



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 12:03 PM UTC

PDB ID : 2XQ8 / pdb_00002xq8
Title : Pentameric ligand gated ion channel GLIC in complex with zinc ion (Zn²⁺)
Authors : Hilf, R.J.C.; Bertozzi, C.; Zimmermann, I.; Reiter, A.; Trauner, D.; Dutzler, R.
Deposited on : 2010-09-01
Resolution : 3.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

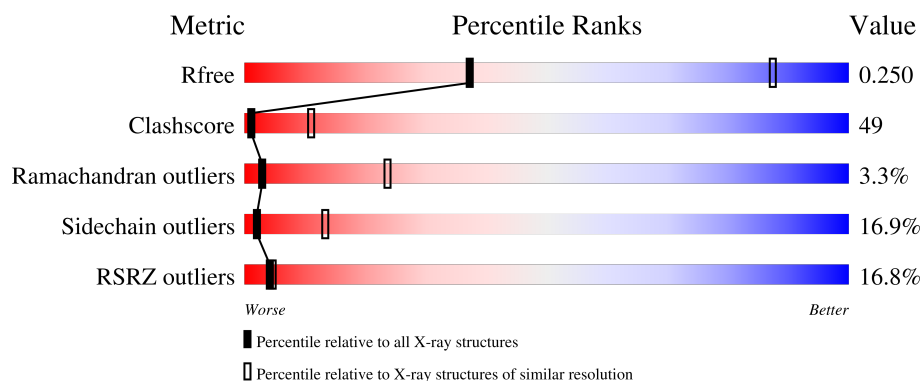
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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

Mol	Chain	Length	Quality of chain
1	A	317	16% 30% 51% 15% ..
1	B	317	15% 29% 53% 15% ..
1	C	317	16% 32% 49% 16% ..
1	D	317	18% 29% 52% 16% ..
1	E	317	17% 31% 50% 16% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ZN	C	1318	-	-	-	X

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12653 atoms, of which 0 are hydrogens and 0 are deuteriums.

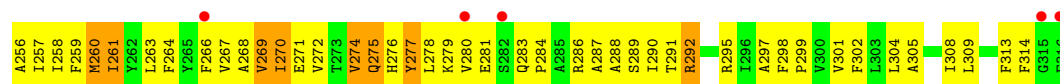
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called GLR4197 PROTEIN.

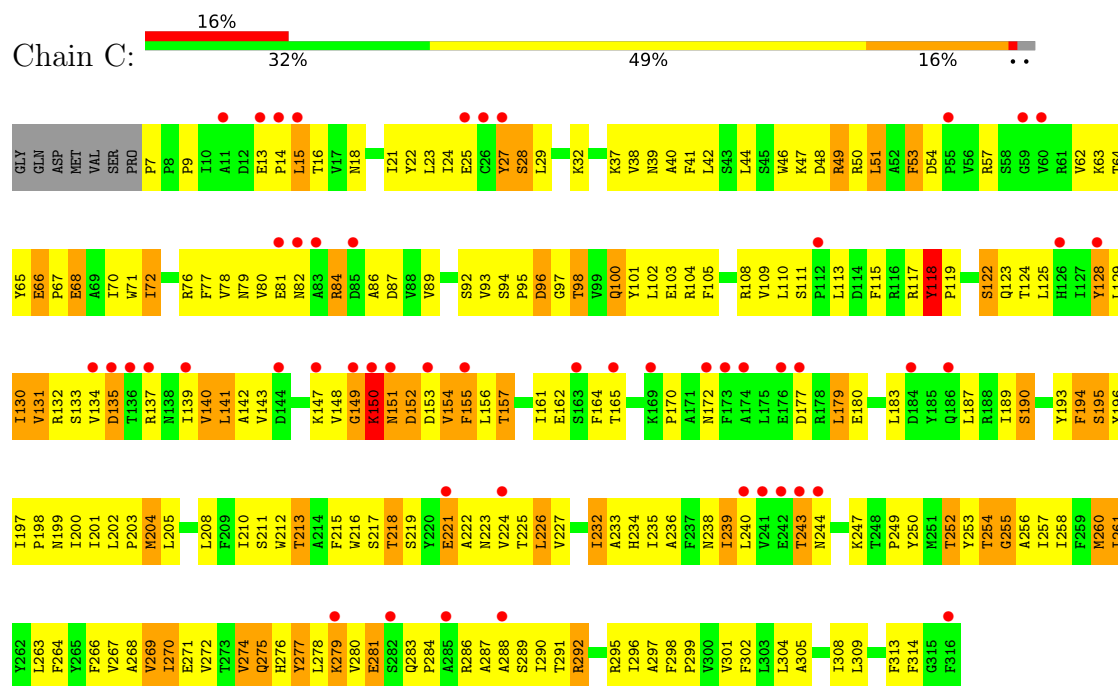
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	1	0
			2530	1667	404	455	4			
1	B	310	Total	C	N	O	S	0	1	0
			2530	1667	404	455	4			
1	C	310	Total	C	N	O	S	0	1	0
			2530	1667	404	455	4			
1	D	310	Total	C	N	O	S	0	1	0
			2530	1667	404	455	4			
1	E	310	Total	C	N	O	S	0	1	0
			2530	1667	404	455	4			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

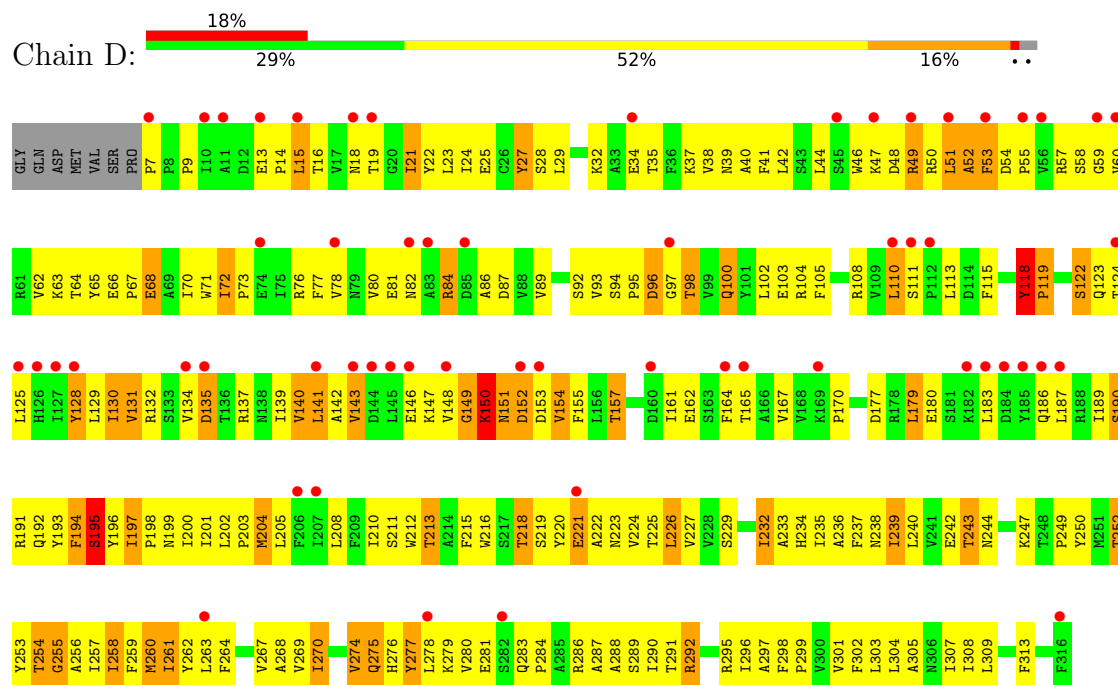
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	2	Total	Zn	0	0
			2	2		
2	D	1	Total	Zn	0	0
			1	1		



• Molecule 1: GLR4197 PROTEIN

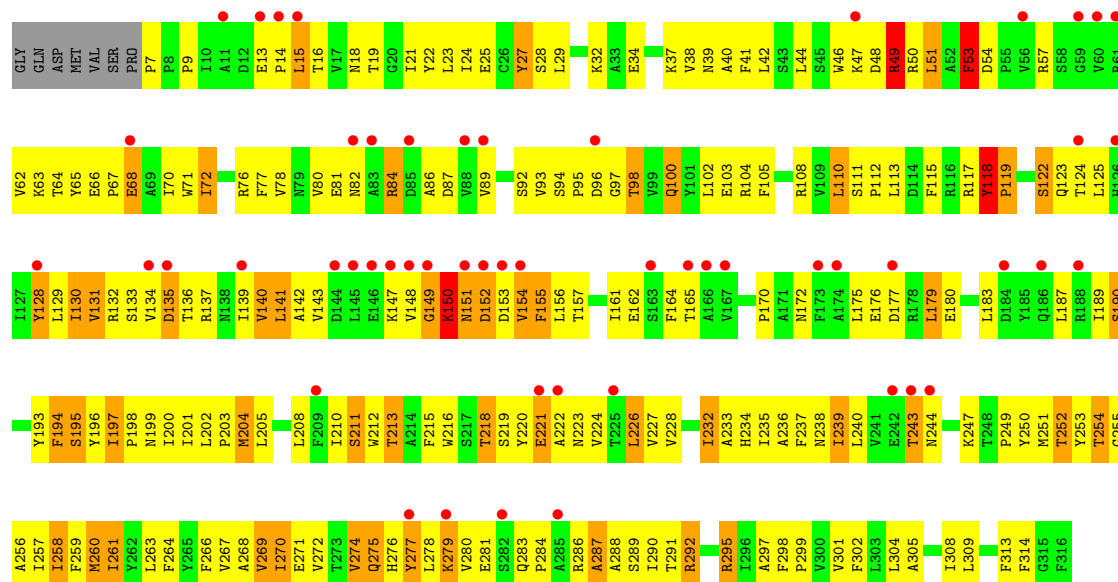


• Molecule 1: GLR4197 PROTEIN



• 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)	40.20 – 3.60 40.20 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.6 (40.20-3.60) 99.7 (40.20-3.60)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.48 (at 3.57Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.238 , 0.248 0.240 , 0.250	Depositor DCC
R_{free} test set	2172 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	94.3	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 98.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	12653	wwPDB-VP
Average B, all atoms (Å ²)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.86% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.67	1/2598 (0.0%)	1.07	17/3547 (0.5%)
1	B	0.67	1/2598 (0.0%)	1.09	17/3547 (0.5%)
1	C	0.67	0/2598	1.08	17/3547 (0.5%)
1	D	0.70	1/2598 (0.0%)	1.09	20/3547 (0.6%)
1	E	0.68	0/2598	1.09	17/3547 (0.5%)
All	All	0.68	3/12990 (0.0%)	1.08	88/17735 (0.5%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	143	VAL	CA-CB	5.44	1.60	1.53
1	B	143	VAL	CA-CB	5.17	1.60	1.53
1	A	272	VAL	CA-CB	5.16	1.60	1.54

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	128	TYR	N-CA-C	7.78	122.85	111.02
1	B	128	TYR	N-CA-C	7.71	122.45	112.12
1	E	128	TYR	N-CA-C	7.63	122.35	112.12
1	A	281	GLU	N-CA-C	-7.43	98.82	109.96
1	D	281	GLU	N-CA-C	-7.42	98.83	109.96
1	B	281	GLU	N-CA-C	-7.41	98.84	109.96
1	C	281	GLU	N-CA-C	-7.40	98.86	109.96
1	E	281	GLU	N-CA-C	-7.39	98.88	109.96
1	A	128	TYR	N-CA-C	7.16	122.01	111.34
1	A	118	TYR	CA-C-N	-7.11	112.46	119.64
1	A	118	TYR	C-N-CA	-7.11	112.46	119.64
1	E	111	SER	CA-C-N	7.04	127.21	120.31
1	E	111	SER	C-N-CA	7.04	127.21	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	128	TYR	N-CA-C	6.94	121.68	111.34
1	C	111	SER	CA-C-N	6.83	127.00	120.31
1	C	111	SER	C-N-CA	6.83	127.00	120.31
1	B	118	TYR	CA-C-N	-6.73	112.84	119.64
1	B	118	TYR	C-N-CA	-6.73	112.84	119.64
1	B	111	SER	CA-C-N	6.69	126.87	120.31
1	B	111	SER	C-N-CA	6.69	126.87	120.31
1	A	255	GLY	N-CA-C	-6.66	104.44	113.37
1	D	111	SER	CA-C-N	6.27	126.45	120.31
1	D	111	SER	C-N-CA	6.27	126.45	120.31
1	C	255	GLY	N-CA-C	-6.26	104.99	113.37
1	A	87	ASP	N-CA-C	-6.25	100.00	109.95
1	B	87	ASP	N-CA-C	-6.25	100.01	109.95
1	C	87	ASP	N-CA-C	-6.24	100.02	109.95
1	E	87	ASP	N-CA-C	-6.24	100.03	109.95
1	D	87	ASP	N-CA-C	-6.23	100.04	109.95
1	D	118	TYR	CA-C-N	-6.21	112.61	119.19
1	D	118	TYR	C-N-CA	-6.21	112.61	119.19
1	C	118	TYR	CA-C-N	-6.13	112.70	119.19
1	C	118	TYR	C-N-CA	-6.13	112.70	119.19
1	E	136	THR	N-CA-C	-5.97	99.92	109.96
1	D	255	GLY	N-CA-C	-5.93	105.43	113.37
1	A	111	SER	CA-C-N	5.92	126.11	120.31
1	A	111	SER	C-N-CA	5.92	126.11	120.31
1	D	60	VAL	N-CA-C	5.82	115.92	108.82
1	A	27	TYR	CB-CA-C	-5.82	100.48	110.95
1	D	167	VAL	CB-CA-C	-5.81	105.64	111.80
1	E	149	GLY	N-CA-C	5.81	126.95	113.18
1	C	149	GLY	N-CA-C	5.80	126.93	113.18
1	A	149	GLY	N-CA-C	5.80	126.93	113.18
1	B	149	GLY	N-CA-C	5.80	126.92	113.18
1	C	135	ASP	N-CA-C	-5.80	105.47	113.18
1	D	149	GLY	N-CA-C	5.79	126.91	113.18
1	E	135	ASP	N-CA-C	-5.79	105.48	113.18
1	D	52	ALA	N-CA-C	-5.78	102.90	110.53
1	A	135	ASP	N-CA-C	-5.78	105.49	113.18
1	B	135	ASP	N-CA-C	-5.77	105.50	113.18
1	D	135	ASP	N-CA-C	-5.77	105.50	113.18
1	D	195	SER	N-CA-C	-5.72	105.39	112.38
1	B	136	THR	N-CA-C	-5.62	100.53	109.96
1	B	255	GLY	N-CA-C	-5.60	105.87	113.37
1	D	186	GLN	N-CA-C	5.56	117.47	108.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	118	TYR	CA-C-N	-5.50	113.36	119.19
1	E	118	TYR	C-N-CA	-5.50	113.36	119.19
1	A	186	GLN	N-CA-C	5.47	117.33	108.41
1	B	27	TYR	CB-CA-C	-5.47	101.10	110.95
1	D	119	PRO	N-CA-C	-5.45	106.43	113.57
1	C	152	ASP	N-CA-C	-5.43	107.22	112.97
1	C	279	LYS	N-CA-C	-5.42	106.39	114.64
1	D	27	TYR	CB-CA-C	-5.42	101.20	110.95
1	A	279	LYS	N-CA-C	-5.40	106.44	114.64
1	E	279	LYS	N-CA-C	-5.38	106.46	114.64
1	C	150	LYS	N-CA-C	-5.37	99.37	110.80
1	A	150	LYS	N-CA-C	-5.36	99.38	110.80
1	C	27	TYR	CB-CA-C	-5.36	101.30	110.95
1	D	150	LYS	N-CA-C	-5.35	99.39	110.80
1	E	150	LYS	N-CA-C	-5.35	99.41	110.80
1	B	150	LYS	N-CA-C	-5.33	99.45	110.80
1	A	249	PRO	N-CA-C	-5.26	107.78	114.35
1	E	152	ASP	N-CA-C	-5.21	107.10	112.93
1	D	21	ILE	N-CA-C	5.20	115.53	107.78
1	B	66	GLU	CA-C-N	5.17	125.47	119.47
1	B	66	GLU	C-N-CA	5.17	125.47	119.47
1	E	27	TYR	CB-CA-C	-5.13	101.71	110.95
1	B	152	ASP	N-CA-C	-5.08	107.24	112.93
1	E	119	PRO	N-CA-C	-5.06	106.94	113.57
1	C	66	GLU	CA-C-N	5.06	125.09	119.32
1	C	66	GLU	C-N-CA	5.06	125.09	119.32
1	D	152	ASP	N-CA-C	-5.06	107.39	113.21
1	C	155	PHE	N-CA-C	5.04	121.53	110.80
1	A	53	PHE	N-CA-C	5.04	121.52	110.80
1	E	155	PHE	N-CA-C	5.03	121.52	110.80
1	B	167	VAL	CB-CA-C	-5.02	106.48	111.80
1	A	119	PRO	N-CA-C	-5.01	107.21	114.18
1	E	53	PHE	N-CA-C	5.01	121.47	110.80

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	2530	0	2542	290	0
1	B	2530	0	2542	283	0
1	C	2530	0	2542	263	0
1	D	2530	0	2542	288	0
1	E	2530	0	2542	261	0
2	C	2	0	0	0	0
2	D	1	0	0	0	0
All	All	12653	0	12710	1248	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 49.

