CD2	2.36	0.56
1:B:276:HIS:C	1:B:278:LEU:H	2.13	0.56
1:A:78:VAL:HG22	1:A:130:ILE:HG12	1.87	0.56
1:B:53:PHE:CD1	1:B:53:PHE:C	2.84	0.56
1:C:23:LEU:HD22	1:C:38:VAL:HG21	1.86	0.56
1:C:222:ALA:HA	1:D:221:GLU:OE1	2.06	0.56
1:A:23:LEU:HD22	1:A:38:VAL:HG21	1.88	0.56
1:D:19:THR:HG22	1:D:44:LEU:CD2	2.35	0.56
1:C:264:PHE:CE2	1:C:302:PHE:HB2	2.41	0.56
1:D:47:LYS:HD3	1:D:49:ARG:NH2	2.21	0.56
1:E:267:VAL:HG23	1:E:298:PHE:CZ	2.40	0.56
1:B:84:ARG:HH11	1:B:84:ARG:HB3	1.70	0.56
1:B:215:PHE:O	1:B:291:THR:HG22	2.06	0.56
1:B:218:THR:HG22	1:B:279:LYS:HE2	1.88	0.56
1:B:274:VAL:O	1:B:276:HIS:N	2.38	0.56
1:C:76:ARG:NH2	1:C:130:ILE:CD1	2.66	0.56
1:D:157:THR:CG2	1:E:34:GLU:OE1	2.53	0.56
1:D:249:PRO:HD2	1:D:250:TYR:CD1	2.41	0.56
1:A:21:ILE:O	1:A:149:GLY:HA3	2.05	0.56
1:C:76:ARG:HH22	1:C:130:ILE:CD1	2.14	0.56
1:C:274:VAL:C	1:C:276:HIS:N	2.64	0.56
1:D:264:PHE:HZ	1:D:301:VAL:HG12	1.71	0.56
1:D:215:PHE:HZ	1:D:298:PHE:CD1	2.24	0.55
1:D:267:VAL:HG23	1:D:298:PHE:CZ	2.41	0.55
1:B:297:ALA:O	1:B:301:VAL:HG23	2.07	0.55
1:E:23:LEU:HA	1:E:40:ALA:HB2	1.88	0.55
1:C:243:THR:HG22	1:C:244:ASN:HD22	1.70	0.55
1:A:104:ARG:NH2	1:B:77:PHE:O	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:ARG:HA	1:B:180:GLU:HG2	1.88	0.55
1:A:238:ASN:HA	1:A:258:ILE:CD1	2.37	0.55
1:B:29:LEU:HB2	1:B:156:LEU:HD11	1.89	0.55
1:C:215:PHE:O	1:C:291:THR:HG22	2.06	0.55
1:E:53:PHE:CD1	1:E:53:PHE:C	2.82	0.55
1:E:132:ARG:HA	1:E:180:GLU:HG2	1.88	0.55
1:A:221:GLU:OE1	1:A:221:GLU:CA	2.54	0.55
1:B:84:ARG:HA	1:B:107:ALA:HB2	1.89	0.55
1:C:75:ILE:HD13	1:C:131:VAL:HB	1.89	0.55
1:A:81:GLU:HG3	1:A:108:ARG:CG	2.36	0.55
1:A:84:ARG:CB	1:A:84:ARG:HH11	2.19	0.55
1:A:137:ARG:HD2	1:A:179:LEU:HG	1.89	0.55
1:A:192:GLN:CD	1:B:249:PRO:HB3	2.32	0.55
1:D:192:GLN:CD	1:E:249:PRO:HB3	2.32	0.55
1:D:76:ARG:O	1:D:129:LEU:HA	2.07	0.55
1:D:84:ARG:HH11	1:D:84:ARG:HB3	1.72	0.55
1:D:215:PHE:O	1:D:291:THR:HG22	2.07	0.55
1:A:19:THR:HG22	1:A:44:LEU:HD23	1.89	0.55
1:A:243:THR:HG22	1:A:244:ASN:HD22	1.72	0.55
1:C:194:PHE:C	1:C:196:TYR:H	2.14	0.55
1:C:264:PHE:HE2	1:C:302:PHE:HB2	1.70	0.55
1:C:314:PHE:CD1	1:C:314:PHE:N	2.74	0.55
1:D:23:LEU:HD22	1:D:38:VAL:HG21	1.89	0.55
1:A:70:ILE:HD13	1:A:70:ILE:N	2.22	0.54
1:A:104:ARG:HH22	1:B:78:VAL:HA	1.71	0.54
1:C:219:SER:OG	1:C:222:ALA:HB3	2.06	0.54
1:C:222:ALA:O	1:C:226:LEU:HB2	2.06	0.54
1:C:300:VAL:O	1:C:304:LEU:HB2	2.06	0.54
1:E:287:ALA:C	1:E:289:SER:H	2.16	0.54
1:A:314:PHE:CD1	1:A:314:PHE:N	2.73	0.54
1:B:54:ASP:HB2	1:B:57:ARG:HB2	1.89	0.54
1:B:123:GLN:HB2	1:B:189:ILE:HG13	1.89	0.54
1:B:264:PHE:HE2	1:B:302:PHE:HB2	1.70	0.54
1:C:84:ARG:HH11	1:C:84:ARG:CB	2.20	0.54
1:C:157:THR:HG21	1:D:34:GLU:HG3	1.88	0.54
1:E:215:PHE:HZ	1:E:298:PHE:CD1	2.25	0.54
1:A:274:VAL:O	1:A:276:HIS:N	2.37	0.54
1:B:23:LEU:HD22	1:B:38:VAL:HG21	1.89	0.54
1:B:78:VAL:HB	1:B:128:TYR:HB2	1.89	0.54
1:A:264:PHE:HZ	1:A:301:VAL:HG12	1.71	0.54
1:C:19:THR:HG22	1:C:44:LEU:CD2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:LEU:HA	1:C:40:ALA:HB2	1.90	0.54
1:A:76:ARG:NH2	1:A:130:ILE:CD1	2.69	0.54
1:B:75:ILE:HD13	1:B:131:VAL:HB	1.88	0.54
1:E:194:PHE:C	1:E:196:TYR:H	2.15	0.54
1:A:264:PHE:HE2	1:A:302:PHE:HB2	1.73	0.54
1:D:75:ILE:HD13	1:D:131:VAL:HB	1.88	0.54
1:A:253:TYR:HB2	1:A:313:PHE:HD2	1.70	0.54
1:D:123:GLN:HB2	1:D:189:ILE:HG13	1.88	0.54
1:D:275:GLN:O	1:D:275:GLN:HG2	2.08	0.54
1:C:123:GLN:HB2	1:C:189:ILE:HG13	1.90	0.54
1:D:23:LEU:HG	1:D:164:PHE:CE1	2.43	0.54
1:E:314:PHE:CD1	1:E:314:PHE:N	2.76	0.54
1:A:149:GLY:O	1:A:164:PHE:CD1	2.50	0.54
1:C:276:HIS:C	1:C:278:LEU:H	2.15	0.54
1:A:215:PHE:O	1:A:291:THR:HG22	2.08	0.54
1:C:179:LEU:HD12	1:C:179:LEU:C	2.33	0.54
1:D:194:PHE:C	1:D:196:TYR:H	2.15	0.54
1:A:229:SER:HB3	1:B:228:VAL:CG1	2.38	0.53
1:B:179:LEU:HD12	1:B:179:LEU:C	2.33	0.53
1:C:21:ILE:O	1:C:149:GLY:HA3	2.08	0.53
1:C:54:ASP:HB2	1:C:57:ARG:HB2	1.90	0.53
1:D:225:THR:HG22	1:E:224:VAL:HG23	1.88	0.53
1:E:179:LEU:HD12	1:E:179:LEU:C	2.32	0.53
1:A:53:PHE:CD1	1:A:53:PHE:C	2.83	0.53
1:B:76:ARG:HH12	1:B:130:ILE:HD11	1.72	0.53
1:B:215:PHE:CZ	1:B:298:PHE:CD1	2.96	0.53
1:D:274:VAL:O	1:D:276:HIS:N	2.42	0.53
1:A:147:LYS:HE2	1:A:165:THR:HA	1.89	0.53
1:A:151:ASN:C	1:A:153:ASP:N	2.66	0.53
1:B:21:ILE:O	1:B:149:GLY:HA3	2.09	0.53
1:D:65:TYR:CD1	1:D:70:ILE:HD11	2.44	0.53
1:E:264:PHE:O	1:E:268:ALA:HB2	2.08	0.53
1:B:249:PRO:HD2	1:B:250:TYR:CE1	2.43	0.53
1:C:53:PHE:CE2	1:C:63:LYS:CB	2.83	0.53
1:A:96:ASP:OD1	1:A:98:THR:HB	2.09	0.53
1:A:155:PHE:CE1	1:B:112:PRO:CB	2.83	0.53
1:B:300:VAL:O	1:B:304:LEU:HB2	2.08	0.53
1:B:314:PHE:N	1:B:314:PHE:CD1	2.76	0.53
1:E:123:GLN:HB2	1:E:189:ILE:HG13	1.91	0.53
1:A:215:PHE:CZ	1:A:298:PHE:CD1	2.96	0.53
1:A:297:ALA:O	1:A:301:VAL:HG23	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:GLN:HB2	1:A:189:ILE:HG13	1.90	0.53
1:A:193:TYR:O	1:A:194:PHE:HB2	2.09	0.53
1:B:271:GLU:OE2	1:B:272:VAL:N	2.42	0.53
1:D:21:ILE:O	1:D:149:GLY:HA3	2.09	0.53
1:D:213:THR:HG22	1:D:226:LEU:CD1	2.38	0.53
1:E:300:VAL:O	1:E:304:LEU:HB2	2.07	0.53
1:A:179:LEU:HD12	1:A:179:LEU:C	2.34	0.53
1:C:53:PHE:CD1	1:C:53:PHE:C	2.83	0.53
1:D:264:PHE:CE2	1:D:302:PHE:HB2	2.43	0.53
1:E:82:ASN:O	1:E:83:ALA:C	2.52	0.53
1:E:84:ARG:HH11	1:E:84:ARG:HB3	1.74	0.53
1:A:275:GLN:O	1:A:275:GLN:HG2	2.09	0.53
1:A:276:HIS:C	1:A:278:LEU:H	2.17	0.52
1:C:147:LYS:HE2	1:C:165:THR:HA	1.90	0.52
