



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:55 PM UTC

PDB ID : 1CN1 / pdb_00001cn1
Title : CRYSTAL STRUCTURE OF DEMETALLIZED CONCAVALIN A. THE METAL-BINDING REGION
Authors : Shoham, M.; Yonath, A.; Sussman, J.L.; Moulton, J.; Traub, W.; Gilboa(Kalb), A.J.
Deposited on : 1981-12-21
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

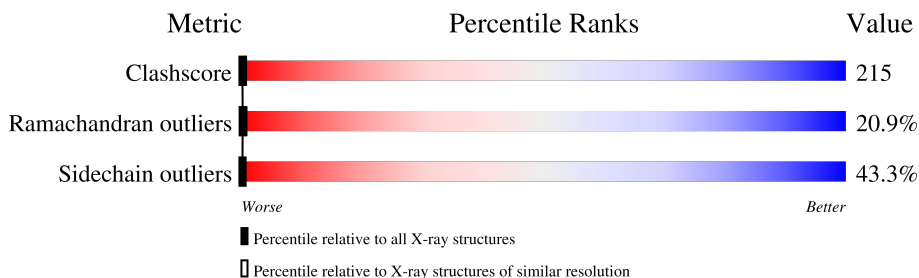
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	237	 • 18% 46% 35%
1	B	237	 • 19% 39% 41%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3612 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called CONCANAVALLIN A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	0	0
			1806	1139	300	365	2			
1	B	237	Total	C	N	O	S	0	0	0
			1806	1139	300	365	2			

There are 4 discrepancies between the modelled and reference sequences:

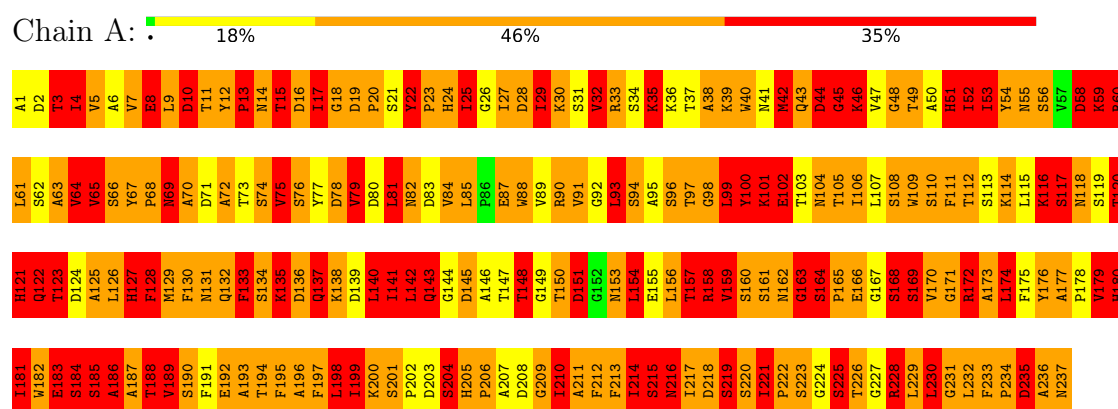
Chain	Residue	Modelled	Actual	Comment	Reference
A	186	ALA	-	insertion	UNP P02866
A	?	-	ALA	deletion	UNP P02866
B	186	ALA	-	insertion	UNP P02866
B	?	-	ALA	deletion	UNP P02866

3 Residue-property plots

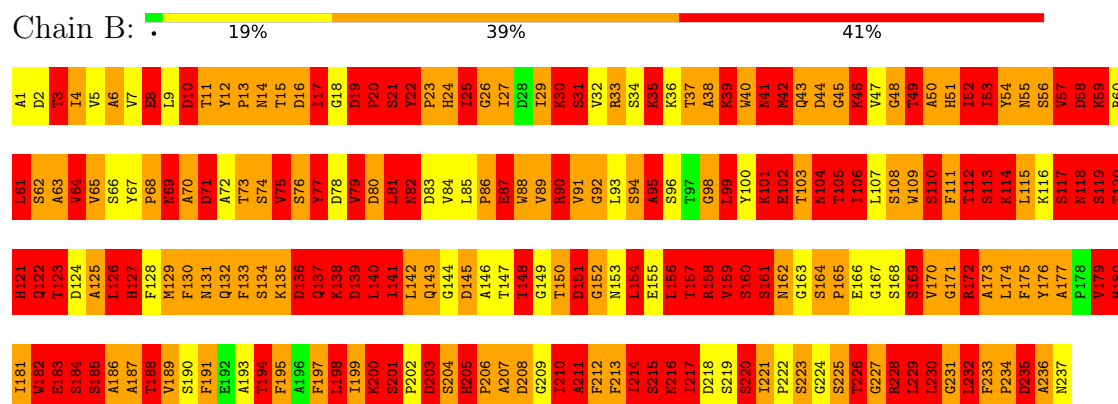
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

• Molecule 1: CONCAVALIN A



• Molecule 1: CONCAVALIN A



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α , β , γ	84.30Å 91.20Å 61.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.20	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3612	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

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	2.98	163/1848 (8.8%)	2.99	210/2519 (8.3%)
1	B	2.87	164/1848 (8.9%)	2.99	215/2519 (8.5%)
All	All	2.93	327/3696 (8.8%)	2.99	425/5038 (8.4%)

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	B	0	1

All (327) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	121	HIS	ND1-CE1	15.55	1.48	1.32
1	A	40	TRP	NE1-CE2	-15.08	1.20	1.37
1	B	40	TRP	NE1-CE2	-13.21	1.23	1.37
1	A	51	HIS	CE1-NE2	12.47	1.45	1.32
1	A	127	HIS	ND1-CE1	11.43	1.44	1.32
1	A	109	TRP	NE1-CE2	-11.37	1.25	1.37
1	B	24	HIS	CE1-NE2	11.08	1.43	1.32
1	A	71	ASP	C-N	-10.92	1.24	1.33
1	B	51	HIS	ND1-CE1	10.38	1.43	1.32
1	A	228	ARG	C-O	10.17	1.36	1.24
1	B	127	HIS	CE1-NE2	10.03	1.42	1.32
1	A	20	PRO	N-CD	9.96	1.61	1.47
1	A	24	HIS	C-O	9.91	1.36	1.24
1	B	121	HIS	C-O	9.91	1.36	1.24
1	A	180	HIS	CE1-NE2	9.67	1.42	1.32
1	B	51	HIS	CE1-NE2	9.67	1.42	1.32
1	A	81	LEU	N-CA	9.59	1.58	1.46
1	B	50	ALA	C-N	-9.58	1.21	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	100	TYR	N-CA	9.45	1.56	1.45
1	A	24	HIS	CB-CG	9.35	1.63	1.50
1	A	205	HIS	ND1-CE1	9.32	1.41	1.32
1	A	193	ALA	N-CA	9.29	1.56	1.45
1	A	229	LEU	C-O	9.03	1.35	1.24
1	B	130	PHE	N-CA	8.99	1.57	1.45
1	A	33	ARG	NE-CZ	8.98	1.43	1.33
1	B	232	LEU	CA-C	-8.93	1.40	1.52
1	A	154	LEU	CA-C	8.91	1.63	1.52
1	A	159	VAL	C-N	-8.84	1.22	1.33
1	A	24	HIS	CG-CD2	-8.82	1.26	1.35
1	A	24	HIS	C-N	-8.78	1.21	1.33
1	B	230	LEU	C-O	8.73	1.34	1.24
1	B	201	SER	C-N	8.71	1.42	1.34
1	A	24	HIS	ND1-CE1	8.61	1.41	1.32
1	B	180	HIS	ND1-CE1	8.61	1.41	1.32
1	A	235	ASP	C-N	-8.61	1.23	1.33
1	B	25	ILE	CA-CB	-8.56	1.45	1.54
1	B	112	THR	N-CA	8.54	1.55	1.46
1	B	114	LYS	C-N	-8.54	1.21	1.33
1	A	140	LEU	N-CA	8.50	1.57	1.46
1	B	163	GLY	CA-C	-8.36	1.40	1.51
1	B	22	TYR	CA-C	8.26	1.63	1.52
1	A	124	ASP	CA-C	-8.21	1.42	1.52
1	A	143	GLN	CA-C	8.17	1.61	1.52
1	A	22	TYR	CA-C	-8.14	1.42	1.52
1	B	88	TRP	NE1-CE2	-8.12	1.28	1.37
1	B	230	LEU	N-CA	8.11	1.56	1.46
1	B	209	GLY	C-O	8.09	1.34	1.23
1	A	8	GLU	C-O	8.08	1.33	1.23
1	A	58	ASP	CA-C	-7.99	1.45	1.53
1	B	103	THR	C-N	-7.98	1.22	1.33
1	A	23	PRO	N-CD	7.95	1.58	1.47
1	A	163	GLY	C-O	7.92	1.34	1.23
1	A	4	ILE	C-O	7.92	1.33	1.24
1	A	121	HIS	ND1-CE1	7.90	1.40	1.32
1	B	23	PRO	N-CA	7.86	1.56	1.47
1	A	164	SER	CA-C	-7.82	1.43	1.52
1	B	24	HIS	CB-CG	7.80	1.61	1.50
1	B	124	ASP	N-CA	7.77	1.55	1.46
1	A	88	TRP	NE1-CE2	-7.77	1.28	1.37
1	B	24	HIS	CD2-NE2	7.77	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	121	HIS	CD2-NE2	7.77	1.46	1.37
1	B	92	GLY	N-CA	7.75	1.54	1.45
1	B	89	VAL	N-CA	-7.72	1.37	1.46
1	B	127	HIS	CG-ND1	7.72	1.46	1.38
1	B	210	ILE	CA-CB	-7.71	1.44	1.54
1	A	105	THR	CA-CB	7.70	1.64	1.53
1	A	98	GLY	C-N	-7.69	1.23	1.33
1	A	43	GLN	N-CA	7.68	1.54	1.46
1	A	198	LEU	CA-C	-7.67	1.45	1.53
1	B	169	SER	C-O	7.66	1.33	1.23
1	A	90	ARG	CD-NE	7.66	1.56	1.46
1	B	49	THR	CA-C	7.60	1.61	1.52
1	B	44	ASP	N-CA	7.59	1.56	1.45
1	B	144	GLY	N-CA	7.56	1.56	1.45
1	B	53	ILE	C-O	-7.56	1.16	1.23
1	B	78	ASP	CA-CB	7.50	1.64	1.53
1	B	206	PRO	N-CD	7.50	1.58	1.47
1	A	196	ALA	CA-CB	-7.47	1.43	1.53
1	B	173	ALA	CA-C	-7.42	1.43	1.52
1	A	104	ASN	CA-C	-7.41	1.45	1.53
1	A	65	VAL	CA-CB	-7.39	1.43	1.53
1	A	51	HIS	CG-CD2	-7.38	1.27	1.35
1	B	12	TYR	C-N	7.36	1.42	1.33
1	A	161	SER	N-CA	7.33	1.55	1.46
1	A	178	PRO	N-CD	7.27	1.57	1.47
1	B	234	PRO	N-CD	7.27	1.57	1.47
1	A	225	SER	C-O	7.25	1.33	1.24
1	B	194	THR	C-O	-7.20	1.15	1.24
1	B	180	HIS	CE1-NE2	7.18	1.39	1.32
1	B	62	SER	C-O	7.15	1.32	1.23
1	A	31	SER	N-CA	7.13	1.54	1.46
1	B	14	ASN	C-N	-7.11	1.23	1.33
1	A	142	LEU	CA-C	-7.10	1.43	1.53
1	B	33	ARG	NE-CZ	7.05	1.40	1.33
1	B	179	VAL	CA-C	7.04	1.61	1.52
1	A	56	SER	CA-CB	7.03	1.64	1.53
1	A	177	ALA	CA-C	-7.01	1.45	1.53
1	B	74	SER	C-N	-6.98	1.24	1.33
1	B	90	ARG	C-N	-6.98	1.24	1.33
1	B	27	ILE	C-O	6.97	1.32	1.24
1	B	159	VAL	C-O	6.97	1.32	1.24
1	A	231	GLY	CA-C	6.94	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	51	HIS	CA-C	6.93	1.60	1.52
1	B	119	SER	C-O	-6.86	1.15	1.24
1	B	226	THR	C-O	6.85	1.30	1.24
1	B	48	GLY	CA-C	-6.85	1.42	1.51
1	A	176	TYR	C-O	-6.81	1.16	1.24
1	B	85	LEU	C-O	6.81	1.32	1.23
1	A	55	ASN	CA-C	-6.80	1.44	1.52
1	B	142	LEU	N-CA	6.78	1.54	1.45
1	A	74	SER	C-O	-6.77	1.17	1.23
1	B	171	GLY	CA-C	6.74	1.61	1.51
1	B	46	LYS	C-N	6.74	1.42	1.33
1	A	197	PHE	CA-CB	-6.74	1.43	1.53
1	B	75	VAL	N-CA	6.70	1.54	1.46
1	A	189	VAL	CA-CB	-6.69	1.45	1.54
1	B	214	ILE	CA-CB	-6.69	1.45	1.54
1	A	45	GLY	C-N	-6.68	1.24	1.33
1	A	151	ASP	C-O	6.65	1.32	1.24
1	B	113	SER	N-CA	6.61	1.54	1.46
1	B	198	LEU	N-CA	6.61	1.54	1.46
1	B	88	TRP	N-CA	6.61	1.54	1.46
1	B	37	THR	CA-CB	-6.61	1.45	1.53
1	B	117	SER	C-N	6.60	1.43	1.33
1	B	213	PHE	C-O	6.60	1.31	1.23
1	A	116	LYS	CA-C	-6.56	1.44	1.52
1	B	95	ALA	CA-C	-6.56	1.44	1.52
1	B	138	LYS	CA-C	-6.56	1.44	1.52
1	A	180	HIS	CD2-NE2	6.52	1.45	1.37
1	A	109	TRP	CA-C	6.48	1.60	1.52
1	B	110	SER	C-O	6.44	1.31	1.23
1	B	157	THR	CA-CB	6.42	1.62	1.53
1	A	61	LEU	N-CA	6.41	1.54	1.46
1	B	225	SER	N-CA	-6.41	1.38	1.46
1	B	54	TYR	CA-C	-6.40	1.44	1.52
1	B	121	HIS	CG-ND1	-6.39	1.31	1.38
1	A	15	THR	N-CA	6.36	1.54	1.46
1	A	102	GLU	N-CA	6.36	1.54	1.46
1	A	221	ILE	N-CA	6.36	1.54	1.46
1	A	102	GLU	C-O	6.35	1.31	1.24
1	A	172	ARG	C-O	6.35	1.31	1.24
1	A	100	TYR	C-O	6.34	1.31	1.23
1	A	189	VAL	CA-C	6.31	1.60	1.52
1	B	169	SER	C-N	-6.29	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	108	SER	C-O	6.26	1.31	1.23
1	A	155	GLU	CA-C	-6.26	1.45	1.52
1	A	133	PHE	C-N	-6.24	1.25	1.33
1	A	181	ILE	C-N	-6.24	1.25	1.33
1	B	183	GLU	CA-CB	-6.24	1.43	1.53
1	B	148	THR	C-N	6.22	1.42	1.33
1	A	141	ILE	C-N	6.21	1.42	1.33
1	A	83	ASP	CA-C	-6.16	1.45	1.53
1	A	234	PRO	CA-CB	-6.16	1.45	1.53
1	A	1	ALA	N-CA	6.15	1.57	1.46
1	A	7	VAL	C-O	-6.14	1.17	1.24
1	B	230	LEU	C-N	-6.13	1.24	1.33
1	A	214	ILE	CA-C	-6.12	1.46	1.52
1	A	99	LEU	N-CA	6.11	1.54	1.46
1	B	103	THR	C-O	6.10	1.31	1.23
1	A	179	VAL	CA-C	-6.09	1.45	1.52
1	A	172	ARG	NE-CZ	6.08	1.39	1.33
1	A	228	ARG	NE-CZ	6.08	1.39	1.33
1	B	172	ARG	CD-NE	6.05	1.54	1.46
1	B	39	LYS	C-O	6.05	1.31	1.24
1	A	10	ASP	CA-C	-6.04	1.44	1.52
1	A	49	THR	C-O	6.04	1.29	1.23
1	A	186	ALA	CA-C	-6.04	1.44	1.52
1	A	2	ASP	N-CA	6.03	1.53	1.46
1	A	84	VAL	CA-CB	-6.03	1.46	1.54
1	A	155	GLU	C-O	6.03	1.31	1.24
1	A	122	GLN	CD-OE1	6.02	1.34	1.23
1	A	182	TRP	NE1-CE2	-6.01	1.30	1.37
1	A	142	LEU	N-CA	6.00	1.53	1.45
1	B	72	ALA	N-CA	6.00	1.53	1.45
1	B	25	ILE	C-O	6.00	1.32	1.24
1	A	120	THR	CA-C	5.96	1.60	1.52
1	B	82	ASN	CA-C	5.96	1.60	1.52
1	B	180	HIS	CG-CD2	-5.96	1.29	1.35
1	A	178	PRO	CA-CB	5.96	1.60	1.54
1	A	219	SER	CA-C	5.94	1.61	1.53
1	A	52	ILE	CA-CB	-5.93	1.46	1.54
1	B	94	SER	CA-C	-5.93	1.45	1.53
1	A	23	PRO	N-CA	-5.93	1.39	1.47
1	B	217	ILE	C-O	5.93	1.31	1.24
1	A	70	ALA	N-CA	5.92	1.52	1.45
1	A	104	ASN	N-CA	5.91	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	110	SER	C-N	5.89	1.41	1.33
1	B	70	ALA	C-N	-5.88	1.25	1.33
1	A	8	GLU	C-N	-5.87	1.24	1.34
1	B	46	LYS	N-CA	5.86	1.53	1.45
1	B	15	THR	N-CA	5.86	1.53	1.46
1	B	158	ARG	CA-C	-5.86	1.45	1.52
1	B	58	ASP	CG-OD1	5.85	1.36	1.25
1	A	121	HIS	C-N	5.84	1.41	1.33
1	A	183	GLU	C-N	5.84	1.41	1.33
1	B	55	ASN	N-CA	5.81	1.53	1.46
1	B	13	PRO	CA-CB	-5.81	1.45	1.53
1	A	169	SER	C-N	-5.80	1.25	1.33
1	B	10	ASP	N-CA	5.80	1.53	1.46
1	A	205	HIS	CG-CD2	5.79	1.42	1.35
1	B	39	LYS	CA-C	-5.79	1.45	1.52
1	B	172	ARG	CZ-NH1	5.75	1.40	1.32
1	B	71	ASP	CA-C	-5.75	1.45	1.53
1	B	127	HIS	ND1-CE1	5.74	1.38	1.32
1	B	162	ASN	C-N	5.73	1.41	1.33
1	B	170	VAL	C-N	5.73	1.41	1.33
1	A	79	VAL	N-CA	-5.73	1.40	1.46
1	A	103	THR	N-CA	-5.73	1.39	1.46
1	B	141	ILE	C-O	5.68	1.30	1.24
1	A	61	LEU	C-O	5.68	1.30	1.24
1	A	36	LYS	C-O	-5.68	1.17	1.24
1	B	118	ASN	C-N	-5.67	1.25	1.33
1	B	109	TRP	NE1-CE2	-5.67	1.31	1.37
1	B	52	ILE	CB-CG1	5.66	1.64	1.53
1	B	159	VAL	N-CA	5.66	1.53	1.46
1	B	96	SER	CA-C	-5.65	1.45	1.52
1	A	16	ASP	N-CA	5.64	1.53	1.46
1	B	35	LYS	N-CA	5.64	1.53	1.46
1	B	220	SER	C-N	5.63	1.39	1.33
1	A	38	ALA	CA-C	5.63	1.59	1.52
1	A	54	TYR	C-N	5.62	1.40	1.33
1	B	8	GLU	CA-C	-5.61	1.45	1.52
1	B	133	PHE	CB-CG	5.61	1.63	1.50
1	B	197	PHE	CB-CG	5.61	1.63	1.50
1	A	205	HIS	N-CA	5.59	1.53	1.46
1	B	68	PRO	CA-CB	5.58	1.61	1.53
1	A	65	VAL	CA-C	5.58	1.59	1.52
1	A	29	ILE	CA-C	5.57	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	47	VAL	N-CA	-5.56	1.39	1.46
1	B	121	HIS	CB-CG	5.56	1.57	1.50
1	A	52	ILE	CA-C	-5.54	1.45	1.52
1	A	126	LEU	CA-C	-5.54	1.46	1.52
1	B	23	PRO	CA-C	5.53	1.59	1.52
1	A	183	GLU	CA-C	-5.53	1.45	1.52
1	A	229	LEU	CA-C	-5.53	1.45	1.52
1	B	154	LEU	N-CA	5.49	1.53	1.46
1	B	83	ASP	C-O	5.46	1.30	1.24
1	B	204	SER	C-O	5.46	1.30	1.24
1	A	160	SER	N-CA	5.45	1.53	1.45
1	B	3	THR	C-O	5.45	1.30	1.23
1	A	234	PRO	CA-C	-5.44	1.44	1.52
1	A	78	ASP	C-O	5.44	1.30	1.24
1	A	136	ASP	C-O	5.44	1.30	1.24
1	B	136	ASP	C-O	5.44	1.30	1.24
1	B	131	ASN	CG-OD1	5.43	1.33	1.23
1	B	202	PRO	N-CA	-5.42	1.40	1.47
1	A	165	PRO	CA-CB	5.42	1.60	1.53
1	A	158	ARG	CA-C	-5.41	1.45	1.53
1	B	11	THR	C-O	5.41	1.31	1.24
1	A	145	ASP	N-CA	5.39	1.52	1.46
1	B	229	LEU	C-N	-5.39	1.26	1.33
1	A	180	HIS	ND1-CE1	5.38	1.38	1.32
1	B	205	HIS	CE1-NE2	5.38	1.38	1.32
1	B	3	THR	CA-C	-5.37	1.46	1.52
1	B	236	ALA	CA-CB	-5.37	1.45	1.53
1	B	52	ILE	C-O	5.36	1.30	1.24
1	A	146	ALA	CA-C	-5.35	1.46	1.53
1	A	150	THR	N-CA	5.35	1.53	1.46
1	A	187	ALA	N-CA	5.35	1.53	1.46
1	A	195	PHE	C-O	5.34	1.30	1.23
1	A	147	THR	C-O	5.33	1.30	1.23
1	B	231	GLY	N-CA	5.33	1.53	1.45
1	A	159	VAL	CA-CB	5.32	1.61	1.54
1	B	168	SER	CA-CB	5.32	1.61	1.53
1	B	202	PRO	C-O	5.32	1.30	1.24
1	B	212	PHE	C-O	5.30	1.30	1.24
1	B	14	ASN	CA-CB	5.29	1.60	1.53
1	A	35	LYS	CA-C	-5.28	1.46	1.53
1	B	228	ARG	N-CA	-5.28	1.39	1.46
1	A	13	PRO	N-CA	5.28	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	25	ILE	CA-C	-5.27	1.46	1.52
1	A	42	MET	CA-C	-5.27	1.45	1.52
1	A	158	ARG	C-N	5.27	1.40	1.33
1	B	78	ASP	C-N	5.27	1.40	1.33
1	A	87	GLU	CD-OE2	5.27	1.35	1.25
1	A	134	SER	CA-C	5.26	1.59	1.52
1	A	235	ASP	CA-C	5.26	1.59	1.52
1	A	67	TYR	C-O	-5.26	1.17	1.24
1	A	112	THR	C-N	-5.25	1.26	1.33
1	B	139	ASP	CA-CB	5.25	1.62	1.53
1	B	3	THR	CA-CB	-5.24	1.45	1.53
1	B	107	LEU	CA-C	-5.24	1.46	1.52
1	A	72	ALA	N-CA	5.21	1.51	1.46
1	A	217	ILE	C-O	-5.21	1.18	1.24
1	B	130	PHE	CA-CB	-5.20	1.45	1.53
1	A	148	THR	C-O	-5.20	1.18	1.23
1	A	210	ILE	C-O	-5.20	1.17	1.23
1	B	52	ILE	CA-CB	-5.18	1.47	1.54
1	A	232	LEU	CA-C	-5.17	1.45	1.52
1	A	22	TYR	C-O	5.16	1.30	1.24
1	A	15	THR	C-O	-5.14	1.17	1.24
1	B	61	LEU	C-O	-5.14	1.17	1.24
1	B	87	GLU	C-O	-5.14	1.17	1.24
1	A	187	ALA	C-O	5.13	1.30	1.24
1	B	77	TYR	C-O	5.13	1.30	1.24
1	B	207	ALA	C-O	-5.13	1.17	1.23
1	B	164	SER	C-O	-5.13	1.18	1.24
1	A	171	GLY	C-O	5.12	1.30	1.23
1	B	163	GLY	C-O	5.12	1.30	1.23
1	A	165	PRO	CA-C	-5.09	1.46	1.52
1	B	13	PRO	C-N	-5.08	1.23	1.34
1	A	59	LYS	C-N	5.08	1.40	1.33
1	B	58	ASP	C-N	5.08	1.40	1.33
1	B	94	SER	C-N	5.08	1.40	1.33
1	B	142	LEU	C-N	5.08	1.40	1.33
1	B	184	SER	C-O	-5.08	1.18	1.24
1	A	63	ALA	C-N	-5.08	1.28	1.33
1	B	24	HIS	CA-C	5.06	1.58	1.52
1	A	39	LYS	C-N	-5.06	1.27	1.33
1	A	42	MET	C-N	-5.06	1.27	1.33
1	A	48	GLY	C-N	5.05	1.40	1.33
1	A	78	ASP	CA-CB	5.05	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	203	ASP	CA-CB	5.05	1.62	1.53
1	B	23	PRO	C-N	-5.03	1.27	1.33
1	B	188	THR	C-N	5.03	1.39	1.33
1	B	72	ALA	CA-CB	-5.02	1.45	1.53
1	B	170	VAL	N-CA	5.01	1.52	1.46
1	A	173	ALA	C-N	5.01	1.39	1.33
1	B	79	VAL	N-CA	-5.01	1.40	1.46
1	A	60	ARG	N-CA	-5.00	1.39	1.46
1	A	120	THR	N-CA	-5.00	1.39	1.46
1	B	39	LYS	N-CA	-5.00	1.39	1.46
1	B	84	VAL	CA-C	-5.00	1.46	1.52
1	A	24	HIS	CA-CB	-5.00	1.45	1.53
1	B	140	LEU	CA-CB	-5.00	1.45	1.53
1	B	162	ASN	CA-CB	-5.00	1.45	1.53
1	B	229	LEU	CA-CB	-5.00	1.45	1.53

