



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 07:18 PM UTC

PDB ID : 3ZX9 / pdb_00003zx9
EMDB ID : EMD-1864
Title : Cryo-EM reconstruction of native and expanded Turnip Crinkle virus
Authors : Bakker, S.E.; Robottom, J.; Pearson, A.R.; Stockley, P.G.; Ranson, N.A.
Deposited on : 2011-08-08
Resolution : 17.00 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>

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:

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

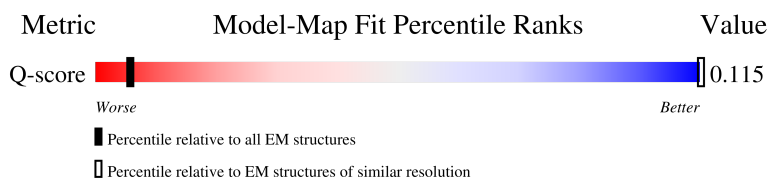
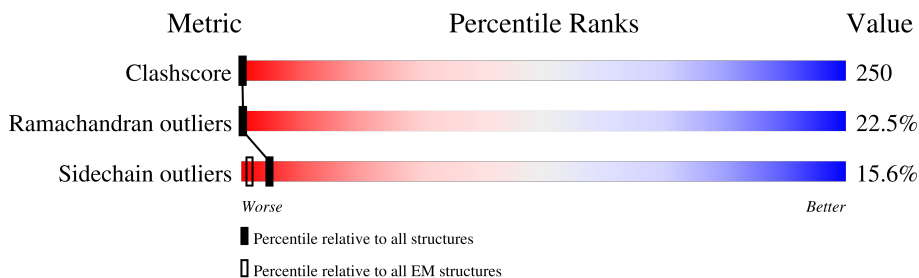
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 17.00 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)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	38 (16.50 - 17.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	347	10% 5% 29% 30% 13% 23%
1	B	347	11% 5% 30% 29% 12% 23%
1	C	347	13% • 33% 33% 15% 15%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6284 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 CAPSID PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	267	Total	C	N	O	S	0	0
			2024	1280	343	396	5		
1	B	267	Total	C	N	O	S	0	0
			2024	1280	343	396	5		
1	C	295	Total	C	N	O	S	0	0
			2236	1409	386	436	5		

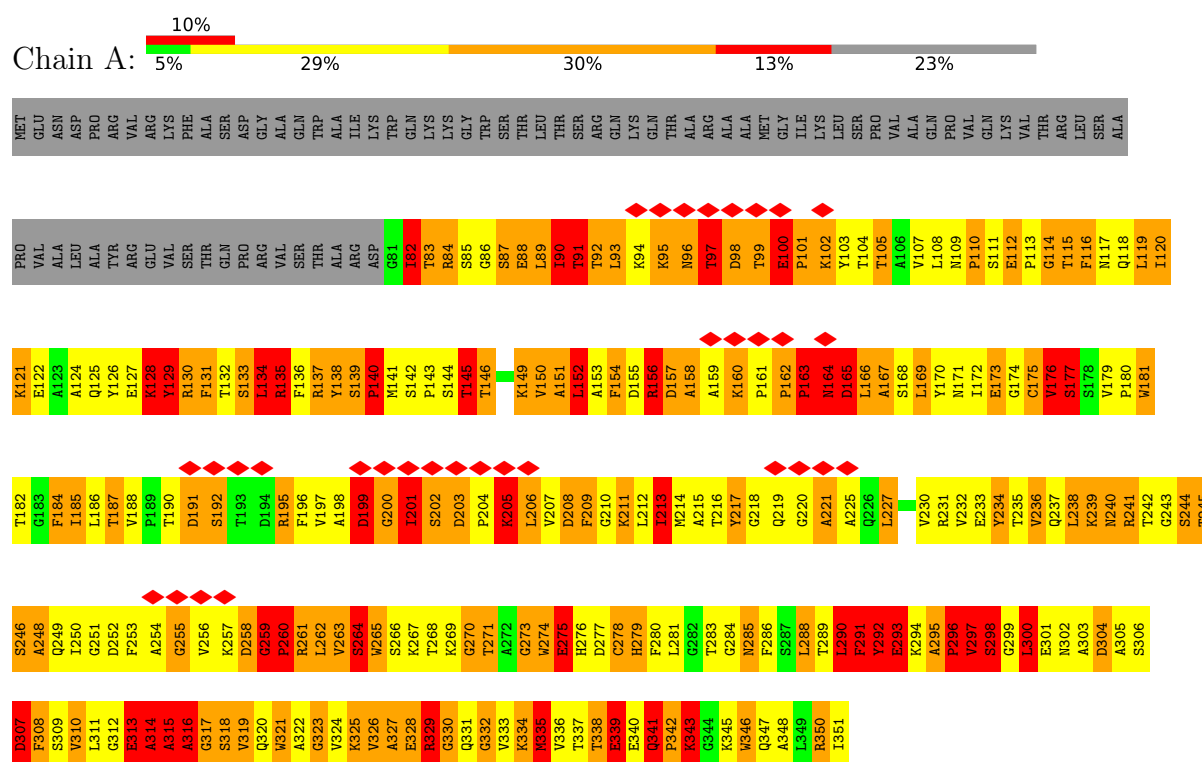
There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ASN	deletion	UNP P06663
A	?	-	ASP	deletion	UNP P06663
A	?	-	ALA	deletion	UNP P06663
A	?	-	ASP	deletion	UNP P06663
A	346	TRP	LEU	variant	UNP P06663
B	?	-	ASN	deletion	UNP P06663
B	?	-	ASP	deletion	UNP P06663
B	?	-	ALA	deletion	UNP P06663
B	?	-	ASP	deletion	UNP P06663
B	346	TRP	LEU	variant	UNP P06663
C	?	-	ASN	deletion	UNP P06663
C	?	-	ASP	deletion	UNP P06663
C	?	-	ALA	deletion	UNP P06663
C	?	-	ASP	deletion	UNP P06663
C	346	TRP	LEU	variant	UNP P06663

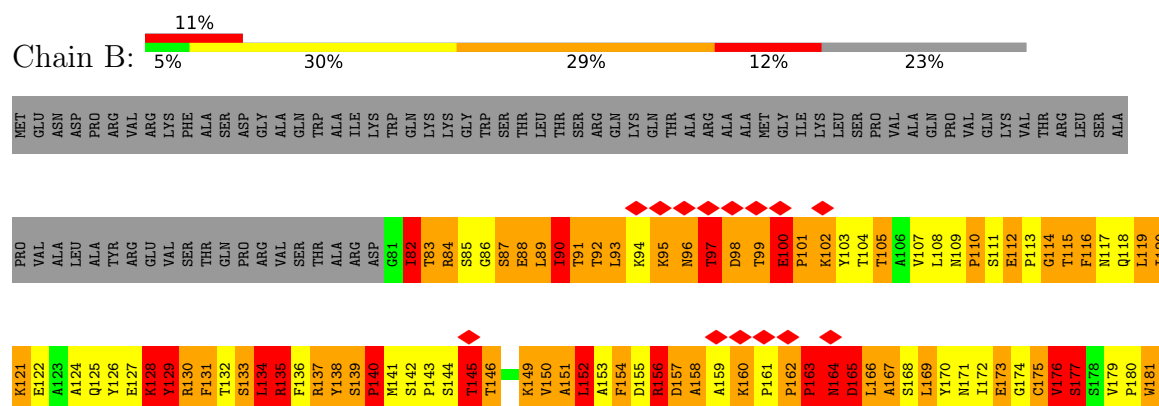
3 Residue-property plots

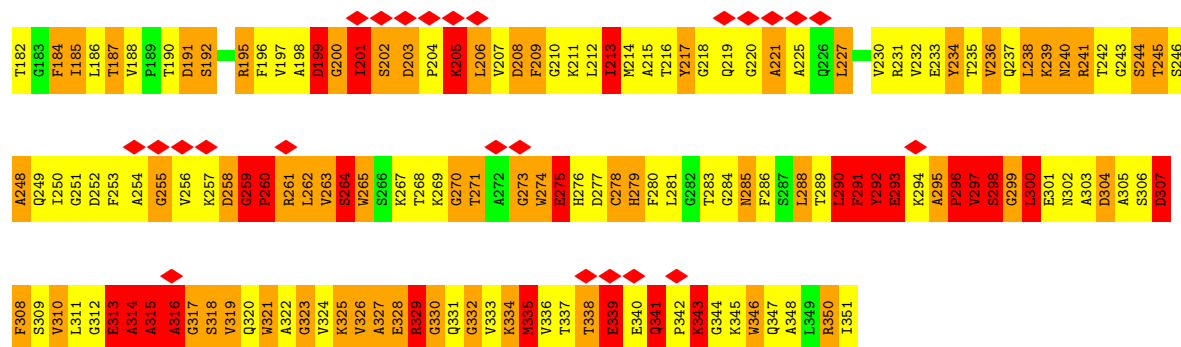
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: CAPSID PROTEIN

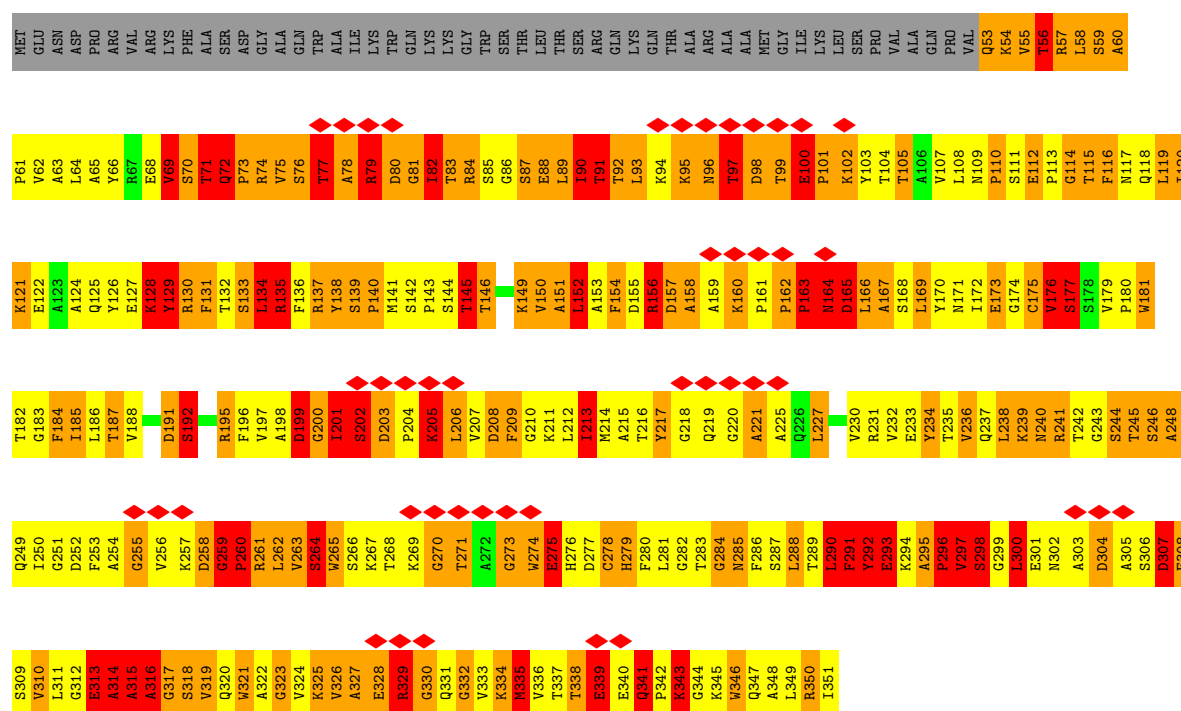


• Molecule 1: CAPSID PROTEIN





Molecule 1: CAPSID PROTEIN



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	5121	Depositor
Resolution determination method	Not provided	
CTF correction method	PHASE-FLIPPING EACH PARTICLE	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	15	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	52911	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	4.173	Depositor
Minimum map value	-1.868	Depositor
Average map value	0.162	Depositor
Map value standard deviation	1.486	Depositor
Recommended contour level	3.2	Depositor
Map size ($\text{\AA}$)	453.6, 453.6, 453.6	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.89, 1.89, 1.89	Depositor

5 Model quality

5.1 Standard geometry

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	3.34	81/2068 (3.9%)	3.03	161/2804 (5.7%)
1	B	3.34	80/2068 (3.9%)	3.03	160/2804 (5.7%)
1	C	3.46	100/2282 (4.4%)	2.99	185/3096 (6.0%)
All	All	3.38	261/6418 (4.1%)	3.02	506/8704 (5.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8
1	B	0	8
1	C	0	10
All	All	0	26

All (261) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	201	ILE	C-N	-69.31	0.36	1.33
1	C	201	ILE	C-N	-69.31	0.36	1.33
1	A	201	ILE	C-N	-69.30	0.36	1.33
1	B	93	LEU	N-CA	-50.26	0.64	1.45
1	C	93	LEU	N-CA	-50.25	0.64	1.45
1	A	93	LEU	N-CA	-50.24	0.64	1.45
1	B	82	ILE	C-N	33.86	1.81	1.33
1	A	82	ILE	C-N	33.84	1.81	1.33
1	C	82	ILE	C-N	33.82	1.81	1.33
1	A	288	LEU	C-N	-28.22	0.94	1.33
1	B	288	LEU	C-N	-28.13	0.94	1.33
1	C	288	LEU	C-N	-28.10	0.94	1.33
1	A	279	HIS	C-N	27.19	1.74	1.33
1	B	279	HIS	C-N	27.12	1.74	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	279	HIS	C-N	27.08	1.74	1.33
1	A	259	GLY	C-N	27.02	1.97	1.33
1	C	259	GLY	C-N	27.00	1.97	1.33
1	B	259	GLY	C-N	26.98	1.97	1.33
1	A	291	PHE	C-N	26.86	1.71	1.33
1	C	291	PHE	C-N	26.84	1.71	1.33
1	B	291	PHE	C-N	26.79	1.71	1.33
1	A	264	SER	C-N	25.11	1.68	1.33
1	C	264	SER	C-N	25.09	1.68	1.33
1	B	264	SER	C-N	25.08	1.68	1.33
1	C	297	VAL	C-N	-23.54	1.00	1.33
1	B	297	VAL	C-N	-23.49	1.00	1.33
1	A	297	VAL	C-N	-23.47	1.00	1.33
1	C	76	SER	N-CA	23.35	1.76	1.45
1	C	53	GLN	C-N	23.13	1.67	1.33
1	A	319	VAL	C-N	22.24	1.61	1.33
1	B	319	VAL	C-N	22.23	1.61	1.33
1	C	319	VAL	C-N	22.22	1.61	1.33
1	C	177	SER	C-N	-21.24	1.04	1.33
1	B	177	SER	C-N	-21.23	1.04	1.33
1	A	177	SER	C-N	-21.12	1.04	1.33
1	C	75	VAL	C-N	20.62	1.60	1.33
1	C	133	SER	CB-OG	19.46	1.81	1.42
1	B	133	SER	CB-OG	19.46	1.81	1.42
1	A	133	SER	CB-OG	19.41	1.80	1.42
1	B	339	GLU	C-N	18.93	1.68	1.34
1	A	339	GLU	C-N	18.91	1.68	1.34
1	C	339	GLU	C-N	18.91	1.68	1.34
1	C	75	VAL	CA-C	18.42	1.76	1.52
1	C	76	SER	CA-C	18.34	1.75	1.52
1	C	75	VAL	N-CA	17.39	1.68	1.46
1	C	308	PHE	C-N	-16.27	1.11	1.33
1	B	308	PHE	C-N	-16.26	1.11	1.33
1	A	308	PHE	C-N	-16.26	1.11	1.33
1	B	149	LYS	CD-CE	15.84	2.00	1.52
1	C	149	LYS	CD-CE	15.81	1.99	1.52
1	A	149	LYS	CD-CE	15.78	1.99	1.52
1	A	200	GLY	C-N	-15.57	1.12	1.33
1	C	200	GLY	C-N	-15.55	1.12	1.33
1	B	200	GLY	C-N	-15.52	1.12	1.33
1	B	91	THR	N-CA	14.55	1.65	1.46
1	C	91	THR	N-CA	14.50	1.64	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	91	THR	N-CA	14.47	1.64	1.46
1	A	315	ALA	C-N	-13.94	1.14	1.33
1	C	315	ALA	C-N	-13.92	1.14	1.33
1	B	315	ALA	C-N	-13.92	1.14	1.33
1	C	74	ARG	CA-C	13.87	1.69	1.52
1	C	74	ARG	C-N	13.86	1.52	1.33
1	C	77	THR	N-CA	13.59	1.63	1.46
1	B	90	ILE	CA-C	12.97	1.69	1.52
1	A	90	ILE	CA-C	12.96	1.69	1.52
1	B	303	ALA	C-N	12.96	1.50	1.33
1	A	260	PRO	C-N	-12.96	1.15	1.33
1	C	260	PRO	C-N	-12.93	1.15	1.33
1	C	90	ILE	CA-C	12.92	1.69	1.52
1	B	260	PRO	C-N	-12.91	1.15	1.33
1	C	303	ALA	C-N	12.91	1.50	1.33
1	A	303	ALA	C-N	12.85	1.50	1.33
1	C	290	LEU	C-N	12.76	1.51	1.33
1	B	290	LEU	C-N	12.75	1.51	1.33
1	C	323	GLY	C-N	-12.74	1.16	1.33
1	B	323	GLY	C-N	-12.73	1.16	1.33
1	A	290	LEU	C-N	12.69	1.51	1.33
1	A	323	GLY	C-N	-12.65	1.16	1.33
1	B	330	GLY	C-N	12.54	1.50	1.33
1	A	330	GLY	C-N	12.49	1.50	1.33
1	C	330	GLY	C-N	12.47	1.50	1.33
1	C	300	LEU	N-CA	-11.60	1.31	1.46
1	B	298	SER	C-N	-11.58	1.16	1.33
1	B	300	LEU	N-CA	-11.56	1.31	1.46
1	C	298	SER	C-N	-11.56	1.16	1.33
1	A	300	LEU	N-CA	-11.54	1.31	1.46
1	A	298	SER	C-N	-11.52	1.16	1.33
1	A	299	GLY	C-N	-11.22	1.18	1.33
1	B	299	GLY	C-N	-11.18	1.18	1.33
1	C	76	SER	C-N	11.16	1.49	1.33
1	C	299	GLY	C-N	-11.16	1.18	1.33
1	C	72	GLN	C-N	11.15	1.47	1.33
1	C	140	PRO	N-CD	-10.91	1.32	1.47
1	A	140	PRO	N-CD	-10.88	1.32	1.47
1	B	140	PRO	N-CD	-10.78	1.32	1.47
1	C	74	ARG	N-CA	10.69	1.59	1.45
1	A	175	CYS	C-N	-10.49	1.19	1.33
1	C	175	CYS	C-N	-10.47	1.19	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	175	CYS	C-N	-10.43	1.19	1.33
1	B	175	CYS	CA-C	-10.38	1.38	1.52
1	C	175	CYS	CA-C	-10.35	1.38	1.52
1	A	175	CYS	CA-C	-10.29	1.38	1.52
1	A	121	LYS	CE-NZ	9.96	1.79	1.49
1	B	121	LYS	CE-NZ	9.96	1.79	1.49
1	C	121	LYS	CE-NZ	9.94	1.79	1.49
1	B	221	ALA	C-N	9.86	1.47	1.33
1	A	221	ALA	C-N	9.85	1.47	1.33
1	C	221	ALA	C-N	9.81	1.47	1.33
1	A	299	GLY	CA-C	-9.68	1.38	1.51
1	C	299	GLY	CA-C	-9.64	1.38	1.51
1	B	299	GLY	CA-C	-9.60	1.38	1.51
1	B	139	SER	C-N	-9.23	1.12	1.33
1	A	139	SER	C-N	-9.19	1.12	1.33
1	C	139	SER	C-N	-9.13	1.12	1.33
1	B	299	GLY	N-CA	-8.89	1.32	1.45
1	C	299	GLY	N-CA	-8.86	1.32	1.45
1	A	299	GLY	N-CA	-8.85	1.32	1.45
1	A	284	GLY	N-CA	8.83	1.54	1.45
1	A	140	PRO	CA-CB	-8.81	1.41	1.53
1	B	140	PRO	CA-CB	-8.78	1.41	1.53
1	B	284	GLY	N-CA	8.78	1.53	1.45
1	C	70	SER	C-N	-8.78	1.21	1.33
1	C	140	PRO	CA-CB	-8.76	1.41	1.53
1	C	284	GLY	N-CA	8.74	1.53	1.45
1	C	332	GLY	C-N	8.65	1.45	1.33
1	A	332	GLY	C-N	8.61	1.45	1.33
1	B	332	GLY	C-N	8.61	1.45	1.33
1	C	176	VAL	N-CA	-8.42	1.35	1.46
1	A	288	LEU	CA-C	-8.40	1.41	1.53
1	C	162	PRO	CA-C	-8.38	1.44	1.52
1	C	58	LEU	C-N	-8.37	1.22	1.33
1	A	176	VAL	N-CA	-8.36	1.35	1.46
1	B	176	VAL	N-CA	-8.36	1.35	1.46
1	B	162	PRO	CA-C	-8.32	1.44	1.52
1	C	288	LEU	CA-C	-8.32	1.41	1.53
1	B	288	LEU	CA-C	-8.31	1.41	1.53
1	A	162	PRO	CA-C	-8.31	1.44	1.52
1	C	163	PRO	N-CA	-8.10	1.36	1.47
1	B	163	PRO	N-CA	-8.10	1.36	1.47
1	A	163	PRO	N-CA	-8.04	1.37	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	57	ARG	CA-C	-7.99	1.42	1.52
1	B	138	TYR	CA-C	-7.95	1.43	1.53
1	A	138	TYR	CA-C	-7.93	1.43	1.53
1	C	138	TYR	CA-C	-7.89	1.43	1.53
1	A	284	GLY	CA-C	7.69	1.59	1.51
1	A	99	THR	N-CA	7.65	1.55	1.46
1	C	284	GLY	CA-C	7.60	1.59	1.51
1	B	284	GLY	CA-C	7.57	1.59	1.51
1	B	99	THR	N-CA	7.55	1.54	1.46
1	C	99	THR	N-CA	7.47	1.54	1.46
1	A	270	GLY	C-N	-7.44	1.23	1.33
1	C	270	GLY	C-N	-7.43	1.23	1.33
1	C	54	LYS	C-N	-7.39	1.23	1.33
1	B	270	GLY	C-N	-7.39	1.23	1.33
1	C	298	SER	CA-C	-7.35	1.43	1.52
1	C	73	PRO	C-N	7.30	1.43	1.33
1	A	298	SER	CA-C	-7.29	1.43	1.52
1	B	298	SER	CA-C	-7.29	1.43	1.52
1	B	259	GLY	CA-C	7.24	1.62	1.51
1	C	259	GLY	CA-C	7.16	1.62	1.51
1	A	259	GLY	CA-C	7.11	1.62	1.51
1	B	187	THR	C-N	7.00	1.41	1.33
1	C	187	THR	C-N	6.99	1.41	1.33
1	A	187	THR	C-N	6.98	1.41	1.33
1	C	56	THR	C-N	-6.92	1.23	1.33
1	A	213	ILE	C-N	-6.90	1.24	1.33
1	C	213	ILE	C-N	-6.84	1.24	1.33
1	B	163	PRO	C-N	-6.81	1.24	1.33
1	C	181	TRP	N-CA	6.80	1.54	1.46
1	C	163	PRO	C-N	-6.80	1.24	1.33
1	B	213	ILE	C-N	-6.80	1.24	1.33
1	A	163	PRO	C-N	-6.80	1.24	1.33
1	B	181	TRP	N-CA	6.80	1.54	1.46
1	A	181	TRP	N-CA	6.72	1.54	1.46
1	B	300	LEU	C-N	6.68	1.42	1.33
1	A	300	LEU	C-N	6.66	1.42	1.33
1	C	300	LEU	C-N	6.64	1.42	1.33
1	B	176	VAL	CA-C	-6.64	1.44	1.52
1	B	327	ALA	C-N	-6.62	1.24	1.33
1	A	327	ALA	C-N	-6.58	1.24	1.33
1	B	139	SER	N-CA	-6.57	1.36	1.46
1	A	139	SER	N-CA	-6.56	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	176	VAL	CA-C	-6.52	1.44	1.52
1	A	176	VAL	CA-C	-6.52	1.44	1.52
1	C	139	SER	N-CA	-6.52	1.36	1.46
1	C	327	ALA	C-N	-6.50	1.24	1.33
1	B	335	MET	C-N	-6.48	1.24	1.33
1	C	335	MET	C-N	-6.48	1.24	1.33
1	A	335	MET	C-N	-6.40	1.25	1.33
1	B	164	ASN	N-CA	-6.37	1.38	1.46
1	C	164	ASN	N-CA	-6.36	1.38	1.46
1	A	164	ASN	N-CA	-6.33	1.38	1.46
1	A	329	ARG	N-CA	-6.10	1.38	1.46
1	C	329	ARG	N-CA	-6.04	1.38	1.46
1	B	329	ARG	N-CA	-6.02	1.38	1.46
1	A	271	THR	C-N	6.01	1.42	1.33
1	A	317	GLY	N-CA	6.01	1.53	1.45
1	B	317	GLY	N-CA	5.99	1.53	1.45
1	B	271	THR	C-N	5.94	1.42	1.33
1	C	317	GLY	N-CA	5.94	1.53	1.45
1	C	316	ALA	C-N	5.92	1.41	1.33
1	C	271	THR	C-N	5.92	1.42	1.33
1	B	316	ALA	C-N	5.89	1.41	1.33
1	B	285	ASN	N-CA	5.89	1.53	1.46
1	A	285	ASN	N-CA	5.87	1.53	1.46
1	C	274	TRP	NE1-CE2	-5.86	1.31	1.37
1	C	285	ASN	N-CA	5.84	1.53	1.46
1	A	316	ALA	C-N	5.84	1.41	1.33
1	A	88	GLU	C-N	-5.84	1.21	1.34
1	B	274	TRP	NE1-CE2	-5.82	1.31	1.37
1	A	293	GLU	N-CA	5.79	1.53	1.46
1	B	88	GLU	C-N	-5.78	1.21	1.34
1	C	98	ASP	CA-C	5.78	1.59	1.52
1	C	88	GLU	C-N	-5.77	1.21	1.34
1	B	274	TRP	C-N	-5.76	1.26	1.33
1	A	274	TRP	NE1-CE2	-5.76	1.31	1.37
1	C	293	GLU	N-CA	5.76	1.53	1.46
1	B	181	TRP	NE1-CE2	-5.74	1.31	1.37
1	C	181	TRP	NE1-CE2	-5.74	1.31	1.37
1	A	274	TRP	C-N	-5.73	1.26	1.33
1	B	98	ASP	CA-C	5.72	1.59	1.52
1	A	181	TRP	NE1-CE2	-5.71	1.31	1.37
1	A	328	GLU	CA-C	-5.68	1.46	1.52
1	C	274	TRP	C-N	-5.67	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	293	GLU	N-CA	5.64	1.53	1.46
1	C	328	GLU	CA-C	-5.64	1.46	1.52
1	B	328	GLU	CA-C	-5.62	1.46	1.52
1	C	313	GLU	C-N	-5.61	1.25	1.33
1	A	184	PHE	C-N	-5.59	1.26	1.33
1	A	98	ASP	CA-C	5.59	1.59	1.52
1	A	313	GLU	C-N	-5.55	1.25	1.33
1	B	184	PHE	C-N	-5.54	1.26	1.33
1	B	90	ILE	C-N	5.51	1.41	1.33
1	B	313	GLU	C-N	-5.50	1.25	1.33
1	C	184	PHE	C-N	-5.48	1.26	1.33
1	C	90	ILE	C-N	5.47	1.41	1.33
1	C	63	ALA	N-CA	-5.47	1.39	1.46
1	A	265	TRP	NE1-CE2	-5.46	1.31	1.37
1	C	265	TRP	NE1-CE2	-5.45	1.31	1.37
1	A	90	ILE	C-N	5.44	1.41	1.33
1	C	346	TRP	NE1-CE2	-5.42	1.31	1.37
1	B	321	TRP	NE1-CE2	-5.41	1.31	1.37
1	A	328	GLU	N-CA	-5.39	1.39	1.46
1	B	265	TRP	NE1-CE2	-5.39	1.31	1.37
1	A	346	TRP	NE1-CE2	-5.38	1.31	1.37
1	C	328	GLU	N-CA	-5.38	1.39	1.46
1	B	328	GLU	N-CA	-5.38	1.39	1.46
1	B	346	TRP	NE1-CE2	-5.36	1.31	1.37
1	A	321	TRP	NE1-CE2	-5.36	1.31	1.37
1	C	192	SER	N-CA	-5.35	1.38	1.46
1	A	192	SER	N-CA	-5.33	1.38	1.46
1	B	192	SER	N-CA	-5.33	1.38	1.46
1	A	327	ALA	N-CA	-5.29	1.39	1.46
1	C	321	TRP	NE1-CE2	-5.28	1.31	1.37
1	C	327	ALA	N-CA	-5.24	1.39	1.46
1	B	327	ALA	N-CA	-5.17	1.39	1.46
1	A	140	PRO	CA-C	5.09	1.59	1.52
1	C	191	ASP	CA-C	-5.07	1.47	1.53
1	C	140	PRO	CA-C	5.06	1.59	1.52
1	B	140	PRO	CA-C	5.04	1.59	1.52
1	A	332	GLY	N-CA	5.03	1.51	1.45