1:E:200:ILE:CD1	1:E:240:LEU:HD23	2.36	0.52
1:B:253:TYR:HB2	1:B:313:PHE:HD2	1.73	0.52
1:D:229:SER:CB	1:E:228:VAL:HG11	2.39	0.52
1:E:78:VAL:HB	1:E:128:TYR:HB2	1.90	0.52
1:E:234:HIS:CE1	1:E:261:ILE:CG2	2.90	0.52
1:E:274:VAL:C	1:E:276:HIS:N	2.67	0.52
1:A:264:PHE:CE2	1:A:302:PHE:HB2	2.43	0.52
1:B:70:ILE:HG22	1:B:71:TRP:O	2.10	0.52
1:B:213:THR:HG22	1:B:226:LEU:HD11	1.91	0.52
1:D:68:GLU:CD	1:D:68:GLU:H	2.16	0.52
1:D:225:THR:HG21	1:E:224:VAL:HG23	1.89	0.52
1:D:297:ALA:O	1:D:301:VAL:HG23	2.09	0.52
1:E:84:ARG:HA	1:E:107:ALA:HB2	1.91	0.52
1:D:158:GLY:HA2	1:D:192:GLN:OE1	2.10	0.52
1:A:234:HIS:CE1	1:A:261:ILE:CG2	2.90	0.52
1:D:96:ASP:OD1	1:D:98:THR:HB	2.10	0.52
1:C:65:TYR:CD1	1:C:70:ILE:HD11	2.45	0.52
1:E:151:ASN:C	1:E:153:ASP:N	2.66	0.52
1:E:275:GLN:O	1:E:275:GLN:HG2	2.09	0.52
1:B:119:PRO:O	1:B:193:TYR:HB3	2.10	0.52
1:B:213:THR:HG22	1:B:226:LEU:CD1	2.39	0.52
1:B:235:ILE:HG22	1:B:239:ILE:HD12	1.91	0.52
1:C:25:GLU:OE1	1:C:25:GLU:HA	2.09	0.52
1:C:297:ALA:O	1:C:301:VAL:HG23	2.09	0.52
1:A:157:THR:HG21	1:B:34:GLU:OE1	2.10	0.52
1:B:215:PHE:HZ	1:B:298:PHE:CD1	2.28	0.52
1:C:193:TYR:O	1:C:194:PHE:HB2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:278:LEU:HD21	1:C:286:ARG:HB3	1.90	0.52
1:E:54:ASP:HB2	1:E:57:ARG:HB2	1.91	0.52
1:A:215:PHE:HZ	1:A:298:PHE:CD1	2.28	0.52
1:A:314:PHE:N	1:A:314:PHE:HD1	2.07	0.52
1:B:287:ALA:C	1:B:289:SER:H	2.18	0.52
1:B:53:PHE:CE2	1:B:63:LYS:CB	2.81	0.51
1:B:151:ASN:C	1:B:153:ASP:N	2.64	0.51
1:D:129:LEU:HD12	1:D:129:LEU:N	2.25	0.51
1:A:54:ASP:HB2	1:A:57:ARG:HB2	1.92	0.51
1:A:271:GLU:OE2	1:A:272:VAL:N	2.43	0.51
1:B:47:LYS:HD3	1:B:49:ARG:NH2	2.26	0.51
1:B:123:GLN:HA	1:B:123:GLN:NE2	2.25	0.51
1:B:194:PHE:C	1:B:196:TYR:H	2.18	0.51
1:A:23:LEU:HG	1:A:164:PHE:CE1	2.46	0.51
1:C:23:LEU:HD22	1:C:38:VAL:CG2	2.40	0.51
1:C:202:LEU:HD12	1:D:259:PHE:CZ	2.46	0.51
1:C:256:ALA:HB1	1:C:309:LEU:HD21	1.92	0.51
1:D:264:PHE:HE2	1:D:302:PHE:HB2	1.75	0.51
1:E:274:VAL:O	1:E:276:HIS:N	2.41	0.51
1:B:13:GLU:HB3	1:B:14:PRO:CD	2.41	0.51
1:E:213:THR:HG22	1:E:226:LEU:CD1	2.40	0.51
1:E:253:TYR:HB2	1:E:313:PHE:HD2	1.74	0.51
1:A:65:TYR:CD1	1:A:70:ILE:HD11	2.46	0.51
1:B:141:LEU:HD23	1:B:142:ALA:H	1.74	0.51
1:D:253:TYR:HB2	1:D:313:PHE:HD2	1.75	0.51
1:E:193:TYR:O	1:E:194:PHE:HB2	2.11	0.51
1:A:89:VAL:HG23	1:B:76:ARG:HD3	1.92	0.51
1:D:119:PRO:O	1:D:193:TYR:HB3	2.11	0.51
1:D:193:TYR:O	1:D:194:PHE:HB2	2.10	0.51
1:D:210:ILE:HG13	1:E:266:PHE:CE1	2.46	0.51
1:D:276:HIS:C	1:D:278:LEU:N	2.69	0.51
1:E:86:ALA:HB2	1:E:105:PHE:HB3	1.93	0.51
1:E:137:ARG:HD2	1:E:179:LEU:HG	1.93	0.51
1:C:226:LEU:HD21	1:D:224:VAL:HB	1.92	0.51
1:A:287:ALA:C	1:A:289:SER:H	2.17	0.51
1:E:25:GLU:OE1	1:E:25:GLU:HA	2.10	0.51
1:C:155:PHE:HD1	1:D:110:LEU:CD2	2.24	0.51
1:D:25:GLU:HA	1:D:25:GLU:OE1	2.11	0.51
1:E:65:TYR:CD1	1:E:70:ILE:HD11	2.46	0.51
1:C:157:THR:HG22	1:D:34:GLU:OE1	2.11	0.51
1:C:287:ALA:C	1:C:289:SER:H	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:253:TYR:CA	1:E:313:PHE:HE2	2.23	0.51
1:A:76:ARG:HH22	1:A:130:ILE:CD1	2.18	0.50
1:B:194:PHE:C	1:B:196:TYR:N	2.63	0.50
1:B:275:GLN:HG2	1:B:275:GLN:O	2.10	0.50
1:A:193:TYR:O	1:A:193:TYR:CG	2.63	0.50
1:D:53:PHE:CD1	1:D:53:PHE:C	2.88	0.50
1:D:95:PRO:C	1:D:97:GLY:H	2.18	0.50
1:E:297:ALA:O	1:E:301:VAL:HG23	2.10	0.50
1:A:203:PRO:HB3	1:B:262:TYR:CE1	2.47	0.50
1:C:89:VAL:CG2	1:D:76:ARG:HD3	2.42	0.50
1:E:23:LEU:HG	1:E:164:PHE:CE1	2.46	0.50
1:A:226:LEU:HD22	1:B:228:VAL:HG21	1.92	0.50
1:B:264:PHE:HZ	1:B:301:VAL:HG12	1.76	0.50
1:C:314:PHE:N	1:C:314:PHE:HD1	2.10	0.50
1:E:76:ARG:HH12	1:E:130:ILE:HD11	1.77	0.50
1:E:275:GLN:HG3	1:E:291:THR:OG1	2.11	0.50
1:A:84:ARG:HH11	1:A:84:ARG:HB3	1.76	0.50
1:A:249:PRO:HD2	1:A:250:TYR:CE1	2.47	0.50
1:B:65:TYR:CD1	1:B:70:ILE:HD11	2.46	0.50
1:C:275:GLN:O	1:C:275:GLN:HG2	2.11	0.50
1:E:21:ILE:O	1:E:149:GLY:HA3	2.10	0.50
1:E:47:LYS:HD3	1:E:49:ARG:NH2	2.27	0.50
1:E:276:HIS:C	1:E:278:LEU:N	2.70	0.50
1:E:314:PHE:N	1:E:314:PHE:HD1	2.10	0.50
1:B:82:ASN:O	1:B:83:ALA:C	2.52	0.50
1:C:29:LEU:HB2	1:C:156:LEU:HD11	1.94	0.50
1:D:213:THR:HG22	1:D:226:LEU:HD11	1.93	0.50
1:C:29:LEU:HD23	1:C:30:ASP:N	2.27	0.50
1:C:46:TRP:HH2	1:C:72:ILE:HG23	1.77	0.50
1:B:193:TYR:O	1:B:194:PHE:HB2	2.12	0.50
1:B:282:SER:C	1:B:284:PRO:HD3	2.37	0.50
1:C:82:ASN:O	1:C:83:ALA:C	2.54	0.50
1:D:77:PHE:CZ	1:D:129:LEU:HD11	2.46	0.50
1:D:287:ALA:C	1:D:289:SER:H	2.20	0.50
1:D:300:VAL:O	1:D:304:LEU:HB2	2.11	0.50
1:A:274:VAL:C	1:A:276:HIS:N	2.66	0.50
1:A:300:VAL:O	1:A:304:LEU:HB2	2.12	0.50
1:C:68:GLU:H	1:C:68:GLU:CD	2.20	0.50
1:D:51:LEU:HD11	1:D:70:ILE:HD12	1.94	0.50
1:E:53:PHE:O	1:E:54:ASP:C	2.55	0.50
1:A:255:GLY:O	1:A:258:ILE:HG22	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:229:SER:HB3	1:E:228:VAL:CG1	2.41	0.49
1:D:234:HIS:CE1	1:D:261:ILE:CG2	2.89	0.49
1:D:274:VAL:C	1:D:276:HIS:N	2.67	0.49
1:E:197:ILE:CB	1:E:198:PRO:HD3	2.41	0.49
1:A:94:SER:OG	1:A:95:PRO:HD2	2.11	0.49
1:C:94:SER:OG	1:C:95:PRO:HD2	2.12	0.49
1:B:214:ALA:HB1	1:B:223:ASN:CG	2.37	0.49
1:D:23:LEU:HD22	1:D:38:VAL:CG2	2.42	0.49
1:E:235:ILE:HG22	1:E:239:ILE:HD12	1.93	0.49
1:A:23:LEU:HD22	1:A:38:VAL:CG2	2.43	0.49
1:A:51:LEU:HD11	1:A:70:ILE:HD12	1.94	0.49
1:A:278:LEU:HD21	1:A:286:ARG:HB3	1.94	0.49
1:B:29:LEU:HD23	1:B:30:ASP:N	2.28	0.49
1:D:271:GLU:OE2	1:D:272:VAL:N	2.45	0.49
1:E:278:LEU:HD21	1:E:286:ARG:HB3	1.93	0.49