All (1248) 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	1.66	1.09
1:D:76:ARG:NH2	1:D:130:ILE:HD12	1.68	1.09
1:D:210:ILE:HG23	1:E:269:VAL:HG11	1.31	1.06
1:E:76:ARG:NH2	1:E:130:ILE:HD12	1.70	1.06
1:A:76:ARG:NH2	1:A:130:ILE:HD12	1.71	1.05
1:A:27:TYR:HB3	1:B:110:LEU:HD11	1.40	1.03
1:B:76:ARG:HH22	1:B:130:ILE:HD12	1.18	1.03
1:C:222:ALA:HA	1:D:221[A]:GLU:OE1	1.58	1.03
1:A:240:LEU:HD13	1:B:239:ILE:HG12	1.40	1.03
1:C:78:VAL:HG22	1:C:130:ILE:HG12	1.38	1.03
1:A:210:ILE:HG23	1:B:269:VAL:HG11	1.40	1.03
1:C:22:TYR:HA	1:C:149:GLY:HA3	1.41	1.02
1:B:22:TYR:HA	1:B:149:GLY:HA3	1.42	1.02
1:C:76:ARG:NH2	1:C:130:ILE:HD12	1.74	1.02
1:C:53:PHE:HE2	1:C:63:LYS:HB3	1.25	1.01
1:A:22:TYR:HA	1:A:149:GLY:HA3	1.42	1.01
1:D:22:TYR:HA	1:D:149:GLY:HA3	1.41	1.01
1:A:53:PHE:HE2	1:A:63:LYS:HB3	1.24	1.00
1:D:53:PHE:HE2	1:D:63:LYS:HB3	1.26	1.00
1:B:53:PHE:HE2	1:B:63:LYS:HB3	1.27	1.00
1:B:78:VAL:HG22	1:B:130:ILE:HG12	1.42	0.99
1:A:78:VAL:HG22	1:A:130:ILE:HG12	1.42	0.98
1:E:76:ARG:HH22	1:E:130:ILE:HD12	1.24	0.98
1:A:222:ALA:HB2	1:B:221[A]:GLU:HA	1.44	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:78:VAL:HG22	1:E:130:ILE:HG12	1.40	0.98
1:D:78:VAL:HG22	1:D:130:ILE:HG12	1.44	0.97
1:E:22:TYR:HA	1:E:149:GLY:HA3	1.47	0.97
1:A:76:ARG:HH22	1:A:130:ILE:HD12	1.31	0.96
1:A:221[A]:GLU:HB3	1:B:221[A]:GLU:HG2	1.47	0.96
1:E:53:PHE:HE2	1:E:63:LYS:HB3	1.28	0.95
1:C:76:ARG:HH22	1:C:130:ILE:HD12	1.32	0.94
1:A:221[B]:GLU:HG2	1:E:222:ALA:HB2	1.48	0.93
1:D:76:ARG:HH22	1:D:130:ILE:HD12	1.27	0.93
1:A:155:PHE:CE1	1:B:112:PRO:HB3	2.05	0.91
1:C:27:TYR:HB3	1:D:110:LEU:HD11	1.53	0.90
1:E:147:LYS:C	1:E:149:GLY:H	1.80	0.89
1:C:222:ALA:HB2	1:D:221[B]:GLU:HG2	1.55	0.89
1:D:225:THR:CG2	1:E:224:VAL:HG23	2.03	0.88
1:E:219:SER:OG	1:E:222:ALA:HB3	1.74	0.87
1:A:222:ALA:HB2	1:B:221[B]:GLU:HA	1.52	0.87
1:E:89:VAL:HG11	1:E:102:LEU:HD23	1.53	0.87
1:C:222:ALA:CA	1:D:221[A]:GLU:OE1	2.23	0.87
1:D:22:TYR:CD1	1:D:149:GLY:HA2	2.09	0.87
1:A:27:TYR:CB	1:B:110:LEU:HD11	2.03	0.86
1:C:219:SER:OG	1:C:222:ALA:HB3	1.75	0.86
1:B:147:LYS:C	1:B:149:GLY:H	1.83	0.85
1:D:219:SER:OG	1:D:222:ALA:HB3	1.77	0.85
1:D:89:VAL:HG11	1:D:102:LEU:HD23	1.58	0.84
1:C:89:VAL:HG11	1:C:102:LEU:HD23	1.59	0.84
1:C:147:LYS:C	1:C:149:GLY:H	1.85	0.83
1:A:89:VAL:HG11	1:A:102:LEU:HD23	1.57	0.83
1:B:22:TYR:CD1	1:B:149:GLY:HA2	2.13	0.83
1:A:219:SER:OG	1:A:222:ALA:HB3	1.77	0.83
1:B:219:SER:OG	1:B:222:ALA:HB3	1.78	0.83
1:A:150:LYS:HG3	1:A:154:VAL:HG21	1.61	0.82
1:D:155:PHE:CE1	1:E:112:PRO:HB3	2.14	0.82
1:A:221[A]:GLU:HB3	1:B:221[A]:GLU:CG	2.09	0.82
1:D:22:TYR:HA	1:D:149:GLY:CA	2.10	0.82
1:E:149:GLY:O	1:E:164:PHE:HD1	1.62	0.82
1:B:22:TYR:HA	1:B:149:GLY:CA	2.10	0.82
1:E:22:TYR:CD1	1:E:149:GLY:HA2	2.15	0.82
1:D:225:THR:HG21	1:E:224:VAL:HG23	1.60	0.82
1:C:22:TYR:HA	1:C:149:GLY:CA	2.09	0.81
1:A:147:LYS:C	1:A:149:GLY:H	1.89	0.81
1:C:22:TYR:CD1	1:C:149:GLY:HA2	2.15	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:VAL:HG11	1:B:102:LEU:HD23	1.62	0.81
1:C:149:GLY:O	1:C:164:PHE:HD1	1.63	0.81
1:A:22:TYR:HA	1:A:149:GLY:CA	2.11	0.80
1:D:257:ILE:HG22	1:D:309:LEU:HD23	1.63	0.80
1:D:141:LEU:HD23	1:D:142:ALA:H	1.47	0.80
1:A:22:TYR:CD1	1:A:149:GLY:HA2	2.17	0.80
1:C:53:PHE:CE2	1:C:63:LYS:HB3	2.16	0.80
1:C:225:THR:HG21	1:D:225:THR:OG1	1.82	0.79
1:D:147:LYS:C	1:D:149:GLY:H	1.89	0.79
1:D:150:LYS:HG3	1:D:154:VAL:HG21	1.65	0.79
1:D:229:SER:HB3	1:E:228:VAL:HG11	1.65	0.79
1:A:202:LEU:HD12	1:B:259:PHE:CZ	2.18	0.79
1:C:222:ALA:HB2	1:D:221[A]:GLU:HA	1.65	0.78
1:A:53:PHE:CE2	1:A:63:LYS:HB3	2.14	0.78
1:B:149:GLY:O	1:B:164:PHE:HD1	1.66	0.78
1:A:257:ILE:HG22	1:A:309:LEU:HD23	1.66	0.78
1:C:150:LYS:HG3	1:C:154:VAL:HG21	1.64	0.78
1:E:150:LYS:HG3	1:E:154:VAL:HG21	1.64	0.77
1:D:149:GLY:O	1:D:164:PHE:HD1	1.67	0.77
1:E:257:ILE:HG22	1:E:309:LEU:HD23	1.67	0.77
1:A:149:GLY:O	1:A:164:PHE:HD1	1.67	0.77
1:C:274:VAL:C	1:C:276:HIS:H	1.93	0.77
1:A:157:THR:CG2	1:B:34:GLU:OE1	2.33	0.76
1:C:199:ASN:HB3	1:D:242:GLU:CD	2.10	0.76
1:D:66:GLU:HG3	1:D:67:PRO:HD2	1.68	0.76
1:A:274:VAL:C	1:A:276:HIS:H	1.94	0.76
1:E:84:ARG:HH11	1:E:84:ARG:HB2	1.51	0.76
1:B:274:VAL:C	1:B:276:HIS:H	1.93	0.76
1:C:65:TYR:CG	1:C:70:ILE:HD11	2.21	0.75
1:C:257:ILE:HG22	1:C:309:LEU:HD23	1.67	0.75
1:B:66:GLU:HG3	1:B:67:PRO:HD2	1.66	0.75
1:D:274:VAL:C	1:D:276:HIS:H	1.94	0.74
1:D:84:ARG:NH1	1:D:84:ARG:HB2	2.01	0.74
1:E:22:TYR:HA	1:E:149:GLY:CA	2.15	0.74
1:E:274:VAL:C	1:E:276:HIS:H	1.94	0.74
1:A:24:ILE:HD13	1:A:104:ARG:HE	1.52	0.74
1:D:240:LEU:HD13	1:E:239:ILE:HG12	1.69	0.74
1:D:65:TYR:CG	1:D:70:ILE:HD11	2.22	0.74
1:C:24:ILE:HD13	1:C:104:ARG:HE	1.51	0.74
1:D:81:GLU:HG3	1:D:108:ARG:HG3	1.70	0.74
1:E:24:ILE:HD13	1:E:104:ARG:HE	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:TYR:CG	1:B:70:ILE:HD11	2.22	0.74
1:D:24:ILE:HD13	1:D:104:ARG:HE	1.53	0.74
1:C:222:ALA:CB	1:D:221[A]:GLU:OE1	2.35	0.74
1:D:229:SER:CB	1:E:228:VAL:HG11	2.18	0.74
1:A:65:TYR:CG	1:A:70:ILE:HD11	2.22	0.73
1:B:24:ILE:HD13	1:B:104:ARG:HE	1.52	0.73
1:B:257:ILE:HG22	1:B:309:LEU:HD23	1.69	0.73
1:B:249:PRO:HD2	1:B:250:TYR:CD1	2.24	0.73
1:E:53:PHE:CE2	1:E:63:LYS:HB3	2.19	0.73
1:E:66:GLU:HG3	1:E:67:PRO:HD2	1.70	0.73
1:E:65:TYR:CG	1:E:70:ILE:HD11	2.23	0.73
1:E:100:GLN:HA	1:E:100:GLN:HE21	1.54	0.73
1:A:217:SER:OG	1:B:220:TYR:CE2	2.41	0.73
1:C:84:ARG:HB2	1:C:84:ARG:HH11	1.54	0.73
1:B:100:GLN:HE21	1:B:100:GLN:HA	1.54	0.73
1:B:254:THR:O	1:B:258:ILE:HB	1.88	0.73
1:D:53:PHE:CE2	1:D:63:LYS:HB3	2.17	0.73
1:A:66:GLU:HG3	1:A:67:PRO:HD2	1.71	0.72
1:B:53:PHE:CE2	1:B:63:LYS:HB3	2.18	0.72
1:E:254:THR:O	1:E:258:ILE:HB	1.90	0.72
1:A:157:THR:HG21	1:B:34:GLU:OE1	1.89	0.72
1:E:84:ARG:HB2	1:E:84:ARG:NH1	2.04	0.72
1:D:96:ASP:OD1	1:D:98:THR:HB	1.90	0.72
1:C:66:GLU:HG3	1:C:67:PRO:HD2	1.72	0.72
1:D:100:GLN:HE21	1:D:100:GLN:HA	1.53	0.72
1:C:267:VAL:HG23	1:C:298:PHE:CZ	2.26	0.71
1:D:229:SER:HB3	1:E:228:VAL:CG1	2.21	0.71
1:A:62:VAL:HG11	1:A:92:SER:HB3	1.73	0.71
1:E:238:ASN:HA	1:E:258:ILE:HD11	1.72	0.71
1:A:96:ASP:OD1	1:A:98:THR:HB	1.91	0.71
1:B:141:LEU:HD23	1:B:142:ALA:H	1.55	0.71
1:E:62:VAL:HG11	1:E:92:SER:HB3	1.73	0.71
1:D:84:ARG:HB2	1:D:84:ARG:HH11	1.55	0.71
1:A:225:THR:HG22	1:B:224:VAL:HG23	1.73	0.71
1:A:240:LEU:CD1	1:B:239:ILE:HG12	2.17	0.71
1:D:238:ASN:HA	1:D:258:ILE:HD11	1.71	0.71
1:B:81:GLU:HG3	1:B:108:ARG:HG3	1.73	0.70
1:C:234:HIS:CE1	1:C:261:ILE:HG21	2.26	0.70
1:C:222:ALA:HB2	1:D:221[B]:GLU:HA	1.71	0.70
1:D:253:TYR:O	1:D:256:ALA:HB3	1.92	0.70
1:A:225:THR:CG2	1:B:224:VAL:HG23	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:ARG:HB2	1:C:84:ARG:NH1	2.06	0.70
1:D:210:ILE:CG2	1:E:269:VAL:HG11	2.16	0.70
1:D:254:THR:O	1:D:258:ILE:HB	1.91	0.70
1:A:226:LEU:CD2	1:B:224:VAL:HB	2.21	0.70
1:C:147:LYS:HG2	1:C:147:LYS:O	1.91	0.69
1:C:202:LEU:HD12	1:D:259:PHE:CE1	2.27	0.69
1:D:95:PRO:C	1:D:97:GLY:H	2.00	0.69
1:A:202:LEU:HD12	1:B:259:PHE:CE1	2.28	0.69
1:B:62:VAL:HG11	1:B:92:SER:HB3	1.73	0.69
1:A:223:ASN:O	1:A:227:VAL:HG23	1.93	0.69
1:B:267:VAL:HG23	1:B:298:PHE:CZ	2.27	0.69
1:E:243:THR:HG22	1:E:244:ASN:HD22	1.57	0.69
1:A:222:ALA:O	1:A:226:LEU:HB2	1.92	0.69
1:A:254:THR:O	1:A:258:ILE:HB	1.92	0.69
1:B:223:ASN:O	1:B:227:VAL:HG23	1.93	0.69
1:C:226:LEU:CD2	1:D:224:VAL:HB	2.23	0.69
1:E:128:TYR:O	1:E:129:LEU:HB2	1.92	0.69
1:A:222:ALA:HB2	1:B:221[A]:GLU:CA	2.21	0.69
1:B:243:THR:HG22	1:B:244:ASN:HD22	1.57	0.69
1:B:276:HIS:C	1:B:278:LEU:H	2.00	0.69
1:A:155:PHE:CZ	1:B:112:PRO:HB3	2.28	0.69
1:D:276:HIS:C	1:D:278:LEU:H	2.01	0.69
1:C:249:PRO:HD2	1:C:250:TYR:CD1	2.29	0.68
1:E:249:PRO:HD2	1:E:250:TYR:CD1	2.28	0.68
1:A:53:PHE:HE2	1:A:63:LYS:CB	2.05	0.68
1:A:84:ARG:NH1	1:A:84:ARG:HB2	2.07	0.68
1:A:249:PRO:HD2	1:A:250:TYR:CD1	2.29	0.68
1:D:62:VAL:HG11	1:D:92:SER:HB3	1.75	0.68
1:E:81:GLU:HG3	1:E:108:ARG:HG3	1.75	0.68
1:A:238:ASN:HA	1:A:258:ILE:HD11	1.76	0.68
1:C:238:ASN:HA	1:C:258:ILE:HD11	1.76	0.68
1:A:137:ARG:HD2	1:A:179:LEU:HG	1.76	0.68
1:C:149:GLY:O	1:C:164:PHE:CD1	2.45	0.68
1:E:276:HIS:C	1:E:278:LEU:H	2.01	0.68
1:A:141:LEU:HD23	1:A:142:ALA:H	1.59	0.67
1:E:149:GLY:O	1:E:164:PHE:CD1	2.45	0.67
1:C:200:ILE:HD11	1:C:240:LEU:HD23	1.76	0.67
1:D:84:ARG:HH11	1:D:84:ARG:CB	2.06	0.67
1:D:222:ALA:O	1:D:226:LEU:HB2	1.95	0.67
1:E:137:ARG:HD2	1:E:179:LEU:HG	1.76	0.67
1:A:267:VAL:HG23	1:A:298:PHE:CZ	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:GLU:HG3	1:C:108:ARG:HG3	1.76	0.67
1:E:118:TYR:CD1	1:E:118:TYR:C	2.72	0.67
1:A:149:GLY:O	1:A:164:PHE:CD1	2.48	0.67
1:B:147:LYS:C	1:B:149:GLY:N	2.52	0.67
1:C:276:HIS:C	1:C:278:LEU:H	2.02	0.67
1:C:100:GLN:HE21	1:C:100:GLN:HA	1.59	0.67
1:D:128:TYR:O	1:D:129:LEU:HB2	1.93	0.67
1:B:84:ARG:NH1	1:B:84:ARG:HB2	2.10	0.67
1:D:223:ASN:O	1:D:227:VAL:HG23	1.94	0.67
1:A:81:GLU:HG3	1:A:108:ARG:HG3	1.77	0.66
1:A:253:TYR:O	1:A:256:ALA:HB3	1.95	0.66
1:B:222:ALA:O	1:B:226:LEU:HB2	1.95	0.66
1:C:62:VAL:HG11	1:C:92:SER:HB3	1.76	0.66
1:B:23:LEU:HA	1:B:40:ALA:HB2	1.78	0.66
1:C:219:SER:HB2	1:D:221[B]:GLU:OE2	1.95	0.66
1:E:222:ALA:O	1:E:226:LEU:HB2	1.95	0.66
1:E:147:LYS:C	1:E:149:GLY:N	2.49	0.66
1:C:254:THR:O	1:C:258:ILE:HB	1.94	0.66
1:E:238:ASN:HA	1:E:258:ILE:CD1	2.25	0.66
1:D:297:ALA:O	1:D:301:VAL:HG23	1.96	0.66
1:A:147:LYS:O	1:A:147:LYS:HG2	1.95	0.66
1:D:221[A]:GLU:HB3	1:E:221[A]:GLU:HG2	1.77	0.66
1:E:96:ASP:OD1	1:E:98:THR:HB	1.94	0.66
1:E:200:ILE:HD11	1:E:240:LEU:HD23	1.77	0.66
1:A:229:SER:HB3	1:B:228:VAL:CG1	2.26	0.66
1:D:137:ARG:HD2	1:D:179:LEU:HG	1.78	0.66
1:A:128:TYR:O	1:A:129:LEU:HB2	1.95	0.66
1:D:267:VAL:HG23	1:D:298:PHE:CZ	2.30	0.66
1:B:118:TYR:CD1	1:B:118:TYR:C	2.72	0.66
1:C:53:PHE:O	1:C:53:PHE:CD1	2.48	0.66
1:E:283:GLN:N	1:E:284:PRO:HD3	2.11	0.65
1:A:276:HIS:C	1:A:278:LEU:H	2.02	0.65
1:C:29:LEU:C	1:C:29:LEU:HD23	2.22	0.65
1:C:222:ALA:HB2	1:D:221[A]:GLU:CG	2.27	0.65
1:E:84:ARG:HH11	1:E:84:ARG:CB	2.08	0.65
1:B:150:LYS:HG3	1:B:154:VAL:HG21	1.77	0.65
1:E:218:THR:HG22	1:E:279:LYS:HE2	1.78	0.65
1:B:149:GLY:O	1:B:164:PHE:CD1	2.49	0.65
1:D:47:LYS:HD2	1:D:49:ARG:HH21	1.61	0.65
1:E:234:HIS:CE1	1:E:261:ILE:HG21	2.31	0.65
1:C:223:ASN:O	1:C:227:VAL:HG23	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:249:PRO:HD2	1:D:250:TYR:CD1	2.32	0.65
1:B:84:ARG:HB2	1:B:84:ARG:HH11	1.60	0.65
1:A:118:TYR:CD1	1:A:118:TYR:C	2.70	0.65
1:B:238:ASN:HA	1:B:258:ILE:HD11	1.78	0.65
1:E:223:ASN:O	1:E:227:VAL:HG23	1.97	0.65
1:B:264:PHE:CE2	1:B:302:PHE:HB2	2.32	0.65
1:C:222:ALA:O	1:C:226:LEU:HB2	1.96	0.65
1:D:243:THR:HG22	1:D:244:ASN:HD22	1.61	0.65
1:B:54:ASP:HB2	1:B:57:ARG:HB2	1.79	0.65
1:C:283:GLN:N	1:C:284:PRO:HD3	2.12	0.65
1:D:149:GLY:O	1:D:164:PHE:CD1	2.49	0.65
1:E:264:PHE:CE2	1:E:302:PHE:HB2	2.31	0.65
1:A:218:THR:HG22	1:A:279:LYS:HE2	1.79	0.64
1:B:47:LYS:HD2	1:B:49:ARG:HH21	1.61	0.64
1:C:147:LYS:C	1:C:149:GLY:N	2.53	0.64
1:C:253:TYR:O	1:C:256:ALA:HB3	1.97	0.64
1:E:267:VAL:HG23	1:E:298:PHE:CZ	2.31	0.64
1:A:100:GLN:HE21	1:A:100:GLN:HA	1.60	0.64
1:C:218:THR:HG22	1:C:279:LYS:HE2	1.80	0.64
1:D:234:HIS:CE1	1:D:261:ILE:HG21	2.33	0.64
1:B:283:GLN:N	1:B:284:PRO:HD3	2.12	0.64
1:D:253:TYR:HA	1:D:313:PHE:CE2	2.33	0.64
1:E:147:LYS:O	1:E:147:LYS:HG2	1.95	0.64
1:A:84:ARG:HB2	1:A:84:ARG:HH11	1.60	0.64
1:C:238:ASN:HA	1:C:258:ILE:CD1	2.28	0.64
1:D:291:THR:O	1:D:295:ARG:HG3	1.97	0.64
1:E:53:PHE:O	1:E:53:PHE:CD1	2.50	0.64
1:D:54:ASP:HB2	1:D:57:ARG:HB2	1.80	0.64
1:A:226:LEU:HD23	1:B:224:VAL:HB	1.79	0.64
1:C:131:VAL:HG11	1:C:140:VAL:HG13	1.79	0.64
1:B:253:TYR:O	1:B:256:ALA:HB3	1.98	0.64
1:E:291:THR:O	1:E:295:ARG:HG3	1.98	0.64
1:C:222:ALA:CB	1:D:221[B]:GLU:HG2	2.27	0.64
1:D:283:GLN:N	1:D:284:PRO:HD3	2.13	0.64
1:E:224:VAL:C	1:E:226:LEU:H	2.05	0.64
1:A:147:LYS:HE2	1:A:165:THR:HA	1.79	0.63
1:A:297:ALA:O	1:A:301:VAL:HG23	1.97	0.63
1:C:96:ASP:OD1	1:C:98:THR:HB	1.97	0.63
1:C:128:TYR:O	1:C:129:LEU:HB2	1.99	0.63
1:D:218:THR:HG22	1:D:279:LYS:HE2	1.81	0.63
1:E:53:PHE:HE2	1:E:63:LYS:CB	2.09	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:TYR:HB3	1:B:110:LEU:CD1	2.24	0.63
1:A:77:PHE:H	1:A:84:ARG:HD3	1.62	0.63
1:A:104:ARG:NH2	1:B:78:VAL:HA	2.13	0.63
1:C:53:PHE:HE2	1:C:63:LYS:CB	2.07	0.63
1:C:118:TYR:CD1	1:C:118:TYR:C	2.74	0.63
1:B:218:THR:HG22	1:B:279:LYS:HE2	1.81	0.63
1:E:253:TYR:HA	1:E:313:PHE:CE2	2.33	0.63
1:A:104:ARG:HH22	1:B:78:VAL:HA	1.64	0.63
1:B:115:PHE:O	1:B:252:THR:HG22	1.98	0.63
1:D:221[B]:GLU:HB2	1:E:221[B]:GLU:OE2	1.99	0.63
1:A:192:GLN:CD	1:B:249:PRO:HB3	2.24	0.63
1:C:243:THR:HG22	1:C:244:ASN:HD22	1.64	0.63
1:D:76:ARG:CZ	1:D:130:ILE:HD12	2.29	0.63
1:B:297:ALA:O	1:B:301:VAL:HG23	1.99	0.63
1:C:137:ARG:HD2	1:C:179:LEU:HG	1.80	0.63
1:E:297:ALA:O	1:E:301:VAL:HG23	1.99	0.63
1:A:243:THR:HG22	1:A:244:ASN:HD22	1.63	0.62
1:A:253:TYR:HA	1:A:313:PHE:CE2	2.33	0.62
1:D:147:LYS:C	1:D:149:GLY:N	2.57	0.62
1:D:157:THR:HG21	1:E:34:GLU:OE1	1.97	0.62
1:E:76:ARG:CZ	1:E:130:ILE:HD12	2.29	0.62
1:D:238:ASN:HA	1:D:258:ILE:CD1	2.29	0.62
1:C:222:ALA:CB	1:D:221[A]:GLU:HA	2.29	0.62
1:C:147:LYS:HE2	1:C:165:THR:HA	1.81	0.62
1:C:84:ARG:HH11	1:C:84:ARG:CB	2.11	0.62
1:C:291:THR:O	1:C:295:ARG:HG3	1.99	0.62
1:D:225:THR:HG22	1:E:224:VAL:HG23	1.80	0.62
1:E:54:ASP:HB2	1:E:57:ARG:HB2	1.82	0.62
1:B:95:PRO:C	1:B:97:GLY:H	2.08	0.61
1:C:118:TYR:HB3	1:C:119:PRO:HD3	1.82	0.61
1:A:104:ARG:NH2	1:B:77:PHE:O	2.31	0.61
1:A:255:GLY:O	1:A:258:ILE:HG22	1.99	0.61
1:C:54:ASP:HB2	1:C:57:ARG:HB2	1.82	0.61
1:A:54:ASP:HB2	1:A:57:ARG:HB2	1.82	0.61
1:B:128:TYR:O	1:B:129:LEU:HB2	1.98	0.61
1:E:95:PRO:C	1:E:97:GLY:H	2.09	0.61
1:A:283:GLN:N	1:A:284:PRO:HD3	2.13	0.61
1:B:53:PHE:O	1:B:53:PHE:CD1	2.53	0.61
1:C:253:TYR:HA	1:C:313:PHE:CE2	2.35	0.61
1:D:27:TYR:HB3	1:E:110:LEU:HD11	1.83	0.61