All (506) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	201	ILE	O-C-N	-75.45	28.25	122.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	201	ILE	O-C-N	-75.44	28.27	122.57
1	C	201	ILE	O-C-N	-75.36	28.37	122.57
1	C	307	ASP	CA-C-N	22.09	156.76	121.86
1	C	307	ASP	C-N-CA	22.09	156.76	121.86
1	B	307	ASP	CA-C-N	22.05	156.70	121.86
1	B	307	ASP	C-N-CA	22.05	156.70	121.86
1	A	307	ASP	CA-C-N	22.05	156.69	121.86
1	A	307	ASP	C-N-CA	22.05	156.69	121.86
1	A	82	ILE	O-C-N	-21.45	95.75	122.57
1	C	82	ILE	O-C-N	-21.43	95.78	122.57
1	B	82	ILE	O-C-N	-21.43	95.78	122.57
1	C	129	TYR	O-C-N	21.40	143.38	123.26
1	C	338	THR	O-C-N	21.35	147.72	122.75
1	B	338	THR	O-C-N	21.34	147.72	122.75
1	A	129	TYR	O-C-N	21.31	143.29	123.26
1	B	129	TYR	O-C-N	21.31	143.29	123.26
1	A	338	THR	O-C-N	21.25	147.62	122.75
1	C	93	LEU	N-CA-C	-19.41	76.80	109.80
1	A	93	LEU	N-CA-C	-19.34	76.93	109.80
1	B	93	LEU	N-CA-C	-19.31	76.97	109.80
1	B	300	LEU	O-C-N	17.58	145.97	122.59
1	A	300	LEU	O-C-N	17.52	145.90	122.59
1	C	300	LEU	O-C-N	17.52	145.89	122.59
1	B	264	SER	O-C-N	17.31	142.59	123.03
1	C	264	SER	O-C-N	17.25	142.53	123.03
1	A	264	SER	O-C-N	17.20	142.47	123.03
1	B	100	GLU	O-C-N	-15.65	103.32	121.32
1	C	100	GLU	O-C-N	-15.64	103.34	121.32
1	A	100	GLU	O-C-N	-15.60	103.38	121.32
1	C	307	ASP	O-C-N	-15.37	102.14	122.59
1	A	307	ASP	O-C-N	-15.34	102.19	122.59
1	B	307	ASP	O-C-N	-15.33	102.20	122.59
1	A	297	VAL	CA-C-N	-15.32	92.28	121.54
1	A	297	VAL	C-N-CA	-15.32	92.28	121.54
1	B	297	VAL	CA-C-N	-15.32	92.29	121.54
1	B	297	VAL	C-N-CA	-15.32	92.29	121.54
1	C	297	VAL	CA-C-N	-15.29	92.34	121.54
1	C	297	VAL	C-N-CA	-15.29	92.34	121.54
1	B	290	LEU	O-C-N	15.05	142.60	122.59
1	A	290	LEU	O-C-N	14.98	142.52	122.59
1	C	290	LEU	O-C-N	14.98	142.51	122.59
1	B	330	GLY	O-C-N	-14.94	103.28	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	330	GLY	O-C-N	-14.90	103.33	122.70
1	A	330	GLY	O-C-N	-14.88	103.35	122.70
1	B	299	GLY	O-C-N	14.72	141.83	122.70
1	C	299	GLY	O-C-N	14.72	141.83	122.70
1	A	299	GLY	O-C-N	14.70	141.81	122.70
1	B	200	GLY	O-C-N	13.76	142.66	123.67
1	C	200	GLY	O-C-N	13.72	142.60	123.67
1	A	200	GLY	O-C-N	13.69	142.57	123.67
1	B	339	GLU	CA-C-N	-13.52	90.83	122.20
1	B	339	GLU	C-N-CA	-13.52	90.83	122.20
1	C	339	GLU	CA-C-N	-13.51	90.86	122.20
1	C	339	GLU	C-N-CA	-13.51	90.86	122.20
1	A	339	GLU	CA-C-N	-13.51	90.86	122.20
1	A	339	GLU	C-N-CA	-13.51	90.86	122.20
1	A	275	GLU	N-CA-C	-13.48	88.03	108.52
1	C	275	GLU	N-CA-C	-13.44	88.10	108.52
1	B	275	GLU	N-CA-C	-13.41	88.14	108.52
1	C	200	GLY	CA-C-N	13.32	145.95	121.97
1	C	200	GLY	C-N-CA	13.32	145.95	121.97
1	B	200	GLY	CA-C-N	13.31	145.94	121.97
1	B	200	GLY	C-N-CA	13.31	145.94	121.97
1	A	200	GLY	CA-C-N	13.31	145.93	121.97
1	A	200	GLY	C-N-CA	13.31	145.93	121.97
1	A	273	GLY	CA-C-N	-12.74	102.85	120.82
1	A	273	GLY	C-N-CA	-12.74	102.85	120.82
1	B	273	GLY	CA-C-N	-12.72	102.88	120.82
1	B	273	GLY	C-N-CA	-12.72	102.88	120.82
1	C	273	GLY	CA-C-N	-12.72	102.89	120.82
1	C	273	GLY	C-N-CA	-12.72	102.89	120.82
1	B	203	ASP	O-C-N	-12.33	106.00	121.29
1	A	203	ASP	O-C-N	-12.31	106.02	121.29
1	C	203	ASP	O-C-N	-12.25	106.09	121.29
1	C	325	LYS	CA-C-N	-11.93	100.50	121.97
1	C	325	LYS	C-N-CA	-11.93	100.50	121.97
1	A	325	LYS	CA-C-N	-11.89	100.56	121.97
1	A	325	LYS	C-N-CA	-11.89	100.56	121.97
1	B	325	LYS	CA-C-N	-11.89	100.57	121.97
1	B	325	LYS	C-N-CA	-11.89	100.57	121.97
1	C	264	SER	CA-C-N	-11.87	98.88	121.54
1	C	264	SER	C-N-CA	-11.87	98.88	121.54
1	B	264	SER	CA-C-N	-11.86	98.89	121.54
1	B	264	SER	C-N-CA	-11.86	98.89	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	264	SER	CA-C-N	-11.85	98.90	121.54
1	A	264	SER	C-N-CA	-11.85	98.90	121.54
1	C	76	SER	N-CA-C	11.76	127.00	109.24
1	C	313	GLU	O-C-N	11.76	138.23	122.59
1	B	313	GLU	O-C-N	11.75	138.22	122.59
1	A	313	GLU	O-C-N	11.74	138.21	122.59
1	C	328	GLU	O-C-N	11.70	136.59	123.13
1	B	328	GLU	O-C-N	11.70	136.58	123.13
1	A	328	GLU	O-C-N	11.67	136.56	123.13
1	A	175	CYS	CA-C-N	-11.63	101.03	121.97
1	A	175	CYS	C-N-CA	-11.63	101.03	121.97
1	B	175	CYS	CA-C-N	-11.63	101.03	121.97
1	B	175	CYS	C-N-CA	-11.63	101.03	121.97
1	C	175	CYS	CA-C-N	-11.62	101.06	121.97
1	C	175	CYS	C-N-CA	-11.62	101.06	121.97
1	A	341	GLN	O-C-N	-11.55	108.03	121.32
1	B	341	GLN	O-C-N	-11.55	108.03	121.32
1	C	341	GLN	O-C-N	-11.50	108.09	121.32
1	B	90	ILE	O-C-N	-10.72	109.17	122.57
1	A	90	ILE	O-C-N	-10.71	109.18	122.57
1	A	279	HIS	O-C-N	-10.71	107.34	122.76
1	B	279	HIS	O-C-N	-10.71	107.34	122.76
1	C	279	HIS	O-C-N	-10.71	107.34	122.76
1	C	90	ILE	O-C-N	-10.70	109.19	122.57
1	C	314	ALA	N-CA-C	-10.59	88.25	110.80
1	A	314	ALA	N-CA-C	-10.57	88.28	110.80
1	B	314	ALA	N-CA-C	-10.57	88.29	110.80
1	B	199	ASP	N-CA-C	-10.53	101.81	112.97
1	C	199	ASP	N-CA-C	-10.51	101.83	112.97
1	A	199	ASP	N-CA-C	-10.46	101.88	112.97
1	C	162	PRO	O-C-N	-9.72	109.99	121.46
1	B	163	PRO	O-C-N	9.70	135.74	122.64
1	B	296	PRO	O-C-N	9.69	135.73	122.64
1	A	162	PRO	O-C-N	-9.68	110.03	121.46
1	A	296	PRO	O-C-N	9.66	135.68	122.64
1	B	162	PRO	O-C-N	-9.66	110.06	121.46
1	C	296	PRO	O-C-N	9.66	135.68	122.64
1	C	163	PRO	O-C-N	9.66	135.68	122.64
1	A	163	PRO	O-C-N	9.65	135.67	122.64
1	C	273	GLY	O-C-N	9.48	135.03	122.70
1	A	273	GLY	O-C-N	9.48	135.03	122.70
1	B	273	GLY	O-C-N	9.44	134.97	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	191	ASP	O-C-N	9.42	134.12	121.78
1	B	140	PRO	N-CD-CG	-9.39	89.11	103.20
1	A	191	ASP	O-C-N	9.38	134.07	121.78
1	C	140	PRO	N-CD-CG	-9.38	89.13	103.20
1	A	140	PRO	N-CD-CG	-9.37	89.15	103.20
1	C	176	VAL	O-C-N	9.35	134.26	122.57
1	A	176	VAL	O-C-N	9.30	134.20	122.57
1	B	338	THR	N-CA-C	9.30	122.61	110.43
1	C	191	ASP	O-C-N	9.29	133.95	121.78
1	A	338	THR	N-CA-C	9.26	122.56	110.43
1	C	338	THR	N-CA-C	9.24	122.53	110.43
1	B	176	VAL	O-C-N	9.21	134.09	122.57
1	C	57	ARG	O-C-N	9.19	134.45	123.33
1	A	274	TRP	O-C-N	9.14	134.28	122.95
1	C	274	TRP	O-C-N	9.13	134.27	122.95
1	C	72	GLN	CA-C-N	9.12	129.54	120.52
1	C	72	GLN	C-N-CA	9.12	129.54	120.52
1	C	140	PRO	CA-N-CD	9.09	124.73	112.00
1	C	63	ALA	O-C-N	9.08	134.61	123.44
1	B	274	TRP	O-C-N	9.08	134.21	122.95
1	A	338	THR	CA-C-N	9.03	138.78	121.54
1	A	338	THR	C-N-CA	9.03	138.78	121.54
1	A	162	PRO	N-CA-C	-9.02	99.69	110.70
1	B	162	PRO	N-CA-C	-9.02	99.70	110.70
1	A	140	PRO	CA-N-CD	9.01	124.62	112.00
1	C	162	PRO	N-CA-C	-9.01	99.71	110.70
1	C	202	SER	CB-CA-C	-9.00	92.51	110.42
1	A	202	SER	CB-CA-C	-8.99	92.53	110.42
1	B	338	THR	CA-C-N	8.99	138.71	121.54
1	B	338	THR	C-N-CA	8.99	138.71	121.54
1	C	338	THR	CA-C-N	8.99	138.71	121.54
1	C	338	THR	C-N-CA	8.99	138.71	121.54
1	B	140	PRO	CA-N-CD	8.98	124.58	112.00
1	B	202	SER	CB-CA-C	-8.98	92.54	110.42
1	C	199	ASP	O-C-N	8.98	134.09	122.06
1	A	199	ASP	O-C-N	8.98	134.09	122.06
1	B	199	ASP	O-C-N	8.97	134.07	122.06
1	A	82	ILE	CA-C-N	8.96	138.66	121.54
1	A	82	ILE	C-N-CA	8.96	138.66	121.54
1	B	82	ILE	CA-C-N	8.96	138.65	121.54
1	B	82	ILE	C-N-CA	8.96	138.65	121.54
1	C	82	ILE	CA-C-N	8.95	138.63	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	82	ILE	C-N-CA	8.95	138.63	121.54
1	C	140	PRO	N-CA-CB	-8.85	93.96	103.25
1	A	140	PRO	N-CA-CB	-8.76	94.06	103.25
1	B	140	PRO	N-CA-CB	-8.75	94.06	103.25
1	B	329	ARG	O-C-N	8.67	134.12	122.59
1	C	313	GLU	CA-C-N	8.67	138.09	121.54
1	C	313	GLU	C-N-CA	8.67	138.09	121.54
1	A	329	ARG	O-C-N	8.66	134.11	122.59
1	A	313	GLU	CA-C-N	8.66	138.08	121.54
1	A	313	GLU	C-N-CA	8.66	138.08	121.54
1	B	288	LEU	O-C-N	8.66	132.72	122.85
1	B	313	GLU	CA-C-N	8.65	138.06	121.54
1	B	313	GLU	C-N-CA	8.65	138.06	121.54
1	C	288	LEU	O-C-N	8.65	132.71	122.85
1	B	165	ASP	O-C-N	8.61	133.78	123.27
1	C	329	ARG	O-C-N	8.61	134.04	122.59
1	A	165	ASP	O-C-N	8.61	133.77	123.27
1	C	165	ASP	O-C-N	8.60	133.76	123.27
1	A	288	LEU	O-C-N	8.59	132.64	122.85
1	C	69	VAL	O-C-N	-8.55	111.89	122.57
1	C	202	SER	O-C-N	8.44	133.82	122.59
1	A	202	SER	O-C-N	8.44	133.81	122.59
1	B	202	SER	O-C-N	8.43	133.80	122.59
1	C	291	PHE	N-CA-CB	-8.36	96.36	110.49
1	A	202	SER	N-CA-C	8.36	128.61	110.80
1	B	291	PHE	N-CA-CB	-8.35	96.39	110.49
1	A	291	PHE	N-CA-CB	-8.33	96.41	110.49
1	B	202	SER	N-CA-C	8.33	128.55	110.80
1	C	202	SER	N-CA-C	8.32	128.53	110.80
1	C	325	LYS	O-C-N	8.31	132.09	123.62
1	A	325	LYS	O-C-N	8.26	132.04	123.62
1	B	325	LYS	O-C-N	8.21	132.00	123.62
1	A	326	VAL	O-C-N	8.18	132.79	122.57
1	C	175	CYS	CB-CA-C	-8.16	97.72	110.04
1	C	53	GLN	C-N-CA	-8.15	110.03	122.09
1	B	326	VAL	O-C-N	8.14	132.75	122.57
1	A	175	CYS	CB-CA-C	-8.14	97.75	110.04
1	B	308	PHE	CA-C-N	-8.13	110.65	122.44
1	B	308	PHE	C-N-CA	-8.13	110.65	122.44
1	C	308	PHE	CA-C-N	-8.13	110.64	122.44
1	C	308	PHE	C-N-CA	-8.13	110.64	122.44
1	C	326	VAL	O-C-N	8.13	132.74	122.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	308	PHE	CA-C-N	-8.11	110.68	122.44
1	A	308	PHE	C-N-CA	-8.11	110.68	122.44
1	B	175	CYS	CB-CA-C	-8.09	97.82	110.04
1	A	164	ASN	N-CA-C	-7.99	103.49	113.55
1	C	164	ASN	N-CA-C	-7.95	103.53	113.55
1	B	164	ASN	N-CA-C	-7.94	103.55	113.55
1	C	62	VAL	O-C-N	7.93	129.56	121.87
1	C	317	GLY	O-C-N	-7.81	113.32	122.38
1	B	317	GLY	O-C-N	-7.81	113.32	122.38
1	A	91	THR	N-CA-CB	7.77	123.63	110.49
1	A	317	GLY	O-C-N	-7.77	113.36	122.38
1	C	91	THR	N-CA-CB	7.73	123.56	110.49
1	B	91	THR	N-CA-CB	7.72	123.54	110.49
1	C	175	CYS	O-C-N	-7.51	114.34	122.00
1	B	175	CYS	O-C-N	-7.49	114.36	122.00
1	A	175	CYS	O-C-N	-7.45	114.40	122.00
1	A	339	GLU	O-C-N	7.31	132.31	122.59
1	B	339	GLU	O-C-N	7.28	132.27	122.59
1	C	339	GLU	O-C-N	7.27	132.26	122.59
1	B	274	TRP	CA-C-N	7.27	138.15	121.87
1	B	274	TRP	C-N-CA	7.27	138.15	121.87
1	C	274	TRP	CA-C-N	7.23	138.07	121.87
1	C	274	TRP	C-N-CA	7.23	138.07	121.87
1	A	274	TRP	CA-C-N	7.22	138.05	121.87
1	A	274	TRP	C-N-CA	7.22	138.05	121.87
1	A	90	ILE	N-CA-C	7.22	124.36	109.34
1	C	90	ILE	N-CA-C	7.22	124.36	109.34
1	B	90	ILE	N-CA-C	7.20	124.32	109.34
1	C	62	VAL	CB-CA-C	-7.19	102.44	112.14
1	A	82	ILE	N-CA-CB	-7.10	99.52	111.23
1	B	82	ILE	N-CA-CB	-7.10	99.52	111.23
1	C	82	ILE	N-CA-CB	-7.09	99.52	111.23
1	C	56	THR	CB-CA-C	-7.07	96.35	110.42
1	B	278	CYS	CA-CB-SG	-7.07	98.15	114.40
1	B	305	ALA	O-C-N	7.06	131.71	123.17
1	A	278	CYS	CA-CB-SG	-7.06	98.17	114.40
1	C	278	CYS	CA-CB-SG	-7.04	98.21	114.40
1	C	71	THR	N-CA-CB	-7.03	98.61	110.49
1	C	305	ALA	O-C-N	7.01	131.66	123.17
1	C	323	GLY	CA-C-N	7.00	134.58	121.97
1	C	323	GLY	C-N-CA	7.00	134.58	121.97
1	A	305	ALA	O-C-N	7.00	131.64	123.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	323	GLY	CA-C-N	7.00	134.56	121.97
1	A	323	GLY	C-N-CA	7.00	134.56	121.97
1	B	323	GLY	CA-C-N	6.97	134.51	121.97
1	B	323	GLY	C-N-CA	6.97	134.51	121.97
1	A	315	ALA	O-C-N	-6.95	113.35	122.59
1	B	290	LEU	CB-CA-C	-6.94	96.61	110.42
1	A	290	LEU	CB-CA-C	-6.92	96.66	110.42
1	B	315	ALA	O-C-N	-6.92	113.39	122.59
1	C	290	LEU	CB-CA-C	-6.91	96.67	110.42
1	C	315	ALA	O-C-N	-6.90	113.41	122.59
1	C	310	VAL	O-C-N	6.89	130.50	123.20
1	B	176	VAL	N-CA-CB	-6.88	99.87	111.23
1	B	129	TYR	CA-C-N	6.88	134.68	121.54
1	B	129	TYR	C-N-CA	6.88	134.68	121.54
1	A	310	VAL	O-C-N	6.86	130.47	123.20
1	C	129	TYR	CA-C-N	6.86	134.65	121.54
1	C	129	TYR	C-N-CA	6.86	134.65	121.54
1	C	176	VAL	N-CA-CB	-6.86	99.91	111.23
1	A	129	TYR	CA-C-N	6.86	134.64	121.54
1	A	129	TYR	C-N-CA	6.86	134.64	121.54
1	A	176	VAL	N-CA-CB	-6.86	99.92	111.23
1	C	76	SER	CB-CA-C	-6.86	94.98	110.07
1	B	310	VAL	O-C-N	6.84	130.45	123.20
1	B	317	GLY	N-CA-C	-6.83	105.45	115.63
1	A	317	GLY	N-CA-C	-6.82	105.46	115.63
1	C	316	ALA	CA-C-N	6.82	131.98	122.29
1	C	316	ALA	C-N-CA	6.82	131.98	122.29
1	A	290	LEU	CA-C-N	6.82	134.57	121.54
1	A	290	LEU	C-N-CA	6.82	134.57	121.54
1	C	290	LEU	CA-C-N	6.81	134.56	121.54
1	C	290	LEU	C-N-CA	6.81	134.56	121.54
1	A	316	ALA	CA-C-N	6.80	131.94	122.29
1	A	316	ALA	C-N-CA	6.80	131.94	122.29
1	C	317	GLY	N-CA-C	-6.79	105.51	115.63
1	B	316	ALA	CA-C-N	6.79	131.93	122.29
1	B	316	ALA	C-N-CA	6.79	131.93	122.29
1	A	305	ALA	N-CA-C	6.78	119.48	109.24
1	B	290	LEU	CA-C-N	6.78	134.49	121.54
1	B	290	LEU	C-N-CA	6.78	134.49	121.54
1	B	220	GLY	N-CA-C	-6.77	104.14	111.93
1	C	305	ALA	N-CA-C	6.77	119.46	109.24
1	C	220	GLY	N-CA-C	-6.72	104.20	111.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	305	ALA	N-CA-C	6.72	119.38	109.24
1	A	220	GLY	N-CA-C	-6.70	104.22	111.93
1	B	304	ASP	O-C-N	6.67	131.04	122.71
1	A	175	CYS	CA-CB-SG	-6.66	99.07	114.40
1	C	175	CYS	CA-CB-SG	-6.66	99.08	114.40
1	B	175	CYS	CA-CB-SG	-6.65	99.11	114.40
1	A	304	ASP	O-C-N	6.61	130.97	122.71
1	C	304	ASP	O-C-N	6.59	130.94	122.71
1	A	102	LYS	CB-CA-C	6.50	123.35	110.42
1	A	130	ARG	N-CA-C	6.47	124.59	110.80
1	C	102	LYS	CB-CA-C	6.47	123.31	110.42
1	B	102	LYS	CB-CA-C	6.46	123.28	110.42
1	B	290	LEU	N-CA-C	6.46	124.56	110.80
1	C	290	LEU	N-CA-C	6.46	124.55	110.80
1	B	130	ARG	N-CA-C	6.45	124.54	110.80
1	C	130	ARG	N-CA-C	6.44	124.53	110.80
1	A	290	LEU	N-CA-C	6.44	124.51	110.80
1	A	112	GLU	O-C-N	-6.32	114.05	121.32
1	C	112	GLU	O-C-N	-6.30	114.08	121.32
1	B	112	GLU	O-C-N	-6.28	114.10	121.32
1	C	275	GLU	O-C-N	-6.26	116.92	123.56
1	A	275	GLU	O-C-N	-6.22	116.96	123.56
1	C	318	SER	N-CA-C	6.22	124.06	110.80
1	A	318	SER	N-CA-C	6.21	124.03	110.80
1	B	318	SER	N-CA-C	6.21	124.02	110.80
1	B	275	GLU	O-C-N	-6.20	116.99	123.56
1	C	53	GLN	O-C-N	-6.13	113.19	123.00
1	A	201	ILE	CA-C-N	-6.09	109.91	121.54
1	A	201	ILE	C-N-CA	-6.09	109.91	121.54
1	A	330	GLY	CA-C-N	6.06	131.45	121.39
1	A	330	GLY	C-N-CA	6.06	131.45	121.39
1	B	201	ILE	CA-C-N	-6.05	109.98	121.54
1	B	201	ILE	C-N-CA	-6.05	109.98	121.54
1	C	330	GLY	CA-C-N	6.05	131.44	121.39
1	C	330	GLY	C-N-CA	6.05	131.44	121.39
1	B	330	GLY	CA-C-N	6.04	131.42	121.39
1	B	330	GLY	C-N-CA	6.04	131.42	121.39
1	A	176	VAL	CB-CA-C	6.03	121.19	111.29
1	B	176	VAL	CB-CA-C	6.02	121.16	111.29
1	A	140	PRO	CB-CA-C	-6.01	101.65	111.56
1	C	140	PRO	CB-CA-C	-6.00	101.67	111.56
1	A	298	SER	CA-C-N	-5.98	109.69	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	298	SER	C-N-CA	-5.98	109.69	121.41
1	C	298	SER	CA-C-N	-5.98	109.70	121.41
1	C	298	SER	C-N-CA	-5.98	109.70	121.41
1	B	264	SER	CB-CA-C	-5.97	99.94	109.80
1	B	140	PRO	CB-CA-C	-5.97	101.70	111.56
1	A	264	SER	CB-CA-C	-5.97	99.95	109.80
1	C	176	VAL	CB-CA-C	5.97	121.08	111.29
1	B	298	SER	CA-C-N	-5.96	109.72	121.41
1	B	298	SER	C-N-CA	-5.96	109.72	121.41
1	A	258	ASP	CA-C-O	5.96	121.40	117.94
1	C	201	ILE	CA-C-N	-5.96	110.16	121.54
1	C	201	ILE	C-N-CA	-5.96	110.16	121.54
1	C	264	SER	CB-CA-C	-5.93	100.02	109.80
1	B	258	ASP	CA-C-O	5.92	121.37	117.94
1	C	75	VAL	N-CA-C	5.91	121.64	109.34
1	C	258	ASP	CA-C-O	5.91	121.37	117.94
1	C	81	GLY	O-C-N	5.91	130.49	123.46
1	B	338	THR	CB-CA-C	-5.89	97.45	109.65
1	C	338	THR	CB-CA-C	-5.89	97.45	109.65
1	A	338	THR	CB-CA-C	-5.88	97.48	109.65
1	A	99	THR	CB-CA-C	-5.85	101.28	110.94
1	B	99	THR	CB-CA-C	-5.85	101.29	110.94
1	C	99	THR	CB-CA-C	-5.83	101.31	110.94
1	A	130	ARG	CB-CA-C	-5.80	98.88	110.42
1	C	130	ARG	CB-CA-C	-5.79	98.90	110.42
1	B	273	GLY	N-CA-C	-5.78	99.48	113.18
1	B	262	LEU	CA-C-N	5.78	132.37	121.97
1	B	262	LEU	C-N-CA	5.78	132.37	121.97
1	C	273	GLY	N-CA-C	-5.78	99.48	113.18
1	B	130	ARG	CB-CA-C	-5.76	98.95	110.42
1	A	273	GLY	N-CA-C	-5.76	99.53	113.18
1	C	262	LEU	CA-C-N	5.75	132.32	121.97
1	C	262	LEU	C-N-CA	5.75	132.32	121.97
1	C	110	PRO	CB-CA-C	5.74	121.03	111.56
1	A	262	LEU	CA-C-N	5.73	132.28	121.97
1	A	262	LEU	C-N-CA	5.73	132.28	121.97
1	B	271	THR	O-C-N	5.73	130.03	123.27
1	A	201	ILE	N-CA-C	5.72	121.25	109.34
1	B	110	PRO	CB-CA-C	5.71	120.99	111.56
1	A	271	THR	O-C-N	5.71	130.00	123.27
1	C	271	THR	O-C-N	5.70	130.00	123.27
1	B	201	ILE	N-CA-C	5.69	121.18	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	75	VAL	O-C-N	-5.69	115.46	122.57
1	C	350	ARG	NE-CZ-NH2	5.69	124.32	119.20
1	C	201	ILE	N-CA-C	5.69	121.17	109.34
1	C	327	ALA	CA-C-N	-5.68	114.63	122.30
1	C	327	ALA	C-N-CA	-5.68	114.63	122.30
1	A	110	PRO	CB-CA-C	5.67	120.92	111.56
1	B	350	ARG	NE-CZ-NH2	5.67	124.31	119.20
1	A	350	ARG	NE-CZ-NH2	5.67	124.30	119.20
1	B	327	ALA	CA-C-N	-5.65	114.68	122.30
1	B	327	ALA	C-N-CA	-5.65	114.68	122.30
1	B	236	VAL	O-C-N	5.65	127.94	122.69
1	C	236	VAL	O-C-N	5.65	127.94	122.69
1	B	308	PHE	CB-CA-C	-5.64	102.00	110.24
1	A	236	VAL	O-C-N	5.64	127.93	122.69
1	A	327	ALA	CA-C-N	-5.64	114.69	122.30
1	A	327	ALA	C-N-CA	-5.64	114.69	122.30
1	C	74	ARG	NE-CZ-NH2	5.63	124.26	119.20
1	C	308	PHE	CB-CA-C	-5.60	102.06	110.24
1	A	308	PHE	CB-CA-C	-5.60	102.06	110.24
1	B	303	ALA	O-C-N	-5.57	115.18	122.59
1	B	248	ALA	CB-CA-C	-5.56	102.16	110.50
1	B	300	LEU	CA-C-N	-5.55	113.07	122.67
1	B	300	LEU	C-N-CA	-5.55	113.07	122.67
1	A	300	LEU	CA-C-N	-5.54	113.09	122.67
1	A	300	LEU	C-N-CA	-5.54	113.09	122.67
1	A	248	ALA	CB-CA-C	-5.54	102.20	110.50
1	A	303	ALA	O-C-N	-5.53	115.24	122.59
1	C	248	ALA	CB-CA-C	-5.53	102.21	110.50
1	C	303	ALA	O-C-N	-5.53	115.24	122.59
1	C	300	LEU	CA-C-N	-5.52	113.11	122.67
1	C	300	LEU	C-N-CA	-5.52	113.11	122.67
1	B	162	PRO	CA-C-N	-5.49	112.98	119.84
1	B	162	PRO	C-N-CA	-5.49	112.98	119.84
1	C	319	VAL	CA-C-N	-5.47	113.01	122.10
1	C	319	VAL	C-N-CA	-5.47	113.01	122.10
1	A	319	VAL	CA-C-N	-5.47	113.03	122.10
1	A	319	VAL	C-N-CA	-5.47	113.03	122.10
1	C	239	LYS	O-C-N	5.46	128.57	121.79
1	A	162	PRO	CA-C-N	-5.46	113.02	119.84
1	A	162	PRO	C-N-CA	-5.46	113.02	119.84
1	B	93	LEU	N-CA-CB	-5.46	99.44	109.10
1	A	239	LYS	O-C-N	5.45	128.55	121.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	93	LEU	N-CA-CB	-5.45	99.45	109.10
1	B	319	VAL	CA-C-N	-5.45	113.05	122.10
1	B	319	VAL	C-N-CA	-5.45	113.05	122.10
1	C	162	PRO	CA-C-N	-5.44	113.04	119.84
1	C	162	PRO	C-N-CA	-5.44	113.04	119.84
1	C	93	LEU	N-CA-CB	-5.43	99.48	109.10
1	B	239	LYS	O-C-N	5.42	128.51	121.79
1	A	343	LYS	O-C-N	5.41	129.78	122.59
1	A	84	ARG	NE-CZ-NH2	5.40	124.06	119.20
1	C	343	LYS	O-C-N	5.39	129.76	122.59
1	A	261	ARG	NE-CZ-NH2	5.39	124.05	119.20
1	C	57	ARG	NE-CZ-NH2	5.39	124.05	119.20
1	C	334	LYS	O-C-N	5.38	129.39	123.25
1	A	135	ARG	NE-CZ-NH2	5.38	124.04	119.20
1	A	334	LYS	O-C-N	5.38	129.38	123.25
1	C	135	ARG	NE-CZ-NH2	5.38	124.04	119.20
1	B	84	ARG	NE-CZ-NH2	5.38	124.04	119.20
1	C	241	ARG	NE-CZ-NH2	5.38	124.04	119.20
1	C	338	THR	N-CA-CB	5.38	117.95	110.26
1	B	135	ARG	NE-CZ-NH2	5.38	124.04	119.20
1	B	338	THR	N-CA-CB	5.38	117.95	110.26
1	A	241	ARG	NE-CZ-NH2	5.36	124.03	119.20
1	B	261	ARG	NE-CZ-NH2	5.36	124.02	119.20
1	A	195	ARG	NE-CZ-NH2	5.35	124.02	119.20
1	B	130	ARG	NE-CZ-NH2	5.35	124.01	119.20
1	A	329	ARG	NE-CZ-NH2	5.34	124.00	119.20
1	B	343	LYS	O-C-N	5.34	129.69	122.59
1	C	195	ARG	NE-CZ-NH2	5.34	124.00	119.20
1	C	261	ARG	NE-CZ-NH2	5.34	124.00	119.20
1	C	84	ARG	NE-CZ-NH2	5.33	124.00	119.20
1	C	130	ARG	NE-CZ-NH2	5.33	124.00	119.20
1	B	334	LYS	O-C-N	5.33	129.32	123.25
1	C	56	THR	O-C-N	-5.32	115.51	122.59
1	A	156	ARG	NE-CZ-NH2	5.32	123.99	119.20
1	A	338	THR	N-CA-CB	5.32	117.86	110.26
1	C	329	ARG	NE-CZ-NH2	5.32	123.99	119.20
1	B	241	ARG	NE-CZ-NH2	5.32	123.98	119.20
1	B	195	ARG	NE-CZ-NH2	5.31	123.98	119.20
1	A	239	LYS	N-CA-CB	5.30	118.40	110.39
1	A	130	ARG	NE-CZ-NH2	5.30	123.97	119.20
1	B	239	LYS	N-CA-CB	5.28	118.36	110.39
1	C	239	LYS	N-CA-CB	5.28	118.36	110.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	156	ARG	NE-CZ-NH2	5.27	123.94	119.20
1	C	78	ALA	O-C-N	5.27	129.60	122.59
1	C	60	ALA	O-C-N	5.26	127.37	121.32
1	B	291	PHE	CB-CA-C	5.26	120.89	110.42
1	B	329	ARG	NE-CZ-NH2	5.26	123.93	119.20
1	C	156	ARG	NE-CZ-NH2	5.25	123.93	119.20
1	C	79	ARG	NE-CZ-NH2	5.25	123.93	119.20
1	C	291	PHE	CB-CA-C	5.25	120.87	110.42
1	A	221	ALA	O-C-N	5.23	129.18	123.27
1	A	291	PHE	CB-CA-C	5.23	120.83	110.42
1	C	341	GLN	N-CA-C	5.22	121.34	109.81
1	B	341	GLN	N-CA-C	5.20	121.31	109.81
1	B	259	GLY	CA-C-O	-5.20	114.08	121.52
1	A	341	GLN	N-CA-C	5.20	121.30	109.81
1	C	259	GLY	CA-C-O	-5.18	114.11	121.52
1	A	211	LYS	N-CA-CB	5.17	117.46	110.38
1	A	258	ASP	CB-CA-C	-5.17	109.63	117.07
1	A	259	GLY	CA-C-O	-5.17	114.13	121.52
1	C	221	ALA	O-C-N	5.15	129.09	123.27
1	A	202	SER	CA-C-N	5.15	131.40	122.28
1	A	202	SER	C-N-CA	5.15	131.40	122.28
1	B	202	SER	CA-C-N	5.15	131.40	122.28
1	B	202	SER	C-N-CA	5.15	131.40	122.28
1	C	258	ASP	CB-CA-C	-5.14	109.66	117.07
1	A	343	LYS	CB-CA-C	-5.12	100.24	110.42
1	B	221	ALA	O-C-N	5.12	129.05	123.27
1	B	258	ASP	CB-CA-C	-5.11	109.71	117.07
1	C	202	SER	CA-C-N	5.11	131.32	122.28
1	C	202	SER	C-N-CA	5.11	131.32	122.28
1	C	76	SER	CA-C-N	5.10	131.28	121.54
1	C	76	SER	C-N-CA	5.10	131.28	121.54
1	B	343	LYS	CB-CA-C	-5.10	100.28	110.42
1	C	343	LYS	CB-CA-C	-5.09	100.29	110.42
1	C	74	ARG	O-C-N	-5.09	117.02	123.17
1	B	334	LYS	N-CA-C	5.06	116.76	109.07
1	A	334	LYS	N-CA-C	5.04	116.73	109.07
1	C	334	LYS	N-CA-C	5.04	116.73	109.07
1	C	192	SER	N-CA-C	5.04	117.26	110.06
1	A	137	ARG	NE-CZ-NH2	5.02	123.72	119.20
1	C	137	ARG	NE-CZ-NH2	5.02	123.72	119.20
1	B	137	ARG	NE-CZ-NH2	5.01	123.71	119.20
1	B	192	SER	N-CA-C	5.01	117.23	110.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	342	PRO	O-C-N	5.00	129.21	123.01

There are no chirality outliers.

All (26) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	GLU	Mainchain
1	A	177	SER	Mainchain
1	A	201	ILE	Mainchain
1	A	260	PRO	Mainchain
1	A	307	ASP	Mainchain
1	A	330	GLY	Mainchain
1	A	335	MET	Mainchain
1	A	92	THR	Peptide
1	B	100	GLU	Mainchain
1	B	177	SER	Mainchain
1	B	201	ILE	Mainchain
1	B	260	PRO	Mainchain
1	B	307	ASP	Mainchain
1	B	330	GLY	Mainchain
1	B	335	MET	Mainchain
1	B	92	THR	Peptide
1	C	100	GLU	Mainchain
1	C	177	SER	Mainchain
1	C	201	ILE	Mainchain
1	C	260	PRO	Mainchain
1	C	307	ASP	Mainchain
1	C	330	GLY	Mainchain
1	C	335	MET	Mainchain
1	C	59	SER	Mainchain
1	C	69	VAL	Mainchain
1	C	92	THR	Peptide

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	2024	0	1970	972	0
1	B	2024	0	1969	966	0
1	C	2236	0	2188	1166	0
All	All	6284	0	6127	3104	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 250.

All (3104) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:TYR:CB	1:A:184:PHE:CE1	1.75	1.66
1:C:138:TYR:CB	1:C:184:PHE:CE1	1.75	1.65
1:C:138:TYR:HB2	1:C:184:PHE:CZ	1.15	1.64
1:A:138:TYR:HB2	1:A:184:PHE:CZ	1.15	1.64
1:B:101:PRO:CD	1:B:166:LEU:CD1	1.75	1.64
1:B:138:TYR:CB	1:B:184:PHE:CE1	1.75	1.64
1:C:101:PRO:CD	1:C:166:LEU:HD11	1.21	1.63
1:A:101:PRO:CD	1:A:166:LEU:CD1	1.75	1.63
1:B:138:TYR:HB2	1:B:184:PHE:CZ	1.15	1.62
1:C:76:SER:CA	1:C:76:SER:C	1.75	1.59
1:B:101:PRO:CD	1:B:166:LEU:HD11	1.22	1.57
1:C:75:VAL:CA	1:C:75:VAL:C	1.76	1.57
1:A:248:ALA:CB	1:A:264:SER:C	1.75	1.57
1:A:101:PRO:CD	1:A:166:LEU:HD11	1.21	1.56
1:B:130:ARG:CD	1:B:237:GLN:CB	1.82	1.56
1:A:130:ARG:CD	1:A:237:GLN:CB	1.81	1.54
1:C:101:PRO:CD	1:C:166:LEU:CD1	1.75	1.53
1:C:130:ARG:CD	1:C:237:GLN:CB	1.82	1.53
1:A:278:CYS:H	1:A:334:LYS:CD	1.21	1.53
1:C:278:CYS:H	1:C:334:LYS:CD	1.21	1.52
1:A:339:GLU:C	1:A:340:GLU:N	1.68	1.52
1:C:159:ALA:HB1	1:C:328:GLU:CB	1.32	1.52
1:B:278:CYS:H	1:B:334:LYS:CD	1.21	1.51
1:A:101:PRO:HD3	1:A:166:LEU:CD1	1.34	1.51
1:C:75:VAL:CA	1:C:75:VAL:N	1.68	1.51
1:C:101:PRO:HD3	1:C:166:LEU:CD1	1.34	1.50
1:B:339:GLU:C	1:B:340:GLU:N	1.68	1.50
1:C:76:SER:CA	1:C:76:SER:N	1.76	1.49
1:C:185:ILE:HD12	1:C:186:LEU:N	1.18	1.49
1:A:264:SER:C	1:A:265:TRP:N	1.68	1.48
1:C:153:ALA:CB	1:C:174:GLY:HA3	1.43	1.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:ALA:CB	1:A:174:GLY:HA3	1.43	1.47
1:B:264:SER:C	1:B:265:TRP:N	1.68	1.47
1:C:200:GLY:N	1:C:265:TRP:CD1	1.82	1.47
1:A:130:ARG:CD	1:A:237:GLN:HB2	0.98	1.46
1:C:291:PHE:C	1:C:292:TYR:N	1.71	1.46
1:C:80:ASP:HA	1:C:241:ARG:NH2	1.24	1.46
1:A:121:LYS:NZ	1:A:121:LYS:CE	1.79	1.45
1:B:153:ALA:CB	1:B:174:GLY:HA3	1.43	1.45
1:C:130:ARG:CD	1:C:237:GLN:HB2	0.98	1.45
1:C:207:VAL:CG1	1:C:329:ARG:CZ	1.93	1.45
1:C:264:SER:C	1:C:265:TRP:N	1.68	1.45
1:B:130:ARG:CD	1:B:237:GLN:HB2	0.98	1.45
1:B:279:HIS:C	1:B:280:PHE:N	1.74	1.45
1:B:291:PHE:C	1:B:292:TYR:N	1.71	1.44
1:C:339:GLU:C	1:C:340:GLU:N	1.68	1.44
1:A:291:PHE:C	1:A:292:TYR:N	1.71	1.43
1:B:101:PRO:HD3	1:B:166:LEU:CD1	1.34	1.43
1:B:121:LYS:NZ	1:B:121:LYS:CE	1.79	1.43
1:C:134:LEU:CA	1:C:233:GLU:O	1.66	1.43
1:C:207:VAL:N	1:C:329:ARG:HH22	0.96	1.43
1:A:269:LYS:O	1:A:277:ASP:CB	1.67	1.43
1:A:296:PRO:CG	1:A:337:THR:HG22	0.96	1.43
1:C:207:VAL:HG12	1:C:329:ARG:NH2	1.27	1.43
1:C:296:PRO:CG	1:C:337:THR:HG22	0.96	1.43
1:A:248:ALA:HB3	1:A:264:SER:C	1.01	1.42
1:C:279:HIS:C	1:C:280:PHE:N	1.74	1.42
1:B:185:ILE:HD12	1:B:186:LEU:N	1.18	1.42
1:B:269:LYS:O	1:B:277:ASP:CB	1.67	1.42
1:C:121:LYS:NZ	1:C:121:LYS:CE	1.79	1.42
1:C:207:VAL:HG12	1:C:329:ARG:CZ	0.96	1.42
1:C:207:VAL:H	1:C:329:ARG:NH2	1.11	1.42
1:B:296:PRO:CG	1:B:337:THR:HG22	0.96	1.42
1:C:197:VAL:CG2	1:C:350:ARG:HH22	1.30	1.42
1:B:185:ILE:CD1	1:B:186:LEU:H	1.32	1.41
1:C:269:LYS:O	1:C:277:ASP:CB	1.67	1.41
1:C:203:ASP:OD1	1:C:205:LYS:CD	1.68	1.41
1:A:134:LEU:CA	1:A:233:GLU:O	1.66	1.41
1:A:279:HIS:C	1:A:280:PHE:N	1.74	1.41
1:A:203:ASP:OD1	1:A:205:LYS:CD	1.68	1.40
1:C:207:VAL:CG1	1:C:329:ARG:NH2	1.81	1.40
1:B:149:LYS:CD	1:B:149:LYS:CE	2.00	1.39

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ILE:HD12	1:A:186:LEU:N	1.18	1.39
1:B:82:ILE:C	1:B:83:THR:N	1.81	1.39
1:C:185:ILE:CD1	1:C:186:LEU:H	1.32	1.39
1:A:130:ARG:HD2	1:A:237:GLN:CB	1.47	1.39
1:A:149:LYS:CE	1:A:149:LYS:CD	1.99	1.39
1:B:115:THR:O	1:B:116:PHE:CD1	1.75	1.39
1:A:82:ILE:C	1:A:83:THR:N	1.81	1.39
1:B:350:ARG:O	1:B:351:ILE:CG2	1.71	1.39
1:A:185:ILE:CD1	1:A:186:LEU:H	1.32	1.39
1:C:82:ILE:C	1:C:83:THR:N	1.81	1.39
1:C:149:LYS:CD	1:C:149:LYS:CE	1.99	1.39
1:A:115:THR:O	1:A:116:PHE:CD1	1.76	1.38
1:B:138:TYR:CB	1:B:184:PHE:CZ	1.96	1.38
1:B:203:ASP:OD1	1:B:205:LYS:CD	1.68	1.38
1:B:134:LEU:CA	1:B:233:GLU:O	1.66	1.38
1:C:350:ARG:O	1:C:351:ILE:CG2	1.71	1.38
1:B:149:LYS:CD	1:B:170:TYR:OH	1.72	1.37
1:A:149:LYS:CD	1:A:170:TYR:OH	1.72	1.37
1:C:204:PRO:HG2	1:C:328:GLU:CG	1.54	1.37
1:C:115:THR:O	1:C:116:PHE:CD1	1.75	1.37
1:C:149:LYS:CD	1:C:170:TYR:OH	1.72	1.36
1:A:138:TYR:CG	1:A:184:PHE:CE1	2.12	1.36
1:B:130:ARG:HD3	1:B:237:GLN:CB	1.46	1.36
1:A:350:ARG:O	1:A:351:ILE:CG2	1.71	1.36
1:C:138:TYR:CG	1:C:184:PHE:CE1	2.12	1.36
1:C:138:TYR:CB	1:C:184:PHE:CZ	1.96	1.35
1:C:165:ASP:O	1:C:168:SER:HB2	1.25	1.35
1:C:159:ALA:CB	1:C:328:GLU:HB2	1.54	1.35
1:C:296:PRO:HG2	1:C:337:THR:CG2	0.89	1.34
1:A:296:PRO:HG2	1:A:337:THR:CG2	0.89	1.34
1:B:138:TYR:CG	1:B:184:PHE:CE1	2.12	1.34
1:B:278:CYS:N	1:B:334:LYS:CD	1.87	1.34
1:B:296:PRO:HG2	1:B:337:THR:CG2	0.88	1.34
1:A:309:SER:O	1:A:322:ALA:HA	1.19	1.34
1:B:291:PHE:HA	1:B:345:LYS:O	1.23	1.34
1:C:278:CYS:N	1:C:334:LYS:CD	1.87	1.34
1:B:153:ALA:HB1	1:B:174:GLY:CA	1.57	1.34
1:B:278:CYS:H	1:B:334:LYS:CE	1.41	1.34
1:C:153:ALA:HB1	1:C:174:GLY:CA	1.57	1.34
1:A:153:ALA:HB1	1:A:174:GLY:CA	1.57	1.33
1:A:278:CYS:N	1:A:334:LYS:CD	1.87	1.33