1:A:13:GLU:HB3	1:A:14:PRO:CD	2.43	0.49
1:A:253:TYR:CA	1:A:313:PHE:HE2	2.24	0.49
1:B:51:LEU:HD11	1:B:70:ILE:HD12	1.93	0.49
1:C:53:PHE:O	1:C:54:ASP:C	2.56	0.49
1:E:84:ARG:HB2	1:E:84:ARG:NH1	2.27	0.49
1:E:219:SER:OG	1:E:222:ALA:HB3	2.12	0.49
1:E:298:PHE:HB2	1:E:299:PRO:HD3	1.95	0.49
1:D:222:ALA:CB	1:E:220:TYR:CD2	2.96	0.49
1:A:158:GLY:HA2	1:A:192:GLN:OE1	2.12	0.49
1:B:137:ARG:HD2	1:B:179:LEU:HG	1.93	0.49
1:C:290:ILE:HG22	1:C:291:THR:N	2.28	0.49
1:D:314:PHE:CD1	1:D:314:PHE:N	2.79	0.49
1:A:53:PHE:CE2	1:A:63:LYS:CB	2.79	0.49
1:A:260:MET:HE2	1:A:309:LEU:HD22	1.94	0.49
1:C:264:PHE:O	1:C:268:ALA:HB2	2.12	0.49
1:D:282:SER:C	1:D:284:PRO:HD3	2.38	0.49
1:E:13:GLU:HB3	1:E:14:PRO:CD	2.43	0.49
1:C:65:TYR:CD2	1:C:70:ILE:HD11	2.48	0.48
1:C:147:LYS:C	1:C:149:GLY:N	2.55	0.48
1:E:158:GLY:HA2	1:E:192:GLN:OE1	2.13	0.48
1:C:212:TRP:HZ3	1:C:264:PHE:HD2	1.61	0.48
1:D:123:GLN:HA	1:D:123:GLN:NE2	2.28	0.48
1:E:23:LEU:HD22	1:E:38:VAL:CG2	2.43	0.48
1:E:249:PRO:HD2	1:E:250:TYR:CE1	2.48	0.48
1:A:200:ILE:CD1	1:A:240:LEU:HD23	2.40	0.48
1:B:53:PHE:O	1:B:54:ASP:C	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:PHE:N	1:B:314:PHE:HD1	2.10	0.48
1:D:221:GLU:OE2	1:E:221:GLU:OE2	2.30	0.48
1:A:65:TYR:CD2	1:A:70:ILE:HD11	2.49	0.48
1:A:141:LEU:HD23	1:A:142:ALA:H	1.78	0.48
1:B:11:ALA:HB3	1:B:136:THR:HG21	1.94	0.48
1:D:219:SER:OG	1:D:222:ALA:HB3	2.12	0.48
1:C:253:TYR:CA	1:C:313:PHE:HE2	2.26	0.48
1:B:193:TYR:O	1:B:193:TYR:CG	2.65	0.48
1:C:264:PHE:CZ	1:C:301:VAL:HG12	2.48	0.48
1:D:54:ASP:HB2	1:D:57:ARG:CB	2.43	0.48
1:D:84:ARG:NH1	1:D:84:ARG:HB2	2.28	0.48
1:E:68:GLU:CD	1:E:68:GLU:H	2.21	0.48
1:E:141:LEU:HD23	1:E:142:ALA:H	1.79	0.48
1:E:53:PHE:CE2	1:E:63:LYS:CB	2.85	0.48
1:E:291:THR:O	1:E:295:ARG:HG3	2.14	0.48
1:B:234:HIS:CE1	1:B:261:ILE:CG2	2.95	0.48
1:D:275:GLN:HG3	1:D:291:THR:OG1	2.14	0.48
1:E:215:PHE:O	1:E:291:THR:CG2	2.61	0.48
1:B:47:LYS:CD	1:B:49:ARG:NH2	2.77	0.48
1:B:243:THR:HG22	1:B:244:ASN:ND2	2.28	0.48
1:C:271:GLU:OE2	1:C:272:VAL:N	2.47	0.48
1:E:70:ILE:HG22	1:E:71:TRP:O	2.14	0.48
1:E:290:ILE:HG22	1:E:291:THR:N	2.29	0.48
1:A:47:LYS:HD3	1:A:49:ARG:NH2	2.29	0.48
1:A:68:GLU:H	1:A:68:GLU:CD	2.21	0.48
1:C:215:PHE:HB2	1:C:216:TRP:CE3	2.49	0.48
1:D:157:THR:HG21	1:E:34:GLU:OE1	2.14	0.48
1:E:65:TYR:CD2	1:E:70:ILE:HD11	2.48	0.48
1:E:213:THR:HG22	1:E:226:LEU:HD11	1.95	0.48
1:A:82:ASN:O	1:A:83:ALA:C	2.57	0.47
1:A:253:TYR:O	1:A:256:ALA:HB3	2.13	0.47
1:A:290:ILE:HG22	1:A:291:THR:N	2.27	0.47
1:B:137:ARG:HA	1:B:137:ARG:HD3	1.55	0.47
1:C:253:TYR:HB2	1:C:313:PHE:CD2	2.49	0.47
1:D:156:LEU:HD12	1:D:156:LEU:HA	1.71	0.47
1:D:227:VAL:CG1	1:D:269:VAL:HG23	2.44	0.47
1:B:215:PHE:O	1:B:291:THR:CG2	2.62	0.47
1:D:212:TRP:HZ3	1:D:264:PHE:HD2	1.61	0.47
1:D:249:PRO:HD2	1:D:250:TYR:CE1	2.50	0.47
1:E:44:LEU:HD12	1:E:101:TYR:CD2	2.49	0.47
1:E:84:ARG:CB	1:E:84:ARG:NH1	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:193:TYR:O	1:E:193:TYR:CG	2.66	0.47
1:E:224:VAL:O	1:E:226:LEU:N	2.47	0.47
1:A:282:SER:C	1:A:284:PRO:HD3	2.40	0.47
1:B:25:GLU:HA	1:B:25:GLU:OE1	2.13	0.47
1:C:23:LEU:HG	1:C:164:PHE:CE1	2.49	0.47
1:C:131:VAL:CG1	1:C:140:VAL:HG13	2.41	0.47
1:C:215:PHE:O	1:C:291:THR:CG2	2.62	0.47
1:C:276:HIS:C	1:C:278:LEU:N	2.72	0.47
1:E:260:MET:HE2	1:E:309:LEU:HD22	1.95	0.47
1:C:158:GLY:HA2	1:C:192:GLN:OE1	2.14	0.47
1:C:249:PRO:HD2	1:C:250:TYR:CE1	2.50	0.47
1:D:193:TYR:O	1:D:193:TYR:CG	2.67	0.47
1:E:243:THR:HG22	1:E:244:ASN:ND2	2.28	0.47
1:C:197:ILE:CB	1:C:198:PRO:HD3	2.43	0.47
1:C:275:GLN:HG3	1:C:291:THR:OG1	2.14	0.47
1:D:70:ILE:N	1:D:70:ILE:HD13	2.29	0.47
1:D:82:ASN:O	1:D:83:ALA:C	2.56	0.47
1:E:147:LYS:HE2	1:E:165:THR:HA	1.95	0.47
1:C:298:PHE:HB2	1:C:299:PRO:HD3	1.97	0.47
1:D:84:ARG:CB	1:D:84:ARG:NH1	2.76	0.47
1:A:119:PRO:O	1:A:193:TYR:HB3	2.14	0.47
1:A:226:LEU:HD23	1:B:224:VAL:CB	2.38	0.47
1:B:212:TRP:HZ3	1:B:264:PHE:HD2	1.63	0.47
1:B:276:HIS:C	1:B:278:LEU:N	2.70	0.47
1:C:19:THR:HG22	1:C:44:LEU:HD23	1.96	0.47
1:C:44:LEU:HD12	1:C:101:TYR:CD2	2.49	0.47
1:C:78:VAL:HB	1:C:128:TYR:CB	2.44	0.47
1:C:261:ILE:CD1	1:C:302:PHE:HE1	2.28	0.47
1:D:47:LYS:CD	1:D:49:ARG:NH2	2.75	0.47
1:D:78:VAL:HB	1:D:128:TYR:CB	2.45	0.47
1:D:253:TYR:CA	1:D:313:PHE:HE2	2.25	0.47
1:E:282:SER:C	1:E:284:PRO:HD3	2.39	0.47
1:B:100:GLN:HE21	1:B:100:GLN:HA	1.79	0.47
1:C:291:THR:O	1:C:295:ARG:HG3	2.14	0.47
1:D:137:ARG:HD2	1:D:179:LEU:HG	1.96	0.47
1:E:11:ALA:HB3	1:E:136:THR:HG21	1.97	0.47
1:B:158:GLY:HA2	1:B:192:GLN:OE1	2.14	0.47
1:B:191:ARG:CG	1:B:192:GLN:N	2.76	0.47
1:B:268:ALA:HA	1:B:298:PHE:HE1	1.80	0.47
1:D:53:PHE:O	1:D:54:ASP:C	2.57	0.47
1:D:260:MET:HE2	1:D:309:LEU:HD22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:29:LEU:HD23	1:E:30:ASP:N	2.30	0.47
1:A:78:VAL:HB	1:A:128:TYR:CB	2.45	0.46
1:A:215:PHE:HB2	1:A:216:TRP:CE3	2.50	0.46
1:A:227:VAL:CG1	1:A:269:VAL:HG23	2.46	0.46
1:C:27:TYR:CE1	1:D:81:GLU:CD	2.93	0.46
1:C:193:TYR:O	1:C:193:TYR:CG	2.68	0.46
1:D:104:ARG:NH2	1:E:78:VAL:HA	2.30	0.46
1:D:192:GLN:OE1	1:E:249:PRO:HB3	2.14	0.46
1:D:214:ALA:HB1	1:D:223:ASN:CG	2.40	0.46
1:C:119:PRO:O	1:C:193:TYR:HB3	2.15	0.46
1:D:29:LEU:HD23	1:D:30:ASP:N	2.29	0.46
1:B:65:TYR:CD2	1:B:70:ILE:HD11	2.50	0.46
1:B:200:ILE:CD1	1:B:240:LEU:HD23	2.40	0.46
1:C:137:ARG:HD2	1:C:179:LEU:HG	1.97	0.46
1:D:195:SER:HB3	1:E:248:THR:O	2.15	0.46
1:B:76:ARG:NH1	1:B:130:ILE:HD11	2.30	0.46
