



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 09:07 PM UTC

PDB ID : 2XQ6 / pdb_00002xq6
Title : Pentameric ligand gated ion channel GLIC in complex with cesium ion (Cs+)
Authors : Hilf, R.J.C.; Bertozzi, C.; Zimmermann, I.; Reiter, A.; Trauner, D.; Dutzler, R.
Deposited on : 2010-09-01
Resolution : 3.70 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

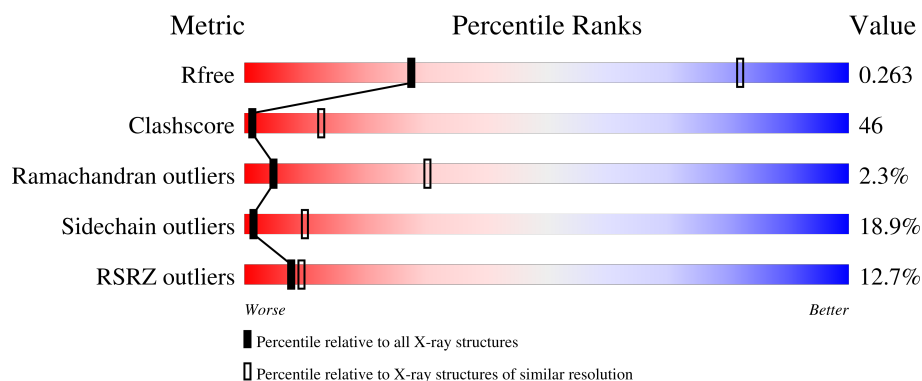
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)

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	13% 31% 54% 12% ..
1	B	317	13% 31% 50% 16% ..
1	C	317	10% 32% 51% 14% ..
1	D	317	13% 30% 53% 15% ..
1	E	317	13% 31% 52% 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.

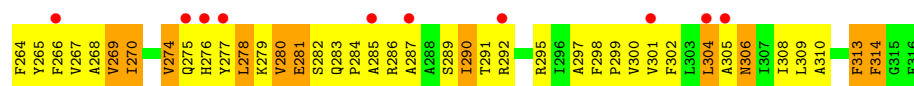
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called GLR4197 PROTEIN.

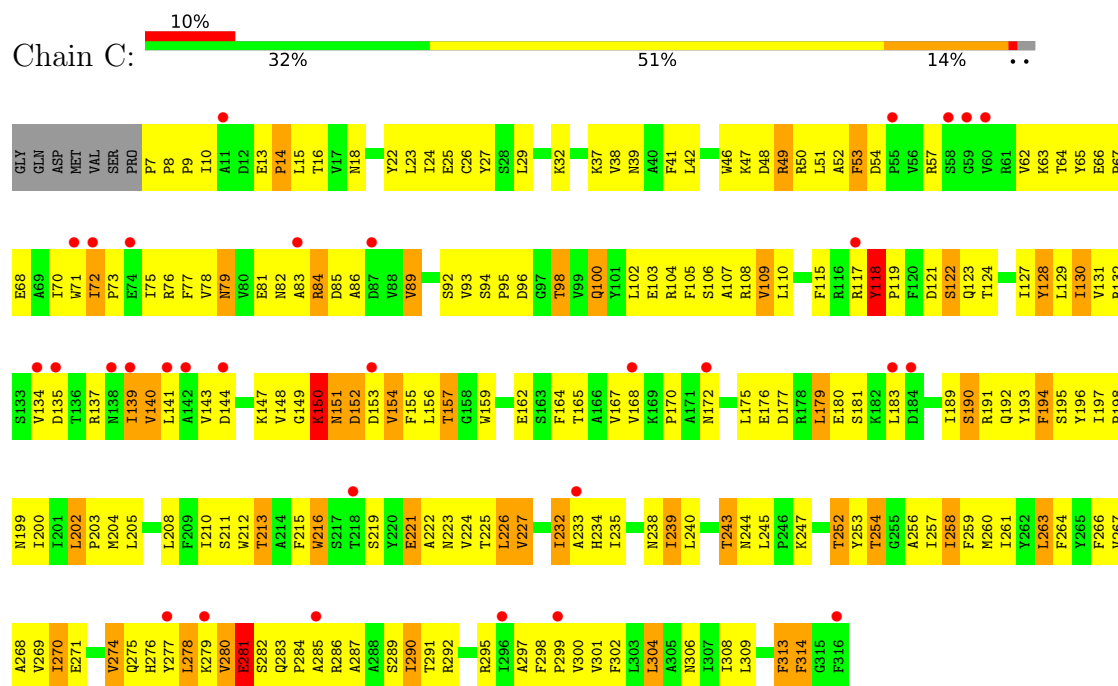
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2521	1662	403	452	4			
1	B	310	Total	C	N	O	S	0	0	0
			2521	1662	403	452	4			
1	C	310	Total	C	N	O	S	0	0	0
			2521	1662	403	452	4			
1	D	310	Total	C	N	O	S	0	0	0
			2521	1662	403	452	4			
1	E	310	Total	C	N	O	S	0	0	0
			2521	1662	403	452	4			

- Molecule 2 is CESIUM ION (CCD ID: CS) (formula: Cs).

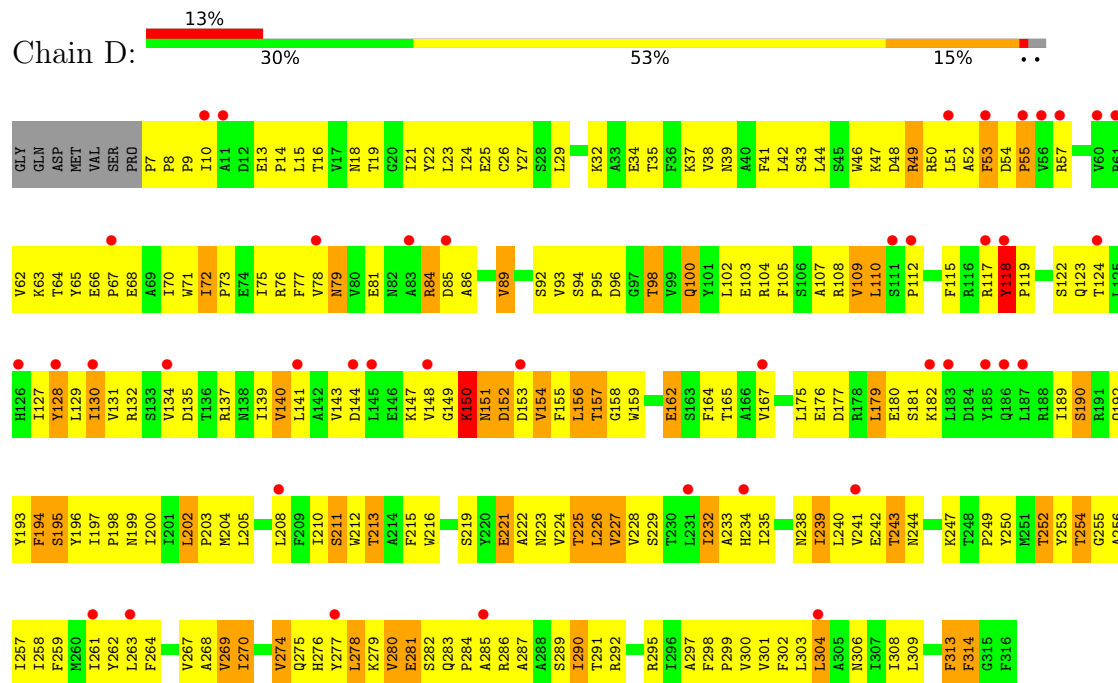
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total	Cs	0	0
			1	1		



• Molecule 1: GLR4197 PROTEIN

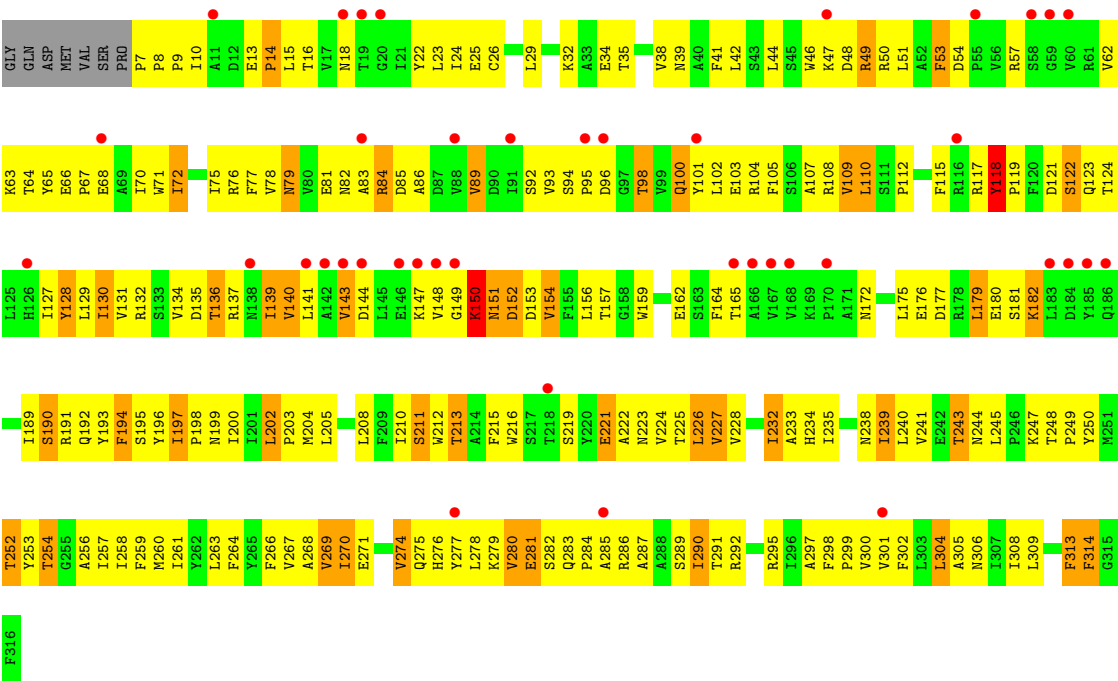


• Molecule 1: GLR4197 PROTEIN



• 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)	39.87 – 3.70 39.87 – 3.70	Depositor EDS
% Data completeness (in resolution range)	97.6 (39.87-3.70) 97.5 (39.87-3.70)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 3.66Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.246 , 0.258 0.252 , 0.263	Depositor DCC
R_{free} test set	2018 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	108.1	Xtriage
Anisotropy	0.329	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 110.5	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)	135.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% 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: CS

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	0.64	0/2589	1.09	17/3535 (0.5%)
1	B	0.68	1/2589 (0.0%)	1.11	22/3535 (0.6%)
1	C	0.66	0/2589	1.09	16/3535 (0.5%)
1	D	0.67	1/2589 (0.0%)	1.10	18/3535 (0.5%)
1	E	0.70	1/2589 (0.0%)	1.10	17/3535 (0.5%)
All	All	0.67	3/12945 (0.0%)	1.10	90/17675 (0.5%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	143	VAL	CA-CB	5.75	1.60	1.53
1	D	55	PRO	C-N	-5.38	1.27	1.33
1	B	143	VAL	CA-CB	5.18	1.59	1.53

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	281	GLU	N-CA-C	-9.42	94.84	109.25
1	D	281	GLU	N-CA-C	-9.42	94.84	109.25
1	A	281	GLU	N-CA-C	-9.41	94.84	109.25
1	E	281	GLU	N-CA-C	-9.40	94.86	109.25
1	C	280	VAL	N-CA-C	-9.10	103.03	111.67
1	A	128	TYR	N-CA-C	8.72	123.81	112.12
1	B	128	TYR	N-CA-C	8.72	123.80	112.12
1	D	128	TYR	N-CA-C	8.71	123.80	112.12
1	C	128	TYR	N-CA-C	8.71	123.78	112.12
1	E	128	TYR	N-CA-C	8.70	123.78	112.12
1	B	280	VAL	N-CA-C	-7.38	105.58	112.96
1	A	280	VAL	N-CA-C	-7.35	105.61	112.96
1	E	280	VAL	N-CA-C	-7.35	105.61	112.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	280	VAL	N-CA-C	-7.33	105.63	112.96
1	B	7	PRO	CA-C-N	7.22	124.86	119.66
1	B	7	PRO	C-N-CA	7.22	124.86	119.66
1	C	281	GLU	N-CA-C	-6.99	99.54	109.96
1	E	7	PRO	CA-C-N	6.90	124.63	119.66
1	E	7	PRO	C-N-CA	6.90	124.63	119.66
1	A	53	PHE	N-CA-C	6.89	120.51	109.83
1	C	7	PRO	CA-C-N	6.71	124.49	119.66
1	C	7	PRO	C-N-CA	6.71	124.49	119.66
1	D	118	TYR	CA-C-N	-6.69	112.80	119.56
1	D	118	TYR	C-N-CA	-6.69	112.80	119.56
1	D	7	PRO	CA-C-N	6.68	124.47	119.66
1	D	7	PRO	C-N-CA	6.68	124.47	119.66
1	B	118	TYR	CA-C-N	-6.66	112.83	119.56
1	B	118	TYR	C-N-CA	-6.66	112.83	119.56
1	C	118	TYR	CA-C-N	-6.66	112.84	119.56
1	C	118	TYR	C-N-CA	-6.66	112.84	119.56
1	A	118	TYR	CA-C-N	-6.63	112.86	119.56
1	A	118	TYR	C-N-CA	-6.63	112.86	119.56
1	E	118	TYR	CA-C-N	-6.63	112.87	119.56
1	E	118	TYR	C-N-CA	-6.63	112.87	119.56
1	B	152	ASP	N-CA-C	-6.33	106.26	112.97
1	E	245	LEU	CA-C-N	6.30	126.25	120.21
1	E	245	LEU	C-N-CA	6.30	126.25	120.21
1	E	152	ASP	N-CA-C	-6.29	106.31	112.97
1	A	7	PRO	CA-C-N	6.22	124.14	119.66
1	A	7	PRO	C-N-CA	6.22	124.14	119.66
1	D	167	VAL	CB-CA-C	-6.19	105.24	111.80
1	D	135	ASP	N-CA-CB	-6.16	102.16	111.15
1	B	135	ASP	N-CA-CB	-6.15	102.17	111.15
1	A	135	ASP	N-CA-CB	-6.13	102.20	111.15
1	C	245	LEU	CA-C-N	6.05	126.02	120.21
1	C	245	LEU	C-N-CA	6.05	126.02	120.21
1	D	152	ASP	N-CA-C	-6.02	106.59	112.97
1	E	279	LYS	N-CA-C	-6.00	105.28	114.16
1	D	21	ILE	N-CA-C	5.97	116.47	107.75
1	B	279	LYS	N-CA-C	-5.97	105.32	114.16
1	D	279	LYS	N-CA-C	-5.97	105.32	114.16
1	A	279	LYS	N-CA-C	-5.97	105.33	114.16
1	C	279	LYS	N-CA-C	-5.96	105.34	114.16
1	B	150	LYS	N-CA-C	-5.95	98.13	110.80
1	E	150	LYS	N-CA-C	-5.93	98.16	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	150	LYS	N-CA-C	-5.93	98.18	110.80
1	A	150	LYS	N-CA-C	-5.92	98.18	110.80
1	D	150	LYS	N-CA-C	-5.92	98.19	110.80
1	B	224	VAL	N-CA-C	-5.87	106.09	111.67
1	C	8	PRO	N-CA-C	5.77	116.75	110.58
1	B	134	VAL	CB-CA-C	5.68	120.60	111.29
1	D	134	VAL	CB-CA-C	5.65	120.56	111.29
1	A	134	VAL	CB-CA-C	5.64	120.55	111.29
1	C	134	VAL	CB-CA-C	5.64	120.55	111.29
1	E	134	VAL	CB-CA-C	5.63	120.52	111.29
1	E	135	ASP	N-CA-CB	-5.57	102.20	111.06
1	A	152	ASP	N-CA-C	-5.57	107.07	112.97
1	C	135	ASP	N-CA-CB	-5.56	102.22	111.06
1	D	195	SER	N-CA-C	-5.54	106.22	112.87
1	B	167	VAL	CB-CA-C	-5.54	105.93	111.80
1	B	265	TYR	N-CA-C	-5.50	106.70	113.41
1	D	8	PRO	N-CA-C	5.46	116.42	110.58
1	B	21	ILE	N-CA-C	5.45	115.84	107.77
1	B	220	TYR	N-CA-C	-5.44	105.00	111.69
1	A	8	PRO	N-CA-C	5.40	116.36	110.58
1	E	136	THR	N-CA-C	-5.37	101.53	110.17
1	B	245	LEU	CA-C-N	5.26	125.26	120.21
1	B	245	LEU	C-N-CA	5.26	125.26	120.21
1	C	152	ASP	N-CA-C	-5.22	107.44	112.97
1	B	195	SER	N-CA-C	-5.15	106.69	112.87
1	C	85	ASP	N-CA-C	5.13	116.40	109.11
1	B	85	ASP	N-CA-C	5.13	116.40	109.11
1	A	85	ASP	N-CA-C	5.12	116.39	109.11
1	E	85	ASP	N-CA-C	5.12	116.38	109.11
1	B	136	THR	N-CA-C	-5.10	101.40	109.76
1	D	85	ASP	N-CA-C	5.10	116.35	109.11
1	D	52	ALA	N-CA-C	-5.08	103.44	110.35
1	A	21	ILE	N-CA-C	5.07	115.16	107.75
1	A	166	ALA	N-CA-C	5.03	116.06	108.46
1	E	8	PRO	N-CA-C	5.01	115.94	110.58

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	261	0
1	B	2521	0	2537	256	0
1	C	2521	0	2537	240	0
1	D	2521	0	2537	274	0
1	E	2521	0	2537	251	0
2	C	1	0	0	0	0
All	All	12606	0	12685	1176	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 46.