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:ALA:HB3	1:B:331:GLN:CD	1.53	1.33
1:C:138:TYR:CD2	1:C:184:PHE:HE1	1.46	1.33
1:C:278:CYS:H	1:C:334:LYS:CE	1.41	1.33
1:A:278:CYS:H	1:A:334:LYS:CE	1.41	1.33
1:C:130:ARG:HD3	1:C:237:GLN:CB	1.46	1.33
1:B:130:ARG:HD2	1:B:237:GLN:CB	1.47	1.32
1:B:138:TYR:CD2	1:B:184:PHE:HE1	1.46	1.32
1:A:138:TYR:CD2	1:A:184:PHE:HE1	1.46	1.32
1:A:130:ARG:HD3	1:A:237:GLN:CB	1.46	1.32
1:C:265:TRP:CZ3	1:C:348:ALA:O	1.82	1.32
1:A:133:SER:O	1:A:234:TYR:HA	1.28	1.32
1:A:198:ALA:HB1	1:A:200:GLY:O	1.17	1.32
1:A:304:ASP:O	1:A:331:GLN:HB3	1.14	1.32
1:A:265:TRP:CZ3	1:A:348:ALA:O	1.82	1.32
1:C:130:ARG:HD2	1:C:237:GLN:CB	1.47	1.32
1:B:165:ASP:O	1:B:168:SER:HB2	1.26	1.31
1:B:265:TRP:CZ3	1:B:348:ALA:O	1.82	1.31
1:C:149:LYS:HG2	1:C:177:SER:OG	1.22	1.31
1:A:165:ASP:O	1:A:168:SER:HB2	1.26	1.30
1:C:71:THR:CG2	1:C:87:SER:OG	1.78	1.30
1:C:291:PHE:CA	1:C:345:LYS:O	1.78	1.30
1:A:138:TYR:CB	1:A:184:PHE:CZ	1.96	1.30
1:C:159:ALA:HB1	1:C:328:GLU:CG	1.60	1.30
1:C:327:ALA:HB3	1:C:331:GLN:CD	1.53	1.30
1:A:291:PHE:HA	1:A:345:LYS:O	1.22	1.30
1:A:327:ALA:HB3	1:A:331:GLN:CD	1.53	1.30
1:A:248:ALA:CB	1:A:264:SER:OG	1.81	1.29
1:C:204:PRO:CG	1:C:328:GLU:HG2	1.59	1.29
1:B:291:PHE:CA	1:B:345:LYS:O	1.79	1.29
1:A:313:GLU:HG3	1:A:318:SER:CB	1.63	1.29
1:C:154:PHE:CD1	1:C:155:ASP:N	2.01	1.29
1:A:291:PHE:CA	1:A:345:LYS:O	1.78	1.29
1:B:88:GLU:O	1:B:231:ARG:HB2	1.19	1.29
1:C:309:SER:O	1:C:322:ALA:HA	1.19	1.29
1:A:333:VAL:O	1:A:334:LYS:HD3	1.30	1.29
1:C:313:GLU:HG3	1:C:318:SER:CB	1.63	1.28
1:A:119:LEU:CD2	1:A:234:TYR:OH	1.82	1.28
1:A:154:PHE:CD1	1:A:155:ASP:N	2.01	1.28
1:B:154:PHE:CD1	1:B:155:ASP:N	2.01	1.28
1:C:88:GLU:O	1:C:231:ARG:HB2	1.19	1.28
1:B:105:THR:OG1	1:B:211:LYS:CD	1.82	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:SER:OG	1:B:133:SER:CB	1.81	1.28
1:B:149:LYS:HG2	1:B:177:SER:OG	1.23	1.28
1:A:154:PHE:HD1	1:A:155:ASP:N	1.32	1.28
1:C:291:PHE:HA	1:C:345:LYS:O	1.23	1.27
1:B:119:LEU:CD2	1:B:234:TYR:OH	1.82	1.27
1:C:78:ALA:O	1:C:80:ASP:N	1.63	1.27
1:B:198:ALA:HB1	1:B:200:GLY:O	1.17	1.27
1:C:133:SER:O	1:C:234:TYR:HA	1.28	1.27
1:C:304:ASP:O	1:C:331:GLN:HB3	1.15	1.27
1:C:105:THR:OG1	1:C:211:LYS:CD	1.82	1.27
1:A:133:SER:CB	1:A:133:SER:OG	1.81	1.27
1:C:159:ALA:CB	1:C:328:GLU:CB	2.08	1.27
1:C:198:ALA:HB1	1:C:200:GLY:O	1.16	1.27
1:A:105:THR:OG1	1:A:211:LYS:CD	1.82	1.26
1:C:133:SER:OG	1:C:133:SER:CB	1.81	1.26
1:A:149:LYS:HG2	1:A:177:SER:OG	1.23	1.26
1:B:309:SER:O	1:B:322:ALA:HA	1.19	1.26
1:B:313:GLU:HG3	1:B:318:SER:CB	1.63	1.26
1:C:119:LEU:CD2	1:C:234:TYR:OH	1.82	1.26
1:A:156:ARG:O	1:A:210:GLY:HA3	1.36	1.25
1:B:133:SER:O	1:B:234:TYR:HA	1.28	1.25
1:C:80:ASP:CA	1:C:241:ARG:HH22	1.49	1.25
1:C:138:TYR:HB3	1:C:184:PHE:CE1	1.51	1.25
1:C:179:VAL:HG11	1:C:181:TRP:CD1	1.71	1.25
1:A:88:GLU:O	1:A:231:ARG:HB2	1.18	1.25
1:A:138:TYR:HB3	1:A:184:PHE:CE1	1.51	1.25
1:B:154:PHE:HD1	1:B:155:ASP:N	1.32	1.25
1:B:288:LEU:HD11	1:B:290:LEU:CD2	1.67	1.25
1:C:201:ILE:HB	1:C:265:TRP:O	1.12	1.25
1:C:156:ARG:O	1:C:210:GLY:HA3	1.37	1.24
1:A:248:ALA:HB1	1:A:264:SER:OG	1.20	1.24
1:B:328:GLU:O	1:B:329:ARG:O	1.55	1.24
1:A:96:ASN:O	1:A:98:ASP:N	1.70	1.24
1:A:179:VAL:HG11	1:A:181:TRP:CD1	1.71	1.24
1:C:204:PRO:HG3	1:C:328:GLU:C	1.61	1.24
1:C:138:TYR:OH	1:C:227:LEU:HB3	1.38	1.24
1:C:159:ALA:CB	1:C:328:GLU:CG	2.15	1.24
1:C:333:VAL:O	1:C:334:LYS:HD3	1.30	1.24
1:B:304:ASP:O	1:B:331:GLN:HB3	1.15	1.23
1:A:101:PRO:C	1:A:102:LYS:HG3	1.57	1.23
1:B:138:TYR:HB3	1:B:184:PHE:CE1	1.51	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:ARG:O	1:B:210:GLY:HA3	1.36	1.23
1:B:179:VAL:HG11	1:B:181:TRP:CD1	1.71	1.23
1:B:259:GLY:C	1:B:260:PRO:N	1.97	1.23
1:A:248:ALA:CB	1:A:264:SER:O	1.87	1.23
1:A:288:LEU:HD11	1:A:290:LEU:CD2	1.66	1.23
1:B:101:PRO:C	1:B:102:LYS:HG3	1.57	1.23
1:B:293:GLU:O	1:B:317:GLY:N	1.72	1.23
1:B:333:VAL:O	1:B:334:LYS:HD3	1.30	1.23
1:C:259:GLY:C	1:C:260:PRO:N	1.97	1.23
1:C:96:ASN:O	1:C:98:ASP:N	1.70	1.22
1:B:96:ASN:O	1:B:98:ASP:N	1.70	1.22
1:C:90:ILE:HD11	1:C:232:VAL:CG2	1.69	1.22
1:C:154:PHE:HD1	1:C:155:ASP:N	1.32	1.22
1:C:197:VAL:CG2	1:C:350:ARG:NH2	2.01	1.22
1:C:101:PRO:O	1:C:102:LYS:CG	1.88	1.22
1:C:288:LEU:HD11	1:C:290:LEU:CD2	1.66	1.22
1:C:293:GLU:O	1:C:317:GLY:N	1.72	1.22
1:A:293:GLU:O	1:A:317:GLY:N	1.72	1.22
1:C:328:GLU:O	1:C:329:ARG:O	1.55	1.21
1:C:149:LYS:HB3	1:C:217:TYR:CE1	1.75	1.21
1:A:259:GLY:C	1:A:260:PRO:N	1.97	1.21
1:A:328:GLU:O	1:A:329:ARG:O	1.55	1.21
1:A:327:ALA:CB	1:A:331:GLN:OE1	1.88	1.21
1:C:201:ILE:CB	1:C:265:TRP:O	1.87	1.21
1:C:207:VAL:HG12	1:C:329:ARG:NE	1.52	1.21
1:A:90:ILE:HD11	1:A:232:VAL:CG2	1.69	1.20
1:B:294:LYS:O	1:B:296:PRO:HD3	1.04	1.20
1:A:294:LYS:O	1:A:296:PRO:HD3	1.04	1.20
1:B:327:ALA:CB	1:B:331:GLN:OE1	1.88	1.20
1:C:327:ALA:CB	1:C:331:GLN:OE1	1.88	1.20
1:C:200:GLY:C	1:C:282:GLY:CA	2.08	1.20
1:B:90:ILE:HD11	1:B:232:VAL:CG2	1.69	1.20
1:C:200:GLY:HA2	1:C:265:TRP:CB	1.70	1.20
1:C:200:GLY:CA	1:C:265:TRP:CD1	2.25	1.19
1:A:149:LYS:HB3	1:A:217:TYR:CE1	1.75	1.19
1:B:101:PRO:O	1:B:102:LYS:CG	1.88	1.19
1:B:149:LYS:HB3	1:B:217:TYR:CE1	1.75	1.19
1:C:294:LYS:O	1:C:296:PRO:HD3	1.04	1.19
1:A:101:PRO:O	1:A:102:LYS:CG	1.88	1.19
1:B:164:ASN:HD22	1:B:164:ASN:N	1.19	1.18
1:C:204:PRO:CG	1:C:329:ARG:N	2.06	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:TYR:HB3	1:C:184:PHE:CD1	1.78	1.18
1:B:326:VAL:CG1	1:B:327:ALA:H	1.54	1.18
1:A:295:ALA:N	1:A:316:ALA:HA	1.51	1.18
1:C:138:TYR:CG	1:C:184:PHE:HE1	1.56	1.17
1:B:138:TYR:OH	1:B:227:LEU:HB3	1.38	1.17
1:A:138:TYR:OH	1:A:227:LEU:HB3	1.38	1.17
1:A:326:VAL:CG1	1:A:327:ALA:H	1.54	1.17
1:C:101:PRO:C	1:C:102:LYS:HG3	1.57	1.17
1:B:138:TYR:HB3	1:B:184:PHE:CD1	1.78	1.17
1:C:295:ALA:N	1:C:316:ALA:HA	1.51	1.17
1:A:101:PRO:HD2	1:A:166:LEU:CD1	1.68	1.17
1:A:138:TYR:HB3	1:A:184:PHE:CD1	1.78	1.17
1:A:149:LYS:HD3	1:A:170:TYR:HH	1.05	1.17
1:A:248:ALA:CB	1:A:265:TRP:HA	1.73	1.17
1:C:120:ILE:HD11	1:C:351:ILE:C	1.69	1.17
1:A:326:VAL:HG12	1:A:327:ALA:N	1.60	1.16
1:B:88:GLU:O	1:B:231:ARG:CB	1.93	1.15
1:B:309:SER:O	1:B:322:ALA:CA	1.94	1.15
1:C:88:GLU:O	1:C:231:ARG:CB	1.93	1.15
1:C:204:PRO:HG3	1:C:329:ARG:N	1.13	1.15
1:A:88:GLU:O	1:A:231:ARG:CB	1.93	1.15
1:A:179:VAL:HG11	1:A:181:TRP:NE1	1.61	1.15
1:C:105:THR:OG1	1:C:211:LYS:HD3	0.98	1.15
1:C:179:VAL:HG11	1:C:181:TRP:NE1	1.61	1.15
1:A:313:GLU:HG3	1:A:318:SER:HB2	1.28	1.15
1:B:138:TYR:CD2	1:B:184:PHE:CE1	2.34	1.15
1:C:138:TYR:CD2	1:C:184:PHE:CE1	2.34	1.15
1:B:116:PHE:O	1:B:120:ILE:HG21	1.46	1.14
1:B:151:ALA:HA	1:B:177:SER:HB2	1.28	1.14
1:C:199:ASP:C	1:C:265:TRP:CD1	2.25	1.14
1:A:116:PHE:O	1:A:120:ILE:HG21	1.46	1.14
1:A:277:ASP:CA	1:A:334:LYS:HD2	1.77	1.14
1:A:294:LYS:O	1:A:296:PRO:CD	1.96	1.14
1:B:277:ASP:CA	1:B:334:LYS:HD2	1.77	1.14
1:B:294:LYS:O	1:B:296:PRO:CD	1.96	1.14
1:C:101:PRO:CD	1:C:166:LEU:HD12	1.73	1.14
1:C:204:PRO:CG	1:C:328:GLU:CG	2.20	1.14
1:C:204:PRO:CB	1:C:328:GLU:HG3	1.77	1.14
1:A:105:THR:OG1	1:A:211:LYS:HD3	0.98	1.14
1:A:309:SER:O	1:A:322:ALA:CA	1.94	1.14
1:A:101:PRO:HG3	1:A:217:TYR:CE2	1.83	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:GLY:HA2	1:B:234:TYR:CD1	1.83	1.14
1:B:112:GLU:HG3	1:B:329:ARG:NH2	1.61	1.14
1:C:86:GLY:HA2	1:C:234:TYR:CD1	1.83	1.14
1:C:294:LYS:O	1:C:296:PRO:CD	1.96	1.14
1:C:297:VAL:HB	1:C:336:VAL:O	1.47	1.14
1:B:105:THR:OG1	1:B:211:LYS:HD3	0.98	1.13
1:B:179:VAL:HG11	1:B:181:TRP:NE1	1.61	1.13
1:C:277:ASP:CA	1:C:334:LYS:HD2	1.77	1.13
1:A:297:VAL:HB	1:A:336:VAL:HG13	1.26	1.13
1:A:265:TRP:HZ3	1:A:348:ALA:O	1.20	1.13
1:C:116:PHE:O	1:C:120:ILE:HG21	1.46	1.13
1:C:101:PRO:HG3	1:C:217:TYR:CE2	1.83	1.12
1:A:126:TYR:CA	1:A:242:THR:HG22	1.80	1.12
1:A:248:ALA:HB2	1:A:265:TRP:HA	1.31	1.12
1:B:297:VAL:HB	1:B:336:VAL:HG13	1.27	1.12
1:C:249:GLN:NE2	1:C:265:TRP:CE3	2.15	1.12
1:C:309:SER:O	1:C:322:ALA:CA	1.94	1.12
1:A:86:GLY:HA2	1:A:234:TYR:CD1	1.83	1.12
1:A:119:LEU:HD22	1:A:234:TYR:CZ	1.85	1.12
1:B:101:PRO:O	1:B:102:LYS:HG3	0.95	1.12
1:B:101:PRO:HG3	1:B:217:TYR:CE2	1.83	1.12
1:B:301:GLU:O	1:B:333:VAL:HG13	1.50	1.12
1:C:164:ASN:HD22	1:C:164:ASN:N	1.19	1.12
1:A:248:ALA:HB3	1:A:264:SER:CA	1.79	1.12
1:B:126:TYR:CA	1:B:242:THR:HG22	1.80	1.12
1:B:297:VAL:HB	1:B:336:VAL:O	1.47	1.12
1:C:265:TRP:HZ3	1:C:348:ALA:O	1.20	1.12
1:C:301:GLU:O	1:C:333:VAL:HG13	1.50	1.12
1:C:326:VAL:HG12	1:C:327:ALA:N	1.60	1.12
1:B:295:ALA:H	1:B:316:ALA:CA	1.63	1.11
1:B:295:ALA:N	1:B:316:ALA:HA	1.51	1.11
1:C:198:ALA:CB	1:C:200:GLY:O	1.96	1.11
1:A:101:PRO:O	1:A:102:LYS:HG3	0.95	1.11
1:B:119:LEU:HD22	1:B:234:TYR:CZ	1.85	1.11
1:B:149:LYS:HD2	1:B:170:TYR:OH	1.44	1.11
1:C:126:TYR:CA	1:C:242:THR:HG22	1.80	1.11
1:C:248:ALA:HB1	1:C:287:SER:O	1.48	1.11
1:A:198:ALA:CB	1:A:200:GLY:O	1.97	1.11
1:A:339:GLU:C	1:A:340:GLU:CA	2.24	1.11
1:C:295:ALA:H	1:C:316:ALA:CA	1.63	1.11
1:A:151:ALA:HA	1:A:177:SER:HB2	1.28	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:ALA:H	1:A:316:ALA:CA	1.63	1.11
1:C:120:ILE:CD1	1:C:351:ILE:C	2.24	1.11
1:C:151:ALA:HA	1:C:177:SER:HB2	1.28	1.11
1:A:297:VAL:HB	1:A:336:VAL:O	1.47	1.10
1:C:80:ASP:CA	1:C:241:ARG:NH2	2.10	1.10
1:C:313:GLU:HG3	1:C:318:SER:HB2	1.28	1.10
1:A:301:GLU:O	1:A:333:VAL:HG13	1.50	1.10
1:B:198:ALA:CB	1:B:200:GLY:O	1.97	1.10
1:C:101:PRO:O	1:C:102:LYS:HG3	0.95	1.10
1:C:116:PHE:O	1:C:120:ILE:CG2	2.00	1.10
1:C:119:LEU:HD22	1:C:234:TYR:CZ	1.85	1.10
1:C:326:VAL:CG1	1:C:327:ALA:H	1.54	1.10
1:A:164:ASN:N	1:A:164:ASN:ND2	1.88	1.10
1:A:248:ALA:HB3	1:A:264:SER:O	1.45	1.10
1:A:315:ALA:CB	1:A:318:SER:HB3	1.82	1.10
1:C:101:PRO:HD2	1:C:166:LEU:CD1	1.68	1.10
1:A:116:PHE:O	1:A:120:ILE:CG2	2.00	1.10
1:B:313:GLU:HG3	1:B:318:SER:HB2	1.28	1.10
1:C:164:ASN:N	1:C:164:ASN:ND2	1.88	1.10
1:C:315:ALA:CB	1:C:318:SER:HB3	1.82	1.10
1:A:288:LEU:HD11	1:A:290:LEU:HD21	1.31	1.09
1:B:116:PHE:O	1:B:120:ILE:CG2	2.00	1.09
1:B:138:TYR:CG	1:B:184:PHE:HE1	1.56	1.09
1:A:86:GLY:CA	1:A:234:TYR:CD1	2.34	1.09
1:A:89:LEU:C	1:A:89:LEU:HD23	1.78	1.09
1:B:86:GLY:CA	1:B:234:TYR:CD1	2.34	1.09
1:B:101:PRO:CD	1:B:166:LEU:HD12	1.73	1.09
1:B:339:GLU:C	1:B:340:GLU:CA	2.24	1.09
1:C:249:GLN:HB3	1:C:265:TRP:HZ3	1.17	1.09
1:C:339:GLU:C	1:C:340:GLU:CA	2.24	1.09
1:A:101:PRO:CD	1:A:166:LEU:HD12	1.73	1.09
1:A:138:TYR:CG	1:A:184:PHE:HE1	1.56	1.09
1:B:89:LEU:HD23	1:B:89:LEU:C	1.77	1.09
1:C:86:GLY:CA	1:C:234:TYR:CD1	2.34	1.09
1:C:160:LYS:HG3	1:C:161:PRO:HD2	1.11	1.09
1:C:204:PRO:HB2	1:C:328:GLU:HG3	1.15	1.09
1:A:149:LYS:CG	1:A:177:SER:OG	2.01	1.09
1:B:101:PRO:HD2	1:B:166:LEU:CD1	1.68	1.09
1:B:149:LYS:CG	1:B:177:SER:OG	2.01	1.09
1:B:315:ALA:HB1	1:B:318:SER:N	1.67	1.09
1:C:179:VAL:CG2	1:C:180:PRO:HD2	1.83	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:TYR:CD2	1:A:184:PHE:CE1	2.34	1.08
1:A:149:LYS:HD2	1:A:170:TYR:OH	1.44	1.08
1:A:315:ALA:HB1	1:A:318:SER:N	1.67	1.08
1:B:179:VAL:CG2	1:B:180:PRO:HD2	1.83	1.08
1:B:248:ALA:O	1:B:263:VAL:HB	1.54	1.08
1:B:315:ALA:CB	1:B:318:SER:HB3	1.82	1.08
1:C:134:LEU:HD21	1:C:188:VAL:HG21	1.08	1.08
1:C:297:VAL:HB	1:C:336:VAL:HG13	1.27	1.08
1:C:315:ALA:HB1	1:C:318:SER:N	1.67	1.08
1:A:179:VAL:CG2	1:A:180:PRO:HD2	1.83	1.08
1:B:278:CYS:HB3	1:B:333:VAL:O	1.52	1.08
1:C:71:THR:HG21	1:C:87:SER:OG	0.92	1.08
1:C:130:ARG:HD3	1:C:237:GLN:CA	1.83	1.08
1:C:297:VAL:HB	1:C:336:VAL:C	1.78	1.08
1:A:297:VAL:HB	1:A:336:VAL:C	1.78	1.08
1:B:255:GLY:HA2	1:B:342:PRO:HB3	1.33	1.08
1:B:278:CYS:N	1:B:334:LYS:HD2	1.68	1.08
1:C:197:VAL:HG23	1:C:350:ARG:HH22	1.17	1.08
1:C:200:GLY:C	1:C:282:GLY:HA3	1.51	1.08
1:C:244:SER:O	1:C:245:THR:HG22	1.54	1.08
1:A:130:ARG:HD3	1:A:237:GLN:CA	1.84	1.07
1:C:89:LEU:HD23	1:C:89:LEU:C	1.78	1.07
1:C:200:GLY:HA2	1:C:265:TRP:CG	1.88	1.07
1:C:327:ALA:N	1:C:331:GLN:OE1	1.87	1.07
1:A:125:GLN:HA	1:A:243:GLY:HA2	1.37	1.07
1:B:249:GLN:HB3	1:B:265:TRP:HZ3	1.17	1.07
1:C:69:VAL:HG12	1:C:70:SER:H	1.09	1.07
1:C:130:ARG:HB2	1:C:237:GLN:HB3	1.07	1.07
1:C:149:LYS:CG	1:C:177:SER:OG	2.01	1.07
1:A:244:SER:O	1:A:245:THR:HG22	1.54	1.07
1:A:288:LEU:HD11	1:A:290:LEU:CG	1.84	1.07
1:B:297:VAL:HB	1:B:336:VAL:C	1.78	1.07
1:C:149:LYS:HD3	1:C:170:TYR:OH	1.43	1.07
1:C:172:ILE:O	1:C:173:GLU:O	1.72	1.07
1:B:297:VAL:CB	1:B:336:VAL:HG13	1.41	1.07
1:C:296:PRO:CG	1:C:337:THR:CG2	1.76	1.07
1:A:86:GLY:HA2	1:A:234:TYR:CE1	1.90	1.07
1:A:166:LEU:O	1:A:169:LEU:N	1.88	1.07
1:B:125:GLN:HA	1:B:243:GLY:HA2	1.37	1.07
1:B:149:LYS:HD3	1:B:170:TYR:HH	0.94	1.07
1:B:166:LEU:O	1:B:169:LEU:N	1.88	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:ASP:HA	1:B:334:LYS:HD2	1.34	1.07
1:B:327:ALA:N	1:B:331:GLN:OE1	1.87	1.07
1:A:327:ALA:N	1:A:331:GLN:OE1	1.87	1.06
1:B:156:ARG:O	1:B:210:GLY:CA	2.03	1.06
1:B:244:SER:O	1:B:245:THR:HG22	1.54	1.06
1:C:149:LYS:HD2	1:C:170:TYR:OH	1.44	1.06
1:C:152:LEU:HD22	1:C:186:LEU:CD1	1.85	1.06
1:A:156:ARG:O	1:A:210:GLY:CA	2.03	1.06
1:B:86:GLY:HA2	1:B:234:TYR:CE1	1.90	1.06
1:B:288:LEU:HD11	1:B:290:LEU:CG	1.84	1.06
1:B:288:LEU:HD11	1:B:290:LEU:HD21	1.31	1.06
1:C:149:LYS:HD3	1:C:170:TYR:HH	1.07	1.06
1:C:288:LEU:HD11	1:C:290:LEU:CG	1.84	1.06
1:A:252:ASP:OD2	1:A:345:LYS:HE2	1.55	1.06
1:A:315:ALA:HB1	1:A:318:SER:H	1.16	1.06
1:B:252:ASP:OD2	1:B:345:LYS:HE2	1.55	1.06
1:B:291:PHE:CB	1:B:345:LYS:O	2.03	1.06
1:C:201:ILE:HG22	1:C:265:TRP:HA	1.38	1.06
1:C:278:CYS:HB3	1:C:333:VAL:O	1.53	1.06
1:A:160:LYS:HG3	1:A:161:PRO:HD2	1.11	1.06
1:A:304:ASP:O	1:A:331:GLN:CB	2.04	1.06
1:B:86:GLY:CA	1:B:234:TYR:HD1	1.68	1.06
1:B:326:VAL:HG12	1:B:327:ALA:N	1.60	1.06
1:C:69:VAL:HG12	1:C:70:SER:N	1.66	1.06
1:C:156:ARG:O	1:C:210:GLY:CA	2.03	1.06
1:C:278:CYS:N	1:C:334:LYS:HD2	1.68	1.06
1:A:134:LEU:HD21	1:A:188:VAL:HG21	1.08	1.06
1:B:160:LYS:HG3	1:B:161:PRO:HD2	1.11	1.06
1:B:248:ALA:O	1:B:263:VAL:CB	2.03	1.06
1:C:207:VAL:N	1:C:329:ARG:NH2	1.78	1.06
1:C:288:LEU:HD11	1:C:290:LEU:HD21	1.31	1.06
1:A:152:LEU:HD22	1:A:186:LEU:CD1	1.85	1.05
1:A:172:ILE:O	1:A:173:GLU:O	1.72	1.05
1:A:203:ASP:CG	1:A:205:LYS:HD3	1.81	1.05
1:B:152:LEU:HD22	1:B:186:LEU:CD1	1.85	1.05
1:B:265:TRP:HZ3	1:B:348:ALA:O	1.20	1.05
1:A:278:CYS:N	1:A:334:LYS:HD2	1.68	1.05
1:A:278:CYS:HB3	1:A:333:VAL:O	1.53	1.05
1:B:130:ARG:HD3	1:B:237:GLN:CA	1.84	1.05
1:C:255:GLY:HA2	1:C:342:PRO:HB3	1.33	1.05
1:C:277:ASP:HA	1:C:334:LYS:HD2	1.35	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:ASN:OD1	1:A:216:THR:O	1.74	1.05
1:A:255:GLY:HA2	1:A:342:PRO:HB3	1.33	1.05
1:B:172:ILE:O	1:B:173:GLU:O	1.72	1.05
1:B:304:ASP:O	1:B:331:GLN:CB	2.04	1.05
1:B:327:ALA:HB3	1:B:331:GLN:OE1	1.48	1.05
1:C:86:GLY:HA2	1:C:234:TYR:CE1	1.90	1.05
1:C:166:LEU:O	1:C:169:LEU:N	1.88	1.05
1:C:291:PHE:CB	1:C:345:LYS:O	2.03	1.05
1:C:327:ALA:HB3	1:C:331:GLN:OE1	1.48	1.05
1:A:130:ARG:HB2	1:A:237:GLN:HB3	1.07	1.04
1:A:249:GLN:HB3	1:A:265:TRP:HZ3	1.17	1.04
1:A:291:PHE:CB	1:A:345:LYS:O	2.03	1.04
1:B:134:LEU:HD21	1:B:188:VAL:HG21	1.08	1.04
1:A:179:VAL:CG1	1:A:181:TRP:CD1	2.40	1.04
1:B:96:ASN:OD1	1:B:216:THR:O	1.74	1.04
1:C:96:ASN:OD1	1:C:216:THR:O	1.74	1.04
1:A:164:ASN:N	1:A:164:ASN:HD22	1.19	1.04
1:B:179:VAL:CG1	1:B:181:TRP:CD1	2.40	1.04
1:B:278:CYS:N	1:B:334:LYS:HD3	1.71	1.04
1:B:315:ALA:HB2	1:B:318:SER:HB3	1.36	1.04
1:C:159:ALA:HB2	1:C:328:GLU:HB2	1.35	1.04
1:C:315:ALA:HB2	1:C:318:SER:HB3	1.36	1.04
1:B:203:ASP:CG	1:B:205:LYS:HD3	1.82	1.04
1:B:269:LYS:C	1:B:277:ASP:HB3	1.82	1.04
1:C:159:ALA:HB1	1:C:328:GLU:CD	1.80	1.04
1:C:252:ASP:OD2	1:C:345:LYS:HE2	1.55	1.04
1:A:269:LYS:C	1:A:277:ASP:HB3	1.82	1.04
1:A:277:ASP:HA	1:A:334:LYS:HD2	1.35	1.04
1:A:315:ALA:HB2	1:A:318:SER:HB3	1.36	1.04
1:C:304:ASP:O	1:C:331:GLN:CB	2.04	1.04
1:B:296:PRO:CG	1:B:337:THR:CG2	1.76	1.03
1:C:179:VAL:CG1	1:C:181:TRP:CD1	2.40	1.03
1:B:130:ARG:HB2	1:B:237:GLN:CB	1.88	1.03
1:B:130:ARG:HB2	1:B:237:GLN:HB3	1.07	1.03
1:C:207:VAL:CA	1:C:329:ARG:NH2	2.21	1.03
1:C:315:ALA:HB1	1:C:318:SER:H	1.16	1.03
1:A:119:LEU:HD22	1:A:234:TYR:OH	0.86	1.03
1:A:252:ASP:CG	1:A:345:LYS:HG2	1.84	1.03
1:B:252:ASP:CG	1:B:345:LYS:HG2	1.84	1.03
1:C:119:LEU:HD22	1:C:234:TYR:OH	0.86	1.03
1:C:130:ARG:HB2	1:C:237:GLN:CB	1.88	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:GLY:CA	1:A:234:TYR:HD1	1.68	1.03
1:A:254:ALA:O	1:A:256:VAL:N	1.91	1.03
1:B:119:LEU:HD22	1:B:234:TYR:OH	0.86	1.03
1:B:290:LEU:HD22	1:B:346:TRP:HB2	1.41	1.03
1:C:203:ASP:CG	1:C:205:LYS:HD3	1.81	1.03
1:C:252:ASP:CG	1:C:345:LYS:HG2	1.84	1.03
1:C:290:LEU:HD22	1:C:346:TRP:HB2	1.41	1.03
1:A:308:PHE:CE2	1:A:310:VAL:CG2	2.42	1.02
1:A:327:ALA:HB3	1:A:331:GLN:OE1	1.48	1.02
1:B:174:GLY:C	1:B:175:CYS:SG	2.42	1.02
1:C:254:ALA:O	1:C:256:VAL:N	1.91	1.02
1:C:269:LYS:C	1:C:277:ASP:HB3	1.82	1.02
1:C:277:ASP:C	1:C:334:LYS:HD2	1.84	1.02
1:A:286:PHE:HA	1:A:351:ILE:CG2	1.89	1.02
1:B:164:ASN:N	1:B:164:ASN:ND2	1.88	1.02
1:B:248:ALA:O	1:B:263:VAL:CG1	2.08	1.02
1:B:315:ALA:O	1:B:316:ALA:C	2.00	1.02
1:C:308:PHE:CE2	1:C:310:VAL:CG2	2.42	1.02
1:B:277:ASP:C	1:B:334:LYS:HD2	1.84	1.02
1:B:308:PHE:CE2	1:B:310:VAL:CG2	2.42	1.02
1:C:174:GLY:C	1:C:175:CYS:SG	2.42	1.02
1:C:326:VAL:HG12	1:C:327:ALA:H	1.18	1.02
1:A:338:THR:OG1	1:A:339:GLU:HB2	1.60	1.01
1:B:254:ALA:O	1:B:256:VAL:N	1.91	1.01
1:B:338:THR:OG1	1:B:339:GLU:HB2	1.60	1.01
1:C:286:PHE:HA	1:C:351:ILE:CG2	1.89	1.01
1:C:338:THR:OG1	1:C:339:GLU:HB2	1.60	1.01
1:A:85:SER:HA	1:A:234:TYR:O	1.60	1.01
1:A:130:ARG:HB2	1:A:237:GLN:CB	1.88	1.01
1:A:154:PHE:CE1	1:A:155:ASP:C	2.39	1.01
1:A:174:GLY:C	1:A:175:CYS:SG	2.42	1.01
1:B:154:PHE:CE1	1:B:155:ASP:C	2.39	1.01
1:B:165:ASP:O	1:B:168:SER:CB	2.07	1.01
1:C:86:GLY:CA	1:C:234:TYR:HD1	1.68	1.01
1:A:86:GLY:N	1:A:234:TYR:CD1	2.29	1.01
1:A:165:ASP:O	1:A:168:SER:CB	2.07	1.01
1:A:277:ASP:C	1:A:334:LYS:HD2	1.84	1.01
1:B:86:GLY:N	1:B:234:TYR:CD1	2.29	1.01
1:B:134:LEU:HD21	1:B:188:VAL:CG2	1.91	1.01
1:B:286:PHE:HA	1:B:351:ILE:CG2	1.89	1.01
1:C:68:GLU:OE2	1:C:137:ARG:NH2	1.94	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:PHE:CE1	1:C:155:ASP:C	2.39	1.01
1:C:165:ASP:O	1:C:168:SER:CB	2.07	1.01
1:C:200:GLY:HA2	1:C:265:TRP:CD1	1.90	1.01
1:A:350:ARG:C	1:A:351:ILE:HG22	1.86	1.01
1:B:315:ALA:HB1	1:B:318:SER:H	1.16	1.01
1:C:135:ARG:HG3	1:C:233:GLU:HB3	1.43	1.01
1:C:200:GLY:HA2	1:C:265:TRP:HB3	1.42	1.01
1:A:134:LEU:CD2	1:A:188:VAL:HG21	1.91	1.01
1:C:85:SER:HA	1:C:234:TYR:O	1.60	1.01
1:C:86:GLY:N	1:C:234:TYR:CD1	2.29	1.01
1:A:278:CYS:H	1:A:334:LYS:HD3	1.25	1.00
1:C:278:CYS:N	1:C:334:LYS:HD3	1.71	1.00
1:B:253:PHE:HA	1:B:258:ASP:HA	1.44	1.00
1:C:133:SER:O	1:C:234:TYR:CA	2.09	1.00
1:C:253:PHE:HA	1:C:258:ASP:HA	1.44	1.00
1:C:315:ALA:O	1:C:316:ALA:C	2.00	1.00
1:A:253:PHE:HA	1:A:258:ASP:HA	1.44	1.00
1:B:85:SER:HA	1:B:234:TYR:O	1.60	1.00
1:B:134:LEU:CD2	1:B:188:VAL:HG21	1.91	1.00
1:C:159:ALA:CB	1:C:328:GLU:CD	2.33	1.00
1:C:278:CYS:H	1:C:334:LYS:HE2	1.27	1.00
1:C:125:GLN:HA	1:C:243:GLY:HA2	1.36	1.00
1:A:249:GLN:HB3	1:A:265:TRP:CZ3	1.97	1.00
1:A:297:VAL:CB	1:A:336:VAL:HG13	1.41	1.00
1:C:197:VAL:HG21	1:C:350:ARG:HH22	1.20	1.00
1:B:133:SER:O	1:B:234:TYR:CA	2.09	1.00
1:A:133:SER:O	1:A:234:TYR:CA	2.09	0.99
1:A:135:ARG:HG3	1:A:233:GLU:HB3	1.43	0.99
1:A:134:LEU:HD21	1:A:188:VAL:CG2	1.91	0.99
1:A:326:VAL:HG12	1:A:327:ALA:H	1.18	0.99
1:C:308:PHE:CE2	1:C:310:VAL:HG23	1.97	0.99
1:A:185:ILE:CD1	1:A:186:LEU:N	2.05	0.99
1:B:248:ALA:C	1:B:263:VAL:HG12	1.88	0.99
1:B:249:GLN:HB3	1:B:265:TRP:CZ3	1.97	0.99
1:B:350:ARG:C	1:B:351:ILE:HG22	1.86	0.99
1:C:79:ARG:O	1:C:80:ASP:HB2	1.61	0.99
1:C:297:VAL:CB	1:C:336:VAL:HG13	1.41	0.99
1:B:278:CYS:H	1:B:334:LYS:HE2	1.27	0.99
1:A:160:LYS:HG3	1:A:161:PRO:CD	1.93	0.99
1:C:134:LEU:CD2	1:C:188:VAL:HG21	1.91	0.99
1:C:350:ARG:C	1:C:351:ILE:HG22	1.86	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:LEU:HD22	1:A:346:TRP:HB2	1.41	0.98
1:B:160:LYS:HG3	1:B:161:PRO:CD	1.93	0.98
1:C:249:GLN:HB3	1:C:265:TRP:CZ3	1.97	0.98
1:B:152:LEU:HD22	1:B:186:LEU:HD13	1.45	0.98
1:B:179:VAL:HG23	1:B:180:PRO:HD2	1.46	0.98
1:C:152:LEU:HD22	1:C:186:LEU:HD13	1.45	0.98
1:A:308:PHE:CE2	1:A:310:VAL:HG23	1.97	0.98
1:B:135:ARG:HG3	1:B:233:GLU:HB3	1.43	0.98
1:C:134:LEU:HD21	1:C:188:VAL:CG2	1.91	0.98
1:A:296:PRO:CG	1:A:337:THR:CG2	1.76	0.98
1:A:278:CYS:N	1:A:334:LYS:HE2	1.78	0.98
1:B:89:LEU:C	1:B:89:LEU:CD2	2.37	0.98
1:B:308:PHE:CE2	1:B:310:VAL:HG23	1.97	0.98
1:C:160:LYS:HG3	1:C:161:PRO:CD	1.93	0.98
1:C:200:GLY:HA3	1:C:265:TRP:HA	1.43	0.98
1:C:89:LEU:C	1:C:89:LEU:CD2	2.37	0.98
1:C:278:CYS:CB	1:C:333:VAL:O	2.12	0.98
1:B:290:LEU:CD2	1:B:346:TRP:HB2	1.94	0.97
1:B:185:ILE:CD1	1:B:186:LEU:N	2.05	0.97
1:B:269:LYS:HG2	1:B:270:GLY:N	1.75	0.97
1:C:143:PRO:O	1:C:146:THR:CG2	2.13	0.97
1:C:269:LYS:HG2	1:C:270:GLY:N	1.75	0.97
1:C:278:CYS:N	1:C:334:LYS:HE2	1.78	0.97
1:A:138:TYR:HB2	1:A:184:PHE:CE2	1.99	0.97
1:B:101:PRO:HG3	1:B:217:TYR:HE2	1.28	0.97
1:A:155:ASP:HB2	1:A:172:ILE:HD11	1.47	0.97
1:A:278:CYS:N	1:A:334:LYS:HD3	1.72	0.97
1:C:101:PRO:HD2	1:C:166:LEU:HD12	1.37	0.97
1:A:278:CYS:H	1:A:334:LYS:HE2	1.26	0.97
1:C:290:LEU:CD2	1:C:346:TRP:HB2	1.94	0.97
1:A:248:ALA:HB2	1:A:264:SER:C	1.89	0.97
1:A:278:CYS:CB	1:A:333:VAL:O	2.12	0.97
1:B:278:CYS:CB	1:B:333:VAL:O	2.12	0.97
1:B:119:LEU:HD22	1:B:234:TYR:HH	1.20	0.97
1:A:269:LYS:HG2	1:A:270:GLY:N	1.75	0.97
1:A:294:LYS:C	1:A:296:PRO:HD3	1.90	0.97
1:B:138:TYR:HB2	1:B:184:PHE:CE2	1.99	0.97
1:B:155:ASP:HB2	1:B:172:ILE:HD11	1.47	0.97
1:C:95:LYS:NZ	1:C:221:ALA:HA	1.80	0.97
1:C:150:VAL:O	1:C:150:VAL:HG12	1.65	0.96
1:C:294:LYS:C	1:C:296:PRO:HD3	1.90	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:185:ILE:CD1	1:C:186:LEU:N	2.05	0.96
1:C:274:TRP:NE1	1:C:339:GLU:O	1.98	0.96
1:B:294:LYS:C	1:B:296:PRO:HD3	1.90	0.96
1:A:179:VAL:HG23	1:A:180:PRO:HD2	1.45	0.96
1:A:290:LEU:CD2	1:A:346:TRP:HB2	1.94	0.96
1:C:113:PRO:O	1:C:115:THR:N	1.99	0.96
1:C:278:CYS:H	1:C:334:LYS:HD3	1.25	0.96
1:A:86:GLY:N	1:A:234:TYR:HD1	1.62	0.96
1:A:101:PRO:HG3	1:A:217:TYR:HE2	1.28	0.96
1:C:163:PRO:C	1:C:164:ASN:HD22	1.73	0.96
1:A:326:VAL:HG12	1:A:327:ALA:O	1.65	0.96
1:C:138:TYR:HB2	1:C:184:PHE:CE2	2.00	0.96
1:B:163:PRO:C	1:B:164:ASN:HD22	1.73	0.96
1:B:350:ARG:O	1:B:351:ILE:HG22	0.78	0.96
1:C:77:THR:HG22	1:C:78:ALA:N	1.78	0.96
1:B:105:THR:HG1	1:B:211:LYS:CD	1.70	0.96
1:C:206:LEU:O	1:C:206:LEU:HD12	1.66	0.96
1:A:95:LYS:NZ	1:A:221:ALA:HA	1.80	0.96
1:A:285:ASN:O	1:A:351:ILE:HG23	1.66	0.96
1:A:350:ARG:O	1:A:351:ILE:HG22	0.78	0.96
1:C:296:PRO:HG2	1:C:337:THR:CB	1.95	0.96
1:A:248:ALA:HB3	1:A:264:SER:CB	1.96	0.95
1:B:95:LYS:NZ	1:B:221:ALA:HA	1.80	0.95
1:B:149:LYS:CB	1:B:217:TYR:HE1	1.79	0.95
1:B:274:TRP:NE1	1:B:339:GLU:O	1.98	0.95
1:C:113:PRO:C	1:C:115:THR:H	1.74	0.95
1:C:285:ASN:O	1:C:351:ILE:HG23	1.66	0.95
1:C:326:VAL:HG12	1:C:327:ALA:O	1.65	0.95
1:A:143:PRO:O	1:A:146:THR:CG2	2.13	0.95
1:A:149:LYS:CB	1:A:217:TYR:HE1	1.79	0.95
1:A:206:LEU:HD12	1:A:206:LEU:O	1.66	0.95
1:B:143:PRO:O	1:B:146:THR:CG2	2.13	0.95
1:A:149:LYS:HB3	1:A:217:TYR:HE1	1.11	0.95
1:B:130:ARG:NH1	1:B:236:VAL:O	2.00	0.95
1:B:149:LYS:HB3	1:B:217:TYR:HE1	1.11	0.95
1:C:207:VAL:CA	1:C:329:ARG:HH22	1.79	0.95
1:A:291:PHE:CE1	1:A:335:MET:HE1	2.01	0.95
1:B:206:LEU:HD12	1:B:206:LEU:O	1.66	0.95
1:C:130:ARG:CB	1:C:237:GLN:HB3	1.97	0.95
1:C:149:LYS:CB	1:C:217:TYR:HE1	1.79	0.95
1:C:291:PHE:CE1	1:C:335:MET:HE1	2.02	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:LEU:HD22	1:A:186:LEU:HD13	1.45	0.95
1:A:274:TRP:NE1	1:A:339:GLU:O	1.98	0.95
1:B:326:VAL:HG12	1:B:327:ALA:O	1.65	0.95
1:C:350:ARG:O	1:C:351:ILE:HG22	0.78	0.95
1:A:163:PRO:C	1:A:164:ASN:HD22	1.73	0.95
1:B:291:PHE:HB2	1:B:346:TRP:HB3	1.48	0.95
1:C:291:PHE:HB2	1:C:346:TRP:HB3	1.48	0.95
1:A:130:ARG:NH1	1:A:236:VAL:O	2.00	0.95
1:B:150:VAL:O	1:B:150:VAL:HG12	1.65	0.95
1:A:150:VAL:O	1:A:150:VAL:HG12	1.65	0.95
1:A:277:ASP:OD1	1:A:334:LYS:HE2	1.67	0.95
1:B:278:CYS:N	1:B:334:LYS:HE2	1.78	0.95
1:C:155:ASP:HB2	1:C:172:ILE:HD11	1.47	0.95
1:A:130:ARG:CB	1:A:237:GLN:HB3	1.96	0.94
1:B:277:ASP:OD1	1:B:334:LYS:HE2	1.67	0.94
1:C:264:SER:C	1:C:265:TRP:CA	2.40	0.94
1:A:113:PRO:O	1:A:115:THR:N	1.99	0.94
1:A:296:PRO:HG2	1:A:337:THR:CB	1.95	0.94
1:C:205:LYS:H	1:C:329:ARG:CZ	1.79	0.94
1:B:113:PRO:O	1:B:115:THR:N	1.99	0.94
1:B:141:MET:HG3	1:B:141:MET:O	1.66	0.94
1:B:296:PRO:HG2	1:B:337:THR:CB	1.95	0.94
1:C:101:PRO:HG3	1:C:217:TYR:HE2	1.28	0.94
1:C:130:ARG:NH1	1:C:236:VAL:O	2.00	0.94
1:A:269:LYS:O	1:A:277:ASP:HB3	0.76	0.94
1:B:285:ASN:O	1:B:351:ILE:HG23	1.66	0.94
1:C:179:VAL:HG23	1:C:180:PRO:HD2	1.46	0.94
1:B:291:PHE:CE1	1:B:335:MET:HE1	2.01	0.94
1:A:101:PRO:CG	1:A:166:LEU:CD1	2.45	0.94
1:A:291:PHE:HB2	1:A:346:TRP:HB3	1.48	0.94
1:B:86:GLY:N	1:B:234:TYR:HD1	1.63	0.94
1:B:101:PRO:CG	1:B:166:LEU:CD1	2.46	0.94
1:B:130:ARG:CB	1:B:237:GLN:HB3	1.96	0.94
1:C:277:ASP:OD1	1:C:334:LYS:HE2	1.67	0.94
1:A:289:THR:HG23	1:A:321:TRP:CE3	2.03	0.94
1:A:315:ALA:CB	1:A:318:SER:CB	2.46	0.94
1:C:204:PRO:HB3	1:C:329:ARG:HG3	1.47	0.94
1:B:326:VAL:CG1	1:B:327:ALA:N	2.19	0.93
1:C:101:PRO:CG	1:C:166:LEU:CD1	2.45	0.93
1:A:265:TRP:O	1:A:281:LEU:N	2.02	0.93
1:B:163:PRO:CA	1:B:164:ASN:HD22	1.82	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:LYS:O	1:B:277:ASP:HB3	0.76	0.93
1:B:289:THR:HG23	1:B:321:TRP:CE3	2.03	0.93
1:A:89:LEU:C	1:A:89:LEU:CD2	2.37	0.93
1:C:112:GLU:HA	1:C:284:GLY:HA3	1.50	0.93
1:C:141:MET:HG3	1:C:141:MET:O	1.66	0.93
1:C:269:LYS:O	1:C:277:ASP:HB3	0.76	0.93
1:A:119:LEU:HD22	1:A:234:TYR:HH	1.19	0.93
1:A:141:MET:HG3	1:A:141:MET:O	1.66	0.93
1:B:315:ALA:CB	1:B:318:SER:CB	2.46	0.93
1:A:264:SER:C	1:A:265:TRP:CA	2.40	0.93
1:A:315:ALA:O	1:A:316:ALA:C	2.00	0.93
1:B:264:SER:C	1:B:265:TRP:CA	2.40	0.93
1:C:207:VAL:CG1	1:C:329:ARG:HH21	1.75	0.93
1:B:124:ALA:HB1	1:B:245:THR:HG22	1.51	0.93
1:C:265:TRP:O	1:C:281:LEU:N	2.02	0.93
1:C:86:GLY:N	1:C:234:TYR:HD1	1.63	0.93
1:C:149:LYS:HB3	1:C:217:TYR:HE1	1.11	0.93
1:C:289:THR:HG23	1:C:321:TRP:CE3	2.03	0.93
1:A:113:PRO:C	1:A:115:THR:H	1.74	0.93
1:B:82:ILE:HD11	1:B:122:GLU:OE2	1.69	0.93
1:B:154:PHE:HB2	1:B:212:LEU:CD1	1.99	0.93
1:A:124:ALA:HB1	1:A:245:THR:HG22	1.51	0.92
1:A:154:PHE:HB2	1:A:212:LEU:CD1	1.99	0.92
1:C:154:PHE:HB2	1:C:212:LEU:CD1	1.99	0.92
1:C:333:VAL:O	1:C:334:LYS:CD	2.18	0.92
1:A:134:LEU:HA	1:A:233:GLU:C	1.95	0.92
1:A:130:ARG:HD3	1:A:237:GLN:N	1.84	0.92
1:A:333:VAL:O	1:A:334:LYS:CD	2.18	0.92
1:B:285:ASN:O	1:B:351:ILE:CG2	2.17	0.92
1:C:159:ALA:HB1	1:C:328:GLU:HB3	1.50	0.92
1:C:315:ALA:CB	1:C:318:SER:CB	2.46	0.92
1:A:82:ILE:HD11	1:A:122:GLU:OE2	1.69	0.92
1:B:333:VAL:O	1:B:334:LYS:CD	2.18	0.92
1:B:338:THR:OG1	1:B:339:GLU:N	1.94	0.92
1:C:204:PRO:CB	1:C:329:ARG:HG3	1.60	0.92
1:A:163:PRO:CA	1:A:164:ASN:HD22	1.82	0.92
1:B:113:PRO:C	1:B:115:THR:H	1.74	0.92
1:C:342:PRO:O	1:C:343:LYS:HD3	1.70	0.92
1:A:278:CYS:N	1:A:334:LYS:CE	2.20	0.92
1:C:76:SER:C	1:C:76:SER:CB	2.43	0.92
1:C:82:ILE:HD11	1:C:122:GLU:OE2	1.69	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:LEU:HA	1:C:233:GLU:C	1.94	0.92
1:B:265:TRP:O	1:B:281:LEU:N	2.02	0.92
1:B:308:PHE:HE2	1:B:310:VAL:HG21	1.34	0.91
1:C:83:THR:HG22	1:C:84:ARG:H	1.34	0.91
1:A:286:PHE:HA	1:A:351:ILE:HG22	1.52	0.91
1:A:342:PRO:O	1:A:343:LYS:HD3	1.70	0.91
1:C:126:TYR:HA	1:C:242:THR:HG22	1.50	0.91
1:A:83:THR:HG22	1:A:84:ARG:H	1.34	0.91
1:B:150:VAL:O	1:B:150:VAL:CG1	2.18	0.91
1:C:163:PRO:CA	1:C:164:ASN:HD22	1.82	0.91
1:A:143:PRO:O	1:A:146:THR:HG23	1.71	0.91
1:A:296:PRO:CB	1:A:337:THR:HG22	2.00	0.91
1:C:296:PRO:CB	1:C:337:THR:HG22	2.00	0.91
1:A:313:GLU:CG	1:A:318:SER:CB	2.49	0.91
1:B:134:LEU:HA	1:B:233:GLU:C	1.94	0.91
1:B:296:PRO:CB	1:B:337:THR:HG22	2.00	0.91
1:A:130:ARG:HD3	1:A:237:GLN:HB2	0.97	0.91
1:A:296:PRO:CD	1:A:337:THR:HG22	2.01	0.91
1:C:124:ALA:HB1	1:C:245:THR:HG22	1.51	0.91
1:C:338:THR:OG1	1:C:339:GLU:N	1.94	0.91
1:B:164:ASN:ND2	1:B:164:ASN:H	1.47	0.91
1:B:342:PRO:O	1:B:343:LYS:HD3	1.70	0.91
1:C:159:ALA:CB	1:C:328:GLU:HG3	2.01	0.91
1:C:207:VAL:CB	1:C:329:ARG:NH2	2.34	0.91
1:A:285:ASN:O	1:A:351:ILE:CG2	2.17	0.91
1:B:83:THR:HG22	1:B:84:ARG:H	1.34	0.91
1:B:130:ARG:HD3	1:B:237:GLN:N	1.84	0.91
1:C:313:GLU:CG	1:C:318:SER:CB	2.49	0.91
1:C:134:LEU:HA	1:C:233:GLU:O	0.73	0.91
1:C:285:ASN:O	1:C:351:ILE:CG2	2.17	0.91
1:B:286:PHE:HA	1:B:351:ILE:HG22	1.52	0.90
1:B:300:LEU:HG	1:B:308:PHE:CZ	2.06	0.90
1:C:130:ARG:HH11	1:C:237:GLN:HA	1.36	0.90
1:A:126:TYR:N	1:A:242:THR:HG22	1.86	0.90
1:A:134:LEU:HA	1:A:233:GLU:O	0.73	0.90
1:A:150:VAL:O	1:A:150:VAL:CG1	2.18	0.90
1:A:296:PRO:HG2	1:A:337:THR:HG21	1.51	0.90
1:C:130:ARG:HD3	1:C:237:GLN:N	1.84	0.90
1:B:296:PRO:CD	1:B:337:THR:HG22	2.01	0.90
1:C:198:ALA:C	1:C:200:GLY:H	1.78	0.90
1:B:134:LEU:CD2	1:B:188:VAL:CG2	2.49	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:TYR:N	1:C:242:THR:HG22	1.86	0.90
1:A:277:ASP:HA	1:A:334:LYS:CD	2.02	0.90
1:C:150:VAL:O	1:C:150:VAL:CG1	2.18	0.90
1:A:186:LEU:HD23	1:A:187:THR:N	1.87	0.90
1:B:130:ARG:HH11	1:B:237:GLN:HA	1.36	0.90
1:B:134:LEU:HA	1:B:233:GLU:O	0.73	0.90
1:A:90:ILE:HD11	1:A:232:VAL:HG23	1.53	0.90
1:A:164:ASN:ND2	1:A:164:ASN:H	1.47	0.90
1:B:89:LEU:CD2	1:B:89:LEU:O	2.20	0.90
1:B:277:ASP:HA	1:B:334:LYS:CD	2.02	0.90
1:C:207:VAL:CG1	1:C:329:ARG:NE	2.17	0.90
1:A:126:TYR:HA	1:A:242:THR:HG22	1.50	0.90
1:B:126:TYR:HA	1:B:242:THR:HG22	1.50	0.90
1:B:186:LEU:HD23	1:B:187:THR:N	1.87	0.90
1:C:246:SER:O	1:C:350:ARG:N	2.05	0.90
1:C:300:LEU:HG	1:C:308:PHE:CZ	2.06	0.90
1:C:308:PHE:HE2	1:C:310:VAL:HG21	1.34	0.90
1:C:274:TRP:CD1	1:C:339:GLU:O	2.25	0.89
1:B:248:ALA:O	1:B:263:VAL:HG12	1.70	0.89
1:C:115:THR:O	1:C:116:PHE:HD1	1.48	0.89
1:C:134:LEU:CD2	1:C:188:VAL:CG2	2.49	0.89
1:C:143:PRO:O	1:C:146:THR:HG23	1.71	0.89
1:A:89:LEU:CD2	1:A:89:LEU:O	2.20	0.89
1:A:95:LYS:NZ	1:A:221:ALA:CA	2.35	0.89
1:A:308:PHE:HE2	1:A:310:VAL:HG21	1.34	0.89
1:B:203:ASP:OD1	1:B:205:LYS:HD3	0.71	0.89
1:C:204:PRO:CB	1:C:328:GLU:CG	2.48	0.89
1:C:200:GLY:CA	1:C:265:TRP:HD1	1.76	0.89
1:C:304:ASP:OD2	1:C:331:GLN:HA	1.72	0.89
1:A:300:LEU:HG	1:A:308:PHE:CZ	2.07	0.89
1:B:90:ILE:HD11	1:B:232:VAL:HG23	1.53	0.89
1:B:143:PRO:O	1:B:146:THR:HG23	1.71	0.89
1:B:304:ASP:OD2	1:B:331:GLN:HA	1.73	0.89
1:C:164:ASN:ND2	1:C:164:ASN:H	1.47	0.89
1:C:203:ASP:OD1	1:C:205:LYS:HD3	0.71	0.89
1:C:277:ASP:HA	1:C:334:LYS:CD	2.02	0.89
1:C:89:LEU:CD2	1:C:89:LEU:O	2.20	0.89
1:C:244:SER:O	1:C:245:THR:CG2	2.21	0.89
1:C:286:PHE:HA	1:C:351:ILE:HG22	1.52	0.89
1:A:134:LEU:CD2	1:A:188:VAL:CG2	2.49	0.89
1:A:203:ASP:OD1	1:A:205:LYS:HD3	0.71	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:THR:O	1:B:116:PHE:HD1	1.48	0.89
1:B:126:TYR:N	1:B:242:THR:HG22	1.86	0.89
1:B:114:GLY:HA3	1:B:329:ARG:HE	1.38	0.89
1:C:204:PRO:CG	1:C:328:GLU:C	2.43	0.89
1:C:95:LYS:NZ	1:C:221:ALA:CA	2.35	0.89
1:A:274:TRP:CD1	1:A:339:GLU:O	2.25	0.88
1:B:154:PHE:HB2	1:B:212:LEU:HD12	1.56	0.88
1:B:274:TRP:CD1	1:B:339:GLU:O	2.26	0.88
1:C:130:ARG:HD3	1:C:237:GLN:HB2	0.97	0.88
1:C:133:SER:C	1:C:234:TYR:HA	1.99	0.88
1:B:249:GLN:CB	1:B:265:TRP:CZ3	2.56	0.88
1:B:308:PHE:CE2	1:B:310:VAL:HG21	2.07	0.88
1:C:119:LEU:HD22	1:C:234:TYR:HH	1.29	0.88
1:A:304:ASP:OD2	1:A:331:GLN:HA	1.73	0.88
1:B:328:GLU:C	1:B:329:ARG:O	2.14	0.88
1:C:249:GLN:CB	1:C:265:TRP:CZ3	2.56	0.88
1:C:296:PRO:CD	1:C:337:THR:HG22	2.01	0.88
1:C:328:GLU:C	1:C:329:ARG:O	2.14	0.88
1:A:130:ARG:HH11	1:A:237:GLN:HA	1.36	0.88
1:B:95:LYS:NZ	1:B:221:ALA:CA	2.35	0.88
1:B:326:VAL:HG12	1:B:327:ALA:H	1.18	0.88
1:A:105:THR:HG1	1:A:211:LYS:CD	1.74	0.88
1:A:249:GLN:CB	1:A:265:TRP:CZ3	2.56	0.88
1:B:313:GLU:CG	1:B:318:SER:CB	2.49	0.88
1:C:231:ARG:HG3	1:C:232:VAL:N	1.87	0.88
1:C:154:PHE:HB2	1:C:212:LEU:HD12	1.56	0.88
1:C:186:LEU:HD23	1:C:187:THR:N	1.87	0.88
1:A:154:PHE:HB2	1:A:212:LEU:HD12	1.56	0.88
1:A:244:SER:O	1:A:245:THR:CG2	2.21	0.88
1:B:244:SER:O	1:B:245:THR:CG2	2.21	0.88
1:C:296:PRO:HG2	1:C:337:THR:HG21	1.51	0.88
1:A:120:ILE:HD12	1:A:329:ARG:NH2	1.88	0.87
1:C:90:ILE:HD11	1:C:232:VAL:HG23	1.53	0.87
1:C:152:LEU:O	1:C:186:LEU:HD12	1.74	0.87
1:A:133:SER:C	1:A:234:TYR:HA	1.99	0.87
1:A:149:LYS:HD3	1:A:170:TYR:OH	1.43	0.87
1:B:109:ASN:OD1	1:B:110:PRO:HD2	1.74	0.87
1:C:78:ALA:C	1:C:80:ASP:H	1.82	0.87
1:C:308:PHE:CE2	1:C:310:VAL:HG21	2.07	0.87
1:C:56:THR:HG23	1:C:57:ARG:N	1.89	0.87
1:A:82:ILE:HG21	1:A:238:LEU:HB2	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:THR:HG21	1:C:87:SER:CB	2.04	0.87
1:C:251:GLY:O	1:C:346:TRP:CD2	2.28	0.87
1:B:130:ARG:HD3	1:B:237:GLN:HB2	0.97	0.87
1:B:251:GLY:O	1:B:346:TRP:CD2	2.28	0.87
1:C:130:ARG:HH11	1:C:237:GLN:CA	1.88	0.87
1:A:138:TYR:C	1:A:139:SER:O	2.16	0.87