All (425) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	160	SER	CA-C-N	19.31	149.66	120.31
1	A	160	SER	C-N-CA	19.31	149.66	120.31
1	A	203	ASP	CA-C-N	19.07	146.28	120.54
1	A	203	ASP	C-N-CA	19.07	146.28	120.54
1	B	57	VAL	CA-C-N	16.09	152.27	121.54
1	B	57	VAL	C-N-CA	16.09	152.27	121.54
1	B	46	LYS	CA-C-N	14.73	140.79	122.37
1	B	46	LYS	C-N-CA	14.73	140.79	122.37
1	A	205	HIS	O-C-N	14.03	134.09	121.32
1	A	117	SER	CA-C-N	13.65	147.61	121.54
1	A	117	SER	C-N-CA	13.65	147.61	121.54
1	B	118	ASN	CA-C-N	13.53	147.38	121.54
1	B	118	ASN	C-N-CA	13.53	147.38	121.54
1	B	80	ASP	CA-C-N	13.38	143.11	122.78
1	B	80	ASP	C-N-CA	13.38	143.11	122.78
1	A	174	LEU	CA-C-N	13.00	139.14	120.82
1	A	174	LEU	C-N-CA	13.00	139.14	120.82
1	B	104	ASN	CA-C-N	12.96	146.29	121.54
1	B	104	ASN	C-N-CA	12.96	146.29	121.54
1	B	218	ASP	CA-C-N	12.49	139.23	121.24
1	B	218	ASP	C-N-CA	12.49	139.23	121.24
1	A	135	LYS	CA-C-N	12.32	145.07	121.54
1	A	135	LYS	C-N-CA	12.32	145.07	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	235	ASP	CA-C-N	12.26	144.11	121.06
1	B	235	ASP	C-N-CA	12.26	144.11	121.06
1	A	55	ASN	CA-C-N	12.20	137.61	120.29
1	A	55	ASN	C-N-CA	12.20	137.61	120.29
1	A	190	SER	CA-C-N	12.00	146.27	121.91
1	A	190	SER	C-N-CA	12.00	146.27	121.91
1	B	17	ILE	O-C-N	-12.00	111.24	122.16
1	A	68	PRO	CA-C-N	11.95	144.37	121.54
1	A	68	PRO	C-N-CA	11.95	144.37	121.54
1	A	221	ILE	O-C-N	11.90	134.67	121.10
1	B	58	ASP	CA-C-N	10.98	142.51	121.54
1	B	58	ASP	C-N-CA	10.98	142.51	121.54
1	B	26	GLY	CA-C-N	10.97	141.71	121.97
1	B	26	GLY	C-N-CA	10.97	141.71	121.97
1	B	206	PRO	CA-C-N	10.84	141.83	122.64
1	B	206	PRO	C-N-CA	10.84	141.83	122.64
1	B	169	SER	CA-C-N	10.74	137.70	122.23
1	B	169	SER	C-N-CA	10.74	137.70	122.23
1	B	212	PHE	CA-CB-CG	-10.71	103.09	113.80
1	A	17	ILE	CA-C-N	10.48	141.96	121.41
1	A	17	ILE	C-N-CA	10.48	141.96	121.41
1	A	209	GLY	CA-C-N	10.41	137.19	123.03
1	A	209	GLY	C-N-CA	10.41	137.19	123.03
1	B	96	SER	CA-C-N	10.16	138.26	122.11
1	B	96	SER	C-N-CA	10.16	138.26	122.11
1	B	21	SER	O-C-N	-10.02	109.27	122.59
1	B	68	PRO	CA-C-N	9.72	140.11	121.54
1	B	68	PRO	C-N-CA	9.72	140.11	121.54
1	B	20	PRO	CA-C-N	9.71	140.09	121.54
1	B	20	PRO	C-N-CA	9.71	140.09	121.54
1	A	230	LEU	O-C-N	-9.69	109.70	122.59
1	A	109	TRP	O-C-N	9.67	134.50	123.19
1	A	195	PHE	CA-CB-CG	-9.38	104.42	113.80
1	B	182	TRP	CA-C-N	9.23	139.17	121.54
1	B	182	TRP	C-N-CA	9.23	139.17	121.54
1	B	177	ALA	CA-C-N	9.23	129.28	119.78
1	B	177	ALA	C-N-CA	9.23	129.28	119.78
1	B	175	PHE	CA-CB-CG	-9.20	104.60	113.80
1	B	150	THR	O-C-N	-9.17	110.40	122.59
1	A	213	PHE	CA-C-N	9.13	135.46	121.85
1	A	213	PHE	C-N-CA	9.13	135.46	121.85
1	A	30	LYS	CA-C-N	-9.09	110.18	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	30	LYS	C-N-CA	-9.09	110.18	123.00
1	B	215	SER	CA-C-N	9.09	138.90	121.54
1	B	215	SER	C-N-CA	9.09	138.90	121.54
1	A	184	SER	CA-C-N	8.96	138.66	121.54
1	A	184	SER	C-N-CA	8.96	138.66	121.54
1	A	204	SER	CA-C-N	-8.77	110.97	122.98
1	A	204	SER	C-N-CA	-8.77	110.97	122.98
1	A	236	ALA	O-C-N	8.71	134.38	123.32
1	A	11	THR	N-CA-C	-8.69	102.69	113.38
1	A	38	ALA	O-C-N	8.65	132.73	123.56
1	A	66	SER	CA-C-N	8.64	142.89	121.80
1	A	66	SER	C-N-CA	8.64	142.89	121.80
1	B	79	VAL	O-C-N	-8.56	111.87	122.57
1	A	49	THR	O-C-N	-8.56	115.63	123.50
1	A	96	SER	CA-C-N	8.53	135.35	122.65
1	A	96	SER	C-N-CA	8.53	135.35	122.65
1	B	233	PHE	CA-CB-CG	-8.50	105.30	113.80
1	B	77	TYR	CA-C-N	8.39	133.49	121.50
1	B	77	TYR	C-N-CA	8.39	133.49	121.50
1	B	114	LYS	CA-C-N	8.31	135.20	123.07
1	B	114	LYS	C-N-CA	8.31	135.20	123.07
1	A	120	THR	O-C-N	8.28	133.60	122.59
1	A	189	VAL	O-C-N	8.26	132.90	122.57
1	A	91	VAL	O-C-N	-8.20	114.57	123.18
1	B	14	ASN	CA-CB-CG	-8.18	104.42	112.60
1	B	99	LEU	O-C-N	-8.08	111.84	122.59
1	A	24	HIS	CA-C-N	8.05	136.46	121.97
1	A	24	HIS	C-N-CA	8.05	136.46	121.97
1	B	89	VAL	O-C-N	8.05	131.76	123.07
1	B	82	ASN	O-C-N	8.03	133.27	122.59
1	A	128	PHE	O-C-N	-8.02	114.27	123.42
1	B	23	PRO	O-C-N	8.01	132.71	123.10
1	A	147	THR	CA-C-N	-8.00	107.97	121.89
1	A	147	THR	C-N-CA	-8.00	107.97	121.89
1	A	150	THR	CA-C-N	-8.00	106.26	121.54
1	A	150	THR	C-N-CA	-8.00	106.26	121.54
1	A	97	THR	O-C-N	-7.93	113.91	123.19
1	B	191	PHE	CA-CB-CG	-7.87	105.94	113.80
1	B	211	ALA	CA-C-N	7.84	133.10	121.72
1	B	211	ALA	C-N-CA	7.84	133.10	121.72
1	A	33	ARG	CA-C-N	7.76	136.37	121.54
1	A	33	ARG	C-N-CA	7.76	136.37	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	133	PHE	CA-CB-CG	-7.76	106.04	113.80
1	A	229	LEU	CA-C-N	7.73	136.31	121.54
1	A	229	LEU	C-N-CA	7.73	136.31	121.54
1	B	195	PHE	CA-CB-CG	-7.72	106.08	113.80
1	A	168	SER	CA-C-N	-7.69	106.86	121.54
1	A	168	SER	C-N-CA	-7.69	106.86	121.54
1	A	2	ASP	O-C-N	7.67	132.17	123.27
1	B	65	VAL	O-C-N	-7.66	113.00	122.57
1	A	212	PHE	CA-CB-CG	-7.65	106.15	113.80
1	A	64	VAL	CA-C-O	7.64	128.14	120.96
1	B	197	PHE	CA-CB-CG	-7.61	106.19	113.80
1	B	6	ALA	CA-C-N	7.61	134.67	122.50
1	B	6	ALA	C-N-CA	7.61	134.67	122.50
1	B	14	ASN	CA-C-N	7.58	136.02	121.54
1	B	14	ASN	C-N-CA	7.58	136.02	121.54
1	A	199	ILE	CA-C-N	7.58	134.85	121.75
1	A	199	ILE	C-N-CA	7.58	134.85	121.75
1	B	101	LYS	O-C-N	7.57	132.66	122.59
1	A	220	SER	CA-C-N	-7.56	108.14	122.13
1	A	220	SER	C-N-CA	-7.56	108.14	122.13
1	A	22	TYR	CA-C-N	7.56	129.29	119.84
1	A	22	TYR	C-N-CA	7.56	129.29	119.84
1	A	177	ALA	O-C-N	-7.54	113.23	121.53
1	B	165	PRO	CA-C-N	7.53	135.38	122.12
1	B	165	PRO	C-N-CA	7.53	135.38	122.12
1	A	151	ASP	CA-C-N	7.52	136.15	121.41
1	A	151	ASP	C-N-CA	7.52	136.15	121.41
1	A	231	GLY	N-CA-C	-7.46	104.91	115.43
1	B	113	SER	O-C-N	7.46	132.83	123.28
1	A	213	PHE	CA-CB-CG	-7.41	106.39	113.80
1	A	140	LEU	CA-C-N	-7.40	113.50	123.12
1	A	140	LEU	C-N-CA	-7.40	113.50	123.12
1	B	176	TYR	N-CA-C	-7.38	103.74	112.89
1	B	74	SER	CA-C-O	-7.35	112.93	121.82
1	B	25	ILE	O-C-N	-7.31	114.75	122.57
1	B	156	LEU	CA-C-N	-7.20	109.78	123.32
1	B	156	LEU	C-N-CA	-7.20	109.78	123.32
1	B	70	ALA	O-C-N	7.19	131.16	122.75
1	A	169	SER	CA-C-N	7.19	134.91	121.97
1	A	169	SER	C-N-CA	7.19	134.91	121.97
1	B	37	THR	CA-C-N	7.18	135.26	121.54
1	B	37	THR	C-N-CA	7.18	135.26	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	146	ALA	CA-C-N	7.17	131.68	121.42
1	A	146	ALA	C-N-CA	7.17	131.68	121.42
1	A	145	ASP	O-C-N	-7.13	112.99	122.19
1	B	11	THR	N-CA-C	-7.13	102.60	112.30
1	A	116	LYS	CA-C-N	-7.13	112.64	123.04
1	A	116	LYS	C-N-CA	-7.13	112.64	123.04
1	B	69	ASN	CA-C-N	7.12	132.91	120.87
1	B	69	ASN	C-N-CA	7.12	132.91	120.87
1	B	184	SER	O-C-N	7.12	130.82	122.20
1	B	69	ASN	CA-CB-CG	-7.11	105.49	112.60
1	A	61	LEU	O-C-N	-7.10	114.73	123.04
1	A	117	SER	CB-CA-C	-7.06	107.63	117.23
1	B	148	THR	CA-C-N	-7.05	107.59	121.41
1	B	148	THR	C-N-CA	-7.05	107.59	121.41
1	A	187	ALA	CA-C-N	7.02	133.11	122.93
1	A	187	ALA	C-N-CA	7.02	133.11	122.93
1	A	173	ALA	CA-C-O	7.01	128.27	120.70
1	B	161	SER	CA-C-N	7.00	134.91	121.54
1	B	161	SER	C-N-CA	7.00	134.91	121.54
1	A	20	PRO	N-CD-CG	-6.98	92.72	103.20
1	A	93	LEU	CA-C-O	-6.96	113.19	120.99
1	A	199	ILE	O-C-N	6.94	130.60	122.69
1	B	131	ASN	CA-C-N	6.94	132.66	122.39
1	B	131	ASN	C-N-CA	6.94	132.66	122.39
1	A	211	ALA	CA-C-O	-6.93	114.01	121.36
1	B	61	LEU	CA-C-N	-6.87	111.01	121.86
1	B	61	LEU	C-N-CA	-6.87	111.01	121.86
1	A	93	LEU	O-C-N	6.85	131.07	123.33
1	B	214	ILE	O-C-N	6.85	131.14	122.57
1	A	9	LEU	CA-C-N	6.85	134.62	121.54
1	A	9	LEU	C-N-CA	6.85	134.62	121.54
1	B	160	SER	CA-C-N	6.84	134.61	121.54
1	B	160	SER	C-N-CA	6.84	134.61	121.54
1	A	125	ALA	CA-C-N	6.84	133.55	122.81
1	A	125	ALA	C-N-CA	6.84	133.55	122.81
1	B	137	GLN	O-C-N	-6.84	113.23	122.19
1	A	79	VAL	CA-C-O	-6.83	114.61	121.45
1	B	92	GLY	O-C-N	-6.81	118.15	123.80
1	A	206	PRO	N-CD-CG	-6.79	93.02	103.20
1	B	20	PRO	O-C-N	6.78	131.80	122.64
1	B	108	SER	O-C-N	-6.76	116.39	123.56
1	B	206	PRO	N-CD-CG	-6.76	93.06	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	113	SER	CA-C-N	6.73	132.01	122.72
1	B	113	SER	C-N-CA	6.73	132.01	122.72
1	B	160	SER	O-C-N	6.73	130.62	122.68
1	B	74	SER	O-C-N	6.72	130.53	122.20
1	A	178	PRO	N-CD-CG	-6.72	93.12	103.20
1	A	159	VAL	O-C-N	6.70	130.94	122.57
1	A	94	SER	O-C-N	6.69	130.97	123.48
1	B	111	PHE	CA-CB-CG	-6.67	107.13	113.80
1	A	147	THR	O-C-N	-6.67	115.14	123.01
1	A	52	ILE	O-C-N	-6.67	114.24	122.57
1	B	179	VAL	CA-C-N	-6.64	108.86	121.54
1	B	179	VAL	C-N-CA	-6.64	108.86	121.54
1	B	24	HIS	ND1-CG-CD2	6.61	112.71	106.10
1	A	182	TRP	CG-CD2-CE3	-6.57	127.33	133.90
1	B	125	ALA	CA-C-N	6.57	133.68	122.37
1	B	125	ALA	C-N-CA	6.57	133.68	122.37
1	A	87	GLU	O-C-N	-6.57	114.53	122.22
1	B	186	ALA	CA-C-N	6.56	134.07	121.54
1	B	186	ALA	C-N-CA	6.56	134.07	121.54
1	A	234	PRO	N-CD-CG	-6.56	93.36	103.20
1	B	70	ALA	CA-C-N	6.54	132.86	120.97