All (1176) 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:76:ARG:NH2	1:B:130:ILE:HD12	1.71	1.06
1:B:76:ARG:HH22	1:B:130:ILE:HD12	1.16	1.05
1:E:76:ARG:HH22	1:E:130:ILE:HD12	1.22	1.04
1:D:210:ILE:HG23	1:E:269:VAL:HG11	1.41	1.02
1:E:76:ARG:NH2	1:E:130:ILE:HD12	1.79	0.97
1:D:76:ARG:HH22	1:D:130:ILE:HD12	1.26	0.97
1:C:76:ARG:HH22	1:C:130:ILE:HD12	1.30	0.95
1:C:76:ARG:NH2	1:C:130:ILE:HD12	1.83	0.94
1:B:78:VAL:HG22	1:B:130:ILE:HG12	1.48	0.93
1:D:76:ARG:NH2	1:D:130:ILE:HD12	1.83	0.93
1:A:240:LEU:HD13	1:B:239:ILE:HG12	1.50	0.92
1:A:76:ARG:HH22	1:A:130:ILE:HD12	1.32	0.92
1:C:22:TYR:CD1	1:C:149:GLY:HA2	2.04	0.92
1:B:22:TYR:CD1	1:B:149:GLY:HA2	2.05	0.92
1:E:89:VAL:HG11	1:E:102:LEU:HD23	1.52	0.92
1:A:155:PHE:CE1	1:B:112:PRO:HB3	2.04	0.91
1:A:76:ARG:NH2	1:A:130:ILE:HD12	1.84	0.91
1:A:89:VAL:HG11	1:A:102:LEU:HD23	1.51	0.91
1:A:221:GLU:HB3	1:B:221:GLU:HG2	1.50	0.91
1:C:22:TYR:HA	1:C:149:GLY:HA3	1.51	0.91
1:B:89:VAL:HG11	1:B:102:LEU:HD23	1.51	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:ILE:HG23	1:B:269:VAL:HG11	1.51	0.90
1:E:78:VAL:HG22	1:E:130:ILE:HG12	1.53	0.90
1:B:22:TYR:HA	1:B:149:GLY:HA3	1.54	0.89
1:A:24:ILE:HD13	1:A:104:ARG:HE	1.38	0.89
1:D:22:TYR:CD1	1:D:149:GLY:HA2	2.06	0.89
1:D:89:VAL:HG11	1:D:102:LEU:HD23	1.52	0.89
1:A:27:TYR:CB	1:B:110:LEU:HD11	2.03	0.89
1:A:155:PHE:CZ	1:B:112:PRO:HB3	2.08	0.88
1:D:78:VAL:HG22	1:D:130:ILE:HG12	1.56	0.88
1:D:253:TYR:HD1	1:D:313:PHE:HD2	1.17	0.88
1:A:253:TYR:HD1	1:A:313:PHE:HD2	1.20	0.88
1:C:89:VAL:HG11	1:C:102:LEU:HD23	1.56	0.87
1:A:22:TYR:HA	1:A:149:GLY:HA3	1.54	0.87
1:D:22:TYR:HA	1:D:149:GLY:HA3	1.53	0.87
1:E:22:TYR:CD1	1:E:149:GLY:HA2	2.09	0.87
1:A:22:TYR:CD1	1:A:149:GLY:HA2	2.09	0.87
1:D:253:TYR:HA	1:D:313:PHE:CE2	2.10	0.87
1:D:253:TYR:HA	1:D:313:PHE:HE2	1.40	0.86
1:C:78:VAL:HG22	1:C:130:ILE:HG12	1.56	0.86
1:D:24:ILE:HD13	1:D:104:ARG:HE	1.38	0.86
1:A:78:VAL:HG22	1:A:130:ILE:HG12	1.56	0.86
1:B:253:TYR:HD1	1:B:313:PHE:HD2	1.23	0.85
1:A:253:TYR:HA	1:A:313:PHE:HE2	1.40	0.85
1:C:253:TYR:HD1	1:C:313:PHE:HD2	1.24	0.85
1:E:253:TYR:HA	1:E:313:PHE:CE2	2.12	0.85
1:D:155:PHE:CE1	1:E:112:PRO:HB3	2.10	0.85
1:A:253:TYR:HA	1:A:313:PHE:CE2	2.11	0.84
1:A:104:ARG:HH22	1:B:78:VAL:HA	1.41	0.84
1:A:222:ALA:HB2	1:B:221:GLU:HA	1.58	0.84
1:C:27:TYR:HB3	1:D:110:LEU:HD11	1.58	0.84
1:C:200:ILE:HD11	1:C:240:LEU:HD23	1.61	0.83
1:B:24:ILE:HD13	1:B:104:ARG:HE	1.44	0.83
1:C:199:ASN:HB3	1:D:242:GLU:CD	2.04	0.83
1:C:253:TYR:HA	1:C:313:PHE:CE2	2.12	0.83
1:B:253:TYR:HA	1:B:313:PHE:HE2	1.44	0.83
1:E:22:TYR:HA	1:E:149:GLY:HA3	1.59	0.83
1:B:253:TYR:HA	1:B:313:PHE:CE2	2.14	0.82
1:C:253:TYR:HA	1:C:313:PHE:HE2	1.42	0.82
1:E:253:TYR:HD1	1:E:313:PHE:HD2	1.23	0.82
1:E:253:TYR:HA	1:E:313:PHE:HE2	1.43	0.82
1:D:221:GLU:OE2	1:E:221:GLU:CD	2.23	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:210:ILE:CG2	1:E:269:VAL:HG11	2.11	0.81
1:C:24:ILE:HD13	1:C:104:ARG:HE	1.46	0.80
1:D:257:ILE:HG22	1:D:309:LEU:HD23	1.65	0.79
1:E:200:ILE:HD11	1:E:240:LEU:HD23	1.65	0.79
1:B:47:LYS:HD3	1:B:49:ARG:HH21	1.48	0.79
1:E:47:LYS:HD3	1:E:49:ARG:HH21	1.48	0.79
1:E:24:ILE:HD13	1:E:104:ARG:HE	1.47	0.79
1:A:104:ARG:NH2	1:B:78:VAL:HA	1.97	0.79
1:E:238:ASN:HA	1:E:258:ILE:HD11	1.63	0.79
1:A:257:ILE:HG22	1:A:309:LEU:HD23	1.65	0.78
1:B:257:ILE:HG22	1:B:309:LEU:HD23	1.66	0.78
1:D:238:ASN:HA	1:D:258:ILE:HD11	1.66	0.78
1:B:47:LYS:CD	1:B:49:ARG:HH21	1.97	0.78
1:B:238:ASN:HA	1:B:258:ILE:HD11	1.65	0.78
1:E:238:ASN:HA	1:E:258:ILE:CD1	2.13	0.77
1:A:27:TYR:HB3	1:B:110:LEU:HD11	1.67	0.77
1:A:202:LEU:HD12	1:B:259:PHE:CZ	2.20	0.77
1:C:65:TYR:CG	1:C:70:ILE:HD11	2.20	0.76
1:A:62:VAL:HG11	1:A:92:SER:HB3	1.68	0.76
1:E:47:LYS:CD	1:E:49:ARG:HH21	1.99	0.76
1:C:257:ILE:HG22	1:C:309:LEU:HD23	1.66	0.76
1:D:147:LYS:O	1:D:147:LYS:HG2	1.86	0.76
1:A:147:LYS:O	1:A:147:LYS:HG2	1.86	0.76
1:D:215:PHE:HB2	1:D:216:TRP:CZ3	2.21	0.76
1:E:257:ILE:HG22	1:E:309:LEU:HD23	1.67	0.76
1:A:47:LYS:HD3	1:A:49:ARG:HH21	1.50	0.76
1:C:215:PHE:HB2	1:C:216:TRP:CZ3	2.20	0.76
1:D:253:TYR:CD1	1:D:313:PHE:HD2	2.03	0.76
1:A:226:LEU:HD23	1:B:224:VAL:HB	1.67	0.75
1:D:225:THR:HG21	1:E:224:VAL:HG23	1.68	0.75
1:E:147:LYS:O	1:E:147:LYS:HG2	1.86	0.75
1:A:27:TYR:CG	1:B:110:LEU:HD11	2.22	0.75
1:C:147:LYS:HG2	1:C:147:LYS:O	1.86	0.75
1:C:222:ALA:HB2	1:D:221:GLU:HA	1.68	0.75
1:B:215:PHE:HB2	1:B:216:TRP:CZ3	2.22	0.74
1:B:65:TYR:CG	1:B:70:ILE:HD11	2.23	0.74
1:A:47:LYS:CD	1:A:49:ARG:HH21	2.00	0.74
1:D:65:TYR:CG	1:D:70:ILE:HD11	2.23	0.74
1:E:65:TYR:CG	1:E:70:ILE:HD11	2.22	0.74
1:D:47:LYS:HD3	1:D:49:ARG:HH21	1.50	0.74
1:C:23:LEU:HG	1:C:164:PHE:CE1	2.23	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:LYS:HD3	1:B:49:ARG:NH2	2.03	0.74
1:D:240:LEU:HD13	1:E:239:ILE:HG12	1.70	0.74
1:C:215:PHE:HB2	1:C:216:TRP:CE3	2.22	0.73
1:E:47:LYS:HD3	1:E:49:ARG:NH2	2.03	0.73
1:B:147:LYS:O	1:B:147:LYS:HG2	1.86	0.73
1:A:65:TYR:CG	1:A:70:ILE:HD11	2.23	0.73
1:B:238:ASN:HA	1:B:258:ILE:CD1	2.19	0.73
1:C:149:GLY:O	1:C:164:PHE:HD1	1.71	0.73
1:E:15:LEU:HD11	1:E:46:TRP:HB2	1.71	0.73
1:A:149:GLY:O	1:A:164:PHE:HD1	1.71	0.73
1:C:238:ASN:HA	1:C:258:ILE:CD1	2.19	0.73
1:E:215:PHE:HB2	1:E:216:TRP:CZ3	2.24	0.73
1:C:234:HIS:CE1	1:C:261:ILE:HG21	2.23	0.73
1:D:215:PHE:HB2	1:D:216:TRP:CE3	2.24	0.73
1:B:15:LEU:HD11	1:B:46:TRP:HB2	1.71	0.73
1:B:89:VAL:CG1	1:B:102:LEU:HD23	2.19	0.73
1:B:257:ILE:O	1:B:261:ILE:HG12	1.88	0.73
1:B:200:ILE:O	1:B:204:MET:HB2	1.88	0.72
1:E:150:LYS:HG3	1:E:154:VAL:HG21	1.71	0.72
1:B:215:PHE:HB2	1:B:216:TRP:CE3	2.24	0.72
1:B:235:ILE:HG22	1:B:239:ILE:HD12	1.71	0.72
1:A:215:PHE:HB2	1:A:216:TRP:CZ3	2.24	0.72
1:A:253:TYR:CD1	1:A:313:PHE:HD2	2.05	0.72
1:C:47:LYS:HD3	1:C:49:ARG:HH21	1.54	0.72
1:C:150:LYS:HG3	1:C:154:VAL:HG21	1.71	0.72
1:A:200:ILE:O	1:A:204:MET:HB2	1.89	0.72
1:C:238:ASN:HA	1:C:258:ILE:HD11	1.70	0.72
1:E:23:LEU:HG	1:E:164:PHE:CE1	2.25	0.72
1:A:215:PHE:HB2	1:A:216:TRP:CE3	2.25	0.72
1:D:200:ILE:HD11	1:D:240:LEU:HD23	1.71	0.72
1:B:253:TYR:CD1	1:B:313:PHE:HD2	2.08	0.72
1:A:229:SER:HB3	1:B:228:VAL:CG1	2.19	0.72
1:A:150:LYS:HG3	1:A:154:VAL:HG21	1.71	0.72
1:E:253:TYR:CD1	1:E:313:PHE:HD2	2.07	0.72
1:E:200:ILE:O	1:E:204:MET:HB2	1.90	0.71
1:E:283:GLN:N	1:E:284:PRO:HD3	2.05	0.71
1:C:47:LYS:CD	1:C:49:ARG:HH21	2.02	0.71
1:D:229:SER:HB3	1:E:228:VAL:HG11	1.71	0.71
1:D:257:ILE:O	1:D:261:ILE:HG12	1.89	0.71
1:E:149:GLY:O	1:E:164:PHE:HD1	1.73	0.71
1:E:235:ILE:HG22	1:E:239:ILE:HD12	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:47:LYS:CD	1:D:49:ARG:HH21	2.02	0.71
1:E:18:ASN:HB3	1:E:143:VAL:HG23	1.72	0.71
1:A:200:ILE:HD11	1:A:240:LEU:HD23	1.72	0.71
1:D:89:VAL:CG1	1:D:102:LEU:HD23	2.20	0.71
1:E:215:PHE:HB2	1:E:216:TRP:CE3	2.25	0.71
1:B:283:GLN:N	1:B:284:PRO:HD3	2.06	0.71
1:D:229:SER:CB	1:E:228:VAL:HG11	2.21	0.71
1:E:264:PHE:HE2	1:E:302:PHE:HB2	1.56	0.71
1:D:238:ASN:HA	1:D:258:ILE:CD1	2.20	0.71
1:A:147:LYS:C	1:A:149:GLY:H	1.99	0.70
1:A:157:THR:CG2	1:B:34:GLU:OE1	2.39	0.70
1:A:47:LYS:HD3	1:A:49:ARG:NH2	2.06	0.70
1:B:150:LYS:HG3	1:B:154:VAL:HG21	1.71	0.70
1:D:18:ASN:HB3	1:D:143:VAL:HG23	1.73	0.70
1:B:200:ILE:HD11	1:B:240:LEU:HD23	1.71	0.70
1:B:264:PHE:HE2	1:B:302:PHE:HB2	1.56	0.70
1:A:238:ASN:HA	1:A:258:ILE:HD11	1.72	0.70
1:C:18:ASN:HB3	1:C:143:VAL:HG23	1.73	0.70
1:D:47:LYS:HD3	1:D:49:ARG:NH2	2.06	0.70
1:D:150:LYS:HG3	1:D:154:VAL:HG21	1.71	0.70
1:A:283:GLN:N	1:A:284:PRO:HD3	2.06	0.70
1:D:155:PHE:CZ	1:E:112:PRO:HB3	2.26	0.70
1:D:253:TYR:HD1	1:D:313:PHE:CD2	2.06	0.70
1:A:192:GLN:CD	1:B:249:PRO:HB3	2.16	0.70
1:C:283:GLN:N	1:C:284:PRO:HD3	2.06	0.70
1:D:276:HIS:O	1:D:280:VAL:HG22	1.92	0.70
1:E:257:ILE:O	1:E:261:ILE:HG12	1.91	0.70
1:B:76:ARG:HH22	1:B:130:ILE:CD1	2.01	0.70
1:A:276:HIS:O	1:A:280:VAL:HG22	1.92	0.70
1:C:200:ILE:O	1:C:204:MET:HB2	1.92	0.70
1:C:147:LYS:C	1:C:149:GLY:H	1.99	0.69
1:D:77:PHE:CD1	1:D:84:ARG:HD2	2.27	0.69
1:D:192:GLN:CD	1:E:249:PRO:HB3	2.17	0.69
1:D:283:GLN:N	1:D:284:PRO:HD3	2.06	0.69
1:E:147:LYS:C	1:E:149:GLY:H	1.99	0.69
1:A:202:LEU:HD12	1:B:259:PHE:HZ	1.57	0.69
1:A:18:ASN:HB3	1:A:143:VAL:HG23	1.74	0.69
1:E:53:PHE:HE2	1:E:63:LYS:HB3	1.57	0.69
1:E:276:HIS:O	1:E:280:VAL:HG22	1.92	0.69
1:A:77:PHE:CD1	1:A:84:ARG:HD2	2.27	0.69
1:B:147:LYS:C	1:B:149:GLY:H	1.99	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:225:THR:CG2	1:E:224:VAL:HG23	2.22	0.69
1:A:257:ILE:O	1:A:261:ILE:HG12	1.92	0.69
1:A:89:VAL:CG1	1:A:102:LEU:HD23	2.22	0.69
1:C:253:TYR:CD1	1:C:313:PHE:HD2	2.08	0.69
1:D:54:ASP:HB2	1:D:57:ARG:HG3	1.73	0.69
1:D:149:GLY:O	1:D:164:PHE:HD1	1.75	0.69
1:A:238:ASN:HA	1:A:258:ILE:CD1	2.23	0.69
1:A:23:LEU:HG	1:A:164:PHE:CE1	2.28	0.68
1:B:18:ASN:HB3	1:B:143:VAL:HG23	1.75	0.68
1:B:276:HIS:O	1:B:280:VAL:HG22	1.92	0.68
1:C:276:HIS:O	1:C:280:VAL:HG22	1.92	0.68
1:A:229:SER:CB	1:B:228:VAL:HG11	2.24	0.68
1:C:89:VAL:CG1	1:C:102:LEU:HD23	2.23	0.68
1:D:81:GLU:HG3	1:D:108:ARG:HG3	1.76	0.68
1:C:267:VAL:HG23	1:C:298:PHE:CZ	2.29	0.68
1:C:15:LEU:HD11	1:C:46:TRP:HB2	1.76	0.68
1:E:89:VAL:CG1	1:E:102:LEU:HD23	2.22	0.68
1:D:23:LEU:HG	1:D:164:PHE:CE1	2.28	0.68
1:C:47:LYS:HD3	1:C:49:ARG:NH2	2.09	0.68
1:D:15:LEU:HD11	1:D:46:TRP:HB2	1.76	0.68
1:B:264:PHE:CE2	1:B:302:PHE:HB2	2.28	0.68
1:C:264:PHE:HE2	1:C:302:PHE:HB2	1.58	0.68
1:D:200:ILE:O	1:D:204:MET:HB2	1.94	0.68
1:D:264:PHE:HE2	1:D:302:PHE:HB2	1.59	0.68
1:C:257:ILE:O	1:C:261:ILE:HG12	1.94	0.68
1:C:200:ILE:CD1	1:C:240:LEU:HD23	2.24	0.67
1:B:23:LEU:HG	1:B:164:PHE:CE1	2.28	0.67
1:A:67:PRO:O	1:A:72:ILE:HD11	1.95	0.67
1:D:147:LYS:C	1:D:149:GLY:H	1.99	0.67
1:B:81:GLU:HG3	1:B:108:ARG:HG3	1.76	0.67
1:B:149:GLY:O	1:B:164:PHE:HD1	1.77	0.67
1:A:15:LEU:HD11	1:A:46:TRP:HB2	1.75	0.67
1:D:132:ARG:HA	1:D:180:GLU:HG2	1.77	0.67
1:E:234:HIS:CE1	1:E:261:ILE:HG21	2.30	0.67
1:E:81:GLU:HG3	1:E:108:ARG:HG3	1.77	0.67
1:B:53:PHE:HE2	1:B:63:LYS:HB3	1.58	0.67
1:E:62:VAL:HG11	1:E:92:SER:HB3	1.77	0.67
1:E:264:PHE:CE2	1:E:302:PHE:HB2	2.30	0.67
1:C:27:TYR:CB	1:D:110:LEU:HD11	2.25	0.66
1:D:53:PHE:HE2	1:D:63:LYS:HB3	1.60	0.66
1:C:62:VAL:HG11	1:C:92:SER:HB3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:267:VAL:HA	1:E:270:ILE:HB	1.77	0.66
1:C:132:ARG:HA	1:C:180:GLU:HG2	1.77	0.66
1:D:264:PHE:CE2	1:D:302:PHE:HB2	2.31	0.66
1:A:132:ARG:HA	1:A:180:GLU:HG2	1.76	0.66
1:A:235:ILE:HG22	1:A:239:ILE:HD12	1.78	0.66
1:D:104:ARG:HH22	1:E:78:VAL:HA	1.60	0.66
1:E:304:LEU:O	1:E:308:ILE:HG12	1.96	0.66
1:A:81:GLU:HG3	1:A:108:ARG:HG3	1.77	0.65
1:E:253:TYR:HD1	1:E:313:PHE:CD2	2.10	0.65
1:A:119:PRO:HB3	1:A:196:TYR:HD2	1.61	0.65
1:B:194:PHE:C	1:B:196:TYR:H	2.03	0.65
1:A:42:LEU:HB3	1:A:103:GLU:HG3	1.79	0.65
1:A:253:TYR:HD1	1:A:313:PHE:CD2	2.08	0.65
1:C:54:ASP:HB2	1:C:57:ARG:HG3	1.78	0.65
1:C:264:PHE:CE2	1:C:302:PHE:HB2	2.32	0.65
1:D:67:PRO:O	1:D:72:ILE:HD11	1.96	0.65
1:C:67:PRO:O	1:C:72:ILE:HD11	1.97	0.65
1:D:62:VAL:HG11	1:D:92:SER:HB3	1.79	0.65
1:C:297:ALA:O	1:C:301:VAL:HG23	1.95	0.65
1:C:77:PHE:CD1	1:C:84:ARG:HD2	2.32	0.65
1:D:297:ALA:O	1:D:301:VAL:HG23	1.97	0.65
1:E:54:ASP:HB2	1:E:57:ARG:HG3	1.78	0.65
1:B:62:VAL:HG11	1:B:92:SER:HB3	1.78	0.65
1:B:267:VAL:HA	1:B:270:ILE:HB	1.79	0.65
1:D:192:GLN:OE1	1:E:249:PRO:HB3	1.97	0.65
1:D:235:ILE:HG22	1:D:239:ILE:HD12	1.78	0.65
1:B:77:PHE:CD1	1:B:84:ARG:HD2	2.31	0.65
1:C:53:PHE:HE2	1:C:63:LYS:HB3	1.59	0.65
1:D:194:PHE:C	1:D:196:TYR:N	2.54	0.65
1:D:119:PRO:HB3	1:D:196:TYR:HD2	1.61	0.65
1:A:159:TRP:CE3	1:A:189:ILE:HD12	2.32	0.64
1:E:77:PHE:CD1	1:E:84:ARG:HD2	2.32	0.64
1:B:304:LEU:O	1:B:308:ILE:HG12	1.97	0.64
1:B:42:LEU:HB3	1:B:103:GLU:HG3	1.78	0.64
1:A:131:VAL:HG11	1:A:140:VAL:HG13	1.80	0.64
1:B:67:PRO:O	1:B:72:ILE:HD11	1.98	0.64
1:B:253:TYR:HD1	1:B:313:PHE:CD2	2.11	0.64
1:A:54:ASP:HB2	1:A:57:ARG:HG3	1.78	0.64
1:A:96:ASP:OD1	1:A:98:THR:HB	1.98	0.64
1:B:54:ASP:HB2	1:B:57:ARG:HG3	1.78	0.64
1:E:224:VAL:C	1:E:226:LEU:H	2.05	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:67:PRO:O	1:E:72:ILE:HD11	1.97	0.64
1:A:297:ALA:O	1:A:301:VAL:HG23	1.98	0.64
1:C:23:LEU:HD22	1:C:38:VAL:HG21	1.79	0.64
1:B:254:THR:O	1:B:258:ILE:HB	1.97	0.64
1:C:194:PHE:C	1:C:196:TYR:N	2.54	0.64
1:C:194:PHE:C	1:C:196:TYR:H	2.03	0.64
1:A:219:SER:OG	1:A:222:ALA:HB3	1.98	0.64
1:B:297:ALA:O	1:B:301:VAL:HG23	1.98	0.64
1:C:131:VAL:HG11	1:C:140:VAL:HG13	1.78	0.64
1:E:200:ILE:CD1	1:E:240:LEU:HD23	2.27	0.64
1:A:157:THR:HG21	1:B:34:GLU:OE1	1.98	0.63
1:B:131:VAL:HG11	1:B:140:VAL:HG13	1.80	0.63
1:D:194:PHE:C	1:D:196:TYR:H	2.04	0.63
1:A:264:PHE:HE2	1:A:302:PHE:HB2	1.62	0.63
1:D:229:SER:HB3	1:E:228:VAL:CG1	2.29	0.63
1:B:215:PHE:HZ	1:B:298:PHE:CE1	2.17	0.63
1:B:224:VAL:C	1:B:226:LEU:H	2.06	0.63
1:C:213:THR:HG22	1:C:226:LEU:CD1	2.28	0.63
1:D:77:PHE:H	1:D:84:ARG:HD3	1.63	0.63
1:A:53:PHE:HE2	1:A:63:LYS:HB3	1.62	0.63
1:A:240:LEU:CD1	1:B:239:ILE:HG12	2.25	0.63
1:E:194:PHE:C	1:E:196:TYR:H	2.06	0.63
1:E:215:PHE:HZ	1:E:298:PHE:CE1	2.17	0.63