1:D:48:ASP:C	1:D:50:ARG:N	2.70	0.46
1:A:283:GLN:N	1:A:284:PRO:CD	2.78	0.46
1:B:23:LEU:HD22	1:B:38:VAL:CG2	2.46	0.46
1:B:147:LYS:HE2	1:B:165:THR:HA	1.97	0.46
1:C:96:ASP:OD1	1:C:98:THR:HB	2.15	0.46
1:C:253:TYR:O	1:C:256:ALA:HB3	2.15	0.46
1:D:215:PHE:HB2	1:D:216:TRP:CE3	2.51	0.46
1:D:243:THR:HG22	1:D:244:ASN:ND2	2.31	0.46
1:D:283:GLN:N	1:D:284:PRO:CD	2.77	0.46
1:E:212:TRP:HB2	1:E:215:PHE:CE1	2.51	0.46
1:B:256:ALA:HB1	1:B:309:LEU:HD21	1.97	0.46
1:B:264:PHE:O	1:B:268:ALA:HB2	2.15	0.46
1:D:204:MET:HE2	1:D:204:MET:HB3	1.59	0.46
1:E:51:LEU:HD11	1:E:70:ILE:HD12	1.97	0.46
1:E:119:PRO:O	1:E:193:TYR:HB3	2.15	0.46
1:A:118:TYR:CZ	1:A:196:TYR:HE2	2.34	0.46
1:D:13:GLU:HB3	1:D:14:PRO:CD	2.44	0.46
1:E:179:LEU:C	1:E:179:LEU:CD1	2.89	0.46
1:A:147:LYS:CE	1:A:165:THR:HA	2.45	0.46
1:A:225:THR:HG22	1:B:224:VAL:HG23	1.96	0.46
1:B:19:THR:HG22	1:B:44:LEU:HD23	1.96	0.46
1:B:125:LEU:HB2	1:B:187:LEU:HB3	1.97	0.46
1:B:255:GLY:O	1:B:258:ILE:HG22	2.15	0.46
1:B:290:ILE:HG22	1:B:291:THR:N	2.29	0.46
1:C:95:PRO:C	1:C:97:GLY:H	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:179:LEU:C	1:D:179:LEU:CD1	2.89	0.46
1:D:309:LEU:HD12	1:D:309:LEU:HA	1.77	0.46
1:E:48:ASP:C	1:E:50:ARG:N	2.73	0.46
1:A:46:TRP:HH2	1:A:72:ILE:HG23	1.80	0.46
1:B:235:ILE:CG2	1:B:239:ILE:HD12	2.46	0.46
1:C:41:PHE:HZ	1:D:76:ARG:NH2	2.14	0.46
1:D:41:PHE:HE2	1:E:175:LEU:HD23	1.80	0.46
1:D:76:ARG:HH12	1:D:130:ILE:HD11	1.81	0.46
1:A:22:TYR:HB3	1:A:41:PHE:HB2	1.98	0.46
1:A:70:ILE:HG22	1:A:71:TRP:O	2.15	0.46
1:B:23:LEU:HG	1:B:164:PHE:CE1	2.50	0.46
1:C:282:SER:C	1:C:284:PRO:HD3	2.41	0.46
1:D:19:THR:HG22	1:D:44:LEU:HD23	1.98	0.46
1:E:147:LYS:CE	1:E:165:THR:HA	2.46	0.46
1:A:202:LEU:O	1:A:203:PRO:C	2.58	0.45
1:B:309:LEU:HD12	1:B:309:LEU:HA	1.71	0.45
1:C:288:ALA:O	1:C:292:ARG:HB2	2.16	0.45
1:D:48:ASP:O	1:D:50:ARG:N	2.48	0.45
1:E:53:PHE:O	1:E:53:PHE:CG	2.69	0.45
1:E:94:SER:OG	1:E:95:PRO:HD2	2.16	0.45
1:A:53:PHE:O	1:A:54:ASP:C	2.59	0.45
1:A:76:ARG:HH12	1:A:130:ILE:HD11	1.81	0.45
1:A:253:TYR:HB2	1:A:313:PHE:CD2	2.51	0.45
1:A:298:PHE:HB2	1:A:299:PRO:HD3	1.98	0.45
1:B:95:PRO:C	1:B:97:GLY:H	2.24	0.45
1:E:29:LEU:HB2	1:E:156:LEU:HD11	1.98	0.45
1:C:149:GLY:O	1:C:164:PHE:CD1	2.54	0.45
1:C:226:LEU:HD23	1:D:224:VAL:HB	1.98	0.45
1:E:271:GLU:OE2	1:E:272:VAL:N	2.49	0.45
1:A:222:ALA:HA	1:B:221:GLU:OE1	2.16	0.45
1:A:261:ILE:CD1	1:A:302:PHE:HE1	2.29	0.45
1:B:204:MET:HB3	1:B:204:MET:HE2	1.68	0.45
1:D:235:ILE:HG22	1:D:239:ILE:HD12	1.98	0.45
1:D:264:PHE:O	1:D:268:ALA:HB2	2.16	0.45
1:E:214:ALA:HB1	1:E:223:ASN:CG	2.40	0.45
1:E:268:ALA:HA	1:E:298:PHE:HE1	1.80	0.45
1:A:240:LEU:CD1	1:B:239:ILE:HG12	2.39	0.45
1:B:226:LEU:HD22	1:B:226:LEU:HA	1.61	0.45
1:B:275:GLN:HG3	1:B:291:THR:OG1	2.17	0.45
1:C:123:GLN:HA	1:C:123:GLN:NE2	2.32	0.45
1:C:213:THR:CG2	1:C:226:LEU:HD11	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:48:ASP:C	1:D:50:ARG:H	2.23	0.45
1:D:65:TYR:CD2	1:D:70:ILE:HD11	2.52	0.45
1:E:212:TRP:HZ3	1:E:264:PHE:HD2	1.64	0.45
1:A:131:VAL:CG1	1:A:140:VAL:HG13	2.43	0.45
1:A:197:ILE:CB	1:A:198:PRO:HD3	2.45	0.45
1:A:276:HIS:C	1:A:278:LEU:N	2.74	0.45
1:B:68:GLU:CD	1:B:68:GLU:H	2.23	0.45
1:B:305:ALA:O	1:B:309:LEU:HB2	2.17	0.45
1:C:27:TYR:CD1	1:D:81:GLU:OE2	2.70	0.45
1:C:47:LYS:HD3	1:C:49:ARG:NH2	2.31	0.45
1:C:137:ARG:HA	1:C:137:ARG:HD3	1.48	0.45
1:D:291:THR:O	1:D:295:ARG:HG3	2.16	0.45
1:E:96:ASP:OD1	1:E:98:THR:HB	2.17	0.45
1:A:47:LYS:CD	1:A:49:ARG:NH2	2.80	0.45
1:C:13:GLU:HB3	1:C:14:PRO:CD	2.44	0.45
1:C:86:ALA:HB2	1:C:105:PHE:HB3	1.97	0.45
1:C:155:PHE:CD1	1:D:110:LEU:CD2	3.00	0.45
1:E:95:PRO:C	1:E:97:GLY:H	2.23	0.45
1:E:261:ILE:CD1	1:E:302:PHE:HE1	2.29	0.45
1:A:29:LEU:HD23	1:A:30:ASP:N	2.30	0.45
1:A:221:GLU:OE2	1:B:221:GLU:OE2	2.34	0.45
1:A:275:GLN:HG3	1:A:291:THR:OG1	2.16	0.45
1:B:84:ARG:CB	1:B:84:ARG:NH1	2.79	0.45
1:B:298:PHE:HB2	1:B:299:PRO:HD3	1.99	0.45
1:D:100:GLN:HE21	1:D:100:GLN:HA	1.82	0.45
1:D:314:PHE:N	1:D:314:PHE:HD1	2.14	0.45
1:E:19:THR:HG22	1:E:44:LEU:HD23	1.97	0.45
1:E:215:PHE:HB2	1:E:216:TRP:CE3	2.52	0.45
1:A:18:ASN:HB3	1:A:143:VAL:CG2	2.47	0.45
1:A:137:ARG:HD3	1:A:137:ARG:HA	1.58	0.45
1:B:44:LEU:HD12	1:B:101:TYR:CD2	2.52	0.45
1:B:215:PHE:HB2	1:B:216:TRP:CE3	2.51	0.45
1:D:70:ILE:HG22	1:D:71:TRP:O	2.17	0.45
1:D:94:SER:OG	1:D:95:PRO:HD2	2.17	0.45
1:D:255:GLY:O	1:D:258:ILE:HG22	2.16	0.45
1:E:48:ASP:O	1:E:51:LEU:HD23	2.17	0.45
1:E:137:ARG:HD3	1:E:137:ARG:HA	1.57	0.45
1:A:215:PHE:O	1:A:291:THR:CG2	2.64	0.45
1:A:291:THR:O	1:A:295:ARG:HG3	2.16	0.45
1:B:48:ASP:C	1:B:50:ARG:N	2.75	0.45
1:B:53:PHE:C	1:B:53:PHE:HD1	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:LEU:O	1:B:211:SER:HB3	2.16	0.45
1:C:29:LEU:C	1:C:29:LEU:CD2	2.90	0.45
1:C:179:LEU:C	1:C:179:LEU:CD1	2.90	0.45
1:D:52:ALA:HB1	1:D:95:PRO:O	2.17	0.45
1:D:212:TRP:HB2	1:D:215:PHE:CE1	2.51	0.45
1:E:204:MET:HE2	1:E:204:MET:HB3	1.63	0.45
1:E:226:LEU:HA	1:E:226:LEU:HD22	1.58	0.45
1:E:283:GLN:N	1:E:284:PRO:CD	2.79	0.45
1:B:80:VAL:HG12	1:B:82:ASN:O	2.18	0.44
1:C:155:PHE:CE1	1:D:112:PRO:HB3	2.52	0.44
1:C:283:GLN:N	1:C:284:PRO:CD	2.80	0.44
1:D:215:PHE:O	1:D:291:THR:CG2	2.65	0.44
1:D:290:ILE:HG22	1:D:291:THR:N	2.30	0.44
1:E:80:VAL:HG12	1:E:82:ASN:O	2.17	0.44
1:E:98:THR:O	1:E:98:THR:HG22	2.17	0.44
1:A:80:VAL:HG12	1:A:82:ASN:O	2.17	0.44
1:B:23:LEU:HA	1:B:40:ALA:CB	2.45	0.44