1	B	70	ALA	C-N-CA	6.54	132.86	120.97
1	A	46	LYS	O-C-N	6.51	131.05	123.30
1	A	108	SER	CA-C-N	6.48	132.31	122.65
1	A	108	SER	C-N-CA	6.48	132.31	122.65
1	A	133	PHE	O-C-N	-6.47	113.98	122.59
1	B	69	ASN	OD1-CG-ND2	6.47	129.07	122.60
1	B	229	LEU	CA-C-N	6.44	133.84	121.54
1	B	229	LEU	C-N-CA	6.44	133.84	121.54
1	B	17	ILE	CA-C-O	6.44	126.11	119.35
1	A	90	ARG	NE-CZ-NH2	-6.44	113.41	119.20
1	B	40	TRP	O-C-N	-6.41	116.30	123.48
1	A	203	ASP	O-C-N	6.39	130.55	123.01
1	B	218	ASP	CA-CB-CG	6.39	118.99	112.60
1	B	19	ASP	O-C-N	6.36	128.63	121.32
1	B	200	LYS	O-C-N	-6.35	114.14	122.59
1	B	120	THR	CA-C-O	6.35	126.70	119.27
1	A	195	PHE	CA-C-N	6.34	130.85	122.42
1	A	195	PHE	C-N-CA	6.34	130.85	122.42
1	B	229	LEU	O-C-N	6.34	131.02	122.59
1	A	137	GLN	N-CA-C	-6.31	105.72	113.41
1	A	223	SER	CA-C-N	6.29	133.74	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	223	SER	C-N-CA	6.29	133.74	121.41
1	A	45	GLY	CA-C-N	6.26	131.81	122.99
1	A	45	GLY	C-N-CA	6.26	131.81	122.99
1	B	213	PHE	CA-C-N	6.22	133.17	121.97
1	B	213	PHE	C-N-CA	6.22	133.17	121.97
1	A	155	GLU	CA-C-N	-6.21	112.71	122.65
1	A	155	GLU	C-N-CA	-6.21	112.71	122.65
1	B	24	HIS	O-C-N	6.20	130.49	123.42
1	A	14	ASN	N-CA-CB	6.19	118.25	110.45
1	B	175	PHE	O-C-N	-6.19	115.62	123.24
1	A	131	ASN	CA-CB-CG	-6.18	106.42	112.60
1	A	63	ALA	O-C-N	6.18	129.46	123.04
1	B	228	ARG	NE-CZ-NH1	-6.14	115.36	121.50
1	A	162	ASN	N-CA-C	-6.12	103.75	112.13
1	A	134	SER	CA-C-N	6.12	131.35	122.85
1	A	134	SER	C-N-CA	6.12	131.35	122.85
1	A	130	PHE	CA-CB-CG	-6.08	107.72	113.80
1	B	38	ALA	CA-C-N	6.06	133.11	121.54
1	B	38	ALA	C-N-CA	6.06	133.11	121.54
1	A	128	PHE	CA-CB-CG	-6.02	107.78	113.80
1	B	183	GLU	CA-C-N	6.02	130.76	121.19
1	B	183	GLU	C-N-CA	6.02	130.76	121.19
1	B	133	PHE	O-C-N	-6.00	115.02	122.82
1	A	88	TRP	CG-CD2-CE3	-5.99	127.91	133.90
1	A	227	GLY	CA-C-N	5.98	130.81	120.58
1	A	227	GLY	C-N-CA	5.98	130.81	120.58
1	A	4	ILE	O-C-N	-5.97	115.11	122.57
1	B	6	ALA	O-C-N	5.96	129.88	123.56
1	A	121	HIS	CA-C-N	-5.95	110.17	121.54
1	A	121	HIS	C-N-CA	-5.95	110.17	121.54
1	A	181	ILE	O-C-N	5.95	130.01	122.57
1	B	31	SER	O-C-N	-5.95	114.68	122.59
1	A	16	ASP	CA-C-N	5.93	132.64	121.97
1	A	16	ASP	C-N-CA	5.93	132.64	121.97
1	A	14	ASN	CA-CB-CG	-5.92	106.68	112.60
1	B	126	LEU	CA-C-N	-5.91	109.05	121.81
1	B	126	LEU	C-N-CA	-5.91	109.05	121.81
1	B	62	SER	CA-C-N	5.90	133.08	122.64
1	B	62	SER	C-N-CA	5.90	133.08	122.64
1	B	121	HIS	ND1-CG-CD2	5.87	111.97	106.10
1	B	136	ASP	O-C-N	-5.87	114.79	122.59
1	A	161	SER	N-CA-C	-5.86	105.03	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	216	ASN	CA-CB-CG	-5.85	106.75	112.60
1	B	202	PRO	N-CD-CG	-5.84	94.44	103.20
1	A	59	LYS	O-C-N	-5.83	114.83	122.59
1	B	107	LEU	O-C-N	-5.83	114.55	122.19
1	B	55	ASN	CA-C-N	5.82	130.44	121.19
1	B	55	ASN	C-N-CA	5.82	130.44	121.19
1	B	46	LYS	N-CA-C	-5.81	100.52	109.52
1	A	90	ARG	CA-C-N	5.80	130.38	123.19
1	A	90	ARG	C-N-CA	5.80	130.38	123.19
1	A	131	ASN	O-C-N	-5.79	114.89	122.59
1	B	209	GLY	CA-C-N	5.78	132.37	121.97
1	B	209	GLY	C-N-CA	5.78	132.37	121.97
1	A	162	ASN	CA-CB-CG	-5.76	106.84	112.60
1	B	86	PRO	N-CD-CG	-5.76	94.56	103.20
1	B	121	HIS	CB-CG-CD2	-5.74	123.74	131.20
1	A	38	ALA	CA-C-N	5.73	129.40	120.75
1	A	38	ALA	C-N-CA	5.73	129.40	120.75
1	B	106	ILE	O-C-N	5.73	128.94	122.98
1	A	3	THR	O-C-N	5.70	130.45	123.10
1	A	157	THR	O-C-N	5.69	130.06	123.17
1	B	124	ASP	CA-C-N	-5.69	113.66	122.59
1	B	124	ASP	C-N-CA	-5.69	113.66	122.59
1	B	139	ASP	CA-C-N	5.68	132.40	121.54
1	B	139	ASP	C-N-CA	5.68	132.40	121.54
1	A	85	LEU	O-C-N	5.66	127.83	121.32
1	B	1	ALA	CA-C-N	-5.66	114.91	122.72
1	B	1	ALA	C-N-CA	-5.66	114.91	122.72
1	A	24	HIS	ND1-CG-CD2	5.64	111.74	106.10
1	B	33	ARG	NH1-CZ-NH2	5.64	126.63	119.30
1	B	56	SER	CA-C-N	5.63	132.11	121.97
1	B	56	SER	C-N-CA	5.63	132.11	121.97
1	A	23	PRO	N-CD-CG	-5.60	94.80	103.20
1	A	24	HIS	CB-CG-ND1	-5.59	114.31	122.70
1	B	185	SER	CA-C-N	-5.59	113.04	123.05
1	B	185	SER	C-N-CA	-5.59	113.04	123.05
1	A	32	VAL	CA-C-N	-5.58	115.00	122.42
1	A	32	VAL	C-N-CA	-5.58	115.00	122.42
1	B	89	VAL	CA-C-N	5.58	131.61	122.07
1	B	89	VAL	C-N-CA	5.58	131.61	122.07
1	A	98	GLY	O-C-N	5.57	129.94	122.70
1	B	64	VAL	CA-C-N	-5.56	111.96	121.97
1	B	64	VAL	C-N-CA	-5.56	111.96	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	142	LEU	O-C-N	-5.55	114.85	122.23
1	B	168	SER	N-CA-CB	-5.54	103.89	111.65
1	A	188	THR	CA-C-N	-5.54	111.99	121.97
1	A	188	THR	C-N-CA	-5.54	111.99	121.97
1	A	83	ASP	CA-C-N	5.54	129.38	120.30
1	A	83	ASP	C-N-CA	5.54	129.38	120.30
1	A	84	VAL	CA-C-N	-5.53	108.31	121.80
1	A	84	VAL	C-N-CA	-5.53	108.31	121.80
1	B	51	HIS	ND1-CE1-NE2	-5.53	102.87	108.40
1	B	168	SER	O-C-N	5.53	128.84	121.99
1	B	41	ASN	CA-CB-CG	-5.51	107.09	112.60
1	B	115	LEU	CA-C-N	-5.50	111.04	121.54
1	B	115	LEU	C-N-CA	-5.50	111.04	121.54
1	B	81	LEU	CA-C-N	5.49	132.02	121.54
1	B	81	LEU	C-N-CA	5.49	132.02	121.54
1	A	101	LYS	O-C-N	5.48	129.88	122.59
1	B	145	ASP	N-CA-C	-5.46	105.25	112.34
1	B	204	SER	N-CA-C	-5.45	105.64	114.09
1	B	139	ASP	N-CA-C	-5.44	105.51	111.82
1	B	63	ALA	CA-C-O	-5.43	114.82	121.88
1	A	7	VAL	CA-C-N	5.41	128.92	120.75
1	A	7	VAL	C-N-CA	5.41	128.92	120.75
1	B	102	GLU	CB-CG-CD	-5.40	103.42	112.60
1	A	11	THR	O-C-N	-5.39	115.35	122.42
1	B	105	THR	O-C-N	-5.39	115.42	122.59
1	A	64	VAL	CA-C-N	-5.38	116.28	123.17
1	A	64	VAL	C-N-CA	-5.38	116.28	123.17
1	B	212	PHE	CA-C-N	5.38	130.92	122.21
1	B	212	PHE	C-N-CA	5.38	130.92	122.21
1	B	13	PRO	CA-C-O	-5.36	115.48	121.32
1	A	40	TRP	CE2-CD2-CE3	5.35	124.15	118.80
1	A	217	ILE	O-C-N	5.35	128.85	121.90
1	B	10	ASP	CA-CB-CG	-5.33	107.27	112.60
1	A	233	PHE	CA-CB-CG	-5.33	108.47	113.80
1	B	161	SER	N-CA-CB	-5.32	101.50	110.49
1	A	143	GLN	OE1-CD-NE2	5.32	127.92	122.60
1	A	14	ASN	O-C-N	5.32	130.01	122.68
1	A	31	SER	CA-C-N	5.30	131.51	121.97
1	A	31	SER	C-N-CA	5.30	131.51	121.97
1	A	104	ASN	CA-C-N	-5.30	113.92	121.50
1	A	104	ASN	C-N-CA	-5.30	113.92	121.50
1	B	43	GLN	CA-C-N	-5.30	112.07	121.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	43	GLN	C-N-CA	-5.30	112.07	121.29
1	A	232	LEU	O-C-N	-5.28	115.14	121.64
1	A	204	SER	CB-CA-C	-5.26	102.39	110.81
1	B	233	PHE	CA-C-N	5.26	126.42	119.84
1	B	233	PHE	C-N-CA	5.26	126.42	119.84
1	B	170	VAL	O-C-N	-5.26	117.22	123.00
1	A	78	ASP	CA-C-N	-5.25	115.63	122.51
1	A	78	ASP	C-N-CA	-5.25	115.63	122.51
1	B	59	LYS	O-C-N	-5.25	115.61	122.59
1	B	99	LEU	CA-C-N	5.23	132.31	122.84
1	B	99	LEU	C-N-CA	5.23	132.31	122.84
1	B	152	GLY	CA-C-N	5.22	131.57	122.81
1	B	152	GLY	C-N-CA	5.22	131.57	122.81
1	B	138	LYS	O-C-N	-5.21	115.66	122.59
1	A	148	THR	O-C-N	5.21	129.85	123.44
1	A	28	ASP	O-C-N	-5.21	116.72	122.86
1	A	68	PRO	N-CD-CG	-5.21	95.39	103.20
1	B	48	GLY	O-C-N	-5.20	115.94	122.70
1	B	30	LYS	CA-C-N	5.20	131.46	121.54
1	B	30	LYS	C-N-CA	5.20	131.46	121.54
1	B	72	ALA	N-CA-C	-5.19	101.79	109.94
1	A	222	PRO	O-C-N	5.19	129.65	122.64
1	A	141	ILE	O-C-N	-5.18	117.03	123.10
1	B	42	MET	CA-C-N	-5.18	115.76	123.11
1	B	42	MET	C-N-CA	-5.18	115.76	123.11
1	A	141	ILE	CA-C-O	5.17	126.07	120.53
1	A	156	LEU	N-CA-C	-5.17	106.56	112.92
1	A	192	GLU	CA-C-N	-5.16	113.74	122.67
1	A	192	GLU	C-N-CA	-5.16	113.74	122.67
1	B	204	SER	CB-CA-C	-5.16	101.50	109.80
1	A	148	THR	CA-C-N	5.15	131.51	121.41
1	A	148	THR	C-N-CA	5.15	131.51	121.41
1	A	111	PHE	CA-C-N	-5.15	113.73	121.86
1	A	111	PHE	C-N-CA	-5.15	113.73	121.86
1	A	28	ASP	N-CA-C	-5.15	103.24	110.50
1	B	228	ARG	NE-CZ-NH2	5.13	123.82	119.20
1	A	132	GLN	CA-C-N	5.13	131.33	121.54
1	A	132	GLN	C-N-CA	5.13	131.33	121.54
1	B	44	ASP	N-CA-C	-5.12	103.84	110.19
1	B	51	HIS	O-C-N	5.12	128.99	123.10
1	B	50	ALA	CA-C-O	-5.10	116.18	121.99
1	B	142	LEU	CA-C-O	5.09	127.63	121.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	91	VAL	CA-C-N	5.08	128.58	120.55
1	B	91	VAL	C-N-CA	5.08	128.58	120.55
1	B	218	ASP	N-CA-CB	-5.08	103.99	111.51
1	A	60	ARG	CA-C-N	-5.08	114.24	121.50
1	A	60	ARG	C-N-CA	-5.08	114.24	121.50
1	B	6	ALA	CA-C-O	-5.07	115.07	120.75
1	B	223	SER	CA-C-N	-5.07	111.47	121.41
1	B	223	SER	C-N-CA	-5.07	111.47	121.41
1	A	48	GLY	N-CA-C	-5.07	102.88	112.10
1	B	33	ARG	O-C-N	5.07	129.10	122.87
1	A	88	TRP	CE2-CD2-CG	5.06	113.27	107.20
1	A	44	ASP	CA-C-N	5.05	131.32	121.41
1	A	44	ASP	C-N-CA	5.05	131.32	121.41
1	A	69	ASN	CA-C-N	5.05	131.01	122.12
1	A	69	ASN	C-N-CA	5.05	131.01	122.12
1	A	153	ASN	CA-C-N	5.05	130.45	123.07
1	A	153	ASN	C-N-CA	5.05	130.45	123.07
1	B	55	ASN	CA-CB-CG	-5.05	107.55	112.60
1	A	229	LEU	O-C-N	-5.03	115.90	122.59
1	B	121	HIS	CA-C-N	-5.03	111.93	121.54
1	B	121	HIS	C-N-CA	-5.03	111.93	121.54
1	A	162	ASN	CA-C-N	5.02	131.25	121.41
1	A	162	ASN	C-N-CA	5.02	131.25	121.41
1	B	236	ALA	O-C-N	5.02	128.77	122.65