1:B:231:ARG:HG3	1:B:232:VAL:N	1.87	0.87
1:C:109:ASN:OD1	1:C:110:PRO:HD2	1.74	0.87
1:A:130:ARG:HH11	1:A:237:GLN:CA	1.88	0.87
1:B:82:ILE:HG21	1:B:238:LEU:HB2	1.56	0.87
1:C:278:CYS:N	1:C:334:LYS:CE	2.20	0.87
1:A:101:PRO:HD2	1:A:166:LEU:HD12	1.37	0.86
1:A:338:THR:OG1	1:A:339:GLU:N	1.94	0.86
1:B:296:PRO:CG	1:B:337:THR:CB	2.52	0.86
1:C:264:SER:CA	1:C:265:TRP:N	2.38	0.86
1:B:152:LEU:O	1:B:186:LEU:HD12	1.74	0.86
1:C:130:ARG:NE	1:C:237:GLN:HB2	1.90	0.86
1:B:138:TYR:C	1:B:139:SER:O	2.16	0.86
1:C:59:SER:O	1:C:61:PRO:HD3	1.74	0.86
1:C:105:THR:HG1	1:C:211:LYS:CD	1.75	0.86
1:A:248:ALA:CB	1:A:265:TRP:CA	2.53	0.86
1:B:264:SER:CA	1:B:265:TRP:N	2.38	0.86
1:C:68:GLU:HG2	1:C:137:ARG:HH22	1.38	0.86
1:C:288:LEU:CD1	1:C:290:LEU:CD2	2.53	0.86
1:A:130:ARG:NE	1:A:237:GLN:HB2	1.90	0.86
1:A:251:GLY:O	1:A:346:TRP:CD2	2.28	0.86
1:A:288:LEU:HD11	1:A:290:LEU:HG	1.58	0.86
1:A:328:GLU:C	1:A:329:ARG:O	2.14	0.86
1:A:198:ALA:C	1:A:200:GLY:H	1.77	0.86
1:A:327:ALA:CB	1:A:331:GLN:CD	2.39	0.86
1:B:130:ARG:HH11	1:B:237:GLN:CA	1.88	0.86
1:C:89:LEU:O	1:C:89:LEU:HD22	1.75	0.86
1:A:109:ASN:OD1	1:A:110:PRO:HD2	1.74	0.86
1:A:115:THR:O	1:A:116:PHE:HD1	1.48	0.86
1:A:231:ARG:HG3	1:A:232:VAL:N	1.87	0.86
1:C:72:GLN:HE21	1:C:72:GLN:HA	1.39	0.86
1:B:101:PRO:CG	1:B:166:LEU:HD11	2.06	0.86
1:B:133:SER:C	1:B:234:TYR:HA	1.99	0.86
1:C:318:SER:OG	1:C:319:VAL:N	2.07	0.86
1:A:101:PRO:CG	1:A:166:LEU:HD11	2.06	0.86
1:C:77:THR:HG22	1:C:78:ALA:H	1.37	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:PHE:HE1	1:C:155:ASP:O	1.59	0.85
1:B:112:GLU:CG	1:B:329:ARG:NH2	2.39	0.85
1:C:125:GLN:HA	1:C:243:GLY:CA	2.06	0.85
1:C:149:LYS:HG2	1:C:177:SER:HG	1.39	0.85
1:A:264:SER:CA	1:A:265:TRP:N	2.38	0.85
1:B:130:ARG:NE	1:B:237:GLN:HB2	1.90	0.85
1:B:154:PHE:HE1	1:B:155:ASP:O	1.59	0.85
1:B:296:PRO:HG2	1:B:337:THR:HG21	1.51	0.85
1:B:296:PRO:CG	1:B:337:THR:HG21	2.06	0.85
1:C:90:ILE:HD11	1:C:232:VAL:HG21	1.58	0.85
1:C:200:GLY:N	1:C:265:TRP:HD1	1.36	0.85
1:A:89:LEU:O	1:A:89:LEU:HD22	1.75	0.85
1:A:136:PHE:CE1	1:A:232:VAL:HG22	2.12	0.85
1:B:89:LEU:O	1:B:89:LEU:HD22	1.75	0.85
1:B:198:ALA:C	1:B:200:GLY:H	1.77	0.85
1:A:90:ILE:HD11	1:A:232:VAL:HG21	1.58	0.85
1:C:277:ASP:OD1	1:C:279:HIS:ND1	2.10	0.85
1:A:296:PRO:CG	1:A:337:THR:CB	2.52	0.85
1:A:308:PHE:CE2	1:A:310:VAL:HG21	2.07	0.85
1:C:95:LYS:HZ2	1:C:221:ALA:HA	1.41	0.85
1:C:101:PRO:CG	1:C:166:LEU:HD11	2.06	0.85
1:A:125:GLN:HA	1:A:243:GLY:CA	2.06	0.85
1:A:130:ARG:HD2	1:A:237:GLN:HB2	0.85	0.85
1:A:152:LEU:O	1:A:186:LEU:HD12	1.74	0.85
1:B:149:LYS:HD3	1:B:170:TYR:OH	1.43	0.85
1:C:136:PHE:CE1	1:C:232:VAL:HG22	2.12	0.85
1:C:138:TYR:C	1:C:139:SER:O	2.16	0.85
1:A:277:ASP:OD1	1:A:279:HIS:ND1	2.10	0.85
1:B:149:LYS:HG2	1:B:177:SER:HG	1.37	0.85
1:B:315:ALA:HB1	1:B:318:SER:CB	2.07	0.85
1:C:82:ILE:HG21	1:C:238:LEU:HB2	1.56	0.85
1:C:179:VAL:HG22	1:C:180:PRO:HD2	1.58	0.85
1:A:149:LYS:HG2	1:A:177:SER:HG	1.37	0.84
1:B:174:GLY:C	1:B:175:CYS:HG	1.80	0.84
1:B:318:SER:OG	1:B:319:VAL:N	2.07	0.84
1:A:119:LEU:CD2	1:A:234:TYR:CZ	2.54	0.84
1:B:327:ALA:CB	1:B:331:GLN:CD	2.39	0.84
1:C:80:ASP:HA	1:C:241:ARG:CZ	2.07	0.84
1:C:197:VAL:HG23	1:C:350:ARG:NH2	1.79	0.84
1:A:154:PHE:HE1	1:A:155:ASP:O	1.59	0.84
1:B:119:LEU:CD2	1:B:234:TYR:CE2	2.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:VAL:HG12	1:B:327:ALA:C	2.02	0.84
1:B:288:LEU:CD1	1:B:290:LEU:CD2	2.53	0.84
1:C:288:LEU:HD11	1:C:290:LEU:HG	1.57	0.84
1:B:136:PHE:CE1	1:B:232:VAL:HG22	2.12	0.84
1:C:53:GLN:C	1:C:53:GLN:N	2.35	0.84
1:A:288:LEU:HD21	1:A:290:LEU:HD11	1.60	0.84
1:B:90:ILE:HD11	1:B:232:VAL:HG21	1.58	0.84
1:B:130:ARG:HD2	1:B:237:GLN:HB2	0.85	0.84
1:C:201:ILE:CG2	1:C:265:TRP:C	2.51	0.84
1:A:315:ALA:HB1	1:A:318:SER:CA	2.08	0.84
1:B:277:ASP:OD1	1:B:279:HIS:ND1	2.10	0.84
1:C:119:LEU:CD2	1:C:234:TYR:CE2	2.60	0.84
1:C:149:LYS:HD3	1:C:217:TYR:OH	1.78	0.84
1:C:207:VAL:H	1:C:329:ARG:CZ	1.90	0.84
1:A:291:PHE:O	1:A:292:TYR:HB3	1.78	0.84
1:B:125:GLN:HA	1:B:243:GLY:CA	2.06	0.84
1:B:149:LYS:HD3	1:B:217:TYR:OH	1.78	0.84
1:B:179:VAL:HG22	1:B:180:PRO:HD2	1.58	0.84
1:B:291:PHE:O	1:B:292:TYR:HB3	1.78	0.84
1:C:315:ALA:HB1	1:C:318:SER:CA	2.08	0.84
1:C:327:ALA:CA	1:C:331:GLN:OE1	2.26	0.84
1:A:119:LEU:CD2	1:A:234:TYR:CE2	2.60	0.83
1:C:130:ARG:HD2	1:C:237:GLN:HB2	0.85	0.83
1:C:288:LEU:CD1	1:C:290:LEU:HD21	2.08	0.83
1:C:296:PRO:CG	1:C:337:THR:CB	2.52	0.83
1:A:152:LEU:HD22	1:A:186:LEU:HD12	1.61	0.83
1:A:315:ALA:HB1	1:A:318:SER:CB	2.07	0.83
1:C:338:THR:HG1	1:C:339:GLU:HB2	1.43	0.83
1:B:288:LEU:HD11	1:B:290:LEU:HG	1.58	0.83
1:C:326:VAL:HG12	1:C:327:ALA:C	2.02	0.83
1:A:295:ALA:HB1	1:A:315:ALA:N	1.93	0.83
1:B:327:ALA:CA	1:B:331:GLN:OE1	2.26	0.83
1:B:339:GLU:C	1:B:340:GLU:HA	2.04	0.83
1:C:295:ALA:HB1	1:C:315:ALA:N	1.93	0.83
1:C:315:ALA:HB1	1:C:318:SER:CB	2.08	0.83
1:A:296:PRO:CG	1:A:337:THR:HG21	2.06	0.83
1:C:251:GLY:O	1:C:346:TRP:CE3	2.31	0.83
1:A:90:ILE:HG22	1:A:90:ILE:O	1.78	0.83
1:A:288:LEU:CD1	1:A:290:LEU:HD21	2.08	0.83
1:A:326:VAL:HG12	1:A:327:ALA:C	2.02	0.83
1:B:251:GLY:O	1:B:346:TRP:CE3	2.31	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:288:LEU:HG	1:C:289:THR:N	1.94	0.83
1:A:149:LYS:HD3	1:A:217:TYR:OH	1.78	0.83
1:A:153:ALA:CB	1:A:174:GLY:CA	2.35	0.83
1:B:169:LEU:HD23	1:B:169:LEU:C	2.04	0.83
1:B:278:CYS:H	1:B:334:LYS:HD3	1.25	0.83
1:C:55:VAL:HG22	1:C:56:THR:N	1.93	0.83
1:C:249:GLN:HE22	1:C:265:TRP:N	1.77	0.83
1:C:291:PHE:O	1:C:292:TYR:HB3	1.78	0.83
1:A:169:LEU:HD23	1:A:169:LEU:C	2.04	0.83
1:A:179:VAL:HG22	1:A:180:PRO:HD2	1.58	0.83
1:A:269:LYS:HG2	1:A:270:GLY:H	1.42	0.83
1:B:288:LEU:HG	1:B:289:THR:N	1.94	0.83
1:C:79:ARG:O	1:C:80:ASP:CB	2.27	0.83
1:C:201:ILE:HG22	1:C:265:TRP:CA	2.09	0.83
1:C:207:VAL:HG13	1:C:329:ARG:HH21	1.44	0.83
1:A:288:LEU:HG	1:A:289:THR:N	1.94	0.82
1:B:295:ALA:HB1	1:B:315:ALA:N	1.93	0.82
1:C:339:GLU:C	1:C:340:GLU:HA	2.04	0.82
1:A:339:GLU:C	1:A:340:GLU:HA	2.04	0.82
1:B:153:ALA:CB	1:B:174:GLY:CA	2.35	0.82
1:B:152:LEU:HD22	1:B:186:LEU:HD12	1.60	0.82
1:C:69:VAL:CG1	1:C:70:SER:N	2.38	0.82
1:C:200:GLY:CA	1:C:265:TRP:HA	2.09	0.82
1:C:277:ASP:OD1	1:C:334:LYS:CE	2.27	0.82
1:A:277:ASP:OD1	1:A:334:LYS:CE	2.27	0.82
1:B:248:ALA:C	1:B:249:GLN:HB2	2.04	0.82
1:C:69:VAL:CG1	1:C:70:SER:H	1.81	0.82
1:C:90:ILE:HG22	1:C:90:ILE:O	1.78	0.82
1:C:249:GLN:NE2	1:C:265:TRP:HE3	1.78	0.82
1:A:251:GLY:O	1:A:346:TRP:CE3	2.31	0.82
1:A:327:ALA:CA	1:A:331:GLN:OE1	2.26	0.82
1:B:288:LEU:HD21	1:B:290:LEU:HD11	1.60	0.82
1:C:66:TYR:CE2	1:C:183:GLY:HA3	2.15	0.82
1:A:169:LEU:O	1:A:172:ILE:HG22	1.80	0.82
1:A:340:GLU:O	1:A:342:PRO:HD2	1.79	0.82
1:B:90:ILE:O	1:B:90:ILE:HG22	1.78	0.82
1:B:169:LEU:O	1:B:172:ILE:HG22	1.80	0.82
1:B:300:LEU:HD11	1:B:333:VAL:CG1	2.09	0.82
1:A:300:LEU:HD11	1:A:333:VAL:CG1	2.09	0.82
1:B:204:PRO:C	1:B:205:LYS:HD2	2.05	0.82
1:B:315:ALA:HB1	1:B:318:SER:CA	2.08	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:95:LYS:HZ3	1:C:225:ALA:H	1.25	0.82
1:C:170:TYR:CE1	1:C:217:TYR:OH	2.32	0.82
1:A:126:TYR:N	1:A:242:THR:CG2	2.43	0.82
1:A:318:SER:OG	1:A:319:VAL:N	2.07	0.82
1:B:277:ASP:OD1	1:B:334:LYS:CE	2.27	0.82
1:C:204:PRO:C	1:C:205:LYS:HD2	2.05	0.82
1:C:288:LEU:HD21	1:C:290:LEU:HD11	1.60	0.82
1:C:300:LEU:HD11	1:C:333:VAL:CG1	2.09	0.82
1:A:128:LYS:HA	1:A:195:ARG:O	1.80	0.81
1:B:128:LYS:HA	1:B:195:ARG:O	1.80	0.81
1:C:269:LYS:HG2	1:C:270:GLY:H	1.42	0.81
1:B:285:ASN:ND2	1:B:324:VAL:O	2.13	0.81
1:B:95:LYS:NZ	1:B:225:ALA:N	2.28	0.81
1:B:126:TYR:N	1:B:242:THR:CG2	2.43	0.81
1:B:251:GLY:O	1:B:346:TRP:CE2	2.34	0.81
1:C:101:PRO:CG	1:C:166:LEU:HD12	2.10	0.81
1:C:169:LEU:O	1:C:172:ILE:HG22	1.80	0.81
1:C:296:PRO:CG	1:C:337:THR:HG21	2.06	0.81
1:A:204:PRO:C	1:A:205:LYS:HD2	2.05	0.81
1:B:164:ASN:HD22	1:B:164:ASN:H	0.82	0.81
1:B:340:GLU:O	1:B:342:PRO:HD2	1.80	0.81
1:A:95:LYS:NZ	1:A:225:ALA:N	2.28	0.81
1:A:112:GLU:O	1:A:115:THR:HG22	1.81	0.81
1:B:315:ALA:CB	1:B:318:SER:H	1.94	0.81
1:C:130:ARG:HD2	1:C:237:GLN:HE21	1.46	0.81
1:A:288:LEU:CD1	1:A:290:LEU:CD2	2.53	0.81
1:C:169:LEU:C	1:C:169:LEU:HD23	2.04	0.81
1:C:206:LEU:H	1:C:329:ARG:NH1	1.79	0.81
1:A:170:TYR:CE1	1:A:217:TYR:OH	2.32	0.81
1:A:296:PRO:HG3	1:A:337:THR:CG2	2.07	0.81
1:C:249:GLN:HE22	1:C:265:TRP:H	1.29	0.81
1:C:285:ASN:ND2	1:C:324:VAL:O	2.13	0.81
1:A:251:GLY:O	1:A:346:TRP:CE2	2.34	0.81
1:B:288:LEU:CD1	1:B:290:LEU:HD21	2.08	0.81
1:B:296:PRO:HG3	1:B:337:THR:CG2	2.07	0.81
1:B:107:VAL:O	1:B:115:THR:HG21	1.81	0.81
1:B:170:TYR:CE1	1:B:217:TYR:OH	2.32	0.81
1:B:278:CYS:N	1:B:334:LYS:CE	2.20	0.81
1:C:107:VAL:O	1:C:115:THR:HG21	1.81	0.81
1:B:90:ILE:CD1	1:B:232:VAL:CG2	2.58	0.81
1:B:119:LEU:CD2	1:B:234:TYR:CZ	2.55	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:SER:C	1:C:146:THR:H	1.89	0.81
1:A:285:ASN:ND2	1:A:324:VAL:O	2.13	0.80
1:B:286:PHE:HA	1:B:351:ILE:HG21	1.61	0.80
1:C:340:GLU:O	1:C:342:PRO:HD2	1.80	0.80
1:B:96:ASN:HD21	1:B:102:LYS:HD3	1.45	0.80
1:B:101:PRO:CG	1:B:166:LEU:HD12	2.10	0.80
1:C:152:LEU:HD22	1:C:186:LEU:HD12	1.60	0.80
1:C:251:GLY:O	1:C:346:TRP:CE2	2.34	0.80
1:C:300:LEU:HD11	1:C:333:VAL:HG12	1.63	0.80
1:A:96:ASN:HD21	1:A:102:LYS:HD3	1.45	0.80
1:A:101:PRO:HG3	1:A:217:TYR:CD2	2.17	0.80
1:A:300:LEU:HD11	1:A:333:VAL:HG12	1.63	0.80
1:C:59:SER:C	1:C:61:PRO:HD3	2.06	0.80
1:C:96:ASN:HD21	1:C:102:LYS:HD3	1.45	0.80
1:C:138:TYR:O	1:C:139:SER:C	2.25	0.80
1:C:315:ALA:CB	1:C:318:SER:H	1.94	0.80
1:C:327:ALA:CB	1:C:331:GLN:CD	2.39	0.80
1:A:90:ILE:CD1	1:A:232:VAL:CG2	2.58	0.80
1:A:248:ALA:HB1	1:A:265:TRP:HA	1.60	0.80
1:C:95:LYS:NZ	1:C:225:ALA:N	2.28	0.80
1:C:71:THR:HG21	1:C:87:SER:HG	0.98	0.80
1:C:128:LYS:HA	1:C:195:ARG:O	1.80	0.80
1:C:201:ILE:CG2	1:C:265:TRP:O	2.29	0.80
1:C:227:LEU:H	1:C:227:LEU:HD12	1.47	0.80
1:A:164:ASN:HD22	1:A:164:ASN:H	0.82	0.80
1:C:126:TYR:N	1:C:242:THR:CG2	2.43	0.80
1:A:248:ALA:CB	1:A:264:SER:CB	2.54	0.80
1:B:95:LYS:HZ2	1:B:221:ALA:HA	1.42	0.80
1:B:95:LYS:HZ1	1:B:225:ALA:N	1.79	0.80
1:B:112:GLU:O	1:B:115:THR:HG22	1.81	0.80
1:B:130:ARG:HD2	1:B:237:GLN:HE21	1.46	0.80
1:A:95:LYS:HZ1	1:A:225:ALA:N	1.79	0.80
1:B:291:PHE:HB2	1:B:345:LYS:O	1.82	0.80
1:B:300:LEU:HD11	1:B:333:VAL:HG12	1.63	0.80
1:A:286:PHE:HA	1:A:351:ILE:HG21	1.61	0.80
1:B:101:PRO:HD2	1:B:166:LEU:HD12	1.37	0.80
1:C:101:PRO:HG3	1:C:217:TYR:CD2	2.17	0.80
1:B:95:LYS:NZ	1:B:225:ALA:H	1.80	0.79
1:C:199:ASP:C	1:C:265:TRP:NE1	2.40	0.79
1:C:296:PRO:HG3	1:C:337:THR:CG2	2.07	0.79
1:A:121:LYS:NZ	1:A:350:ARG:HH12	1.80	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:GLN:HB3	1:A:348:ALA:O	1.83	0.79
1:C:164:ASN:HD22	1:C:164:ASN:H	0.82	0.79
1:A:291:PHE:HB2	1:A:345:LYS:O	1.82	0.79
1:C:112:GLU:O	1:C:115:THR:HG22	1.81	0.79
1:C:153:ALA:CB	1:C:174:GLY:CA	2.35	0.79
1:C:199:ASP:HA	1:C:265:TRP:HE1	1.47	0.79
1:A:95:LYS:NZ	1:A:225:ALA:H	1.80	0.79
1:A:227:LEU:H	1:A:227:LEU:HD12	1.47	0.79
1:C:119:LEU:CD2	1:C:234:TYR:CZ	2.55	0.79
1:C:249:GLN:HB3	1:C:348:ALA:O	1.83	0.79
1:A:95:LYS:HZ2	1:A:221:ALA:HA	1.42	0.79
1:B:101:PRO:HG3	1:B:217:TYR:CD2	2.17	0.79
1:B:133:SER:HB3	1:B:235:THR:HG22	1.64	0.79
1:C:95:LYS:NZ	1:C:225:ALA:H	1.80	0.79
1:A:315:ALA:CB	1:A:318:SER:H	1.94	0.79
1:A:133:SER:HB3	1:A:235:THR:HG22	1.64	0.79
1:A:310:VAL:C	1:A:311:LEU:HD12	2.08	0.79
1:C:293:GLU:O	1:C:317:GLY:CA	2.31	0.79
1:C:300:LEU:CD1	1:C:333:VAL:HG12	2.13	0.79
1:A:248:ALA:HB2	1:A:264:SER:O	1.77	0.79
1:B:175:CYS:HB2	1:B:176:VAL:HB	1.65	0.79
1:A:101:PRO:CG	1:A:166:LEU:HD12	2.10	0.79
1:B:300:LEU:CD1	1:B:333:VAL:HG12	2.13	0.79
1:C:133:SER:HB3	1:C:235:THR:HG22	1.64	0.79
1:A:107:VAL:O	1:A:115:THR:HG21	1.81	0.78
1:B:269:LYS:HG2	1:B:270:GLY:H	1.42	0.78
1:C:291:PHE:HB2	1:C:345:LYS:O	1.82	0.78
1:C:296:PRO:CD	1:C:337:THR:CG2	2.60	0.78
1:C:90:ILE:CD1	1:C:232:VAL:CG2	2.58	0.78
1:A:121:LYS:HZ2	1:A:350:ARG:HH12	1.30	0.78
1:A:138:TYR:O	1:A:139:SER:C	2.24	0.78
1:C:78:ALA:C	1:C:80:ASP:N	2.32	0.78
1:A:134:LEU:O	1:A:134:LEU:HG	1.83	0.78
1:A:293:GLU:O	1:A:317:GLY:CA	2.31	0.78
1:B:134:LEU:HG	1:B:134:LEU:O	1.83	0.78
1:B:227:LEU:H	1:B:227:LEU:HD12	1.47	0.78
1:C:179:VAL:HG11	1:C:181:TRP:HE1	1.49	0.78
1:C:286:PHE:HA	1:C:351:ILE:HG21	1.61	0.78
1:B:249:GLN:HB3	1:B:348:ALA:O	1.83	0.78
1:B:289:THR:O	1:B:290:LEU:HB3	1.83	0.78
1:C:249:GLN:O	1:C:348:ALA:N	2.17	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:GLN:O	1:B:348:ALA:N	2.17	0.78
1:C:133:SER:N	1:C:235:THR:HG22	1.99	0.78
1:B:236:VAL:HG12	1:B:238:LEU:HD12	1.66	0.78
1:C:204:PRO:HG2	1:C:328:GLU:HG2	0.80	0.78
1:A:130:ARG:HD2	1:A:237:GLN:HE21	1.46	0.78
1:A:249:GLN:O	1:A:348:ALA:N	2.17	0.78
1:B:293:GLU:O	1:B:317:GLY:CA	2.31	0.78
1:C:97:THR:HA	1:C:219:GLN:CA	2.14	0.78
1:B:117:ASN:O	1:B:117:ASN:ND2	2.17	0.78
1:C:179:VAL:CG2	1:C:180:PRO:CD	2.62	0.78
1:C:310:VAL:C	1:C:311:LEU:HD12	2.08	0.78
1:A:117:ASN:O	1:A:117:ASN:ND2	2.17	0.77
1:B:276:HIS:CG	1:B:277:ASP:H	2.03	0.77
1:A:300:LEU:CD1	1:A:333:VAL:HG12	2.13	0.77
1:B:135:ARG:HB2	1:B:185:ILE:HD11	1.67	0.77
1:A:109:ASN:HD21	1:A:197:VAL:HG23	1.50	0.77
1:A:149:LYS:HE2	1:A:151:ALA:HA	1.66	0.77
1:B:133:SER:N	1:B:235:THR:HG22	1.99	0.77
1:B:310:VAL:C	1:B:311:LEU:HD12	2.08	0.77
1:C:205:LYS:H	1:C:329:ARG:NH1	1.82	0.77
1:A:133:SER:N	1:A:235:THR:HG22	1.99	0.77
1:A:149:LYS:CB	1:A:217:TYR:CE1	2.60	0.77
1:A:296:PRO:CD	1:A:337:THR:CG2	2.60	0.77
1:C:76:SER:C	1:C:76:SER:OG	2.26	0.77
1:C:124:ALA:O	1:C:244:SER:N	2.18	0.77
1:C:159:ALA:HB3	1:C:328:GLU:CG	2.11	0.77
1:C:86:GLY:CA	1:C:234:TYR:CE1	2.66	0.77
1:C:200:GLY:CA	1:C:265:TRP:CB	2.58	0.77
1:A:236:VAL:HG12	1:A:238:LEU:HD12	1.66	0.77
1:B:296:PRO:CD	1:B:337:THR:CG2	2.60	0.77
1:A:135:ARG:HB2	1:A:185:ILE:HD11	1.67	0.77
1:A:179:VAL:CG2	1:A:180:PRO:CD	2.62	0.77
1:B:144:SER:C	1:B:146:THR:H	1.89	0.77
1:A:175:CYS:HB2	1:A:176:VAL:HB	1.65	0.77
1:B:185:ILE:HD12	1:B:186:LEU:CA	2.16	0.76
1:B:315:ALA:O	1:B:317:GLY:N	2.18	0.76
1:C:134:LEU:HG	1:C:134:LEU:O	1.83	0.76
1:C:163:PRO:CA	1:C:164:ASN:ND2	2.47	0.76
1:C:251:GLY:O	1:C:346:TRP:CZ3	2.38	0.76
1:C:289:THR:O	1:C:290:LEU:HB3	1.83	0.76
1:A:251:GLY:O	1:A:346:TRP:CZ3	2.38	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:THR:HA	1:B:219:GLN:CA	2.15	0.76
1:C:97:THR:HA	1:C:218:GLY:O	1.85	0.76
1:C:207:VAL:HG13	1:C:329:ARG:NH2	1.94	0.76
1:C:236:VAL:HG12	1:C:238:LEU:HD12	1.66	0.76
1:C:313:GLU:HB2	1:C:315:ALA:N	2.00	0.76
1:A:149:LYS:NZ	1:A:170:TYR:CE1	2.52	0.76
1:B:156:ARG:O	1:B:158:ALA:N	2.18	0.76
1:C:149:LYS:HE2	1:C:151:ALA:HA	1.66	0.76
1:A:156:ARG:O	1:A:158:ALA:N	2.18	0.76
1:A:179:VAL:HG11	1:A:181:TRP:HE1	1.49	0.76
1:A:289:THR:O	1:A:290:LEU:HB3	1.83	0.76
1:B:248:ALA:HB3	1:B:348:ALA:O	1.86	0.76
1:C:154:PHE:CD1	1:C:154:PHE:C	2.62	0.76
1:A:313:GLU:HB2	1:A:315:ALA:N	2.00	0.76
1:B:109:ASN:HD21	1:B:197:VAL:HG23	1.50	0.76
1:B:149:LYS:CB	1:B:217:TYR:CE1	2.60	0.76
1:A:97:THR:HA	1:A:218:GLY:O	1.85	0.76
1:B:163:PRO:CA	1:B:164:ASN:ND2	2.47	0.76
1:C:117:ASN:ND2	1:C:117:ASN:O	2.17	0.76
1:C:156:ARG:O	1:C:158:ALA:N	2.18	0.76
1:C:175:CYS:HB2	1:C:176:VAL:HB	1.65	0.76
1:A:97:THR:HA	1:A:219:GLN:CA	2.14	0.76
1:A:163:PRO:CA	1:A:164:ASN:ND2	2.47	0.76
1:A:276:HIS:CG	1:A:277:ASP:H	2.03	0.76
1:A:300:LEU:CD1	1:A:333:VAL:CG1	2.64	0.76
1:B:149:LYS:HE2	1:B:151:ALA:HA	1.66	0.76
1:A:315:ALA:O	1:A:317:GLY:N	2.18	0.76
1:C:135:ARG:HB2	1:C:185:ILE:HD11	1.67	0.76
1:C:248:ALA:CB	1:C:287:SER:O	2.32	0.76
1:A:185:ILE:HD12	1:A:186:LEU:CA	2.16	0.76
1:A:314:ALA:O	1:A:315:ALA:CB	2.34	0.76
1:B:310:VAL:HA	1:B:321:TRP:O	1.86	0.76
1:C:149:LYS:HB3	1:C:217:TYR:CD1	2.20	0.76
1:C:314:ALA:O	1:C:315:ALA:CB	2.34	0.76
1:A:95:LYS:HZ3	1:A:225:ALA:H	1.34	0.75
1:C:276:HIS:CG	1:C:277:ASP:H	2.03	0.75
1:C:109:ASN:HD21	1:C:197:VAL:HG23	1.50	0.75
1:B:95:LYS:HZ3	1:B:225:ALA:H	1.34	0.75
1:B:179:VAL:HG11	1:B:181:TRP:HE1	1.49	0.75
1:B:251:GLY:O	1:B:346:TRP:CZ3	2.39	0.75
1:B:313:GLU:HB2	1:B:315:ALA:N	2.00	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:THR:HG22	1:C:84:ARG:N	2.01	0.75
1:C:279:HIS:CA	1:C:280:PHE:N	2.50	0.75
1:C:301:GLU:O	1:C:333:VAL:CG1	2.34	0.75
1:A:83:THR:HG22	1:A:84:ARG:N	2.01	0.75
1:A:144:SER:C	1:A:146:THR:H	1.89	0.75
1:B:179:VAL:CG2	1:B:180:PRO:CD	2.62	0.75
1:B:300:LEU:CD1	1:B:333:VAL:CG1	2.64	0.75
1:C:306:SER:HB3	1:C:325:LYS:HB3	1.69	0.75
1:A:167:ALA:O	1:A:171:ASN:CG	2.30	0.75
1:B:306:SER:HB3	1:B:325:LYS:HB3	1.69	0.75
1:C:115:THR:O	1:C:116:PHE:CG	2.40	0.75
1:C:136:PHE:CZ	1:C:212:LEU:HD22	2.22	0.75
1:C:300:LEU:CD1	1:C:333:VAL:CG1	2.64	0.75
1:A:136:PHE:CZ	1:A:212:LEU:HD22	2.22	0.75
1:A:292:TYR:HB2	1:A:318:SER:O	1.86	0.75
1:B:326:VAL:CG1	1:B:331:GLN:HG3	2.17	0.75
1:C:277:ASP:OD1	1:C:334:LYS:NZ	2.20	0.75
1:C:288:LEU:CD1	1:C:290:LEU:HG	2.17	0.75
1:B:138:TYR:CG	1:B:184:PHE:CZ	2.62	0.75
1:B:277:ASP:OD1	1:B:334:LYS:NZ	2.20	0.75
1:A:279:HIS:CA	1:A:280:PHE:N	2.50	0.74
1:B:279:HIS:CA	1:B:280:PHE:N	2.50	0.74
1:A:241:ARG:HD2	1:A:241:ARG:N	2.03	0.74
1:B:154:PHE:HE1	1:B:155:ASP:C	1.95	0.74
1:B:289:THR:O	1:B:290:LEU:CB	2.35	0.74
1:B:301:GLU:O	1:B:333:VAL:CG1	2.34	0.74
1:C:68:GLU:HG2	1:C:137:ARG:NH2	2.02	0.74
1:C:167:ALA:O	1:C:171:ASN:CG	2.30	0.74
1:A:277:ASP:OD1	1:A:334:LYS:NZ	2.20	0.74
1:B:97:THR:HA	1:B:218:GLY:O	1.85	0.74
1:B:167:ALA:O	1:B:171:ASN:CG	2.30	0.74
1:B:241:ARG:N	1:B:241:ARG:HD2	2.03	0.74
1:B:271:THR:HG21	1:B:275:GLU:OE2	1.87	0.74
1:C:310:VAL:HA	1:C:321:TRP:O	1.86	0.74
1:A:133:SER:CB	1:A:235:THR:HG22	2.17	0.74
1:C:136:PHE:CD1	1:C:232:VAL:HG22	2.23	0.74
1:C:271:THR:HG21	1:C:275:GLU:OE2	1.87	0.74
1:A:126:TYR:CA	1:A:242:THR:CG2	2.64	0.74
1:B:136:PHE:CZ	1:B:212:LEU:HD22	2.22	0.74
1:B:292:TYR:HB2	1:B:318:SER:O	1.86	0.74
1:B:138:TYR:O	1:B:139:SER:C	2.24	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:ALA:O	1:B:315:ALA:CB	2.34	0.74
1:C:159:ALA:HB3	1:C:328:GLU:CD	2.11	0.74
1:A:154:PHE:CD1	1:A:154:PHE:C	2.62	0.74
1:C:292:TYR:HB2	1:C:318:SER:O	1.86	0.74
1:A:310:VAL:HA	1:A:321:TRP:O	1.86	0.74
1:A:313:GLU:HG3	1:A:318:SER:HB3	1.69	0.74
1:A:326:VAL:CG1	1:A:331:GLN:HG3	2.17	0.74
1:B:258:ASP:CG	1:B:259:GLY:H	1.95	0.74
1:C:75:VAL:N	1:C:75:VAL:CB	2.51	0.74
1:C:174:GLY:O	1:C:175:CYS:SG	2.45	0.74
1:A:154:PHE:HD1	1:A:155:ASP:H	0.75	0.74
1:B:83:THR:HG22	1:B:84:ARG:N	2.01	0.74
1:B:133:SER:CB	1:B:235:THR:HG22	2.17	0.74
1:C:85:SER:CA	1:C:234:TYR:O	2.36	0.74
1:C:333:VAL:C	1:C:334:LYS:HD3	2.12	0.74
1:A:124:ALA:O	1:A:244:SER:N	2.18	0.74
1:A:135:ARG:HB3	1:A:186:LEU:O	1.88	0.74
1:A:248:ALA:HB2	1:A:265:TRP:CA	2.13	0.74
1:B:130:ARG:HD2	1:B:237:GLN:HB3	1.64	0.74
1:B:149:LYS:HB3	1:B:217:TYR:CD1	2.20	0.74
1:B:174:GLY:O	1:B:175:CYS:SG	2.45	0.74
1:C:76:SER:N	1:C:76:SER:HA	2.01	0.74
1:C:109:ASN:HA	1:C:129:TYR:OH	1.88	0.74
1:C:197:VAL:HG22	1:C:350:ARG:NH2	2.01	0.74
1:A:94:LYS:O	1:A:95:LYS:O	2.06	0.73
1:A:130:ARG:HD2	1:A:237:GLN:HB3	1.63	0.73
1:A:149:LYS:HB3	1:A:217:TYR:CD1	2.20	0.73
1:A:174:GLY:O	1:A:175:CYS:SG	2.45	0.73
1:A:288:LEU:CD1	1:A:290:LEU:HG	2.17	0.73
1:B:288:LEU:CD1	1:B:290:LEU:HG	2.18	0.73
1:C:71:THR:OG1	1:C:87:SER:HB2	1.87	0.73
1:C:315:ALA:O	1:C:317:GLY:N	2.18	0.73
1:A:136:PHE:CD1	1:A:232:VAL:HG22	2.23	0.73
1:A:271:THR:HG21	1:A:275:GLU:OE2	1.87	0.73
1:B:126:TYR:CA	1:B:242:THR:CG2	2.64	0.73
1:B:333:VAL:C	1:B:334:LYS:HD3	2.12	0.73
1:C:75:VAL:C	1:C:75:VAL:CB	2.59	0.73
1:A:86:GLY:CA	1:A:234:TYR:CE1	2.66	0.73
1:B:154:PHE:HD1	1:B:155:ASP:H	0.75	0.73
1:B:94:LYS:O	1:B:95:LYS:O	2.06	0.73
1:B:136:PHE:CD1	1:B:232:VAL:HG22	2.23	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:LYS:HD3	1:B:217:TYR:CE1	2.23	0.73
1:C:159:ALA:C	1:C:328:GLU:OE1	2.31	0.73
1:C:326:VAL:CG1	1:C:331:GLN:HG3	2.17	0.73
1:B:115:THR:O	1:B:116:PHE:CG	2.40	0.73
1:C:94:LYS:O	1:C:95:LYS:O	2.06	0.73
1:C:149:LYS:HE2	1:C:151:ALA:CA	2.19	0.73
1:C:283:THR:OG1	1:C:329:ARG:HG2	1.89	0.73
1:A:253:PHE:CD2	1:A:346:TRP:HZ3	2.07	0.73
1:C:133:SER:CB	1:C:235:THR:HG22	2.17	0.73
1:C:185:ILE:HD12	1:C:186:LEU:CA	2.16	0.73
1:C:297:VAL:O	1:C:298:SER:OG	2.07	0.73
1:A:149:LYS:HD3	1:A:217:TYR:CE1	2.24	0.73
1:A:306:SER:HB3	1:A:325:LYS:HB3	1.69	0.73
1:B:283:THR:OG1	1:B:329:ARG:HG2	1.89	0.73
1:C:241:ARG:N	1:C:241:ARG:HD2	2.03	0.73
1:B:135:ARG:HB3	1:B:186:LEU:O	1.88	0.73
1:B:289:THR:C	1:B:290:LEU:HG	2.14	0.73
1:C:90:ILE:CD1	1:C:232:VAL:HG23	2.19	0.73
1:C:208:ASP:N	1:C:329:ARG:HH21	1.85	0.73
1:A:109:ASN:HA	1:A:129:TYR:OH	1.88	0.73
1:A:258:ASP:CG	1:A:259:GLY:H	1.95	0.73
1:C:135:ARG:HB3	1:C:186:LEU:O	1.88	0.73
1:A:127:GLU:O	1:A:128:LYS:HB2	1.89	0.73
1:C:205:LYS:N	1:C:329:ARG:CZ	2.51	0.73
1:A:90:ILE:CD1	1:A:232:VAL:HG23	2.19	0.72
1:A:288:LEU:CG	1:A:289:THR:N	2.50	0.72
1:B:241:ARG:HD2	1:B:241:ARG:H	1.54	0.72
1:C:149:LYS:HD3	1:C:217:TYR:CE1	2.24	0.72
1:A:252:ASP:OD2	1:A:345:LYS:CE	2.37	0.72
1:B:127:GLU:O	1:B:128:LYS:HB2	1.89	0.72
1:C:95:LYS:HZ1	1:C:225:ALA:N	1.87	0.72
1:C:201:ILE:CD1	1:C:280:PHE:O	2.10	0.72
1:C:313:GLU:HG3	1:C:318:SER:HB3	1.69	0.72
1:A:120:ILE:CD1	1:A:329:ARG:NH2	2.53	0.72
1:A:149:LYS:HE2	1:A:151:ALA:CA	2.19	0.72
1:B:85:SER:CA	1:B:234:TYR:O	2.36	0.72
1:B:109:ASN:HA	1:B:129:TYR:OH	1.88	0.72
1:A:115:THR:O	1:A:116:PHE:CG	2.40	0.72
1:A:241:ARG:HD2	1:A:241:ARG:H	1.54	0.72
1:A:301:GLU:O	1:A:333:VAL:CG1	2.34	0.72
1:B:90:ILE:CD1	1:B:232:VAL:HG23	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:VAL:HG13	1:A:331:GLN:CG	2.20	0.72
1:A:333:VAL:C	1:A:334:LYS:HD3	2.12	0.72
1:B:113:PRO:HB2	1:B:283:THR:O	1.88	0.72
1:B:124:ALA:O	1:B:244:SER:N	2.18	0.72
1:B:253:PHE:CD2	1:B:346:TRP:HZ3	2.07	0.72
1:B:308:PHE:HE2	1:B:310:VAL:CG2	1.92	0.72
1:A:283:THR:OG1	1:A:329:ARG:HG2	1.89	0.72
1:B:132:THR:HG22	1:B:235:THR:O	1.89	0.72
1:C:126:TYR:CA	1:C:242:THR:CG2	2.64	0.72
1:C:200:GLY:O	1:C:282:GLY:CA	2.38	0.72
1:C:201:ILE:HD11	1:C:280:PHE:O	1.88	0.72
1:C:241:ARG:HD2	1:C:241:ARG:H	1.54	0.72
1:B:179:VAL:HG22	1:B:180:PRO:CD	2.19	0.72
1:B:267:LYS:O	1:B:279:HIS:HB2	1.90	0.72
1:B:339:GLU:CA	1:B:340:GLU:N	2.53	0.72
1:A:95:LYS:HZ2	1:A:221:ALA:CA	2.01	0.72
1:B:101:PRO:C	1:B:102:LYS:CG	2.42	0.72
1:C:200:GLY:O	1:C:282:GLY:HA3	1.89	0.72
1:C:339:GLU:CA	1:C:340:GLU:N	2.53	0.72
1:A:169:LEU:HD23	1:A:169:LEU:O	1.89	0.72
1:A:289:THR:C	1:A:290:LEU:HG	2.14	0.72
1:B:104:THR:O	1:B:105:THR:C	2.33	0.72
1:B:113:PRO:C	1:B:115:THR:N	2.43	0.72
1:B:149:LYS:HE2	1:B:151:ALA:CA	2.19	0.72
1:C:253:PHE:CD2	1:C:346:TRP:HZ3	2.07	0.72
1:A:132:THR:HG22	1:A:235:THR:O	1.89	0.72
1:A:179:VAL:HG22	1:A:180:PRO:CD	2.19	0.72
1:C:206:LEU:H	1:C:329:ARG:HH12	1.37	0.72
1:C:208:ASP:N	1:C:329:ARG:NH2	2.38	0.72
1:C:288:LEU:CG	1:C:289:THR:N	2.50	0.72
1:C:295:ALA:CB	1:C:315:ALA:N	2.53	0.72
1:C:326:VAL:HG13	1:C:331:GLN:CG	2.20	0.72
1:B:112:GLU:HG3	1:B:329:ARG:HH22	1.53	0.71
1:C:55:VAL:CG2	1:C:56:THR:H	2.03	0.71
1:C:104:THR:O	1:C:105:THR:C	2.33	0.71
1:C:138:TYR:CG	1:C:184:PHE:CZ	2.62	0.71
1:C:149:LYS:CB	1:C:217:TYR:CE1	2.60	0.71
1:C:308:PHE:CD2	1:C:310:VAL:HG23	2.25	0.71
1:B:308:PHE:CD2	1:B:310:VAL:HG23	2.25	0.71
1:B:326:VAL:HG13	1:B:327:ALA:H	1.54	0.71
1:C:132:THR:HG22	1:C:235:THR:O	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:208:ASP:H	1:C:329:ARG:NH2	1.87	0.71
1:C:290:LEU:HD22	1:C:346:TRP:CB	2.20	0.71
1:A:297:VAL:O	1:A:298:SER:OG	2.07	0.71
1:A:308:PHE:CD2	1:A:310:VAL:HG23	2.25	0.71
1:B:179:VAL:HG21	1:B:181:TRP:HD1	1.55	0.71
1:B:326:VAL:HG13	1:B:331:GLN:CG	2.20	0.71
1:C:258:ASP:CG	1:C:259:GLY:H	1.95	0.71
1:A:242:THR:HG23	1:A:243:GLY:N	2.05	0.71
1:B:242:THR:HG23	1:B:243:GLY:N	2.05	0.71
1:B:252:ASP:OD2	1:B:345:LYS:CE	2.37	0.71
1:C:112:GLU:HA	1:C:284:GLY:CA	2.19	0.71
1:C:267:LYS:O	1:C:279:HIS:HB2	1.90	0.71
1:B:297:VAL:O	1:B:298:SER:OG	2.07	0.71
1:C:127:GLU:O	1:C:128:LYS:HB2	1.89	0.71
1:A:104:THR:O	1:A:105:THR:C	2.33	0.71
1:B:179:VAL:CG2	1:B:181:TRP:HD1	2.03	0.71
1:B:242:THR:HG23	1:B:243:GLY:H	1.56	0.71
1:B:276:HIS:ND1	1:B:277:ASP:N	2.38	0.71
1:C:252:ASP:OD2	1:C:345:LYS:CE	2.37	0.71
1:A:101:PRO:C	1:A:102:LYS:CG	2.42	0.71
1:A:198:ALA:HB1	1:A:200:GLY:C	2.14	0.71
1:A:238:LEU:HD12	1:A:238:LEU:N	2.05	0.71
1:B:169:LEU:HD23	1:B:169:LEU:O	1.90	0.71
1:B:295:ALA:CB	1:B:315:ALA:N	2.53	0.71
1:C:56:THR:HG23	1:C:57:ARG:H	1.56	0.71
1:C:238:LEU:HD12	1:C:238:LEU:N	2.05	0.71
1:C:276:HIS:ND1	1:C:277:ASP:N	2.38	0.71
1:A:295:ALA:CB	1:A:315:ALA:N	2.53	0.71
1:B:238:LEU:HD12	1:B:238:LEU:N	2.05	0.71
1:C:179:VAL:CG2	1:C:181:TRP:HD1	2.03	0.71
1:C:286:PHE:HA	1:C:350:ARG:O	1.91	0.71
1:A:179:VAL:CG2	1:A:181:TRP:HD1	2.03	0.71
1:A:267:LYS:O	1:A:279:HIS:HB2	1.90	0.71
1:B:198:ALA:HB1	1:B:200:GLY:C	2.14	0.71
1:C:289:THR:C	1:C:290:LEU:HG	2.14	0.71
1:B:124:ALA:HB1	1:B:245:THR:CG2	2.20	0.71
1:C:200:GLY:CA	1:C:265:TRP:CG	2.58	0.71
1:A:124:ALA:HB1	1:A:245:THR:CG2	2.20	0.70
1:A:252:ASP:OD1	1:A:253:PHE:N	2.24	0.70
1:B:236:VAL:HG12	1:B:237:GLN:N	2.05	0.70
1:C:116:PHE:O	1:C:120:ILE:HG22	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:179:VAL:HG22	1:C:180:PRO:CD	2.19	0.70
1:C:242:THR:HG23	1:C:243:GLY:N	2.05	0.70
1:B:130:ARG:HD2	1:B:237:GLN:NE2	2.06	0.70
1:B:154:PHE:CD1	1:B:154:PHE:C	2.62	0.70
1:B:86:GLY:CA	1:B:234:TYR:CE1	2.66	0.70
1:B:101:PRO:CG	1:B:217:TYR:CD2	2.75	0.70
1:C:130:ARG:HD2	1:C:237:GLN:NE2	2.06	0.70
1:B:286:PHE:HA	1:B:350:ARG:O	1.91	0.70
1:B:288:LEU:CG	1:B:289:THR:N	2.50	0.70
1:C:137:ARG:O	1:C:230:VAL:HG13	1.91	0.70
1:A:130:ARG:HD2	1:A:237:GLN:NE2	2.06	0.70
1:C:242:THR:HG23	1:C:243:GLY:H	1.56	0.70
1:A:85:SER:CA	1:A:234:TYR:O	2.36	0.70
1:A:236:VAL:HG12	1:A:237:GLN:N	2.05	0.70
1:C:149:LYS:NZ	1:C:170:TYR:CE1	2.52	0.70
1:C:236:VAL:HG12	1:C:237:GLN:N	2.05	0.70
1:A:242:THR:HG23	1:A:243:GLY:H	1.56	0.70
1:C:124:ALA:HB1	1:C:245:THR:CG2	2.20	0.70
1:C:313:GLU:CG	1:C:318:SER:OG	2.40	0.70
1:A:138:TYR:CG	1:A:184:PHE:CZ	2.62	0.70
1:A:300:LEU:C	1:A:308:PHE:HZ	2.00	0.70
1:A:338:THR:OG1	1:A:339:GLU:CB	2.37	0.70
1:B:154:PHE:CE1	1:B:155:ASP:O	2.41	0.70
1:B:313:GLU:CG	1:B:318:SER:OG	2.40	0.70
1:B:326:VAL:HG13	1:B:331:GLN:HG3	1.74	0.70
1:C:101:PRO:CG	1:C:217:TYR:CD2	2.75	0.70
1:C:156:ARG:O	1:C:210:GLY:N	2.25	0.70
1:C:169:LEU:O	1:C:169:LEU:HD23	1.90	0.70
1:A:103:TYR:HE1	1:A:169:LEU:HD12	1.56	0.70
1:A:129:TYR:HA	1:A:237:GLN:O	1.92	0.70
1:C:55:VAL:CG2	1:C:56:THR:N	2.52	0.70
1:B:95:LYS:HZ2	1:B:221:ALA:CA	2.01	0.69
1:C:120:ILE:HD12	1:C:351:ILE:C	2.17	0.69
1:C:159:ALA:HB1	1:C:328:GLU:OE1	1.90	0.69
1:C:200:GLY:H	1:C:265:TRP:HD1	1.36	0.69
1:A:170:TYR:OH	1:A:217:TYR:OH	2.10	0.69
1:A:276:HIS:ND1	1:A:277:ASP:N	2.38	0.69
1:A:295:ALA:H	1:A:316:ALA:HA	0.69	0.69
1:B:156:ARG:O	1:B:210:GLY:N	2.25	0.69
1:A:101:PRO:CG	1:A:217:TYR:CD2	2.75	0.69
1:A:156:ARG:O	1:A:210:GLY:N	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:GLU:CG	1:A:318:SER:OG	2.40	0.69
1:B:122:GLU:O	1:B:122:GLU:HG2	1.93	0.69
1:B:137:ARG:O	1:B:230:VAL:HG13	1.92	0.69
1:C:244:SER:O	1:C:245:THR:CB	2.41	0.69
1:A:137:ARG:O	1:A:230:VAL:HG13	1.91	0.69
1:A:179:VAL:HG21	1:A:181:TRP:HD1	1.56	0.69
1:B:129:TYR:HA	1:B:237:GLN:O	1.92	0.69
1:B:252:ASP:OD1	1:B:253:PHE:N	2.24	0.69
1:C:66:TYR:CZ	1:C:183:GLY:HA3	2.27	0.69
1:C:103:TYR:HE1	1:C:169:LEU:HD12	1.56	0.69
1:C:179:VAL:HG21	1:C:181:TRP:HD1	1.55	0.69
1:A:244:SER:O	1:A:245:THR:CB	2.41	0.69
1:B:170:TYR:OH	1:B:217:TYR:OH	2.11	0.69
1:C:72:GLN:HA	1:C:72:GLN:NE2	2.04	0.69
1:C:166:LEU:O	1:C:167:ALA:C	2.36	0.69
1:C:207:VAL:HG13	1:C:208:ASP:CG	2.18	0.69
1:C:252:ASP:OD1	1:C:253:PHE:N	2.24	0.69
1:C:326:VAL:HG13	1:C:331:GLN:HG3	1.74	0.69
1:A:286:PHE:HA	1:A:350:ARG:O	1.91	0.69
1:A:290:LEU:HD22	1:A:346:TRP:CB	2.20	0.69
1:C:129:TYR:HA	1:C:237:GLN:O	1.92	0.69
1:C:300:LEU:C	1:C:308:PHE:HZ	2.00	0.69
1:C:326:VAL:HG13	1:C:327:ALA:H	1.54	0.69
1:A:125:GLN:C	1:A:242:THR:CG2	2.66	0.69
1:A:289:THR:O	1:A:290:LEU:CB	2.35	0.69
1:B:103:TYR:HE1	1:B:169:LEU:HD12	1.56	0.69
1:B:244:SER:O	1:B:245:THR:CB	2.41	0.69
1:B:112:GLU:CG	1:B:329:ARG:HH22	2.05	0.69
1:B:125:GLN:C	1:B:242:THR:CG2	2.66	0.69
1:B:155:ASP:CB	1:B:172:ILE:HD11	2.23	0.69
1:B:166:LEU:O	1:B:167:ALA:C	2.35	0.69
1:B:172:ILE:O	1:B:173:GLU:C	2.36	0.69
1:B:290:LEU:HD12	1:B:290:LEU:O	1.93	0.69
1:C:80:ASP:HA	1:C:241:ARG:HH22	0.70	0.69
1:C:125:GLN:C	1:C:242:THR:CG2	2.66	0.69
1:C:278:CYS:CA	1:C:333:VAL:O	2.41	0.69
1:C:327:ALA:HB3	1:C:331:GLN:NE2	2.07	0.69
1:C:338:THR:OG1	1:C:339:GLU:CB	2.37	0.69
1:A:290:LEU:HD12	1:A:290:LEU:O	1.93	0.69
1:B:300:LEU:C	1:B:308:PHE:HZ	2.00	0.69
1:C:200:GLY:CA	1:C:265:TRP:CA	2.70	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:289:THR:O	1:C:290:LEU:CB	2.35	0.69
1:A:166:LEU:O	1:A:167:ALA:C	2.36	0.69
1:A:172:ILE:O	1:A:173:GLU:C	2.36	0.69
1:B:169:LEU:HD22	1:B:170:TYR:HD1	1.58	0.69
1:B:173:GLU:HG3	1:B:174:GLY:N	2.08	0.69
1:B:338:THR:OG1	1:B:339:GLU:CB	2.37	0.69
1:B:207:VAL:HG13	1:B:208:ASP:CG	2.18	0.68
1:C:143:PRO:O	1:C:146:THR:HG22	1.93	0.68
1:C:154:PHE:HD1	1:C:155:ASP:H	0.75	0.68
1:C:155:ASP:CB	1:C:172:ILE:HD11	2.23	0.68
1:A:154:PHE:CE1	1:A:155:ASP:O	2.41	0.68
1:B:327:ALA:HB3	1:B:331:GLN:NE2	2.08	0.68
1:C:151:ALA:CA	1:C:177:SER:HB2	2.17	0.68
1:C:172:ILE:O	1:C:173:GLU:C	2.36	0.68
1:A:173:GLU:HG3	1:A:174:GLY:N	2.08	0.68
1:B:170:TYR:CZ	1:B:217:TYR:OH	2.45	0.68
1:A:122:GLU:HG2	1:A:122:GLU:O	1.92	0.68
1:B:124:ALA:O	1:B:243:GLY:HA2	1.93	0.68
1:C:170:TYR:OH	1:C:217:TYR:OH	2.11	0.68
1:A:339:GLU:CA	1:A:340:GLU:N	2.53	0.68
1:C:251:GLY:O	1:C:346:TRP:CH2	2.47	0.68
1:A:124:ALA:O	1:A:243:GLY:HA2	1.93	0.68
1:A:170:TYR:CZ	1:A:217:TYR:OH	2.45	0.68
1:A:251:GLY:O	1:A:346:TRP:CH2	2.47	0.68
1:B:155:ASP:O	1:B:156:ARG:C	2.36	0.68
1:C:127:GLU:O	1:C:128:LYS:CB	2.41	0.68
1:A:230:VAL:HG12	1:A:231:ARG:N	2.09	0.68
1:C:173:GLU:HG3	1:C:174:GLY:N	2.08	0.68
1:C:230:VAL:HG12	1:C:231:ARG:N	2.09	0.68
1:A:207:VAL:HG13	1:A:208:ASP:CG	2.18	0.68
1:A:254:ALA:N	1:A:257:LYS:O	2.27	0.68
1:A:278:CYS:CA	1:A:333:VAL:O	2.41	0.68
1:B:313:GLU:HG3	1:B:318:SER:HB3	1.69	0.68
1:C:83:THR:O	1:C:84:ARG:HG2	1.94	0.68
1:C:125:GLN:C	1:C:242:THR:HG22	2.19	0.68
1:A:155:ASP:O	1:A:156:ARG:C	2.36	0.68
1:A:248:ALA:C	1:A:264:SER:HB3	2.19	0.68
1:B:143:PRO:O	1:B:146:THR:HG22	1.92	0.68
1:C:124:ALA:O	1:C:243:GLY:HA2	1.93	0.68
1:C:149:LYS:HD3	1:C:217:TYR:CZ	2.29	0.68
1:A:156:ARG:O	1:A:209:PHE:C	2.37	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:ARG:HG3	1:A:261:ARG:O	1.94	0.68
1:B:230:VAL:HG12	1:B:231:ARG:N	2.09	0.68
1:B:251:GLY:O	1:B:346:TRP:CH2	2.47	0.68
1:C:68:GLU:CD	1:C:137:ARG:NH2	2.51	0.68
1:C:295:ALA:H	1:C:316:ALA:HA	0.69	0.68
1:A:127:GLU:O	1:A:128:LYS:CB	2.42	0.67
1:B:251:GLY:O	1:B:346:TRP:CZ2	2.48	0.67
1:C:170:TYR:C	1:C:171:ASN:HD22	2.02	0.67
1:C:290:LEU:HD12	1:C:290:LEU:O	1.93	0.67
1:A:125:GLN:C	1:A:242:THR:HG22	2.19	0.67
1:A:169:LEU:HD22	1:A:170:TYR:HD1	1.58	0.67
1:A:269:LYS:HE2	1:A:270:GLY:O	1.94	0.67
1:B:127:GLU:O	1:B:128:LYS:CB	2.42	0.67
1:B:291:PHE:CZ	1:B:335:MET:HE1	2.30	0.67
1:C:156:ARG:O	1:C:209:PHE:C	2.37	0.67
1:A:291:PHE:C	1:A:292:TYR:CA	2.67	0.67
1:C:169:LEU:HD22	1:C:170:TYR:HD1	1.58	0.67
1:B:340:GLU:O	1:B:342:PRO:CD	2.43	0.67
1:C:251:GLY:O	1:C:346:TRP:CZ2	2.47	0.67
1:B:107:VAL:HB	1:B:329:ARG:HH12	1.58	0.67
1:C:155:ASP:O	1:C:156:ARG:C	2.36	0.67
1:B:253:PHE:CE2	1:B:346:TRP:CZ3	2.83	0.67
1:B:278:CYS:CA	1:B:333:VAL:O	2.41	0.67
1:C:340:GLU:O	1:C:342:PRO:CD	2.43	0.67
1:A:83:THR:O	1:A:84:ARG:HG2	1.94	0.67
1:A:326:VAL:HG13	1:A:331:GLN:HG3	1.74	0.67
1:A:327:ALA:HB3	1:A:331:GLN:NE2	2.08	0.67
1:B:149:LYS:HD3	1:B:217:TYR:CZ	2.29	0.67
1:B:286:PHE:CA	1:B:351:ILE:HG21	2.25	0.67
1:C:198:ALA:HB1	1:C:200:GLY:C	2.14	0.67
1:A:143:PRO:O	1:A:146:THR:HG22	1.93	0.67
1:A:170:TYR:C	1:A:171:ASN:HD22	2.02	0.67
1:B:156:ARG:O	1:B:209:PHE:C	2.37	0.67
1:C:95:LYS:O	1:C:96:ASN:HB2	1.95	0.67
1:C:135:ARG:HG3	1:C:233:GLU:CB	2.23	0.67
1:C:269:LYS:HE2	1:C:270:GLY:O	1.94	0.67
1:A:340:GLU:O	1:A:342:PRO:CD	2.43	0.67
1:B:254:ALA:N	1:B:257:LYS:O	2.27	0.67
1:A:96:ASN:ND2	1:A:102:LYS:HD3	2.10	0.67
1:A:126:TYR:O	1:A:242:THR:HG21	1.95	0.67
1:B:83:THR:O	1:B:84:ARG:HG2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:ALA:C	1:B:263:VAL:O	2.38	0.67
1:B:269:LYS:HE2	1:B:270:GLY:O	1.94	0.67
1:C:122:GLU:O	1:C:122:GLU:HG2	1.93	0.67
1:C:163:PRO:HA	1:C:164:ASN:ND2	2.10	0.67
1:A:121:LYS:HD3	1:A:350:ARG:HH22	1.61	0.66
1:A:149:LYS:HD3	1:A:217:TYR:CZ	2.29	0.66
1:C:185:ILE:HD13	1:C:186:LEU:H	1.53	0.66
1:C:253:PHE:CE2	1:C:346:TRP:CZ3	2.83	0.66
1:A:136:PHE:HE1	1:A:232:VAL:HG22	1.59	0.66
1:A:253:PHE:CE2	1:A:346:TRP:CZ3	2.83	0.66
1:C:186:LEU:HD23	1:C:186:LEU:C	2.20	0.66
1:A:136:PHE:CE1	1:A:212:LEU:HD22	2.31	0.66
1:A:237:GLN:C	1:A:238:LEU:HD12	2.21	0.66
1:B:96:ASN:ND2	1:B:102:LYS:HD3	2.10	0.66
1:C:95:LYS:HZ2	1:C:221:ALA:CA	2.04	0.66
1:C:254:ALA:N	1:C:257:LYS:O	2.27	0.66