1:C:47:LYS:HD2	1:C:49:ARG:HH21	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:ARG:CZ	1:B:130:ILE:HD12	2.31	0.61
1:D:77:PHE:H	1:D:84:ARG:HD3	1.65	0.61
1:E:141:LEU:HD23	1:E:142:ALA:H	1.63	0.61
1:A:291:THR:O	1:A:295:ARG:HG3	2.00	0.61
1:B:253:TYR:HA	1:B:313:PHE:CE2	2.35	0.61
1:B:96:ASP:OD1	1:B:98:THR:HB	2.00	0.61
1:A:53:PHE:O	1:A:53:PHE:CD1	2.54	0.61
1:D:264:PHE:CE2	1:D:302:PHE:HB2	2.36	0.61
1:E:115:PHE:O	1:E:252:THR:HG22	2.01	0.61
1:D:192:GLN:CD	1:E:249:PRO:HB3	2.25	0.61
1:A:118:TYR:HB3	1:A:119:PRO:HD3	1.83	0.60
1:B:81:GLU:HG3	1:B:108:ARG:CG	2.31	0.60
1:C:222:ALA:HB2	1:D:221[B]:GLU:CG	2.30	0.60
1:B:234:HIS:CE1	1:B:261:ILE:HG21	2.37	0.60
1:D:147:LYS:O	1:D:147:LYS:HG2	2.00	0.60
1:D:210:ILE:HD11	1:E:266:PHE:HD1	1.66	0.60
1:A:222:ALA:CB	1:B:221[A]:GLU:HA	2.23	0.60
1:C:78:VAL:CG2	1:C:130:ILE:HG12	2.25	0.60
1:D:48:ASP:C	1:D:50:ARG:H	2.09	0.60
1:B:131:VAL:HG11	1:B:140:VAL:HG13	1.82	0.60
1:D:23:LEU:HA	1:D:40:ALA:HB2	1.82	0.60
1:B:84:ARG:HH11	1:B:84:ARG:CB	2.15	0.60
1:E:224:VAL:C	1:E:226:LEU:N	2.58	0.60
1:A:29:LEU:C	1:A:29:LEU:HD23	2.26	0.60
1:B:13:GLU:HB3	1:B:14:PRO:HD2	1.84	0.60
1:B:224:VAL:C	1:B:226:LEU:H	2.10	0.60
1:C:297:ALA:O	1:C:301:VAL:HG23	2.01	0.60
1:C:202:LEU:HD12	1:D:259:PHE:HE1	1.65	0.60
1:D:118:TYR:CD1	1:D:118:TYR:C	2.75	0.60
1:C:95:PRO:C	1:C:97:GLY:H	2.10	0.60
1:E:47:LYS:HD2	1:E:49:ARG:HH21	1.66	0.60
1:D:200:ILE:HD11	1:D:240:LEU:HD23	1.84	0.59
1:A:86:ALA:HB2	1:A:105:PHE:HB3	1.84	0.59
1:C:81:GLU:HG3	1:C:108:ARG:CG	2.32	0.59
1:E:267:VAL:HA	1:E:270:ILE:HB	1.84	0.59
1:A:222:ALA:HA	1:B:221[A]:GLU:OE1	2.01	0.59
1:B:238:ASN:HA	1:B:258:ILE:CD1	2.32	0.59
1:C:28:SER:CB	1:C:37:LYS:HD2	2.32	0.59
1:A:84:ARG:HH11	1:A:84:ARG:CB	2.14	0.59
1:A:264:PHE:CE2	1:A:302:PHE:HB2	2.37	0.59
1:B:29:LEU:HD23	1:B:29:LEU:C	2.28	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:LYS:O	1:B:147:LYS:HG2	2.01	0.59
1:C:264:PHE:CE2	1:C:302:PHE:HB2	2.36	0.59
1:A:81:GLU:HG3	1:A:108:ARG:CG	2.32	0.59
1:A:229:SER:HB2	1:B:228:VAL:HG11	1.84	0.59
1:A:234:HIS:CE1	1:A:261:ILE:HG21	2.37	0.59
1:E:253:TYR:O	1:E:256:ALA:HB3	2.03	0.59
1:E:278:LEU:HD21	1:E:286:ARG:HB3	1.84	0.59
1:A:47:LYS:HD2	1:A:49:ARG:HH21	1.67	0.59
1:D:157:THR:CG2	1:E:34:GLU:OE1	2.51	0.59
1:D:304:LEU:O	1:D:308:ILE:HG12	2.03	0.59
1:E:29:LEU:C	1:E:29:LEU:HD23	2.28	0.59
1:A:226:LEU:HD23	1:B:224:VAL:CB	2.33	0.59
1:D:29:LEU:HD23	1:D:29:LEU:C	2.28	0.59
1:D:197:ILE:HA	1:D:201:ILE:HB	1.84	0.59
1:E:118:TYR:HB3	1:E:119:PRO:HD3	1.84	0.59
1:E:147:LYS:O	1:E:149:GLY:N	2.35	0.59
1:B:197:ILE:HA	1:B:201:ILE:HB	1.84	0.59
1:C:200:ILE:CD1	1:C:240:LEU:HD23	2.32	0.59
1:D:278:LEU:HD21	1:D:286:ARG:HB3	1.85	0.59
1:E:15:LEU:HD11	1:E:46:TRP:HB2	1.85	0.59
1:B:291:THR:O	1:B:295:ARG:HG3	2.02	0.58
1:D:123:GLN:HA	1:D:123:GLN:NE2	2.18	0.58
1:E:13:GLU:HB3	1:E:14:PRO:HD2	1.85	0.58
1:A:200:ILE:HD11	1:A:240:LEU:HD23	1.85	0.58
1:D:53:PHE:HE2	1:D:63:LYS:CB	2.08	0.58
1:B:225:THR:HG21	1:C:224:VAL:HG23	1.85	0.58
1:A:42:LEU:HB3	1:A:103:GLU:HG3	1.86	0.58
1:C:104:ARG:NH2	1:D:77:PHE:O	2.35	0.58
1:E:81:GLU:HG3	1:E:108:ARG:CG	2.33	0.58
1:A:224:VAL:C	1:A:226:LEU:N	2.61	0.58
1:A:274:VAL:O	1:A:276:HIS:N	2.37	0.58
1:B:53:PHE:CE1	1:B:95:PRO:HA	2.39	0.58
1:B:137:ARG:HD2	1:B:179:LEU:HG	1.84	0.58
1:C:27:TYR:CE1	1:C:37:LYS:HB3	2.39	0.58
1:D:53:PHE:HE1	1:D:95:PRO:HG3	1.67	0.58
1:D:275:GLN:O	1:D:275:GLN:HG2	2.03	0.58
1:E:283:GLN:HE21	1:E:286:ARG:HB2	1.69	0.58
1:B:15:LEU:HD11	1:B:46:TRP:HB2	1.86	0.58
1:C:53:PHE:CE1	1:C:95:PRO:HA	2.39	0.58
1:A:229:SER:CB	1:B:228:VAL:HG11	2.33	0.58
1:B:118:TYR:HB3	1:B:119:PRO:HD3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:VAL:C	1:B:226:LEU:N	2.61	0.58
1:C:222:ALA:HB2	1:D:221[A]:GLU:OE1	2.02	0.58
1:D:224:VAL:C	1:D:226:LEU:H	2.10	0.58
1:A:131:VAL:HG11	1:A:140:VAL:HG13	1.84	0.58
1:A:275:GLN:O	1:A:275:GLN:HG2	2.03	0.58
1:B:53:PHE:HE2	1:B:63:LYS:CB	2.09	0.58
1:B:119:PRO:O	1:B:193:TYR:HB3	2.04	0.58
1:D:81:GLU:HG3	1:D:108:ARG:CG	2.32	0.58
1:E:48:ASP:C	1:E:50:ARG:H	2.12	0.58
1:E:77:PHE:H	1:E:84:ARG:HD3	1.69	0.58
1:A:283:GLN:HE21	1:A:286:ARG:HB2	1.69	0.58
1:C:53:PHE:CD1	1:C:53:PHE:C	2.81	0.58
1:D:53:PHE:CE1	1:D:95:PRO:HA	2.39	0.57
1:E:53:PHE:CE1	1:E:95:PRO:HA	2.39	0.57
1:E:200:ILE:CD1	1:E:240:LEU:HD23	2.33	0.57
1:B:274:VAL:O	1:B:276:HIS:N	2.36	0.57
1:C:86:ALA:HB2	1:C:105:PHE:HB3	1.84	0.57
1:B:123:GLN:HA	1:B:123:GLN:NE2	2.20	0.57
1:B:257:ILE:O	1:B:261:ILE:HG12	2.03	0.57
1:B:283:GLN:HE21	1:B:286:ARG:HB2	1.68	0.57
1:E:202:LEU:HB2	1:E:203:PRO:HD3	1.86	0.57
1:A:238:ASN:HA	1:A:258:ILE:CD1	2.33	0.57
1:B:86:ALA:HB2	1:B:105:PHE:HB3	1.87	0.57
1:C:224:VAL:C	1:C:226:LEU:N	2.62	0.57
1:B:77:PHE:H	1:B:84:ARG:HD3	1.69	0.57
1:D:86:ALA:HB2	1:D:105:PHE:HB3	1.86	0.57
1:B:27:TYR:CE1	1:B:37:LYS:HB3	2.39	0.57
1:B:200:ILE:HD11	1:B:240:LEU:HD23	1.85	0.57
1:C:141:LEU:HD23	1:C:142:ALA:H	1.69	0.57
1:A:95:PRO:C	1:A:97:GLY:H	2.12	0.57
1:C:222:ALA:HB2	1:D:221[A]:GLU:HG2	1.87	0.57
1:E:274:VAL:C	1:E:276:HIS:N	2.62	0.57
1:B:21:ILE:O	1:B:149:GLY:HA3	2.05	0.57
1:C:257:ILE:O	1:C:261:ILE:HG12	2.05	0.57
1:B:235:ILE:HG22	1:B:239:ILE:HD12	1.86	0.57
1:C:42:LEU:HB3	1:C:103:GLU:HG3	1.87	0.57
1:C:77:PHE:H	1:C:84:ARG:HD3	1.69	0.57
1:D:267:VAL:HA	1:D:270:ILE:HB	1.87	0.57
1:E:53:PHE:CD1	1:E:53:PHE:C	2.81	0.57
1:E:147:LYS:HE2	1:E:165:THR:HA	1.87	0.57
1:E:275:GLN:O	1:E:275:GLN:HG2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:267:VAL:HA	1:B:270:ILE:HB	1.87	0.56
1:D:53:PHE:CD1	1:D:53:PHE:O	2.58	0.56
1:E:25:GLU:HB2	1:E:39:ASN:HB3	1.87	0.56
1:A:51:LEU:CD1	1:A:70:ILE:HD12	2.35	0.56
1:B:278:LEU:HD21	1:B:286:ARG:HB3	1.86	0.56
1:C:155:PHE:HD1	1:D:110:LEU:CD2	2.18	0.56
1:D:13:GLU:HB3	1:D:14:PRO:HD2	1.87	0.56
1:C:283:GLN:HE21	1:C:286:ARG:HB2	1.68	0.56
1:D:224:VAL:C	1:D:226:LEU:N	2.61	0.56
1:D:255:GLY:O	1:D:258:ILE:HG22	2.04	0.56
1:E:23:LEU:HA	1:E:40:ALA:HB2	1.87	0.56
1:A:170:PRO:HB3	1:A:183:LEU:HD23	1.88	0.56
1:B:147:LYS:O	1:B:149:GLY:N	2.38	0.56
1:B:243:THR:HG22	1:B:244:ASN:ND2	2.19	0.56
1:C:267:VAL:HA	1:C:270:ILE:HB	1.87	0.56
1:A:23:LEU:HA	1:A:40:ALA:HB2	1.88	0.56
1:A:119:PRO:O	1:A:193:TYR:HB3	2.05	0.56
1:C:93:VAL:HG12	1:C:94:SER:O	2.05	0.56
1:E:264:PHE:HE2	1:E:302:PHE:HB2	1.69	0.56
1:A:157:THR:HG22	1:B:34:GLU:OE1	2.04	0.56
1:A:221[B]:GLU:HB2	1:B:221[B]:GLU:CD	2.30	0.56
1:A:277:TYR:HA	1:A:280:VAL:HG22	1.88	0.56
1:C:274:VAL:O	1:C:276:HIS:N	2.37	0.56
1:C:224:VAL:C	1:C:226:LEU:H	2.12	0.56
1:D:131:VAL:HG11	1:D:140:VAL:HG13	1.87	0.56
1:D:194:PHE:C	1:D:196:TYR:N	2.63	0.56
1:B:51:LEU:CD1	1:B:70:ILE:HD12	2.36	0.56
1:D:283:GLN:HE21	1:D:286:ARG:HB2	1.70	0.56
1:E:131:VAL:HG11	1:E:140:VAL:HG13	1.86	0.56
1:A:78:VAL:CG2	1:A:130:ILE:HG12	2.27	0.56
1:C:122:SER:OG	1:C:190:SER:HB2	2.06	0.56
1:C:202:LEU:HB2	1:C:203:PRO:HD3	1.88	0.56
1:C:275:GLN:O	1:C:275:GLN:HG2	2.04	0.56
1:D:202:LEU:HD12	1:E:259:PHE:CZ	2.41	0.56
1:A:215:PHE:HB2	1:A:216:TRP:CE3	2.42	0.55
1:C:13:GLU:HB3	1:C:14:PRO:HD2	1.88	0.55
1:D:257:ILE:O	1:D:261:ILE:HG12	2.07	0.55
1:E:86:ALA:HB2	1:E:105:PHE:HB3	1.87	0.55
1:A:304:LEU:O	1:A:308:ILE:HG12	2.06	0.55
1:A:53:PHE:CD1	1:A:53:PHE:C	2.83	0.55
1:B:53:PHE:CD1	1:B:53:PHE:C	2.83	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:ILE:O	1:B:204:MET:HB2	2.06	0.55
1:C:215:PHE:HZ	1:C:298:PHE:CE1	2.24	0.55
1:D:21:ILE:O	1:D:149:GLY:HA3	2.05	0.55
1:E:274:VAL:O	1:E:276:HIS:N	2.36	0.55
1:A:224:VAL:C	1:A:226:LEU:H	2.14	0.55
1:D:51:LEU:CD1	1:D:70:ILE:HD12	2.36	0.55
1:D:147:LYS:HE2	1:D:165:THR:HA	1.88	0.55
1:E:21:ILE:O	1:E:149:GLY:HA3	2.07	0.55
1:E:89:VAL:CG1	1:E:102:LEU:HD23	2.29	0.55
1:B:23:LEU:HD22	1:B:38:VAL:HG21	1.89	0.55
1:C:21:ILE:O	1:C:149:GLY:HA3	2.07	0.55
1:D:42:LEU:HB3	1:D:103:GLU:HG3	1.87	0.55
1:A:93:VAL:HG12	1:A:94:SER:O	2.06	0.55
1:C:65:TYR:CD2	1:C:70:ILE:HD11	2.42	0.55
1:C:76:ARG:CZ	1:C:130:ILE:HD12	2.37	0.55
1:E:243:THR:HG22	1:E:244:ASN:ND2	2.22	0.55
1:E:304:LEU:O	1:E:308:ILE:HG12	2.07	0.55
1:A:274:VAL:C	1:A:276:HIS:N	2.62	0.55
1:B:264:PHE:HE2	1:B:302:PHE:HB2	1.69	0.55
1:C:89:VAL:CG1	1:C:102:LEU:HD23	2.35	0.55
1:D:78:VAL:CG2	1:D:130:ILE:HG12	2.29	0.55
1:D:93:VAL:HG12	1:D:94:SER:O	2.07	0.55
1:D:215:PHE:HZ	1:D:298:PHE:CE1	2.25	0.55
1:E:235:ILE:HG22	1:E:239:ILE:HD12	1.88	0.55
1:A:28:SER:CB	1:A:37:LYS:HD2	2.37	0.55
1:A:76:ARG:CZ	1:A:130:ILE:HD12	2.35	0.55
1:B:215:PHE:HB2	1:B:216:TRP:CZ3	2.42	0.55
1:B:53:PHE:CD1	1:B:95:PRO:HA	2.42	0.55
1:D:53:PHE:O	1:D:54:ASP:C	2.50	0.55
1:E:264:PHE:O	1:E:268:ALA:HB2	2.07	0.55
1:A:221[A]:GLU:OE2	1:B:221[A]:GLU:OE2	2.24	0.55
1:D:18:ASN:HB3	1:D:143:VAL:HG23	1.88	0.55
1:D:202:LEU:HB2	1:D:203:PRO:HD3	1.87	0.55
1:D:274:VAL:O	1:D:276:HIS:N	2.40	0.55
1:E:215:PHE:HZ	1:E:298:PHE:CE1	2.25	0.55
1:B:261:ILE:CD1	1:B:302:PHE:HE1	2.20	0.54
1:B:305:ALA:O	1:B:309:LEU:HB2	2.07	0.54
1:C:215:PHE:HB2	1:C:216:TRP:CE3	2.42	0.54
1:C:278:LEU:HD21	1:C:286:ARG:HB3	1.88	0.54
1:D:139:ILE:HG22	1:D:140:VAL:O	2.07	0.54
1:D:215:PHE:HB2	1:D:216:TRP:CE3	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:53:PHE:CD1	1:E:95:PRO:HA	2.42	0.54
1:E:122:SER:HA	1:E:190:SER:HA	1.88	0.54
1:B:274:VAL:C	1:B:276:HIS:N	2.61	0.54
1:B:275:GLN:HG2	1:B:275:GLN:O	2.06	0.54
1:C:51:LEU:CD1	1:C:70:ILE:HD12	2.37	0.54
1:C:115:PHE:O	1:C:252:THR:HG22	2.07	0.54
1:D:48:ASP:O	1:D:50:ARG:N	2.40	0.54
1:D:89:VAL:CG1	1:D:102:LEU:HD23	2.33	0.54
1:E:27:TYR:CE1	1:E:37:LYS:HB3	2.42	0.54
1:A:267:VAL:HA	1:A:270:ILE:HB	1.89	0.54
1:D:23:LEU:HD22	1:D:38:VAL:HG21	1.90	0.54
1:A:13:GLU:HB3	1:A:14:PRO:HD2	1.88	0.54
1:A:15:LEU:HD11	1:A:46:TRP:HB2	1.89	0.54
1:A:260:MET:HE3	1:A:309:LEU:HD22	1.89	0.54
1:C:197:ILE:HA	1:C:201:ILE:HB	1.89	0.54
1:E:23:LEU:HD22	1:E:38:VAL:HG21	1.90	0.54
1:B:25:GLU:HB2	1:B:39:ASN:HB3	1.88	0.54
1:B:215:PHE:HB2	1:B:216:TRP:CE3	2.42	0.54
1:B:255:GLY:O	1:B:258:ILE:HG22	2.07	0.54
1:A:53:PHE:CE1	1:A:95:PRO:HA	2.43	0.54
1:C:147:LYS:O	1:C:149:GLY:N	2.40	0.54
1:E:257:ILE:O	1:E:261:ILE:HG12	2.07	0.54
1:A:202:LEU:HB2	1:A:203:PRO:HD3	1.89	0.54
1:E:51:LEU:CD1	1:E:70:ILE:HD12	2.38	0.54
1:A:21:ILE:O	1:A:149:GLY:HA3	2.07	0.54
1:A:104:ARG:NH1	1:B:77:PHE:O	2.40	0.54
1:A:225:THR:HG21	1:B:225:THR:OG1	2.08	0.54
1:A:226:LEU:HD23	1:B:224:VAL:CG1	2.38	0.54
1:D:215:PHE:HB2	1:D:216:TRP:CZ3	2.43	0.54
1:E:215:PHE:HB2	1:E:216:TRP:CE3	2.43	0.54
1:B:53:PHE:HE1	1:B:95:PRO:HG3	1.73	0.54
1:C:288:ALA:O	1:C:292:ARG:HB2	2.07	0.54
1:B:202:LEU:HB2	1:B:203:PRO:HD3	1.89	0.53
1:E:53:PHE:HE1	1:E:95:PRO:HG3	1.72	0.53
1:E:202:LEU:O	1:E:203:PRO:C	2.50	0.53
1:D:53:PHE:CD1	1:D:53:PHE:C	2.85	0.53
1:D:53:PHE:CD1	1:D:95:PRO:HA	2.43	0.53
1:E:42:LEU:HB3	1:E:103:GLU:HG3	1.91	0.53
1:C:15:LEU:HD11	1:C:46:TRP:HB2	1.89	0.53
1:C:23:LEU:HA	1:C:40:ALA:HB2	1.91	0.53
1:C:42:LEU:HB3	1:C:103:GLU:CG	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:TYR:HE1	1:D:247:LYS:HG3	1.73	0.53
1:A:86:ALA:HA	1:A:105:PHE:HA	1.91	0.53
1:A:215:PHE:HB2	1:A:216:TRP:CZ3	2.43	0.53
1:A:215:PHE:HZ	1:A:298:PHE:CE1	2.27	0.53
1:B:18:ASN:HB3	1:B:143:VAL:HG23	1.90	0.53
1:D:15:LEU:HD11	1:D:46:TRP:HB2	1.90	0.53
1:B:86:ALA:HA	1:B:105:PHE:HA	1.90	0.53
1:C:264:PHE:O	1:C:268:ALA:HB2	2.08	0.53
1:D:86:ALA:HA	1:D:105:PHE:HA	1.91	0.53
1:A:65:TYR:CD2	1:A:70:ILE:HD11	2.43	0.53
1:A:122:SER:HA	1:A:190:SER:HA	1.91	0.53
1:B:122:SER:HA	1:B:190:SER:HA	1.90	0.53
1:B:147:LYS:HE2	1:B:165:THR:HA	1.90	0.53
1:B:200:ILE:CD1	1:B:240:LEU:HD23	2.39	0.53
1:A:147:LYS:O	1:A:149:GLY:N	2.42	0.53
1:A:197:ILE:HA	1:A:201:ILE:HB	1.90	0.53
1:C:215:PHE:HB2	1:C:216:TRP:CZ3	2.43	0.53
1:E:70:ILE:HD13	1:E:70:ILE:N	2.24	0.53
1:A:198:PRO:CG	1:B:251:MET:HE1	2.39	0.53
1:C:53:PHE:CD1	1:C:95:PRO:HA	2.44	0.53
1:C:261:ILE:CD1	1:C:302:PHE:HE1	2.22	0.53
1:E:93:VAL:HG12	1:E:94:SER:O	2.08	0.53
1:A:94:SER:HB2	1:A:98:THR:HG22	1.91	0.53
1:A:193:TYR:O	1:A:194:PHE:HB2	2.09	0.53
1:A:222:ALA:CB	1:B:221[B]:GLU:HA	2.33	0.53
1:B:139:ILE:HG22	1:B:140:VAL:O	2.08	0.53
1:B:304:LEU:O	1:B:308:ILE:HG12	2.09	0.53
1:D:264:PHE:O	1:D:268:ALA:HB2	2.09	0.53
1:E:78:VAL:CG2	1:E:130:ILE:HG12	2.27	0.53
1:E:255:GLY:O	1:E:258:ILE:HG22	2.09	0.53
1:A:288:ALA:O	1:A:292:ARG:HB2	2.08	0.52
1:B:249:PRO:HD2	1:B:250:TYR:HD1	1.72	0.52
1:C:194:PHE:C	1:C:196:TYR:N	2.65	0.52
1:E:305:ALA:O	1:E:309:LEU:HB2	2.09	0.52
1:A:194:PHE:C	1:A:196:TYR:N	2.66	0.52
1:A:260:MET:CE	1:A:309:LEU:HD22	2.38	0.52
1:B:53:PHE:O	1:B:54:ASP:C	2.51	0.52
1:D:122:SER:HA	1:D:190:SER:HA	1.91	0.52
1:D:215:PHE:O	1:D:291:THR:CG2	2.57	0.52
1:D:264:PHE:HE2	1:D:302:PHE:HB2	1.74	0.52
1:E:123:GLN:NE2	1:E:123:GLN:HA	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:298:PHE:HB2	1:E:299:PRO:HD3	1.91	0.52
1:A:27:TYR:CE1	1:A:37:LYS:HB3	2.45	0.52
1:B:42:LEU:HB3	1:B:103:GLU:HG3	1.91	0.52
1:C:23:LEU:HD22	1:C:38:VAL:HG21	1.91	0.52
1:D:210:ILE:O	1:D:213:THR:HB	2.10	0.52
1:C:25:GLU:OE1	1:C:25:GLU:HA	2.09	0.52
1:C:86:ALA:HA	1:C:105:PHE:HA	1.91	0.52
1:C:264:PHE:HE2	1:C:302:PHE:HB2	1.74	0.52
1:C:215:PHE:O	1:C:291:THR:CG2	2.57	0.52
1:D:192:GLN:OE1	1:E:249:PRO:HB3	2.09	0.52
1:D:27:TYR:CE1	1:D:37:LYS:HB3	2.44	0.52
1:D:161:ILE:HA	1:D:189:ILE:HG22	1.91	0.52
1:D:235:ILE:HG22	1:D:239:ILE:HD12	1.92	0.52
1:E:197:ILE:HA	1:E:201:ILE:HB	1.91	0.52
1:A:23:LEU:HD22	1:A:38:VAL:HG21	1.91	0.52
1:A:235:ILE:HG22	1:A:239:ILE:HD12	1.91	0.52
1:B:78:VAL:CG2	1:B:130:ILE:HG12	2.27	0.52
1:C:18:ASN:HB3	1:C:143:VAL:HG23	1.92	0.52
1:D:42:LEU:HB3	1:D:103:GLU:CG	2.40	0.52
1:D:76:ARG:HH22	1:D:130:ILE:CD1	2.11	0.52
1:D:95:PRO:C	1:D:97:GLY:N	2.67	0.52
1:E:194:PHE:C	1:E:196:TYR:N	2.66	0.52
1:E:215:PHE:HB2	1:E:216:TRP:CZ3	2.44	0.52
1:A:233:ALA:O	1:A:236:ALA:HB3	2.10	0.52
1:B:65:TYR:CD2	1:B:70:ILE:HD11	2.45	0.52
1:B:215:PHE:HZ	1:B:298:PHE:CE1	2.28	0.52