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	57	VAL	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	1806	0	1745	825	5
1	B	1806	0	1744	733	23

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3612	0	3489	1525	23

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 215.

All (1525) 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:180:HIS:HB2	1:A:182:TRP:CZ3	1.17	1.69
1:A:180:HIS:CB	1:A:182:TRP:CZ3	1.95	1.46
1:A:222:PRO:CG	1:A:225:SER:HB3	1.43	1.45
1:A:115:LEU:HD22	1:A:180:HIS:NE2	1.39	1.35
1:A:222:PRO:HG2	1:A:225:SER:CB	1.53	1.35
1:B:6:ALA:CB	1:B:213:PHE:HA	1.57	1.33
1:A:180:HIS:HB2	1:A:182:TRP:CH2	1.65	1.32
1:A:29:ILE:HG12	1:A:35:LYS:CE	1.60	1.29
1:A:115:LEU:HD13	1:A:180:HIS:CE1	1.66	1.28
1:A:225:SER:HB2	1:A:231:GLY:CA	1.65	1.27
1:A:180:HIS:HB2	1:A:182:TRP:CE3	1.70	1.26
1:A:198:LEU:O	1:A:198:LEU:HD23	1.09	1.25
1:A:180:HIS:CB	1:A:182:TRP:CH2	2.17	1.23
1:B:6:ALA:HB2	1:B:213:PHE:HA	1.23	1.19
1:B:88:TRP:CE2	1:B:182:TRP:HH2	1.61	1.19
1:A:166:GLU:HG2	1:A:167:GLY:N	1.55	1.18
1:B:38:ALA:HB2	1:B:75:VAL:CG1	1.74	1.18
1:A:22:TYR:HB2	1:A:23:PRO:CD	1.76	1.16
1:B:22:TYR:HB2	1:B:23:PRO:CD	1.71	1.16
1:A:59:LYS:HE2	1:A:78:ASP:HB3	1.25	1.16
1:B:137:GLN:HB3	1:B:140:LEU:HB2	1.21	1.16
1:A:48:GLY:HA3	1:A:197:PHE:CE2	1.82	1.15
1:A:29:ILE:CG1	1:A:35:LYS:HE3	1.76	1.15
1:A:56:SER:HB2	1:A:188:THR:HA	1.20	1.15
1:B:4:ILE:HD12	1:B:4:ILE:C	1.70	1.14
1:A:45:GLY:H	1:A:200:LYS:HG3	1.06	1.14
1:B:88:TRP:CE2	1:B:182:TRP:CH2	2.35	1.14
1:B:141:ILE:O	1:B:173:ALA:HA	1.48	1.13
1:B:141:ILE:HG22	1:B:174:LEU:H	1.08	1.13
1:A:59:LYS:O	1:A:59:LYS:HG3	1.47	1.11
1:A:22:TYR:HE1	1:A:39:LYS:HA	1.07	1.10
1:A:106:ILE:HD13	1:A:154:LEU:HD13	1.18	1.10
1:A:53:ILE:N	1:A:53:ILE:HD12	1.64	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:VAL:HG23	1:B:214:ILE:HA	1.20	1.10
1:A:122:GLN:HG2	1:B:131:ASN:HB3	1.15	1.10
1:B:210:ILE:HG22	1:B:211:ALA:H	1.15	1.10
1:A:27:ILE:HG22	1:A:29:ILE:HD11	1.34	1.09
1:A:44:ASP:O	1:A:46:LYS:HD2	1.50	1.09
1:A:51:HIS:C	1:A:52:ILE:HD13	1.76	1.09
1:B:22:TYR:HB2	1:B:23:PRO:HD2	1.12	1.09
1:B:32:VAL:HA	1:B:233:PHE:HE2	1.17	1.09
1:B:92:GLY:HA2	1:B:109:TRP:HH2	1.10	1.08
1:A:15:THR:HG22	1:A:21:SER:HA	1.18	1.08
1:A:116:LYS:HD2	1:A:116:LYS:N	1.58	1.08
1:B:6:ALA:HB1	1:B:212:PHE:O	1.53	1.08
1:B:38:ALA:HB2	1:B:75:VAL:HG11	1.28	1.08
1:B:207:ALA:HB1	1:B:208:ASP:HA	1.18	1.08
1:A:106:ILE:HD11	1:A:156:LEU:HG	1.31	1.08
1:A:180:HIS:C	1:A:180:HIS:HD1	1.60	1.08
1:A:211:ALA:HB2	1:A:230:LEU:HD12	1.22	1.08
1:B:38:ALA:CB	1:B:75:VAL:HG11	1.84	1.08
1:A:157:THR:OG1	1:A:169:SER:HB2	1.54	1.07
1:B:156:LEU:O	1:B:171:GLY:HA3	1.52	1.07
1:A:158:ARG:HG2	1:A:158:ARG:NH1	1.57	1.07
1:B:14:ASN:H	1:B:19:ASP:HB3	0.91	1.07
1:B:222:PRO:HG2	1:B:225:SER:OG	1.55	1.07
1:B:166:GLU:HG2	1:B:167:GLY:H	1.11	1.06
1:A:91:VAL:HG23	1:A:179:VAL:HG21	1.37	1.06
1:A:198:LEU:O	1:A:198:LEU:CD2	2.02	1.06
1:B:173:ALA:C	1:B:174:LEU:HD23	1.80	1.06
1:A:9:LEU:HD23	1:A:25:ILE:CG2	1.85	1.06
1:A:14:ASN:HB3	1:A:228:ARG:CZ	1.84	1.06
1:B:22:TYR:CB	1:B:23:PRO:HD2	1.84	1.06
1:B:121:HIS:C	1:B:122:GLN:HG3	1.79	1.06
1:A:9:LEU:HD23	1:A:25:ILE:HG22	1.39	1.05
1:A:87:GLU:CD	1:A:182:TRP:HB2	1.81	1.05
1:B:207:ALA:CB	1:B:208:ASP:HA	1.80	1.05
1:A:174:LEU:HD23	1:A:174:LEU:N	1.67	1.05
1:B:14:ASN:N	1:B:19:ASP:HB3	1.73	1.04
1:B:92:GLY:HA2	1:B:109:TRP:CH2	1.91	1.04
1:A:225:SER:CB	1:A:231:GLY:HA2	1.86	1.04
1:B:137:GLN:HA	1:B:137:GLN:NE2	1.56	1.04
1:A:158:ARG:HH11	1:A:158:ARG:CG	1.69	1.04
1:B:42:MET:HE1	1:B:206:PRO:O	1.57	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:LEU:HD22	1:B:25:ILE:HG22	1.40	1.03
1:B:56:SER:HB2	1:B:189:VAL:N	1.72	1.03
1:A:115:LEU:C	1:A:116:LYS:HD2	1.83	1.03
1:B:87:GLU:HG2	1:B:182:TRP:CD2	1.93	1.03
1:B:95:ALA:HB2	1:B:210:ILE:HG23	1.37	1.03
1:A:115:LEU:HD13	1:A:180:HIS:HE1	0.88	1.03
1:A:112:THR:HG23	1:A:127:HIS:HB2	1.07	1.03
1:B:6:ALA:HB1	1:B:213:PHE:HA	1.41	1.02
1:B:88:TRP:CZ2	1:B:182:TRP:HH2	1.77	1.02
1:B:141:ILE:HG22	1:B:174:LEU:N	1.74	1.02
1:A:115:LEU:CD1	1:A:180:HIS:HE1	1.72	1.02
1:A:180:HIS:HB3	1:A:182:TRP:CH2	1.93	1.02
1:B:137:GLN:HE21	1:B:137:GLN:CA	1.72	1.02
1:A:22:TYR:CB	1:A:23:PRO:HD2	1.84	1.01
1:B:7:VAL:HG22	1:B:212:PHE:HB3	1.42	1.01
1:A:4:ILE:HD12	1:A:232:LEU:HB3	1.40	1.01
1:B:56:SER:CB	1:B:188:THR:HA	1.90	1.01
1:A:92:GLY:HA3	1:A:174:LEU:HB3	1.37	1.01
1:A:52:ILE:HG12	1:A:193:ALA:HB3	1.40	1.00
1:A:22:TYR:CE1	1:A:39:LYS:HA	1.97	1.00
1:B:159:VAL:HA	1:B:165:PRO:HA	1.41	1.00
1:A:225:SER:CA	1:A:229:LEU:HB3	1.91	1.00
1:B:2:ASP:HA	1:B:216:ASN:HD21	1.25	1.00
1:B:53:ILE:HD11	1:B:62:SER:HB2	1.39	1.00
1:A:54:TYR:HB3	1:A:191:PHE:CE2	1.96	1.00
1:B:61:LEU:HD22	1:B:81:LEU:HD13	1.43	1.00
1:B:158:ARG:HD3	1:B:166:GLU:OE2	1.60	1.00
1:B:226:THR:H	1:B:229:LEU:HD13	1.23	1.00
1:B:89:VAL:HG13	1:B:215:SER:O	1.63	0.99
1:B:4:ILE:HD12	1:B:4:ILE:O	1.63	0.99
1:A:122:GLN:HE22	1:B:132:GLN:HE22	1.04	0.98
1:A:67:TYR:O	1:A:70:ALA:HB3	1.62	0.98
1:A:106:ILE:HD13	1:A:154:LEU:CD1	1.93	0.97
1:A:115:LEU:CD1	1:A:180:HIS:CE1	2.46	0.97
1:A:106:ILE:HD11	1:A:156:LEU:CG	1.91	0.97
1:A:27:ILE:HG22	1:A:29:ILE:CD1	1.94	0.97
1:B:98:GLY:O	1:B:99:LEU:HD22	1.65	0.97
1:B:137:GLN:HA	1:B:137:GLN:HE21	0.80	0.97
1:A:29:ILE:HG12	1:A:35:LYS:HE3	0.98	0.97
1:B:7:VAL:CG2	1:B:212:PHE:HB3	1.94	0.97
1:A:56:SER:HB2	1:A:188:THR:CA	1.94	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:ALA:CB	1:B:213:PHE:CA	2.42	0.97
1:A:106:ILE:CD1	1:A:154:LEU:HD22	1.95	0.96
1:A:15:THR:CG2	1:A:21:SER:HA	1.94	0.96
1:A:66:SER:HA	1:A:72:ALA:HB2	1.46	0.96
1:A:225:SER:HB2	1:A:231:GLY:HA2	0.98	0.96
1:A:13:PRO:HB3	1:A:21:SER:C	1.91	0.96
1:A:112:THR:CG2	1:A:127:HIS:HB2	1.93	0.96
1:A:172:ARG:HH11	1:A:232:LEU:HD22	1.29	0.96
1:A:115:LEU:CD2	1:A:180:HIS:NE2	2.29	0.96
1:A:137:GLN:HA	1:A:137:GLN:OE1	1.65	0.96
1:A:166:GLU:HG2	1:A:167:GLY:H	1.19	0.96
1:A:88:TRP:CD2	1:B:138:LYS:HD2	2.01	0.96
1:B:56:SER:HB3	1:B:188:THR:HA	1.46	0.95
1:B:23:PRO:HB2	1:B:40:TRP:HB3	1.45	0.95
1:A:122:GLN:HE22	1:B:132:GLN:NE2	1.65	0.95
1:A:62:SER:HB3	1:A:76:SER:HA	1.48	0.95
1:A:91:VAL:CG2	1:A:179:VAL:HG21	1.96	0.95
1:A:172:ARG:NH1	1:A:232:LEU:HD22	1.82	0.95
1:B:207:ALA:HB1	1:B:208:ASP:CA	1.97	0.95
1:A:42:MET:HG2	1:A:43:GLN:H	1.32	0.94
1:B:101:LYS:N	1:B:101:LYS:HD2	1.80	0.94
1:B:112:THR:HG23	1:B:127:HIS:HB2	1.48	0.94
1:B:58:ASP:C	1:B:59:LYS:HG3	1.88	0.94
1:A:112:THR:HG23	1:A:127:HIS:CB	1.96	0.94
1:A:50:ALA:HB3	1:A:195:PHE:CZ	2.03	0.94
1:A:116:LYS:HG2	1:A:117:SER:H	1.32	0.94
1:A:122:GLN:CG	1:B:131:ASN:HB3	1.97	0.94
1:B:180:HIS:CD2	1:B:182:TRP:CH2	2.54	0.94
1:A:17:ILE:HG13	1:A:17:ILE:O	1.65	0.94
1:B:180:HIS:CG	1:B:182:TRP:CZ3	2.56	0.94
1:A:115:LEU:HD12	1:A:189:VAL:HG22	1.49	0.94
1:A:16:ASP:HB2	1:A:228:ARG:NH1	1.80	0.94
1:B:137:GLN:CB	1:B:140:LEU:HB2	1.97	0.94
1:A:48:GLY:HA3	1:A:197:PHE:CZ	2.02	0.93
1:B:55:ASN:HB3	1:B:58:ASP:HB2	1.48	0.93
1:B:7:VAL:HG21	1:B:52:ILE:HD11	1.48	0.93
1:B:101:LYS:N	1:B:101:LYS:CD	2.29	0.93
1:B:225:SER:HA	1:B:229:LEU:HD22	1.49	0.93
1:B:9:LEU:HD13	1:B:40:TRP:CH2	2.04	0.93
1:A:11:THR:HG23	1:A:209:GLY:HA2	1.51	0.93
1:B:4:ILE:C	1:B:4:ILE:CD1	2.41	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:ILE:HD13	1:A:52:ILE:N	1.84	0.92
1:A:55:ASN:HB2	1:A:58:ASP:HB2	1.49	0.92
1:A:106:ILE:HB	1:A:154:LEU:HB3	1.48	0.92
1:A:87:GLU:O	1:A:182:TRP:HE3	1.52	0.92
1:A:182:TRP:CD1	1:A:183:GLU:H	1.88	0.91
1:B:8:GLU:HA	1:B:211:ALA:CB	2.00	0.91
1:A:45:GLY:N	1:A:200:LYS:HG3	1.84	0.91
1:B:92:GLY:HA3	1:B:174:LEU:HA	1.52	0.91
1:A:174:LEU:N	1:A:174:LEU:CD2	2.34	0.91
1:B:74:SER:O	1:B:75:VAL:HG13	1.71	0.91
1:B:122:GLN:HE21	1:B:122:GLN:N	1.68	0.91
1:B:25:ILE:HD13	1:B:25:ILE:O	1.69	0.91
1:A:106:ILE:HD11	1:A:156:LEU:CD2	2.00	0.90
1:A:143:GLN:NE2	1:A:143:GLN:C	2.28	0.90
1:B:25:ILE:HD12	1:B:25:ILE:H	1.36	0.90
1:B:111:PHE:CD2	1:B:112:THR:N	2.40	0.90
1:A:211:ALA:HB2	1:A:230:LEU:CD1	2.00	0.90
1:B:222:PRO:HG3	1:B:232:LEU:C	1.97	0.90
1:A:56:SER:CB	1:A:188:THR:HA	2.00	0.90
1:B:137:GLN:HG3	1:B:140:LEU:HD22	1.53	0.90
1:B:32:VAL:HG22	1:B:233:PHE:HD2	1.33	0.89
1:B:91:VAL:HG23	1:B:214:ILE:CA	2.03	0.89
1:B:95:ALA:CB	1:B:210:ILE:HA	2.02	0.89
1:B:32:VAL:HG22	1:B:233:PHE:CD2	2.08	0.89
1:A:180:HIS:C	1:A:180:HIS:ND1	2.20	0.89
1:A:13:PRO:HB3	1:A:22:TYR:HA	1.55	0.89
1:A:231:GLY:C	1:A:232:LEU:HD23	1.97	0.89
1:A:229:LEU:CD2	1:A:235:ASP:HA	2.03	0.89
1:A:229:LEU:HD21	1:A:235:ASP:HA	1.54	0.89
1:A:137:GLN:HG3	1:A:140:LEU:HB2	1.55	0.88
1:B:201:SER:CB	1:B:206:PRO:HB3	2.02	0.88
1:A:172:ARG:HD2	1:A:213:PHE:CZ	2.08	0.88
1:B:127:HIS:ND1	1:B:127:HIS:C	2.31	0.88
1:A:66:SER:HA	1:A:72:ALA:CB	2.04	0.88
1:B:38:ALA:CB	1:B:75:VAL:CG1	2.47	0.88
1:B:121:HIS:O	1:B:122:GLN:HG3	1.72	0.88
1:A:105:THR:HG21	1:A:198:LEU:HD22	1.53	0.88
1:B:139:ASP:O	1:B:176:TYR:HB2	1.73	0.88
1:A:88:TRP:CH2	1:A:182:TRP:CH2	2.61	0.88
1:A:91:VAL:HG23	1:A:179:VAL:CG2	2.04	0.88
1:A:92:GLY:CA	1:A:174:LEU:HB3	2.03	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:ILE:CD1	1:A:232:LEU:HB3	2.04	0.88
1:A:158:ARG:HG2	1:A:158:ARG:HH11	0.76	0.88
1:A:45:GLY:HA2	1:A:200:LYS:HD2	1.55	0.88
1:B:172:ARG:HH21	1:B:220:SER:C	1.82	0.88
1:A:224:GLY:HA3	1:A:229:LEU:HD23	1.55	0.87
1:A:28:ASP:C	1:A:29:ILE:HD13	1.99	0.87
1:A:22:TYR:HB2	1:A:23:PRO:HD2	0.92	0.87
1:A:229:LEU:HD21	1:A:235:ASP:CB	2.03	0.87
1:B:55:ASN:HB2	1:B:58:ASP:CB	2.04	0.87
1:B:141:ILE:HG21	1:B:174:LEU:HB2	1.54	0.87
1:A:32:VAL:HG22	1:A:233:PHE:CD2	2.09	0.87
1:A:84:VAL:C	1:A:85:LEU:HD23	1.99	0.87
1:B:32:VAL:HA	1:B:233:PHE:CE2	2.08	0.87
1:A:118:ASN:HA	1:A:185:SER:HB2	1.55	0.87
1:A:135:LYS:HA	1:A:148:THR:O	1.74	0.87
1:A:235:ASP:CG	1:A:236:ALA:H	1.81	0.87
1:B:104:ASN:HB3	1:B:210:ILE:HD11	1.56	0.87