1:C:84:ARG:HB2	1:C:84:ARG:NH1	2.32	0.44
1:C:268:ALA:HA	1:C:298:PHE:HE1	1.81	0.44
1:D:29:LEU:HB2	1:D:156:LEU:HD11	1.98	0.44
1:D:54:ASP:O	1:D:54:ASP:OD1	2.35	0.44
1:D:131:VAL:CG1	1:D:140:VAL:HG13	2.43	0.44
1:C:48:ASP:O	1:C:51:LEU:HD23	2.17	0.44
1:A:25:GLU:OE1	1:A:25:GLU:HA	2.16	0.44
1:A:217:SER:OG	1:B:220:TYR:CE2	2.65	0.44
1:A:235:ILE:HG22	1:A:239:ILE:HD12	1.99	0.44
1:B:13:GLU:OE1	1:B:14:PRO:HD3	2.18	0.44
1:C:76:ARG:HH12	1:C:130:ILE:HD11	1.82	0.44
1:C:243:THR:HG22	1:C:244:ASN:ND2	2.32	0.44
1:D:253:TYR:O	1:D:256:ALA:HB3	2.16	0.44
1:D:261:ILE:CD1	1:D:302:PHE:HE1	2.31	0.44
1:E:123:GLN:NE2	1:E:123:GLN:HA	2.33	0.44
1:A:264:PHE:CZ	1:A:301:VAL:HG12	2.51	0.44
1:A:268:ALA:HA	1:A:298:PHE:HE1	1.81	0.44
1:B:118:TYR:CZ	1:B:196:TYR:HE2	2.36	0.44
1:B:274:VAL:C	1:B:276:HIS:N	2.66	0.44
1:C:227:VAL:CG1	1:C:269:VAL:HG23	2.47	0.44
1:A:157:THR:HG21	1:B:34:GLU:HG3	1.99	0.44
1:C:42:LEU:HD23	1:C:103:GLU:OE1	2.17	0.44
1:C:84:ARG:HH11	1:C:84:ARG:HB3	1.82	0.44
1:D:268:ALA:HA	1:D:298:PHE:HE1	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:PHE:O	1:A:53:PHE:CG	2.70	0.44
1:A:155:PHE:HB3	1:A:156:LEU:H	1.66	0.44
1:A:212:TRP:HZ3	1:A:264:PHE:HD2	1.65	0.44
1:B:54:ASP:HB2	1:B:57:ARG:CB	2.47	0.44
1:B:253:TYR:O	1:B:256:ALA:HB3	2.17	0.44
1:D:151:ASN:C	1:D:153:ASP:N	2.68	0.44
1:E:264:PHE:CZ	1:E:301:VAL:HG12	2.50	0.44
1:A:305:ALA:O	1:A:309:LEU:HB2	2.18	0.44
1:B:250:TYR:CD1	1:B:250:TYR:N	2.86	0.44
1:C:53:PHE:C	1:C:53:PHE:HD1	2.25	0.44
1:C:54:ASP:HB2	1:C:57:ARG:CB	2.48	0.44
1:D:197:ILE:HA	1:D:201:ILE:HB	1.99	0.44
1:D:270:ILE:HD13	1:D:270:ILE:HA	1.64	0.44
1:E:118:TYR:HB3	1:E:119:PRO:HD3	2.00	0.44
1:A:86:ALA:HB2	1:A:105:PHE:HB3	1.99	0.44
1:C:118:TYR:HB3	1:C:119:PRO:HD3	1.99	0.44
1:D:210:ILE:HG13	1:E:266:PHE:HE1	1.82	0.44
1:B:10:ILE:H	1:B:10:ILE:HG13	1.47	0.43
1:B:86:ALA:HB2	1:B:105:PHE:HB3	2.00	0.43
1:B:224:VAL:O	1:B:226:LEU:N	2.51	0.43
1:B:227:VAL:CG1	1:B:269:VAL:HG23	2.48	0.43
1:B:291:THR:O	1:B:295:ARG:HG3	2.18	0.43
1:C:191:ARG:CG	1:C:192:GLN:N	2.81	0.43
1:D:196:TYR:N	1:D:196:TYR:HD1	2.16	0.43
1:A:44:LEU:HD12	1:A:101:TYR:CD2	2.53	0.43
1:B:27:TYR:CE1	1:B:37:LYS:HB3	2.53	0.43
1:B:212:TRP:HB2	1:B:215:PHE:CE1	2.54	0.43
1:B:288:ALA:O	1:B:292:ARG:HB2	2.18	0.43
1:C:118:TYR:CZ	1:C:196:TYR:HE2	2.36	0.43
1:D:298:PHE:HB2	1:D:299:PRO:HD3	1.99	0.43
1:E:53:PHE:C	1:E:53:PHE:HD1	2.24	0.43
1:E:100:GLN:HA	1:E:100:GLN:HE21	1.83	0.43
1:E:202:LEU:O	1:E:203:PRO:C	2.60	0.43
1:E:274:VAL:HG12	1:E:275:GLN:N	2.33	0.43
1:A:179:LEU:C	1:A:179:LEU:CD1	2.91	0.43
1:B:25:GLU:HB2	1:B:39:ASN:HB3	2.00	0.43
1:B:179:LEU:C	1:B:179:LEU:CD1	2.91	0.43
1:D:212:TRP:CZ3	1:D:264:PHE:HD2	2.36	0.43
1:D:261:ILE:O	1:D:262:TYR:C	2.62	0.43
1:A:203:PRO:HB3	1:B:262:TYR:CZ	2.53	0.43
1:A:229:SER:CB	1:B:228:VAL:HG11	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:118:TYR:CZ	1:D:196:TYR:HE2	2.35	0.43
1:E:25:GLU:HB2	1:E:39:ASN:HB3	1.98	0.43
1:E:46:TRP:HH2	1:E:72:ILE:HG23	1.83	0.43
1:B:210:ILE:HD11	1:C:266:PHE:HD1	1.84	0.43
1:C:70:ILE:HG22	1:C:71:TRP:O	2.19	0.43
1:C:167:VAL:O	1:C:168:VAL:C	2.62	0.43
1:D:196:TYR:N	1:D:196:TYR:CD1	2.86	0.43
1:E:89:VAL:HG12	1:E:102:LEU:HB3	2.01	0.43
1:A:95:PRO:C	1:A:97:GLY:H	2.27	0.43
1:A:260:MET:CE	1:A:309:LEU:HD22	2.49	0.43
1:B:261:ILE:CD1	1:B:302:PHE:HE1	2.32	0.43
1:D:48:ASP:O	1:D:51:LEU:HD23	2.19	0.43
1:D:146:GLU:HG3	1:E:176:GLU:HG2	2.00	0.43
1:D:305:ALA:O	1:D:309:LEU:HB2	2.17	0.43
1:E:267:VAL:HA	1:E:270:ILE:HB	2.00	0.43
1:B:253:TYR:CA	1:B:313:PHE:HE2	2.26	0.43
1:D:147:LYS:HE2	1:D:165:THR:HA	2.01	0.43
1:A:104:ARG:NH1	1:B:77:PHE:O	2.50	0.43
1:A:287:ALA:C	1:A:289:SER:N	2.77	0.43
1:B:78:VAL:HB	1:B:128:TYR:CB	2.48	0.43
1:B:84:ARG:NH1	1:B:84:ARG:HB2	2.34	0.43
1:D:250:TYR:CD1	1:D:250:TYR:N	2.86	0.43
1:A:9:PRO:HD3	1:A:71:TRP:CE3	2.53	0.43
1:B:94:SER:OG	1:B:95:PRO:HD2	2.19	0.43
1:B:96:ASP:OD1	1:B:98:THR:HB	2.19	0.43
1:C:147:LYS:CE	1:C:165:THR:HA	2.47	0.43
1:E:210:ILE:O	1:E:211:SER:C	2.62	0.43
1:E:235:ILE:CG2	1:E:239:ILE:HD12	2.49	0.43
1:A:48:ASP:O	1:A:51:LEU:HD23	2.19	0.43
1:B:18:ASN:HB3	1:B:143:VAL:CG2	2.47	0.43
1:B:131:VAL:CG1	1:B:140:VAL:HG13	2.42	0.43
1:B:196:TYR:N	1:B:196:TYR:HD1	2.17	0.43
1:B:283:GLN:N	1:B:284:PRO:CD	2.79	0.43
1:C:212:TRP:HB2	1:C:215:PHE:CE1	2.54	0.43
1:D:256:ALA:HB1	1:D:309:LEU:HD21	2.00	0.43
1:D:264:PHE:CZ	1:D:301:VAL:HG12	2.52	0.43
1:E:54:ASP:HB2	1:E:57:ARG:CB	2.49	0.43
1:E:156:LEU:HA	1:E:156:LEU:HD12	1.70	0.43
1:E:202:LEU:HB2	1:E:203:PRO:HD3	2.01	0.43
1:E:227:VAL:CG1	1:E:269:VAL:HG23	2.49	0.43
1:E:287:ALA:C	1:E:289:SER:N	2.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:ARG:CG	1:A:192:GLN:N	2.81	0.42
1:A:224:VAL:O	1:A:226:LEU:N	2.52	0.42
1:C:202:LEU:O	1:C:203:PRO:C	2.61	0.42
1:E:10:ILE:H	1:E:10:ILE:HG13	1.50	0.42
1:A:242:GLU:CD	1:E:199:ASN:HB3	2.44	0.42
1:B:196:TYR:N	1:B:196:TYR:CD1	2.87	0.42
1:C:235:ILE:HG22	1:C:239:ILE:HD12	2.00	0.42
1:A:42:LEU:HD23	1:A:103:GLU:OE1	2.18	0.42
1:A:84:ARG:CB	1:A:84:ARG:NH1	2.81	0.42
1:A:84:ARG:NH1	1:A:84:ARG:HB2	2.33	0.42
1:A:156:LEU:HD12	1:A:156:LEU:HA	1.70	0.42
1:A:212:TRP:HB2	1:A:215:PHE:CE1	2.53	0.42
1:A:226:LEU:HD22	1:A:226:LEU:HA	1.58	0.42
1:C:240:LEU:HD22	1:D:239:ILE:HG12	2.00	0.42
1:D:44:LEU:HD12	1:D:101:TYR:CD2	2.53	0.42
1:D:253:TYR:CA	1:D:313:PHE:CE2	2.99	0.42
1:A:54:ASP:HB2	1:A:57:ARG:CB	2.49	0.42
1:A:195:SER:HB3	1:B:248:THR:O	2.18	0.42