1:C:249:PRO:HD2	1:C:250:TYR:HD1	1.75	0.52
1:D:147:LYS:O	1:D:149:GLY:N	2.43	0.52
1:E:65:TYR:CD2	1:E:70:ILE:HD11	2.44	0.52
1:E:215:PHE:O	1:E:291:THR:CG2	2.58	0.52
1:C:210:ILE:O	1:C:213:THR:HB	2.10	0.52
1:D:27:TYR:CB	1:E:110:LEU:HD11	2.40	0.52
1:D:243:THR:HG22	1:D:244:ASN:ND2	2.25	0.52
1:E:155:PHE:C	1:E:155:PHE:CD2	2.87	0.52
1:A:278:LEU:HD21	1:A:286:ARG:HB3	1.93	0.51
1:A:41:PHE:HZ	1:B:76:ARG:NH2	2.08	0.51
1:A:123:GLN:HA	1:A:123:GLN:NE2	2.26	0.51
1:A:229:SER:CB	1:B:228:VAL:CG1	2.88	0.51
1:B:288:ALA:O	1:B:292:ARG:HB2	2.09	0.51
1:C:215:PHE:HZ	1:C:298:PHE:CD1	2.28	0.51
1:D:25:GLU:HB2	1:D:39:ASN:HB3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:PHE:O	1:A:268:ALA:HB2	2.11	0.51
1:D:65:TYR:CD2	1:D:70:ILE:HD11	2.45	0.51
1:D:286:ARG:O	1:D:289:SER:HB3	2.11	0.51
1:E:48:ASP:C	1:E:50:ARG:N	2.67	0.51
1:E:249:PRO:HD2	1:E:250:TYR:HD1	1.75	0.51
1:E:277:TYR:HA	1:E:280:VAL:HG22	1.92	0.51
1:A:48:ASP:C	1:A:50:ARG:H	2.18	0.51
1:A:298:PHE:HB2	1:A:299:PRO:HD3	1.92	0.51
1:D:261:ILE:CD1	1:D:302:PHE:HE1	2.23	0.51
1:C:193:TYR:O	1:C:194:PHE:HB2	2.10	0.51
1:C:194:PHE:O	1:C:198:PRO:HD3	2.11	0.51
1:E:147:LYS:CE	1:E:165:THR:HA	2.40	0.51
1:E:161:ILE:HA	1:E:189:ILE:HG22	1.92	0.51
1:D:115:PHE:O	1:D:252:THR:HG22	2.10	0.51
1:D:193:TYR:O	1:D:194:PHE:HB2	2.11	0.51
1:E:18:ASN:HB3	1:E:143:VAL:HG23	1.93	0.51
1:E:94:SER:HB2	1:E:98:THR:HG22	1.92	0.51
1:A:139:ILE:HG22	1:A:140:VAL:O	2.10	0.51
1:A:215:PHE:O	1:A:291:THR:CG2	2.59	0.51
1:C:255:GLY:O	1:C:258:ILE:HG22	2.10	0.51
1:B:89:VAL:CG1	1:B:102:LEU:HD23	2.37	0.51
1:B:276:HIS:C	1:B:278:LEU:N	2.67	0.51
1:D:260:MET:CE	1:D:309:LEU:HD22	2.41	0.51
1:D:277:TYR:HA	1:D:280:VAL:HG22	1.92	0.51
1:D:288:ALA:O	1:D:292:ARG:HB2	2.11	0.51
1:C:122:SER:HA	1:C:190:SER:HA	1.93	0.51
1:C:222:ALA:CB	1:D:221[B]:GLU:HA	2.38	0.51
1:E:23:LEU:HG	1:E:164:PHE:CE1	2.46	0.51
1:E:288:ALA:O	1:E:292:ARG:HB2	2.10	0.51
1:A:217:SER:OG	1:B:220:TYR:HE2	1.87	0.51
1:C:123:GLN:HA	1:C:123:GLN:NE2	2.25	0.51
1:A:264:PHE:HE2	1:A:302:PHE:HB2	1.76	0.50
1:A:305:ALA:O	1:A:309:LEU:HB2	2.11	0.50
1:B:48:ASP:C	1:B:50:ARG:H	2.18	0.50
1:D:260:MET:HE3	1:D:309:LEU:HD22	1.91	0.50
1:E:122:SER:OG	1:E:190:SER:HB2	2.10	0.50
1:B:202:LEU:O	1:B:203:PRO:C	2.54	0.50
1:D:48:ASP:C	1:D:50:ARG:N	2.64	0.50
1:D:118:TYR:HB3	1:D:119:PRO:HD3	1.92	0.50
1:D:221[A]:GLU:OE2	1:E:221[A]:GLU:OE2	2.28	0.50
1:E:53:PHE:O	1:E:54:ASP:C	2.53	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:170:PRO:HB3	1:E:183:LEU:HD23	1.93	0.50
1:A:200:ILE:CD1	1:A:240:LEU:HD23	2.41	0.50
1:A:202:LEU:HD12	1:B:259:PHE:HZ	1.75	0.50
1:B:29:LEU:HB2	1:B:156:LEU:HD11	1.94	0.50
1:B:264:PHE:O	1:B:268:ALA:HB2	2.11	0.50
1:C:23:LEU:HB2	1:C:150:LYS:HA	1.93	0.50
1:C:147:LYS:CE	1:C:165:THR:HA	2.41	0.50
1:A:25:GLU:HB2	1:A:39:ASN:HB3	1.93	0.50
1:A:89:VAL:CG1	1:A:102:LEU:HD23	2.34	0.50
1:C:195:SER:O	1:C:199:ASN:HB2	2.11	0.50
1:C:243:THR:HG22	1:C:244:ASN:ND2	2.27	0.50
1:D:65:TYR:CD1	1:D:70:ILE:HD11	2.46	0.50
1:D:212:TRP:HZ3	1:D:264:PHE:HD2	1.60	0.50
1:E:274:VAL:HG12	1:E:275:GLN:N	2.26	0.50
1:A:243:THR:HG22	1:A:244:ASN:ND2	2.27	0.50
1:A:286:ARG:O	1:A:289:SER:HB3	2.12	0.50
1:B:42:LEU:HB3	1:B:103:GLU:CG	2.42	0.50
1:E:86:ALA:HA	1:E:105:PHE:HA	1.93	0.50
1:E:193:TYR:O	1:E:194:PHE:HB2	2.12	0.50
1:E:197:ILE:HB	1:E:198:PRO:HD3	1.92	0.50
1:A:257:ILE:O	1:A:261:ILE:HG12	2.12	0.50
1:C:202:LEU:O	1:C:203:PRO:C	2.52	0.50
1:C:215:PHE:O	1:C:291:THR:HG22	2.12	0.50
1:D:200:ILE:O	1:D:204:MET:HB2	2.12	0.50
1:E:261:ILE:CD1	1:E:302:PHE:HE1	2.24	0.50
1:A:115:PHE:O	1:A:252:THR:HG22	2.11	0.50
1:B:215:PHE:O	1:B:291:THR:CG2	2.60	0.50
1:B:260:MET:HE3	1:B:309:LEU:HD22	1.93	0.50
1:C:200:ILE:O	1:C:204:MET:HB2	2.12	0.50
1:D:249:PRO:HD2	1:D:250:TYR:HD1	1.77	0.50
1:A:18:ASN:HB3	1:A:143:VAL:HG23	1.94	0.50
1:A:122:SER:OG	1:A:190:SER:HB2	2.12	0.50
1:A:200:ILE:O	1:A:204:MET:HB2	2.11	0.50
1:A:226:LEU:HD23	1:B:224:VAL:HG11	1.94	0.50
1:E:42:LEU:HB3	1:E:103:GLU:CG	2.42	0.50
1:B:65:TYR:CD1	1:B:70:ILE:HD11	2.47	0.49
1:B:233:ALA:O	1:B:236:ALA:HB3	2.12	0.49
1:B:277:TYR:HA	1:B:280:VAL:HG22	1.93	0.49
1:C:25:GLU:HB2	1:C:39:ASN:HB3	1.93	0.49
1:B:7:PRO:O	1:B:50:ARG:NH1	2.43	0.49
1:B:286:ARG:O	1:B:289:SER:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:28:SER:CB	1:D:37:LYS:HD2	2.41	0.49
1:D:215:PHE:HZ	1:D:298:PHE:CD1	2.30	0.49
1:D:298:PHE:HB2	1:D:299:PRO:HD3	1.94	0.49
1:A:42:LEU:HB3	1:A:103:GLU:CG	2.41	0.49
1:B:76:ARG:HH22	1:B:130:ILE:CD1	2.07	0.49
1:C:170:PRO:HB3	1:C:183:LEU:HD23	1.95	0.49
1:C:212:TRP:HZ3	1:C:264:PHE:HD2	1.60	0.49
1:C:304:LEU:O	1:C:308:ILE:HG12	2.12	0.49
1:E:25:GLU:OE1	1:E:25:GLU:HA	2.12	0.49
1:E:76:ARG:HH12	1:E:130:ILE:HD11	1.77	0.49
1:E:286:ARG:O	1:E:289:SER:HB3	2.13	0.49
1:B:194:PHE:O	1:B:198:PRO:HD3	2.11	0.49
1:C:298:PHE:HB2	1:C:299:PRO:HD3	1.94	0.49
1:A:53:PHE:CD1	1:A:95:PRO:HA	2.47	0.49
1:A:147:LYS:CE	1:A:165:THR:HA	2.41	0.49
1:B:193:TYR:O	1:B:194:PHE:HB2	2.13	0.49
1:C:157:THR:HG22	1:D:34:GLU:OE1	2.12	0.49
1:E:195:SER:O	1:E:199:ASN:HB2	2.13	0.49
1:E:215:PHE:O	1:E:291:THR:HG22	2.13	0.49
1:A:195:SER:O	1:A:199:ASN:HB2	2.13	0.49
1:A:202:LEU:O	1:A:203:PRO:C	2.52	0.49
1:A:290:ILE:HG22	1:A:291:THR:N	2.27	0.49
1:C:234:HIS:CE1	1:C:261:ILE:CG2	2.94	0.49
1:E:151:ASN:HD22	1:E:152:ASP:H	1.60	0.49
1:A:215:PHE:HZ	1:A:298:PHE:CD1	2.31	0.49
1:B:48:ASP:C	1:B:50:ARG:N	2.70	0.49
1:B:212:TRP:HZ3	1:B:264:PHE:HD2	1.59	0.49
1:C:277:TYR:HA	1:C:280:VAL:HG22	1.94	0.49
1:E:80:VAL:HG12	1:E:82:ASN:O	2.13	0.49
1:A:249:PRO:HD2	1:A:250:TYR:HD1	1.75	0.49
1:B:161:ILE:HA	1:B:189:ILE:HG22	1.93	0.49
1:D:23:LEU:HB2	1:D:150:LYS:HA	1.95	0.49
1:D:47:LYS:CD	1:D:49:ARG:NH2	2.76	0.49
1:A:147:LYS:C	1:A:149:GLY:N	2.57	0.49
1:A:222:ALA:HB2	1:B:221[B]:GLU:HG2	1.95	0.49
1:B:151:ASN:HD22	1:B:152:ASP:H	1.61	0.49
1:C:23:LEU:HG	1:C:164:PHE:CE1	2.48	0.49
1:D:215:PHE:O	1:D:291:THR:HG22	2.12	0.49
1:D:222:ALA:CB	1:E:220:TYR:CD2	2.96	0.49
1:E:155:PHE:C	1:E:155:PHE:HD2	2.20	0.49
1:E:200:ILE:O	1:E:204:MET:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:VAL:HG12	1:B:94:SER:O	2.13	0.49
1:C:155:PHE:CD1	1:D:110:LEU:CD2	2.96	0.49
1:C:215:PHE:CZ	1:C:298:PHE:CD1	3.01	0.48
1:D:305:ALA:O	1:D:309:LEU:HB2	2.12	0.48
1:A:215:PHE:O	1:A:291:THR:HG22	2.13	0.48
1:B:298:PHE:HB2	1:B:299:PRO:HD3	1.94	0.48
1:C:305:ALA:O	1:C:309:LEU:HB2	2.12	0.48
1:D:68:GLU:CD	1:D:68:GLU:H	2.20	0.48
1:B:28:SER:CB	1:B:37:LYS:HD2	2.44	0.48
1:B:125:LEU:HB2	1:B:187:LEU:HB3	1.95	0.48
1:C:155:PHE:HD2	1:C:155:PHE:C	2.21	0.48
1:C:286:ARG:O	1:C:289:SER:HB3	2.13	0.48
1:A:155:PHE:CE1	1:B:112:PRO:CB	2.89	0.48
1:A:48:ASP:C	1:A:50:ARG:N	2.70	0.48
1:B:274:VAL:HG12	1:B:275:GLN:N	2.28	0.48
1:D:23:LEU:HG	1:D:164:PHE:CE1	2.48	0.48
1:A:276:HIS:O	1:A:280:VAL:HG22	2.14	0.48
1:B:47:LYS:HD2	1:B:49:ARG:NH2	2.28	0.48
1:B:76:ARG:HH12	1:B:130:ILE:HD11	1.79	0.48
1:C:155:PHE:C	1:C:155:PHE:CD2	2.89	0.48
1:E:80:VAL:CG1	1:E:82:ASN:O	2.62	0.48
1:C:274:VAL:HG12	1:C:275:GLN:N	2.29	0.48
1:E:215:PHE:HZ	1:E:298:PHE:CD1	2.31	0.48
1:A:23:LEU:HB2	1:A:150:LYS:HA	1.94	0.48
1:A:205:LEU:O	1:A:208:LEU:HB3	2.14	0.48
1:B:215:PHE:O	1:B:291:THR:HG22	2.14	0.48
1:C:80:VAL:HG12	1:C:82:ASN:O	2.14	0.48
1:C:287:ALA:C	1:C:289:SER:H	2.22	0.48
1:E:28:SER:CB	1:E:37:LYS:HD2	2.44	0.48
1:A:53:PHE:O	1:A:54:ASP:C	2.57	0.48
1:D:94:SER:HB2	1:D:98:THR:HG22	1.95	0.48
1:D:215:PHE:CZ	1:D:298:PHE:CD1	3.02	0.48
1:A:212:TRP:HZ3	1:A:264:PHE:HD2	1.61	0.48
1:B:170:PRO:HB3	1:B:183:LEU:HD23	1.96	0.48
1:C:205:LEU:O	1:C:208:LEU:HB3	2.13	0.48
1:D:226:LEU:HD23	1:E:224:VAL:HG11	1.96	0.48
1:C:41:PHE:HZ	1:D:76:ARG:NH2	2.12	0.47
1:C:53:PHE:O	1:C:54:ASP:C	2.56	0.47
1:D:200:ILE:CD1	1:D:240:LEU:HD23	2.44	0.47
1:A:15:LEU:O	1:A:15:LEU:HG	2.08	0.47
1:A:125:LEU:HB2	1:A:187:LEU:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:ALA:C	1:A:289:SER:H	2.22	0.47
1:B:249:PRO:HD2	1:B:250:TYR:CE1	2.49	0.47
1:A:27:TYR:CG	1:B:110:LEU:HD11	2.49	0.47
1:A:42:LEU:HD23	1:A:103:GLU:OE1	2.13	0.47
1:A:161:ILE:HA	1:A:189:ILE:HG22	1.96	0.47
1:A:274:VAL:HG12	1:A:275:GLN:N	2.29	0.47
1:A:314:PHE:CD1	1:A:314:PHE:N	2.82	0.47
1:C:161:ILE:HA	1:C:189:ILE:HG22	1.97	0.47
1:D:78:VAL:HB	1:D:128:TYR:HB2	1.96	0.47
1:D:155:PHE:C	1:D:155:PHE:CD2	2.91	0.47
1:A:19:THR:HG22	1:A:44:LEU:CD2	2.45	0.47
1:C:65:TYR:CD1	1:C:70:ILE:HD11	2.49	0.47
1:E:48:ASP:O	1:E:50:ARG:N	2.47	0.47
1:E:65:TYR:CD1	1:E:70:ILE:HD11	2.49	0.47
1:A:9:PRO:HD3	1:A:71:TRP:CE3	2.49	0.47
1:A:159:TRP:CE3	1:A:189:ILE:HD12	2.50	0.47
1:A:209:PHE:HB2	1:B:266:PHE:HE1	1.79	0.47
1:B:94:SER:HB2	1:B:98:THR:HG22	1.95	0.47
1:C:290:ILE:HG22	1:C:291:THR:N	2.29	0.47
1:E:212:TRP:HZ3	1:E:264:PHE:HD2	1.62	0.47
1:A:222:ALA:HB2	1:B:221[B]:GLU:CA	2.26	0.47
1:B:147:LYS:CE	1:B:165:THR:HA	2.44	0.47
1:C:76:ARG:HH22	1:C:130:ILE:CD1	2.17	0.47
1:D:196:TYR:O	1:D:201:ILE:HG12	2.15	0.47
1:E:29:LEU:HB2	1:E:156:LEU:HD11	1.95	0.47
1:E:139:ILE:HG12	1:E:172:ASN:HD21	1.80	0.47
1:A:65:TYR:CD1	1:A:70:ILE:HD11	2.49	0.47
1:A:210:ILE:O	1:A:213:THR:HB	2.14	0.47
1:B:47:LYS:CD	1:B:49:ARG:NH2	2.77	0.47
1:B:122:SER:OG	1:B:190:SER:HB2	2.14	0.47
1:B:260:MET:CE	1:B:309:LEU:HD22	2.44	0.47
1:C:48:ASP:C	1:C:50:ARG:H	2.23	0.47
1:C:132:ARG:HA	1:C:180:GLU:HG2	1.97	0.47
1:C:260:MET:CE	1:C:309:LEU:HD22	2.45	0.47
1:D:41:PHE:HE2	1:E:175:LEU:HD23	1.79	0.47
1:D:198:PRO:CG	1:E:251:MET:HE1	2.45	0.47
1:A:146:GLU:HG3	1:B:176:GLU:HG2	1.96	0.47
1:A:155:PHE:C	1:A:155:PHE:CD2	2.92	0.47
1:B:70:ILE:N	1:B:70:ILE:HD13	2.29	0.47
1:C:133:SER:HB3	1:C:137:ARG:HA	1.97	0.47
1:A:27:TYR:CG	1:B:110:LEU:CD1	2.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:276:HIS:C	1:D:278:LEU:N	2.68	0.47
1:A:170:PRO:HB3	1:A:183:LEU:CD2	2.45	0.47
1:A:261:ILE:CD1	1:A:302:PHE:HE1	2.27	0.47
1:B:9:PRO:HD3	1:B:71:TRP:CE3	2.50	0.47
1:B:70:ILE:HG22	1:B:71:TRP:N	2.30	0.47
1:C:46:TRP:HH2	1:C:72:ILE:HG23	1.79	0.47
1:C:47:LYS:HD2	1:C:49:ARG:NH2	2.30	0.47
1:C:197:ILE:HB	1:C:198:PRO:HD3	1.96	0.47
1:B:25:GLU:HA	1:B:25:GLU:OE1	2.14	0.46
1:B:95:PRO:C	1:B:97:GLY:N	2.73	0.46
1:C:28:SER:HB2	1:C:37:LYS:HD2	1.96	0.46
1:C:94:SER:HB2	1:C:98:THR:HG22	1.96	0.46
1:C:270:ILE:HD13	1:C:270:ILE:HA	1.66	0.46
1:D:195:SER:O	1:D:199:ASN:HB2	2.16	0.46
1:E:137:ARG:HD3	1:E:137:ARG:HA	1.58	0.46
1:E:194:PHE:O	1:E:198:PRO:HD3	2.16	0.46
1:A:194:PHE:O	1:A:198:PRO:HD3	2.15	0.46
1:A:197:ILE:HB	1:A:198:PRO:HD3	1.97	0.46
1:D:202:LEU:O	1:D:203:PRO:C	2.58	0.46
1:E:7:PRO:O	1:E:50:ARG:NH1	2.47	0.46
1:B:196:TYR:O	1:B:201:ILE:HG12	2.15	0.46
1:B:287:ALA:C	1:B:289:SER:H	2.22	0.46
1:C:53:PHE:HE1	1:C:95:PRO:HG3	1.81	0.46
1:A:54:ASP:HB2	1:A:57:ARG:HG3	1.97	0.46
1:A:215:PHE:CZ	1:A:298:PHE:CD1	3.03	0.46
1:E:9:PRO:HD3	1:E:71:TRP:CE3	2.50	0.46
1:D:9:PRO:HD3	1:D:71:TRP:CE3	2.51	0.46
1:D:122:SER:OG	1:D:190:SER:HB2	2.15	0.46
1:B:78:VAL:HB	1:B:128:TYR:HB2	1.97	0.46
1:B:137:ARG:HA	1:B:137:ARG:HD3	1.57	0.46
1:C:78:VAL:HB	1:C:128:TYR:HB2	1.98	0.46
1:D:155:PHE:CZ	1:E:112:PRO:HB3	2.50	0.46
1:E:47:LYS:CD	1:E:49:ARG:NH2	2.79	0.46
1:E:215:PHE:CZ	1:E:298:PHE:CD1	3.03	0.46
1:A:196:TYR:O	1:A:201:ILE:HG12	2.15	0.46
1:B:191:ARG:HG2	1:B:192:GLN:N	2.30	0.46
1:B:194:PHE:C	1:B:196:TYR:N	2.69	0.46
1:B:215:PHE:HZ	1:B:298:PHE:CD1	2.34	0.46
1:C:80:VAL:CG1	1:C:82:ASN:O	2.64	0.46
1:C:137:ARG:HA	1:C:137:ARG:HD3	1.56	0.46
1:C:222:ALA:HB2	1:D:221[A]:GLU:CA	2.38	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:235:ILE:HG22	1:C:239:ILE:HD12	1.98	0.46
1:D:53:PHE:CE1	1:D:95:PRO:CA	2.98	0.46
1:D:132:ARG:HA	1:D:180:GLU:HG2	1.97	0.46
1:D:237:PHE:O	1:D:238:ASN:C	2.58	0.46
1:A:151:ASN:C	1:A:153:ASP:H	2.24	0.46
1:A:212:TRP:HB2	1:A:215:PHE:CE1	2.51	0.46
1:C:314:PHE:CD1	1:C:314:PHE:N	2.84	0.46
1:E:260:MET:CE	1:E:309:LEU:HD22	2.46	0.46
1:E:287:ALA:C	1:E:289:SER:H	2.23	0.46
1:C:260:MET:HE3	1:C:309:LEU:HD22	1.96	0.46
1:D:233:ALA:O	1:D:236:ALA:HB3	2.15	0.46
1:E:276:HIS:O	1:E:280:VAL:HG22	2.16	0.46
1:A:132:ARG:HA	1:A:180:GLU:HG2	1.98	0.46
1:B:13:GLU:HB3	1:B:14:PRO:CD	2.46	0.46
1:C:48:ASP:C	1:C:50:ARG:N	2.73	0.46
1:D:66:GLU:HG3	1:D:67:PRO:CD	2.43	0.46
1:E:53:PHE:C	1:E:53:PHE:HD1	2.23	0.46
1:E:132:ARG:HA	1:E:180:GLU:HG2	1.98	0.46
1:A:51:LEU:HD13	1:A:70:ILE:HD12	1.98	0.45
1:B:23:LEU:HG	1:B:164:PHE:CE1	2.51	0.45
1:C:27:TYR:CE1	1:C:37:LYS:CB	2.99	0.45
1:C:274:VAL:C	1:C:276:HIS:N	2.61	0.45
1:D:25:GLU:OE1	1:D:25:GLU:HA	2.15	0.45
1:D:155:PHE:C	1:D:155:PHE:HD2	2.23	0.45
1:D:270:ILE:HD13	1:D:270:ILE:HA	1.64	0.45
1:B:222:ALA:HA	1:B:225:THR:HB	1.99	0.45
1:C:29:LEU:HB2	1:C:156:LEU:HD11	1.98	0.45
1:C:53:PHE:C	1:C:53:PHE:HD1	2.23	0.45
1:C:125:LEU:HB2	1:C:187:LEU:HB3	1.99	0.45
1:C:217:SER:HB2	1:D:220:TYR:CE2	2.52	0.45
1:D:104:ARG:HH22	1:E:78:VAL:HA	1.82	0.45
1:D:212:TRP:HB2	1:D:215:PHE:CE1	2.51	0.45
1:E:270:ILE:HG22	1:E:271:GLU:N	2.30	0.45
1:E:314:PHE:CD1	1:E:314:PHE:N	2.84	0.45
1:C:42:LEU:HD23	1:C:103:GLU:OE1	2.15	0.45
1:C:155:PHE:HD1	1:D:110:LEU:HD22	1.82	0.45
1:C:276:HIS:O	1:C:280:VAL:HG22	2.15	0.45
1:E:98:THR:HG22	1:E:98:THR:O	2.16	0.45
1:E:233:ALA:O	1:E:236:ALA:HB3	2.17	0.45
1:A:217:SER:CB	1:B:220:TYR:CE2	2.99	0.45
1:B:9:PRO:HD3	1:B:71:TRP:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:ASP:O	1:B:154:VAL:C	2.60	0.45
1:B:205:LEU:O	1:B:208:LEU:HB3	2.16	0.45
1:E:70:ILE:HG22	1:E:71:TRP:N	2.30	0.45
1:E:205:LEU:O	1:E:208:LEU:HB3	2.16	0.45
1:E:260:MET:HE3	1:E:309:LEU:HD22	1.97	0.45
1:A:23:LEU:HG	1:A:164:PHE:CE1	2.51	0.45
1:A:78:VAL:HB	1:A:128:TYR:HB2	1.98	0.45
1:A:247:LYS:HA	1:A:247:LYS:HD3	1.77	0.45
1:B:132:ARG:HA	1:B:180:GLU:HG2	1.98	0.45
1:B:232:ILE:HG22	1:B:233:ALA:N	2.31	0.45
1:D:48:ASP:O	1:D:51:LEU:HD23	2.17	0.45
1:D:52:ALA:HB1	1:D:95:PRO:O	2.17	0.45
1:E:23:LEU:HB2	1:E:150:LYS:HA	1.98	0.45