1:A:300:LEU:CG	1:A:308:PHE:CZ	2.78	0.66
1:B:109:ASN:HB2	1:B:208:ASP:HB3	1.77	0.66
1:B:136:PHE:CE1	1:B:212:LEU:HD22	2.31	0.66
1:B:237:GLN:C	1:B:238:LEU:HD12	2.21	0.66
1:B:290:LEU:HD22	1:B:346:TRP:CB	2.20	0.66
1:B:300:LEU:C	1:B:308:PHE:CZ	2.74	0.66
1:C:201:ILE:HG21	1:C:265:TRP:C	2.20	0.66
1:C:291:PHE:CZ	1:C:335:MET:HE1	2.30	0.66
1:A:268:THR:HG23	1:A:268:THR:O	1.96	0.66
1:B:116:PHE:O	1:B:120:ILE:HG22	1.89	0.66
1:B:125:GLN:C	1:B:242:THR:HG22	2.19	0.66
1:C:64:LEU:HD12	1:C:65:ALA:H	1.60	0.66
1:C:126:TYR:O	1:C:242:THR:HG21	1.95	0.66
1:C:130:ARG:HD2	1:C:237:GLN:HB3	1.64	0.66
1:C:170:TYR:CZ	1:C:217:TYR:OH	2.45	0.66
1:A:291:PHE:CZ	1:A:335:MET:HE1	2.30	0.66
1:B:163:PRO:HA	1:B:164:ASN:ND2	2.10	0.66
1:C:136:PHE:CE1	1:C:212:LEU:HD22	2.31	0.66
1:C:199:ASP:HA	1:C:265:TRP:NE1	2.09	0.66
1:C:261:ARG:HG3	1:C:261:ARG:O	1.94	0.66
1:C:286:PHE:CA	1:C:351:ILE:HG21	2.25	0.66
1:C:308:PHE:HE2	1:C:310:VAL:CG2	1.92	0.66
1:A:109:ASN:HB2	1:A:208:ASP:HB3	1.77	0.66
1:B:186:LEU:HD23	1:B:186:LEU:C	2.20	0.66
1:B:261:ARG:O	1:B:261:ARG:HG3	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:PRO:C	1:C:102:LYS:CG	2.42	0.66
1:B:236:VAL:HG12	1:B:238:LEU:CD1	2.26	0.66
1:B:291:PHE:C	1:B:292:TYR:CA	2.67	0.66
1:C:300:LEU:C	1:C:308:PHE:CZ	2.74	0.66
1:A:144:SER:C	1:A:146:THR:N	2.54	0.66
1:A:297:VAL:CB	1:A:336:VAL:O	2.36	0.66
1:A:300:LEU:C	1:A:308:PHE:CZ	2.74	0.66
1:A:326:VAL:HG13	1:A:327:ALA:H	1.54	0.66
1:B:124:ALA:CB	1:B:245:THR:CG2	2.74	0.66
1:B:144:SER:C	1:B:146:THR:N	2.54	0.66
1:A:116:PHE:O	1:A:120:ILE:HG22	1.90	0.66
1:A:124:ALA:CB	1:A:245:THR:CG2	2.74	0.66
1:A:251:GLY:O	1:A:346:TRP:CZ2	2.47	0.66
1:B:126:TYR:O	1:B:242:THR:HG21	1.95	0.66
1:C:85:SER:C	1:C:234:TYR:CE1	2.74	0.66
1:C:236:VAL:HG12	1:C:238:LEU:CD1	2.26	0.66
1:C:268:THR:HG23	1:C:268:THR:O	1.96	0.66
1:A:95:LYS:O	1:A:96:ASN:HB2	1.95	0.65
1:A:249:GLN:HB2	1:A:265:TRP:CZ3	2.30	0.65
1:A:290:LEU:CD1	1:A:290:LEU:C	2.69	0.65
1:B:170:TYR:C	1:B:171:ASN:HD22	2.02	0.65
1:B:312:GLY:HA3	1:B:320:GLN:HG2	1.78	0.65
1:C:124:ALA:CB	1:C:245:THR:CG2	2.74	0.65
1:A:85:SER:C	1:A:234:TYR:CE1	2.74	0.65
1:C:297:VAL:CB	1:C:336:VAL:O	2.36	0.65
1:A:163:PRO:HA	1:A:164:ASN:ND2	2.10	0.65
1:B:82:ILE:O	1:B:83:THR:N	2.29	0.65
1:B:290:LEU:C	1:B:290:LEU:CD1	2.69	0.65
1:B:295:ALA:H	1:B:316:ALA:HA	0.69	0.65
1:C:68:GLU:CG	1:C:137:ARG:NH2	2.59	0.65
1:C:200:GLY:C	1:C:282:GLY:HA2	2.16	0.65
1:C:306:SER:O	1:C:307:ASP:C	2.40	0.65
1:A:286:PHE:CA	1:A:351:ILE:HG21	2.25	0.65
1:B:85:SER:C	1:B:234:TYR:CE1	2.74	0.65
1:B:306:SER:O	1:B:307:ASP:C	2.40	0.65
1:C:290:LEU:CD1	1:C:290:LEU:C	2.69	0.65
1:C:326:VAL:HG12	1:C:327:ALA:CA	2.27	0.65
1:A:264:SER:C	1:A:265:TRP:HA	2.22	0.65
1:B:119:LEU:CD2	1:B:234:TYR:HE2	2.10	0.65
1:B:249:GLN:HB2	1:B:265:TRP:CZ3	2.31	0.65
1:C:66:TYR:OH	1:C:183:GLY:HA3	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:GLN:O	1:C:119:LEU:HB2	1.97	0.65
1:A:121:LYS:NZ	1:A:350:ARG:NH1	2.44	0.65
1:A:205:LYS:HD2	1:A:205:LYS:N	2.12	0.65
1:A:306:SER:O	1:A:307:ASP:C	2.40	0.65
1:B:130:ARG:NH1	1:B:237:GLN:HA	2.10	0.65
1:B:149:LYS:NZ	1:B:170:TYR:CE1	2.52	0.65
1:B:205:LYS:HD2	1:B:205:LYS:N	2.12	0.65
1:A:236:VAL:HG12	1:A:238:LEU:CD1	2.26	0.65
1:C:291:PHE:C	1:C:292:TYR:CA	2.67	0.65
1:C:306:SER:O	1:C:307:ASP:O	2.14	0.65
1:A:119:LEU:CD2	1:A:234:TYR:HE2	2.10	0.65
1:A:130:ARG:HD2	1:A:237:GLN:CG	2.27	0.65
1:A:186:LEU:HD23	1:A:186:LEU:C	2.20	0.65
1:B:268:THR:HG23	1:B:268:THR:O	1.96	0.65
1:C:96:ASN:ND2	1:C:102:LYS:HD3	2.10	0.65
1:C:200:GLY:HA2	1:C:265:TRP:CA	2.26	0.65
1:C:237:GLN:C	1:C:238:LEU:HD12	2.21	0.65
1:C:309:SER:O	1:C:321:TRP:O	2.15	0.65
1:A:312:GLY:HA3	1:A:320:GLN:HG2	1.78	0.65
1:B:296:PRO:HG3	1:B:337:THR:CB	2.27	0.65
1:B:300:LEU:CG	1:B:308:PHE:CZ	2.78	0.65
1:B:309:SER:O	1:B:321:TRP:O	2.15	0.65
1:C:109:ASN:HB2	1:C:208:ASP:HB3	1.77	0.65
1:C:153:ALA:HA	1:C:186:LEU:HD11	1.78	0.65
1:A:306:SER:O	1:A:307:ASP:O	2.14	0.64
1:A:326:VAL:HG12	1:A:327:ALA:CA	2.27	0.64
1:A:342:PRO:C	1:A:343:LYS:HD3	2.23	0.64
1:B:196:PHE:O	1:B:207:VAL:HG23	1.97	0.64
1:B:306:SER:O	1:B:307:ASP:O	2.14	0.64
1:C:169:LEU:C	1:C:169:LEU:CD2	2.70	0.64
1:C:300:LEU:CG	1:C:308:PHE:CZ	2.78	0.64
1:C:306:SER:HB3	1:C:325:LYS:CB	2.27	0.64
1:A:253:PHE:CD2	1:A:346:TRP:CZ3	2.85	0.64
1:A:274:TRP:NE1	1:A:340:GLU:OE1	2.31	0.64
1:B:95:LYS:O	1:B:96:ASN:HB2	1.95	0.64
1:B:96:ASN:C	1:B:98:ASP:N	2.55	0.64
1:B:277:ASP:CG	1:B:334:LYS:HZ3	2.05	0.64
1:C:68:GLU:OE2	1:C:139:SER:OG	2.14	0.64
1:C:144:SER:C	1:C:146:THR:N	2.54	0.64
1:A:118:GLN:O	1:A:119:LEU:HB2	1.97	0.64
1:B:118:GLN:O	1:B:119:LEU:HB2	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:ALA:HA	1:B:186:LEU:HD11	1.78	0.64
1:B:253:PHE:CD2	1:B:346:TRP:CZ3	2.85	0.64
1:B:297:VAL:CB	1:B:336:VAL:O	2.36	0.64
1:C:264:SER:C	1:C:265:TRP:HA	2.21	0.64
1:A:153:ALA:HA	1:A:186:LEU:HD11	1.78	0.64
1:C:196:PHE:O	1:C:207:VAL:HG23	1.97	0.64
1:A:196:PHE:O	1:A:207:VAL:HG23	1.97	0.64
1:A:135:ARG:HG3	1:A:233:GLU:CB	2.23	0.64
1:B:136:PHE:HE1	1:B:232:VAL:HG22	1.59	0.64
1:B:309:SER:O	1:B:322:ALA:CB	2.46	0.64
1:C:112:GLU:OE2	1:C:283:THR:HG22	1.97	0.64
1:A:82:ILE:O	1:A:83:THR:N	2.29	0.64
1:B:264:SER:C	1:B:265:TRP:HA	2.22	0.64
1:B:306:SER:HB3	1:B:325:LYS:CB	2.27	0.64
1:C:152:LEU:CD2	1:C:186:LEU:HD13	2.25	0.64
1:C:154:PHE:CZ	1:C:156:ARG:HA	2.33	0.64
1:C:309:SER:O	1:C:322:ALA:CB	2.46	0.64
1:A:152:LEU:CD2	1:A:186:LEU:HD13	2.25	0.64
1:C:253:PHE:CD2	1:C:346:TRP:CZ3	2.85	0.64
1:C:327:ALA:HB2	1:C:331:GLN:OE1	1.96	0.64
1:B:248:ALA:HB3	1:B:249:GLN:CB	2.28	0.64
1:C:163:PRO:HG3	1:C:168:SER:HB3	1.80	0.64
1:C:246:SER:O	1:C:349:LEU:C	2.40	0.64
1:C:249:GLN:O	1:C:347:GLN:HA	1.98	0.64
1:A:138:TYR:O	1:A:139:SER:O	2.15	0.63
1:A:155:ASP:CB	1:A:172:ILE:HD11	2.23	0.63
1:B:169:LEU:C	1:B:169:LEU:CD2	2.70	0.63
1:C:61:PRO:HD2	1:C:181:TRP:CZ3	2.33	0.63
1:C:199:ASP:CA	1:C:265:TRP:NE1	2.61	0.63
1:C:205:LYS:HD2	1:C:205:LYS:N	2.12	0.63
1:C:206:LEU:O	1:C:206:LEU:CD1	2.45	0.63
1:C:249:GLN:HB2	1:C:265:TRP:CZ3	2.30	0.63
1:A:151:ALA:CA	1:A:177:SER:HB2	2.17	0.63
1:C:136:PHE:HE1	1:C:232:VAL:HG22	1.59	0.63
1:C:246:SER:O	1:C:349:LEU:CA	2.42	0.63
1:B:138:TYR:O	1:B:139:SER:O	2.15	0.63
1:C:312:GLY:HA3	1:C:320:GLN:HG2	1.78	0.63
1:A:306:SER:HB3	1:A:325:LYS:CB	2.27	0.63
1:A:309:SER:O	1:A:321:TRP:O	2.15	0.63
1:B:152:LEU:CD2	1:B:186:LEU:HD13	2.25	0.63
1:C:154:PHE:CE1	1:C:155:ASP:O	2.41	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ARG:O	1:A:230:VAL:HG22	1.98	0.63
1:A:249:GLN:O	1:A:347:GLN:HA	1.98	0.63
1:B:249:GLN:O	1:B:347:GLN:HA	1.98	0.63
1:A:135:ARG:CB	1:A:186:LEU:O	2.47	0.63
1:A:154:PHE:CZ	1:A:156:ARG:HA	2.33	0.63
1:B:109:ASN:ND2	1:B:197:VAL:HG23	2.14	0.63
1:B:135:ARG:CB	1:B:186:LEU:O	2.47	0.63
1:B:206:LEU:O	1:B:206:LEU:CD1	2.45	0.63
1:B:292:TYR:CB	1:B:318:SER:O	2.47	0.63
1:C:83:THR:CG2	1:C:84:ARG:H	2.08	0.63
1:C:86:GLY:N	1:C:234:TYR:O	2.31	0.63
1:A:292:TYR:CB	1:A:318:SER:O	2.47	0.63
1:A:309:SER:O	1:A:322:ALA:CB	2.46	0.63
1:B:154:PHE:CZ	1:B:156:ARG:HA	2.33	0.63
1:C:207:VAL:CG1	1:C:329:ARG:HE	2.12	0.63
1:C:213:ILE:C	1:C:214:MET:HG3	2.24	0.63
1:B:86:GLY:N	1:B:234:TYR:O	2.31	0.63
1:B:137:ARG:O	1:B:230:VAL:HG22	1.98	0.63
1:B:154:PHE:CE1	1:B:156:ARG:N	2.66	0.63
1:B:185:ILE:HD13	1:B:186:LEU:H	1.53	0.63
1:C:154:PHE:CE1	1:C:156:ARG:N	2.66	0.63
1:A:169:LEU:C	1:A:169:LEU:CD2	2.70	0.63
1:A:206:LEU:O	1:A:206:LEU:CD1	2.45	0.63
1:B:326:VAL:HG12	1:B:327:ALA:CA	2.27	0.63
1:B:342:PRO:C	1:B:343:LYS:HD3	2.23	0.63
1:C:82:ILE:O	1:C:83:THR:N	2.29	0.63
1:C:119:LEU:CD2	1:C:234:TYR:HE2	2.10	0.63
1:B:166:LEU:O	1:B:168:SER:N	2.32	0.62
1:B:274:TRP:NE1	1:B:340:GLU:OE1	2.31	0.62
1:B:296:PRO:HG3	1:B:337:THR:HB	1.81	0.62
1:C:135:ARG:CB	1:C:186:LEU:O	2.47	0.62
1:A:83:THR:CG2	1:A:84:ARG:H	2.08	0.62
1:A:86:GLY:N	1:A:234:TYR:O	2.31	0.62
1:A:166:LEU:O	1:A:168:SER:N	2.32	0.62
1:B:83:THR:HG23	1:B:236:VAL:O	2.00	0.62
1:B:163:PRO:HG3	1:B:168:SER:HB3	1.80	0.62
1:C:68:GLU:CG	1:C:137:ARG:HH22	2.12	0.62
1:C:137:ARG:O	1:C:230:VAL:HG22	1.98	0.62
1:C:166:LEU:O	1:C:168:SER:N	2.32	0.62
1:C:296:PRO:HG3	1:C:337:THR:HB	1.81	0.62
1:C:342:PRO:C	1:C:343:LYS:HD3	2.23	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:THR:CG2	1:B:84:ARG:H	2.08	0.62
1:B:112:GLU:O	1:B:113:PRO:C	2.41	0.62
1:C:55:VAL:HG22	1:C:56:THR:H	1.60	0.62
1:C:82:ILE:HG23	1:C:83:THR:N	2.15	0.62
1:C:130:ARG:NH1	1:C:237:GLN:HA	2.10	0.62
1:C:206:LEU:N	1:C:329:ARG:HH12	1.96	0.62
1:C:231:ARG:HG3	1:C:232:VAL:H	1.63	0.62
1:A:83:THR:HG23	1:A:236:VAL:O	2.00	0.62
1:A:248:ALA:HB1	1:A:264:SER:HG	1.54	0.62
1:B:213:ILE:O	1:B:214:MET:HG3	2.00	0.62
1:C:292:TYR:CB	1:C:318:SER:O	2.47	0.62
1:B:82:ILE:HG23	1:B:83:THR:N	2.15	0.62
1:B:135:ARG:HG3	1:B:233:GLU:CB	2.23	0.62
1:C:163:PRO:C	1:C:164:ASN:ND2	2.44	0.62
1:A:136:PHE:CE2	1:A:212:LEU:HD11	2.35	0.62
1:C:136:PHE:CE2	1:C:212:LEU:HD11	2.35	0.62
1:C:157:ASP:OD1	1:C:157:ASP:O	2.18	0.62
1:A:124:ALA:HB1	1:A:244:SER:O	2.00	0.62
1:A:157:ASP:OD1	1:A:157:ASP:O	2.18	0.62
1:C:109:ASN:ND2	1:C:197:VAL:HG23	2.14	0.62
1:C:159:ALA:HB3	1:C:328:GLU:HG3	1.72	0.62
1:A:109:ASN:ND2	1:A:197:VAL:HG23	2.14	0.62
1:A:163:PRO:HG3	1:A:168:SER:HB3	1.80	0.62
1:A:308:PHE:HE2	1:A:310:VAL:CG2	1.92	0.62
1:C:112:GLU:O	1:C:114:GLY:N	2.33	0.62
1:A:112:GLU:O	1:A:114:GLY:N	2.33	0.62
1:A:154:PHE:CE1	1:A:156:ARG:N	2.66	0.62
1:B:136:PHE:CE2	1:B:212:LEU:HD11	2.35	0.62
1:B:112:GLU:O	1:B:114:GLY:N	2.33	0.61
1:C:83:THR:HG23	1:C:236:VAL:O	2.00	0.61
1:C:124:ALA:HB1	1:C:244:SER:O	2.00	0.61
1:C:236:VAL:CG1	1:C:237:GLN:N	2.62	0.61
1:A:124:ALA:HB2	1:A:245:THR:HG21	1.82	0.61
1:A:154:PHE:CD1	1:A:155:ASP:C	2.78	0.61
1:A:213:ILE:C	1:A:214:MET:HG3	2.24	0.61
1:B:124:ALA:HB2	1:B:245:THR:HG21	1.82	0.61
1:B:188:VAL:HG23	1:B:188:VAL:O	1.99	0.61
1:B:236:VAL:CG1	1:B:237:GLN:N	2.62	0.61
1:C:98:ASP:OD1	1:C:99:THR:N	2.33	0.61
1:C:154:PHE:CD1	1:C:155:ASP:C	2.78	0.61
1:A:120:ILE:CD1	1:A:329:ARG:HH21	2.13	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ILE:HD13	1:A:186:LEU:H	1.53	0.61
1:B:124:ALA:HB1	1:B:244:SER:O	2.00	0.61
1:B:157:ASP:O	1:B:157:ASP:OD1	2.18	0.61
1:A:82:ILE:HG23	1:A:83:THR:N	2.15	0.61
1:A:83:THR:HG23	1:A:130:ARG:NH1	2.15	0.61
1:A:130:ARG:NH1	1:A:237:GLN:HA	2.10	0.61
1:A:236:VAL:CG1	1:A:237:GLN:N	2.62	0.61
1:B:130:ARG:HB3	1:B:237:GLN:H	1.66	0.61
1:B:290:LEU:HD12	1:B:290:LEU:C	2.26	0.61
1:C:111:SER:N	1:C:350:ARG:NH2	2.45	0.61
1:A:136:PHE:CE2	1:A:212:LEU:CD1	2.84	0.61
1:A:290:LEU:HD12	1:A:290:LEU:C	2.26	0.61
1:A:296:PRO:HG3	1:A:337:THR:HB	1.81	0.61
1:B:134:LEU:HD23	1:B:188:VAL:CG2	2.31	0.61
1:B:169:LEU:HD22	1:B:170:TYR:CD1	2.36	0.61
1:A:112:GLU:O	1:A:113:PRO:C	2.41	0.61
1:A:130:ARG:HB3	1:A:237:GLN:H	1.66	0.61
1:C:188:VAL:HG23	1:C:188:VAL:O	1.99	0.61
1:C:213:ILE:O	1:C:214:MET:HG3	2.00	0.61
1:A:188:VAL:HG23	1:A:188:VAL:O	1.99	0.61
1:C:136:PHE:CE2	1:C:212:LEU:CD1	2.84	0.61
1:B:83:THR:HG23	1:B:130:ARG:NH1	2.15	0.61
1:B:156:ARG:NH1	1:B:173:GLU:OE1	2.34	0.61
1:A:213:ILE:O	1:A:214:MET:HG3	2.00	0.61
1:A:291:PHE:HB2	1:A:346:TRP:CB	2.29	0.61
1:B:311:LEU:HD12	1:B:311:LEU:N	2.16	0.61
1:C:120:ILE:HD12	1:C:351:ILE:O	2.01	0.61
1:C:130:ARG:HD2	1:C:237:GLN:CG	2.27	0.61
1:A:311:LEU:HD12	1:A:311:LEU:N	2.16	0.61
1:B:213:ILE:C	1:B:214:MET:HG3	2.24	0.61
1:C:274:TRP:NE1	1:C:340:GLU:OE1	2.31	0.61
1:C:286:PHE:CD2	1:C:350:ARG:HA	2.35	0.61
1:A:286:PHE:CD2	1:A:350:ARG:HA	2.35	0.60
1:B:136:PHE:CE2	1:B:212:LEU:CD1	2.84	0.60
1:B:154:PHE:CD1	1:B:155:ASP:C	2.78	0.60
1:C:95:LYS:NZ	1:C:221:ALA:CB	2.64	0.60
1:A:105:THR:HG1	1:A:211:LYS:HD3	0.78	0.60
1:A:258:ASP:CG	1:A:259:GLY:N	2.58	0.60
1:A:277:ASP:CG	1:A:334:LYS:HZ3	2.09	0.60
1:A:338:THR:HG1	1:A:339:GLU:HB2	1.64	0.60
1:B:231:ARG:HG3	1:B:232:VAL:H	1.63	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:TYR:O	1:C:139:SER:O	2.15	0.60
1:C:105:THR:HG1	1:C:211:LYS:HD3	0.79	0.60
1:C:109:ASN:ND2	1:C:350:ARG:HH21	1.99	0.60
1:C:124:ALA:HB2	1:C:245:THR:HG21	1.82	0.60
1:C:311:LEU:HD12	1:C:311:LEU:N	2.16	0.60
1:B:129:TYR:CB	1:B:237:GLN:O	2.49	0.60
1:B:162:PRO:C	1:B:163:PRO:O	2.42	0.60
1:C:314:ALA:O	1:C:315:ALA:HB2	2.01	0.60
1:A:129:TYR:CB	1:A:237:GLN:O	2.49	0.60
1:A:217:TYR:CD1	1:A:217:TYR:N	2.69	0.60
1:B:130:ARG:CB	1:B:237:GLN:CB	2.68	0.60
1:B:136:PHE:CD2	1:B:212:LEU:HD21	2.36	0.60
1:B:286:PHE:CD2	1:B:350:ARG:HA	2.35	0.60
1:C:156:ARG:NH1	1:C:173:GLU:OE1	2.34	0.60
1:C:201:ILE:CG2	1:C:265:TRP:CA	2.80	0.60
1:A:156:ARG:NH1	1:A:173:GLU:OE1	2.34	0.60
1:A:162:PRO:C	1:A:163:PRO:O	2.42	0.60
1:A:274:TRP:CD1	1:A:339:GLU:C	2.80	0.60
1:A:120:ILE:O	1:A:120:ILE:CG1	2.50	0.60
1:A:134:LEU:HD23	1:A:188:VAL:CG2	2.31	0.60
1:A:269:LYS:CG	1:A:270:GLY:N	2.58	0.60
1:B:130:ARG:HD2	1:B:237:GLN:CG	2.27	0.60
1:B:163:PRO:C	1:B:164:ASN:ND2	2.44	0.60
1:B:327:ALA:HB2	1:B:331:GLN:OE1	1.96	0.60
1:C:200:GLY:HA3	1:C:201:ILE:HG22	1.83	0.60
1:A:136:PHE:CD2	1:A:212:LEU:HD21	2.37	0.60
1:B:95:LYS:NZ	1:B:221:ALA:CB	2.64	0.60
1:B:120:ILE:O	1:B:120:ILE:CG1	2.50	0.60
1:B:179:VAL:HG21	1:B:181:TRP:CD1	2.36	0.60
1:B:217:TYR:CD1	1:B:217:TYR:N	2.69	0.60
1:C:130:ARG:CB	1:C:237:GLN:CB	2.68	0.60
1:C:134:LEU:HD23	1:C:188:VAL:CG2	2.31	0.60
1:C:169:LEU:HD22	1:C:170:TYR:CD1	2.36	0.60
1:A:179:VAL:HG21	1:A:181:TRP:CD1	2.37	0.60
1:B:149:LYS:CD	1:B:177:SER:OG	2.50	0.60
1:C:83:THR:HG23	1:C:130:ARG:NH1	2.15	0.60
1:C:290:LEU:HD12	1:C:290:LEU:C	2.26	0.60
1:A:95:LYS:NZ	1:A:221:ALA:CB	2.64	0.60
1:A:169:LEU:HD22	1:A:170:TYR:CD1	2.36	0.60
1:A:314:ALA:O	1:A:315:ALA:HB2	2.01	0.59
1:B:98:ASP:OD1	1:B:99:THR:N	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:PHE:CD2	1:C:212:LEU:HD21	2.37	0.59
1:C:274:TRP:CD1	1:C:339:GLU:C	2.80	0.59
1:B:126:TYR:C	1:B:242:THR:CG2	2.75	0.59
1:B:163:PRO:CB	1:B:164:ASN:HD22	2.15	0.59
1:C:96:ASN:C	1:C:98:ASP:N	2.55	0.59
1:C:138:TYR:HD2	1:C:184:PHE:CE1	2.16	0.59
1:A:126:TYR:C	1:A:242:THR:CG2	2.75	0.59
1:A:277:ASP:HA	1:A:334:LYS:CE	2.32	0.59
1:C:97:THR:CA	1:C:218:GLY:O	2.50	0.59
1:C:112:GLU:O	1:C:113:PRO:C	2.41	0.59
1:C:129:TYR:CB	1:C:237:GLN:O	2.49	0.59
1:C:163:PRO:HB2	1:C:165:ASP:H	1.67	0.59
1:C:277:ASP:HA	1:C:334:LYS:CE	2.32	0.59
1:A:97:THR:CA	1:A:218:GLY:O	2.50	0.59
1:A:130:ARG:CB	1:A:237:GLN:CB	2.68	0.59
1:A:163:PRO:CB	1:A:164:ASN:HD22	2.15	0.59
1:A:327:ALA:HB2	1:A:331:GLN:OE1	1.96	0.59
1:B:304:ASP:CG	1:B:332:GLY:H	2.11	0.59
1:C:258:ASP:CG	1:C:259:GLY:N	2.58	0.59
1:A:163:PRO:HB2	1:A:165:ASP:H	1.66	0.59
1:A:203:ASP:O	1:A:205:LYS:N	2.34	0.59
1:B:163:PRO:HB2	1:B:165:ASP:H	1.67	0.59
1:C:203:ASP:O	1:C:205:LYS:N	2.35	0.59
1:C:206:LEU:N	1:C:329:ARG:NH1	2.48	0.59
1:A:163:PRO:C	1:A:164:ASN:ND2	2.44	0.59
1:A:231:ARG:HG3	1:A:232:VAL:H	1.63	0.59
1:A:248:ALA:N	1:A:264:SER:O	2.36	0.59
1:A:307:ASP:O	1:A:323:GLY:O	2.21	0.59
1:B:97:THR:CA	1:B:218:GLY:O	2.50	0.59
1:C:95:LYS:HZ1	1:C:221:ALA:CA	2.13	0.59
1:C:162:PRO:C	1:C:163:PRO:O	2.42	0.59
1:A:98:ASP:OD1	1:A:99:THR:N	2.33	0.59
1:A:138:TYR:HE2	1:A:180:PRO:HA	1.68	0.59
1:A:207:VAL:HG13	1:A:208:ASP:OD2	2.03	0.59
1:C:230:VAL:HG12	1:C:231:ARG:H	1.68	0.59
1:B:207:VAL:HG13	1:B:208:ASP:OD2	2.03	0.59
1:B:300:LEU:HB3	1:B:310:VAL:HG21	1.84	0.59
1:B:336:VAL:HG13	1:B:336:VAL:O	2.03	0.59
1:C:120:ILE:O	1:C:120:ILE:CG1	2.50	0.59
1:C:154:PHE:HE1	1:C:155:ASP:C	1.95	0.59
1:A:200:GLY:HA3	1:A:201:ILE:HG22	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:TRP:CD1	1:B:339:GLU:C	2.80	0.59
1:B:300:LEU:HD11	1:B:333:VAL:HG11	1.85	0.59
1:B:307:ASP:O	1:B:323:GLY:O	2.21	0.59
1:C:113:PRO:C	1:C:115:THR:N	2.43	0.59
1:C:126:TYR:C	1:C:242:THR:CG2	2.75	0.59
1:C:163:PRO:CB	1:C:164:ASN:HD22	2.15	0.59
1:A:265:TRP:CH2	1:A:348:ALA:O	2.52	0.58
1:C:304:ASP:CG	1:C:332:GLY:H	2.11	0.58
1:C:307:ASP:O	1:C:323:GLY:O	2.21	0.58
1:A:304:ASP:CG	1:A:332:GLY:H	2.11	0.58
1:B:113:PRO:CB	1:B:283:THR:O	2.51	0.58
1:B:179:VAL:HG13	1:B:181:TRP:CD1	2.38	0.58
1:B:200:GLY:HA3	1:B:201:ILE:HG22	1.83	0.58
1:B:203:ASP:O	1:B:205:LYS:N	2.34	0.58
1:B:258:ASP:CG	1:B:259:GLY:N	2.58	0.58
1:C:130:ARG:HB3	1:C:237:GLN:H	1.66	0.58
1:A:179:VAL:HG13	1:A:181:TRP:CD1	2.38	0.58
1:A:336:VAL:HG13	1:A:336:VAL:O	2.03	0.58
1:C:85:SER:C	1:C:234:TYR:CD1	2.82	0.58
1:C:202:SER:HA	1:C:281:LEU:HG	1.85	0.58
1:A:113:PRO:C	1:A:115:THR:N	2.43	0.58
1:A:179:VAL:CG1	1:A:181:TRP:HD1	2.14	0.58
1:A:230:VAL:HG12	1:A:231:ARG:H	1.68	0.58
1:A:300:LEU:HB3	1:A:310:VAL:HG21	1.84	0.58
1:B:230:VAL:HG12	1:B:231:ARG:H	1.68	0.58
1:B:138:TYR:HE2	1:B:180:PRO:HA	1.68	0.58
1:B:227:LEU:H	1:B:227:LEU:CD1	2.17	0.58
1:B:277:ASP:HA	1:B:334:LYS:CE	2.32	0.58
1:B:315:ALA:HA	1:B:318:SER:HB2	1.84	0.58
1:C:113:PRO:HD2	1:C:285:ASN:N	2.19	0.58
1:C:179:VAL:HG21	1:C:181:TRP:CD1	2.36	0.58
1:C:291:PHE:HB2	1:C:346:TRP:CB	2.29	0.58
1:C:300:LEU:HB3	1:C:310:VAL:HG21	1.84	0.58
1:C:313:GLU:HB2	1:C:314:ALA:C	2.29	0.58
1:B:314:ALA:O	1:B:315:ALA:HB2	2.01	0.58
1:C:172:ILE:O	1:C:172:ILE:HG23	2.03	0.58
1:C:207:VAL:HG13	1:C:208:ASP:OD2	2.03	0.58
1:C:217:TYR:CD1	1:C:217:TYR:N	2.69	0.58
1:C:296:PRO:HG3	1:C:337:THR:CB	2.27	0.58
1:A:296:PRO:HG3	1:A:337:THR:CB	2.27	0.58
1:C:138:TYR:HE2	1:C:180:PRO:HA	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:185:ILE:HD12	1:C:186:LEU:H	0.65	0.58
1:A:174:GLY:C	1:A:175:CYS:HG	2.08	0.58
1:B:83:THR:HA	1:B:236:VAL:O	2.04	0.58
1:B:105:THR:HG1	1:B:211:LYS:HD3	0.75	0.58
1:B:179:VAL:CG1	1:B:181:TRP:HD1	2.14	0.58
1:C:197:VAL:HG21	1:C:350:ARG:NH2	1.95	0.58
1:C:315:ALA:HA	1:C:318:SER:HB2	1.84	0.58
1:B:172:ILE:O	1:B:172:ILE:HG23	2.03	0.57
1:B:280:PHE:HD2	1:B:331:GLN:O	1.86	0.57
1:C:113:PRO:HD2	1:C:285:ASN:O	2.04	0.57
1:C:174:GLY:C	1:C:175:CYS:HG	2.04	0.57
1:C:340:GLU:HA	1:C:340:GLU:OE1	2.04	0.57
1:A:136:PHE:HB3	1:A:230:VAL:HG11	1.87	0.57
1:A:340:GLU:HA	1:A:340:GLU:OE1	2.03	0.57
1:C:302:ASN:CB	1:C:333:VAL:HG22	2.34	0.57
1:C:336:VAL:O	1:C:336:VAL:HG13	2.03	0.57
1:A:83:THR:HA	1:A:236:VAL:O	2.04	0.57
1:A:85:SER:C	1:A:234:TYR:CD1	2.82	0.57
1:A:172:ILE:O	1:A:172:ILE:HG23	2.03	0.57
1:A:250:ILE:HA	1:A:347:GLN:HA	1.87	0.57
1:B:302:ASN:CB	1:B:333:VAL:HG22	2.34	0.57
1:B:138:TYR:HD2	1:B:184:PHE:CE1	2.16	0.57
1:B:313:GLU:CG	1:B:318:SER:HB2	2.19	0.57
1:C:61:PRO:HD2	1:C:181:TRP:HZ3	1.67	0.57
1:C:83:THR:HA	1:C:236:VAL:O	2.03	0.57
1:A:138:TYR:HA	1:A:230:VAL:HG22	1.86	0.57
1:A:315:ALA:HA	1:A:318:SER:HB2	1.84	0.57
1:B:85:SER:C	1:B:234:TYR:CD1	2.82	0.57
1:B:151:ALA:CA	1:B:177:SER:HB2	2.17	0.57
1:B:238:LEU:N	1:B:238:LEU:CD1	2.67	0.57
1:C:136:PHE:HB3	1:C:230:VAL:HG11	1.86	0.57
1:A:313:GLU:HG3	1:A:318:SER:OG	2.01	0.57
1:B:95:LYS:HZ2	1:B:221:ALA:CB	2.17	0.57
1:B:295:ALA:HB1	1:B:314:ALA:C	2.30	0.57
1:B:340:GLU:HA	1:B:340:GLU:OE1	2.04	0.57
1:C:238:LEU:N	1:C:238:LEU:CD1	2.67	0.57
1:A:95:LYS:HZ2	1:A:221:ALA:CB	2.17	0.57
1:B:291:PHE:HB2	1:B:346:TRP:CB	2.29	0.57
1:C:78:ALA:O	1:C:80:ASP:CA	2.52	0.57
1:C:94:LYS:O	1:C:95:LYS:C	2.48	0.57
1:C:197:VAL:CG2	1:C:350:ARG:CZ	2.80	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:280:PHE:HD2	1:C:331:GLN:O	1.86	0.57
1:A:227:LEU:H	1:A:227:LEU:CD1	2.17	0.57
1:B:136:PHE:HB3	1:B:230:VAL:HG11	1.87	0.57
1:C:126:TYR:C	1:C:242:THR:HG22	2.30	0.57
1:C:197:VAL:HG21	1:C:350:ARG:HH12	1.69	0.57
1:C:250:ILE:HA	1:C:347:GLN:HA	1.87	0.57
1:A:280:PHE:HD2	1:A:331:GLN:O	1.86	0.57
1:A:302:ASN:CB	1:A:333:VAL:HG22	2.34	0.57
1:B:124:ALA:CB	1:B:245:THR:HG21	2.35	0.57
1:A:95:LYS:HZ1	1:A:221:ALA:CA	2.16	0.57
1:A:124:ALA:CB	1:A:245:THR:HG21	2.35	0.57
1:B:149:LYS:CE	1:B:151:ALA:HA	2.35	0.57
1:B:302:ASN:HB2	1:B:333:VAL:HG22	1.87	0.57
1:C:152:LEU:CD1	1:C:184:PHE:HE2	2.18	0.57
1:C:166:LEU:C	1:C:168:SER:N	2.61	0.57
1:A:149:LYS:CE	1:A:151:ALA:HA	2.35	0.56
1:C:82:ILE:CG2	1:C:238:LEU:HB2	2.32	0.56
1:C:302:ASN:HB2	1:C:333:VAL:HG22	1.87	0.56
1:B:86:GLY:N	1:B:234:TYR:CE1	2.74	0.56
1:B:152:LEU:HD12	1:B:184:PHE:HE2	1.70	0.56
1:B:313:GLU:HB2	1:B:314:ALA:C	2.29	0.56
1:C:265:TRP:CH2	1:C:348:ALA:O	2.52	0.56
1:A:125:GLN:C	1:A:242:THR:HG23	2.30	0.56
1:A:138:TYR:HD2	1:A:184:PHE:CE1	2.16	0.56
1:B:285:ASN:HD22	1:B:286:PHE:N	2.03	0.56
1:C:125:GLN:C	1:C:242:THR:HG23	2.30	0.56
1:C:138:TYR:HA	1:C:230:VAL:HG22	1.86	0.56
1:C:138:TYR:HH	1:C:227:LEU:HB3	1.66	0.56
1:C:198:ALA:CA	1:C:200:GLY:O	2.54	0.56
1:A:185:ILE:HD12	1:A:185:ILE:C	2.14	0.56
1:A:238:LEU:N	1:A:238:LEU:CD1	2.67	0.56
1:A:295:ALA:HB1	1:A:314:ALA:C	2.30	0.56
1:B:250:ILE:HA	1:B:347:GLN:HA	1.87	0.56
1:B:300:LEU:HD12	1:B:333:VAL:CG1	2.36	0.56
1:C:77:THR:CG2	1:C:78:ALA:N	2.49	0.56
1:C:95:LYS:HZ1	1:C:221:ALA:HB1	1.70	0.56
1:A:300:LEU:HD11	1:A:333:VAL:HG11	1.85	0.56
1:A:326:VAL:CG1	1:A:327:ALA:O	2.48	0.56
1:B:94:LYS:O	1:B:95:LYS:C	2.48	0.56
1:B:138:TYR:HA	1:B:230:VAL:HG22	1.86	0.56
1:B:152:LEU:CD1	1:B:184:PHE:HE2	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:208:ASP:H	1:C:329:ARG:HH21	1.46	0.56
1:C:285:ASN:HD22	1:C:286:PHE:N	2.04	0.56
1:A:152:LEU:HD12	1:A:184:PHE:HE2	1.71	0.56
1:B:248:ALA:O	1:B:263:VAL:C	2.48	0.56
1:C:200:GLY:O	1:C:282:GLY:HA2	2.06	0.56
1:A:145:THR:CG2	1:A:145:THR:O	2.54	0.56
1:A:166:LEU:C	1:A:168:SER:N	2.61	0.56
1:B:95:LYS:HZ1	1:B:221:ALA:CA	2.17	0.56
1:A:94:LYS:O	1:A:95:LYS:C	2.48	0.56
1:A:152:LEU:CD1	1:A:184:PHE:HE2	2.18	0.56
1:C:295:ALA:HB1	1:C:314:ALA:C	2.30	0.56
1:A:82:ILE:CG2	1:A:238:LEU:HB2	2.32	0.56
1:A:300:LEU:CA	1:A:308:PHE:HZ	2.19	0.56
1:B:120:ILE:O	1:B:120:ILE:HG13	2.05	0.56
1:B:125:GLN:C	1:B:242:THR:HG23	2.30	0.56
1:C:152:LEU:HD12	1:C:184:PHE:HE2	1.70	0.56
1:A:302:ASN:HB2	1:A:333:VAL:HG22	1.87	0.56
1:A:120:ILE:O	1:A:120:ILE:HG13	2.05	0.55
1:C:120:ILE:O	1:C:120:ILE:HG13	2.06	0.55
1:C:277:ASP:HA	1:C:334:LYS:HZ2	1.71	0.55
1:C:277:ASP:HA	1:C:334:LYS:NZ	2.21	0.55
1:C:289:THR:HG23	1:C:321:TRP:CZ3	2.41	0.55
1:B:104:THR:O	1:B:105:THR:O	2.24	0.55
1:B:145:THR:O	1:B:145:THR:CG2	2.54	0.55
1:B:149:LYS:CD	1:B:170:TYR:HH	1.67	0.55
1:B:170:TYR:HE1	1:B:217:TYR:OH	1.86	0.55
1:B:326:VAL:CG1	1:B:327:ALA:O	2.48	0.55
1:C:145:THR:CG2	1:C:145:THR:O	2.54	0.55
1:C:200:GLY:H	1:C:265:TRP:CD1	2.07	0.55
1:A:244:SER:C	1:A:245:THR:HG22	2.31	0.55
1:B:82:ILE:CG2	1:B:238:LEU:HB2	2.32	0.55
1:B:277:ASP:HA	1:B:334:LYS:NZ	2.21	0.55
1:C:71:THR:CG2	1:C:87:SER:CB	2.77	0.55
1:C:124:ALA:CB	1:C:245:THR:HG21	2.35	0.55
1:C:300:LEU:HD11	1:C:333:VAL:HG11	1.85	0.55
1:A:121:LYS:HZ3	1:A:350:ARG:NH1	2.03	0.55
1:A:313:GLU:HB2	1:A:314:ALA:C	2.29	0.55
1:C:149:LYS:CE	1:C:151:ALA:HA	2.35	0.55
1:C:153:ALA:HB1	1:C:174:GLY:HA3	0.62	0.55
1:C:207:VAL:C	1:C:329:ARG:NH2	2.64	0.55
1:C:300:LEU:CA	1:C:308:PHE:HZ	2.19	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:PHE:HE2	1:A:234:TYR:CE2	2.24	0.55
1:A:170:TYR:HE1	1:A:217:TYR:OH	1.87	0.55
1:A:289:THR:HG23	1:A:321:TRP:CZ3	2.41	0.55
1:B:126:TYR:C	1:B:242:THR:HG22	2.30	0.55
1:B:274:TRP:CD1	1:B:339:GLU:HA	2.42	0.55
1:A:86:GLY:N	1:A:234:TYR:CE1	2.74	0.55
1:A:157:ASP:OD1	1:A:157:ASP:C	2.50	0.55
1:B:116:PHE:HE2	1:B:234:TYR:CE2	2.24	0.55
1:B:300:LEU:CA	1:B:308:PHE:HZ	2.19	0.55
1:C:179:VAL:CG1	1:C:181:TRP:HD1	2.14	0.55
1:A:274:TRP:CD1	1:A:339:GLU:HA	2.42	0.55
1:A:313:GLU:CG	1:A:318:SER:HB2	2.19	0.55
1:B:133:SER:HB3	1:B:235:THR:CG2	2.35	0.55
1:C:104:THR:O	1:C:105:THR:O	2.24	0.55
1:C:116:PHE:HE2	1:C:234:TYR:CE2	2.24	0.55
1:C:149:LYS:CD	1:C:177:SER:OG	2.50	0.55
1:B:198:ALA:CA	1:B:200:GLY:O	2.54	0.55
1:C:227:LEU:H	1:C:227:LEU:CD1	2.17	0.55
1:C:297:VAL:HB	1:C:336:VAL:CG1	1.98	0.55
1:A:104:THR:O	1:A:105:THR:O	2.24	0.55
1:A:198:ALA:C	1:A:200:GLY:N	2.55	0.55
1:A:300:LEU:HD12	1:A:333:VAL:CG1	2.36	0.55
1:B:300:LEU:CB	1:B:308:PHE:HZ	2.20	0.55
1:C:197:VAL:HG22	1:C:198:ALA:H	1.72	0.55
1:C:201:ILE:CG2	1:C:264:SER:OG	2.55	0.55
1:C:300:LEU:CB	1:C:308:PHE:HZ	2.20	0.55
1:C:326:VAL:CG1	1:C:327:ALA:O	2.48	0.55
1:A:154:PHE:CD1	1:A:155:ASP:CA	2.90	0.55
1:A:198:ALA:CA	1:A:200:GLY:O	2.54	0.55
1:B:97:THR:O	1:B:97:THR:OG1	2.25	0.55
1:B:157:ASP:OD1	1:B:157:ASP:C	2.50	0.55
1:C:100:GLU:O	1:C:101:PRO:O	2.25	0.55
1:A:109:ASN:CA	1:A:129:TYR:OH	2.55	0.54
1:A:197:VAL:HG22	1:A:198:ALA:H	1.72	0.54
1:A:277:ASP:HA	1:A:334:LYS:NZ	2.21	0.54
1:A:126:TYR:C	1:A:242:THR:HG22	2.30	0.54
1:B:197:VAL:HG22	1:B:198:ALA:N	2.23	0.54
1:B:350:ARG:O	1:B:351:ILE:CB	2.53	0.54
1:C:113:PRO:HD2	1:C:285:ASN:H	1.72	0.54
1:B:341:GLN:O	1:B:343:LYS:HG2	2.07	0.54
1:C:274:TRP:CD1	1:C:339:GLU:HA	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:VAL:HG22	1:A:198:ALA:N	2.23	0.54
1:A:300:LEU:CB	1:A:308:PHE:HZ	2.20	0.54
1:C:113:PRO:HG3	1:C:351:ILE:HG13	1.90	0.54
1:C:156:ARG:O	1:C:209:PHE:O	2.26	0.54
1:C:157:ASP:OD1	1:C:157:ASP:C	2.50	0.54
1:C:191:ASP:OD1	1:C:209:PHE:CZ	2.61	0.54
1:A:191:ASP:OD1	1:A:209:PHE:CZ	2.61	0.54
1:B:191:ASP:OD1	1:B:209:PHE:CZ	2.61	0.54
1:C:179:VAL:CG1	1:C:181:TRP:NE1	2.54	0.54
1:C:197:VAL:HG22	1:C:198:ALA:N	2.23	0.54
1:C:199:ASP:OD1	1:C:199:ASP:N	2.40	0.54
1:C:306:SER:HB2	1:C:325:LYS:H	1.72	0.54
1:A:120:ILE:HD13	1:A:329:ARG:HH21	1.71	0.54
1:A:339:GLU:O	1:A:340:GLU:HA	2.08	0.54
1:A:149:LYS:CD	1:A:177:SER:OG	2.50	0.54
1:A:271:THR:CG2	1:A:275:GLU:OE2	2.56	0.54
1:A:306:SER:HB2	1:A:325:LYS:H	1.72	0.54
1:B:300:LEU:O	1:B:308:PHE:CZ	2.61	0.54
1:C:133:SER:HB3	1:C:235:THR:CG2	2.35	0.54
1:A:130:ARG:O	1:A:131:PHE:HB2	2.08	0.54
1:A:300:LEU:O	1:A:308:PHE:CZ	2.61	0.54
1:B:130:ARG:O	1:B:131:PHE:HB2	2.08	0.54
1:B:289:THR:HG23	1:B:321:TRP:CZ3	2.41	0.54
1:B:306:SER:HB2	1:B:325:LYS:H	1.72	0.54
1:C:95:LYS:NZ	1:C:221:ALA:HB1	2.22	0.54
1:C:100:GLU:O	1:C:101:PRO:C	2.48	0.54
1:C:300:LEU:HD12	1:C:333:VAL:CG1	2.36	0.54
1:B:153:ALA:HB1	1:B:174:GLY:HA3	0.62	0.54
1:B:244:SER:C	1:B:245:THR:HG22	2.31	0.54
1:B:309:SER:C	1:B:322:ALA:HA	2.20	0.54
1:C:173:GLU:HG3	1:C:174:GLY:H	1.73	0.54
1:C:213:ILE:O	1:C:214:MET:CG	2.56	0.54
1:A:100:GLU:O	1:A:101:PRO:C	2.48	0.54
1:A:153:ALA:HB1	1:A:174:GLY:HA3	0.62	0.54
1:A:156:ARG:O	1:A:209:PHE:O	2.26	0.54
1:A:285:ASN:HD22	1:A:286:PHE:N	2.04	0.54
1:B:136:PHE:CZ	1:B:212:LEU:CD2	2.91	0.54
1:B:248:ALA:O	1:B:263:VAL:O	2.25	0.54
1:C:333:VAL:C	1:C:334:LYS:CD	2.78	0.54
1:C:339:GLU:O	1:C:340:GLU:HA	2.08	0.54
1:A:100:GLU:O	1:A:101:PRO:O	2.25	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:VAL:HG22	1:B:198:ALA:H	1.72	0.53
1:C:109:ASN:O	1:C:110:PRO:C	2.51	0.53
1:C:231:ARG:CG	1:C:232:VAL:N	2.61	0.53
1:C:326:VAL:CG1	1:C:327:ALA:N	2.19	0.53
1:A:179:VAL:HG13	1:A:182:THR:HG22	1.90	0.53
1:A:213:ILE:O	1:A:214:MET:CG	2.56	0.53
1:B:213:ILE:O	1:B:214:MET:CG	2.56	0.53
1:B:248:ALA:C	1:B:263:VAL:C	2.75	0.53
1:C:97:THR:O	1:C:97:THR:OG1	2.25	0.53
1:A:136:PHE:CZ	1:A:212:LEU:CD2	2.91	0.53
1:A:276:HIS:CG	1:A:277:ASP:N	2.74	0.53
1:B:154:PHE:CD1	1:B:155:ASP:CA	2.90	0.53
1:B:179:VAL:HG22	1:B:180:PRO:N	2.23	0.53
1:C:341:GLN:O	1:C:343:LYS:HG2	2.08	0.53
1:A:248:ALA:CB	1:A:265:TRP:N	2.70	0.53
1:A:341:GLN:O	1:A:343:LYS:HG2	2.07	0.53
1:B:95:LYS:NZ	1:B:221:ALA:HB1	2.22	0.53
1:B:130:ARG:HH11	1:B:236:VAL:C	2.16	0.53
1:B:265:TRP:CH2	1:B:348:ALA:O	2.52	0.53
1:C:244:SER:O	1:C:245:THR:HB	2.08	0.53
1:C:291:PHE:C	1:C:292:TYR:HB3	2.33	0.53
1:A:291:PHE:C	1:A:292:TYR:HB3	2.33	0.53
1:A:333:VAL:C	1:A:334:LYS:CD	2.78	0.53
1:B:109:ASN:CA	1:B:129:TYR:OH	2.55	0.53
1:B:293:GLU:O	1:B:317:GLY:HA2	2.09	0.53
1:C:130:ARG:O	1:C:131:PHE:HB2	2.08	0.53
1:C:170:TYR:HE1	1:C:217:TYR:OH	1.87	0.53
1:C:269:LYS:HB3	1:C:277:ASP:OD2	2.09	0.53
1:B:166:LEU:C	1:B:168:SER:N	2.61	0.53
1:B:339:GLU:O	1:B:340:GLU:HA	2.08	0.53
1:C:90:ILE:O	1:C:90:ILE:CG2	2.54	0.53
1:C:142:SER:HB3	1:C:227:LEU:O	2.09	0.53
1:C:300:LEU:O	1:C:308:PHE:CZ	2.61	0.53
1:A:84:ARG:HG3	1:A:119:LEU:HD11	1.91	0.53
1:A:150:VAL:O	1:A:151:ALA:C	2.52	0.53
1:A:154:PHE:CB	1:A:212:LEU:HD12	2.35	0.53
1:A:179:VAL:HG22	1:A:180:PRO:N	2.23	0.53
1:A:293:GLU:HA	1:A:317:GLY:HA2	1.91	0.53
1:B:142:SER:HB3	1:B:227:LEU:O	2.09	0.53
1:B:150:VAL:O	1:B:151:ALA:C	2.52	0.53
1:B:156:ARG:O	1:B:209:PHE:O	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:PRO:HG3	1:C:120:ILE:CD1	2.39	0.53
1:C:150:VAL:O	1:C:151:ALA:C	2.52	0.53
1:C:269:LYS:CG	1:C:270:GLY:N	2.58	0.53
1:C:271:THR:CG2	1:C:275:GLU:OE2	2.56	0.53
1:B:179:VAL:HG13	1:B:182:THR:HG22	1.90	0.53
1:B:199:ASP:OD1	1:B:199:ASP:N	2.40	0.53
1:B:291:PHE:C	1:B:292:TYR:HB3	2.33	0.53
1:B:339:GLU:O	1:B:340:GLU:OE1	2.27	0.53
1:A:130:ARG:HH11	1:A:236:VAL:C	2.16	0.53
1:A:269:LYS:HB3	1:A:277:ASP:OD2	2.09	0.53
1:B:84:ARG:HG3	1:B:119:LEU:HD11	1.91	0.53
1:B:293:GLU:HA	1:B:317:GLY:HA2	1.91	0.53
1:C:179:VAL:HG22	1:C:180:PRO:N	2.23	0.53
1:A:133:SER:HB3	1:A:235:THR:CG2	2.35	0.53
1:A:179:VAL:CG1	1:A:182:THR:HG22	2.39	0.53
1:A:288:LEU:C	1:A:289:THR:OG1	2.49	0.53
1:B:129:TYR:CA	1:B:237:GLN:O	2.57	0.53
1:B:173:GLU:HG3	1:B:174:GLY:H	1.73	0.53
1:C:82:ILE:HG12	1:C:83:THR:N	2.24	0.53
1:C:135:ARG:CB	1:C:185:ILE:HD11	2.38	0.53
1:A:82:ILE:HD12	1:A:126:TYR:CE2	2.44	0.52
1:A:82:ILE:HG12	1:A:83:THR:N	2.24	0.52
1:A:95:LYS:NZ	1:A:221:ALA:HB1	2.22	0.52
1:A:129:TYR:CA	1:A:237:GLN:O	2.57	0.52
1:B:100:GLU:O	1:B:101:PRO:O	2.25	0.52
1:B:112:GLU:HB3	1:B:115:THR:CG2	2.40	0.52
1:B:113:PRO:HG3	1:B:120:ILE:CD1	2.39	0.52
1:B:244:SER:O	1:B:245:THR:HB	2.08	0.52
1:B:300:LEU:CG	1:B:308:PHE:HZ	2.20	0.52
1:C:107:VAL:O	1:C:115:THR:CG2	2.56	0.52
1:C:136:PHE:CZ	1:C:212:LEU:CD2	2.91	0.52
1:B:82:ILE:HD12	1:B:126:TYR:CE2	2.44	0.52
1:B:149:LYS:HE2	1:B:151:ALA:CB	2.39	0.52
1:B:179:VAL:CG1	1:B:182:THR:HG22	2.39	0.52
1:C:179:VAL:CG1	1:C:182:THR:HG22	2.39	0.52
1:A:115:THR:C	1:A:116:PHE:CD1	2.78	0.52
1:A:152:LEU:HD12	1:A:184:PHE:CE2	2.45	0.52
1:B:152:LEU:HD12	1:B:184:PHE:CE2	2.44	0.52
1:B:185:ILE:CD1	1:B:186:LEU:O	2.58	0.52
1:A:95:LYS:HZ1	1:A:221:ALA:C	2.18	0.52
1:A:236:VAL:CG1	1:A:237:GLN:H	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:ARG:O	1:A:351:ILE:CB	2.53	0.52
1:B:95:LYS:HZ1	1:B:221:ALA:C	2.18	0.52
1:B:135:ARG:CB	1:B:185:ILE:HD11	2.38	0.52
1:B:154:PHE:CB	1:B:212:LEU:HD12	2.35	0.52
1:C:112:GLU:HB3	1:C:115:THR:CG2	2.39	0.52
1:C:115:THR:C	1:C:116:PHE:CD1	2.78	0.52
1:C:244:SER:C	1:C:245:THR:HG22	2.31	0.52
1:C:293:GLU:HA	1:C:317:GLY:HA2	1.91	0.52
1:C:339:GLU:O	1:C:340:GLU:OE1	2.27	0.52
1:A:112:GLU:HB3	1:A:115:THR:CG2	2.39	0.52
1:A:304:ASP:OD2	1:A:332:GLY:N	2.43	0.52
1:C:128:LYS:O	1:C:129:TYR:HB3	2.10	0.52
1:C:152:LEU:HD12	1:C:184:PHE:CE2	2.45	0.52
1:C:179:VAL:HG13	1:C:182:THR:HG22	1.90	0.52
1:A:142:SER:HB3	1:A:227:LEU:O	2.09	0.52
1:A:244:SER:O	1:A:245:THR:HB	2.08	0.52
1:A:248:ALA:C	1:A:264:SER:CB	2.82	0.52
1:C:56:THR:CG2	1:C:57:ARG:N	2.58	0.52
1:C:78:ALA:O	1:C:81:GLY:N	2.42	0.52
1:C:82:ILE:HD12	1:C:126:TYR:CE2	2.44	0.52
1:C:109:ASN:CA	1:C:129:TYR:OH	2.55	0.52
1:C:350:ARG:O	1:C:351:ILE:CB	2.53	0.52
1:A:93:LEU:HD12	1:A:138:TYR:HE1	1.75	0.52
1:A:149:LYS:HE2	1:A:151:ALA:CB	2.39	0.52
1:A:300:LEU:CG	1:A:308:PHE:HZ	2.21	0.52
1:B:269:LYS:HB3	1:B:277:ASP:OD2	2.09	0.52
1:B:338:THR:HG1	1:B:339:GLU:HB2	1.69	0.52
1:C:54:LYS:O	1:C:55:VAL:HB	2.08	0.52
1:C:130:ARG:HH11	1:C:236:VAL:C	2.16	0.52
1:C:239:LYS:O	1:C:240:ASN:O	2.28	0.52
1:A:113:PRO:HG3	1:A:120:ILE:CD1	2.39	0.52
1:B:236:VAL:CG1	1:B:237:GLN:H	2.23	0.52
1:C:90:ILE:HD11	1:C:232:VAL:HG22	1.83	0.52
1:C:149:LYS:HE2	1:C:151:ALA:CB	2.39	0.52
1:C:304:ASP:OD2	1:C:332:GLY:N	2.43	0.52
1:A:339:GLU:O	1:A:340:GLU:OE1	2.27	0.52
1:B:93:LEU:HD12	1:B:138:TYR:HE1	1.75	0.52
1:B:304:ASP:OD2	1:B:332:GLY:N	2.43	0.52
1:C:149:LYS:HD3	1:C:217:TYR:HE1	1.73	0.52
1:A:295:ALA:HB2	1:A:315:ALA:CB	2.37	0.52
1:C:138:TYR:CZ	1:C:150:VAL:HG21	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:185:ILE:CD1	1:C:186:LEU:O	2.58	0.52
1:A:185:ILE:CD1	1:A:186:LEU:O	2.58	0.51
1:A:235:THR:O	1:A:235:THR:HG23	2.09	0.51
1:A:273:GLY:O	1:A:274:TRP:C	2.53	0.51
1:B:136:PHE:HB3	1:B:230:VAL:CG1	2.40	0.51
1:C:300:LEU:O	1:C:308:PHE:CE2	2.63	0.51
1:A:138:TYR:CZ	1:A:150:VAL:HG21	2.45	0.51
1:A:144:SER:O	1:A:146:THR:N	2.44	0.51
1:B:144:SER:O	1:B:146:THR:N	2.44	0.51
1:B:295:ALA:N	1:B:316:ALA:CA	2.40	0.51
1:C:84:ARG:HG3	1:C:119:LEU:HD11	1.91	0.51
1:C:179:VAL:HG13	1:C:181:TRP:CD1	2.38	0.51
1:C:236:VAL:CG1	1:C:237:GLN:H	2.23	0.51
1:C:277:ASP:CG	1:C:334:LYS:HZ3	2.17	0.51
1:C:285:ASN:HD22	1:C:286:PHE:H	1.58	0.51
1:A:103:TYR:CD1	1:A:215:ALA:HB2	2.45	0.51
1:A:103:TYR:CE1	1:A:169:LEU:HD12	2.43	0.51
1:A:293:GLU:O	1:A:317:GLY:HA2	2.09	0.51
1:B:82:ILE:O	1:B:83:THR:OG1	2.18	0.51
1:B:82:ILE:HG12	1:B:83:THR:N	2.24	0.51
1:C:185:ILE:HD12	1:C:186:LEU:C	2.36	0.51
1:B:115:THR:C	1:B:116:PHE:CD1	2.78	0.51
1:B:153:ALA:CA	1:B:174:GLY:HA3	2.33	0.51
1:B:239:LYS:O	1:B:240:ASN:O	2.28	0.51
1:C:83:THR:CB	1:C:130:ARG:HH12	2.24	0.51
1:A:230:VAL:CG1	1:A:231:ARG:N	2.74	0.51
1:A:297:VAL:HB	1:A:336:VAL:CG1	1.98	0.51