1:B:172:ARG:NH2	1:B:220:SER:C	2.32	0.87
1:A:118:ASN:CA	1:A:185:SER:HB2	2.04	0.86
1:A:87:GLU:OE2	1:A:182:TRP:HB2	1.74	0.86
1:A:13:PRO:HB3	1:A:22:TYR:N	1.89	0.86
1:A:225:SER:N	1:A:229:LEU:HB3	1.89	0.86
1:A:225:SER:HA	1:A:229:LEU:O	1.75	0.86
1:A:58:ASP:O	1:A:59:LYS:HG2	1.76	0.86
1:B:111:PHE:HD2	1:B:112:THR:N	1.72	0.86
1:B:56:SER:CB	1:B:189:VAL:H	1.88	0.85
1:A:47:VAL:HA	1:A:198:LEU:HB2	1.59	0.85
1:A:108:SER:O	1:A:195:PHE:HA	1.75	0.85
1:B:18:GLY:O	1:B:20:PRO:HD3	1.75	0.85
1:B:103:THR:C	1:B:199:ILE:HG23	2.01	0.85
1:B:122:GLN:O	1:B:123:THR:HB	1.75	0.85
1:A:13:PRO:HB3	1:A:22:TYR:CA	2.05	0.85
1:A:59:LYS:O	1:A:59:LYS:CG	2.24	0.85
1:B:51:HIS:C	1:B:52:ILE:HG12	2.01	0.85
1:B:103:THR:O	1:B:199:ILE:HG23	1.77	0.85
1:B:235:ASP:CG	1:B:236:ALA:H	1.85	0.85
1:A:182:TRP:CD1	1:A:183:GLU:N	2.44	0.85
1:B:104:ASN:CB	1:B:210:ILE:HD11	2.07	0.85
1:A:119:SER:C	1:A:121:HIS:H	1.80	0.85
1:B:55:ASN:CB	1:B:58:ASP:HB2	2.06	0.85
1:B:56:SER:HB2	1:B:189:VAL:H	1.41	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:PRO:HG3	1:A:225:SER:HB3	1.56	0.84
1:A:137:GLN:HB3	1:A:140:LEU:H	1.42	0.84
1:B:22:TYR:CE1	1:B:39:LYS:HD3	2.12	0.84
1:A:88:TRP:CD2	1:A:182:TRP:CZ3	2.66	0.84
1:A:88:TRP:CZ3	1:A:182:TRP:CH2	2.65	0.84
1:B:23:PRO:HG2	1:B:40:TRP:O	1.77	0.84
1:B:117:SER:HB3	1:B:187:ALA:HB3	1.59	0.84
1:B:4:ILE:HG22	1:B:215:SER:HB3	1.59	0.84
1:B:5:VAL:HG11	1:B:81:LEU:HD11	1.57	0.84
1:B:87:GLU:HG3	1:B:182:TRP:CG	2.13	0.84
1:A:93:LEU:HD22	1:A:212:PHE:CD1	2.13	0.83
1:A:122:GLN:HB3	1:B:131:ASN:HB2	1.59	0.83
1:B:148:THR:HG22	1:B:148:THR:O	1.76	0.83
1:A:32:VAL:HG22	1:A:233:PHE:CB	2.07	0.83
1:B:87:GLU:CG	1:B:182:TRP:CD2	2.60	0.83
1:B:205:HIS:N	1:B:206:PRO:CD	2.40	0.83
1:B:225:SER:HA	1:B:229:LEU:HB3	1.60	0.83
1:A:225:SER:CB	1:A:231:GLY:CA	2.51	0.83
1:B:55:ASN:HB2	1:B:58:ASP:HB3	1.60	0.83
1:A:64:VAL:HA	1:A:73:THR:O	1.78	0.83
1:B:2:ASP:HA	1:B:216:ASN:ND2	1.94	0.83
1:B:9:LEU:CD2	1:B:25:ILE:HG22	2.08	0.83
1:B:200:LYS:O	1:B:201:SER:HB3	1.76	0.83
1:A:29:ILE:HG12	1:A:35:LYS:NZ	1.94	0.83
1:B:179:VAL:HG12	1:B:180:HIS:H	1.43	0.83
1:A:105:THR:CG2	1:A:198:LEU:HD22	2.09	0.82
1:A:126:LEU:HD11	1:A:175:PHE:HE1	1.42	0.82
1:A:229:LEU:CG	1:A:235:ASP:HA	2.09	0.82
1:B:205:HIS:N	1:B:206:PRO:HD2	1.95	0.82
1:A:92:GLY:O	1:A:93:LEU:HD23	1.79	0.82
1:B:127:HIS:C	1:B:127:HIS:HD1	1.87	0.82
1:A:5:VAL:HG21	1:A:84:VAL:HG11	1.62	0.82
1:A:32:VAL:HA	1:A:233:PHE:CE2	2.14	0.82
1:B:137:GLN:CG	1:B:140:LEU:HD22	2.09	0.82
1:A:45:GLY:HA3	1:A:200:LYS:CE	2.09	0.81
1:A:45:GLY:HA3	1:A:200:LYS:HE3	1.61	0.81
1:B:14:ASN:H	1:B:19:ASP:CB	1.85	0.81
1:A:50:ALA:HB3	1:A:195:PHE:CE1	2.15	0.81
1:A:137:GLN:C	1:A:139:ASP:H	1.88	0.81
1:A:234:PRO:O	1:A:235:ASP:HB3	1.78	0.81
1:B:22:TYR:CE1	1:B:39:LYS:CD	2.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:SER:HB3	1:B:164:SER:O	1.80	0.81
1:B:210:ILE:HG22	1:B:211:ALA:N	1.92	0.81
1:A:115:LEU:HD23	1:A:183:GLU:OE1	1.80	0.81
1:A:235:ASP:CG	1:A:236:ALA:N	2.35	0.81
1:B:103:THR:C	1:B:105:THR:H	1.88	0.81
1:A:92:GLY:C	1:A:93:LEU:HD23	2.06	0.81
1:A:231:GLY:O	1:A:232:LEU:HD23	1.79	0.81
1:B:55:ASN:CB	1:B:58:ASP:CB	2.58	0.81
1:A:198:LEU:HD23	1:A:198:LEU:C	2.04	0.81
1:B:88:TRP:CZ2	1:B:182:TRP:CH2	2.63	0.81
1:B:181:ILE:HG22	1:B:189:VAL:CG1	2.10	0.81
1:B:9:LEU:HB3	1:B:40:TRP:CH2	2.15	0.81
1:B:226:THR:H	1:B:229:LEU:CD1	1.93	0.81
1:A:127:HIS:ND1	1:A:127:HIS:C	2.39	0.80
1:B:226:THR:N	1:B:229:LEU:HD13	1.96	0.80
1:B:172:ARG:HD2	1:B:174:LEU:HD21	1.63	0.80
1:A:211:ALA:CB	1:A:230:LEU:HD12	2.07	0.80
1:B:225:SER:HA	1:B:229:LEU:CD2	2.12	0.80
1:A:117:SER:OG	1:A:186:ALA:HA	1.81	0.80
1:A:181:ILE:HG22	1:A:189:VAL:HG11	1.62	0.80
1:B:9:LEU:HD13	1:B:40:TRP:HH2	1.43	0.80
1:B:95:ALA:HB2	1:B:210:ILE:CG2	2.10	0.80
1:A:139:ASP:O	1:A:176:TYR:HB2	1.80	0.80
1:B:88:TRP:CD2	1:B:182:TRP:CH2	2.69	0.80
1:A:172:ARG:HH21	1:A:219:SER:HB3	1.45	0.80
1:A:66:SER:CA	1:A:72:ALA:HB2	2.11	0.80
1:A:16:ASP:HB2	1:A:228:ARG:HH12	1.47	0.79
1:B:8:GLU:HB2	1:B:211:ALA:HB2	1.63	0.79
1:A:32:VAL:HG13	1:A:233:PHE:HD2	1.48	0.79
1:B:6:ALA:HB1	1:B:213:PHE:CA	2.11	0.79
1:B:137:GLN:NE2	1:B:137:GLN:CA	2.34	0.79
1:A:84:VAL:O	1:A:85:LEU:HD23	1.81	0.79
1:B:52:ILE:HG13	1:B:212:PHE:CD2	2.17	0.79
1:A:133:PHE:CE1	1:A:154:LEU:HB2	2.17	0.79
1:B:151:ASP:OD2	1:B:153:ASN:HB2	1.82	0.79
1:A:143:GLN:HB3	1:A:172:ARG:HB3	1.63	0.79
1:B:104:ASN:HB3	1:B:210:ILE:CD1	2.12	0.79
1:B:222:PRO:HG3	1:B:232:LEU:O	1.82	0.79
1:A:40:TRP:HA	1:A:73:THR:HG21	1.65	0.79
1:A:45:GLY:HA2	1:A:200:LYS:CD	2.12	0.79
1:B:91:VAL:CG2	1:B:214:ILE:HG23	2.12	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:ILE:CG2	1:B:211:ALA:H	1.93	0.79
1:A:53:ILE:N	1:A:53:ILE:CD1	2.43	0.79
1:B:136:ASP:OD1	1:B:136:ASP:O	2.00	0.78
1:A:88:TRP:CG	1:B:138:LYS:HD2	2.18	0.78
1:B:35:LYS:HD2	1:B:35:LYS:N	1.97	0.78
1:B:181:ILE:HG22	1:B:189:VAL:CG2	2.12	0.78
1:B:21:SER:HB3	1:B:22:TYR:CE2	2.17	0.78
1:B:204:SER:C	1:B:206:PRO:HD2	2.08	0.78
1:A:88:TRP:CZ3	1:A:182:TRP:HH2	2.01	0.78
1:A:16:ASP:C	1:A:18:GLY:H	1.91	0.78
1:A:145:ASP:OD2	1:A:158:ARG:HD2	1.83	0.78
1:A:229:LEU:HD21	1:A:235:ASP:CA	2.12	0.78
1:B:222:PRO:HG2	1:B:225:SER:HG	1.45	0.78
1:B:56:SER:CB	1:B:189:VAL:N	2.44	0.78
1:B:95:ALA:HB1	1:B:210:ILE:HG12	1.65	0.78
1:A:74:SER:O	1:A:75:VAL:HG23	1.84	0.78
1:B:8:GLU:HA	1:B:211:ALA:HB2	1.63	0.78
1:A:115:LEU:HD12	1:A:189:VAL:CG2	2.13	0.78
1:A:229:LEU:HD21	1:A:235:ASP:HB2	1.66	0.78
1:B:228:ARG:O	1:B:230:LEU:N	2.17	0.78
1:A:56:SER:OG	1:A:189:VAL:HB	1.84	0.77
1:A:116:LYS:HB3	1:A:123:THR:HA	1.66	0.77
1:B:158:ARG:O	1:B:159:VAL:HG12	1.83	0.77
1:A:93:LEU:HD21	1:A:109:TRP:CE2	2.17	0.77
1:A:224:GLY:CA	1:A:229:LEU:HD23	2.15	0.77
1:A:118:ASN:HB3	1:A:185:SER:HB2	1.65	0.77
1:A:87:GLU:CD	1:A:182:TRP:CB	2.56	0.77
1:B:137:GLN:HB3	1:B:140:LEU:CB	2.10	0.77
1:B:231:GLY:O	1:B:232:LEU:HG	1.84	0.77
1:B:87:GLU:HG2	1:B:182:TRP:CE3	2.19	0.77
1:A:225:SER:HA	1:A:229:LEU:HB3	1.65	0.77
1:A:118:ASN:HB3	1:A:185:SER:CB	2.15	0.77
1:B:207:ALA:CB	1:B:208:ASP:CA	2.60	0.77
1:A:42:MET:CG	1:A:43:GLN:H	1.97	0.77
1:A:143:GLN:NE2	1:A:144:GLY:N	2.32	0.77
1:A:157:THR:OG1	1:A:169:SER:CB	2.32	0.77
1:A:14:ASN:O	1:A:17:ILE:HG23	1.85	0.76
1:A:17:ILE:CG2	1:A:228:ARG:HD3	2.15	0.76
1:A:45:GLY:CA	1:A:200:LYS:CE	2.64	0.76
1:B:29:ILE:O	1:B:30:LYS:HG3	1.86	0.76
1:B:94:SER:O	1:B:210:ILE:HG23	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:GLY:O	1:B:46:LYS:HD3	1.85	0.76
1:A:20:PRO:CG	1:A:24:HIS:CG	2.69	0.76
1:B:65:VAL:HG23	1:B:73:THR:HG23	1.68	0.76
1:B:102:GLU:OE1	1:B:199:ILE:HG21	1.86	0.76
1:B:10:ASP:HB2	1:B:24:HIS:O	1.85	0.76
1:B:121:HIS:C	1:B:122:GLN:CG	2.59	0.75
1:A:61:LEU:HD12	1:A:62:SER:N	2.01	0.75
1:B:86:PRO:HG2	1:B:89:VAL:HG22	1.68	0.75
1:A:52:ILE:C	1:A:53:ILE:HD12	2.11	0.75
1:A:115:LEU:CD1	1:A:189:VAL:HG22	2.15	0.75
1:B:213:PHE:C	1:B:213:PHE:CD2	2.63	0.75
1:B:62:SER:OG	1:B:76:SER:HB3	1.86	0.75
1:A:137:GLN:CG	1:A:140:LEU:HB2	2.16	0.75
1:B:94:SER:HB3	1:B:172:ARG:HG2	1.66	0.75
1:B:166:GLU:HG2	1:B:167:GLY:N	1.82	0.75
1:B:118:ASN:HB2	1:B:120:THR:OG1	1.87	0.74
1:A:14:ASN:HB3	1:A:228:ARG:NE	2.02	0.74
1:B:14:ASN:HB3	1:B:228:ARG:NH2	2.02	0.74
1:B:86:PRO:O	1:B:89:VAL:HG23	1.85	0.74
1:B:101:LYS:CD	1:B:101:LYS:H	1.99	0.74
1:A:166:GLU:CG	1:A:167:GLY:N	2.44	0.74
1:A:109:TRP:CZ3	1:A:140:LEU:HD11	2.23	0.74
1:A:174:LEU:HD23	1:A:174:LEU:H	1.51	0.74
1:B:2:ASP:OD2	1:B:219:SER:HA	1.87	0.74
1:A:64:VAL:HA	1:A:74:SER:HA	1.69	0.74
1:A:118:ASN:CB	1:A:185:SER:HB2	2.18	0.74
1:B:19:ASP:CG	1:B:24:HIS:HE1	1.95	0.74
1:B:52:ILE:HD13	1:B:63:ALA:HB2	1.68	0.74
1:B:32:VAL:CA	1:B:233:PHE:HE2	1.97	0.74
1:A:49:THR:HA	1:A:195:PHE:O	1.87	0.74
1:A:142:LEU:HD23	1:A:142:LEU:N	2.03	0.74
1:B:95:ALA:HB1	1:B:210:ILE:HA	1.68	0.74
1:A:157:THR:HG23	1:A:158:ARG:O	1.87	0.73
1:A:170:VAL:O	1:A:170:VAL:HG23	1.86	0.73
1:B:9:LEU:CA	1:B:40:TRP:HZ3	2.00	0.73
1:A:56:SER:HB2	1:A:189:VAL:N	2.03	0.73
1:A:97:THR:OG1	1:A:167:GLY:HA2	1.87	0.73
1:B:157:THR:HG23	1:B:158:ARG:N	2.01	0.73
1:A:44:ASP:OD1	1:A:200:LYS:HG2	1.88	0.73
1:A:87:GLU:O	1:A:182:TRP:CE3	2.41	0.73
1:A:115:LEU:HD22	1:A:180:HIS:CE1	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:SER:HB3	1:B:22:TYR:CD2	2.23	0.73
1:B:65:VAL:HG23	1:B:73:THR:CG2	2.19	0.73
1:B:91:VAL:HG21	1:B:214:ILE:HG23	1.71	0.73
1:B:93:LEU:C	1:B:213:PHE:CE1	2.67	0.73
1:A:32:VAL:HG22	1:A:233:PHE:CG	2.23	0.73
1:A:68:PRO:C	1:A:70:ALA:H	1.96	0.73
1:A:180:HIS:HB2	1:A:182:TRP:CD2	2.23	0.73
1:B:174:LEU:CD2	1:B:213:PHE:HZ	2.02	0.73
1:A:4:ILE:CD1	1:A:232:LEU:CB	2.67	0.73
1:A:20:PRO:HG3	1:A:24:HIS:CG	2.24	0.73
1:A:222:PRO:HG2	1:A:225:SER:HB3	0.75	0.73
1:B:25:ILE:N	1:B:25:ILE:CD1	2.51	0.73
1:A:145:ASP:OD1	1:A:169:SER:HA	1.90	0.72
1:B:61:LEU:CD2	1:B:81:LEU:HD13	2.17	0.72
1:A:55:ASN:HB2	1:A:58:ASP:CB	2.20	0.72
1:A:182:TRP:HD1	1:A:183:GLU:H	1.33	0.72
1:A:117:SER:HB3	1:A:186:ALA:C	2.14	0.72
1:B:17:ILE:O	1:B:33:ARG:HG2	1.89	0.72
1:B:145:ASP:HB3	1:B:158:ARG:HG3	1.72	0.72
1:A:32:VAL:HA	1:A:233:PHE:CD2	2.25	0.72
1:A:65:VAL:C	1:A:72:ALA:HB1	2.15	0.72
1:B:25:ILE:H	1:B:25:ILE:CD1	2.02	0.72
1:B:53:ILE:HD12	1:B:53:ILE:O	1.88	0.72
1:A:20:PRO:HG3	1:A:24:HIS:CB	2.19	0.72
1:A:180:HIS:CA	1:A:182:TRP:CZ3	2.71	0.72
1:A:225:SER:HB2	1:A:231:GLY:N	2.05	0.72
1:B:45:GLY:C	1:B:46:LYS:HD3	2.14	0.72
1:A:162:ASN:CG	1:A:163:GLY:N	2.47	0.72
1:B:230:LEU:HD13	1:B:230:LEU:O	1.89	0.72
1:A:180:HIS:C	1:A:181:ILE:HG13	2.13	0.71
1:B:17:ILE:HG22	1:B:237:ASN:OD1	1.89	0.71
1:B:174:LEU:HD23	1:B:174:LEU:N	2.03	0.71
1:A:106:ILE:HD12	1:A:154:LEU:HB3	1.73	0.71
1:B:56:SER:CB	1:B:188:THR:CA	2.66	0.71
1:B:145:ASP:OD2	1:B:169:SER:HB2	1.90	0.71
1:A:122:GLN:HG2	1:B:131:ASN:CB	2.08	0.71
1:B:26:GLY:HA3	1:B:34:SER:OG	1.91	0.71
1:A:17:ILE:HA	1:A:33:ARG:CZ	2.21	0.71