1:E:151:ASN:C	1:E:153:ASP:H	2.25	0.45
1:A:193:TYR:O	1:A:194:PHE:CB	2.65	0.45
1:A:209:PHE:HB2	1:B:266:PHE:CE1	2.52	0.45
1:A:270:ILE:HD13	1:A:270:ILE:HA	1.63	0.45
1:D:49:ARG:HB3	1:D:49:ARG:NH1	2.32	0.45
1:A:22:TYR:HB3	1:A:41:PHE:HB2	1.99	0.45
1:B:131:VAL:CG1	1:B:140:VAL:HG13	2.46	0.45
1:B:276:HIS:O	1:B:280:VAL:HG22	2.17	0.45
1:C:283:GLN:N	1:C:284:PRO:CD	2.79	0.45
1:D:137:ARG:HD3	1:D:137:ARG:HA	1.59	0.45
1:D:151:ASN:C	1:D:153:ASP:H	2.24	0.45
1:D:210:ILE:HG13	1:E:266:PHE:CE1	2.51	0.45
1:A:53:PHE:HE1	1:A:95:PRO:HG3	1.81	0.45
1:A:68:GLU:CD	1:A:68:GLU:H	2.25	0.45
1:A:151:ASN:HD22	1:A:152:ASP:H	1.65	0.45
1:C:117:ARG:O	1:C:118:TYR:C	2.59	0.45
1:D:274:VAL:HG12	1:D:275:GLN:N	2.32	0.45
1:E:133:SER:HB3	1:E:137:ARG:HA	1.97	0.45
1:E:276:HIS:C	1:E:278:LEU:N	2.68	0.45
1:B:237:PHE:O	1:B:238:ASN:C	2.60	0.45
1:C:70:ILE:HD13	1:C:70:ILE:N	2.32	0.45
1:B:131:VAL:O	1:B:131:VAL:HG13	2.17	0.45
1:C:151:ASN:C	1:C:153:ASP:H	2.25	0.45
1:D:80:VAL:HG12	1:D:82:ASN:O	2.16	0.45
1:E:270:ILE:HA	1:E:270:ILE:HD13	1.65	0.45
1:E:290:ILE:HG22	1:E:291:THR:N	2.30	0.45
1:A:62:VAL:CG1	1:A:92:SER:HB3	2.45	0.44
1:A:232:ILE:HG22	1:A:233:ALA:N	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:226:LEU:HD23	1:D:224:VAL:HB	1.96	0.44
1:E:53:PHE:O	1:E:53:PHE:CG	2.70	0.44
1:A:155:PHE:C	1:A:155:PHE:HD2	2.25	0.44
1:A:298:PHE:CB	1:A:299:PRO:HD3	2.47	0.44
1:B:53:PHE:C	1:B:53:PHE:HD1	2.24	0.44
1:B:210:ILE:O	1:B:213:THR:HB	2.16	0.44
1:E:125:LEU:HB2	1:E:187:LEU:HB3	1.99	0.44
1:A:193:TYR:O	1:A:193:TYR:CG	2.71	0.44
1:D:146:GLU:HG3	1:E:176:GLU:HG2	1.99	0.44
1:E:48:ASP:O	1:E:51:LEU:HD23	2.17	0.44
1:E:95:PRO:C	1:E:97:GLY:N	2.75	0.44
1:C:47:LYS:CD	1:C:49:ARG:NH2	2.80	0.44
1:C:68:GLU:CD	1:C:68:GLU:H	2.25	0.44
1:C:270:ILE:HG22	1:C:271:GLU:N	2.32	0.44
1:D:78:VAL:CG2	1:D:128:TYR:HB3	2.47	0.44
1:D:261:ILE:O	1:D:262:TYR:C	2.60	0.44
1:D:274:VAL:O	1:D:278:LEU:HB3	2.18	0.44
1:A:25:GLU:OE1	1:A:25:GLU:HA	2.17	0.44
1:A:132:ARG:NH1	1:A:175:LEU:O	2.41	0.44
1:B:76:ARG:O	1:B:129:LEU:HA	2.18	0.44
1:D:80:VAL:CG1	1:D:82:ASN:O	2.65	0.44
1:D:193:TYR:O	1:D:194:PHE:CB	2.65	0.44
1:D:194:PHE:C	1:D:196:TYR:H	2.25	0.44
1:D:240:LEU:CD1	1:E:239:ILE:HG12	2.42	0.44
1:E:283:GLN:N	1:E:284:PRO:CD	2.80	0.44
1:B:195:SER:O	1:B:199:ASN:HB2	2.18	0.44
1:C:48:ASP:O	1:C:51:LEU:HD23	2.18	0.44
1:C:54:ASP:HB2	1:C:57:ARG:HG3	2.00	0.44
1:D:76:ARG:HH12	1:D:130:ILE:HD11	1.83	0.44
1:D:194:PHE:O	1:D:198:PRO:HD3	2.17	0.44
1:D:296:ILE:O	1:D:299:PRO:HD2	2.18	0.44
1:B:18:ASN:HB3	1:B:143:VAL:CG2	2.47	0.44
1:B:225:THR:CG2	1:C:224:VAL:HG23	2.47	0.44
1:C:157:THR:CG2	1:D:34:GLU:OE1	2.66	0.44
1:D:15:LEU:O	1:D:15:LEU:HG	2.06	0.44
1:B:290:ILE:HG22	1:B:291:THR:N	2.33	0.44
1:D:28:SER:HB2	1:D:37:LYS:HD2	2.00	0.44
1:A:41:PHE:HE2	1:B:175:LEU:HD23	1.83	0.44
1:A:204:MET:HE2	1:A:204:MET:HB3	1.88	0.44
1:A:229:SER:HB3	1:B:228:VAL:HG12	1.97	0.44
1:C:271:GLU:O	1:C:272:VAL:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:13:GLU:HB3	1:E:14:PRO:CD	2.47	0.44
1:E:47:LYS:HD2	1:E:49:ARG:NH2	2.33	0.44
1:B:19:THR:HG22	1:B:44:LEU:CD2	2.48	0.43
1:B:66:GLU:HG3	1:B:67:PRO:CD	2.44	0.43
1:C:9:PRO:HD3	1:C:71:TRP:CE3	2.53	0.43
1:C:22:TYR:HB3	1:C:41:PHE:HB2	2.00	0.43
1:C:29:LEU:C	1:C:29:LEU:CD2	2.91	0.43
1:D:137:ARG:NH1	1:D:179:LEU:H	2.16	0.43
1:D:210:ILE:HG13	1:E:266:PHE:HE1	1.83	0.43
1:D:276:HIS:O	1:D:280:VAL:HG22	2.17	0.43
1:E:247:LYS:HD3	1:E:247:LYS:HA	1.83	0.43
1:A:78:VAL:CG2	1:A:128:TYR:HB3	2.48	0.43
1:A:303:LEU:O	1:A:307:ILE:HD12	2.18	0.43
1:B:53:PHE:CE1	1:B:95:PRO:CA	3.01	0.43
1:B:62:VAL:CG1	1:B:92:SER:HB3	2.46	0.43
1:B:80:VAL:CG1	1:B:82:ASN:O	2.66	0.43
1:B:80:VAL:HG12	1:B:82:ASN:O	2.18	0.43
1:C:51:LEU:HD13	1:C:70:ILE:HD12	1.99	0.43
1:D:53:PHE:HE1	1:D:95:PRO:CG	2.31	0.43
1:D:197:ILE:HB	1:D:198:PRO:HD3	1.99	0.43
1:D:290:ILE:HG22	1:D:291:THR:N	2.33	0.43
1:A:7:PRO:O	1:A:50:ARG:NH2	2.49	0.43
1:A:77:PHE:CD1	1:A:84:ARG:HD2	2.54	0.43
1:A:193:TYR:CD2	1:A:193:TYR:C	2.97	0.43
1:A:274:VAL:O	1:A:278:LEU:HB3	2.18	0.43
1:C:131:VAL:CG1	1:C:140:VAL:HG13	2.45	0.43
1:C:204:MET:HE2	1:C:204:MET:HB3	1.83	0.43
1:C:226:LEU:HD22	1:C:226:LEU:HA	1.81	0.43
1:E:210:ILE:O	1:E:213:THR:HB	2.17	0.43
1:E:275:GLN:HG3	1:E:291:THR:OG1	2.18	0.43
1:E:298:PHE:CB	1:E:299:PRO:HD3	2.48	0.43
1:A:221[A]:GLU:HB3	1:B:221[A]:GLU:HG3	1.99	0.43
1:B:283:GLN:N	1:B:284:PRO:CD	2.80	0.43
1:C:53:PHE:CE1	1:C:95:PRO:CA	3.01	0.43
1:C:232:ILE:HG22	1:C:233:ALA:N	2.32	0.43
1:D:275:GLN:HG3	1:D:291:THR:OG1	2.18	0.43
1:D:298:PHE:CB	1:D:299:PRO:HD3	2.49	0.43
1:E:9:PRO:HD3	1:E:71:TRP:CD2	2.54	0.43
1:E:78:VAL:HB	1:E:128:TYR:HB2	2.00	0.43
1:E:179:LEU:HD12	1:E:179:LEU:O	2.19	0.43
1:B:23:LEU:HA	1:B:40:ALA:CB	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:PHE:C	1:B:155:PHE:CD2	2.96	0.43
1:B:204:MET:HE2	1:B:204:MET:HB3	1.92	0.43
1:B:314:PHE:N	1:B:314:PHE:CD1	2.86	0.43
1:C:78:VAL:CG2	1:C:128:TYR:HB3	2.48	0.43
1:C:179:LEU:O	1:C:179:LEU:HD12	2.19	0.43
1:C:274:VAL:O	1:C:278:LEU:HB3	2.18	0.43
1:D:225:THR:HG22	1:D:225:THR:O	2.18	0.43
1:A:7:PRO:O	1:A:50:ARG:NH1	2.51	0.43
1:D:170:PRO:HB3	1:D:183:LEU:HD23	2.00	0.43
1:A:54:ASP:HB2	1:A:57:ARG:CG	2.48	0.43
1:B:151:ASN:C	1:B:153:ASP:H	2.26	0.43
1:B:197:ILE:HB	1:B:198:PRO:HD3	2.00	0.43
1:C:221[A]:GLU:HA	1:C:221[A]:GLU:OE1	2.18	0.43
1:D:19:THR:HG22	1:D:44:LEU:CD2	2.49	0.43
1:D:179:LEU:HD12	1:D:179:LEU:O	2.19	0.43
1:E:53:PHE:CE1	1:E:95:PRO:CA	3.01	0.43
1:A:179:LEU:O	1:A:179:LEU:HD12	2.19	0.43
1:B:225:THR:HG22	1:B:225:THR:O	2.19	0.43
1:D:47:LYS:HD2	1:D:49:ARG:NH2	2.29	0.43
1:E:234:HIS:CE1	1:E:261:ILE:CG2	3.01	0.43
1:A:137:ARG:NH1	1:A:179:LEU:H	2.17	0.43
1:A:270:ILE:HG22	1:A:271:GLU:N	2.34	0.43
1:B:193:TYR:O	1:B:194:PHE:CB	2.66	0.43
1:B:196:TYR:N	1:B:196:TYR:CD1	2.87	0.43
1:B:210:ILE:HG23	1:C:269:VAL:HG11	2.01	0.43
1:B:215:PHE:CZ	1:B:298:PHE:CD1	3.06	0.43
1:D:76:ARG:O	1:D:129:LEU:HA	2.19	0.43
1:D:274:VAL:C	1:D:276:HIS:N	2.62	0.43
1:D:287:ALA:C	1:D:289:SER:H	2.25	0.43
1:E:78:VAL:CG2	1:E:128:TYR:HB3	2.49	0.43
1:E:131:VAL:HG13	1:E:131:VAL:O	2.19	0.43
1:A:47:LYS:CD	1:A:49:ARG:NH2	2.82	0.43
1:A:146:GLU:HG3	1:B:176:GLU:CG	2.49	0.43
1:B:179:LEU:HD12	1:B:179:LEU:O	2.19	0.43
1:B:275:GLN:HG3	1:B:291:THR:OG1	2.19	0.43
1:D:196:TYR:N	1:D:196:TYR:CD1	2.87	0.43
1:D:205:LEU:O	1:D:208:LEU:HB3	2.19	0.43
1:B:28:SER:HB2	1:B:37:LYS:HD2	1.99	0.42
1:C:298:PHE:CB	1:C:299:PRO:HD3	2.50	0.42
1:D:18:ASN:HB3	1:D:143:VAL:CG2	2.49	0.42
1:D:202:LEU:HD12	1:E:259:PHE:HZ	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:232:ILE:HG22	1:D:233:ALA:N	2.32	0.42
1:E:49:ARG:NH1	1:E:49:ARG:HB3	2.33	0.42
1:A:13:GLU:HB3	1:A:14:PRO:CD	2.49	0.42
1:A:276:HIS:C	1:A:278:LEU:N	2.69	0.42
1:C:139:ILE:HG12	1:C:172:ASN:HD21	1.83	0.42
1:C:193:TYR:O	1:C:194:PHE:CB	2.66	0.42
1:E:131:VAL:CG1	1:E:140:VAL:HG13	2.50	0.42
1:A:70:ILE:N	1:A:70:ILE:HD13	2.34	0.42
1:B:48:ASP:O	1:B:50:ARG:N	2.52	0.42
1:B:49:ARG:HB3	1:B:49:ARG:NH1	2.34	0.42
1:B:212:TRP:HB2	1:B:215:PHE:CE1	2.54	0.42
1:D:55:PRO:O	1:D:58:SER:O	2.37	0.42
1:A:221[A]:GLU:OE1	1:A:221[A]:GLU:HA	2.18	0.42
1:C:46:TRP:CH2	1:C:72:ILE:HG23	2.54	0.42
1:C:70:ILE:HG22	1:C:71:TRP:N	2.35	0.42
1:E:193:TYR:O	1:E:194:PHE:CB	2.66	0.42
1:A:9:PRO:HD3	1:A:71:TRP:CD2	2.54	0.42
1:A:49:ARG:HB3	1:A:49:ARG:NH1	2.34	0.42
1:A:70:ILE:HG22	1:A:71:TRP:N	2.34	0.42
1:B:7:PRO:O	1:B:50:ARG:NH2	2.51	0.42
1:B:68:GLU:CD	1:B:68:GLU:H	2.26	0.42
1:C:13:GLU:HB3	1:C:14:PRO:CD	2.50	0.42
1:C:95:PRO:C	1:C:97:GLY:N	2.77	0.42
1:E:54:ASP:HB2	1:E:57:ARG:HG3	2.02	0.42
1:E:94:SER:CB	1:E:98:THR:HG22	2.49	0.42
1:E:221[A]:GLU:HA	1:E:221[A]:GLU:OE1	2.18	0.42
1:A:80:VAL:HG12	1:A:82:ASN:O	2.20	0.42
1:A:194:PHE:C	1:A:196:TYR:H	2.27	0.42
1:B:78:VAL:CG2	1:B:128:TYR:HB3	2.50	0.42
1:C:53:PHE:O	1:C:53:PHE:CG	2.69	0.42
1:D:283:GLN:N	1:D:284:PRO:CD	2.80	0.42
1:E:28:SER:HB2	1:E:37:LYS:HD2	2.02	0.42
1:E:68:GLU:CD	1:E:68:GLU:H	2.28	0.42
1:E:76:ARG:NH1	1:E:130:ILE:CD1	2.83	0.42
1:A:53:PHE:C	1:A:53:PHE:HD1	2.25	0.42
1:A:119:PRO:HB3	1:A:196:TYR:CD2	2.54	0.42
1:A:133:SER:HB3	1:A:137:ARG:HA	2.00	0.42
1:C:7:PRO:O	1:C:50:ARG:NH1	2.51	0.42
1:E:156:LEU:HD12	1:E:156:LEU:HA	1.74	0.42
1:E:196:TYR:O	1:E:201:ILE:HG12	2.20	0.42
1:E:274:VAL:O	1:E:278:LEU:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:ASP:O	1:A:50:ARG:N	2.52	0.42
1:A:196:TYR:N	1:A:196:TYR:CD1	2.87	0.42
1:B:210:ILE:HD11	1:C:266:PHE:HD1	1.85	0.42
1:C:194:PHE:C	1:C:196:TYR:H	2.27	0.42
1:D:98:THR:HG22	1:D:98:THR:O	2.18	0.42
1:D:191:ARG:HG2	1:D:192:GLN:N	2.33	0.42
1:D:283:GLN:O	1:D:283:GLN:HG2	2.20	0.42
1:E:22:TYR:HB3	1:E:41:PHE:HB2	2.01	0.42
1:E:309:LEU:HD12	1:E:309:LEU:HA	1.82	0.42
1:C:137:ARG:NH1	1:C:179:LEU:H	2.17	0.42
1:C:151:ASN:HD22	1:C:152:ASP:H	1.67	0.42
1:C:156:LEU:HD12	1:C:156:LEU:HA	1.73	0.42
1:D:23:LEU:HA	1:D:40:ALA:CB	2.50	0.42
1:D:35:THR:HG22	1:D:110:LEU:HG	2.01	0.42
1:E:212:TRP:HB2	1:E:215:PHE:CE1	2.55	0.42
1:B:298:PHE:CB	1:B:299:PRO:HD3	2.50	0.42
1:D:151:ASN:HD22	1:D:152:ASP:H	1.66	0.42
1:A:28:SER:HB2	1:A:37:LYS:HD2	2.00	0.41
1:A:130:ILE:HG23	1:A:182:LYS:HB2	2.02	0.41
1:C:212:TRP:HB2	1:C:215:PHE:CE1	2.54	0.41
1:C:217:SER:CB	1:D:220:TYR:HE2	2.33	0.41
1:D:125:LEU:HB2	1:D:187:LEU:HB3	2.01	0.41
1:E:237:PHE:O	1:E:238:ASN:C	2.63	0.41
1:A:98:THR:HG22	1:A:98:THR:O	2.20	0.41
1:B:274:VAL:O	1:B:278:LEU:HB3	2.19	0.41
1:C:196:TYR:O	1:C:201:ILE:HG12	2.21	0.41
1:D:70:ILE:HG22	1:D:71:TRP:N	2.34	0.41
1:D:303:LEU:O	1:D:307:ILE:HD12	2.21	0.41
1:E:15:LEU:O	1:E:15:LEU:HG	2.09	0.41
1:A:104:ARG:HH22	1:B:78:VAL:CA	2.32	0.41
1:A:191:ARG:HG2	1:A:192:GLN:N	2.36	0.41
1:B:283:GLN:O	1:B:283:GLN:HG2	2.20	0.41
1:D:47:LYS:HD3	1:D:49:ARG:NH2	2.35	0.41
1:E:224:VAL:O	1:E:226:LEU:N	2.53	0.41
1:A:48:ASP:O	1:A:51:LEU:HD23	2.21	0.41
1:A:95:PRO:C	1:A:97:GLY:N	2.77	0.41
1:A:196:TYR:CE1	1:B:247:LYS:HD2	2.56	0.41
1:A:271:GLU:O	1:A:272:VAL:C	2.64	0.41
1:A:283:GLN:O	1:A:283:GLN:HG2	2.20	0.41
1:C:240:LEU:HD13	1:D:239:ILE:HG12	2.03	0.41
1:D:7:PRO:O	1:D:50:ARG:NH2	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:137:ARG:NH1	1:E:179:LEU:H	2.19	0.41
1:E:175:LEU:HA	1:E:175:LEU:HD12	1.67	0.41
1:E:201:ILE:HD13	1:E:201:ILE:HA	1.95	0.41
1:E:283:GLN:O	1:E:283:GLN:HG2	2.20	0.41
1:A:46:TRP:HH2	1:A:72:ILE:HG23	1.85	0.41
1:B:54:ASP:HB2	1:B:57:ARG:HG3	2.01	0.41
1:B:210:ILE:O	1:B:211:SER:C	2.63	0.41
1:C:49:ARG:NH1	1:C:49:ARG:HB3	2.35	0.41
1:E:19:THR:HG22	1:E:44:LEU:CD2	2.51	0.41
1:A:131:VAL:CG1	1:A:140:VAL:HG13	2.49	0.41
1:A:137:ARG:HA	1:A:137:ARG:HD3	1.57	0.41
1:A:274:VAL:CG1	1:A:275:GLN:N	2.83	0.41
1:B:133:SER:HB3	1:B:137:ARG:HA	2.02	0.41
1:C:283:GLN:O	1:C:283:GLN:HG2	2.20	0.41
1:E:210:ILE:O	1:E:211:SER:C	2.61	0.41
1:E:271:GLU:O	1:E:272:VAL:C	2.63	0.41
1:A:94:SER:CB	1:A:98:THR:HG22	2.50	0.41
1:B:23:LEU:HB2	1:B:150:LYS:HA	2.02	0.41
1:C:54:ASP:HB2	1:C:57:ARG:CB	2.50	0.41
1:C:193:TYR:O	1:C:193:TYR:CG	2.72	0.41
1:C:275:GLN:HG3	1:C:291:THR:OG1	2.20	0.41
1:D:131:VAL:CG1	1:D:140:VAL:HG13	2.51	0.41
1:D:212:TRP:CE3	1:D:298:PHE:HD1	2.39	0.41
1:E:51:LEU:HD13	1:E:70:ILE:HD12	2.01	0.41
1:A:53:PHE:O	1:A:53:PHE:CG	2.72	0.41
1:A:80:VAL:CG1	1:A:82:ASN:O	2.69	0.41
1:B:132:ARG:NH2	1:B:178:ARG:HB2	2.36	0.41
1:B:271:GLU:OE2	1:B:272:VAL:N	2.54	0.41
1:C:79:ASN:OD1	1:C:109:VAL:HG12	2.21	0.41
1:D:13:GLU:HB3	1:D:14:PRO:CD	2.50	0.41
1:D:22:TYR:HB3	1:D:41:PHE:HB2	2.03	0.41
1:D:42:LEU:HD23	1:D:103:GLU:OE1	2.21	0.41
1:D:53:PHE:O	1:D:53:PHE:CG	2.74	0.41
1:E:117:ARG:O	1:E:118:TYR:C	2.63	0.41
1:E:194:PHE:C	1:E:196:TYR:H	2.28	0.41
1:A:132:ARG:HH22	1:A:176:GLU:HB2	1.86	0.41
1:B:54:ASP:HB2	1:B:57:ARG:CG	2.51	0.41
1:C:15:LEU:O	1:C:15:LEU:HG	2.08	0.41
1:D:296:ILE:O	1:D:297:ALA:C	2.64	0.41
1:C:76:ARG:HH12	1:C:130:ILE:HD11	1.86	0.40
1:C:226:LEU:HD23	1:D:224:VAL:CB	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:70:ILE:N	1:D:70:ILE:HD13	2.37	0.40
1:D:234:HIS:CE1	1:D:261:ILE:CG2	3.03	0.40
1:E:46:TRP:HH2	1:E:72:ILE:HG23	1.84	0.40
1:A:137:ARG:HH12	1:A:178:ARG:HA	1.86	0.40
1:A:210:ILE:HG23	1:B:269:VAL:CG1	2.29	0.40
1:C:44:LEU:HB2	1:C:101:TYR:HB3	2.03	0.40
1:D:225:THR:CG2	1:E:224:VAL:CG2	2.88	0.40
1:E:62:VAL:CG1	1:E:92:SER:HB3	2.45	0.40
1:E:170:PRO:HB3	1:E:183:LEU:CD2	2.51	0.40
1:E:232:ILE:HG22	1:E:233:ALA:N	2.36	0.40
1:A:76:ARG:HH22	1:A:130:ILE:CD1	2.14	0.40
1:A:283:GLN:N	1:A:284:PRO:CD	2.81	0.40
1:B:13:GLU:OE1	1:B:14:PRO:HD3	2.21	0.40
1:B:22:TYR:HB3	1:B:41:PHE:HB2	2.04	0.40
1:C:27:TYR:CE1	1:D:81:GLU:OE1	2.75	0.40
1:C:98:THR:HG22	1:C:98:THR:O	2.20	0.40
1:C:179:LEU:HD12	1:C:179:LEU:C	2.47	0.40
1:C:222:ALA:HB2	1:D:221[A]:GLU:CD	2.47	0.40
1:C:296:ILE:O	1:C:299:PRO:HD2	2.22	0.40
1:A:76:ARG:HH12	1:A:130:ILE:HD11	1.86	0.40
1:A:221[B]:GLU:HB2	1:B:221[B]:GLU:OE2	2.20	0.40
1:B:270:ILE:HG22	1:B:271:GLU:N	2.36	0.40
1:C:224:VAL:HG23	1:C:225:THR:N	2.36	0.40
1:C:281:GLU:O	1:C:283:GLN:N	2.53	0.40
1:D:72:ILE:HG22	1:D:73:PRO:CD	2.51	0.40
1:E:27:TYR:CE1	1:E:37:LYS:CB	3.04	0.40
1:E:193:TYR:O	1:E:193:TYR:CG	2.74	0.40
1:A:261:ILE:O	1:A:262:TYR:C	2.63	0.40
1:C:54:ASP:HB2	1:C:57:ARG:CG	2.51	0.40
1:C:233:ALA:O	1:C:236:ALA:HB3	2.22	0.40
1:C:247:LYS:HA	1:C:247:LYS:HD3	1.82	0.40
1:D:104:ARG:NH2	1:E:78:VAL:HA	2.37	0.40
1:D:131:VAL:HG13	1:D:131:VAL:O	2.21	0.40
1:E:128:TYR:O	1:E:129:LEU:CB	2.64	0.40
1:E:139:ILE:HG22	1:E:140:VAL:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	309/317 (98%)	250 (81%)	49 (16%)	10 (3%)	3	24
1	B	309/317 (98%)	245 (79%)	54 (18%)	10 (3%)	3	24
1	C	309/317 (98%)	250 (81%)	50 (16%)	9 (3%)	3	26
1	D	309/317 (98%)	248 (80%)	50 (16%)	11 (4%)	2	22
1	E	309/317 (98%)	248 (80%)	50 (16%)	11 (4%)	2	22
All	All	1545/1585 (98%)	1241 (80%)	253 (16%)	51 (3%)	3	24