1:B:219:SER:OG	1:B:222:ALA:HB3	2.19	0.42
1:C:18:ASN:HB3	1:C:143:VAL:CG2	2.49	0.42
1:C:149:GLY:O	1:C:150:LYS:HB2	2.19	0.42
1:D:296:ILE:HD13	1:D:296:ILE:HA	1.90	0.42
1:E:253:TYR:O	1:E:256:ALA:HB3	2.19	0.42
1:E:305:ALA:O	1:E:309:LEU:HB2	2.19	0.42
1:A:29:LEU:C	1:A:29:LEU:CD2	2.92	0.42
1:A:29:LEU:HB2	1:A:156:LEU:HD11	2.01	0.42
1:A:53:PHE:C	1:A:53:PHE:HD1	2.25	0.42
1:B:195:SER:HB3	1:C:248:THR:O	2.19	0.42
1:D:210:ILE:CG1	1:E:266:PHE:CD1	3.02	0.42
1:E:118:TYR:CZ	1:E:196:TYR:HE2	2.38	0.42
1:A:41:PHE:HZ	1:B:76:ARG:NH2	2.17	0.42
1:A:303:LEU:O	1:A:307:ILE:HD12	2.19	0.42
1:B:245:LEU:HA	1:B:245:LEU:HD12	1.78	0.42
1:B:267:VAL:HA	1:B:270:ILE:HB	2.02	0.42
1:C:15:LEU:O	1:C:15:LEU:HG	2.11	0.42
1:C:204:MET:HE2	1:C:204:MET:HB3	1.63	0.42
1:C:214:ALA:HB1	1:C:223:ASN:CG	2.45	0.42
1:C:222:ALA:CA	1:D:221:GLU:OE1	2.67	0.42
1:C:287:ALA:C	1:C:289:SER:N	2.78	0.42
1:A:100:GLN:HE21	1:A:100:GLN:HA	1.85	0.42
1:C:51:LEU:HD11	1:C:70:ILE:HD12	1.98	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:260:MET:HE2	1:C:309:LEU:HD22	2.02	0.42
1:D:173:PHE:O	1:D:179:LEU:HB2	2.20	0.42
1:E:84:ARG:H	1:E:84:ARG:HG2	1.33	0.42
1:E:256:ALA:HB1	1:E:309:LEU:HD21	2.01	0.42
1:A:193:TYR:O	1:A:194:PHE:CB	2.67	0.42
1:A:264:PHE:O	1:A:268:ALA:HB2	2.19	0.42
1:C:80:VAL:HG12	1:C:82:ASN:O	2.20	0.42
1:C:84:ARG:CB	1:C:84:ARG:NH1	2.83	0.42
1:C:155:PHE:HB3	1:C:156:LEU:H	1.70	0.42
1:D:94:SER:OG	1:D:95:PRO:CD	2.68	0.42
1:D:191:ARG:CG	1:D:192:GLN:N	2.82	0.42
1:B:253:TYR:HB2	1:B:313:PHE:CD2	2.53	0.42
1:C:94:SER:OG	1:C:95:PRO:CD	2.68	0.42
1:C:151:ASN:C	1:C:153:ASP:N	2.67	0.42
1:C:215:PHE:HB2	1:C:216:TRP:CZ3	2.55	0.42
1:A:62:VAL:CG1	1:A:92:SER:HB3	2.46	0.42
1:A:213:THR:HG22	1:A:226:LEU:HD12	2.02	0.42
1:B:53:PHE:O	1:B:53:PHE:CG	2.71	0.42
1:D:79:ASN:OD1	1:D:79:ASN:O	2.37	0.42
1:E:47:LYS:CD	1:E:49:ARG:NH2	2.80	0.42
1:E:80:VAL:CG1	1:E:82:ASN:O	2.68	0.42
1:A:19:THR:HA	1:A:43:SER:O	2.20	0.41
1:C:253:TYR:CA	1:C:313:PHE:CE2	2.99	0.41
1:D:27:TYR:CB	1:E:110:LEU:HD11	2.50	0.41
1:A:94:SER:OG	1:A:95:PRO:CD	2.67	0.41
1:B:19:THR:HA	1:B:43:SER:O	2.20	0.41
1:B:80:VAL:CG1	1:B:82:ASN:O	2.69	0.41
1:C:47:LYS:CD	1:C:49:ARG:NH2	2.82	0.41
1:D:193:TYR:O	1:D:194:PHE:CB	2.67	0.41
1:A:270:ILE:HD13	1:A:270:ILE:HA	1.61	0.41
1:B:147:LYS:CE	1:B:165:THR:HA	2.50	0.41
1:B:212:TRP:CZ3	1:B:264:PHE:HD2	2.38	0.41
1:B:260:MET:HE2	1:B:309:LEU:HD22	2.01	0.41
1:B:287:ALA:C	1:B:289:SER:N	2.78	0.41
1:C:296:ILE:HD13	1:C:296:ILE:HA	1.91	0.41
1:D:202:LEU:O	1:D:203:PRO:C	2.63	0.41
1:E:131:VAL:CG1	1:E:140:VAL:HG13	2.43	0.41
1:A:27:TYR:CD1	1:B:81:GLU:OE2	2.73	0.41
1:A:52:ALA:HB1	1:A:95:PRO:O	2.20	0.41
1:A:214:ALA:HB1	1:A:223:ASN:CG	2.45	0.41
1:B:155:PHE:HB3	1:B:156:LEU:H	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:125:LEU:HB2	1:D:187:LEU:HB3	2.03	0.41
1:D:200:ILE:CD1	1:D:240:LEU:HD23	2.45	0.41
1:D:288:ALA:O	1:D:292:ARG:HB2	2.20	0.41
1:E:208:LEU:O	1:E:211:SER:HB3	2.20	0.41
1:A:196:TYR:N	1:A:196:TYR:HD1	2.19	0.41
1:E:125:LEU:HB2	1:E:187:LEU:HB3	2.01	0.41
1:E:155:PHE:HB3	1:E:156:LEU:H	1.72	0.41
1:A:80:VAL:CG1	1:A:82:ASN:O	2.69	0.41
1:A:104:ARG:HH22	1:B:78:VAL:CA	2.34	0.41
1:A:204:MET:HB3	1:A:204:MET:HE2	1.64	0.41
1:A:288:ALA:O	1:A:292:ARG:HB2	2.20	0.41
1:B:46:TRP:HH2	1:B:72:ILE:HG23	1.86	0.41
1:D:18:ASN:HB3	1:D:143:VAL:CG2	2.46	0.41
1:E:49:ARG:H	1:E:49:ARG:HG2	1.66	0.41
1:E:193:TYR:O	1:E:194:PHE:CB	2.68	0.41
1:A:48:ASP:C	1:A:50:ARG:N	2.77	0.41
1:D:64:THR:O	1:D:64:THR:HG22	2.20	0.41
1:D:224:VAL:O	1:D:226:LEU:N	2.54	0.41
1:D:253:TYR:HD1	1:D:313:PHE:CD2	2.38	0.41
1:E:19:THR:HA	1:E:43:SER:O	2.20	0.41
1:E:79:ASN:OD1	1:E:79:ASN:O	2.39	0.41
1:E:253:TYR:HB2	1:E:313:PHE:CD2	2.55	0.41
1:E:296:ILE:HD13	1:E:296:ILE:HA	1.89	0.41
1:A:118:TYR:HB3	1:A:119:PRO:HD3	2.02	0.41
1:A:139:ILE:HG12	1:A:172:ASN:HD21	1.86	0.41
1:A:146:GLU:HG3	1:B:176:GLU:CG	2.51	0.41
1:A:225:THR:HG22	1:A:225:THR:O	2.21	0.41
1:A:249:PRO:HD2	1:A:250:TYR:HD1	1.84	0.41
1:A:253:TYR:CA	1:A:313:PHE:CE2	2.99	0.41
1:B:128:TYR:HD1	1:B:128:TYR:HA	1.72	0.41
1:B:197:ILE:HA	1:B:201:ILE:HB	2.02	0.41
1:C:27:TYR:CE1	1:D:81:GLU:OE1	2.73	0.41
1:C:100:GLN:HE21	1:C:100:GLN:HA	1.86	0.41
1:C:141:LEU:HD23	1:C:142:ALA:H	1.85	0.41
1:C:240:LEU:HD13	1:D:239:ILE:HG12	2.03	0.41
1:C:270:ILE:HA	1:C:270:ILE:HD13	1.65	0.41
1:D:19:THR:HA	1:D:43:SER:O	2.21	0.41
1:D:202:LEU:HB2	1:D:203:PRO:HD3	2.03	0.41
1:D:208:LEU:O	1:D:211:SER:HB3	2.21	0.41
1:E:76:ARG:NH1	1:E:130:ILE:HD11	2.35	0.41
1:E:78:VAL:HB	1:E:128:TYR:CB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:98:THR:O	1:C:98:THR:HG22	2.21	0.41
1:C:149:GLY:O	1:C:150:LYS:CB	2.69	0.41
1:D:197:ILE:CB	1:D:198:PRO:HD3	2.48	0.41
1:D:278:LEU:HD23	1:D:287:ALA:HA	2.03	0.41
1:E:167:VAL:O	1:E:168:VAL:C	2.62	0.41
1:E:212:TRP:CZ3	1:E:264:PHE:HD2	2.39	0.41
1:A:25:GLU:HB2	1:A:39:ASN:HB3	2.04	0.40
1:A:27:TYR:CE1	1:B:81:GLU:CD	2.99	0.40
1:A:175:LEU:C	1:A:175:LEU:HD12	2.47	0.40
1:A:196:TYR:N	1:A:196:TYR:CD1	2.88	0.40
1:A:229:SER:HB3	1:B:228:VAL:HG11	2.03	0.40
1:C:226:LEU:HA	1:C:226:LEU:HD22	1.58	0.40
1:D:210:ILE:O	1:D:211:SER:C	2.65	0.40
1:D:287:ALA:C	1:D:289:SER:N	2.79	0.40
1:E:7:PRO:O	1:E:50:ARG:NH1	2.54	0.40
1:E:48:ASP:C	1:E:50:ARG:H	2.28	0.40
1:A:208:LEU:O	1:A:211:SER:HB3	2.21	0.40
1:A:225:THR:CG2	1:B:224:VAL:HG23	2.52	0.40
1:B:9:PRO:HD3	1:B:71:TRP:CE3	2.55	0.40
1:C:267:VAL:HA	1:C:270:ILE:HB	2.03	0.40