1:A:116:LYS:HG2	1:A:117:SER:N	2.06	0.71
1:A:170:VAL:O	1:A:170:VAL:CG2	2.39	0.71
1:B:7:VAL:HG21	1:B:52:ILE:CD1	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:ASP:O	1:B:59:LYS:HG3	1.89	0.71
1:B:143:GLN:NE2	1:B:221:ILE:HB	2.05	0.71
1:A:54:TYR:HB3	1:A:191:PHE:CZ	2.25	0.70
1:A:137:GLN:CB	1:A:140:LEU:HB2	2.20	0.70
1:B:100:TYR:O	1:B:167:GLY:HA3	1.91	0.70
1:A:10:ASP:CB	1:A:24:HIS:CE1	2.73	0.70
1:B:9:LEU:HB3	1:B:40:TRP:HH2	1.56	0.70
1:A:17:ILE:HD11	1:A:19:ASP:OD2	1.91	0.70
1:B:60:ARG:HG2	1:B:62:SER:OG	1.90	0.70
1:B:79:VAL:HG22	1:B:80:ASP:N	2.07	0.70
1:B:141:ILE:CG2	1:B:174:LEU:HB2	2.20	0.70
1:B:52:ILE:HG13	1:B:212:PHE:HD2	1.57	0.70
1:B:60:ARG:HG2	1:B:62:SER:HG	1.56	0.70
1:B:137:GLN:O	1:B:138:LYS:CB	2.39	0.70
1:B:35:LYS:HD2	1:B:35:LYS:H	1.54	0.70
1:B:87:GLU:CG	1:B:182:TRP:CG	2.75	0.70
1:A:52:ILE:O	1:A:53:ILE:HG13	1.91	0.70
1:B:93:LEU:O	1:B:213:PHE:HE1	1.75	0.70
1:A:180:HIS:CD2	1:A:182:TRP:CE2	2.79	0.70
1:B:51:HIS:O	1:B:63:ALA:HB1	1.92	0.70
1:B:180:HIS:CD2	1:B:182:TRP:CZ3	2.78	0.70
1:B:8:GLU:HA	1:B:211:ALA:CA	2.21	0.70
1:A:3:THR:C	1:A:4:ILE:HG22	2.16	0.70
1:B:102:GLU:HG3	1:B:199:ILE:CG2	2.21	0.70
1:A:5:VAL:CG2	1:A:84:VAL:HG11	2.20	0.69
1:A:21:SER:O	1:A:22:TYR:HB3	1.92	0.69
1:A:117:SER:HB3	1:A:187:ALA:N	2.07	0.69
1:A:50:ALA:CB	1:A:195:PHE:CZ	2.75	0.69
1:B:141:ILE:O	1:B:141:ILE:CG2	2.39	0.69
1:B:146:ALA:CB	1:B:156:LEU:HA	2.22	0.69
1:A:118:ASN:HA	1:A:185:SER:CB	2.22	0.69
1:A:59:LYS:HE2	1:A:78:ASP:CB	2.15	0.69
1:A:106:ILE:CD1	1:A:154:LEU:HD13	2.12	0.69
1:A:116:LYS:CG	1:A:117:SER:H	2.03	0.69
1:A:88:TRP:CH2	1:B:137:GLN:O	2.45	0.69
1:B:105:THR:HG22	1:B:105:THR:O	1.93	0.69
1:B:216:ASN:OD1	1:B:216:ASN:N	2.21	0.69
1:A:115:LEU:CD1	1:A:189:VAL:CG2	2.69	0.69
1:B:22:TYR:CB	1:B:23:PRO:CD	2.50	0.69
1:B:101:LYS:H	1:B:101:LYS:HD3	1.57	0.69
1:B:2:ASP:CA	1:B:216:ASN:HD21	2.02	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:ASP:OD2	1:B:169:SER:HA	1.92	0.69
1:A:106:ILE:HD12	1:A:154:LEU:C	2.18	0.69
1:A:119:SER:C	1:A:121:HIS:N	2.48	0.69
1:B:102:GLU:HG3	1:B:103:THR:N	2.08	0.69
1:B:180:HIS:ND1	1:B:182:TRP:CZ3	2.60	0.69
1:A:62:SER:HB2	1:A:75:VAL:O	1.93	0.69
1:B:120:THR:O	1:B:122:GLN:HG3	1.93	0.69
1:A:122:GLN:HB3	1:B:131:ASN:CB	2.22	0.68
1:B:39:LYS:HG3	1:B:40:TRP:H	1.57	0.68
1:A:12:TYR:O	1:A:14:ASN:N	2.26	0.68
1:A:50:ALA:CB	1:A:195:PHE:CE1	2.77	0.68
1:A:157:THR:HG1	1:A:169:SER:HB2	1.58	0.68
1:B:225:SER:OG	1:B:231:GLY:HA2	1.92	0.68
1:A:17:ILE:C	1:A:19:ASP:H	1.99	0.68
1:B:44:ASP:O	1:B:46:LYS:HG2	1.92	0.68
1:B:180:HIS:ND1	1:B:182:TRP:CE3	2.62	0.68
1:A:181:ILE:HG22	1:A:189:VAL:CG1	2.24	0.68
1:A:229:LEU:HG	1:A:235:ASP:HA	1.75	0.68
1:B:179:VAL:HG12	1:B:180:HIS:N	2.08	0.68
1:A:12:TYR:CD2	1:A:14:ASN:ND2	2.62	0.68
1:B:91:VAL:HG22	1:B:92:GLY:H	1.59	0.68
1:B:225:SER:HA	1:B:229:LEU:CB	2.22	0.68
1:A:115:LEU:O	1:A:123:THR:HA	1.92	0.68
1:B:106:ILE:HD11	1:B:156:LEU:HD11	1.76	0.68
1:A:166:GLU:CG	1:A:167:GLY:H	2.00	0.68
1:A:180:HIS:HB3	1:A:182:TRP:CZ3	2.15	0.68
1:B:9:LEU:HA	1:B:40:TRP:HZ3	1.59	0.68
1:B:71:ASP:OD2	1:B:71:ASP:N	2.25	0.68
1:A:52:ILE:N	1:A:52:ILE:CD1	2.57	0.68
1:A:180:HIS:CD2	1:A:182:TRP:CZ2	2.81	0.68
1:A:225:SER:CA	1:A:231:GLY:H	2.07	0.68
1:B:94:SER:HB3	1:B:172:ARG:CG	2.24	0.67
1:B:145:ASP:HB2	1:B:170:VAL:O	1.92	0.67
1:A:26:GLY:C	1:A:27:ILE:HD12	2.19	0.67
1:A:106:ILE:HD12	1:A:154:LEU:HD22	1.75	0.67
1:A:113:SER:HA	1:A:191:PHE:HA	1.76	0.67
1:B:63:ALA:C	1:B:64:VAL:HG12	2.20	0.67
1:A:66:SER:CA	1:A:72:ALA:CB	2.71	0.67
1:A:182:TRP:HD1	1:A:183:GLU:N	1.87	0.67
1:B:95:ALA:HB2	1:B:210:ILE:HA	1.76	0.67
1:A:32:VAL:HG13	1:A:233:PHE:CD2	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:ILE:CG2	1:A:61:LEU:HD11	2.25	0.67
1:A:106:ILE:CD1	1:A:154:LEU:HB3	2.25	0.67
1:B:93:LEU:C	1:B:213:PHE:HE1	2.00	0.67
1:A:93:LEU:CD2	1:A:212:PHE:CD1	2.78	0.67
1:A:140:LEU:HD12	1:A:174:LEU:O	1.95	0.67
1:A:7:VAL:HG23	1:A:7:VAL:O	1.94	0.67
1:A:20:PRO:HG3	1:A:24:HIS:HB3	1.77	0.67
1:A:106:ILE:CD1	1:A:154:LEU:CD2	2.73	0.67
1:A:172:ARG:CD	1:A:213:PHE:CZ	2.78	0.67
1:A:88:TRP:CZ2	1:A:182:TRP:CH2	2.83	0.66
1:B:29:ILE:C	1:B:30:LYS:HG3	2.19	0.66
1:B:112:THR:HG23	1:B:127:HIS:CB	2.24	0.66
1:A:25:ILE:HG13	1:A:38:ALA:O	1.95	0.66
1:A:29:ILE:HG22	1:A:84:VAL:CG1	2.25	0.66
1:A:115:LEU:CG	1:A:180:HIS:CE1	2.78	0.66
1:B:225:SER:HB2	1:B:231:GLY:H	1.60	0.66
1:B:6:ALA:HB2	1:B:213:PHE:CA	2.13	0.66
1:B:25:ILE:HD13	1:B:25:ILE:C	2.17	0.66
1:B:174:LEU:HD21	1:B:213:PHE:HZ	1.61	0.66
1:A:109:TRP:HH2	1:A:174:LEU:HA	1.60	0.66
1:B:45:GLY:C	1:B:46:LYS:HE2	2.21	0.66
1:B:115:LEU:HD21	1:B:183:GLU:HB3	1.76	0.66
1:B:198:LEU:O	1:B:198:LEU:HG	1.95	0.66
1:A:17:ILE:HG21	1:A:228:ARG:HD3	1.76	0.66
1:B:6:ALA:HB1	1:B:212:PHE:C	2.19	0.66
1:B:87:GLU:HG2	1:B:182:TRP:CE2	2.31	0.66
1:A:12:TYR:CD2	1:A:12:TYR:C	2.74	0.66
1:B:89:VAL:O	1:B:179:VAL:HB	1.95	0.66
1:B:225:SER:HB2	1:B:231:GLY:N	2.11	0.66
1:A:27:ILE:HG22	1:A:27:ILE:O	1.95	0.66
1:B:23:PRO:CG	1:B:40:TRP:O	2.44	0.66
1:B:103:THR:H	1:B:199:ILE:HG22	1.59	0.66
1:B:103:THR:OG1	1:B:199:ILE:HA	1.94	0.66
1:B:40:TRP:HD1	1:B:41:ASN:H	1.42	0.66
1:B:158:ARG:HB2	1:B:169:SER:HB3	1.76	0.66
1:B:237:ASN:N	1:B:237:ASN:HD22	1.92	0.66
1:A:52:ILE:O	1:A:53:ILE:HG23	1.96	0.65
1:A:52:ILE:HG22	1:A:53:ILE:H	1.60	0.65
1:A:13:PRO:CB	1:A:21:SER:C	2.68	0.65
1:B:143:GLN:HE22	1:B:221:ILE:HB	1.60	0.65
1:B:221:ILE:HD12	1:B:222:PRO:HD2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:ILE:CD1	1:A:156:LEU:HG	2.19	0.65
1:A:33:ARG:HH21	1:A:237:ASN:HB3	1.60	0.65
1:A:45:GLY:CA	1:A:200:LYS:CD	2.75	0.65
1:A:115:LEU:C	1:A:116:LYS:CD	2.66	0.65
1:A:180:HIS:HB2	1:A:182:TRP:CZ2	2.30	0.65
1:B:8:GLU:O	1:B:25:ILE:HA	1.96	0.65
1:B:184:SER:C	1:B:186:ALA:H	2.05	0.65
1:B:201:SER:OG	1:B:206:PRO:HB3	1.97	0.65
1:A:134:SER:O	1:A:148:THR:HG22	1.97	0.65
1:B:145:ASP:OD2	1:B:158:ARG:HD2	1.97	0.65
1:B:180:HIS:CE1	1:B:182:TRP:CD2	2.84	0.65
1:A:65:VAL:O	1:A:72:ALA:HA	1.97	0.65
1:B:173:ALA:O	1:B:174:LEU:HD23	1.96	0.65
1:A:172:ARG:CZ	1:A:213:PHE:CE2	2.80	0.65
1:B:8:GLU:CB	1:B:211:ALA:HB2	2.26	0.65
1:B:74:SER:O	1:B:75:VAL:HG22	1.97	0.65
1:B:160:SER:HB3	1:B:164:SER:HB2	1.79	0.65
1:A:89:VAL:HG21	1:A:214:ILE:HG22	1.77	0.65
1:B:141:ILE:HG21	1:B:174:LEU:CB	2.27	0.65
1:B:225:SER:CA	1:B:229:LEU:HD22	2.25	0.65
1:A:53:ILE:HD13	1:A:53:ILE:O	1.97	0.64
1:B:48:GLY:O	1:B:197:PHE:CE1	2.50	0.64
1:B:88:TRP:CD2	1:B:182:TRP:HH2	2.10	0.64
1:B:137:GLN:CB	1:B:140:LEU:CB	2.73	0.64
1:B:154:LEU:HD22	1:B:155:GLU:N	2.12	0.64
1:A:137:GLN:O	1:A:139:ASP:N	2.30	0.64
1:B:19:ASP:CG	1:B:24:HIS:CE1	2.75	0.64
1:B:224:GLY:O	1:B:229:LEU:HD22	1.98	0.64
1:B:226:THR:N	1:B:229:LEU:HB2	2.11	0.64
1:A:173:ALA:C	1:A:174:LEU:CD2	2.71	0.64
1:B:110:SER:HB3	1:B:194:THR:CG2	2.28	0.64
1:B:237:ASN:N	1:B:237:ASN:ND2	2.46	0.64
1:A:169:SER:C	1:A:170:VAL:HG13	2.23	0.64
1:A:6:ALA:HA	1:A:212:PHE:O	1.96	0.64
1:A:88:TRP:CE2	1:B:138:LYS:HD2	2.33	0.64
1:A:180:HIS:HD2	1:A:182:TRP:CZ2	2.16	0.64
1:B:18:GLY:O	1:B:20:PRO:CD	2.44	0.64
1:A:29:ILE:N	1:A:35:LYS:HE3	2.12	0.64
1:A:135:LYS:HG3	1:A:149:GLY:HA3	1.79	0.64
1:B:193:ALA:O	1:B:194:THR:HB	1.98	0.64
1:A:95:ALA:HB2	1:A:210:ILE:HG23	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:THR:C	1:A:121:HIS:CG	2.76	0.64
1:A:127:HIS:ND1	1:A:128:PHE:N	2.45	0.64
1:B:100:TYR:C	1:B:101:LYS:HD2	2.23	0.64
1:A:133:PHE:CE2	1:A:154:LEU:HD12	2.32	0.64
1:B:7:VAL:O	1:B:212:PHE:N	2.30	0.64
1:B:22:TYR:HE1	1:B:39:LYS:HB2	1.61	0.64
1:B:110:SER:HB3	1:B:194:THR:HG22	1.79	0.64
1:A:60:ARG:HA	1:A:77:TYR:O	1.98	0.63
1:B:8:GLU:HA	1:B:211:ALA:HA	1.80	0.63
1:B:91:VAL:HG23	1:B:214:ILE:CG2	2.27	0.63
1:A:88:TRP:CE3	1:A:182:TRP:CZ3	2.86	0.63
1:A:93:LEU:HD21	1:A:109:TRP:CZ2	2.34	0.63
1:A:106:ILE:HD12	1:A:154:LEU:CB	2.29	0.63
1:A:141:ILE:HG22	1:A:174:LEU:CD2	2.28	0.63
1:B:122:GLN:N	1:B:122:GLN:NE2	2.45	0.63
1:A:159:VAL:HA	1:A:165:PRO:HA	1.80	0.63
1:A:89:VAL:HG23	1:A:215:SER:O	1.98	0.63
1:B:14:ASN:O	1:B:17:ILE:HG13	1.98	0.63
1:B:74:SER:C	1:B:75:VAL:HG22	2.24	0.63
1:B:88:TRP:CZ3	1:B:180:HIS:HB2	2.34	0.63
1:B:91:VAL:CG2	1:B:214:ILE:CG2	2.77	0.63
1:B:93:LEU:O	1:B:213:PHE:CE1	2.52	0.63
1:A:12:TYR:C	1:A:12:TYR:HD2	2.05	0.63
1:A:8:GLU:O	1:A:25:ILE:HG22	1.98	0.63
1:A:42:MET:CG	1:A:43:GLN:N	2.56	0.63
1:A:122:GLN:O	1:A:123:THR:HG22	1.99	0.63
1:B:180:HIS:ND1	1:B:180:HIS:C	2.56	0.63
1:A:10:ASP:HB2	1:A:24:HIS:CE1	2.34	0.63
1:B:8:GLU:CA	1:B:211:ALA:HB2	2.29	0.63
1:B:162:ASN:CG	1:B:162:ASN:O	2.42	0.63
1:A:93:LEU:HD21	1:A:109:TRP:NE1	2.13	0.62
1:B:55:ASN:O	1:B:59:LYS:HA	1.98	0.62
1:B:141:ILE:O	1:B:173:ALA:CA	2.36	0.62
1:A:23:PRO:HB2	1:A:40:TRP:O	2.00	0.62
1:A:128:PHE:CE2	1:A:175:PHE:CE1	2.86	0.62
1:B:205:HIS:O	1:B:206:PRO:C	2.38	0.62
1:A:20:PRO:HG2	1:A:24:HIS:CG	2.33	0.62
1:A:87:GLU:CG	1:A:182:TRP:CB	2.77	0.62
1:B:63:ALA:O	1:B:64:VAL:HG12	1.99	0.62
1:B:181:ILE:HG22	1:B:189:VAL:HG21	1.81	0.62
1:A:17:ILE:O	1:A:33:ARG:HD3	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:SER:CB	1:A:189:VAL:N	2.63	0.62
1:A:87:GLU:CG	1:A:182:TRP:HB3	2.29	0.62
1:A:141:ILE:O	1:A:141:ILE:CG2	2.48	0.62
1:A:172:ARG:NH1	1:A:213:PHE:CE1	2.68	0.62
1:A:18:GLY:O	1:A:19:ASP:O	2.17	0.62
1:B:74:SER:O	1:B:75:VAL:CG1	2.47	0.62
1:B:95:ALA:CB	1:B:210:ILE:HG12	2.28	0.62
1:A:89:VAL:O	1:A:179:VAL:HG23	1.99	0.62
1:A:137:GLN:HB3	1:A:139:ASP:OD2	1.99	0.62
1:B:51:HIS:O	1:B:63:ALA:CB	2.48	0.62
1:B:90:ARG:HG3	1:B:91:VAL:N	2.14	0.62
1:A:89:VAL:CG2	1:A:214:ILE:HG22	2.30	0.61
1:A:32:VAL:CG1	1:A:233:PHE:HD2	2.12	0.61
1:A:51:HIS:O	1:A:52:ILE:HD13	1.99	0.61
1:B:4:ILE:HG22	1:B:215:SER:CB	2.28	0.61
1:B:39:LYS:CG	1:B:40:TRP:N	2.62	0.61
1:B:82:ASN:OD1	1:B:82:ASN:N	2.33	0.61
1:B:91:VAL:HG22	1:B:213:PHE:O	2.00	0.61