All (51) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
1	B	118	TYR
1	D	148	VAL
1	D	275	GLN
1	E	118	TYR
1	A	49	ARG
1	A	96	ASP
1	C	96	ASP
1	C	277	TYR
1	D	49	ARG
1	D	277	TYR
1	E	49	ARG
1	A	277	TYR
1	B	49	ARG
1	B	277	TYR
1	C	49	ARG
1	E	277	TYR
1	D	96	ASP
1	E	287	ALA
1	E	295	ARG
1	D	131	VAL
1	E	131	VAL
1	A	131	VAL
1	B	59	GLY
1	B	197	ILE
1	C	131	VAL
1	D	59	GLY
1	D	197	ILE
1	A	197	ILE
1	B	131	VAL
1	E	197	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	279/284 (98%)	231 (83%)	48 (17%)	2 12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	279/284 (98%)	232 (83%)	47 (17%)	2	13
1	C	279/284 (98%)	231 (83%)	48 (17%)	2	12
1	D	279/284 (98%)	231 (83%)	48 (17%)	2	12
1	E	279/284 (98%)	230 (82%)	49 (18%)	2	12
All	All	1395/1420 (98%)	1155 (83%)	240 (17%)	2	12

All (240) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	16	THR
1	A	28	SER
1	A	32	LYS
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	98	THR
1	A	100	GLN
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	135	ASP
1	A	140	VAL
1	A	141	LEU
1	A	151	ASN
1	A	154	VAL
1	A	157	THR
1	A	162	GLU
1	A	177	ASP
1	A	179	LEU
1	A	190	SER
1	A	195	SER
1	A	204	MET
1	A	211	SER
1	A	213	THR