1:B:100:GLU:C	1:B:101:PRO:O	2.54	0.51
1:B:221:ALA:O	1:B:225:ALA:HB2	2.10	0.51
1:A:100:GLU:C	1:A:101:PRO:O	2.54	0.51
1:B:128:LYS:HG3	1:B:196:PHE:CD2	2.46	0.51
1:B:243:GLY:O	1:B:244:SER:HB2	2.11	0.51
1:B:285:ASN:HD22	1:B:286:PHE:H	1.58	0.51
1:C:230:VAL:CG1	1:C:231:ARG:N	2.74	0.51
1:C:273:GLY:O	1:C:274:TRP:C	2.53	0.51
1:A:107:VAL:O	1:A:115:THR:CG2	2.56	0.51
1:A:128:LYS:HG3	1:A:196:PHE:CD2	2.46	0.51
1:A:291:PHE:CG	1:A:345:LYS:O	2.64	0.51
1:B:83:THR:CB	1:B:130:ARG:HH12	2.24	0.51
1:B:235:THR:O	1:B:235:THR:HG23	2.09	0.51
1:C:113:PRO:HG2	1:C:285:ASN:HB3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:241:ARG:H	1:C:241:ARG:CD	2.22	0.51
1:C:313:GLU:CG	1:C:318:SER:HB2	2.19	0.51
1:B:103:TYR:CE1	1:B:169:LEU:HD12	2.43	0.51
1:B:300:LEU:O	1:B:308:PHE:CE2	2.63	0.51
1:C:129:TYR:CA	1:C:237:GLN:O	2.57	0.51
1:C:136:PHE:HB3	1:C:230:VAL:CG1	2.40	0.51
1:C:202:SER:N	1:C:281:LEU:HG	2.26	0.51
1:A:185:ILE:HD12	1:A:186:LEU:C	2.36	0.51
1:A:239:LYS:O	1:A:240:ASN:O	2.28	0.51
1:A:243:GLY:O	1:A:244:SER:HB2	2.11	0.51
1:A:285:ASN:HD22	1:A:286:PHE:H	1.58	0.51
1:A:300:LEU:O	1:A:308:PHE:CE2	2.63	0.51
1:B:101:PRO:CB	1:B:217:TYR:CD2	2.94	0.51
1:C:172:ILE:C	1:C:173:GLU:O	2.51	0.51
1:C:188:VAL:CG2	1:C:188:VAL:O	2.59	0.51
1:A:136:PHE:HB3	1:A:230:VAL:CG1	2.40	0.51
1:A:296:PRO:CD	1:A:337:THR:HG21	2.38	0.51
1:B:291:PHE:CG	1:B:345:LYS:O	2.64	0.51
1:B:333:VAL:C	1:B:334:LYS:CD	2.78	0.51
1:C:243:GLY:O	1:C:244:SER:HB2	2.11	0.51
1:C:295:ALA:HB2	1:C:315:ALA:CB	2.37	0.51
1:A:101:PRO:CB	1:A:217:TYR:CD2	2.94	0.50
1:A:107:VAL:HA	1:A:211:LYS:HA	1.93	0.50
1:A:221:ALA:O	1:A:225:ALA:HB2	2.10	0.50
1:B:185:ILE:HD12	1:B:186:LEU:C	2.36	0.50
1:C:85:SER:O	1:C:234:TYR:CE1	2.65	0.50
1:C:109:ASN:ND2	1:C:350:ARG:NH2	2.58	0.50
1:C:128:LYS:HG3	1:C:196:PHE:CD2	2.46	0.50
1:C:158:ALA:C	1:C:211:LYS:H	1.93	0.50
1:C:221:ALA:O	1:C:225:ALA:HB2	2.10	0.50
1:C:235:THR:O	1:C:235:THR:HG23	2.09	0.50
1:A:188:VAL:CG2	1:A:188:VAL:O	2.59	0.50
1:A:314:ALA:O	1:A:315:ALA:HB3	2.11	0.50
1:B:103:TYR:CD1	1:B:215:ALA:HB2	2.46	0.50
1:B:138:TYR:CZ	1:B:150:VAL:HG21	2.45	0.50
1:B:241:ARG:H	1:B:241:ARG:CD	2.22	0.50
1:C:93:LEU:HD12	1:C:138:TYR:HE1	1.75	0.50
1:A:128:LYS:O	1:A:129:TYR:HB3	2.10	0.50
1:A:138:TYR:HH	1:A:227:LEU:HB3	1.66	0.50
1:B:230:VAL:CG1	1:B:231:ARG:N	2.74	0.50
1:C:74:ARG:C	1:C:75:VAL:HG23	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:TYR:C	1:C:242:THR:HG21	2.37	0.50
1:C:130:ARG:CB	1:C:237:GLN:N	2.74	0.50
1:C:153:ALA:CA	1:C:174:GLY:HA3	2.33	0.50
1:C:154:PHE:CB	1:C:212:LEU:HD12	2.35	0.50
1:C:314:ALA:O	1:C:315:ALA:HB3	2.11	0.50
1:A:130:ARG:CB	1:A:237:GLN:N	2.74	0.50
1:B:119:LEU:HD23	1:B:234:TYR:CE2	2.43	0.50
1:B:273:GLY:O	1:B:274:TRP:C	2.53	0.50
1:C:77:THR:CG2	1:C:78:ALA:H	2.03	0.50
1:C:144:SER:O	1:C:146:THR:N	2.44	0.50
1:C:279:HIS:HB3	1:C:280:PHE:N	2.26	0.50
1:C:300:LEU:CG	1:C:308:PHE:HZ	2.20	0.50
1:A:173:GLU:HG3	1:A:174:GLY:H	1.73	0.50
1:A:242:THR:CG2	1:A:243:GLY:H	2.22	0.50
1:B:109:ASN:O	1:B:110:PRO:C	2.51	0.50
1:B:314:ALA:O	1:B:315:ALA:HB3	2.11	0.50
1:C:100:GLU:C	1:C:101:PRO:O	2.54	0.50
1:C:154:PHE:CD1	1:C:155:ASP:CA	2.90	0.50
1:B:188:VAL:CG2	1:B:188:VAL:O	2.59	0.50
1:A:83:THR:CB	1:A:130:ARG:HH12	2.24	0.50
1:B:130:ARG:CB	1:B:237:GLN:H	2.25	0.50
1:B:151:ALA:HA	1:B:177:SER:CB	2.21	0.50
1:C:103:TYR:CD1	1:C:215:ALA:HB2	2.46	0.50
1:B:107:VAL:HA	1:B:211:LYS:HA	1.93	0.50
1:B:128:LYS:O	1:B:129:TYR:HB3	2.10	0.50
1:B:136:PHE:HD1	1:B:231:ARG:O	1.95	0.50
1:B:271:THR:CG2	1:B:275:GLU:OE2	2.56	0.50
1:B:290:LEU:HD23	1:B:346:TRP:HB2	1.90	0.50
1:C:95:LYS:HZ1	1:C:221:ALA:C	2.20	0.50
1:C:101:PRO:CB	1:C:217:TYR:CD2	2.94	0.50
1:A:130:ARG:CB	1:A:237:GLN:H	2.25	0.50
1:A:135:ARG:CB	1:A:185:ILE:HD11	2.38	0.50
1:B:116:PHE:CE2	1:B:234:TYR:CE2	3.00	0.50
1:B:130:ARG:CB	1:B:237:GLN:N	2.74	0.50
1:B:133:SER:N	1:B:235:THR:CG2	2.74	0.50
1:B:279:HIS:HB3	1:B:280:PHE:N	2.27	0.50
1:B:288:LEU:C	1:B:289:THR:OG1	2.49	0.50
1:C:71:THR:OG1	1:C:87:SER:CB	2.59	0.50
1:A:150:VAL:HG23	1:A:227:LEU:HD23	1.94	0.49
1:A:241:ARG:H	1:A:241:ARG:CD	2.22	0.49
1:B:107:VAL:O	1:B:115:THR:CG2	2.56	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:SER:O	1:B:234:TYR:CB	2.60	0.49
1:B:242:THR:CG2	1:B:243:GLY:H	2.22	0.49
1:B:300:LEU:CB	1:B:308:PHE:CZ	2.95	0.49
1:C:130:ARG:CB	1:C:237:GLN:H	2.25	0.49
1:C:293:GLU:O	1:C:317:GLY:HA2	2.09	0.49
1:B:85:SER:O	1:B:234:TYR:CE1	2.65	0.49
1:B:150:VAL:HG23	1:B:227:LEU:HD23	1.94	0.49
1:B:293:GLU:O	1:B:316:ALA:C	2.52	0.49
1:C:107:VAL:HA	1:C:211:LYS:HA	1.93	0.49
1:A:136:PHE:HD1	1:A:231:ARG:O	1.95	0.49
1:A:300:LEU:CB	1:A:308:PHE:CZ	2.95	0.49
1:B:336:VAL:C	1:B:337:THR:HG23	2.37	0.49
1:C:95:LYS:HZ1	1:C:221:ALA:CB	2.25	0.49
1:C:167:ALA:O	1:C:171:ASN:ND2	2.45	0.49
1:A:116:PHE:CE2	1:A:234:TYR:CE2	3.00	0.49
1:A:163:PRO:HB2	1:A:165:ASP:N	2.28	0.49
1:B:100:GLU:O	1:B:101:PRO:C	2.48	0.49
1:B:150:VAL:CG2	1:B:227:LEU:HD23	2.43	0.49
1:A:126:TYR:C	1:A:242:THR:HG21	2.37	0.49
1:B:269:LYS:CG	1:B:270:GLY:N	2.58	0.49
1:C:151:ALA:HA	1:C:177:SER:CB	2.21	0.49
1:C:204:PRO:CB	1:C:329:ARG:N	2.75	0.49
1:A:85:SER:O	1:A:234:TYR:CE1	2.65	0.49
1:A:109:ASN:O	1:A:110:PRO:C	2.51	0.49
1:A:133:SER:O	1:A:234:TYR:CB	2.60	0.49
1:B:167:ALA:O	1:B:171:ASN:ND2	2.45	0.49
1:C:95:LYS:HZ2	1:C:221:ALA:CB	2.25	0.49
1:C:290:LEU:HD23	1:C:346:TRP:HB2	1.90	0.49
1:A:96:ASN:C	1:A:98:ASP:N	2.55	0.49
1:A:119:LEU:HD23	1:A:234:TYR:CE2	2.43	0.49
1:A:167:ALA:O	1:A:171:ASN:ND2	2.45	0.49
1:B:85:SER:O	1:B:234:TYR:HE1	1.96	0.49
1:B:126:TYR:C	1:B:242:THR:HG21	2.37	0.49
1:C:107:VAL:HG11	1:C:283:THR:CG2	2.43	0.49
1:C:116:PHE:CE2	1:C:234:TYR:CE2	3.00	0.49
1:C:150:VAL:CG2	1:C:227:LEU:HD23	2.43	0.49
1:C:288:LEU:C	1:C:289:THR:OG1	2.49	0.49
1:C:291:PHE:CG	1:C:345:LYS:O	2.64	0.49
1:A:264:SER:OG	1:A:265:TRP:N	2.45	0.49
1:A:295:ALA:N	1:A:316:ALA:CA	2.40	0.49
1:B:86:GLY:HA2	1:B:234:TYR:HE1	1.68	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:PRO:HB2	1:B:165:ASP:N	2.28	0.49
1:C:150:VAL:HG23	1:C:227:LEU:HD23	1.94	0.49
1:C:198:ALA:C	1:C:200:GLY:N	2.55	0.49
1:B:278:CYS:CA	1:B:334:LYS:HD3	2.42	0.49
1:B:288:LEU:CD1	1:B:290:LEU:CG	2.70	0.49
1:C:85:SER:O	1:C:234:TYR:HE1	1.96	0.49
1:C:185:ILE:HD12	1:C:185:ILE:C	2.14	0.49
1:A:85:SER:O	1:A:234:TYR:HE1	1.96	0.49
1:B:241:ARG:N	1:B:241:ARG:CD	2.75	0.49
1:B:244:SER:OG	1:B:245:THR:N	2.46	0.49
1:B:264:SER:OG	1:B:265:TRP:N	2.45	0.49
1:C:86:GLY:N	1:C:234:TYR:CE1	2.74	0.49
1:C:119:LEU:HD23	1:C:234:TYR:CE2	2.43	0.49
1:C:136:PHE:HD1	1:C:231:ARG:O	1.95	0.49
1:C:201:ILE:CD1	1:C:281:LEU:CD1	2.90	0.49
1:A:88:GLU:OE2	1:A:118:GLN:HB3	2.13	0.48
1:A:150:VAL:CG2	1:A:227:LEU:HD23	2.43	0.48
1:A:244:SER:OG	1:A:245:THR:N	2.46	0.48
1:A:279:HIS:HB3	1:A:280:PHE:N	2.27	0.48
1:B:92:THR:HG23	1:B:93:LEU:O	2.13	0.48
1:B:291:PHE:C	1:B:292:TYR:CB	2.86	0.48
1:C:241:ARG:N	1:C:241:ARG:CD	2.75	0.48
1:C:278:CYS:CA	1:C:334:LYS:HD3	2.42	0.48
1:A:336:VAL:C	1:A:337:THR:HG23	2.37	0.48
1:B:84:ARG:HD2	1:B:119:LEU:HD13	1.94	0.48
1:B:88:GLU:O	1:B:231:ARG:HB3	2.05	0.48
1:B:88:GLU:OE2	1:B:118:GLN:HB3	2.13	0.48
1:B:158:ALA:C	1:B:211:LYS:H	1.93	0.48
1:C:133:SER:O	1:C:234:TYR:CB	2.60	0.48
1:C:249:GLN:NE2	1:C:265:TRP:N	2.54	0.48
1:C:264:SER:OG	1:C:265:TRP:N	2.45	0.48
1:C:291:PHE:C	1:C:292:TYR:CB	2.86	0.48
1:A:105:THR:O	1:A:105:THR:HG23	2.14	0.48
1:A:152:LEU:O	1:A:186:LEU:CD1	2.55	0.48
1:A:291:PHE:C	1:A:292:TYR:CB	2.86	0.48
1:B:204:PRO:N	1:B:205:LYS:HD2	2.28	0.48
1:C:66:TYR:HE2	1:C:183:GLY:HA3	1.73	0.48
1:C:336:VAL:O	1:C:337:THR:CG2	2.62	0.48
1:C:336:VAL:C	1:C:337:THR:HG23	2.37	0.48
1:B:83:THR:HG23	1:B:130:ARG:CZ	2.44	0.48
1:B:172:ILE:C	1:B:173:GLU:O	2.51	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:GLN:O	1:B:347:GLN:CA	2.61	0.48
1:C:163:PRO:CG	1:C:168:SER:CB	2.92	0.48
1:C:300:LEU:CB	1:C:308:PHE:CZ	2.95	0.48
1:C:339:GLU:O	1:C:340:GLU:CA	2.60	0.48
1:A:84:ARG:HD2	1:A:119:LEU:HD13	1.94	0.48
1:A:172:ILE:C	1:A:173:GLU:O	2.51	0.48
1:A:241:ARG:N	1:A:241:ARG:CD	2.75	0.48
1:B:336:VAL:O	1:B:337:THR:HG23	2.14	0.48
1:C:86:GLY:HA2	1:C:234:TYR:HE1	1.68	0.48
1:C:336:VAL:O	1:C:337:THR:HG23	2.14	0.48
1:C:337:THR:OG1	1:C:343:LYS:NZ	2.42	0.48
1:A:83:THR:HG23	1:A:130:ARG:CZ	2.44	0.48
1:A:158:ALA:C	1:A:211:LYS:H	1.93	0.48
1:C:83:THR:HG23	1:C:130:ARG:CZ	2.44	0.48
1:C:84:ARG:HD2	1:C:119:LEU:HD13	1.94	0.48
1:C:103:TYR:CE1	1:C:169:LEU:HD12	2.43	0.48
1:A:92:THR:HG23	1:A:93:LEU:O	2.14	0.48
1:A:163:PRO:CG	1:A:168:SER:CB	2.92	0.48
1:A:249:GLN:O	1:A:347:GLN:CA	2.61	0.48
1:C:159:ALA:HB1	1:C:328:GLU:HB2	1.18	0.48
1:A:204:PRO:N	1:A:205:LYS:HD2	2.29	0.48
1:A:339:GLU:O	1:A:340:GLU:CA	2.60	0.48
1:B:152:LEU:O	1:B:186:LEU:CD1	2.55	0.48
1:C:101:PRO:CG	1:C:217:TYR:CE2	2.74	0.48
1:C:204:PRO:N	1:C:205:LYS:HD2	2.29	0.48
1:C:293:GLU:O	1:C:316:ALA:C	2.52	0.48
1:A:150:VAL:O	1:A:151:ALA:O	2.32	0.48
1:A:186:LEU:C	1:A:186:LEU:CD2	2.87	0.48
1:A:109:ASN:OD1	1:A:129:TYR:OH	2.32	0.48
1:A:248:ALA:CA	1:A:264:SER:O	2.58	0.48
1:A:290:LEU:HB2	1:A:346:TRP:HA	1.96	0.48
1:A:336:VAL:O	1:A:337:THR:CG2	2.62	0.48
1:B:163:PRO:CG	1:B:168:SER:CB	2.92	0.48
1:B:186:LEU:C	1:B:186:LEU:CD2	2.87	0.48
1:B:296:PRO:CD	1:B:337:THR:HG21	2.38	0.48
1:C:88:GLU:OE2	1:C:118:GLN:HB3	2.14	0.48
1:C:101:PRO:CG	1:C:217:TYR:HD2	2.26	0.48
1:C:163:PRO:HB2	1:C:165:ASP:N	2.28	0.48
1:A:111:SER:HB3	1:A:197:VAL:CG2	2.44	0.47
1:B:105:THR:O	1:B:105:THR:HG23	2.14	0.47
1:B:109:ASN:OD1	1:B:129:TYR:OH	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:SER:HB3	1:B:197:VAL:CG2	2.44	0.47
1:B:141:MET:O	1:B:141:MET:CG	2.46	0.47
1:B:336:VAL:O	1:B:337:THR:CG2	2.62	0.47
1:C:134:LEU:CD2	1:C:188:VAL:HG22	2.41	0.47
1:C:152:LEU:O	1:C:186:LEU:CD1	2.56	0.47
1:B:179:VAL:CG1	1:B:181:TRP:NE1	2.54	0.47
1:C:92:THR:HG23	1:C:93:LEU:O	2.14	0.47
1:C:244:SER:OG	1:C:245:THR:N	2.46	0.47
1:C:269:LYS:HG2	1:C:270:GLY:O	2.14	0.47
1:A:163:PRO:CG	1:A:168:SER:HB3	2.44	0.47
1:B:101:PRO:HG2	1:B:166:LEU:HD12	1.94	0.47
1:B:144:SER:HA	1:B:181:TRP:HB3	1.96	0.47
1:B:163:PRO:CG	1:B:168:SER:HB3	2.44	0.47
1:C:295:ALA:N	1:C:316:ALA:CA	2.40	0.47
1:C:343:LYS:HB2	1:C:344:GLY:H	1.13	0.47
1:C:249:GLN:O	1:C:347:GLN:CA	2.61	0.47
1:A:278:CYS:N	1:A:333:VAL:O	2.48	0.47
1:B:149:LYS:HE2	1:B:151:ALA:HB2	1.96	0.47
1:B:150:VAL:O	1:B:151:ALA:O	2.32	0.47
1:B:185:ILE:HD11	1:B:186:LEU:O	2.15	0.47
1:C:130:ARG:HB3	1:C:237:GLN:N	2.30	0.47
1:C:179:VAL:CG2	1:C:181:TRP:CD1	2.93	0.47
1:C:185:ILE:HD11	1:C:186:LEU:O	2.15	0.47
1:C:278:CYS:N	1:C:333:VAL:O	2.48	0.47
1:C:309:SER:C	1:C:322:ALA:HA	2.20	0.47
1:A:149:LYS:HE2	1:A:151:ALA:HB2	1.96	0.47
1:A:179:VAL:CG1	1:A:181:TRP:NE1	2.54	0.47
1:B:203:ASP:OD1	1:B:205:LYS:CG	2.56	0.47
1:B:341:GLN:O	1:B:342:PRO:C	2.58	0.47
1:A:136:PHE:CE2	1:A:212:LEU:CD2	2.98	0.47
1:A:185:ILE:HD11	1:A:186:LEU:O	2.15	0.47
1:A:293:GLU:O	1:A:316:ALA:C	2.52	0.47
1:B:136:PHE:CE2	1:B:212:LEU:CD2	2.98	0.47
1:B:269:LYS:HG2	1:B:270:GLY:O	2.14	0.47
1:B:278:CYS:N	1:B:333:VAL:O	2.48	0.47
1:B:290:LEU:HB2	1:B:346:TRP:HA	1.96	0.47
1:B:291:PHE:HD2	1:B:346:TRP:HE3	1.63	0.47
1:B:338:THR:OG1	1:B:339:GLU:CA	2.63	0.47
1:C:136:PHE:CE2	1:C:212:LEU:CD2	2.98	0.47
1:C:144:SER:HA	1:C:181:TRP:HB3	1.96	0.47
1:C:150:VAL:O	1:C:151:ALA:O	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:PRO:O	1:C:163:PRO:O	2.33	0.47
1:C:186:LEU:C	1:C:186:LEU:CD2	2.87	0.47
1:A:144:SER:HA	1:A:181:TRP:HB3	1.96	0.47
1:A:169:LEU:C	1:A:171:ASN:H	2.22	0.47
1:C:313:GLU:HG3	1:C:315:ALA:HA	1.97	0.47
1:A:269:LYS:HG2	1:A:270:GLY:O	2.14	0.47
1:B:152:LEU:C	1:B:186:LEU:HD12	2.40	0.47
1:B:170:TYR:C	1:B:171:ASN:ND2	2.72	0.47
1:C:201:ILE:HD13	1:C:266:SER:HA	1.97	0.47
1:C:291:PHE:CD1	1:C:292:TYR:N	2.83	0.47
1:C:296:PRO:CD	1:C:337:THR:HG21	2.39	0.47
1:A:170:TYR:C	1:A:171:ASN:ND2	2.72	0.47
1:A:203:ASP:OD1	1:A:205:LYS:CG	2.56	0.47
1:B:95:LYS:HZ1	1:B:221:ALA:HB1	1.80	0.47
1:B:138:TYR:HH	1:B:227:LEU:HB3	1.66	0.47
1:B:169:LEU:C	1:B:171:ASN:H	2.23	0.47
1:B:291:PHE:CD1	1:B:292:TYR:N	2.83	0.47
1:B:300:LEU:HD12	1:B:300:LEU:HA	1.28	0.47
1:C:105:THR:O	1:C:105:THR:HG23	2.14	0.47
1:C:107:VAL:HG22	1:C:211:LYS:HB3	1.97	0.47
1:C:338:THR:OG1	1:C:339:GLU:CA	2.63	0.47
1:A:153:ALA:CA	1:A:174:GLY:HA3	2.33	0.46
1:A:291:PHE:CD1	1:A:292:TYR:N	2.83	0.46
1:C:149:LYS:O	1:C:216:THR:HA	2.15	0.46
1:A:336:VAL:O	1:A:337:THR:HG23	2.14	0.46
1:B:90:ILE:O	1:B:90:ILE:CG2	2.54	0.46
1:B:162:PRO:O	1:B:163:PRO:O	2.33	0.46
1:B:174:GLY:O	1:B:175:CYS:CB	2.64	0.46
1:B:280:PHE:HZ	1:B:324:VAL:HG21	1.81	0.46
1:C:130:ARG:NH1	1:C:236:VAL:C	2.70	0.46
1:A:130:ARG:HB3	1:A:237:GLN:N	2.30	0.46
1:A:289:THR:O	1:A:290:LEU:HG	2.14	0.46
1:B:101:PRO:CG	1:B:217:TYR:HD2	2.26	0.46
1:B:279:HIS:CB	1:B:280:PHE:N	2.78	0.46
1:C:71:THR:HG23	1:C:71:THR:O	2.16	0.46
1:C:174:GLY:O	1:C:175:CYS:CB	2.63	0.46
1:C:201:ILE:C	1:C:281:LEU:HG	2.39	0.46
1:C:269:LYS:C	1:C:277:ASP:CB	2.63	0.46
1:C:290:LEU:HB2	1:C:346:TRP:HA	1.96	0.46
1:A:162:PRO:O	1:A:163:PRO:O	2.33	0.46
1:A:230:VAL:CG1	1:A:231:ARG:H	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:PHE:HZ	1:A:324:VAL:HG21	1.81	0.46
1:A:290:LEU:HD23	1:A:346:TRP:HB2	1.90	0.46
1:B:89:LEU:HD23	1:B:90:ILE:N	2.28	0.46
1:B:230:VAL:CG1	1:B:231:ARG:H	2.28	0.46
1:B:249:GLN:CG	1:B:263:VAL:O	2.64	0.46
1:B:259:GLY:C	1:B:260:PRO:CD	2.84	0.46
1:B:295:ALA:HB2	1:B:315:ALA:CB	2.38	0.46
1:C:125:GLN:CA	1:C:243:GLY:HA2	2.27	0.46
1:C:234:TYR:CD2	1:C:236:VAL:HG23	2.51	0.46
1:A:291:PHE:HD2	1:A:346:TRP:HE3	1.63	0.46
1:B:112:GLU:HG3	1:B:112:GLU:O	2.16	0.46
1:C:289:THR:O	1:C:290:LEU:HG	2.14	0.46
1:C:292:TYR:CD1	1:C:292:TYR:C	2.93	0.46
1:A:112:GLU:O	1:A:112:GLU:HG3	2.16	0.46
1:B:290:LEU:HD13	1:B:291:PHE:HB3	1.98	0.46
1:B:297:VAL:HG12	1:B:336:VAL:HG11	0.97	0.46
1:C:149:LYS:HE2	1:C:151:ALA:HB2	1.96	0.46
1:C:249:GLN:CG	1:C:263:VAL:O	2.64	0.46
1:A:249:GLN:CG	1:A:263:VAL:O	2.64	0.46
1:A:271:THR:HG23	1:A:275:GLU:HG2	1.97	0.46
1:B:130:ARG:HB3	1:B:237:GLN:N	2.30	0.46
1:C:160:LYS:N	1:C:328:GLU:OE1	2.49	0.46
1:C:197:VAL:HG21	1:C:350:ARG:NH1	2.30	0.46
1:C:201:ILE:CD1	1:C:266:SER:HA	2.46	0.46
1:C:230:VAL:CG1	1:C:231:ARG:H	2.28	0.46
1:A:90:ILE:HD11	1:A:232:VAL:HG22	1.83	0.46
1:B:269:LYS:CE	1:B:270:GLY:O	2.63	0.46
1:B:276:HIS:CG	1:B:277:ASP:N	2.74	0.46
1:C:136:PHE:CE2	1:C:212:LEU:HD21	2.51	0.46
1:A:82:ILE:HG21	1:A:82:ILE:HD13	1.78	0.46
1:A:90:ILE:O	1:A:90:ILE:CG2	2.54	0.46
1:A:174:GLY:O	1:A:175:CYS:CB	2.64	0.46
1:A:185:ILE:HD12	1:A:186:LEU:H	0.65	0.46
1:A:279:HIS:CB	1:A:280:PHE:N	2.78	0.46
1:A:341:GLN:O	1:A:342:PRO:C	2.58	0.46
1:B:271:THR:HG23	1:B:275:GLU:HG2	1.97	0.46
1:B:313:GLU:HG3	1:B:315:ALA:HA	1.97	0.46
1:C:127:GLU:O	1:C:128:LYS:CG	2.64	0.46
1:C:169:LEU:C	1:C:171:ASN:H	2.23	0.46
1:C:207:VAL:H	1:C:329:ARG:NH1	2.13	0.46
1:A:97:THR:O	1:A:97:THR:OG1	2.25	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:TYR:CD2	1:A:236:VAL:HG23	2.50	0.46
1:C:207:VAL:N	1:C:329:ARG:CZ	2.64	0.46
1:B:289:THR:O	1:B:290:LEU:HG	2.14	0.45
1:C:271:THR:HG23	1:C:275:GLU:HG2	1.97	0.45
1:C:279:HIS:CB	1:C:280:PHE:N	2.78	0.45
1:A:101:PRO:CG	1:A:217:TYR:CE2	2.74	0.45
1:A:107:VAL:HG22	1:A:211:LYS:HB3	1.97	0.45
1:B:127:GLU:O	1:B:128:LYS:CG	2.64	0.45
1:B:149:LYS:O	1:B:216:THR:HA	2.15	0.45
1:C:89:LEU:HA	1:C:230:VAL:O	2.16	0.45
1:C:133:SER:CA	1:C:235:THR:HG22	2.46	0.45
1:C:181:TRP:O	1:C:181:TRP:CE3	2.69	0.45
1:A:95:LYS:HZ1	1:A:221:ALA:HB1	1.80	0.45
1:A:181:TRP:O	1:A:181:TRP:CE3	2.69	0.45
1:A:253:PHE:HZ	1:A:268:THR:HG21	1.82	0.45
1:B:292:TYR:C	1:B:292:TYR:CD1	2.94	0.45
1:C:201:ILE:HG23	1:C:281:LEU:HD23	1.93	0.45
1:A:338:THR:OG1	1:A:339:GLU:CA	2.63	0.45
1:C:84:ARG:CD	1:C:119:LEU:HD13	2.46	0.45
1:C:163:PRO:CG	1:C:168:SER:HB3	2.44	0.45
1:C:280:PHE:HZ	1:C:324:VAL:HG21	1.81	0.45
1:A:101:PRO:HG2	1:A:166:LEU:HD12	1.94	0.45
1:A:127:GLU:O	1:A:128:LYS:CG	2.64	0.45
1:A:290:LEU:HD13	1:A:291:PHE:HB3	1.98	0.45
1:A:295:ALA:HB2	1:A:315:ALA:HB3	1.99	0.45
1:A:313:GLU:HG3	1:A:315:ALA:HA	1.97	0.45
1:A:326:VAL:HG13	1:A:331:GLN:OE1	2.17	0.45
1:B:84:ARG:CD	1:B:119:LEU:HD13	2.46	0.45
1:B:234:TYR:CD2	1:B:236:VAL:HG23	2.51	0.45
1:B:295:ALA:HB2	1:B:315:ALA:HB3	1.99	0.45
1:C:60:ALA:HA	1:C:61:PRO:HD2	1.81	0.45
1:C:204:PRO:CG	1:C:328:GLU:HG3	2.05	0.45
1:A:236:VAL:CG1	1:A:238:LEU:CD1	2.94	0.45
1:A:269:LYS:CE	1:A:270:GLY:O	2.63	0.45
1:B:181:TRP:CE3	1:B:181:TRP:O	2.69	0.45
1:C:109:ASN:OD1	1:C:129:TYR:OH	2.32	0.45
1:C:278:CYS:HB3	1:C:333:VAL:C	2.35	0.45
1:A:136:PHE:CE2	1:A:212:LEU:HD21	2.51	0.45
1:A:149:LYS:O	1:A:216:THR:HA	2.15	0.45
1:C:153:ALA:HB2	1:C:175:CYS:N	2.32	0.45
1:C:236:VAL:CG1	1:C:238:LEU:CD1	2.94	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:291:PHE:HD2	1:C:346:TRP:HE3	1.63	0.45
1:C:288:LEU:CD1	1:C:290:LEU:CG	2.70	0.45
1:C:290:LEU:HD13	1:C:291:PHE:HB3	1.98	0.45
1:C:315:ALA:O	1:C:318:SER:N	2.50	0.45
1:A:89:LEU:HA	1:A:230:VAL:O	2.17	0.45
1:A:149:LYS:HD3	1:A:217:TYR:HE1	1.73	0.45
1:A:152:LEU:C	1:A:186:LEU:HD12	2.40	0.45
1:A:269:LYS:O	1:A:277:ASP:CA	2.57	0.45
1:A:278:CYS:CA	1:A:334:LYS:HD3	2.42	0.45
1:A:315:ALA:O	1:A:318:SER:N	2.50	0.45
1:B:90:ILE:HD11	1:B:232:VAL:HG22	1.83	0.45
1:B:271:THR:CG2	1:B:275:GLU:HG2	2.47	0.45
1:C:112:GLU:O	1:C:112:GLU:HG3	2.16	0.45
1:A:109:ASN:CG	1:A:110:PRO:HD2	2.40	0.45
1:A:149:LYS:CG	1:A:217:TYR:HE1	2.29	0.45
1:A:262:LEU:HA	1:A:262:LEU:HD23	1.71	0.45
1:A:277:ASP:HA	1:A:334:LYS:HZ2	1.81	0.45
1:A:292:TYR:CD1	1:A:292:TYR:C	2.94	0.45
1:C:68:GLU:CD	1:C:139:SER:OG	2.59	0.45
1:C:113:PRO:CD	1:C:285:ASN:O	2.65	0.45
1:C:118:GLN:O	1:C:118:GLN:HG2	2.17	0.45
1:A:84:ARG:CD	1:A:119:LEU:HD13	2.46	0.44
1:A:271:THR:CG2	1:A:275:GLU:HG2	2.47	0.44
1:B:89:LEU:HA	1:B:230:VAL:O	2.17	0.44
1:B:107:VAL:HG22	1:B:211:LYS:HB3	1.98	0.44
1:B:133:SER:CA	1:B:235:THR:HG22	2.47	0.44
1:B:134:LEU:C	1:B:233:GLU:O	2.54	0.44
1:B:213:ILE:HG23	1:B:214:MET:N	2.32	0.44
1:C:119:LEU:C	1:C:121:LYS:H	2.25	0.44
1:A:133:SER:N	1:A:235:THR:CG2	2.74	0.44
1:A:309:SER:C	1:A:322:ALA:HA	2.20	0.44
1:B:82:ILE:HG21	1:B:82:ILE:HD13	1.78	0.44
1:B:118:GLN:O	1:B:118:GLN:HG2	2.17	0.44
1:B:149:LYS:CG	1:B:217:TYR:HE1	2.29	0.44
1:B:315:ALA:O	1:B:318:SER:N	2.50	0.44
1:C:101:PRO:CD	1:C:217:TYR:HD2	2.30	0.44
1:C:253:PHE:HZ	1:C:268:THR:HG21	1.82	0.44
1:A:82:ILE:O	1:A:83:THR:OG1	2.18	0.44
1:A:105:THR:HA	1:A:212:LEU:O	2.18	0.44
1:A:122:GLU:O	1:A:122:GLU:CG	2.64	0.44
1:A:133:SER:CA	1:A:235:THR:HG22	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:PRO:HD3	1:B:166:LEU:HD11	0.47	0.44
1:C:105:THR:HA	1:C:212:LEU:O	2.18	0.44
1:C:268:THR:O	1:C:268:THR:CG2	2.66	0.44
1:C:326:VAL:HG13	1:C:331:GLN:OE1	2.17	0.44
1:A:101:PRO:CD	1:A:217:TYR:HD2	2.30	0.44
1:B:136:PHE:CE2	1:B:212:LEU:HD21	2.51	0.44
1:C:111:SER:O	1:C:350:ARG:NE	2.48	0.44
1:A:119:LEU:C	1:A:121:LYS:H	2.25	0.44
1:A:199:ASP:OD1	1:A:199:ASP:N	2.40	0.44
1:B:101:PRO:CD	1:B:217:TYR:HD2	2.30	0.44
1:B:101:PRO:HB3	1:B:217:TYR:CD2	2.53	0.44
1:B:326:VAL:HG13	1:B:331:GLN:OE1	2.17	0.44
1:C:95:LYS:NZ	1:C:221:ALA:C	2.76	0.44
1:C:163:PRO:HG3	1:C:168:SER:CB	2.48	0.44
1:C:333:VAL:C	1:C:334:LYS:CG	2.91	0.44
1:A:333:VAL:C	1:A:334:LYS:CG	2.91	0.44
1:B:109:ASN:CG	1:B:110:PRO:HD2	2.40	0.44
1:C:56:THR:HG23	1:C:57:ARG:HB3	1.99	0.44
1:C:109:ASN:O	1:C:111:SER:N	2.50	0.44
1:C:133:SER:N	1:C:235:THR:CG2	2.74	0.44
1:C:137:ARG:N	1:C:230:VAL:HG13	2.33	0.44
1:C:295:ALA:HB2	1:C:315:ALA:HB3	1.98	0.44
1:C:341:GLN:O	1:C:342:PRO:C	2.58	0.44
1:A:153:ALA:HB2	1:A:175:CYS:N	2.32	0.44
1:B:277:ASP:CG	1:B:279:HIS:HD1	2.18	0.44
1:C:101:PRO:HD3	1:C:166:LEU:HD11	0.47	0.44
1:C:159:ALA:CB	1:C:328:GLU:OE1	2.55	0.44
1:C:213:ILE:HG23	1:C:214:MET:N	2.32	0.44
1:A:96:ASN:O	1:A:97:THR:C	2.52	0.44
1:B:84:ARG:NE	1:B:119:LEU:CD1	2.81	0.44
1:B:105:THR:HA	1:B:212:LEU:O	2.18	0.44
1:B:248:ALA:HB3	1:B:249:GLN:HB3	1.87	0.44
1:C:72:GLN:HE21	1:C:73:PRO:HD2	1.83	0.44
1:C:134:LEU:N	1:C:233:GLU:O	2.44	0.44
1:C:170:TYR:C	1:C:171:ASN:ND2	2.72	0.44
1:A:118:GLN:O	1:A:118:GLN:HG2	2.17	0.44
1:A:252:ASP:OD2	1:A:345:LYS:HG2	2.16	0.44
1:A:300:LEU:HD12	1:A:300:LEU:HA	1.28	0.44
1:B:304:ASP:OD2	1:B:331:GLN:CA	2.57	0.44
1:B:333:VAL:C	1:B:334:LYS:CG	2.91	0.44
1:C:130:ARG:HD2	1:C:237:GLN:CD	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:262:LEU:HD23	1:C:262:LEU:HA	1.71	0.44
1:A:96:ASN:O	1:A:96:ASN:ND2	2.51	0.43
1:B:105:THR:OG1	1:B:211:LYS:HD2	2.03	0.43
1:B:109:ASN:O	1:B:111:SER:N	2.50	0.43
1:B:119:LEU:C	1:B:121:LYS:H	2.25	0.43
1:B:134:LEU:CD2	1:B:188:VAL:HG22	2.41	0.43
1:B:153:ALA:HB2	1:B:175:CYS:N	2.32	0.43
1:B:236:VAL:CG1	1:B:238:LEU:CD1	2.94	0.43
1:C:76:SER:OG	1:C:77:THR:N	2.50	0.43
1:C:113:PRO:HD3	1:C:351:ILE:O	2.18	0.43
1:C:154:PHE:CZ	1:C:156:ARG:CA	3.01	0.43
1:C:197:VAL:HG22	1:C:350:ARG:CZ	2.48	0.43
1:C:271:THR:CG2	1:C:275:GLU:HG2	2.47	0.43
1:A:109:ASN:O	1:A:111:SER:N	2.50	0.43
1:A:326:VAL:CG1	1:A:327:ALA:N	2.19	0.43
1:B:149:LYS:HD3	1:B:217:TYR:HE1	1.73	0.43
1:C:101:PRO:HB3	1:C:217:TYR:CD2	2.53	0.43
1:C:152:LEU:C	1:C:186:LEU:HD12	2.40	0.43
1:C:259:GLY:C	1:C:260:PRO:CD	2.84	0.43
1:A:130:ARG:NH1	1:A:236:VAL:C	2.70	0.43
1:A:203:ASP:CG	1:A:205:LYS:CD	2.64	0.43
1:A:254:ALA:O	1:A:257:LYS:N	2.38	0.43
1:B:163:PRO:HG3	1:B:168:SER:CB	2.47	0.43
1:B:253:PHE:HZ	1:B:268:THR:HG21	1.82	0.43
1:B:269:LYS:O	1:B:277:ASP:CA	2.57	0.43
1:B:339:GLU:O	1:B:340:GLU:CA	2.60	0.43
1:C:149:LYS:CG	1:C:217:TYR:HE1	2.29	0.43
1:C:243:GLY:O	1:C:244:SER:CB	2.67	0.43
1:A:137:ARG:N	1:A:230:VAL:HG13	2.33	0.43
1:B:96:ASN:O	1:B:96:ASN:ND2	2.51	0.43
1:C:70:SER:O	1:C:71:THR:C	2.62	0.43
1:C:121:LYS:HG3	1:C:121:LYS:O	2.19	0.43
1:A:89:LEU:HD23	1:A:90:ILE:N	2.28	0.43
1:A:101:PRO:HB3	1:A:217:TYR:CD2	2.53	0.43
1:A:125:GLN:CA	1:A:243:GLY:HA2	2.27	0.43
1:A:139:SER:HA	1:A:140:PRO:HD3	1.13	0.43
1:A:213:ILE:HG23	1:A:214:MET:N	2.32	0.43
1:A:216:THR:OG1	1:A:227:LEU:HD21	2.18	0.43
1:A:315:ALA:CA	1:A:318:SER:HB2	2.49	0.43
1:A:325:LYS:HG2	1:A:325:LYS:O	2.18	0.43
1:B:137:ARG:N	1:B:230:VAL:HG13	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:ARG:NE	1:C:119:LEU:CD1	2.81	0.43
1:B:112:GLU:HG2	1:B:329:ARG:HH22	1.83	0.43
1:B:121:LYS:O	1:B:121:LYS:HG3	2.19	0.43
1:B:242:THR:CG2	1:B:243:GLY:N	2.73	0.43
1:C:109:ASN:CG	1:C:110:PRO:HD2	2.40	0.43
1:C:203:ASP:CG	1:C:205:LYS:CD	2.64	0.43
1:C:291:PHE:CE1	1:C:335:MET:CE	2.90	0.43
1:A:101:PRO:HD3	1:A:166:LEU:HD11	0.47	0.43
1:A:121:LYS:HG3	1:A:121:LYS:O	2.19	0.43
1:B:96:ASN:O	1:B:97:THR:C	2.53	0.43
1:B:278:CYS:O	1:B:333:VAL:O	2.37	0.43
1:C:254:ALA:O	1:C:257:LYS:N	2.38	0.43
1:B:130:ARG:HD2	1:B:237:GLN:CD	2.43	0.43
1:A:84:ARG:NE	1:A:119:LEU:CD1	2.81	0.43
1:A:150:VAL:C	1:A:151:ALA:O	2.62	0.43
1:A:274:TRP:NE1	1:A:339:GLU:C	2.75	0.43
1:B:216:THR:OG1	1:B:227:LEU:HD21	2.18	0.43
1:C:87:SER:HA	1:C:231:ARG:HD2	2.01	0.43
1:C:95:LYS:HZ3	1:C:225:ALA:N	1.96	0.43
1:B:273:GLY:O	1:B:275:GLU:HB3	2.19	0.43
1:B:288:LEU:O	1:B:289:THR:OG1	2.37	0.43
1:B:311:LEU:N	1:B:311:LEU:CD1	2.82	0.43
1:B:325:LYS:O	1:B:325:LYS:HG2	2.18	0.43
1:C:130:ARG:HD3	1:C:236:VAL:C	2.40	0.43
1:C:154:PHE:CE1	1:C:156:ARG:CA	3.02	0.43
1:C:325:LYS:O	1:C:325:LYS:HG2	2.18	0.43
1:A:130:ARG:HD2	1:A:237:GLN:CD	2.43	0.42
1:B:255:GLY:HA2	1:B:342:PRO:CB	2.25	0.42
1:C:125:GLN:HA	1:C:243:GLY:N	2.34	0.42
1:A:125:GLN:HA	1:A:243:GLY:N	2.34	0.42
1:A:278:CYS:HB3	1:A:333:VAL:C	2.35	0.42
1:A:278:CYS:O	1:A:333:VAL:O	2.37	0.42
1:B:258:ASP:OD1	1:B:259:GLY:N	2.52	0.42
1:C:96:ASN:O	1:C:96:ASN:ND2	2.52	0.42
1:C:137:ARG:O	1:C:230:VAL:HA	2.19	0.42
1:C:266:SER:HA	1:C:280:PHE:HA	2.02	0.42
1:A:113:PRO:HB2	1:A:329:ARG:HG3	1.96	0.42
1:A:137:ARG:O	1:A:230:VAL:HA	2.19	0.42
1:A:242:THR:CG2	1:A:243:GLY:N	2.73	0.42
1:A:293:GLU:CA	1:A:317:GLY:HA2	2.50	0.42
1:A:309:SER:O	1:A:321:TRP:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:SER:HB3	1:B:197:VAL:HG21	2.01	0.42
1:B:278:CYS:HB3	1:B:333:VAL:C	2.35	0.42
1:C:236:VAL:CG1	1:C:238:LEU:HD11	2.50	0.42
1:A:130:ARG:HD3	1:A:236:VAL:C	2.40	0.42
1:A:134:LEU:CD2	1:A:188:VAL:HG22	2.41	0.42
1:A:288:LEU:O	1:A:289:THR:OG1	2.37	0.42
1:B:137:ARG:O	1:B:230:VAL:HA	2.19	0.42
1:B:293:GLU:CA	1:B:317:GLY:HA2	2.50	0.42
1:C:120:ILE:CG1	1:C:351:ILE:C	2.91	0.42
1:C:273:GLY:O	1:C:275:GLU:HB3	2.19	0.42
1:C:302:ASN:HB3	1:C:308:PHE:CE1	2.55	0.42
1:C:304:ASP:OD2	1:C:331:GLN:CA	2.57	0.42
1:A:154:PHE:CE1	1:A:156:ARG:CA	3.02	0.42
1:A:269:LYS:C	1:A:277:ASP:CB	2.63	0.42
1:B:302:ASN:HB3	1:B:308:PHE:CE1	2.55	0.42
1:B:309:SER:O	1:B:321:TRP:C	2.63	0.42
1:C:293:GLU:CA	1:C:317:GLY:HA2	2.50	0.42
1:A:243:GLY:O	1:A:244:SER:CB	2.67	0.42
1:A:266:SER:HA	1:A:280:PHE:HA	2.02	0.42
1:A:268:THR:O	1:A:268:THR:CG2	2.66	0.42
1:B:297:VAL:HB	1:B:336:VAL:CG1	1.98	0.42
1:B:343:LYS:HB2	1:B:344:GLY:H	1.13	0.42
1:C:112:GLU:CA	1:C:284:GLY:CA	2.96	0.42
1:C:201:ILE:HG22	1:C:264:SER:OG	2.20	0.42
1:C:289:THR:CG2	1:C:321:TRP:CZ3	3.03	0.42
1:C:315:ALA:CA	1:C:318:SER:HB2	2.49	0.42
1:A:87:SER:HA	1:A:231:ARG:HD2	2.01	0.42
1:A:273:GLY:O	1:A:275:GLU:HB3	2.19	0.42
1:B:130:ARG:NH1	1:B:236:VAL:C	2.70	0.42
1:B:154:PHE:CE1	1:B:156:ARG:CA	3.02	0.42
1:B:162:PRO:O	1:B:163:PRO:C	2.51	0.42
1:C:94:LYS:C	1:C:95:LYS:O	2.63	0.42
1:C:101:PRO:HG2	1:C:166:LEU:HD12	1.94	0.42
1:C:163:PRO:CG	1:C:168:SER:HB2	2.50	0.42
1:C:216:THR:OG1	1:C:227:LEU:HD21	2.18	0.42
1:C:258:ASP:OD1	1:C:259:GLY:N	2.52	0.42
1:C:269:LYS:CG	1:C:270:GLY:H	2.23	0.42
1:C:276:HIS:CG	1:C:277:ASP:N	2.74	0.42
1:A:94:LYS:C	1:A:95:LYS:O	2.63	0.42
1:A:296:PRO:HD2	1:A:337:THR:CG2	2.49	0.42
1:A:302:ASN:HB3	1:A:308:PHE:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:VAL:C	1:B:151:ALA:O	2.62	0.42
1:B:157:ASP:C	1:B:159:ALA:H	2.27	0.42
1:A:157:ASP:C	1:A:159:ALA:H	2.27	0.42
1:A:163:PRO:CG	1:A:168:SER:HB2	2.50	0.42
1:A:289:THR:CG2	1:A:321:TRP:CZ3	3.03	0.42
1:A:313:GLU:HB2	1:A:315:ALA:CA	2.50	0.42
1:B:87:SER:HA	1:B:231:ARG:HD2	2.01	0.42
1:B:93:LEU:HD12	1:B:138:TYR:CE1	2.54	0.42
1:B:130:ARG:HD3	1:B:236:VAL:C	2.40	0.42
1:B:133:SER:CB	1:B:235:THR:CG2	2.94	0.42
1:B:185:ILE:HD12	1:B:186:LEU:O	2.20	0.42
1:B:243:GLY:O	1:B:244:SER:CB	2.66	0.42
1:B:315:ALA:HB1	1:B:318:SER:HB3	1.72	0.42
1:B:315:ALA:CA	1:B:318:SER:HB2	2.49	0.42
1:B:336:VAL:O	1:B:336:VAL:CG1	2.67	0.42
1:C:75:VAL:HG12	1:C:76:SER:N	2.35	0.42
1:A:93:LEU:HD12	1:A:138:TYR:CE1	2.54	0.42
1:A:101:PRO:CG	1:A:217:TYR:HD2	2.26	0.42
1:A:134:LEU:N	1:A:233:GLU:O	2.44	0.42
1:A:162:PRO:O	1:A:163:PRO:C	2.50	0.42
1:A:185:ILE:HD12	1:A:186:LEU:O	2.20	0.42
1:A:248:ALA:HB1	1:A:265:TRP:CA	2.38	0.42
1:A:258:ASP:OD1	1:A:259:GLY:N	2.52	0.42
1:A:259:GLY:C	1:A:260:PRO:CD	2.84	0.42
1:A:315:ALA:CA	1:A:318:SER:CB	2.97	0.42
1:B:149:LYS:CD	1:B:217:TYR:HE1	2.33	0.42
1:B:236:VAL:CG1	1:B:238:LEU:HD11	2.50	0.42
1:B:315:ALA:C	1:B:318:SER:H	2.28	0.42
1:C:107:VAL:HG11	1:C:283:THR:HG22	2.02	0.42
1:C:157:ASP:C	1:C:159:ALA:H	2.27	0.42
1:C:207:VAL:HG11	1:C:329:ARG:NE	2.24	0.42
1:C:336:VAL:O	1:C:336:VAL:CG1	2.66	0.42
1:A:141:MET:O	1:A:141:MET:CG	2.46	0.41
1:C:150:VAL:C	1:C:151:ALA:O	2.62	0.41
1:C:315:ALA:C	1:C:318:SER:H	2.28	0.41
1:A:130:ARG:HB2	1:A:237:GLN:CA	2.49	0.41
1:A:236:VAL:CG1	1:A:238:LEU:HD11	2.49	0.41
1:B:254:ALA:O	1:B:257:LYS:N	2.38	0.41
1:B:289:THR:CG2	1:B:321:TRP:CZ3	3.03	0.41
1:B:315:ALA:CA	1:B:318:SER:CB	2.97	0.41
1:B:350:ARG:C	1:B:351:ILE:CG2	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:GLU:O	1:C:231:ARG:HB3	2.05	0.41
1:C:264:SER:OG	1:C:265:TRP:CA	2.69	0.41
1:C:269:LYS:CE	1:C:270:GLY:O	2.63	0.41
1:A:149:LYS:CD	1:A:217:TYR:HE1	2.34	0.41
1:A:154:PHE:CZ	1:A:156:ARG:CA	3.01	0.41
1:A:197:VAL:CG2	1:A:198:ALA:H	2.34	0.41
1:A:291:PHE:CD1	1:A:335:MET:HE1	2.53	0.41
1:B:125:GLN:HA	1:B:243:GLY:N	2.34	0.41
1:B:139:SER:HA	1:B:140:PRO:HD3	1.13	0.41
1:C:93:LEU:CD1	1:C:138:TYR:HE1	2.33	0.41
1:C:141:MET:O	1:C:141:MET:CG	2.46	0.41
1:C:326:VAL:HG13	1:C:331:GLN:CD	2.45	0.41
1:A:93:LEU:CD1	1:A:138:TYR:HE1	2.33	0.41
1:A:291:PHE:CD2	1:A:345:LYS:O	2.73	0.41
1:B:264:SER:OG	1:B:265:TRP:CA	2.69	0.41
1:C:309:SER:O	1:C:321:TRP:C	2.63	0.41
1:A:130:ARG:CG	1:A:131:PHE:N	2.79	0.41
1:A:151:ALA:HA	1:A:177:SER:CB	2.21	0.41
1:A:306:SER:HB2	1:A:325:LYS:N	2.33	0.41
1:B:125:GLN:CA	1:B:243:GLY:HA2	2.27	0.41
1:B:154:PHE:CZ	1:B:156:ARG:CA	3.02	0.41
1:B:197:VAL:CG2	1:B:198:ALA:H	2.34	0.41
1:C:66:TYR:HE2	1:C:183:GLY:CA	2.33	0.41
1:C:185:ILE:HD12	1:C:186:LEU:O	2.20	0.41
1:C:278:CYS:O	1:C:333:VAL:O	2.37	0.41
1:A:126:TYR:O	1:A:242:THR:CG2	2.66	0.41
1:A:128:LYS:O	1:A:238:LEU:HA	2.21	0.41
1:A:163:PRO:HG3	1:A:168:SER:CB	2.47	0.41
1:B:136:PHE:CE2	1:B:212:LEU:HD13	2.56	0.41
1:B:203:ASP:CG	1:B:205:LYS:CD	2.64	0.41
1:B:289:THR:O	1:B:290:LEU:CG	2.69	0.41
1:C:135:ARG:N	1:C:233:GLU:O	2.54	0.41
1:A:249:GLN:HG3	1:A:263:VAL:O	2.21	0.41
1:A:297:VAL:HG12	1:A:336:VAL:HG11	0.98	0.41
1:B:120:ILE:HG13	1:B:350:ARG:HH12	1.19	0.41
1:B:249:GLN:HG3	1:B:263:VAL:O	2.21	0.41
1:B:337:THR:OG1	1:B:343:LYS:NZ	2.42	0.41
1:C:269:LYS:O	1:C:277:ASP:CA	2.57	0.41
1:C:315:ALA:CA	1:C:318:SER:CB	2.97	0.41
1:A:253:PHE:CZ	1:A:268:THR:HG21	2.56	0.41
1:A:264:SER:OG	1:A:265:TRP:CA	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:LEU:CD1	1:B:138:TYR:CE1	3.03	0.41
1:B:262:LEU:HA	1:B:262:LEU:HD23	1.71	0.41
1:C:90:ILE:HG21	1:C:90:ILE:HD13	1.83	0.41
1:C:249:GLN:HG3	1:C:263:VAL:O	2.21	0.41
1:C:289:THR:O	1:C:290:LEU:CG	2.69	0.41
1:A:93:LEU:CD1	1:A:138:TYR:CE1	3.03	0.41
1:A:111:SER:HB3	1:A:197:VAL:HG21	2.02	0.41
1:A:135:ARG:N	1:A:233:GLU:O	2.54	0.41
1:A:172:ILE:HD13	1:A:172:ILE:HG21	1.88	0.41
1:A:308:PHE:HE1	1:A:333:VAL:CG1	2.34	0.41
1:A:326:VAL:HG13	1:A:331:GLN:CD	2.45	0.41
1:B:94:LYS:C	1:B:95:LYS:O	2.63	0.41
1:B:128:LYS:O	1:B:238:LEU:HA	2.21	0.41
1:B:130:ARG:CG	1:B:131:PHE:N	2.79	0.41
1:B:248:ALA:CB	1:B:249:GLN:HB2	2.47	0.41
1:B:274:TRP:NE1	1:B:339:GLU:C	2.75	0.41
1:B:296:PRO:HB2	1:B:297:VAL:H	0.85	0.41
1:B:313:GLU:HB2	1:B:315:ALA:CA	2.50	0.41
1:C:55:VAL:O	1:C:57:ARG:N	2.52	0.41
1:C:86:GLY:O	1:C:87:SER:CB	2.69	0.41
1:C:93:LEU:CD1	1:C:138:TYR:CE1	3.03	0.41
1:C:95:LYS:HB3	1:C:96:ASN:H	1.60	0.41
1:C:120:ILE:HG21	1:C:120:ILE:HD13	1.87	0.41
1:C:136:PHE:CG	1:C:212:LEU:HD21	2.56	0.41
1:C:191:ASP:HB2	1:C:192:SER:H	1.41	0.41
1:C:231:ARG:CG	1:C:232:VAL:H	2.27	0.41
1:C:252:ASP:OD2	1:C:345:LYS:HG2	2.16	0.41
1:C:253:PHE:CZ	1:C:268:THR:HG21	2.56	0.41
1:C:291:PHE:CD2	1:C:345:LYS:O	2.73	0.41
1:C:308:PHE:HE1	1:C:333:VAL:CG1	2.34	0.41
1:C:313:GLU:HB2	1:C:315:ALA:CA	2.50	0.41
1:A:289:THR:O	1:A:290:LEU:CG	2.69	0.41
1:B:93:LEU:CD1	1:B:138:TYR:HE1	2.33	0.41
1:C:128:LYS:O	1:C:238:LEU:HA	2.21	0.41
1:C:130:ARG:HB2	1:C:237:GLN:CA	2.49	0.41
1:C:252:ASP:O	1:C:258:ASP:C	2.64	0.41
1:A:302:ASN:HB3	1:A:308:PHE:CD1	2.56	0.40
1:B:134:LEU:N	1:B:233:GLU:O	2.44	0.40
1:B:135:ARG:N	1:B:233:GLU:O	2.54	0.40
1:B:163:PRO:CG	1:B:168:SER:HB2	2.50	0.40
1:B:291:PHE:CD2	1:B:345:LYS:O	2.73	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:LYS:O	1:B:296:PRO:CG	2.65	0.40
1:B:302:ASN:HB3	1:B:308:PHE:CD1	2.56	0.40
1:C:197:VAL:CG2	1:C:198:ALA:H	2.33	0.40
1:A:130:ARG:HB3	1:A:131:PHE:H	1.46	0.40
1:A:176:VAL:O	1:A:176:VAL:CG1	2.69	0.40
1:A:291:PHE:CE1	1:A:335:MET:CE	2.90	0.40
1:A:315:ALA:C	1:A:318:SER:H	2.28	0.40
1:B:95:LYS:HZ1	1:B:221:ALA:CB	2.34	0.40
1:B:95:LYS:HZ3	1:B:221:ALA:HA	1.79	0.40
1:B:244:SER:C	1:B:245:THR:CG2	2.93	0.40
1:B:269:LYS:C	1:B:277:ASP:CB	2.63	0.40
1:C:71:THR:HG23	1:C:87:SER:OG	2.03	0.40
1:C:75:VAL:N	1:C:75:VAL:CG2	2.84	0.40
1:C:82:ILE:HD13	1:C:238:LEU:HD22	2.03	0.40
1:C:176:VAL:O	1:C:176:VAL:CG1	2.69	0.40
1:C:296:PRO:HD2	1:C:337:THR:CG2	2.49	0.40
1:A:136:PHE:CG	1:A:212:LEU:HD21	2.56	0.40
1:A:246:SER:CB	1:A:263:VAL:HG13	2.52	0.40
1:B:136:PHE:CG	1:B:212:LEU:HD21	2.56	0.40
1:B:299:GLY:HA2	1:B:335:MET:HG2	2.03	0.40
1:B:308:PHE:HE1	1:B:333:VAL:CG1	2.34	0.40
1:C:91:THR:HG23	1:C:92:THR:N	2.36	0.40
1:C:302:ASN:HB3	1:C:308:PHE:CD1	2.56	0.40
1:C:313:GLU:H	1:C:313:GLU:HG2	1.62	0.40
1:C:341:GLN:HE21	1:C:341:GLN:HB2	1.72	0.40
1:A:86:GLY:O	1:A:87:SER:CB	2.69	0.40
1:A:190:THR:HG22	1:A:191:ASP:O	2.22	0.40
1:B:149:LYS:HG2	1:B:150:VAL:H	1.87	0.40
1:B:149:LYS:O	1:B:216:THR:OG1	2.36	0.40
1:B:176:VAL:O	1:B:176:VAL:CG1	2.69	0.40
1:B:190:THR:HG22	1:B:191:ASP:O	2.22	0.40
1:C:93:LEU:HD12	1:C:138:TYR:CE1	2.54	0.40
1:C:149:LYS:CD	1:C:217:TYR:HE1	2.33	0.40
1:C:297:VAL:HG12	1:C:336:VAL:HG11	0.98	0.40
1:A:91:THR:HG23	1:A:92:THR:N	2.36	0.40
1:A:256:VAL:HG13	1:A:257:LYS:N	2.37	0.40
1:A:336:VAL:O	1:A:336:VAL:CG1	2.67	0.40
1:B:86:GLY:O	1:B:87:SER:CB	2.69	0.40
1:B:326:VAL:HG13	1:B:331:GLN:CD	2.45	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 PDB entries followed by that with respect to all EM entries.