1:E:255:GLY:O	1:E:258:ILE:HG22	2.22	0.40
1:A:224:VAL:HG23	1:A:225:THR:N	2.36	0.40
1:A:243:THR:HG22	1:A:244:ASN:ND2	2.34	0.40
1:A:261:ILE:O	1:A:262:TYR:C	2.64	0.40
1:C:224:VAL:O	1:C:226:LEU:N	2.54	0.40
1:C:245:LEU:HD12	1:C:245:LEU:HA	1.82	0.40
1:D:22:TYR:HB3	1:D:41:PHE:HB2	2.03	0.40
1:D:41:PHE:HE2	1:E:175:LEU:CD2	2.34	0.40
1:E:9:PRO:HD3	1:E:71:TRP:CE3	2.57	0.40
1:B:7:PRO:O	1:B:50:ARG:NH1	2.51	0.40
1:B:48:ASP:O	1:B:51:LEU:HD23	2.21	0.40
1:C:213:THR:HG22	1:C:226:LEU:HD12	2.03	0.40
1:D:41:PHE:HD1	1:D:41:PHE:HA	1.81	0.40
1:D:79:ASN:OD1	1:D:109:VAL:CG1	2.69	0.40
1:D:215:PHE:HB2	1:D:216:TRP:CZ3	2.57	0.40
1:D:253:TYR:HB2	1:D:313:PHE:CD2	2.55	0.40
1:E:288:ALA:O	1:E:292:ARG:HB2	2.21	0.40
1:B:202:LEU:O	1:B:203:PRO:C	2.61	0.40
1:C:79:ASN:OD1	1:C:109:VAL:CG1	2.70	0.40
1:C:150:LYS:CG	1:C:154:VAL:HG21	2.48	0.40
1:C:250:TYR:CD1	1:C:250:TYR:N	2.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:305:ALA:O	1:C:309:LEU:HB2	2.20	0.40
1:D:128:TYR:HD1	1:D:128:TYR:HA	1.73	0.40
1:E:47:LYS:HE2	1:E:47:LYS:HB3	1.90	0.40
1:E:48:ASP:O	1:E:50:ARG:N	2.54	0.40
1:E:253:TYR:HD1	1:E:313:PHE:CD2	2.39	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%)	247 (80%)	48 (16%)	13 (4%)	2	19
1	B	308/317 (97%)	245 (80%)	49 (16%)	14 (4%)	2	17
1	C	308/317 (97%)	245 (80%)	48 (16%)	15 (5%)	1	16
1	D	308/317 (97%)	248 (80%)	46 (15%)	14 (4%)	2	17
1	E	308/317 (97%)	245 (80%)	49 (16%)	14 (4%)	2	17
All	All	1540/1585 (97%)	1230 (80%)	240 (16%)	70 (4%)	2	17

All (70) 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	A	275	GLN
1	A	282	SER
1	B	118	TYR
1	B	148	VAL
1	B	150	LYS

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Mol	Chain	Res	Type
1	B	194	PHE
1	B	275	GLN
1	B	282	SER
1	C	118	TYR
1	C	148	VAL
1	C	150	LYS
1	C	194	PHE
1	C	275	GLN
1	C	282	SER
1	D	118	TYR
1	D	148	VAL
1	D	150	LYS
1	D	194	PHE
1	D	282	SER
1	E	118	TYR
1	E	148	VAL
1	E	150	LYS
1	E	194	PHE
1	E	275	GLN
1	E	282	SER
1	A	84	ARG
1	B	84	ARG
1	B	287	ALA
1	C	84	ARG
1	C	287	ALA
1	D	84	ARG
1	D	275	GLN
1	E	84	ARG
1	E	287	ALA
1	A	278	LEU
1	A	287	ALA
1	A	288	ALA
1	B	278	LEU
1	B	288	ALA
1	C	225	THR
1	C	278	LEU
1	C	288	ALA
1	D	278	LEU
1	D	287	ALA
1	D	288	ALA
1	E	278	LEU
1	E	288	ALA

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Mol	Chain	Res	Type
1	E	302	PHE
1	B	302	PHE
1	E	225	THR
1	A	225	THR
1	B	155	PHE
1	C	302	PHE
1	D	49	ARG
1	D	131	VAL
1	D	302	PHE
1	E	14	PRO
1	A	131	VAL
1	C	14	PRO
1	C	131	VAL
1	D	14	PRO
1	E	131	VAL
1	B	14	PRO
1	B	131	VAL
1	A	14	PRO
1	C	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%)	227 (82%)	51 (18%)	2	10
1	B	278/284 (98%)	228 (82%)	50 (18%)	2	10
1	C	278/284 (98%)	227 (82%)	51 (18%)	2	10
1	D	278/284 (98%)	229 (82%)	49 (18%)	2	11
1	E	278/284 (98%)	227 (82%)	51 (18%)	2	10
All	All	1390/1420 (98%)	1138 (82%)	252 (18%)	2	10

All (252) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ILE
1	A	15	LEU
1	A	16	THR
1	A	32	LYS
1	A	49	ARG
1	A	51	LEU
1	A	53	PHE
1	A	64	THR
1	A	68	GLU
1	A	72	ILE
1	A	84	ARG
1	A	89	VAL
1	A	98	THR
1	A	110	LEU
1	A	113	LEU
1	A	122	SER
1	A	124	THR
1	A	130	ILE
1	A	134	VAL
1	A	140	VAL
1	A	141	LEU
1	A	150	LYS
1	A	151	ASN
1	A	154	VAL
1	A	157	THR
1	A	162	GLU
1	A	179	LEU
1	A	191	ARG
1	A	202	LEU
1	A	204	MET
1	A	211	SER
1	A	213	THR
1	A	221	GLU
1	A	226	LEU
1	A	239	ILE
1	A	243	THR
1	A	245	LEU
1	A	252	THR
1	A	254	THR
1	A	257	ILE
1	A	263	LEU
1	A	269	VAL
1	A	270	ILE

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Mol	Chain	Res	Type
1	A	274	VAL
1	A	290	ILE
1	A	292	ARG
1	A	296	ILE
1	A	304	LEU
1	A	306	ASN
1	A	307	ILE
1	A	314	PHE
1	B	15	LEU
1	B	16	THR
1	B	32	LYS
1	B	49	ARG
1	B	51	LEU
1	B	53	PHE
1	B	64	THR
1	B	68	GLU
1	B	72	ILE
1	B	84	ARG
1	B	89	VAL
1	B	98	THR
1	B	110	LEU
1	B	113	LEU
1	B	122	SER
1	B	124	THR
1	B	130	ILE
1	B	134	VAL
1	B	140	VAL
1	B	141	LEU
1	B	150	LYS
1	B	151	ASN
1	B	154	VAL
1	B	157	THR
1	B	162	GLU
1	B	179	LEU
1	B	191	ARG
1	B	202	LEU
1	B	204	MET
1	B	211	SER
1	B	213	THR
1	B	221	GLU
1	B	226	LEU
1	B	239	ILE

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Mol	Chain	Res	Type
1	B	243	THR
1	B	245	LEU
1	B	252	THR
1	B	254	THR
1	B	257	ILE
1	B	263	LEU
1	B	269	VAL
1	B	270	ILE
1	B	274	VAL
1	B	290	ILE
1	B	292	ARG
1	B	296	ILE
1	B	304	LEU
1	B	306	ASN
1	B	307	ILE
1	B	314	PHE
1	C	10	ILE
1	C	15	LEU
1	C	16	THR
1	C	32	LYS
1	C	49	ARG
1	C	51	LEU
1	C	53	PHE
1	C	64	THR
1	C	68	GLU
1	C	70	ILE
1	C	72	ILE
1	C	84	ARG
1	C	89	VAL
1	C	98	THR
1	C	110	LEU
1	C	113	LEU
1	C	122	SER
1	C	124	THR
1	C	130	ILE
1	C	134	VAL
1	C	140	VAL
1	C	141	LEU
1	C	151	ASN
1	C	154	VAL
1	C	157	THR
1	C	162	GLU

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Mol	Chain	Res	Type
1	C	179	LEU
1	C	191	ARG
1	C	202	LEU
1	C	204	MET
1	C	211	SER
1	C	213	THR
1	C	221	GLU
1	C	226	LEU
1	C	239	ILE
1	C	243	THR
1	C	245	LEU
1	C	252	THR
1	C	254	THR
1	C	257	ILE
1	C	263	LEU
1	C	269	VAL
1	C	270	ILE
1	C	274	VAL
1	C	290	ILE
1	C	292	ARG
1	C	296	ILE
1	C	304	LEU
1	C	306	ASN
1	C	307	ILE
1	C	314	PHE
1	D	15	LEU
1	D	16	THR
1	D	32	LYS
1	D	49	ARG
1	D	51	LEU
1	D	53	PHE
1	D	64	THR
1	D	68	GLU
1	D	72	ILE
1	D	84	ARG
1	D	89	VAL
1	D	98	THR
1	D	110	LEU
1	D	113	LEU
1	D	122	SER
1	D	124	THR
1	D	130	ILE

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Mol	Chain	Res	Type
1	D	134	VAL
1	D	140	VAL
1	D	141	LEU
1	D	150	LYS
1	D	151	ASN
1	D	154	VAL
1	D	157	THR
1	D	162	GLU