1:C:215:PHE:HZ	1:C:298:PHE:CE1	2.17	0.63
1:C:81:GLU:HG3	1:C:108:ARG:HG3	1.79	0.62
1:D:157:THR:HG21	1:E:34:GLU:OE1	1.98	0.62
1:E:297:ALA:O	1:E:301:VAL:HG23	1.98	0.62
1:D:42:LEU:HB3	1:D:103:GLU:HG3	1.80	0.62
1:D:131:VAL:HG11	1:D:140:VAL:HG13	1.81	0.62
1:B:159:TRP:CE3	1:B:189:ILE:HD12	2.34	0.62
1:E:42:LEU:HB3	1:E:103:GLU:HG3	1.81	0.62
1:A:226:LEU:CD2	1:B:224:VAL:HB	2.29	0.62
1:B:224:VAL:C	1:B:226:LEU:N	2.57	0.62
1:C:253:TYR:HD1	1:C:313:PHE:CD2	2.11	0.62
1:D:210:ILE:HG23	1:E:269:VAL:CG1	2.25	0.62
1:A:23:LEU:HD22	1:A:38:VAL:HG21	1.82	0.62
1:C:267:VAL:HA	1:C:270:ILE:HB	1.81	0.62
1:D:304:LEU:O	1:D:308:ILE:HG12	1.99	0.62
1:A:234:HIS:CE1	1:A:261:ILE:HG21	2.34	0.62
1:E:159:TRP:CE3	1:E:189:ILE:HD12	2.35	0.62
1:A:304:LEU:O	1:A:308:ILE:HG12	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:132:ARG:HA	1:E:180:GLU:HG2	1.81	0.62
1:A:224:VAL:C	1:A:226:LEU:H	2.07	0.62
1:E:18:ASN:HB3	1:E:143:VAL:CG2	2.30	0.62
1:E:267:VAL:HG23	1:E:298:PHE:CZ	2.34	0.62
1:A:25:GLU:HB2	1:A:39:ASN:HB3	1.82	0.62
1:D:215:PHE:HZ	1:D:298:PHE:CE1	2.18	0.62
1:A:217:SER:OG	1:B:220:TYR:CE2	2.53	0.62
1:B:13:GLU:HB3	1:B:14:PRO:HD2	1.82	0.62
1:B:119:PRO:O	1:B:193:TYR:HB3	2.00	0.62
1:A:77:PHE:H	1:A:84:ARG:HD3	1.64	0.61
1:C:219:SER:OG	1:C:222:ALA:HB3	2.00	0.61
1:B:18:ASN:HB3	1:B:143:VAL:CG2	2.30	0.61
1:C:42:LEU:HB3	1:C:103:GLU:HG3	1.82	0.61
1:A:18:ASN:HB3	1:A:143:VAL:CG2	2.30	0.61
1:A:194:PHE:C	1:A:196:TYR:N	2.57	0.61
1:B:200:ILE:CD1	1:B:240:LEU:HD23	2.31	0.61
1:E:224:VAL:C	1:E:226:LEU:N	2.58	0.61
1:A:221:GLU:OE2	1:B:221:GLU:CD	2.44	0.61
1:B:65:TYR:CD1	1:B:70:ILE:HD11	2.36	0.61
1:E:25:GLU:HB2	1:E:39:ASN:HB3	1.81	0.61
1:A:13:GLU:HB3	1:A:14:PRO:HD2	1.82	0.61
1:A:194:PHE:C	1:A:196:TYR:H	2.07	0.61
1:A:27:TYR:CG	1:B:110:LEU:CD1	2.83	0.61
1:A:267:VAL:HG23	1:A:298:PHE:CZ	2.36	0.61
1:D:234:HIS:CE1	1:D:261:ILE:HG21	2.36	0.61
1:E:13:GLU:HB3	1:E:14:PRO:HD2	1.82	0.61
1:B:221:GLU:OE2	1:C:221:GLU:CD	2.44	0.61
1:D:23:LEU:HD22	1:D:38:VAL:HG21	1.82	0.61
1:D:79:ASN:OD1	1:D:109:VAL:HG12	2.01	0.61
1:A:264:PHE:CE2	1:A:302:PHE:HB2	2.35	0.60
1:B:119:PRO:HB3	1:B:196:TYR:HD2	1.66	0.60
1:C:119:PRO:HB3	1:C:196:TYR:HD2	1.65	0.60
1:D:22:TYR:HA	1:D:149:GLY:CA	2.29	0.60
1:D:224:VAL:C	1:D:226:LEU:H	2.06	0.60
1:E:194:PHE:C	1:E:196:TYR:N	2.57	0.60
1:B:132:ARG:HA	1:B:180:GLU:HG2	1.82	0.60
1:C:202:LEU:HD12	1:D:259:PHE:CE1	2.35	0.60
1:C:224:VAL:C	1:C:226:LEU:H	2.07	0.60
1:D:65:TYR:CD1	1:D:70:ILE:HD11	2.36	0.60
1:D:157:THR:CG2	1:E:34:GLU:OE1	2.49	0.60
1:D:224:VAL:C	1:D:226:LEU:N	2.58	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:PHE:HZ	1:A:298:PHE:CE1	2.20	0.60
1:B:267:VAL:HG23	1:B:298:PHE:CZ	2.36	0.60
1:C:18:ASN:HB3	1:C:143:VAL:CG2	2.31	0.60
1:E:23:LEU:HD22	1:E:38:VAL:HG21	1.83	0.60
1:B:25:GLU:HB2	1:B:39:ASN:HB3	1.83	0.60
1:C:23:LEU:HD22	1:C:38:VAL:CG2	2.32	0.60
1:E:119:PRO:HB3	1:E:196:TYR:HD2	1.65	0.60
1:E:131:VAL:HG11	1:E:140:VAL:HG13	1.83	0.60
1:B:96:ASP:OD1	1:B:98:THR:HB	2.02	0.60
1:C:215:PHE:HZ	1:C:298:PHE:CD1	2.20	0.60
1:D:119:PRO:O	1:D:193:TYR:HB3	2.01	0.60
1:D:267:VAL:HA	1:D:270:ILE:HB	1.83	0.60
1:E:96:ASP:OD1	1:E:98:THR:HB	2.01	0.60
1:A:119:PRO:HB3	1:A:196:TYR:CD2	2.36	0.60
1:A:267:VAL:HA	1:A:270:ILE:HB	1.83	0.60
1:B:77:PHE:H	1:B:84:ARG:HD3	1.67	0.60
1:A:224:VAL:C	1:A:226:LEU:N	2.56	0.59
1:C:22:TYR:HA	1:C:149:GLY:CA	2.27	0.59
1:D:119:PRO:HB3	1:D:196:TYR:CD2	2.36	0.59
1:A:157:THR:HG22	1:B:34:GLU:OE1	2.02	0.59
1:A:226:LEU:HD22	1:B:228:VAL:HG21	1.85	0.59
1:C:66:GLU:HG3	1:C:67:PRO:HD2	1.84	0.59
1:E:66:GLU:HG3	1:E:67:PRO:HD2	1.84	0.59
1:A:66:GLU:HG3	1:A:67:PRO:HD2	1.84	0.59
1:D:18:ASN:HB3	1:D:143:VAL:CG2	2.31	0.59
1:D:159:TRP:CE3	1:D:189:ILE:HD12	2.38	0.59
1:A:119:PRO:O	1:A:193:TYR:HB3	2.02	0.59
1:E:197:ILE:HB	1:E:198:PRO:HD3	1.84	0.59
1:B:66:GLU:HG3	1:B:67:PRO:HD2	1.84	0.59
1:B:194:PHE:C	1:B:196:TYR:N	2.54	0.59
1:C:65:TYR:CD1	1:C:70:ILE:HD11	2.38	0.59
1:C:86:ALA:HB2	1:C:105:PHE:HB3	1.85	0.59
1:C:77:PHE:H	1:C:84:ARG:HD3	1.68	0.59
1:C:304:LEU:O	1:C:308:ILE:HG12	2.03	0.59
1:D:13:GLU:HB3	1:D:14:PRO:HD2	1.85	0.59
1:D:202:LEU:HD12	1:E:259:PHE:HZ	1.67	0.59
1:B:22:TYR:HA	1:B:149:GLY:CA	2.31	0.59
1:C:25:GLU:HB2	1:C:39:ASN:HB3	1.83	0.59
1:E:65:TYR:CD1	1:E:70:ILE:HD11	2.38	0.59
1:D:66:GLU:HG3	1:D:67:PRO:HD2	1.84	0.58
1:D:254:THR:O	1:D:258:ILE:HB	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:53:PHE:HE2	1:E:63:LYS:CB	2.16	0.58
1:E:213:THR:HG22	1:E:226:LEU:CD1	2.33	0.58
1:B:274:VAL:C	1:B:276:HIS:H	2.12	0.58
1:D:179:LEU:HD12	1:D:179:LEU:C	2.28	0.58
1:A:200:ILE:CD1	1:A:240:LEU:HD23	2.33	0.58
1:C:215:PHE:CZ	1:C:298:PHE:CD1	2.92	0.58
1:B:215:PHE:HZ	1:B:298:PHE:CD1	2.22	0.58
1:C:25:GLU:OE1	1:C:25:GLU:HA	2.02	0.58
1:C:213:THR:HG22	1:C:226:LEU:HD11	1.85	0.58
1:A:65:TYR:CD1	1:A:70:ILE:HD11	2.39	0.58
1:A:210:ILE:CG2	1:B:269:VAL:HG11	2.28	0.58
1:B:274:VAL:O	1:B:278:LEU:HB3	2.03	0.58
1:E:274:VAL:O	1:E:278:LEU:HB3	2.03	0.58
1:C:197:ILE:HB	1:C:198:PRO:HD3	1.86	0.58
1:A:149:GLY:O	1:A:164:PHE:CD1	2.56	0.58
1:C:13:GLU:HB3	1:C:14:PRO:HD2	1.86	0.58
1:C:119:PRO:HB3	1:C:196:TYR:CD2	2.39	0.58
1:C:96:ASP:OD1	1:C:98:THR:HB	2.03	0.58
1:D:210:ILE:HD11	1:E:266:PHE:HD1	1.69	0.58
1:D:215:PHE:HZ	1:D:298:PHE:CD1	2.22	0.58
1:D:267:VAL:HG23	1:D:298:PHE:CZ	2.39	0.58
1:A:53:PHE:HE2	1:A:63:LYS:CB	2.17	0.57
1:E:77:PHE:H	1:E:84:ARG:HD3	1.69	0.57
1:A:104:ARG:HH22	1:B:78:VAL:CA	2.16	0.57
1:A:274:VAL:O	1:A:278:LEU:HB3	2.03	0.57
1:C:53:PHE:HE2	1:C:63:LYS:CB	2.16	0.57
1:C:235:ILE:HG22	1:C:239:ILE:HD12	1.86	0.57
1:D:274:VAL:O	1:D:278:LEU:HB3	2.03	0.57
1:E:219:SER:O	1:E:223:ASN:HB2	2.04	0.57
1:B:76:ARG:HH12	1:B:130:ILE:HD11	1.69	0.57
1:C:119:PRO:O	1:C:193:TYR:HB3	2.03	0.57
1:C:274:VAL:C	1:C:276:HIS:H	2.12	0.57
1:B:23:LEU:HD22	1:B:38:VAL:HG21	1.86	0.57
1:C:226:LEU:CD2	1:D:224:VAL:HB	2.34	0.57
1:C:274:VAL:O	1:C:278:LEU:HB3	2.03	0.57
1:E:254:THR:O	1:E:258:ILE:HB	2.04	0.57
1:B:219:SER:O	1:B:223:ASN:HB2	2.05	0.57
1:B:234:HIS:CE1	1:B:261:ILE:HG21	2.40	0.57
1:C:42:LEU:HD23	1:C:103:GLU:OE1	2.04	0.57
1:D:25:GLU:HB2	1:D:39:ASN:HB3	1.86	0.57
1:E:298:PHE:HB2	1:E:299:PRO:HD3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:LYS:C	1:A:149:GLY:N	2.63	0.57
1:A:213:THR:HG22	1:A:226:LEU:CD1	2.35	0.57
1:A:226:LEU:HD23	1:B:224:VAL:CB	2.35	0.57
1:B:86:ALA:HB2	1:B:105:PHE:HB3	1.86	0.57
1:C:29:LEU:C	1:C:29:LEU:HD23	2.29	0.57
1:C:76:ARG:HH22	1:C:130:ILE:CD1	2.12	0.57
1:C:147:LYS:C	1:C:149:GLY:N	2.63	0.57
1:D:274:VAL:C	1:D:276:HIS:H	2.12	0.57
1:E:147:LYS:C	1:E:149:GLY:N	2.63	0.57
1:B:235:ILE:CG2	1:B:239:ILE:HD12	2.35	0.57
1:C:149:GLY:O	1:C:164:PHE:CD1	2.56	0.57
1:E:274:VAL:C	1:E:276:HIS:H	2.12	0.57
1:A:42:LEU:HD23	1:A:103:GLU:OE1	2.05	0.57
1:A:290:ILE:HG22	1:A:291:THR:N	2.20	0.57
1:E:119:PRO:HB3	1:E:196:TYR:CD2	2.40	0.57
1:A:219:SER:O	1:A:223:ASN:HB2	2.04	0.57
1:B:119:PRO:HB3	1:B:196:TYR:CD2	2.38	0.57
1:A:86:ALA:HB2	1:A:105:PHE:HB3	1.86	0.57
1:B:79:ASN:OD1	1:B:109:VAL:HG12	2.05	0.57
1:E:235:ILE:CG2	1:E:239:ILE:HD12	2.35	0.57
1:B:147:LYS:C	1:B:149:GLY:N	2.63	0.56
1:D:213:THR:HG22	1:D:226:LEU:CD1	2.35	0.56
1:E:119:PRO:O	1:E:193:TYR:HB3	2.03	0.56
1:E:179:LEU:C	1:E:179:LEU:HD12	2.30	0.56
1:D:53:PHE:HE2	1:D:63:LYS:CB	2.17	0.56
1:E:147:LYS:O	1:E:147:LYS:CG	2.53	0.56
1:A:274:VAL:C	1:A:276:HIS:H	2.12	0.56
1:B:283:GLN:N	1:B:284:PRO:CD	2.69	0.56
1:C:79:ASN:OD1	1:C:109:VAL:HG12	2.04	0.56
1:C:157:THR:HG22	1:D:34:GLU:OE1	2.05	0.56
1:E:215:PHE:HZ	1:E:298:PHE:CD1	2.23	0.56
1:B:194:PHE:O	1:B:198:PRO:HD3	2.06	0.56
1:B:215:PHE:CZ	1:B:298:PHE:CD1	2.93	0.56
1:D:221:GLU:OE2	1:E:221:GLU:OE2	2.23	0.56
1:A:23:LEU:HD22	1:A:38:VAL:CG2	2.35	0.56
1:C:222:ALA:HA	1:D:221:GLU:OE1	2.05	0.56
1:E:79:ASN:HD22	1:E:79:ASN:H	1.53	0.56
1:E:290:ILE:HG22	1:E:291:THR:N	2.20	0.56
1:D:215:PHE:CZ	1:D:298:PHE:CD1	2.94	0.56
1:A:79:ASN:OD1	1:A:109:VAL:HG12	2.06	0.56
1:B:53:PHE:HE2	1:B:63:LYS:CB	2.17	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:VAL:C	1:C:226:LEU:N	2.59	0.56
1:D:210:ILE:HG13	1:E:266:PHE:CE1	2.41	0.56
1:B:53:PHE:CD1	1:B:53:PHE:C	2.84	0.56
1:A:221:GLU:OE2	1:B:221:GLU:OE2	2.24	0.56
1:C:219:SER:O	1:C:223:ASN:HB2	2.06	0.56
1:D:202:LEU:HD12	1:E:259:PHE:CZ	2.41	0.55
1:D:283:GLN:N	1:D:284:PRO:CD	2.69	0.55
1:E:283:GLN:N	1:E:284:PRO:CD	2.68	0.55
1:B:123:GLN:HB2	1:B:189:ILE:HG13	1.88	0.55
1:E:149:GLY:O	1:E:164:PHE:CD1	2.57	0.55
1:E:215:PHE:CZ	1:E:298:PHE:CD1	2.94	0.55
1:E:219:SER:OG	1:E:222:ALA:HB3	2.06	0.55
1:A:225:THR:CG2	1:B:224:VAL:HG23	2.36	0.55
1:C:283:GLN:N	1:C:284:PRO:CD	2.69	0.55
1:E:23:LEU:HD22	1:E:38:VAL:CG2	2.36	0.55
1:E:76:ARG:HH12	1:E:130:ILE:HD11	1.71	0.55
1:E:86:ALA:HB2	1:E:105:PHE:HB3	1.88	0.55
1:A:179:LEU:C	1:A:179:LEU:HD12	2.31	0.55
1:C:179:LEU:C	1:C:179:LEU:HD12	2.31	0.55
1:D:104:ARG:NH2	1:E:78:VAL:HA	2.20	0.55
1:A:215:PHE:HZ	1:A:298:PHE:CD1	2.24	0.55
1:A:22:TYR:HA	1:A:149:GLY:CA	2.30	0.55
1:D:23:LEU:HD22	1:D:38:VAL:CG2	2.36	0.55
1:D:200:ILE:CD1	1:D:240:LEU:HD23	2.36	0.55
1:B:147:LYS:O	1:B:147:LYS:CG	2.53	0.55
1:D:86:ALA:HB2	1:D:105:PHE:HB3	1.89	0.55
1:A:254:THR:O	1:A:258:ILE:HB	2.07	0.55
1:B:115:PHE:O	1:B:252:THR:HG22	2.07	0.55
1:C:147:LYS:O	1:C:147:LYS:CG	2.53	0.55
1:E:216:TRP:CH2	1:E:295:ARG:HB3	2.42	0.55
1:C:159:TRP:CE3	1:C:189:ILE:HD12	2.42	0.54
1:C:290:ILE:HG22	1:C:291:THR:N	2.21	0.54
1:D:147:LYS:O	1:D:147:LYS:CG	2.53	0.54
1:D:147:LYS:C	1:D:149:GLY:N	2.63	0.54
1:D:219:SER:O	1:D:223:ASN:HB2	2.07	0.54
1:E:243:THR:HG22	1:E:244:ASN:HD22	1.72	0.54
1:A:298:PHE:HB2	1:A:299:PRO:HD3	1.88	0.54
1:B:213:THR:HG22	1:B:226:LEU:CD1	2.38	0.54
1:D:53:PHE:CD1	1:D:53:PHE:C	2.84	0.54
1:B:53:PHE:CE2	1:B:63:LYS:HB3	2.41	0.54
1:B:243:THR:HG22	1:B:244:ASN:HD22	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:29:LEU:HD23	1:D:29:LEU:C	2.32	0.54
1:B:100:GLN:HE21	1:B:100:GLN:HA	1.73	0.54
1:C:179:LEU:HD12	1:C:179:LEU:O	2.07	0.54
1:D:298:PHE:HB2	1:D:299:PRO:HD3	1.90	0.54
1:A:215:PHE:CZ	1:A:298:PHE:CD1	2.95	0.54
1:A:283:GLN:N	1:A:284:PRO:CD	2.70	0.54
1:E:79:ASN:OD1	1:E:109:VAL:HG12	2.08	0.54
1:B:42:LEU:HB3	1:B:103:GLU:CG	2.38	0.54
1:B:290:ILE:HG22	1:B:291:THR:N	2.23	0.54
1:C:254:THR:O	1:C:258:ILE:HB	2.07	0.54
1:D:100:GLN:HE21	1:D:100:GLN:HA	1.72	0.54
1:E:215:PHE:O	1:E:291:THR:CG2	2.56	0.54
1:C:298:PHE:HB2	1:C:299:PRO:HD3	1.89	0.54
1:D:123:GLN:HB2	1:D:189:ILE:HG13	1.90	0.54
1:D:193:TYR:O	1:D:194:PHE:HB2	2.08	0.54
1:D:197:ILE:HB	1:D:198:PRO:HD3	1.89	0.54
1:E:25:GLU:OE1	1:E:25:GLU:HA	2.06	0.54
1:E:276:HIS:C	1:E:278:LEU:H	2.16	0.54
1:A:9:PRO:HD3	1:A:71:TRP:CE3	2.43	0.54
1:A:276:HIS:C	1:A:278:LEU:H	2.16	0.54
1:C:215:PHE:O	1:C:291:THR:CG2	2.56	0.54
1:E:238:ASN:HA	1:E:258:ILE:HD13	1.90	0.54
1:A:25:GLU:OE1	1:A:25:GLU:HA	2.08	0.53
1:A:48:ASP:C	1:A:50:ARG:H	2.17	0.53
1:B:179:LEU:HD12	1:B:179:LEU:C	2.32	0.53
1:B:215:PHE:O	1:B:291:THR:CG2	2.56	0.53
1:C:53:PHE:CE2	1:C:63:LYS:HB3	2.41	0.53
1:D:276:HIS:C	1:D:278:LEU:H	2.16	0.53
1:C:53:PHE:CD1	1:C:53:PHE:C	2.84	0.53
1:A:229:SER:HB2	1:B:228:VAL:HG11	1.91	0.53
1:B:23:LEU:HD22	1:B:38:VAL:CG2	2.39	0.53
1:B:140:VAL:HG22	1:B:181:SER:HB3	1.91	0.53
1:C:62:VAL:HG13	1:C:93:VAL:O	2.09	0.53
1:C:314:PHE:CD1	1:C:314:PHE:N	2.76	0.53
1:E:48:ASP:C	1:E:50:ARG:H	2.17	0.53
1:E:53:PHE:CE2	1:E:63:LYS:HB3	2.41	0.53
1:B:48:ASP:C	1:B:50:ARG:H	2.17	0.53
1:D:27:TYR:CB	1:E:110:LEU:HD11	2.39	0.53
1:E:29:LEU:C	1:E:29:LEU:HD23	2.33	0.53
1:A:314:PHE:CD1	1:A:314:PHE:N	2.76	0.53
1:B:25:GLU:HA	1:B:25:GLU:OE1	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:ARG:HH22	1:C:176:GLU:HB2	1.73	0.53
1:A:193:TYR:O	1:A:194:PHE:HB2	2.09	0.53
1:D:232:ILE:HG22	1:D:233:ALA:N	2.23	0.53
1:D:235:ILE:CG2	1:D:239:ILE:HD12	2.38	0.53
1:C:276:HIS:C	1:C:278:LEU:H	2.16	0.53
1:A:140:VAL:HG22	1:A:181:SER:HB3	1.91	0.52
1:A:210:ILE:HG12	1:B:269:VAL:HG11	1.90	0.52
1:B:298:PHE:HB2	1:B:299:PRO:HD3	1.91	0.52
1:E:100:GLN:HA	1:E:100:GLN:HE21	1.73	0.52
1:E:179:LEU:HD12	1:E:179:LEU:O	2.08	0.52
1:E:53:PHE:CD1	1:E:53:PHE:C	2.84	0.52
1:C:193:TYR:O	1:C:194:PHE:HB2	2.09	0.52
1:D:215:PHE:O	1:D:291:THR:CG2	2.58	0.52
1:D:25:GLU:HA	1:D:25:GLU:OE1	2.08	0.52
1:D:243:THR:HG22	1:D:244:ASN:N	2.24	0.52
1:A:128:TYR:O	1:A:129:LEU:HB2	2.10	0.52
1:A:253:TYR:O	1:A:256:ALA:HB3	2.10	0.52
1:B:9:PRO:HD3	1:B:71:TRP:CE3	2.44	0.52
1:C:77:PHE:CE2	1:C:127:ILE:HG23	2.45	0.52
1:C:128:TYR:O	1:C:129:LEU:HB2	2.10	0.52
1:D:79:ASN:H	1:D:79:ASN:HD22	1.57	0.52
1:E:123:GLN:HB2	1:E:189:ILE:HG13	1.92	0.52
1:B:29:LEU:HD23	1:B:29:LEU:C	2.34	0.52
1:C:275:GLN:O	1:C:275:GLN:HG2	2.10	0.52
1:D:48:ASP:C	1:D:50:ARG:H	2.17	0.52
1:A:53:PHE:CE2	1:A:63:LYS:HB3	2.44	0.52
1:B:276:HIS:C	1:B:278:LEU:H	2.16	0.52
1:E:115:PHE:O	1:E:252:THR:HG22	2.09	0.52
1:A:197:ILE:HB	1:A:198:PRO:HD3	1.91	0.51
1:B:76:ARG:NH2	1:B:130:ILE:CD1	2.60	0.51
1:B:128:TYR:O	1:B:129:LEU:HB2	2.10	0.51
1:C:48:ASP:C	1:C:50:ARG:H	2.17	0.51
1:E:275:GLN:O	1:E:275:GLN:HG2	2.10	0.51
1:E:291:THR:O	1:E:295:ARG:HG3	2.11	0.51