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Mol	Chain	Res	Type
1	A	218	THR
1	A	221[A]	GLU
1	A	221[B]	GLU
1	A	226	LEU
1	A	232	ILE
1	A	239	ILE
1	A	243	THR
1	A	252	THR
1	A	254	THR
1	A	260	MET
1	A	261	ILE
1	A	263	LEU
1	A	269	VAL
1	A	270	ILE
1	A	274	VAL
1	A	292	ARG
1	B	15	LEU
1	B	16	THR
1	B	32	LYS
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	98	THR
1	B	100	GLN
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	135	ASP
1	B	140	VAL
1	B	141	LEU
1	B	151	ASN
1	B	154	VAL
1	B	157	THR
1	B	162	GLU
1	B	177	ASP
1	B	179	LEU

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Mol	Chain	Res	Type
1	B	190	SER
1	B	195	SER
1	B	204	MET
1	B	211	SER
1	B	213	THR
1	B	218	THR
1	B	221[A]	GLU
1	B	221[B]	GLU
1	B	226	LEU
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	261	ILE
1	B	263	LEU
1	B	269	VAL
1	B	270	ILE
1	B	274	VAL
1	B	292	ARG
1	C	15	LEU
1	C	16	THR
1	C	28	SER
1	C	32	LYS
1	C	51	LEU
1	C	53	PHE
1	C	64	THR
1	C	68	GLU
1	C	72	ILE
1	C	84	ARG
1	C	98	THR
1	C	100	GLN
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	135	ASP
1	C	140	VAL
1	C	141	LEU