1:B:63:ALA:C	1:B:64:VAL:CG1	2.72	0.61
1:B:157:THR:CG2	1:B:158:ARG:N	2.62	0.61
1:A:54:TYR:CB	1:A:191:PHE:CZ	2.83	0.61
1:A:143:GLN:O	1:A:171:GLY:HA2	2.00	0.61
1:B:187:ALA:O	1:B:188:THR:HG22	2.00	0.61
1:B:225:SER:CA	1:B:229:LEU:HB3	2.29	0.61
1:A:22:TYR:CB	1:A:23:PRO:CD	2.54	0.61
1:A:24:HIS:C	1:A:25:ILE:CG1	2.73	0.61
1:A:35:LYS:HD3	1:A:35:LYS:N	2.16	0.61
1:A:111:PHE:HB3	1:A:128:PHE:CZ	2.36	0.61
1:B:38:ALA:HB2	1:B:75:VAL:HG13	1.76	0.61
1:B:9:LEU:HD22	1:B:25:ILE:CG2	2.25	0.61
1:B:38:ALA:HB3	1:B:75:VAL:HG11	1.80	0.61
1:B:92:GLY:CA	1:B:174:LEU:HA	2.26	0.61
1:B:101:LYS:HB3	1:B:165:PRO:HB2	1.82	0.61
1:A:11:THR:HG23	1:A:209:GLY:CA	2.28	0.61
1:A:122:GLN:NE2	1:B:132:GLN:NE2	2.45	0.61
1:B:31:SER:C	1:B:233:PHE:CE2	2.79	0.61
1:B:54:TYR:OH	1:B:81:LEU:HB3	2.01	0.61
1:B:120:THR:O	1:B:121:HIS:CD2	2.54	0.61
1:B:9:LEU:CD1	1:B:40:TRP:CH2	2.83	0.60
1:B:188:THR:HG23	1:B:188:THR:O	2.01	0.60
1:A:180:HIS:CB	1:A:182:TRP:CE3	2.60	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:SER:HB3	1:B:164:SER:C	2.25	0.60
1:A:42:MET:O	1:A:43:GLN:HG2	2.00	0.60
1:B:122:GLN:HE21	1:B:122:GLN:H	1.47	0.60
1:A:48:GLY:O	1:A:196:ALA:HA	1.99	0.60
1:A:62:SER:CB	1:A:76:SER:HA	2.28	0.60
1:B:9:LEU:CD1	1:B:40:TRP:HH2	2.13	0.60
1:B:120:THR:O	1:B:121:HIS:O	2.20	0.60
1:B:143:GLN:N	1:B:172:ARG:O	2.34	0.60
1:A:29:ILE:HG12	1:A:35:LYS:HZ2	1.65	0.60
1:A:24:HIS:C	1:A:25:ILE:HG13	2.27	0.60
1:A:24:HIS:O	1:A:25:ILE:HG12	2.02	0.60
1:A:29:ILE:CG2	1:A:84:VAL:HG11	2.32	0.60
1:B:44:ASP:O	1:B:46:LYS:CE	2.50	0.60
1:A:13:PRO:CB	1:A:22:TYR:HA	2.30	0.60
1:A:101:LYS:O	1:A:102:GLU:HG2	2.01	0.60
1:B:79:VAL:CG2	1:B:80:ASP:N	2.64	0.60
1:A:92:GLY:O	1:A:212:PHE:CD1	2.55	0.60
1:B:53:ILE:CD1	1:B:62:SER:HB2	2.24	0.60
1:B:212:PHE:C	1:B:212:PHE:CD1	2.70	0.60
1:A:29:ILE:C	1:A:30:LYS:HG3	2.26	0.60
1:A:69:ASN:N	1:A:69:ASN:ND2	2.49	0.59
1:B:94:SER:O	1:B:95:ALA:HB2	2.00	0.59
1:A:61:LEU:HD12	1:A:62:SER:H	1.66	0.59
1:A:224:GLY:C	1:A:226:THR:H	2.09	0.59
1:A:225:SER:O	1:A:231:GLY:N	2.35	0.59
1:B:9:LEU:HB3	1:B:40:TRP:CZ3	2.37	0.59
1:B:181:ILE:HG22	1:B:189:VAL:HG11	1.83	0.59
1:A:27:ILE:O	1:A:29:ILE:CD1	2.51	0.59
1:A:29:ILE:CG1	1:A:35:LYS:CE	2.52	0.59
1:A:29:ILE:O	1:A:30:LYS:HG3	2.02	0.59
1:B:53:ILE:CD1	1:B:62:SER:O	2.51	0.59
1:A:222:PRO:HG2	1:A:225:SER:OG	2.01	0.59
1:B:40:TRP:CD1	1:B:41:ASN:H	2.20	0.59
1:A:65:VAL:O	1:A:72:ALA:CA	2.51	0.59
1:A:195:PHE:O	1:A:195:PHE:CD1	2.56	0.59
1:B:95:ALA:HB2	1:B:210:ILE:CB	2.32	0.59
1:B:180:HIS:CE1	1:B:182:TRP:CE3	2.90	0.59
1:A:116:LYS:HB3	1:A:123:THR:CA	2.31	0.59
1:A:160:SER:HB3	1:A:164:SER:H	1.67	0.59
1:A:10:ASP:HB3	1:A:24:HIS:CE1	2.38	0.59
1:A:93:LEU:HD22	1:A:212:PHE:HD1	1.64	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:LYS:O	1:A:117:SER:CB	2.47	0.59
1:A:117:SER:HA	1:A:187:ALA:HB3	1.83	0.59
1:A:158:ARG:NH1	1:A:158:ARG:CG	2.41	0.59
1:B:154:LEU:HD22	1:B:154:LEU:C	2.27	0.59
1:A:29:ILE:H	1:A:35:LYS:CE	2.15	0.59
1:A:235:ASP:OD1	1:A:236:ALA:N	2.36	0.59
1:B:22:TYR:HE1	1:B:39:LYS:HD3	1.64	0.59
1:A:80:ASP:O	1:A:81:LEU:CB	2.49	0.59
1:A:27:ILE:O	1:A:29:ILE:HD13	2.03	0.59
1:A:117:SER:CB	1:A:187:ALA:N	2.65	0.59
1:A:143:GLN:CB	1:A:172:ARG:HB3	2.32	0.59
1:A:145:ASP:OD1	1:A:169:SER:HB3	2.03	0.59
1:B:172:ARG:HD3	1:B:213:PHE:CZ	2.38	0.59
1:A:11:THR:N	1:A:208:ASP:O	2.32	0.58
1:A:33:ARG:HH21	1:A:237:ASN:CB	2.15	0.58
1:B:34:SER:HB2	1:B:37:THR:HG22	1.85	0.58
1:B:13:PRO:HG3	1:B:22:TYR:HA	1.85	0.58
1:B:39:LYS:HG3	1:B:40:TRP:N	2.17	0.58
1:A:29:ILE:HG22	1:A:84:VAL:HG13	1.86	0.58
1:A:56:SER:HB3	1:A:187:ALA:O	2.03	0.58
1:B:40:TRP:CD1	1:B:41:ASN:N	2.72	0.58
1:B:118:ASN:OD1	1:B:121:HIS:N	2.36	0.58
1:A:17:ILE:HG12	1:A:19:ASP:HB2	1.84	0.58
1:A:107:LEU:HB2	1:A:196:ALA:O	2.03	0.58
1:B:215:SER:HB2	1:B:216:ASN:OD1	2.03	0.58
1:A:56:SER:HB2	1:A:188:THR:C	2.27	0.58
1:A:115:LEU:CD2	1:A:180:HIS:CE1	2.85	0.58
1:A:172:ARG:NH1	1:A:213:PHE:CE2	2.71	0.58
1:B:92:GLY:CA	1:B:109:TRP:HH2	2.01	0.58
1:B:120:THR:HB	1:B:122:GLN:OE1	2.03	0.58
1:A:29:ILE:HD13	1:A:29:ILE:N	2.15	0.58
1:A:118:ASN:CB	1:A:185:SER:CB	2.80	0.58
1:A:180:HIS:CB	1:A:182:TRP:CZ2	2.83	0.58
1:A:52:ILE:O	1:A:53:ILE:CG1	2.51	0.58
1:A:120:THR:HG22	1:A:120:THR:O	2.02	0.58
1:A:88:TRP:CE3	1:A:182:TRP:CH2	2.91	0.58
1:A:137:GLN:HB3	1:A:140:LEU:N	2.17	0.58
1:A:172:ARG:NH1	1:A:213:PHE:CZ	2.71	0.58
1:B:87:GLU:CG	1:B:182:TRP:CE2	2.87	0.58
1:B:141:ILE:CG2	1:B:174:LEU:CB	2.81	0.58
1:A:137:GLN:O	1:B:88:TRP:CH2	2.57	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:TYR:HB2	1:B:207:ALA:HB2	1.86	0.58
1:B:180:HIS:NE2	1:B:182:TRP:CZ2	2.72	0.57
1:A:133:PHE:CZ	1:A:154:LEU:HB2	2.38	0.57
1:B:8:GLU:CA	1:B:211:ALA:CB	2.79	0.57
1:B:128:PHE:CD2	1:B:175:PHE:CZ	2.92	0.57
1:B:180:HIS:NE2	1:B:182:TRP:CH2	2.72	0.57
1:B:201:SER:HB2	1:B:206:PRO:HB3	1.86	0.57
1:A:27:ILE:CG2	1:A:29:ILE:CD1	2.78	0.57
1:A:130:PHE:CE2	1:A:140:LEU:HD22	2.38	0.57
1:B:9:LEU:CB	1:B:40:TRP:CH2	2.87	0.57
1:B:226:THR:H	1:B:229:LEU:HB2	1.69	0.57
1:B:234:PRO:O	1:B:235:ASP:HB3	2.05	0.57
1:A:35:LYS:HB3	1:A:77:TYR:CZ	2.40	0.57
1:A:88:TRP:CE2	1:A:182:TRP:CH2	2.92	0.57
1:A:106:ILE:HD13	1:A:154:LEU:CG	2.33	0.57
1:A:106:ILE:HD11	1:A:156:LEU:HD21	1.83	0.57
1:B:44:ASP:O	1:B:46:LYS:CG	2.52	0.57
1:B:49:THR:CG2	1:B:51:HIS:CE1	2.87	0.57
1:A:6:ALA:CB	1:A:212:PHE:O	2.52	0.57
1:A:17:ILE:HA	1:A:33:ARG:NH2	2.18	0.57
1:A:56:SER:HB2	1:A:189:VAL:H	1.69	0.57
1:A:145:ASP:OD1	1:A:169:SER:CA	2.52	0.57
1:B:7:VAL:HG11	1:B:52:ILE:CD1	2.34	0.57
1:B:141:ILE:O	1:B:141:ILE:HG23	2.03	0.57
1:A:109:TRP:HZ3	1:A:140:LEU:HD11	1.68	0.57
1:A:199:ILE:HD11	1:A:210:ILE:HD11	1.86	0.57
1:B:212:PHE:CD1	1:B:213:PHE:N	2.73	0.57
1:A:6:ALA:CA	1:A:212:PHE:O	2.52	0.57
1:A:113:SER:HB3	1:A:191:PHE:HB3	1.86	0.57
1:A:180:HIS:C	1:A:181:ILE:CG1	2.77	0.57
1:B:32:VAL:CA	1:B:233:PHE:CE2	2.81	0.57
1:B:110:SER:CB	1:B:194:THR:HG23	2.34	0.57
1:A:88:TRP:CG	1:B:138:LYS:CD	2.86	0.57
1:A:32:VAL:CA	1:A:233:PHE:CD2	2.87	0.56
1:A:32:VAL:CG2	1:A:233:PHE:CD2	2.86	0.56
1:A:106:ILE:CB	1:A:154:LEU:HB3	2.31	0.56
1:A:126:LEU:HD11	1:A:175:PHE:CE1	2.33	0.56
1:A:128:PHE:CE2	1:A:175:PHE:CD1	2.93	0.56
1:A:141:ILE:O	1:A:174:LEU:HD23	2.05	0.56
1:B:7:VAL:O	1:B:211:ALA:HB1	2.04	0.56
1:B:134:SER:O	1:B:148:THR:HG23	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:ASP:HB2	1:B:206:PRO:HD3	1.87	0.56
1:A:177:ALA:HB2	1:B:177:ALA:HB2	1.87	0.56
1:B:172:ARG:CD	1:B:174:LEU:HD21	2.35	0.56
1:A:91:VAL:HG22	1:A:214:ILE:HG23	1.87	0.56
1:A:95:ALA:HB1	1:A:104:ASN:ND2	2.20	0.56
1:A:132:GLN:HB3	1:B:183:GLU:OE2	2.04	0.56
1:B:51:HIS:C	1:B:52:ILE:CG1	2.77	0.56
1:B:52:ILE:CG1	1:B:212:PHE:HD2	2.18	0.56
1:B:172:ARG:HH21	1:B:221:ILE:N	2.03	0.56
1:B:217:ILE:HG23	1:B:217:ILE:O	2.06	0.56
1:B:3:THR:O	1:B:4:ILE:CG2	2.54	0.56
1:B:117:SER:HB3	1:B:187:ALA:CB	2.32	0.56
1:B:182:TRP:CG	1:B:183:GLU:N	2.73	0.56
1:A:5:VAL:HG12	1:A:5:VAL:O	2.05	0.56
1:A:28:ASP:O	1:A:29:ILE:HD13	2.05	0.56
1:A:51:HIS:C	1:A:52:ILE:CD1	2.67	0.56
1:A:88:TRP:CE2	1:A:182:TRP:CZ3	2.94	0.56
1:B:52:ILE:CD1	1:B:212:PHE:HD2	2.18	0.56
1:A:93:LEU:CD2	1:A:212:PHE:HD1	2.18	0.56
1:A:106:ILE:CD1	1:A:156:LEU:HD21	2.36	0.56
1:B:9:LEU:HA	1:B:40:TRP:CZ3	2.39	0.56
1:B:14:ASN:C	1:B:16:ASP:H	2.13	0.56
1:A:16:ASP:HB2	1:A:228:ARG:HH11	1.69	0.56
1:A:128:PHE:N	1:A:128:PHE:CD2	2.74	0.56
1:B:30:LYS:O	1:B:31:SER:HB2	2.04	0.56
1:B:34:SER:HB2	1:B:37:THR:CG2	2.36	0.56
1:B:133:PHE:HB3	1:B:153:ASN:O	2.05	0.56
1:B:183:GLU:O	1:B:186:ALA:CB	2.54	0.56
1:B:201:SER:CB	1:B:206:PRO:CB	2.82	0.56
1:A:91:VAL:HG13	1:A:212:PHE:CZ	2.41	0.56
1:B:222:PRO:HG3	1:B:232:LEU:N	2.21	0.56
1:A:133:PHE:CZ	1:A:154:LEU:HD12	2.41	0.55
1:A:233:PHE:O	1:A:234:PRO:C	2.49	0.55
1:B:3:THR:C	1:B:4:ILE:HG23	2.31	0.55
1:B:184:SER:C	1:B:186:ALA:N	2.64	0.55
1:B:151:ASP:OD2	1:B:151:ASP:N	2.40	0.55
1:A:225:SER:C	1:A:229:LEU:HB3	2.31	0.55
1:B:45:GLY:CA	1:B:46:LYS:HE2	2.37	0.55
1:B:61:LEU:CD2	1:B:81:LEU:CD1	2.84	0.55
1:A:111:PHE:HE2	1:A:179:VAL:HG11	1.71	0.55
1:B:231:GLY:C	1:B:232:LEU:HG	2.31	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:THR:HG23	1:A:216:ASN:OD1	2.06	0.55
1:A:139:ASP:OD2	1:A:140:LEU:N	2.39	0.55
1:A:133:PHE:CD1	1:A:154:LEU:HB2	2.42	0.55
1:A:145:ASP:OD1	1:A:169:SER:CB	2.55	0.55
1:B:65:VAL:CG2	1:B:73:THR:CG2	2.85	0.55
1:B:121:HIS:O	1:B:122:GLN:CG	2.52	0.55
1:A:150:THR:OG1	1:A:153:ASN:HB2	2.07	0.55
1:A:173:ALA:C	1:A:174:LEU:HD23	2.29	0.55
1:A:222:PRO:HD2	1:A:231:GLY:O	2.06	0.55
1:B:217:ILE:O	1:B:217:ILE:CG2	2.55	0.55
1:B:9:LEU:CB	1:B:40:TRP:CZ3	2.90	0.55
1:B:103:THR:HG1	1:B:199:ILE:HA	1.70	0.55
1:B:233:PHE:CD1	1:B:233:PHE:N	2.74	0.55
1:B:9:LEU:HD22	1:B:40:TRP:CZ3	2.42	0.54
1:B:34:SER:CB	1:B:37:THR:HG22	2.37	0.54
1:B:38:ALA:CB	1:B:75:VAL:HG13	2.34	0.54
1:B:230:LEU:O	1:B:230:LEU:CD1	2.55	0.54
1:B:74:SER:OG	1:B:75:VAL:N	2.36	0.54
1:B:226:THR:O	1:B:228:ARG:C	2.51	0.54
1:A:24:HIS:O	1:A:25:ILE:CG1	2.56	0.54
1:A:58:ASP:O	1:A:59:LYS:CG	2.53	0.54
1:A:115:LEU:HB2	1:A:180:HIS:CE1	2.43	0.54
1:B:7:VAL:HG22	1:B:212:PHE:CB	2.29	0.54
1:A:27:ILE:CD1	1:A:27:ILE:N	2.71	0.54
1:A:92:GLY:HA2	1:A:174:LEU:HA	1.90	0.54
1:A:116:LYS:CG	1:A:117:SER:N	2.64	0.54
1:A:145:ASP:CB	1:A:169:SER:HB3	2.36	0.54
1:B:65:VAL:CG2	1:B:73:THR:HG23	2.35	0.54
1:B:181:ILE:CG2	1:B:189:VAL:CG2	2.84	0.54
1:B:189:VAL:CG1	1:B:189:VAL:O	2.54	0.54
1:A:184:SER:C	1:A:186:ALA:H	2.15	0.54
1:B:54:TYR:OH	1:B:81:LEU:CB	2.56	0.54
1:B:183:GLU:O	1:B:186:ALA:HB2	2.08	0.54
1:A:6:ALA:HB1	1:A:212:PHE:O	2.07	0.54
1:B:103:THR:O	1:B:105:THR:N	2.40	0.54
1:A:6:ALA:HB2	1:A:213:PHE:HB3	1.89	0.54
1:A:29:ILE:CG1	1:A:35:LYS:NZ	2.70	0.54
1:A:29:ILE:HG22	1:A:84:VAL:HG11	1.88	0.54
1:A:32:VAL:HG22	1:A:233:PHE:HB3	1.89	0.54
1:A:166:GLU:OE1	1:A:168:SER:HB2	2.07	0.54