1:A:53:PHE:CD1	1:A:53:PHE:C	2.84	0.51
1:A:194:PHE:O	1:A:198:PRO:HD3	2.10	0.51
1:A:210:ILE:HG23	1:B:269:VAL:CG1	2.34	0.51
1:C:194:PHE:O	1:C:198:PRO:HD3	2.09	0.51
1:D:149:GLY:O	1:D:164:PHE:CD1	2.59	0.51
1:E:62:VAL:HG13	1:E:93:VAL:O	2.10	0.51
1:D:179:LEU:HD12	1:D:179:LEU:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:275:GLN:O	1:D:275:GLN:HG2	2.10	0.51
1:C:123:GLN:HB2	1:C:189:ILE:HG13	1.92	0.51
1:C:155:PHE:HD1	1:D:110:LEU:CD2	2.23	0.51
1:C:243:THR:HG22	1:C:244:ASN:HD22	1.75	0.51
1:A:179:LEU:HD12	1:A:179:LEU:O	2.11	0.51
1:C:202:LEU:HD12	1:D:259:PHE:HE1	1.75	0.51
1:C:291:THR:O	1:C:295:ARG:HG3	2.11	0.51
1:E:243:THR:HG22	1:E:244:ASN:N	2.26	0.51
1:E:314:PHE:CD1	1:E:314:PHE:N	2.78	0.51
1:A:29:LEU:C	1:A:29:LEU:HD23	2.35	0.51
1:A:229:SER:CB	1:B:228:VAL:CG1	2.85	0.51
1:A:243:THR:HG22	1:A:244:ASN:N	2.25	0.51
1:B:179:LEU:HD12	1:B:179:LEU:O	2.09	0.51
1:C:192:GLN:CD	1:D:249:PRO:HB3	2.36	0.51
1:B:41:PHE:CE1	1:B:104:ARG:HG3	2.45	0.51
1:B:79:ASN:H	1:B:79:ASN:HD22	1.58	0.51
1:B:193:TYR:O	1:B:194:PHE:HB2	2.10	0.51
1:D:291:THR:O	1:D:295:ARG:HG3	2.10	0.51
1:C:79:ASN:HD22	1:C:79:ASN:H	1.57	0.51
1:C:140:VAL:HG22	1:C:181:SER:HB3	1.92	0.51
1:D:132:ARG:HH22	1:D:176:GLU:HB2	1.75	0.51
1:A:215:PHE:O	1:A:291:THR:CG2	2.59	0.51
1:A:223:ASN:O	1:A:227:VAL:HG23	2.11	0.51
1:C:48:ASP:O	1:C:50:ARG:N	2.44	0.51
1:C:195:SER:O	1:C:199:ASN:HB2	2.11	0.51
1:D:48:ASP:O	1:D:50:ARG:N	2.44	0.51
1:D:243:THR:HG22	1:D:244:ASN:HD22	1.75	0.51
1:A:232:ILE:HG22	1:A:233:ALA:N	2.25	0.51
1:B:62:VAL:HG13	1:B:93:VAL:O	2.11	0.51
1:B:149:GLY:O	1:B:164:PHE:CD1	2.61	0.51
1:C:234:HIS:CE1	1:C:261:ILE:CG2	2.93	0.51
1:A:221:GLU:HB3	1:B:221:GLU:CG	2.34	0.50
1:A:275:GLN:O	1:A:275:GLN:HG2	2.10	0.50
1:D:128:TYR:O	1:D:129:LEU:HB2	2.10	0.50
1:E:132:ARG:HH22	1:E:176:GLU:HB2	1.75	0.50
1:A:123:GLN:HB2	1:A:189:ILE:HG13	1.92	0.50
1:A:202:LEU:HD12	1:B:259:PHE:CE1	2.45	0.50
1:D:54:ASP:HB2	1:D:57:ARG:CG	2.40	0.50
1:A:192:GLN:OE1	1:B:249:PRO:HB3	2.12	0.50
1:B:48:ASP:O	1:B:50:ARG:N	2.44	0.50
1:B:243:THR:HG22	1:B:244:ASN:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:41:PHE:HE2	1:E:175:LEU:HD23	1.76	0.50
1:D:257:ILE:CG2	1:D:309:LEU:HD23	2.40	0.50
1:E:48:ASP:O	1:E:50:ARG:N	2.44	0.50
1:A:48:ASP:O	1:A:50:ARG:N	2.44	0.50
1:C:210:ILE:HG12	1:D:269:VAL:HG11	1.94	0.50
1:D:290:ILE:HG22	1:D:291:THR:N	2.25	0.50
1:D:96:ASP:OD1	1:D:98:THR:HB	2.11	0.50
1:D:216:TRP:CH2	1:D:295:ARG:HB3	2.47	0.50
1:E:193:TYR:O	1:E:194:PHE:HB2	2.11	0.50
1:A:104:ARG:NH1	1:B:77:PHE:O	2.42	0.50
1:D:94:SER:OG	1:D:95:PRO:HD2	2.12	0.50
1:B:275:GLN:HG2	1:B:275:GLN:O	2.10	0.50
1:D:210:ILE:HG13	1:E:266:PHE:HE1	1.76	0.50
1:C:48:ASP:C	1:C:50:ARG:N	2.70	0.50
1:E:77:PHE:CE2	1:E:127:ILE:HG23	2.47	0.50
1:E:128:TYR:O	1:E:129:LEU:HB2	2.10	0.50
1:A:13:GLU:HB3	1:A:14:PRO:CD	2.42	0.50
1:D:42:LEU:HB3	1:D:103:GLU:CG	2.42	0.50
1:D:140:VAL:HG22	1:D:181:SER:HB3	1.92	0.50
1:E:264:PHE:HE2	1:E:302:PHE:CB	2.24	0.50
1:A:314:PHE:N	1:A:314:PHE:HD1	2.10	0.49
1:B:94:SER:OG	1:B:95:PRO:HD2	2.12	0.49
1:E:94:SER:OG	1:E:95:PRO:HD2	2.12	0.49
1:B:253:TYR:O	1:B:256:ALA:HB3	2.12	0.49
1:E:9:PRO:HD3	1:E:71:TRP:CE3	2.47	0.49
1:E:144:ASP:HA	1:E:147:LYS:HB3	1.95	0.49
1:E:194:PHE:O	1:E:198:PRO:HD3	2.12	0.49
1:A:249:PRO:HB3	1:E:192:GLN:CD	2.37	0.49
1:C:54:ASP:HB2	1:C:57:ARG:CG	2.42	0.49
1:E:140:VAL:HG22	1:E:181:SER:HB3	1.95	0.49
1:B:48:ASP:C	1:B:50:ARG:N	2.70	0.49
1:C:76:ARG:HH12	1:C:130:ILE:HD11	1.77	0.49
1:E:42:LEU:HB3	1:E:103:GLU:CG	2.42	0.49
1:E:264:PHE:O	1:E:268:ALA:HB2	2.13	0.49
1:A:155:PHE:CE1	1:B:112:PRO:CB	2.87	0.49
1:C:94:SER:OG	1:C:95:PRO:HD2	2.12	0.49
1:D:194:PHE:O	1:D:198:PRO:HD3	2.12	0.49
1:E:76:ARG:HH22	1:E:130:ILE:CD1	2.10	0.49
1:C:253:TYR:O	1:C:256:ALA:HB3	2.13	0.49
1:E:232:ILE:HG22	1:E:233:ALA:N	2.28	0.49
1:E:278:LEU:HD21	1:E:286:ARG:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:SER:OG	1:A:95:PRO:HD2	2.12	0.49
1:A:216:TRP:CH2	1:A:295:ARG:HB3	2.48	0.49
1:A:291:THR:O	1:A:295:ARG:HG3	2.13	0.49
1:B:216:TRP:CH2	1:B:295:ARG:HB3	2.48	0.49
1:D:77:PHE:CE2	1:D:127:ILE:HG23	2.47	0.49
1:A:132:ARG:HH22	1:A:176:GLU:HB2	1.77	0.49
1:B:54:ASP:HB2	1:B:57:ARG:CG	2.42	0.49
1:B:197:ILE:HB	1:B:198:PRO:HD3	1.95	0.49
1:A:195:SER:O	1:A:199:ASN:HB2	2.12	0.49
1:D:193:TYR:O	1:D:194:PHE:CB	2.60	0.49
1:A:79:ASN:HD22	1:A:79:ASN:H	1.61	0.48
1:C:100:GLN:HE21	1:C:100:GLN:HA	1.78	0.48
1:C:281:GLU:O	1:C:283:GLN:N	2.47	0.48
1:D:27:TYR:CG	1:E:110:LEU:HD11	2.48	0.48
1:A:137:ARG:HA	1:A:137:ARG:HD3	1.64	0.48
1:B:77:PHE:CE2	1:B:127:ILE:HG23	2.48	0.48
1:D:137:ARG:HA	1:D:137:ARG:HD3	1.63	0.48
1:D:150:LYS:CG	1:D:154:VAL:HG21	2.43	0.48
1:A:100:GLN:HE21	1:A:100:GLN:HA	1.78	0.48
1:B:132:ARG:HH22	1:B:176:GLU:HB2	1.78	0.48
1:D:223:ASN:O	1:D:227:VAL:HG23	2.14	0.48
1:E:48:ASP:C	1:E:50:ARG:N	2.70	0.48
1:C:9:PRO:HD3	1:C:71:TRP:CE3	2.49	0.48
1:C:238:ASN:HA	1:C:258:ILE:HD13	1.94	0.48
1:D:53:PHE:CE2	1:D:63:LYS:HB3	2.43	0.48
1:D:78:VAL:CG2	1:D:128:TYR:HB3	2.43	0.48
1:D:84:ARG:HA	1:D:107:ALA:HB2	1.95	0.48
1:D:195:SER:HB3	1:E:248:THR:O	2.13	0.48
1:D:253:TYR:O	1:D:256:ALA:HB3	2.14	0.48
1:A:54:ASP:HB2	1:A:57:ARG:CG	2.44	0.48
1:A:213:THR:HG22	1:A:226:LEU:HD11	1.95	0.48
1:B:13:GLU:HB3	1:B:14:PRO:CD	2.43	0.48
1:D:314:PHE:CD1	1:D:314:PHE:N	2.80	0.48
1:A:42:LEU:HB3	1:A:103:GLU:CG	2.44	0.48
1:C:232:ILE:HG22	1:C:233:ALA:N	2.28	0.48
1:D:41:PHE:HE2	1:E:175:LEU:CD2	2.27	0.48
1:D:42:LEU:HD23	1:D:103:GLU:OE1	2.14	0.48
1:D:115:PHE:O	1:D:252:THR:HG22	2.14	0.48
1:A:48:ASP:C	1:A:50:ARG:N	2.70	0.48
1:A:76:ARG:HH12	1:A:130:ILE:HD11	1.79	0.48
1:C:157:THR:HG21	1:D:34:GLU:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:278:LEU:HD21	1:C:286:ARG:HB3	1.95	0.48
1:E:70:ILE:HD13	1:E:70:ILE:N	2.29	0.48
1:B:232:ILE:HG22	1:B:233:ALA:N	2.28	0.48
1:B:314:PHE:N	1:B:314:PHE:CD1	2.81	0.48
1:D:278:LEU:HD21	1:D:286:ARG:HB3	1.95	0.48
1:E:54:ASP:HB2	1:E:57:ARG:CG	2.43	0.48
1:E:282:SER:C	1:E:284:PRO:HD3	2.38	0.48
1:B:47:LYS:HD2	1:B:49:ARG:HH21	1.77	0.47
1:B:53:PHE:CD1	1:B:95:PRO:HA	2.49	0.47
1:B:86:ALA:HB2	1:B:105:PHE:CB	2.44	0.47
1:B:291:THR:O	1:B:295:ARG:HG3	2.14	0.47
1:B:223:ASN:O	1:B:227:VAL:HG23	2.14	0.47
1:C:53:PHE:CD1	1:C:95:PRO:HA	2.49	0.47
1:C:53:PHE:CE1	1:C:95:PRO:HA	2.49	0.47
1:C:264:PHE:HE2	1:C:302:PHE:CB	2.27	0.47
1:D:9:PRO:HD3	1:D:71:TRP:CE3	2.49	0.47
1:D:219:SER:OG	1:D:222:ALA:HB3	2.14	0.47
1:E:13:GLU:HB3	1:E:14:PRO:CD	2.44	0.47
1:E:22:TYR:HA	1:E:149:GLY:CA	2.35	0.47
1:A:278:LEU:HD21	1:A:286:ARG:HB3	1.95	0.47
1:C:193:TYR:O	1:C:194:PHE:CB	2.62	0.47
1:C:226:LEU:HD23	1:D:224:VAL:HB	1.96	0.47
1:D:51:LEU:CD1	1:D:70:ILE:HD12	2.44	0.47
1:D:53:PHE:CD1	1:D:95:PRO:HA	2.49	0.47
1:D:256:ALA:HB1	1:D:309:LEU:HD21	1.96	0.47
1:A:53:PHE:CD1	1:A:95:PRO:HA	2.49	0.47
1:A:243:THR:HG22	1:A:244:ASN:HD22	1.79	0.47
1:A:282:SER:C	1:A:284:PRO:HD3	2.40	0.47
1:B:278:LEU:HD21	1:B:286:ARG:HB3	1.95	0.47
1:C:157:THR:CG2	1:D:34:GLU:OE1	2.61	0.47
1:C:243:THR:HG22	1:C:244:ASN:N	2.29	0.47
1:C:256:ALA:HB1	1:C:309:LEU:HD21	1.97	0.47
1:E:213:THR:HG22	1:E:226:LEU:HD11	1.96	0.47
1:A:53:PHE:CE1	1:A:95:PRO:HA	2.49	0.47
1:A:147:LYS:O	1:A:147:LYS:CG	2.54	0.47
1:A:193:TYR:O	1:A:194:PHE:CB	2.63	0.47
1:A:222:ALA:O	1:A:226:LEU:HB2	2.15	0.47
1:A:270:ILE:HD13	1:A:270:ILE:HA	1.60	0.47
1:C:314:PHE:N	1:C:314:PHE:HD1	2.11	0.47
1:E:259:PHE:C	1:E:259:PHE:CD2	2.92	0.47
1:E:283:GLN:HE21	1:E:286:ARG:HB2	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:SER:HB3	1:B:228:VAL:HG11	1.86	0.47
1:A:259:PHE:C	1:A:259:PHE:CD2	2.93	0.47
1:A:283:GLN:HE21	1:A:286:ARG:HB2	1.80	0.47
1:B:53:PHE:CE1	1:B:95:PRO:HA	2.49	0.47
1:B:70:ILE:HG22	1:B:71:TRP:N	2.30	0.47
1:B:144:ASP:HA	1:B:147:LYS:HB3	1.95	0.47
1:B:305:ALA:O	1:B:309:LEU:HB2	2.15	0.47
1:C:199:ASN:HB3	1:D:242:GLU:OE1	2.15	0.47
1:D:240:LEU:CD1	1:E:239:ILE:HG12	2.41	0.47
1:E:314:PHE:N	1:E:314:PHE:HD1	2.12	0.47
1:A:193:TYR:C	1:A:193:TYR:CD2	2.92	0.47
1:A:212:TRP:HB2	1:A:215:PHE:CE1	2.49	0.47
1:B:193:TYR:O	1:B:194:PHE:CB	2.62	0.47
1:B:219:SER:OG	1:B:222:ALA:HB3	2.15	0.47
1:D:53:PHE:CE1	1:D:95:PRO:HA	2.50	0.47
1:D:75:ILE:HD13	1:D:131:VAL:HB	1.97	0.47
1:D:78:VAL:HB	1:D:128:TYR:HB2	1.96	0.47
1:E:78:VAL:CG2	1:E:128:TYR:HB3	2.45	0.47
1:E:151:ASN:HD22	1:E:152:ASP:H	1.61	0.47
1:E:264:PHE:CE2	1:E:302:PHE:CB	2.98	0.47
1:B:247:LYS:HA	1:B:247:LYS:HD3	1.75	0.47
1:B:264:PHE:HE2	1:B:302:PHE:CB	2.25	0.47
1:D:195:SER:O	1:D:199:ASN:HB2	2.14	0.47
1:B:259:PHE:CD2	1:B:259:PHE:C	2.93	0.47
1:C:193:TYR:CD2	1:C:193:TYR:C	2.93	0.47
1:A:84:ARG:HA	1:A:107:ALA:HB2	1.96	0.46
1:A:226:LEU:HD22	1:A:226:LEU:HA	1.49	0.46
1:B:151:ASN:HD22	1:B:152:ASP:H	1.63	0.46
1:B:282:SER:C	1:B:284:PRO:HD3	2.40	0.46
1:A:51:LEU:CD1	1:A:70:ILE:HD12	2.44	0.46
1:C:78:VAL:CG2	1:C:128:TYR:HB3	2.45	0.46
1:D:76:ARG:HH12	1:D:130:ILE:HD11	1.80	0.46
1:A:224:VAL:O	1:A:226:LEU:N	2.48	0.46
1:C:247:LYS:HA	1:C:247:LYS:HD3	1.72	0.46
1:D:48:ASP:C	1:D:50:ARG:N	2.70	0.46
1:D:222:ALA:O	1:D:226:LEU:HB2	2.16	0.46
1:E:213:THR:HG22	1:E:226:LEU:HD12	1.98	0.46
1:E:223:ASN:O	1:E:227:VAL:HG23	2.16	0.46
1:A:281:GLU:O	1:A:283:GLN:N	2.48	0.46
1:B:42:LEU:HD23	1:B:103:GLU:OE1	2.15	0.46
1:C:86:ALA:HB2	1:C:105:PHE:CB	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:ASN:C	1:C:153:ASP:H	2.24	0.46
1:E:53:PHE:CD1	1:E:95:PRO:HA	2.49	0.46
1:E:287:ALA:C	1:E:289:SER:H	2.24	0.46
1:B:264:PHE:O	1:B:268:ALA:HB2	2.15	0.46
1:B:287:ALA:C	1:B:289:SER:H	2.22	0.46
1:E:35:THR:OG1	1:E:108:ARG:NH2	2.47	0.46
1:E:86:ALA:HB2	1:E:105:PHE:CB	2.46	0.46
1:A:77:PHE:CE2	1:A:127:ILE:HG23	2.50	0.46
1:B:283:GLN:HE21	1:B:286:ARG:HB2	1.80	0.46
1:C:23:LEU:HG	1:C:164:PHE:CD1	2.50	0.46
1:C:196:TYR:HE1	1:D:247:LYS:HG3	1.81	0.46
1:C:213:THR:HG22	1:C:226:LEU:HD12	1.97	0.46
1:C:222:ALA:CA	1:D:221:GLU:OE1	2.62	0.46
1:E:23:LEU:HG	1:E:164:PHE:CD1	2.50	0.46
1:E:53:PHE:CE1	1:E:95:PRO:HA	2.50	0.46
1:A:170:PRO:HB3	1:A:183:LEU:CD2	2.46	0.46
1:A:195:SER:HB3	1:B:248:THR:O	2.16	0.46
1:C:47:LYS:HD2	1:C:49:ARG:HH21	1.80	0.46
1:C:137:ARG:HD3	1:C:137:ARG:HA	1.59	0.46
1:D:13:GLU:HB3	1:D:14:PRO:CD	2.45	0.46
1:E:195:SER:O	1:E:199:ASN:HB2	2.15	0.46
1:A:147:LYS:CE	1:A:165:THR:HA	2.45	0.46
1:B:241:VAL:C	1:B:243:THR:N	2.74	0.46
1:C:216:TRP:CH2	1:C:295:ARG:HB3	2.50	0.46
1:D:156:LEU:HD12	1:D:156:LEU:HA	1.71	0.46
1:D:281:GLU:O	1:D:283:GLN:N	2.48	0.46
1:D:283:GLN:HE21	1:D:286:ARG:HB2	1.80	0.46
1:E:70:ILE:HG22	1:E:71:TRP:N	2.31	0.46
1:D:151:ASN:C	1:D:153:ASP:H	2.24	0.46
1:A:217:SER:OG	1:B:220:TYR:HE2	1.96	0.46
1:A:256:ALA:HB1	1:A:309:LEU:HD21	1.98	0.46
1:B:213:THR:HG22	1:B:226:LEU:HD11	1.98	0.46
1:C:202:LEU:HD12	1:D:259:PHE:CZ	2.51	0.46
1:A:76:ARG:HH22	1:A:130:ILE:CD1	2.16	0.45
1:A:238:ASN:HA	1:A:258:ILE:HD13	1.97	0.45
1:C:75:ILE:HD13	1:C:131:VAL:HB	1.98	0.45
1:C:84:ARG:HA	1:C:107:ALA:HB2	1.96	0.45
1:B:150:LYS:CG	1:B:154:VAL:HG21	2.43	0.45
1:C:13:GLU:HB3	1:C:14:PRO:CD	2.47	0.45
1:C:147:LYS:CE	1:C:165:THR:HA	2.46	0.45
1:A:86:ALA:HB2	1:A:105:PHE:CB	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:ASP:HA	1:C:147:LYS:HB3	1.98	0.45
1:D:226:LEU:HD22	1:D:226:LEU:HA	1.53	0.45
1:E:139:ILE:HG12	1:E:172:ASN:HD21	1.82	0.45
1:A:51:LEU:HD13	1:A:70:ILE:HD12	1.99	0.45
1:A:151:ASN:C	1:A:153:ASP:H	2.24	0.45
1:B:23:LEU:HB2	1:B:150:LYS:HA	1.99	0.45
1:C:194:PHE:HA	1:C:197:ILE:HD12	1.97	0.45
1:D:23:LEU:HB2	1:D:150:LYS:HA	1.98	0.45
1:D:259:PHE:C	1:D:259:PHE:CD2	2.95	0.45
1:E:23:LEU:HB2	1:E:150:LYS:HA	1.99	0.45
1:E:150:LYS:CG	1:E:154:VAL:HG21	2.43	0.45
1:C:115:PHE:O	1:C:252:THR:HG22	2.17	0.45
1:D:225:THR:HB	1:E:224:VAL:HG21	1.99	0.45
1:B:151:ASN:C	1:B:153:ASP:H	2.24	0.45
1:C:223:ASN:O	1:C:227:VAL:HG23	2.16	0.45
1:D:158:GLY:HA2	1:D:192:GLN:OE1	2.16	0.45
1:A:78:VAL:CG2	1:A:128:TYR:HB3	2.46	0.45
1:A:309:LEU:HD12	1:A:309:LEU:HA	1.84	0.45
1:D:62:VAL:HG13	1:D:93:VAL:O	2.17	0.45
1:D:196:TYR:N	1:D:196:TYR:HD1	2.15	0.45
1:E:241:VAL:C	1:E:243:THR:N	2.75	0.45
1:A:235:ILE:CG2	1:A:239:ILE:HD12	2.45	0.45
1:E:256:ALA:HB1	1:E:309:LEU:HD21	1.98	0.45
1:D:98:THR:O	1:D:98:THR:HG22	2.17	0.45
1:A:196:TYR:N	1:A:196:TYR:HD1	2.15	0.44
1:B:123:GLN:HA	1:B:123:GLN:NE2	2.31	0.44
1:C:283:GLN:HE21	1:C:286:ARG:HB2	1.80	0.44
1:E:75:ILE:HD13	1:E:131:VAL:HB	1.99	0.44
1:B:51:LEU:CD1	1:B:70:ILE:HD12	2.46	0.44
1:B:84:ARG:HA	1:B:107:ALA:HB2	1.99	0.44
1:C:282:SER:C	1:C:284:PRO:HD3	2.42	0.44
1:D:282:SER:C	1:D:284:PRO:HD3	2.42	0.44
1:A:78:VAL:HB	1:A:128:TYR:HB2	1.98	0.44
1:B:70:ILE:HG22	1:B:71:TRP:O	2.17	0.44
1:C:23:LEU:HB2	1:C:150:LYS:HA	1.98	0.44
1:D:70:ILE:HG22	1:D:71:TRP:N	2.32	0.44
1:A:23:LEU:HB2	1:A:150:LYS:HA	1.98	0.44
1:D:264:PHE:CE2	1:D:302:PHE:CB	3.00	0.44
1:D:309:LEU:HD12	1:D:309:LEU:HA	1.82	0.44
1:A:38:VAL:O	1:A:106:SER:HA	2.17	0.44
1:A:151:ASN:HD22	1:A:152:ASP:H	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:GLN:CG	1:B:249:PRO:HB3	2.48	0.44
1:C:150:LYS:CG	1:C:154:VAL:HG21	2.43	0.44
1:D:224:VAL:O	1:D:226:LEU:N	2.51	0.44