1	D	179	LEU
1	D	191	ARG
1	D	202	LEU
1	D	204	MET
1	D	211	SER
1	D	213	THR
1	D	221	GLU
1	D	226	LEU
1	D	239	ILE
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	290	ILE
1	D	292	ARG
1	D	296	ILE
1	D	304	LEU
1	D	306	ASN
1	D	307	ILE
1	D	314	PHE
1	E	15	LEU
1	E	16	THR
1	E	32	LYS
1	E	49	ARG
1	E	51	LEU
1	E	53	PHE
1	E	64	THR
1	E	68	GLU
1	E	70	ILE
1	E	72	ILE

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Mol	Chain	Res	Type
1	E	84	ARG
1	E	89	VAL
1	E	98	THR
1	E	110	LEU
1	E	113	LEU
1	E	122	SER
1	E	124	THR
1	E	130	ILE
1	E	134	VAL
1	E	140	VAL
1	E	141	LEU
1	E	150	LYS
1	E	151	ASN
1	E	154	VAL
1	E	157	THR
1	E	162	GLU
1	E	179	LEU
1	E	191	ARG
1	E	202	LEU
1	E	204	MET
1	E	211	SER
1	E	213	THR
1	E	221	GLU
1	E	226	LEU
1	E	239	ILE
1	E	243	THR
1	E	245	LEU
1	E	252	THR
1	E	254	THR
1	E	257	ILE
1	E	263	LEU
1	E	269	VAL
1	E	270	ILE
1	E	274	VAL
1	E	290	ILE
1	E	292	ARG
1	E	296	ILE
1	E	304	LEU
1	E	306	ASN
1	E	307	ILE
1	E	314	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	GLN
1	A	138	ASN
1	A	151	ASN
1	A	244	ASN
1	A	283	GLN
1	B	100	GLN
1	B	138	ASN
1	B	151	ASN
1	B	238	ASN
1	B	244	ASN
1	B	275	GLN
1	B	283	GLN
1	C	100	GLN
1	C	138	ASN
1	C	151	ASN
1	C	244	ASN
1	C	275	GLN
1	D	100	GLN
1	D	151	ASN
1	D	244	ASN
1	D	283	GLN
1	E	100	GLN
1	E	151	ASN
1	E	244	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	310/317 (97%)	0.90	47 (15%) 5 5	69, 112, 168, 218	0
1	B	310/317 (97%)	0.82	35 (11%) 10 7	73, 112, 167, 217	0
1	C	310/317 (97%)	0.68	33 (10%) 11 8	72, 112, 167, 220	0
1	D	310/317 (97%)	0.86	39 (12%) 8 6	70, 111, 167, 218	0
1	E	310/317 (97%)	0.83	40 (12%) 7 6	74, 112, 167, 218	0
All	All	1550/1585 (97%)	0.82	194 (12%) 8 6	69, 112, 168, 220	0

All (194) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	60	VAL	11.4
1	A	59	GLY	7.6
1	D	153	ASP	7.3
1	C	144	ASP	6.6
1	B	148	VAL	5.8
1	B	152	ASP	5.6
1	C	60	VAL	5.4
1	E	148	VAL	5.2
1	E	147	LYS	5.1
1	B	101	TYR	5.1
1	A	58	SER	5.0
1	A	61	ARG	4.9
1	A	62	VAL	4.9
1	B	88	VAL	4.9
1	C	172	ASN	4.9
1	B	153	ASP	4.8
1	B	100	GLN	4.8
1	E	100	GLN	4.7
1	B	47	LYS	4.6
1	A	206	PHE	4.5

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Mol	Chain	Res	Type	RSRZ
1	E	144	ASP	4.5
1	B	144	ASP	4.5
1	A	11	ALA	4.4
1	C	153	ASP	4.4
1	E	146	GLU	4.3
1	A	153	ASP	4.3
1	D	128	TYR	4.2
1	A	13	GLU	4.2
1	B	49	ARG	4.1
1	A	148	VAL	4.0
1	D	78	VAL	4.0
1	A	172	ASN	4.0
1	A	139	ILE	3.9
1	B	136	THR	3.9
1	A	144	ASP	3.9
1	D	57	ARG	3.8
1	D	45	SER	3.7
1	D	11	ALA	3.7
1	D	111	SER	3.7
1	E	45	SER	3.6
1	D	129	LEU	3.6
1	C	277	TYR	3.6
1	D	118	TYR	3.6
1	A	10	ILE	3.5
1	D	85	ASP	3.4
1	C	85	ASP	3.4
1	E	184	ASP	3.4
1	E	47	LYS	3.4
1	D	117	ARG	3.4
1	B	231	LEU	3.3
1	A	7	PRO	3.3
1	B	61	ARG	3.3
1	A	12	ASP	3.3
1	E	149	GLY	3.3
1	B	86	ALA	3.2
1	D	60	VAL	3.2
1	A	64	THR	3.2
1	C	139	ILE	3.2
1	E	101	TYR	3.2
1	D	126	HIS	3.2
1	C	11	ALA	3.1
1	D	7	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	126	HIS	3.1
1	C	135	ASP	3.1
1	B	11	ALA	3.1
1	D	263	LEU	3.1
1	C	147	LYS	3.1
1	A	74	GLU	3.1
1	A	134	VAL	3.0
1	C	173	PHE	3.0
1	D	112	PRO	3.0
1	C	142	ALA	3.0
1	E	242	GLU	3.0
1	E	285	ALA	3.0
1	D	148	VAL	2.9
1	C	285	ALA	2.9
1	C	114	ASP	2.9
1	A	230	THR	2.9
1	A	128	TYR	2.9
1	B	7	PRO	2.9
1	C	13	GLU	2.9
1	D	55	PRO	2.9
1	E	61	ARG	2.9
1	A	145	LEU	2.8
1	C	7	PRO	2.8
1	A	221	GLU	2.8
1	A	79	ASN	2.8
1	C	117	ARG	2.7
1	E	286	ARG	2.7
1	E	139	ILE	2.7
1	D	100	GLN	2.7
1	B	91	ILE	2.7
1	D	83	ALA	2.7
1	E	244	ASN	2.7
1	D	144	ASP	2.7
1	B	56	VAL	2.6
1	D	10	ILE	2.6
1	C	316	PHE	2.6
1	A	47	LYS	2.6
1	B	90	ASP	2.6
1	E	209	PHE	2.6
1	E	88	VAL	2.6
1	C	242	GLU	2.6
1	E	116	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	59	GLY	2.6
1	E	91	ILE	2.5
1	D	47	LYS	2.5
1	B	117	ARG	2.5
1	B	87	ASP	2.5
1	D	316	PHE	2.5
1	A	208	LEU	2.5
1	B	55	PRO	2.5
1	C	59	GLY	2.5
1	D	187	LEU	2.5
1	D	18	ASN	2.5
1	D	82	ASN	2.5
1	E	145	LEU	2.5
1	A	78	VAL	2.5
1	C	233	ALA	2.4
1	C	25	GLU	2.4
1	D	12	ASP	2.4
1	C	279	LYS	2.4
1	D	56	VAL	2.4
1	A	209	PHE	2.4
1	E	243	THR	2.4
1	B	102	LEU	2.4
1	C	169	LYS	2.4
1	E	173	PHE	2.4
1	E	7	PRO	2.4
1	A	53	PHE	2.4
1	B	266	PHE	2.4
1	D	195	SER	2.4
1	E	128	TYR	2.3
1	A	54	ASP	2.3
1	E	282	SER	2.3
1	A	169	LYS	2.3
1	E	83	ALA	2.3
1	E	168	VAL	2.3
1	A	91	ILE	2.3
1	A	211	SER	2.3
1	A	14	PRO	2.3
1	C	168	VAL	2.3
1	E	126	HIS	2.3
1	E	141	LEU	2.3
1	A	187	LEU	2.2
1	B	141	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	174	ALA	2.2
1	B	285	ALA	2.2
1	E	174	ALA	2.2
1	B	216	TRP	2.2
1	A	194	PHE	2.2
1	A	203	PRO	2.2
1	A	90	ASP	2.2
1	A	202	LEU	2.2
1	D	277	TYR	2.2
1	C	74	GLU	2.2
1	E	114	ASP	2.2
1	C	288	ALA	2.1
1	B	154	VAL	2.1
1	D	134	VAL	2.1
1	C	18	ASN	2.1
1	D	244	ASN	2.1
1	A	49	ARG	2.1
1	E	60	VAL	2.1
1	E	18	ASN	2.1
1	A	130	ILE	2.1
1	A	63	LYS	2.1
1	B	96	ASP	2.1
1	A	212	TRP	2.1
1	B	59	GLY	2.1
1	C	14	PRO	2.1
1	A	124	THR	2.1
1	B	165	THR	2.1
1	E	136	THR	2.1
1	E	222	ALA	2.1
1	B	277	TYR	2.1
1	D	152	ASP	2.1
1	E	183	LEU	2.1
1	A	55	PRO	2.1
1	B	149	GLY	2.1
1	D	221	GLU	2.1
1	B	42	LEU	2.1
1	B	145	LEU	2.1
1	C	141	LEU	2.1
1	C	136	THR	2.0
1	D	49	ARG	2.0
1	E	177	ASP	2.0
1	A	186	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	244	ASN	2.0
1	C	55	PRO	2.0
1	E	220	TYR	2.0
1	E	137	ARG	2.0
1	D	285	ALA	2.0
1	D	141	LEU	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	BR	C	1317	1/1	0.90	0.29	171,171,171,171	0

6.5 Other polymers [i](#)

There are no such residues in this entry.