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Mol	Chain	Res	Type
1	C	151	ASN
1	C	154	VAL
1	C	157	THR
1	C	162	GLU
1	C	177	ASP
1	C	179	LEU
1	C	190	SER
1	C	195	SER
1	C	204	MET
1	C	211	SER
1	C	213	THR
1	C	218	THR
1	C	221[A]	GLU
1	C	221[B]	GLU
1	C	226	LEU
1	C	232	ILE
1	C	239	ILE
1	C	243	THR
1	C	252	THR
1	C	254	THR
1	C	260	MET
1	C	261	ILE
1	C	263	LEU
1	C	269	VAL
1	C	270	ILE
1	C	274	VAL
1	C	292	ARG
1	D	15	LEU
1	D	16	THR
1	D	32	LYS
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	98	THR
1	D	100	GLN
1	D	110	LEU
1	D	113	LEU
1	D	122	SER
1	D	124	THR

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Mol	Chain	Res	Type
1	D	130	ILE
1	D	134	VAL
1	D	135	ASP
1	D	140	VAL
1	D	141	LEU
1	D	151	ASN
1	D	154	VAL
1	D	157	THR
1	D	162	GLU
1	D	177	ASP
1	D	179	LEU
1	D	190	SER
1	D	195	SER
1	D	204	MET
1	D	211	SER
1	D	213	THR
1	D	218	THR
1	D	221[A]	GLU
1	D	221[B]	GLU
1	D	226	LEU
1	D	232	ILE
1	D	239	ILE
1	D	243	THR
1	D	252	THR
1	D	254	THR
1	D	258	ILE
1	D	260	MET
1	D	261	ILE
1	D	263	LEU
1	D	269	VAL
1	D	270	ILE
1	D	274	VAL
1	D	292	ARG
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	72	ILE

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Mol	Chain	Res	Type
1	E	84	ARG
1	E	98	THR
1	E	100	GLN
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	135	ASP
1	E	140	VAL
1	E	141	LEU
1	E	151	ASN
1	E	154	VAL
1	E	157	THR
1	E	162	GLU
1	E	177	ASP
1	E	179	LEU
1	E	190	SER
1	E	195	SER
1	E	204	MET
1	E	211	SER
1	E	213	THR
1	E	218	THR
1	E	221[A]	GLU
1	E	221[B]	GLU
1	E	226	LEU
1	E	232	ILE
1	E	239	ILE
1	E	243	THR
1	E	252	THR
1	E	254	THR
1	E	258	ILE
1	E	260	MET
1	E	261	ILE
1	E	263	LEU
1	E	269	VAL
1	E	270	ILE
1	E	274	VAL
1	E	292	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	100	GLN
1	A	151	ASN
1	A	238	ASN
1	A	244	ASN
1	A	275	GLN
1	A	276	HIS
1	A	283	GLN
1	B	100	GLN
1	B	151	ASN
1	B	244	ASN
1	B	275	GLN
1	B	276	HIS
1	B	283	GLN
1	C	100	GLN
1	C	151	ASN
1	C	238	ASN
1	C	244	ASN
1	C	275	GLN
1	C	276	HIS
1	C	283	GLN
1	D	39	ASN
1	D	100	GLN
1	D	151	ASN
1	D	238	ASN
1	D	244	ASN
1	D	275	GLN
1	D	283	GLN
1	E	39	ASN
1	E	100	GLN
1	E	151	ASN
1	E	238	ASN
1	E	244	ASN
1	E	275	GLN
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 [i](#)

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 3 ligands modelled in this entry, 3 are 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%)	0.94	52 (16%) 4 5	63, 102, 160, 213	1 (0%)
1	B	310/317 (97%)	0.88	47 (15%) 5 5	63, 102, 160, 212	1 (0%)
1	C	310/317 (97%)	0.95	51 (16%) 4 5	63, 102, 160, 213	1 (0%)
1	D	310/317 (97%)	1.04	58 (18%) 3 4	63, 102, 160, 213	1 (0%)
1	E	310/317 (97%)	0.98	53 (17%) 4 4	63, 102, 160, 213	1 (0%)
All	All	1550/1585 (97%)	0.96	261 (16%) 4 5	63, 102, 161, 213	5 (0%)

All (261) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	153	ASP	14.9
1	B	153	ASP	14.0
1	B	152	ASP	13.8
1	D	153	ASP	12.1
1	E	184	ASP	7.6
1	E	186	GLN	7.5
1	E	126	HIS	6.7
1	C	153	ASP	6.1
1	D	126	HIS	6.1
1	C	85	ASP	6.0
1	D	186	GLN	5.8
1	B	148	VAL	5.7
1	A	144	ASP	5.7
1	D	111	SER	5.7
1	A	60	VAL	5.6
1	E	60	VAL	5.2
1	C	126	HIS	5.2
1	E	144	ASP	5.1
1	B	101	TYR	5.0
1	D	187	LEU	5.0

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Mol	Chain	Res	Type	RSRZ
1	C	60	VAL	5.0
1	A	221[A]	GLU	4.9
1	B	100	GLN	4.9
1	E	188	ARG	4.9
1	C	244	ASN	4.9
1	A	11	ALA	4.9
1	D	11	ALA	4.8
1	E	146	GLU	4.5
1	A	74	GLU	4.5
1	E	59	GLY	4.5
1	D	85	ASP	4.5
1	E	165	THR	4.5
1	A	152	ASP	4.4
1	C	221[A]	GLU	4.4
1	A	177	ASP	4.4
1	B	154	VAL	4.3
1	C	242	GLU	4.3
1	B	88	VAL	4.3
1	A	172	ASN	4.3
1	D	282	SER	4.2
1	B	282	SER	4.2
1	C	186	GLN	4.2
1	D	83	ALA	4.2
1	E	47	LYS	4.2
1	D	60	VAL	4.1
1	B	242	GLU	4.1
1	D	128	TYR	4.1
1	D	152	ASP	4.1
1	C	243	THR	4.0
1	B	74	GLU	4.0
1	C	13	GLU	4.0
1	B	90	ASP	4.0
1	D	148	VAL	3.9
1	E	148	VAL	3.9
1	D	78	VAL	3.9
1	A	139	ILE	3.9
1	B	60	VAL	3.9
1	A	206	PHE	3.9
1	E	145	LEU	3.9
1	C	83	ALA	3.9
1	E	88	VAL	3.9
1	A	59	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	25	GLU	3.8
1	D	59	GLY	3.7
1	A	169	LYS	3.7
1	C	11	ALA	3.7
1	D	82	ASN	3.7
1	A	13	GLU	3.6
1	B	61	ARG	3.6
1	A	224	VAL	3.6
1	B	59	GLY	3.6
1	C	144	ASP	3.6
1	C	14	PRO	3.6
1	D	124	THR	3.6
1	C	240	LEU	3.5
1	D	49	ARG	3.5
1	D	55	PRO	3.5
1	C	184	ASP	3.5
1	D	144	ASP	3.5
1	E	139	ILE	3.5
1	A	244	ASN	3.4
1	B	243	THR	3.4
1	D	47	LYS	3.4
1	C	172	ASN	3.4
1	B	56	VAL	3.4
1	B	11	ALA	3.4
1	E	124	THR	3.3
1	B	102	LEU	3.3
1	E	285	ALA	3.3
1	E	147	LYS	3.3
1	A	173	PHE	3.3
1	B	91	ILE	3.3
1	C	59	GLY	3.2
1	D	165	THR	3.2
1	E	243	THR	3.1
1	A	155	PHE	3.1
1	C	155	PHE	3.1
1	B	47	LYS	3.1
1	E	244	ASN	3.1
1	C	169	LYS	3.1
1	A	154	VAL	3.1
1	B	89	VAL	3.1
1	C	279	LYS	3.1
1	A	220	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	56	VAL	3.1
1	E	222	ALA	3.1
1	B	222	ALA	3.0
1	C	165	THR	3.0
1	A	148	VAL	3.0
1	C	128	TYR	3.0
1	A	316	PHE	3.0
1	E	225	THR	3.0
1	E	11	ALA	2.9
1	A	55	PRO	2.9
1	E	221[A]	GLU	2.9
1	D	53	PHE	2.9
1	D	263	LEU	2.9
1	E	128	TYR	2.9
1	A	66	GLU	2.9
1	A	209	PHE	2.9
1	D	125	LEU	2.9
1	E	61	ARG	2.9
1	C	316	PHE	2.9
1	A	88	VAL	2.9
1	C	82	ASN	2.9
1	E	152	ASP	2.8
1	D	134	VAL	2.8
1	C	139	ILE	2.8
1	E	83	ALA	2.8
1	D	206	PHE	2.8
1	A	151	ASN	2.8
1	C	173	PHE	2.8
1	A	168	VAL	2.8
1	C	241	VAL	2.8
1	D	19	THR	2.8
1	C	135	ASP	2.8
1	E	282	SER	2.8
1	E	174	ALA	2.8
1	C	177	ASP	2.7
1	D	10	ILE	2.7
1	D	97	GLY	2.7
1	D	146	GLU	2.7
1	E	209	PHE	2.7
1	C	147	LYS	2.7
1	E	134	VAL	2.7
1	E	153	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	145	LEU	2.7
1	D	18	ASN	2.7
1	B	62	VAL	2.7
1	A	145	LEU	2.7
1	B	316	PHE	2.6
1	D	160	ASP	2.6
1	E	82	ASN	2.6
1	C	288	ALA	2.6
1	D	51	LEU	2.6
1	C	163	SER	2.6
1	D	207	ILE	2.6
1	D	13	GLU	2.6
1	A	134	VAL	2.6
1	A	187	LEU	2.6
1	B	145	LEU	2.6
1	D	74	GLU	2.6
1	A	171	ALA	2.6
1	E	242	GLU	2.5
1	A	126	HIS	2.5
1	B	225	THR	2.5
1	D	127	ILE	2.5
1	D	316	PHE	2.5
1	B	155	PHE	2.5
1	A	85	ASP	2.5
1	C	136	THR	2.5
1	B	86	ALA	2.5
1	A	89	VAL	2.5
1	D	141	LEU	2.4
1	B	49	ARG	2.4
1	E	177	ASP	2.4
1	A	163	SER	2.4
1	E	14	PRO	2.4
1	E	149	GLY	2.4
1	C	134	VAL	2.4
1	C	285	ALA	2.4
1	A	208	LEU	2.4
1	D	278	LEU	2.4
1	A	135	ASP	2.4
1	A	7	PRO	2.4
1	B	136	THR	2.4
1	E	151	ASN	2.3
1	B	221[A]	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	47	LYS	2.3
1	D	221[A]	GLU	2.3
1	D	7	PRO	2.3
1	C	224	VAL	2.3
1	C	26	CYS	2.3
1	B	7	PRO	2.3
1	C	55	PRO	2.3
1	D	169	LYS	2.3
1	D	185	TYR	2.3
1	B	103	GLU	2.3
1	B	12	ASP	2.3
1	B	168	VAL	2.3
1	C	137	ARG	2.3
1	A	170	PRO	2.3
1	D	112	PRO	2.3
1	E	167	VAL	2.3
1	D	164	PHE	2.2
1	C	282	SER	2.2
1	D	143	VAL	2.2
1	D	110	LEU	2.2
1	E	96	ASP	2.2
1	B	315	GLY	2.2
1	B	151	ASN	2.2
1	B	169	LYS	2.2
1	C	149	GLY	2.2
1	D	34	GLU	2.2
1	E	68	GLU	2.2
1	D	184	ASP	2.2
1	B	15	LEU	2.2
1	B	280	VAL	2.2
1	B	173	PHE	2.2
1	B	174	ALA	2.2
1	E	15	LEU	2.2
1	B	146	GLU	2.2
1	E	13	GLU	2.2
1	D	182	LYS	2.2
1	E	166	ALA	2.1
1	E	89	VAL	2.1
1	C	112	PRO	2.1
1	A	58	SER	2.1
1	B	241	VAL	2.1
1	E	173	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	81	GLU	2.1
1	A	64	THR	2.1
1	D	45	SER	2.1
1	A	149	GLY	2.1
1	A	203	PRO	2.1
1	A	150	LYS	2.1
1	A	186	GLN	2.1
1	C	27	TYR	2.1
1	D	183	LEU	2.1
1	B	92	SER	2.1
1	C	150	LYS	2.1
1	E	163	SER	2.1
1	A	143	VAL	2.1
1	C	15	LEU	2.1
1	E	135	ASP	2.1
1	B	266	PHE	2.1
1	B	82	ASN	2.1
1	E	56	VAL	2.1
1	E	154	VAL	2.1
1	E	277	TYR	2.0
1	A	162	GLU	2.0
1	C	176	GLU	2.0
1	C	174	ALA	2.0
1	A	240	LEU	2.0
1	E	279	LYS	2.0
1	A	225	THR	2.0
1	A	160	ASP	2.0
1	D	135	ASP	2.0
1	D	15	LEU	2.0
1	C	151	ASN	2.0
1	E	85	ASP	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	ZN	C	1318	1/1	0.42	0.53	186,186,186,186	0
2	ZN	D	1317	1/1	0.77	0.12	176,176,176,176	0
2	ZN	C	1317	1/1	0.92	0.32	130,130,130,130	0

6.5 Other polymers [i](#)

There are no such residues in this entry.