1:E:249:PRO:HD2	1:E:250:TYR:CD1	2.52	0.44
1:A:203:PRO:HB3	1:B:262:TYR:CZ	2.53	0.44
1:B:46:TRP:CH2	1:B:73:PRO:HD3	2.52	0.44
1:D:287:ALA:C	1:D:289:SER:H	2.25	0.44
1:A:70:ILE:HG22	1:A:71:TRP:N	2.32	0.44
1:A:150:LYS:CG	1:A:154:VAL:HG21	2.43	0.44
1:A:196:TYR:N	1:A:196:TYR:CD1	2.85	0.44
1:B:23:LEU:HG	1:B:164:PHE:CD1	2.52	0.44
1:B:130:ILE:CG2	1:B:182:LYS:HB2	2.47	0.44
1:D:84:ARG:CB	1:D:84:ARG:HH11	2.31	0.44
1:E:151:ASN:C	1:E:153:ASP:H	2.24	0.44
1:A:270:ILE:HG22	1:A:271:GLU:N	2.33	0.44
1:C:42:LEU:HB3	1:C:103:GLU:CG	2.46	0.44
1:C:84:ARG:HH11	1:C:84:ARG:CB	2.31	0.44
1:D:277:TYR:HA	1:D:280:VAL:HG22	2.00	0.44
1:E:51:LEU:CD1	1:E:70:ILE:HD12	2.47	0.44
1:E:264:PHE:CD1	1:E:264:PHE:N	2.86	0.44
1:D:213:THR:HG22	1:D:226:LEU:HD11	1.98	0.44
1:E:147:LYS:CE	1:E:165:THR:HA	2.48	0.44
1:E:193:TYR:O	1:E:194:PHE:CB	2.64	0.44
1:A:22:TYR:HB3	1:A:41:PHE:HB2	2.00	0.43
1:A:37:LYS:HG2	1:A:108:ARG:HB3	2.00	0.43
1:B:212:TRP:HB2	1:B:215:PHE:CE1	2.53	0.43
1:B:238:ASN:HA	1:B:258:ILE:HD13	1.97	0.43
1:C:51:LEU:CD1	1:C:70:ILE:HD12	2.48	0.43
1:D:314:PHE:N	1:D:314:PHE:HD1	2.16	0.43
1:E:50:ARG:HE	1:E:50:ARG:HB3	1.56	0.43
1:E:84:ARG:CB	1:E:84:ARG:HH11	2.31	0.43
1:E:212:TRP:HB2	1:E:215:PHE:CE1	2.53	0.43
1:E:277:TYR:HA	1:E:280:VAL:HG22	2.00	0.43
1:B:75:ILE:HD13	1:B:131:VAL:HB	1.99	0.43
1:B:79:ASN:ND2	1:B:128:TYR:HD2	2.15	0.43
1:B:147:LYS:CE	1:B:165:THR:HA	2.48	0.43
1:C:264:PHE:CD1	1:C:264:PHE:N	2.86	0.43
1:D:196:TYR:N	1:D:196:TYR:CD1	2.85	0.43
1:D:197:ILE:CG2	1:D:202:LEU:HG	2.48	0.43
1:D:197:ILE:HG23	1:D:202:LEU:HG	1.99	0.43
1:E:300:VAL:O	1:E:304:LEU:HB2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:ALA:C	1:A:289:SER:H	2.25	0.43
1:B:264:PHE:CE2	1:B:302:PHE:CB	2.98	0.43
1:C:277:TYR:HA	1:C:280:VAL:HG22	2.00	0.43
1:E:42:LEU:HD23	1:E:103:GLU:OE1	2.18	0.43
1:E:98:THR:O	1:E:98:THR:HG22	2.18	0.43
1:E:298:PHE:CB	1:E:299:PRO:HD3	2.47	0.43
1:B:224:VAL:O	1:B:226:LEU:N	2.51	0.43
1:C:51:LEU:HD13	1:C:70:ILE:HD12	2.01	0.43
1:C:263:LEU:O	1:C:266:PHE:N	2.51	0.43
1:E:205:LEU:O	1:E:208:LEU:HB3	2.18	0.43
1:B:10:ILE:H	1:B:10:ILE:HG13	1.65	0.43
1:C:274:VAL:C	1:C:276:HIS:N	2.77	0.43
1:E:70:ILE:HG22	1:E:71:TRP:O	2.19	0.43
1:E:257:ILE:CG2	1:E:309:LEU:HD23	2.44	0.43
1:A:19:THR:HA	1:A:43:SER:O	2.19	0.43
1:A:75:ILE:HD13	1:A:131:VAL:HB	2.00	0.43
1:A:84:ARG:CB	1:A:84:ARG:HH11	2.31	0.43
1:A:264:PHE:O	1:A:268:ALA:HB2	2.19	0.43
1:A:269:VAL:HG11	1:E:210:ILE:HG12	1.99	0.43
1:B:205:LEU:O	1:B:208:LEU:HB3	2.18	0.43
1:B:300:VAL:O	1:B:304:LEU:HB2	2.18	0.43
1:C:70:ILE:HG22	1:C:71:TRP:N	2.33	0.43
1:C:287:ALA:C	1:C:289:SER:H	2.26	0.43
1:D:175:LEU:HD12	1:D:175:LEU:HA	1.69	0.43
1:E:224:VAL:O	1:E:226:LEU:N	2.51	0.43
1:A:157:THR:HG21	1:B:34:GLU:CD	2.42	0.43
1:A:298:PHE:CB	1:A:299:PRO:HD3	2.49	0.43
1:B:225:THR:HG21	1:C:224:VAL:HG23	2.01	0.43
1:C:53:PHE:CD1	1:C:53:PHE:O	2.72	0.43
1:D:264:PHE:O	1:D:268:ALA:HB2	2.19	0.43
1:A:23:LEU:HG	1:A:164:PHE:CD1	2.53	0.43
1:A:53:PHE:CD1	1:A:53:PHE:O	2.72	0.43
1:B:224:VAL:O	1:B:228:VAL:HB	2.18	0.43
1:C:261:ILE:CD1	1:C:302:PHE:HE1	2.31	0.43
1:C:283:GLN:C	1:C:285:ALA:N	2.77	0.43
1:D:264:PHE:HE2	1:D:302:PHE:CB	2.27	0.43
1:E:137:ARG:HD3	1:E:137:ARG:HA	1.63	0.43
1:E:193:TYR:CD2	1:E:193:TYR:C	2.96	0.43
1:B:195:SER:O	1:B:199:ASN:HB2	2.18	0.43
1:B:210:ILE:HD11	1:C:266:PHE:HD1	1.84	0.43
1:B:314:PHE:N	1:B:314:PHE:HD1	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:155:PHE:CZ	1:D:112:PRO:HB3	2.54	0.43
1:C:309:LEU:HD12	1:C:309:LEU:HA	1.82	0.43
1:D:86:ALA:HB2	1:D:105:PHE:CB	2.48	0.43
1:E:53:PHE:CD1	1:E:53:PHE:O	2.72	0.43
1:E:121:ASP:CG	1:E:191:ARG:HH21	2.27	0.43
1:A:274:VAL:C	1:A:276:HIS:N	2.77	0.43
1:B:53:PHE:CD1	1:B:53:PHE:O	2.72	0.43
1:B:84:ARG:CB	1:B:84:ARG:HH11	2.31	0.43
1:B:162:GLU:OE1	1:B:190:SER:HB3	2.19	0.43
1:B:194:PHE:HA	1:B:197:ILE:HD12	2.01	0.43
1:C:179:LEU:C	1:C:179:LEU:CD1	2.91	0.43
1:D:144:ASP:HA	1:D:147:LYS:HB3	2.01	0.43
1:B:193:TYR:CD2	1:B:193:TYR:C	2.97	0.42
1:C:202:LEU:HD22	1:C:202:LEU:HA	1.85	0.42
1:A:46:TRP:CH2	1:A:73:PRO:HD3	2.53	0.42
1:A:264:PHE:HE2	1:A:302:PHE:CB	2.31	0.42
1:A:277:TYR:HA	1:A:280:VAL:HG22	2.00	0.42
1:B:241:VAL:C	1:B:243:THR:H	2.25	0.42
1:B:277:TYR:HA	1:B:280:VAL:HG22	2.00	0.42
1:C:38:VAL:O	1:C:106:SER:HA	2.19	0.42
1:C:298:PHE:CB	1:C:299:PRO:HD3	2.48	0.42
1:D:41:PHE:CE1	1:D:104:ARG:HG3	2.54	0.42
1:E:51:LEU:HD13	1:E:70:ILE:HD12	2.00	0.42
1:E:62:VAL:HG13	1:E:93:VAL:C	2.44	0.42
1:E:270:ILE:HG22	1:E:271:GLU:N	2.34	0.42
1:A:194:PHE:HA	1:A:197:ILE:HD12	2.02	0.42
1:A:264:PHE:N	1:A:264:PHE:CD1	2.87	0.42
1:C:270:ILE:HG22	1:C:271:GLU:N	2.33	0.42
1:D:18:ASN:O	1:D:44:LEU:HA	2.19	0.42
1:D:70:ILE:HG22	1:D:71:TRP:O	2.19	0.42
1:D:213:THR:HG22	1:D:226:LEU:HD12	2.00	0.42
1:D:247:LYS:HA	1:D:247:LYS:HD3	1.71	0.42
1:D:283:GLN:C	1:D:285:ALA:N	2.77	0.42
1:E:226:LEU:HD22	1:E:226:LEU:HA	1.49	0.42
1:E:241:VAL:C	1:E:243:THR:H	2.25	0.42
1:A:62:VAL:HG13	1:A:93:VAL:O	2.19	0.42
1:B:283:GLN:C	1:B:285:ALA:N	2.77	0.42
1:C:253:TYR:HA	1:C:313:PHE:CD2	2.54	0.42
1:D:212:TRP:HB2	1:D:215:PHE:CE1	2.55	0.42
1:E:202:LEU:HB2	1:E:203:PRO:HD3	2.01	0.42
1:E:253:TYR:O	1:E:256:ALA:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:283:GLN:O	1:E:283:GLN:HG2	2.20	0.42
1:B:137:ARG:HA	1:B:137:ARG:HD3	1.63	0.42
1:B:270:ILE:HA	1:B:270:ILE:HD13	1.64	0.42
1:C:122:SER:OG	1:C:190:SER:HB2	2.20	0.42
1:C:270:ILE:HD13	1:C:270:ILE:HA	1.67	0.42
1:D:274:VAL:C	1:D:276:HIS:N	2.77	0.42
1:B:309:LEU:HD12	1:B:309:LEU:HA	1.75	0.42
1:C:62:VAL:HG13	1:C:93:VAL:C	2.44	0.42
1:C:151:ASN:HD22	1:C:152:ASP:H	1.67	0.42
1:E:122:SER:OG	1:E:190:SER:HB2	2.20	0.42
1:A:153:ASP:O	1:A:154:VAL:C	2.62	0.42
1:A:213:THR:HG22	1:A:226:LEU:HD12	2.02	0.42
1:A:283:GLN:C	1:A:285:ALA:N	2.77	0.42
1:B:153:ASP:O	1:B:154:VAL:C	2.62	0.42
1:C:226:LEU:HD22	1:C:226:LEU:HA	1.47	0.42
1:C:300:VAL:O	1:C:304:LEU:HB2	2.19	0.42
1:D:53:PHE:CD1	1:D:53:PHE:O	2.72	0.42
1:E:194:PHE:CD2	1:E:195:SER:N	2.88	0.42
1:E:212:TRP:CZ3	1:E:298:PHE:HB3	2.54	0.42
1:A:18:ASN:O	1:A:44:LEU:HA	2.20	0.42
1:A:47:LYS:HD2	1:A:49:ARG:HH21	1.81	0.42
1:B:170:PRO:HB3	1:B:183:LEU:CD2	2.50	0.42
1:B:263:LEU:O	1:B:266:PHE:N	2.51	0.42
1:C:46:TRP:CH2	1:C:73:PRO:HD3	2.55	0.42
1:C:264:PHE:CE2	1:C:302:PHE:CB	3.01	0.42
1:D:232:ILE:HA	1:D:235:ILE:HD12	2.02	0.42
1:E:47:LYS:HD2	1:E:49:ARG:HH21	1.80	0.42
1:E:119:PRO:HD3	1:E:254:THR:OG1	2.19	0.42
1:E:175:LEU:HD12	1:E:175:LEU:HA	1.69	0.42
1:E:261:ILE:CD1	1:E:302:PHE:HE1	2.32	0.42
1:A:159:TRP:CD2	1:A:189:ILE:HD12	2.54	0.42
1:A:283:GLN:O	1:A:283:GLN:HG2	2.20	0.42
1:A:305:ALA:O	1:A:309:LEU:HB2	2.19	0.42
1:B:117:ARG:O	1:B:118:TYR:C	2.63	0.42
1:B:261:ILE:CD1	1:B:302:PHE:HE1	2.33	0.42
1:D:147:LYS:CE	1:D:165:THR:HA	2.49	0.42
1:D:179:LEU:C	1:D:179:LEU:CD1	2.91	0.42
1:D:193:TYR:CD2	1:D:193:TYR:C	2.96	0.42
1:D:264:PHE:N	1:D:264:PHE:CD1	2.87	0.42
1:D:283:GLN:O	1:D:283:GLN:HG2	2.20	0.42
1:B:264:PHE:CD1	1:B:264:PHE:N	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:19:THR:HA	1:D:43:SER:O	2.20	0.42
1:D:23:LEU:HG	1:D:164:PHE:CD1	2.54	0.42
1:D:84:ARG:H	1:D:84:ARG:HG2	1.41	0.42
1:D:151:ASN:HD22	1:D:152:ASP:H	1.67	0.42
1:D:194:PHE:HA	1:D:197:ILE:HD12	2.02	0.42
1:D:261:ILE:O	1:D:262:TYR:C	2.63	0.42
1:E:196:TYR:N	1:E:196:TYR:HD1	2.18	0.42
1:E:253:TYR:HA	1:E:313:PHE:CD2	2.54	0.42
1:E:305:ALA:O	1:E:309:LEU:HB2	2.20	0.42
1:B:84:ARG:H	1:B:84:ARG:HG2	1.41	0.41
1:B:283:GLN:O	1:B:283:GLN:HG2	2.20	0.41
1:C:226:LEU:HD21	1:D:224:VAL:HB	2.01	0.41
1:B:18:ASN:O	1:B:44:LEU:HA	2.20	0.41
1:C:170:PRO:HB3	1:C:183:LEU:CD2	2.50	0.41
1:D:78:VAL:HB	1:D:128:TYR:CB	2.49	0.41
1:E:84:ARG:HA	1:E:107:ALA:HB2	2.01	0.41
1:A:255:GLY:O	1:A:258:ILE:HG22	2.20	0.41
1:B:19:THR:HA	1:B:43:SER:O	2.21	0.41
1:C:24:ILE:HG21	1:C:104:ARG:HH21	1.85	0.41
1:C:175:LEU:HD12	1:C:175:LEU:HA	1.69	0.41
1:D:57:ARG:H	1:D:57:ARG:HG2	1.73	0.41
1:D:303:LEU:HD23	1:D:303:LEU:C	2.45	0.41
1:B:281:GLU:O	1:B:283:GLN:N	2.48	0.41
1:C:212:TRP:HB2	1:C:215:PHE:CE1	2.55	0.41
1:C:224:VAL:O	1:C:226:LEU:N	2.52	0.41
1:D:77:PHE:HD1	1:D:84:ARG:HD2	1.79	0.41
1:D:123:GLN:NE2	1:D:123:GLN:HA	2.35	0.41
1:D:241:VAL:C	1:D:243:THR:H	2.29	0.41
1:E:130:ILE:CG2	1:E:182:LYS:HB2	2.51	0.41
1:E:247:LYS:HA	1:E:247:LYS:HD3	1.74	0.41
1:B:210:ILE:HG13	1:C:266:PHE:HE1	1.85	0.41
1:D:202:LEU:HB2	1:D:203:PRO:HD3	2.03	0.41
1:E:210:ILE:O	1:E:211:SER:C	2.64	0.41
1:E:274:VAL:C	1:E:276:HIS:N	2.77	0.41
1:A:117:ARG:O	1:A:118:TYR:C	2.63	0.41
1:A:205:LEU:O	1:A:208:LEU:HB3	2.20	0.41
1:C:52:ALA:HA	1:C:95:PRO:O	2.21	0.41
1:D:76:ARG:HH22	1:D:130:ILE:CD1	2.14	0.41
1:E:281:GLU:O	1:E:283:GLN:N	2.49	0.41
1:E:283:GLN:C	1:E:285:ALA:N	2.77	0.41
1:E:313:PHE:HD1	1:E:313:PHE:HA	1.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:VAL:HB	1:A:128:TYR:CB	2.51	0.41
1:A:260:MET:CE	1:A:309:LEU:HD22	2.51	0.41
1:A:300:VAL:O	1:A:304:LEU:HB2	2.21	0.41
1:B:81:GLU:HG3	1:B:108:ARG:CG	2.48	0.41
1:C:139:ILE:HG12	1:C:172:ASN:HD21	1.85	0.41
1:C:170:PRO:HB3	1:C:183:LEU:HD23	2.01	0.41
1:C:196:TYR:O	1:C:200:ILE:HB	2.21	0.41
1:C:222:ALA:O	1:C:226:LEU:HB2	2.20	0.41
1:C:264:PHE:O	1:C:268:ALA:HB2	2.20	0.41
1:C:283:GLN:O	1:C:283:GLN:HG2	2.20	0.41
1:D:153:ASP:O	1:D:154:VAL:C	2.63	0.41
1:E:179:LEU:C	1:E:179:LEU:CD1	2.92	0.41
1:A:261:ILE:CD1	1:A:302:PHE:HE1	2.33	0.41
1:C:41:PHE:CE1	1:C:104:ARG:HG3	2.56	0.41
1:D:24:ILE:HG21	1:D:104:ARG:HH21	1.86	0.41
1:E:309:LEU:HD12	1:E:309:LEU:HA	1.79	0.41
1:A:10:ILE:H	1:A:10:ILE:HG13	1.62	0.41
1:A:121:ASP:CG	1:A:191:ARG:HH21	2.28	0.41
1:A:303:LEU:C	1:A:303:LEU:HD23	2.46	0.41
1:B:78:VAL:CG2	1:B:128:TYR:HB3	2.50	0.41
1:B:139:ILE:HG12	1:B:172:ASN:HD21	1.86	0.41
1:B:226:LEU:HA	1:B:226:LEU:HD22	1.58	0.41
1:B:256:ALA:HB1	1:B:309:LEU:HD21	2.02	0.41
1:C:70:ILE:N	1:C:70:ILE:HD13	2.36	0.41
1:C:197:ILE:HG23	1:C:202:LEU:HG	2.02	0.41
1:C:213:THR:CG2	1:C:226:LEU:HD11	2.48	0.41
1:C:259:PHE:CD2	1:C:259:PHE:C	2.99	0.41
1:D:51:LEU:HD13	1:D:70:ILE:HD12	2.03	0.41
1:D:117:ARG:O	1:D:118:TYR:C	2.63	0.41
1:D:205:LEU:O	1:D:208:LEU:HB3	2.21	0.41
1:D:210:ILE:O	1:D:211:SER:C	2.64	0.41
1:D:224:VAL:HG23	1:D:225:THR:N	2.36	0.41
1:D:241:VAL:C	1:D:243:THR:N	2.78	0.41
1:E:22:TYR:HB3	1:E:41:PHE:HB2	2.02	0.41
1:E:196:TYR:N	1:E:196:TYR:CD1	2.88	0.41
1:A:119:PRO:HD3	1:A:254:THR:OG1	2.21	0.41
1:A:179:LEU:C	1:A:179:LEU:CD1	2.93	0.41
1:A:209:PHE:HB2	1:B:266:PHE:CE1	2.56	0.41
1:C:37:LYS:HG2	1:C:108:ARG:HB3	2.03	0.41
1:C:167:VAL:O	1:C:168:VAL:C	2.64	0.41
1:C:194:PHE:O	1:C:196:TYR:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:51:LEU:HD11	1:E:93:VAL:HG21	2.02	0.41
1:E:264:PHE:N	1:E:264:PHE:HD1	2.19	0.41
1:B:94:SER:OG	1:B:95:PRO:CD	2.69	0.40
1:B:208:LEU:O	1:B:211:SER:HB3	2.21	0.40
1:C:240:LEU:HD13	1:D:239:ILE:HG12	2.02	0.40
1:D:37:LYS:HG2	1:D:108:ARG:HB3	2.02	0.40
1:D:298:PHE:CB	1:D:299:PRO:HD3	2.50	0.40
1:E:159:TRP:CD2	1:E:189:ILE:HD12	2.56	0.40
1:E:261:ILE:HD13	1:E:261:ILE:HA	1.85	0.40
1:A:9:PRO:HD3	1:A:71:TRP:CD2	2.56	0.40
1:B:194:PHE:CD2	1:B:195:SER:N	2.89	0.40
1:C:202:LEU:HB2	1:C:203:PRO:HD3	2.03	0.40
1:C:264:PHE:N	1:C:264:PHE:HD1	2.19	0.40
1:D:77:PHE:HD1	1:D:84:ARG:CD	2.35	0.40
1:D:119:PRO:HD3	1:D:254:THR:OG1	2.21	0.40
1:D:162:GLU:OE1	1:D:190:SER:HB3	2.21	0.40
1:A:144:ASP:HA	1:A:147:LYS:HB3	2.04	0.40
1:B:306:ASN:O	1:B:310:ALA:CB	2.69	0.40
1:C:121:ASP:CG	1:C:191:ARG:HH21	2.30	0.40
1:C:153:ASP:O	1:C:154:VAL:C	2.63	0.40
1:D:35:THR:OG1	1:D:108:ARG:NH2	2.53	0.40
1:D:224:VAL:O	1:D:228:VAL:HB	2.22	0.40
1:D:249:PRO:HD2	1:D:250:TYR:CD1	2.57	0.40
1:A:139:ILE:HG12	1:A:172:ASN:HD21	1.87	0.40
1:A:170:PRO:HB3	1:A:183:LEU:HD23	2.02	0.40
1:C:50:ARG:HE	1:C:50:ARG:HB3	1.56	0.40
1:C:117:ARG:O	1:C:118:TYR:C	2.63	0.40
1:C:205:LEU:O	1:C:208:LEU:HB3	2.20	0.40
1:D:54:ASP:HA	1:D:55:PRO:HD2	1.91	0.40
1:E:44:LEU:HD12	1:E:101:TYR:CD2	2.56	0.40
1:E:53:PHE:C	1:E:53:PHE:HD1	2.30	0.40
1:E:249:PRO:HD2	1:E:250:TYR:CE1	2.56	0.40
1:A:24:ILE:HG21	1:A:104:ARG:HH21	1.87	0.40
1:A:51:LEU:HD11	1:A:93:VAL:HG21	2.03	0.40
1:A:70:ILE:HG22	1:A:71:TRP:O	2.22	0.40
1:A:115:PHE:O	1:A:252:THR:HG22	2.22	0.40
1:A:232:ILE:HA	1:A:235:ILE:HD12	2.03	0.40
1:A:278:LEU:HD23	1:A:287:ALA:HA	2.03	0.40
1:B:249:PRO:HD2	1:B:250:TYR:CD1	2.57	0.40
1:C:22:TYR:HB3	1:C:41:PHE:HB2	2.04	0.40
1:C:82:ASN:O	1:C:83:ALA:C	2.65	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:TRP:CH2	1:D:73:PRO:HD3	2.57	0.40
1:D:76:ARG:O	1:D:129:LEU:HA	2.22	0.40
1:D:255:GLY:O	1:D:258:ILE:HG22	2.21	0.40
1:D:300:VAL:O	1:D:304:LEU:HB2	2.21	0.40
1:E:82:ASN:O	1:E:83:ALA:C	2.65	0.40
1:E:117:ARG:O	1:E:118:TYR:C	2.63	0.40
1:E:222:ALA:O	1:E:226:LEU:HB2	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%)	63 (20%)	6 (2%)	6	33
1	B	308/317 (97%)	241 (78%)	61 (20%)	6 (2%)	6	33
1	C	308/317 (97%)	237 (77%)	63 (20%)	8 (3%)	4	28
1	D	308/317 (97%)	236 (77%)	65 (21%)	7 (2%)	5	30
1	E	308/317 (97%)	237 (77%)	63 (20%)	8 (3%)	4	28
All	All	1540/1585 (97%)	1190 (77%)	315 (20%)	35 (2%)	5	30