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	263/347 (76%)	144 (55%)	60 (23%)	59 (22%)	0	1
1	B	263/347 (76%)	144 (55%)	60 (23%)	59 (22%)	0	1
1	C	291/347 (84%)	161 (55%)	64 (22%)	66 (23%)	0	1
All	All	817/1041 (78%)	449 (55%)	184 (22%)	184 (22%)	0	1

All (184) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	83	THR
1	A	87	SER
1	A	90	ILE
1	A	95	LYS
1	A	96	ASN
1	A	97	THR
1	A	119	LEU
1	A	128	LYS
1	A	140	PRO
1	A	157	ASP
1	A	160	LYS
1	A	166	LEU
1	A	173	GLU
1	A	202	SER
1	A	209	PHE
1	A	227	LEU
1	A	240	ASN
1	A	244	SER
1	A	245	THR
1	A	246	SER
1	A	255	GLY
1	A	290	LEU
1	A	293	GLU
1	A	295	ALA

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Mol	Chain	Res	Type
1	A	307	ASP
1	A	316	ALA
1	A	329	ARG
1	A	339	GLU
1	A	341	GLN
1	B	83	THR
1	B	87	SER
1	B	90	ILE
1	B	95	LYS
1	B	96	ASN
1	B	97	THR
1	B	119	LEU
1	B	128	LYS
1	B	140	PRO
1	B	157	ASP
1	B	160	LYS
1	B	166	LEU
1	B	173	GLU
1	B	202	SER
1	B	209	PHE
1	B	227	LEU
1	B	240	ASN
1	B	244	SER
1	B	245	THR
1	B	246	SER
1	B	255	GLY
1	B	290	LEU
1	B	293	GLU
1	B	295	ALA
1	B	307	ASP
1	B	316	ALA
1	B	329	ARG
1	B	339	GLU
1	B	341	GLN
1	C	55	VAL
1	C	56	THR
1	C	77	THR
1	C	79	ARG
1	C	80	ASP
1	C	83	THR
1	C	87	SER
1	C	90	ILE