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	150	LYS
1	A	194	PHE
1	B	150	LYS
1	B	194	PHE
1	C	150	LYS
1	C	194	PHE
1	D	150	LYS

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Mol	Chain	Res	Type
1	D	194	PHE
1	E	150	LYS
1	E	194	PHE
1	A	49	ARG
1	A	118	TYR
1	B	49	ARG
1	B	118	TYR
1	C	49	ARG
1	C	118	TYR
1	D	49	ARG
1	D	118	TYR
1	E	49	ARG
1	E	118	TYR
1	A	225	THR
1	C	225	THR
1	D	225	THR
1	E	225	THR
1	B	10	ILE
1	A	148	VAL
1	B	148	VAL
1	C	10	ILE
1	C	148	VAL
1	D	148	VAL
1	E	148	VAL
1	D	10	ILE
1	E	10	ILE
1	E	14	PRO
1	C	14	PRO

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	11
1	B	278/284 (98%)	224 (81%)	54 (19%)	1	9
1	C	278/284 (98%)	224 (81%)	54 (19%)	1	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	278/284 (98%)	227 (82%)	51 (18%)	2	11
1	E	278/284 (98%)	225 (81%)	53 (19%)	1	10
All	All	1390/1420 (98%)	1127 (81%)	263 (19%)	1	10

All (263) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	THR
1	A	26	CYS
1	A	32	LYS
1	A	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	109	VAL
1	A	110	LEU
1	A	122	SER
1	A	124	THR
1	A	130	ILE
1	A	139	ILE
1	A	140	VAL
1	A	141	LEU
1	A	151	ASN
1	A	154	VAL
1	A	156	LEU
1	A	157	THR
1	A	162	GLU
1	A	177	ASP
1	A	179	LEU
1	A	182	LYS
1	A	190	SER
1	A	202	LEU
1	A	211	SER
1	A	213	THR
1	A	221	GLU
1	A	226	LEU

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Mol	Chain	Res	Type
1	A	227	VAL
1	A	232	ILE
1	A	239	ILE
1	A	243	THR
1	A	252	THR
1	A	254	THR
1	A	263	LEU
1	A	269	VAL
1	A	270	ILE
1	A	274	VAL
1	A	278	LEU
1	A	290	ILE
1	A	292	ARG
1	A	304	LEU
1	A	306	ASN
1	A	313	PHE
1	A	314	PHE
1	B	16	THR
1	B	26	CYS
1	B	32	LYS
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	109	VAL
1	B	110	LEU
1	B	122	SER
1	B	124	THR
1	B	130	ILE
1	B	136	THR
1	B	139	ILE
1	B	140	VAL
1	B	141	LEU
1	B	151	ASN
1	B	154	VAL
1	B	156	LEU
1	B	157	THR