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Mol	Chain	Res	Type
1	C	95	LYS
1	C	96	ASN
1	C	97	THR
1	C	119	LEU
1	C	128	LYS
1	C	140	PRO
1	C	157	ASP
1	C	160	LYS
1	C	166	LEU
1	C	173	GLU
1	C	202	SER
1	C	209	PHE
1	C	227	LEU
1	C	240	ASN
1	C	244	SER
1	C	245	THR
1	C	246	SER
1	C	255	GLY
1	C	290	LEU
1	C	293	GLU
1	C	295	ALA
1	C	307	ASP
1	C	316	ALA
1	C	329	ARG
1	C	339	GLU
1	C	341	GLN
1	A	101	PRO
1	A	105	THR
1	A	114	GLY
1	A	115	THR
1	A	116	PHE
1	A	151	ALA
1	A	156	ARG
1	A	158	ALA
1	A	167	ALA
1	A	291	PHE
1	A	292	TYR
1	A	296	PRO
1	A	315	ALA
1	B	101	PRO
1	B	105	THR
1	B	114	GLY

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Mol	Chain	Res	Type
1	B	115	THR
1	B	116	PHE
1	B	151	ALA
1	B	156	ARG
1	B	158	ALA
1	B	167	ALA
1	B	291	PHE
1	B	292	TYR
1	B	296	PRO
1	B	315	ALA
1	C	69	VAL
1	C	101	PRO
1	C	105	THR
1	C	114	GLY
1	C	115	THR
1	C	116	PHE
1	C	151	ALA
1	C	156	ARG
1	C	158	ALA
1	C	167	ALA
1	C	291	PHE
1	C	292	TYR
1	C	296	PRO
1	C	315	ALA
1	A	145	THR
1	A	152	LEU
1	A	263	VAL
1	B	145	THR
1	B	152	LEU
1	B	263	VAL
1	C	145	THR
1	C	152	LEU
1	C	263	VAL
1	A	131	PHE
1	A	205	LYS
1	A	298	SER
1	A	343	LYS
1	B	131	PHE
1	B	205	LYS
1	B	298	SER
1	B	343	LYS
1	C	131	PHE

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Mol	Chain	Res	Type
1	C	205	LYS
1	C	298	SER
1	C	343	LYS
1	A	134	LEU
1	A	163	PRO
1	A	201	ILE
1	A	260	PRO
1	A	300	LEU
1	A	314	ALA
1	B	82	ILE
1	B	134	LEU
1	B	163	PRO
1	B	201	ILE
1	B	260	PRO
1	B	300	LEU
1	B	314	ALA
1	C	163	PRO
1	C	201	ILE
1	C	260	PRO
1	C	300	LEU
1	C	314	ALA
1	A	82	ILE
1	A	313	GLU
1	B	313	GLU
1	C	71	THR
1	C	82	ILE
1	C	134	LEU
1	C	313	GLU
1	A	297	VAL
1	B	297	VAL
1	C	297	VAL
1	A	259	GLY
1	B	259	GLY
1	C	259	GLY

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	215/282 (76%)	181 (84%)	34 (16%)	2	11
1	B	215/282 (76%)	181 (84%)	34 (16%)	2	11
1	C	238/282 (84%)	202 (85%)	36 (15%)	3	12
All	All	668/846 (79%)	564 (84%)	104 (16%)	4	12

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	LEU
1	A	91	THR
1	A	97	THR
1	A	108	LEU
1	A	120	ILE
1	A	128	LYS
1	A	129	TYR
1	A	134	LEU
1	A	135	ARG
1	A	145	THR
1	A	146	THR
1	A	150	VAL
1	A	152	LEU
1	A	154	PHE
1	A	164	ASN
1	A	165	ASP
1	A	169	LEU
1	A	176	VAL
1	A	185	ILE
1	A	192	SER
1	A	199	ASP
1	A	205	LYS
1	A	206	LEU
1	A	208	ASP
1	A	213	ILE
1	A	217	TYR
1	A	234	TYR
1	A	238	LEU
1	A	264	SER
1	A	275	GLU
1	A	292	TYR
1	A	300	LEU
1	A	313	GLU
1	A	339	GLU

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Mol	Chain	Res	Type
1	B	89	LEU
1	B	91	THR
1	B	97	THR
1	B	108	LEU
1	B	120	ILE
1	B	128	LYS
1	B	129	TYR
1	B	134	LEU
1	B	135	ARG
1	B	145	THR
1	B	146	THR
1	B	150	VAL
1	B	152	LEU
1	B	154	PHE
1	B	164	ASN
1	B	165	ASP
1	B	169	LEU
1	B	176	VAL
1	B	185	ILE
1	B	192	SER
1	B	199	ASP
1	B	205	LYS
1	B	206	LEU
1	B	208	ASP
1	B	213	ILE
1	B	217	TYR
1	B	234	TYR
1	B	238	LEU
1	B	264	SER
1	B	275	GLU
1	B	292	TYR
1	B	300	LEU
1	B	313	GLU
1	B	339	GLU
1	C	58	LEU
1	C	72	GLN
1	C	89	LEU
1	C	91	THR
1	C	97	THR
1	C	108	LEU
1	C	120	ILE
1	C	128	LYS

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Mol	Chain	Res	Type
1	C	129	TYR
1	C	134	LEU
1	C	135	ARG
1	C	145	THR
1	C	146	THR
1	C	150	VAL
1	C	152	LEU
1	C	154	PHE
1	C	164	ASN
1	C	165	ASP
1	C	169	LEU
1	C	176	VAL
1	C	185	ILE
1	C	192	SER
1	C	199	ASP
1	C	205	LYS
1	C	206	LEU
1	C	208	ASP
1	C	213	ILE
1	C	217	TYR
1	C	234	TYR
1	C	238	LEU
1	C	264	SER
1	C	275	GLU
1	C	292	TYR
1	C	300	LEU
1	C	313	GLU
1	C	339	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	ASN
1	A	164	ASN
1	A	171	ASN
1	A	237	GLN
1	A	240	ASN
1	A	285	ASN
1	A	341	GLN
1	B	96	ASN
1	B	164	ASN
1	B	171	ASN

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Mol	Chain	Res	Type
1	B	237	GLN
1	B	240	ASN
1	B	285	ASN
1	B	341	GLN
1	C	72	GLN
1	C	96	ASN
1	C	109	ASN
1	C	125	GLN
1	C	164	ASN
1	C	171	ASN
1	C	237	GLN
1	C	240	ASN
1	C	249	GLN
1	C	285	ASN
1	C	341	GLN

5.3.3 RNA [i](#)

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	22
1	A	21
1	B	21

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	248:ALA	C	249:GLN	N	10.35
1	C	248:ALA	C	249:GLN	N	4.25
1	B	248:ALA	C	249:GLN	N	4.13
1	A	259:GLY	C	260:PRO	N	1.97
1	B	259:GLY	C	260:PRO	N	1.97
1	C	259:GLY	C	260:PRO	N	1.97
1	A	82:ILE	C	83:THR	N	1.81
1	B	82:ILE	C	83:THR	N	1.81
1	C	82:ILE	C	83:THR	N	1.81
1	A	279:HIS	C	280:PHE	N	1.74
1	B	279:HIS	C	280:PHE	N	1.74
1	C	279:HIS	C	280:PHE	N	1.74
1	A	291:PHE	C	292:TYR	N	1.71
1	B	291:PHE	C	292:TYR	N	1.71
1	C	291:PHE	C	292:TYR	N	1.71
1	A	264:SER	C	265:TRP	N	1.68
1	A	339:GLU	C	340:GLU	N	1.68
1	B	264:SER	C	265:TRP	N	1.68
1	B	339:GLU	C	340:GLU	N	1.68
1	C	264:SER	C	265:TRP	N	1.68
1	C	339:GLU	C	340:GLU	N	1.68
1	C	53:GLN	C	54:LYS	N	1.67
1	A	319:VAL	C	320:GLN	N	1.61
1	B	319:VAL	C	320:GLN	N	1.61
1	C	319:VAL	C	320:GLN	N	1.61
1	A	175:CYS	C	176:VAL	N	1.19
1	B	175:CYS	C	176:VAL	N	1.19
1	C	175:CYS	C	176:VAL	N	1.19
1	A	299:GLY	C	300:LEU	N	1.18
1	B	299:GLY	C	300:LEU	N	1.18
1	C	299:GLY	C	300:LEU	N	1.18
1	A	298:SER	C	299:GLY	N	1.16
1	A	323:GLY	C	324:VAL	N	1.16
1	B	298:SER	C	299:GLY	N	1.16
1	B	323:GLY	C	324:VAL	N	1.16
1	C	298:SER	C	299:GLY	N	1.16
1	C	323:GLY	C	324:VAL	N	1.16

Continued on next page...

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	260:PRO	C	261:ARG	N	1.15
1	B	260:PRO	C	261:ARG	N	1.15
1	C	260:PRO	C	261:ARG	N	1.15
1	A	315:ALA	C	316:ALA	N	1.14
1	B	315:ALA	C	316:ALA	N	1.14
1	C	315:ALA	C	316:ALA	N	1.14
1	A	139:SER	C	140:PRO	N	1.12
1	A	200:GLY	C	201:ILE	N	1.12
1	A	308:PHE	C	309:SER	N	1.12
1	B	139:SER	C	140:PRO	N	1.12
1	B	200:GLY	C	201:ILE	N	1.12
1	B	308:PHE	C	309:SER	N	1.12
1	C	139:SER	C	140:PRO	N	1.12
1	C	200:GLY	C	201:ILE	N	1.12
1	C	308:PHE	C	309:SER	N	1.12
1	A	177:SER	C	178:SER	N	1.04
1	B	177:SER	C	178:SER	N	1.04
1	C	177:SER	C	178:SER	N	1.04
1	A	297:VAL	C	298:SER	N	1.00
1	B	297:VAL	C	298:SER	N	1.00
1	C	297:VAL	C	298:SER	N	1.00
1	A	288:LEU	C	289:THR	N	0.94
1	B	288:LEU	C	289:THR	N	0.94
1	C	288:LEU	C	289:THR	N	0.94
1	A	201:ILE	C	202:SER	N	0.36
1	B	201:ILE	C	202:SER	N	0.36
1	C	201:ILE	C	202:SER	N	0.36

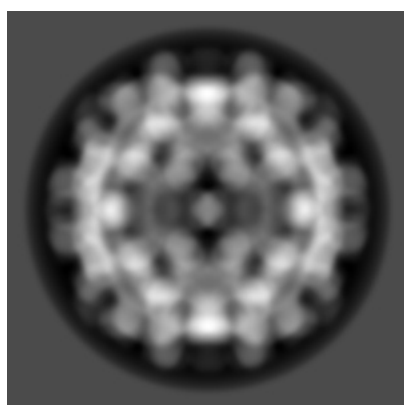
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-1864. These allow visual inspection of the internal detail of the map and identification of artifacts.

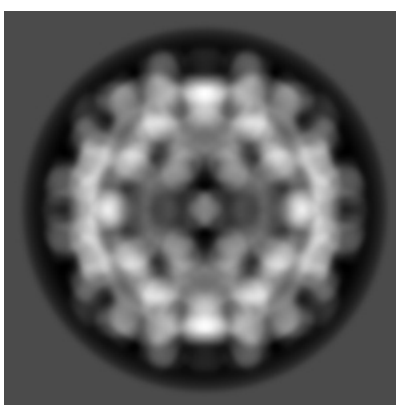
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

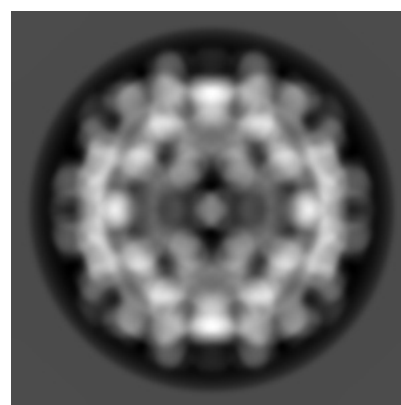
6.1.1 Primary map



X



Y



Z

The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 120



Y Index: 120



Z Index: 120

The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 120



Y Index: 120

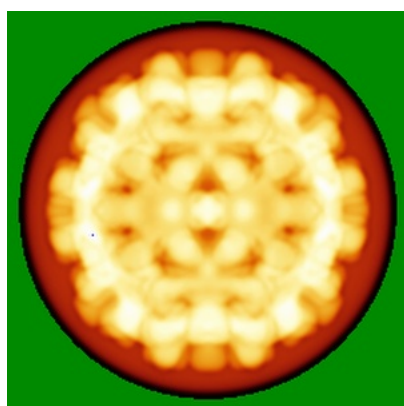


Z Index: 120

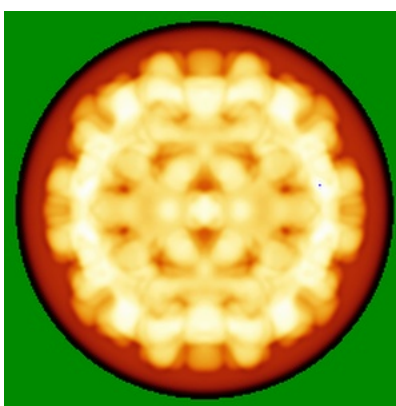
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

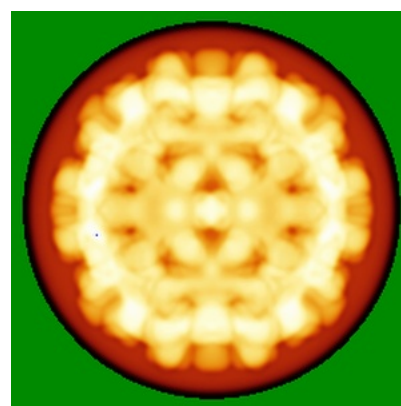
6.4.1 Primary map



X



Y

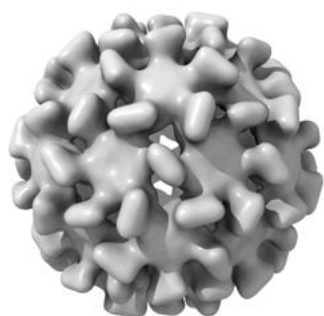


Z

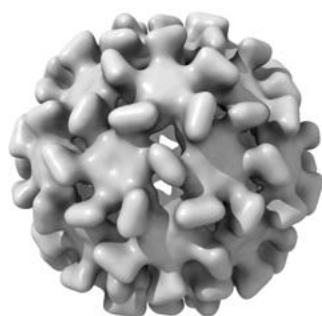
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

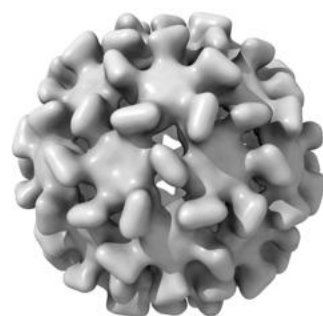
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

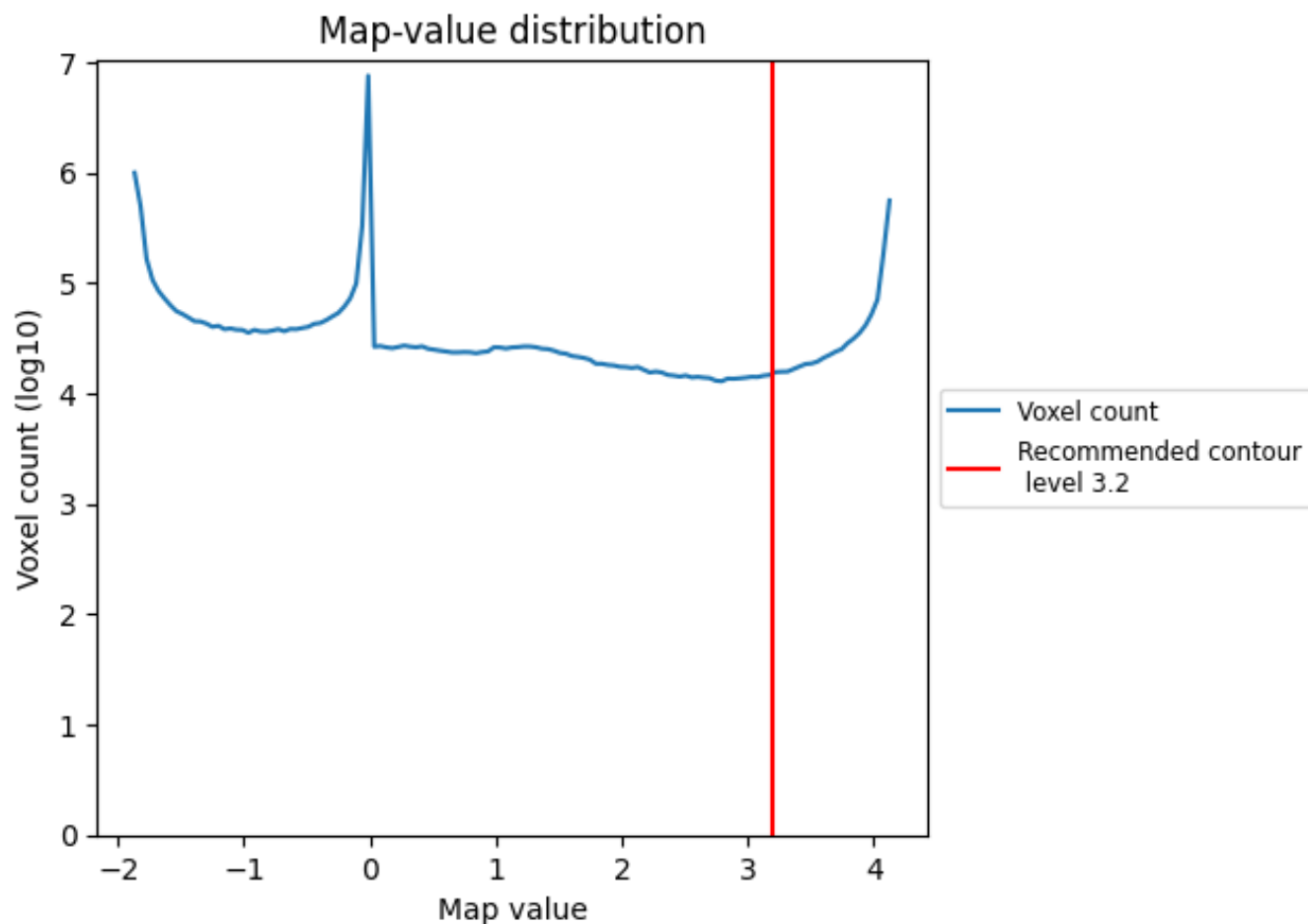
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

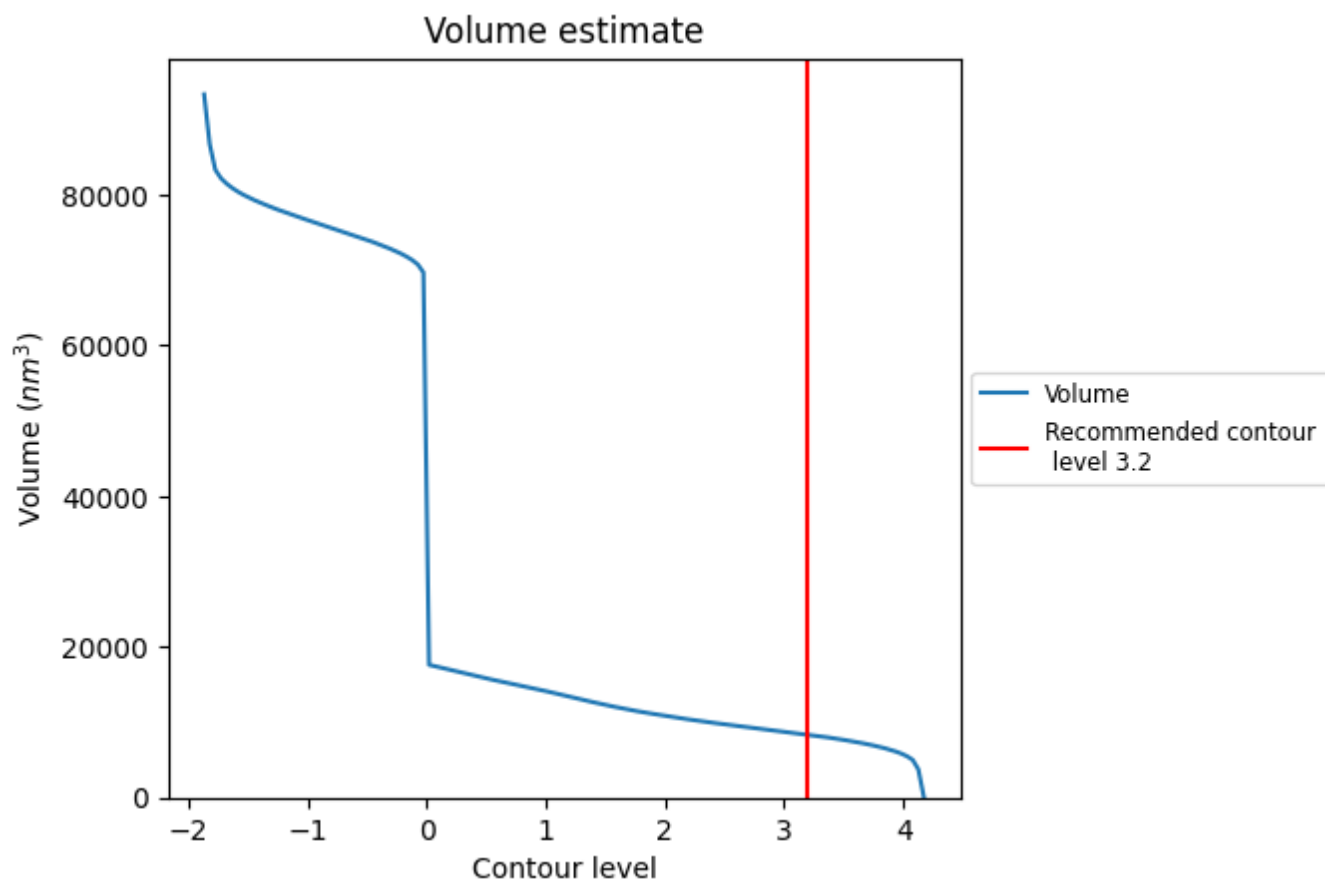
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

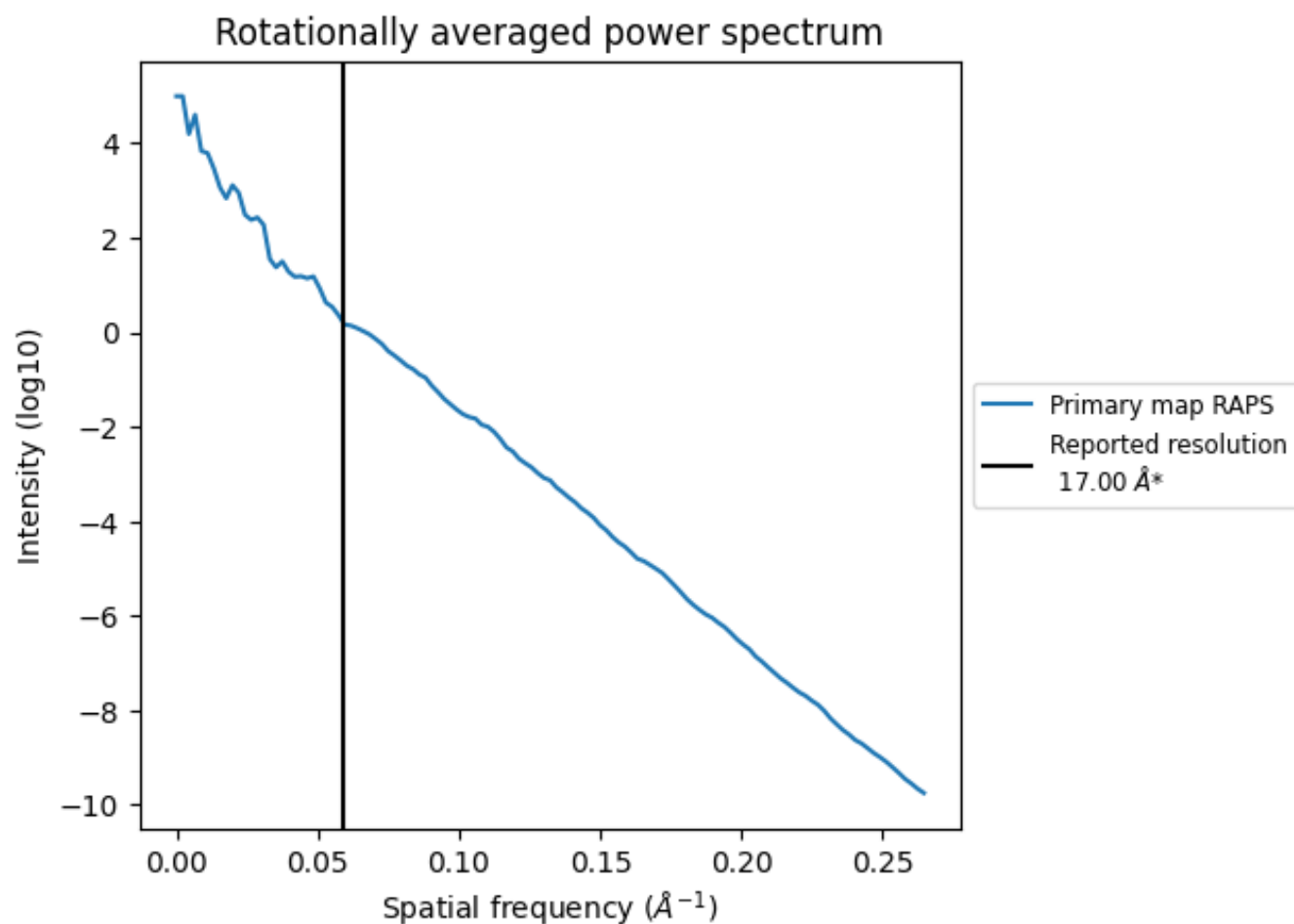
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 8351 nm³; this corresponds to an approximate mass of 7543 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.059 Å⁻¹

8 Fourier-Shell correlation ⓘ

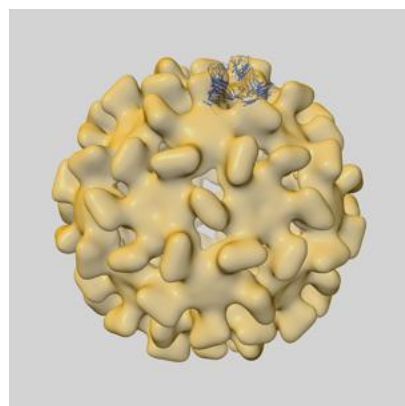
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

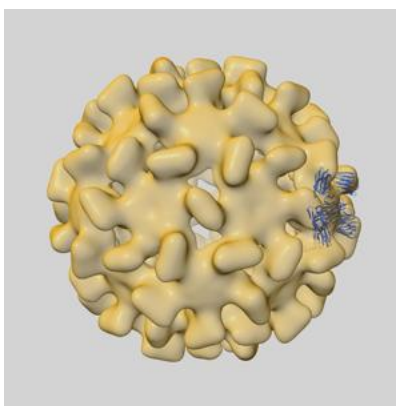
This section contains information regarding the fit between EMDB map EMD-1864 and PDB model 3ZX9. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlays

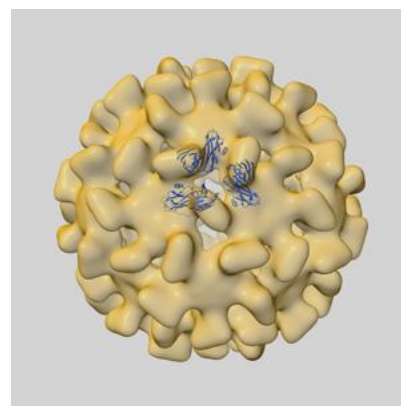
9.1.1 Map-model overlay [i](#)



X

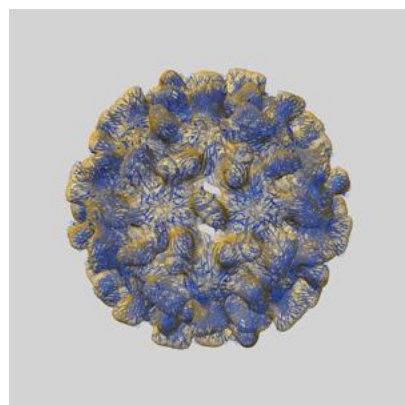


Y

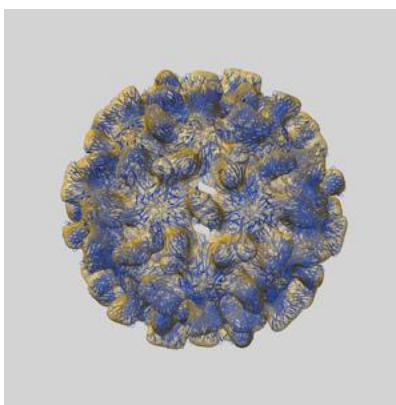


Z

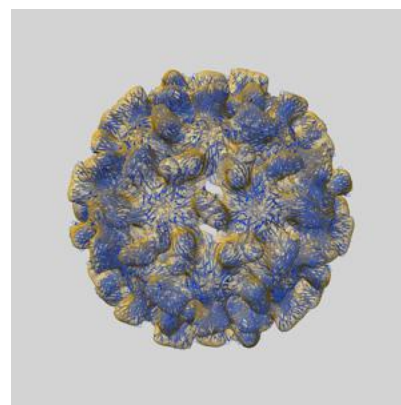
9.1.2 Map-model assembly overlay [i](#)



X



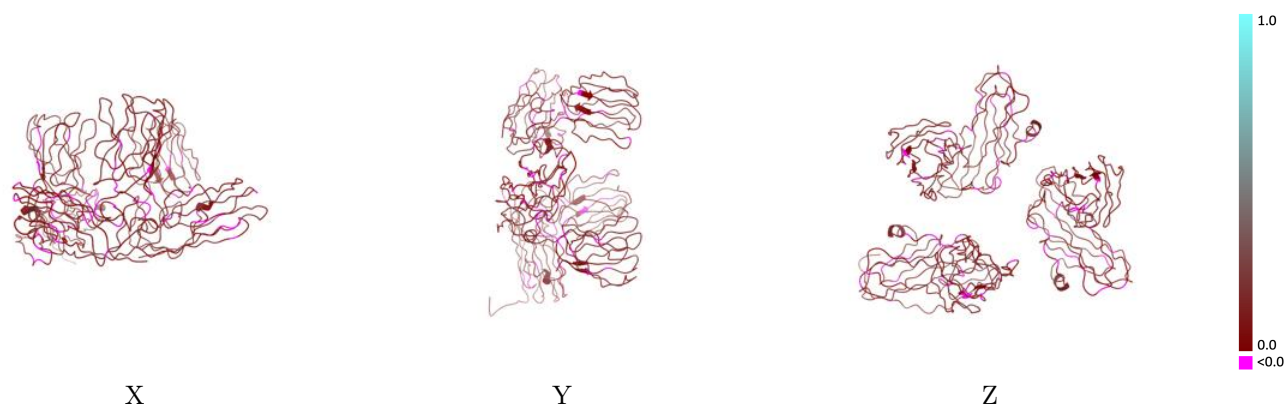
Y



Z

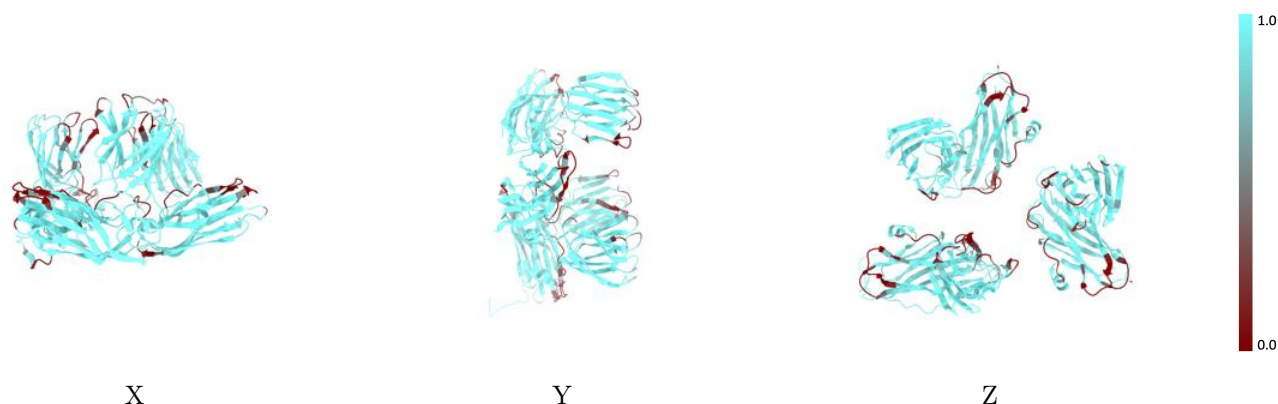
The images above show the 3D surface view of the map at the recommended contour level 3.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



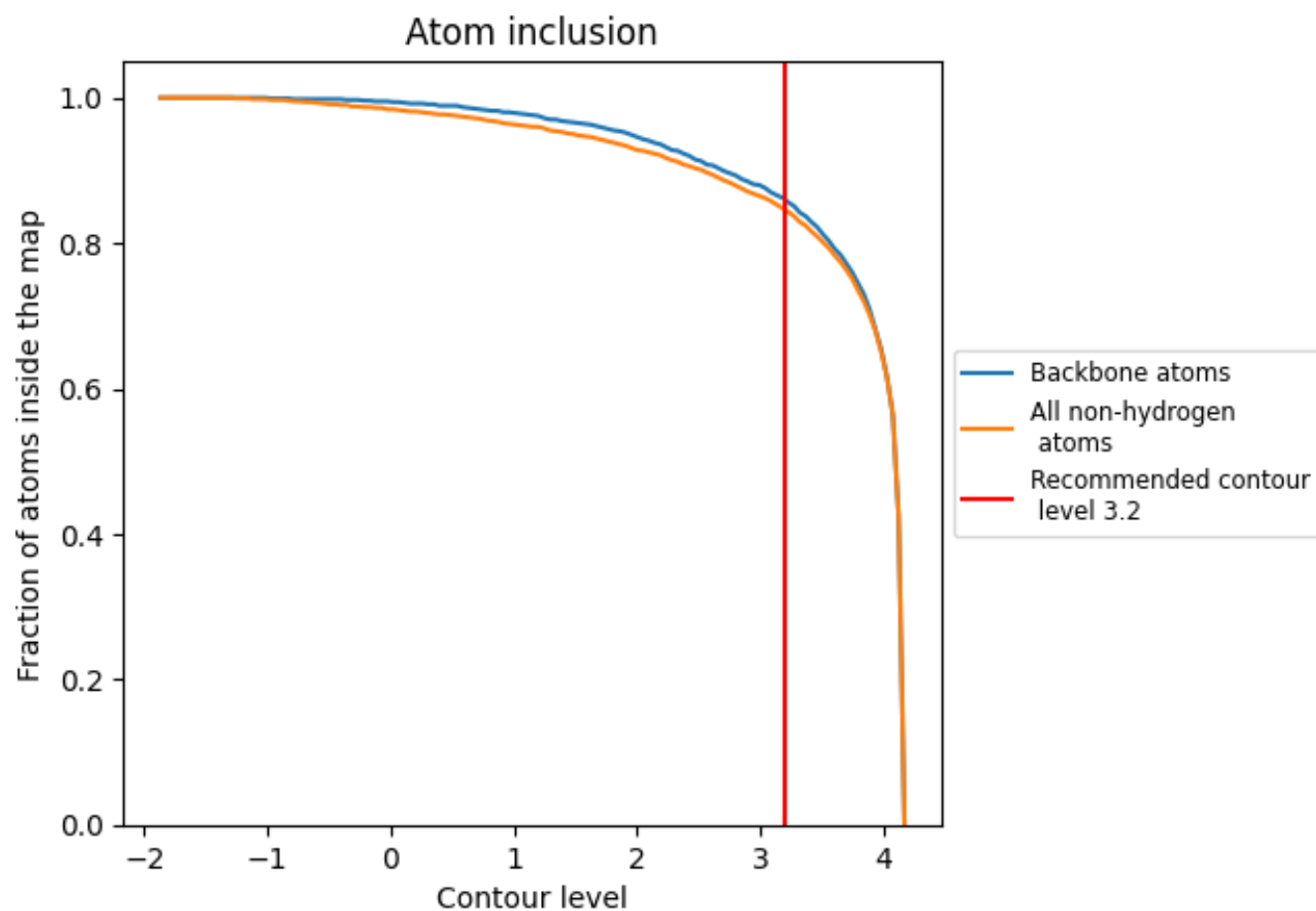
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (3.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8460	0.1150
A	0.8610	0.1130
B	0.8540	0.1200
C	0.8260	0.1130