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Mol	Chain	Res	Type
1	B	162	GLU
1	B	177	ASP
1	B	179	LEU
1	B	182	LYS
1	B	190	SER
1	B	197	ILE
1	B	202	LEU
1	B	211	SER
1	B	213	THR
1	B	221	GLU
1	B	226	LEU
1	B	227	VAL
1	B	232	ILE
1	B	239	ILE
1	B	243	THR
1	B	252	THR
1	B	254	THR
1	B	260	MET
1	B	263	LEU
1	B	269	VAL
1	B	270	ILE
1	B	274	VAL
1	B	278	LEU
1	B	290	ILE
1	B	292	ARG
1	B	304	LEU
1	B	306	ASN
1	B	313	PHE
1	B	314	PHE
1	C	16	THR
1	C	26	CYS
1	C	32	LYS
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	109	VAL

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Mol	Chain	Res	Type
1	C	110	LEU
1	C	122	SER
1	C	124	THR
1	C	130	ILE
1	C	139	ILE
1	C	140	VAL
1	C	141	LEU
1	C	151	ASN
1	C	154	VAL
1	C	156	LEU
1	C	157	THR
1	C	162	GLU
1	C	177	ASP
1	C	179	LEU
1	C	190	SER
1	C	202	LEU
1	C	211	SER
1	C	213	THR
1	C	216	TRP
1	C	221	GLU
1	C	226	LEU
1	C	227	VAL
1	C	232	ILE
1	C	239	ILE
1	C	243	THR
1	C	252	THR
1	C	254	THR
1	C	258	ILE
1	C	260	MET
1	C	263	LEU
1	C	269	VAL
1	C	270	ILE
1	C	274	VAL
1	C	278	LEU
1	C	281	GLU
1	C	290	ILE
1	C	292	ARG
1	C	304	LEU
1	C	306	ASN
1	C	313	PHE
1	C	314	PHE
1	D	16	THR

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Mol	Chain	Res	Type
1	D	26	CYS
1	D	32	LYS
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	109	VAL
1	D	110	LEU
1	D	122	SER
1	D	124	THR
1	D	130	ILE
1	D	139	ILE
1	D	140	VAL
1	D	141	LEU
1	D	151	ASN
1	D	154	VAL
1	D	156	LEU
1	D	157	THR
1	D	162	GLU
1	D	177	ASP
1	D	179	LEU
1	D	182	LYS
1	D	190	SER
1	D	202	LEU
1	D	211	SER
1	D	213	THR
1	D	221	GLU
1	D	226	LEU
1	D	227	VAL
1	D	232	ILE
1	D	239	ILE
1	D	243	THR
1	D	252	THR
1	D	254	THR
1	D	263	LEU
1	D	269	VAL
1	D	270	ILE

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Mol	Chain	Res	Type
1	D	274	VAL
1	D	278	LEU
1	D	290	ILE
1	D	292	ARG
1	D	304	LEU
1	D	306	ASN
1	D	313	PHE
1	D	314	PHE
1	E	16	THR
1	E	26	CYS
1	E	32	LYS
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	109	VAL
1	E	110	LEU
1	E	122	SER
1	E	124	THR
1	E	130	ILE
1	E	136	THR
1	E	139	ILE
1	E	140	VAL
1	E	141	LEU
1	E	151	ASN
1	E	154	VAL
1	E	156	LEU
1	E	157	THR
1	E	162	GLU
1	E	177	ASP
1	E	179	LEU
1	E	182	LYS
1	E	190	SER
1	E	197	ILE
1	E	202	LEU
1	E	211	SER
1	E	213	THR

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Mol	Chain	Res	Type
1	E	221	GLU
1	E	226	LEU
1	E	227	VAL
1	E	232	ILE
1	E	239	ILE
1	E	243	THR
1	E	252	THR
1	E	254	THR
1	E	260	MET
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	304	LEU
1	E	306	ASN
1	E	313	PHE
1	E	314	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	ASN
1	A	100	GLN
1	A	138	ASN
1	A	151	ASN
1	A	172	ASN
1	A	234	HIS
1	A	238	ASN
1	A	244	ASN
1	A	283	GLN
1	B	79	ASN
1	B	100	GLN
1	B	138	ASN
1	B	151	ASN
1	B	172	ASN
1	B	234	HIS
1	B	238	ASN
1	B	244	ASN
1	B	276	HIS
1	B	283	GLN

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Mol	Chain	Res	Type
1	C	79	ASN
1	C	100	GLN
1	C	138	ASN
1	C	151	ASN
1	C	172	ASN
1	C	234	HIS
1	C	238	ASN
1	C	244	ASN
1	C	276	HIS
1	C	283	GLN
1	D	79	ASN
1	D	100	GLN
1	D	123	GLN
1	D	138	ASN
1	D	151	ASN
1	D	172	ASN
1	D	234	HIS
1	D	244	ASN
1	D	276	HIS
1	D	283	GLN
1	E	79	ASN
1	E	100	GLN
1	E	138	ASN
1	E	151	ASN
1	E	172	ASN
1	E	234	HIS
1	E	238	ASN
1	E	244	ASN
1	E	276	HIS
1	E	283	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%)	0.81	42 (13%) 7 8	83, 130, 190, 246	0
1	B	310/317 (97%)	0.88	42 (13%) 7 8	86, 129, 191, 246	0
1	C	310/317 (97%)	0.69	31 (10%) 12 13	86, 129, 191, 246	0
1	D	310/317 (97%)	0.85	42 (13%) 7 8	85, 130, 190, 246	0
1	E	310/317 (97%)	0.87	40 (12%) 7 9	88, 129, 191, 246	0
All	All	1550/1585 (97%)	0.82	197 (12%) 8 9	83, 130, 191, 246	0

All (197) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	60	VAL	9.3
1	B	153	ASP	9.3
1	E	147	LYS	7.3
1	B	152	ASP	6.8
1	C	60	VAL	6.8
1	C	144	ASP	6.7
1	E	144	ASP	6.3
1	D	56	VAL	6.0
1	A	59	GLY	5.8
1	B	47	LYS	5.3
1	D	11	ALA	5.1
1	E	149	GLY	5.0
1	C	59	GLY	5.0
1	E	285	ALA	5.0
1	A	62	VAL	4.8
1	C	153	ASP	4.7
1	A	90	ASP	4.7
1	E	184	ASP	4.7
1	A	144	ASP	4.6
1	A	206	PHE	4.6

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Mol	Chain	Res	Type	RSRZ
1	E	146	GLU	4.5
1	E	186	GLN	4.4
1	E	59	GLY	4.3
1	B	117	ARG	4.2
1	C	218	THR	4.2
1	B	216	TRP	4.2
1	B	74	GLU	4.1
1	D	144	ASP	4.1
1	E	183	LEU	4.1
1	D	57	ARG	4.1
1	A	61	ARG	4.0
1	D	128	TYR	4.0
1	E	148	VAL	3.9
1	D	111	SER	3.9
1	B	144	ASP	3.9
1	A	58	SER	3.9
1	E	168	VAL	3.8
1	A	91	ILE	3.8
1	A	186	GLN	3.7
1	E	88	VAL	3.7
1	A	11	ALA	3.7
1	A	13	GLU	3.6
1	E	47	LYS	3.6
1	D	126	HIS	3.5
1	D	145	LEU	3.5
1	A	153	ASP	3.5
1	B	15	LEU	3.4
1	A	66	GLU	3.4
1	B	132	ARG	3.4
1	A	64	THR	3.3
1	C	11	ALA	3.3
1	A	209	PHE	3.3
1	B	88	VAL	3.3
1	D	51	LEU	3.3
1	C	138	ASN	3.3
1	E	165	THR	3.3
1	A	208	LEU	3.2
1	D	153	ASP	3.2
1	D	183	LEU	3.2
1	D	187	LEU	3.2
1	E	141	LEU	3.2
1	D	61	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	177	ASP	3.1
1	C	74	GLU	3.1
1	B	49	ARG	3.1
1	D	304	LEU	3.1
1	E	218	THR	3.1
1	A	126	HIS	3.1
1	C	183	LEU	3.0
1	C	117	ARG	3.0
1	C	277	TYR	3.0
1	D	10	ILE	3.0
1	A	148	VAL	3.0
1	B	285	ALA	3.0
1	C	142	ALA	3.0
1	E	18	ASN	2.9
1	C	58	SER	2.9
1	E	126	HIS	2.9
1	E	185	TYR	2.9
1	A	139	ILE	2.9
1	E	20	GLY	2.9
1	D	263	LEU	2.9
1	B	154	VAL	2.8
1	C	55	PRO	2.8
1	A	89	VAL	2.8
1	B	136	THR	2.8
1	D	67	PRO	2.8
1	A	124	THR	2.8
1	B	266	PHE	2.8
1	D	130	ILE	2.8
1	B	148	VAL	2.8
1	C	172	ASN	2.8
1	D	186	GLN	2.8
1	A	117	ARG	2.7
1	A	12	ASP	2.7
1	D	148	VAL	2.6
1	A	10	ILE	2.6
1	E	101	TYR	2.6
1	A	47	LYS	2.6
1	B	57	ARG	2.6
1	C	83	ALA	2.6
1	C	233	ALA	2.6
1	E	277	TYR	2.6
1	E	11	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	11	ALA	2.6
1	B	275	GLN	2.6
1	D	124	THR	2.6
1	A	134	VAL	2.6
1	A	15	LEU	2.6
1	E	95	PRO	2.6
1	A	88	VAL	2.5
1	A	145	LEU	2.5
1	A	7	PRO	2.5
1	A	14	PRO	2.5
1	A	285	ALA	2.5
1	B	151	ASN	2.5
1	D	83	ALA	2.5
1	E	142	ALA	2.5
1	D	85	ASP	2.5
1	B	276	HIS	2.5
1	B	277	TYR	2.5
1	E	143	VAL	2.5
1	E	167	VAL	2.5
1	C	141	LEU	2.5
1	C	134	VAL	2.4
1	C	296	ILE	2.4
1	A	142	ALA	2.4
1	A	211	SER	2.4
1	E	60	VAL	2.4
1	D	208	LEU	2.4
1	D	231	LEU	2.4
1	B	141	LEU	2.4
1	C	139	ILE	2.4
1	C	285	ALA	2.4
1	D	234	HIS	2.3
1	D	141	LEU	2.3
1	E	166	ALA	2.3
1	C	72	ILE	2.3
1	E	19	THR	2.3
1	E	91	ILE	2.3
1	D	60	VAL	2.3
1	B	188	ARG	2.3
1	D	277	TYR	2.3
1	E	83	ALA	2.3
1	B	90	ASP	2.3
1	D	55	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	71	TRP	2.2
1	D	285	ALA	2.2
1	D	241	VAL	2.2
1	C	316	PHE	2.2
1	B	48	ASP	2.2
1	B	96	ASP	2.2
1	B	138	ASN	2.2
1	D	117	ARG	2.2
1	E	301	VAL	2.2
1	C	135	ASP	2.2
1	B	305	ALA	2.2
1	D	78	VAL	2.2
1	A	111	SER	2.2
1	B	145	LEU	2.2
1	B	263	LEU	2.2
1	E	116	ARG	2.2
1	B	101	TYR	2.2
1	D	118	TYR	2.2
1	A	74	GLU	2.2
1	B	213	THR	2.1
1	B	304	LEU	2.1
1	B	135	ASP	2.1
1	D	185	TYR	2.1
1	D	112	PRO	2.1
1	E	68	GLU	2.1
1	C	87	ASP	2.1
1	E	55	PRO	2.1
1	B	122	SER	2.1
1	E	96	ASP	2.1
1	B	292	ARG	2.1
1	D	261	ILE	2.1
1	A	167	VAL	2.1
1	D	134	VAL	2.1
1	B	118	TYR	2.1
1	A	184	ASP	2.1
1	C	184	ASP	2.1
1	B	16	THR	2.1
1	E	138	ASN	2.1
1	E	170	PRO	2.0
1	C	279	LYS	2.0
1	A	128	TYR	2.0
1	C	299	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	287	ALA	2.0
1	D	53	PHE	2.0
1	E	58	SER	2.0
1	B	56	VAL	2.0
1	B	301	VAL	2.0
1	C	168	VAL	2.0
1	D	182	LYS	2.0
1	A	221	GLU	2.0
1	D	167	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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	CS	C	1317	1/1	0.91	0.13	212,212,212,212	0

6.5 Other polymers [i](#)

There are no such residues in this entry.