1:A:184:SER:O	1:A:186:ALA:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:TRP:CH2	1:B:180:HIS:HD2	2.26	0.54
1:B:182:TRP:CD1	1:B:183:GLU:N	2.75	0.54
1:B:111:PHE:HE2	1:B:113:SER:HG	1.55	0.54
1:A:55:ASN:HD22	1:A:58:ASP:CG	2.16	0.54
1:A:88:TRP:CZ2	1:A:182:TRP:CZ2	2.96	0.54
1:B:88:TRP:NE1	1:B:182:TRP:CH2	2.72	0.54
1:B:95:ALA:CB	1:B:210:ILE:CG1	2.86	0.54
1:B:141:ILE:HG22	1:B:174:LEU:CA	2.37	0.54
1:B:191:PHE:CD1	1:B:191:PHE:C	2.85	0.54
1:A:27:ILE:HD12	1:A:27:ILE:N	2.23	0.53
1:A:143:GLN:C	1:A:143:GLN:CD	2.75	0.53
1:A:91:VAL:O	1:A:174:LEU:HB2	2.08	0.53
1:B:12:TYR:C	1:B:12:TYR:CD2	2.86	0.53
1:B:19:ASP:OD1	1:B:24:HIS:CE1	2.60	0.53
1:B:29:ILE:C	1:B:30:LYS:CG	2.78	0.53
1:A:44:ASP:OD1	1:A:200:LYS:CG	2.57	0.53
1:A:54:TYR:CB	1:A:191:PHE:CE2	2.84	0.53
1:A:87:GLU:CB	1:A:182:TRP:HB3	2.39	0.53
1:A:141:ILE:HG22	1:A:141:ILE:O	2.08	0.53
1:A:199:ILE:CD1	1:A:210:ILE:HD11	2.38	0.53
1:B:68:PRO:O	1:B:70:ALA:N	2.42	0.53
1:B:112:THR:HA	1:B:127:HIS:HB2	1.90	0.53
1:B:160:SER:CB	1:B:164:SER:O	2.54	0.53
1:A:10:ASP:OD1	1:A:19:ASP:OD2	2.26	0.53
1:A:105:THR:CG2	1:A:198:LEU:CD2	2.84	0.53
1:A:120:THR:CG2	1:A:122:GLN:NE2	2.71	0.53
1:A:213:PHE:CD1	1:A:232:LEU:HD13	2.42	0.53
1:B:81:LEU:C	1:B:82:ASN:OD1	2.50	0.53
1:B:31:SER:O	1:B:233:PHE:CE2	2.62	0.53
1:B:222:PRO:HG2	1:B:225:SER:CB	2.36	0.53
1:A:7:VAL:O	1:A:7:VAL:CG2	2.57	0.53
1:A:14:ASN:HB3	1:A:228:ARG:NH1	2.21	0.53
1:B:92:GLY:HA3	1:B:173:ALA:O	2.08	0.53
1:B:214:ILE:O	1:B:215:SER:HB3	2.08	0.53
1:A:27:ILE:CG2	1:A:29:ILE:HD11	2.23	0.53
1:A:88:TRP:CZ2	1:B:137:GLN:O	2.62	0.53
1:A:32:VAL:CB	1:A:233:PHE:HD2	2.22	0.53
1:A:80:ASP:O	1:A:81:LEU:HB2	2.06	0.53
1:A:137:GLN:C	1:A:139:ASP:N	2.64	0.53
1:B:52:ILE:HD13	1:B:63:ALA:CB	2.36	0.53
1:B:158:ARG:HB2	1:B:169:SER:CB	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:LYS:O	1:A:102:GLU:CB	2.57	0.53
1:A:106:ILE:HD12	1:A:154:LEU:O	2.09	0.53
1:A:17:ILE:CG1	1:A:19:ASP:CG	2.82	0.53
1:A:80:ASP:CG	1:A:82:ASN:ND2	2.67	0.53
1:A:172:ARG:HG3	1:A:213:PHE:HZ	1.73	0.53
1:A:225:SER:H	1:A:229:LEU:HB3	1.73	0.53
1:B:17:ILE:O	1:B:33:ARG:CG	2.57	0.53
1:B:101:LYS:O	1:B:102:GLU:HB3	2.09	0.53
1:B:174:LEU:HD22	1:B:213:PHE:HZ	1.73	0.53
1:A:87:GLU:HG2	1:A:182:TRP:CB	2.38	0.52
1:B:22:TYR:CD1	1:B:39:LYS:HD2	2.44	0.52
1:B:56:SER:HB2	1:B:188:THR:C	2.33	0.52
1:B:117:SER:CB	1:B:187:ALA:N	2.72	0.52
1:A:88:TRP:CD1	1:B:138:LYS:HD2	2.43	0.52
1:A:105:THR:HG22	1:A:198:LEU:CD2	2.39	0.52
1:A:225:SER:C	1:A:231:GLY:H	2.17	0.52
1:A:45:GLY:CA	1:A:200:LYS:HE3	2.32	0.52
1:A:172:ARG:NH1	1:A:213:PHE:CG	2.77	0.52
1:A:20:PRO:CG	1:A:24:HIS:HB3	2.39	0.52
1:A:72:ALA:O	1:A:73:THR:CG2	2.57	0.52
1:A:17:ILE:CD1	1:A:19:ASP:OD2	2.58	0.52
1:B:221:ILE:CG2	1:B:221:ILE:O	2.57	0.52
1:A:172:ARG:NH1	1:A:213:PHE:CD1	2.78	0.52
1:B:142:LEU:HD11	1:B:148:THR:HB	1.91	0.52
1:B:145:ASP:OD2	1:B:169:SER:CB	2.57	0.52
1:B:222:PRO:HG3	1:B:232:LEU:CA	2.40	0.52
1:A:3:THR:C	1:A:4:ILE:CG2	2.82	0.52
1:A:49:THR:N	1:A:197:PHE:CE1	2.78	0.52
1:A:107:LEU:HD23	1:A:153:ASN:OD1	2.08	0.52
1:B:44:ASP:OD2	1:B:200:LYS:HA	2.10	0.52
1:B:56:SER:OG	1:B:188:THR:HA	2.09	0.52
1:B:136:ASP:OD1	1:B:136:ASP:C	2.52	0.52
1:B:230:LEU:HB3	1:B:232:LEU:HD12	1.91	0.52
1:A:115:LEU:HD11	1:A:189:VAL:HG21	1.92	0.52
1:A:162:ASN:OD1	1:A:163:GLY:N	2.43	0.52
1:A:180:HIS:HA	1:A:182:TRP:CZ3	2.43	0.52
1:B:95:ALA:CB	1:B:210:ILE:CA	2.84	0.52
1:B:129:MET:HE2	1:B:131:ASN:OD1	2.10	0.52
1:A:12:TYR:HB2	1:A:207:ALA:HA	1.92	0.52
1:A:106:ILE:CD1	1:A:154:LEU:CG	2.87	0.52
1:A:120:THR:O	1:A:121:HIS:CG	2.63	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:HIS:O	1:B:121:HIS:CD2	2.63	0.52
1:A:17:ILE:HD11	1:A:19:ASP:CG	2.35	0.52
1:A:215:SER:O	1:A:216:ASN:O	2.28	0.52
1:A:222:PRO:CG	1:A:225:SER:CB	2.38	0.52
1:A:12:TYR:HB3	1:A:14:ASN:HD21	1.75	0.51
1:A:137:GLN:O	1:A:138:LYS:HB2	2.09	0.51
1:A:142:LEU:N	1:A:142:LEU:CD2	2.72	0.51
1:A:150:THR:C	1:A:151:ASP:OD1	2.53	0.51
1:A:172:ARG:NH2	1:A:219:SER:HB3	2.19	0.51
1:B:88:TRP:CH2	1:B:182:TRP:HH2	2.27	0.51
1:B:91:VAL:CG2	1:B:213:PHE:O	2.57	0.51
1:B:133:PHE:CD1	1:B:154:LEU:HB2	2.46	0.51
1:B:187:ALA:O	1:B:188:THR:HB	2.09	0.51
1:A:228:ARG:O	1:A:230:LEU:HD23	2.11	0.51
1:B:11:THR:N	1:B:208:ASP:O	2.36	0.51
1:B:91:VAL:HG23	1:B:214:ILE:HG23	1.90	0.51
1:B:99:LEU:O	1:B:100:TYR:CG	2.63	0.51
1:B:137:GLN:HB2	1:B:140:LEU:CD2	2.41	0.51
1:A:120:THR:O	1:A:121:HIS:CD2	2.63	0.51
1:A:137:GLN:HB3	1:A:140:LEU:HB2	1.92	0.51
1:B:12:TYR:C	1:B:12:TYR:HD2	2.18	0.51
1:B:45:GLY:C	1:B:46:LYS:CD	2.82	0.51
1:B:104:ASN:CA	1:B:210:ILE:HD11	2.40	0.51
1:B:145:ASP:OD2	1:B:158:ARG:HG3	2.11	0.51
1:A:9:LEU:CD2	1:A:25:ILE:CG2	2.75	0.51
1:A:29:ILE:CG1	1:A:35:LYS:HZ2	2.24	0.51
1:A:172:ARG:HD2	1:A:213:PHE:CE1	2.44	0.51
1:B:8:GLU:O	1:B:8:GLU:HG2	2.03	0.51
1:B:193:ALA:O	1:B:194:THR:CB	2.58	0.51
1:A:122:GLN:HE22	1:B:132:GLN:CD	2.19	0.51
1:A:173:ALA:C	1:A:174:LEU:HD22	2.34	0.51
1:A:184:SER:C	1:A:186:ALA:N	2.68	0.51
1:B:65:VAL:O	1:B:66:SER:HB3	2.10	0.51
1:B:87:GLU:OE2	1:B:182:TRP:CE2	2.63	0.51
1:B:174:LEU:HD22	1:B:213:PHE:CZ	2.46	0.51
1:A:4:ILE:HA	1:A:215:SER:HB3	1.92	0.51
1:A:20:PRO:O	1:A:22:TYR:N	2.43	0.51
1:A:180:HIS:HB2	1:A:182:TRP:CE2	2.46	0.51
1:B:25:ILE:HD12	1:B:25:ILE:N	2.09	0.51
1:B:143:GLN:CB	1:B:172:ARG:HB3	2.41	0.51
1:A:55:ASN:HB2	1:A:58:ASP:CG	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:ILE:O	1:B:30:LYS:CG	2.57	0.51
1:B:160:SER:CB	1:B:164:SER:HB2	2.39	0.51
1:A:143:GLN:HE22	1:A:144:GLY:CA	2.24	0.51
1:A:158:ARG:HD3	1:A:166:GLU:OE2	2.11	0.51
1:A:169:SER:C	1:A:170:VAL:CG1	2.84	0.50
1:A:224:GLY:O	1:A:226:THR:N	2.44	0.50
1:A:225:SER:CB	1:A:231:GLY:N	2.73	0.50
1:B:128:PHE:CE2	1:B:175:PHE:CZ	2.98	0.50
1:B:172:ARG:HH21	1:B:220:SER:CA	2.24	0.50
1:A:33:ARG:HH21	1:A:237:ASN:CG	2.18	0.50
1:A:52:ILE:HG23	1:A:61:LEU:HD11	1.93	0.50
1:A:115:LEU:HD12	1:A:189:VAL:HG13	1.92	0.50
1:A:122:GLN:CG	1:B:131:ASN:CB	2.81	0.50
1:B:86:PRO:O	1:B:89:VAL:CG2	2.56	0.50
1:B:158:ARG:C	1:B:159:VAL:HG12	2.36	0.50
1:A:29:ILE:H	1:A:35:LYS:HE3	1.76	0.50
1:A:127:HIS:CE1	1:A:129:MET:HG2	2.45	0.50
1:B:22:TYR:CE1	1:B:39:LYS:HD2	2.45	0.50
1:A:8:GLU:HG3	1:A:10:ASP:H	1.75	0.50
1:A:101:LYS:O	1:A:102:GLU:HB3	2.10	0.50
1:A:127:HIS:C	1:A:128:PHE:CD2	2.89	0.50
1:B:49:THR:O	1:B:49:THR:HG22	2.11	0.50
1:A:100:TYR:N	1:A:100:TYR:CD2	2.79	0.50
1:B:9:LEU:CA	1:B:40:TRP:CZ3	2.89	0.50
1:B:11:THR:OG1	1:B:207:ALA:HA	2.11	0.50
1:B:117:SER:HB2	1:B:186:ALA:HA	1.93	0.50
1:A:96:SER:O	1:A:96:SER:OG	2.28	0.50
1:A:106:ILE:CD1	1:A:154:LEU:CB	2.89	0.50
1:B:88:TRP:CE3	1:B:179:VAL:O	2.65	0.50
1:A:117:SER:CB	1:A:186:ALA:C	2.84	0.50
1:B:54:TYR:HB2	1:B:191:PHE:CE2	2.47	0.50
1:B:110:SER:CB	1:B:194:THR:CG2	2.89	0.50
1:A:48:GLY:CA	1:A:197:PHE:CZ	2.87	0.50
1:A:106:ILE:CD1	1:A:156:LEU:CD2	2.81	0.50
1:A:172:ARG:NH1	1:A:213:PHE:CD2	2.79	0.50
1:B:54:TYR:OH	1:B:80:ASP:O	2.30	0.50
1:B:160:SER:OG	1:B:161:SER:N	2.44	0.50
1:B:187:ALA:O	1:B:188:THR:CB	2.59	0.50
1:A:12:TYR:O	1:A:14:ASN:CG	2.55	0.49
1:A:91:VAL:CG1	1:A:212:PHE:CZ	2.95	0.49
1:A:105:THR:HG22	1:A:198:LEU:HD22	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:GLN:O	1:A:123:THR:O	2.30	0.49
1:A:171:GLY:O	1:A:172:ARG:HB2	2.12	0.49
1:B:14:ASN:N	1:B:19:ASP:O	2.45	0.49
1:B:27:ILE:HD13	1:B:77:TYR:HB2	1.93	0.49
1:B:182:TRP:O	1:B:183:GLU:O	2.30	0.49
1:A:117:SER:HG	1:A:186:ALA:HA	1.75	0.49
1:A:122:GLN:NE2	1:B:132:GLN:OE1	2.45	0.49
1:A:141:ILE:C	1:A:142:LEU:HD23	2.36	0.49
1:A:40:TRP:CA	1:A:73:THR:HG21	2.39	0.49
1:A:44:ASP:C	1:A:46:LYS:N	2.69	0.49
1:A:51:HIS:O	1:A:63:ALA:HB1	2.12	0.49
1:A:181:ILE:CG2	1:A:189:VAL:HG11	2.40	0.49
1:A:213:PHE:CD1	1:A:232:LEU:CD1	2.96	0.49
1:B:7:VAL:HG11	1:B:52:ILE:HD12	1.93	0.49
1:B:22:TYR:CD1	1:B:39:LYS:CD	2.94	0.49
1:B:32:VAL:CG2	1:B:233:PHE:HD2	2.15	0.49
1:B:92:GLY:CA	1:B:109:TRP:CH2	2.82	0.49
1:B:137:GLN:O	1:B:138:LYS:HB2	2.10	0.49
1:A:42:MET:HG2	1:A:43:GLN:N	2.06	0.49
1:B:13:PRO:C	1:B:14:ASN:ND2	2.70	0.49
1:B:102:GLU:CG	1:B:103:THR:N	2.74	0.49
1:B:126:LEU:HD23	1:B:179:VAL:HG13	1.94	0.49
1:B:143:GLN:HB2	1:B:172:ARG:HB3	1.92	0.49
1:A:117:SER:OG	1:A:187:ALA:N	2.45	0.49
1:A:118:ASN:C	1:A:120:THR:H	2.20	0.49
1:A:221:ILE:HG13	1:A:222:PRO:HD2	1.95	0.49
1:B:120:THR:C	1:B:122:GLN:HG3	2.37	0.49
1:A:13:PRO:C	1:A:15:THR:H	2.21	0.49
1:A:29:ILE:CB	1:A:35:LYS:HE3	2.42	0.49
1:B:116:LYS:HB2	1:B:188:THR:CG2	2.42	0.49
1:B:180:HIS:CE1	1:B:182:TRP:CZ3	3.00	0.49
1:A:29:ILE:H	1:A:35:LYS:HE2	1.76	0.49
1:A:225:SER:C	1:A:229:LEU:CB	2.86	0.49
1:B:56:SER:OG	1:B:188:THR:CA	2.61	0.49
1:B:111:PHE:O	1:B:112:THR:OG1	2.29	0.49
1:A:4:ILE:O	1:A:5:VAL:HG23	2.12	0.49
1:A:93:LEU:CD2	1:A:212:PHE:CE1	2.96	0.49
1:B:93:LEU:HD23	1:B:212:PHE:HA	1.95	0.49
1:A:32:VAL:CB	1:A:233:PHE:CD2	2.95	0.49
1:B:95:ALA:HB2	1:B:210:ILE:CA	2.41	0.49
1:A:128:PHE:CD2	1:A:175:PHE:CE1	3.01	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:ILE:HD11	1:A:232:LEU:CB	2.43	0.48
1:A:89:VAL:HG22	1:A:215:SER:H	1.77	0.48
1:B:53:ILE:O	1:B:53:ILE:CD1	2.60	0.48
1:B:162:ASN:O	1:B:162:ASN:ND2	2.46	0.48
1:A:14:ASN:C	1:A:16:ASP:H	2.20	0.48
1:A:53:ILE:CD1	1:A:53:ILE:O	2.61	0.48
1:A:59:LYS:O	1:A:78:ASP:HA	2.13	0.48
1:A:122:GLN:NE2	1:B:132:GLN:CD	2.70	0.48
1:B:122:GLN:HE21	1:B:123:THR:H	1.59	0.48
1:B:133:PHE:H	1:B:152:GLY:HA2	1.77	0.48
1:B:158:ARG:C	1:B:159:VAL:CG1	2.86	0.48
1:A:13:PRO:HB3	1:A:21:SER:O	2.13	0.48
1:A:184:SER:HB2	1:A:185:SER:H	1.29	0.48
1:A:14:ASN:C	1:A:16:ASP:N	2.69	0.48
1:A:101:LYS:CG	1:A:102:GLU:N	2.74	0.48
1:A:159:VAL:HG23	1:A:165:PRO:HD3	1.95	0.48
1:B:3:THR:C	1:B:4:ILE:CG2	2.85	0.48
1:B:117:SER:OG	1:B:187:ALA:N	2.46	0.48
1:A:233:PHE:O	1:A:235:ASP:N	2.47	0.48
1:A:91:VAL:O	1:A:174:LEU:CB	2.62	0.48
1:A:195:PHE:CD1	1:A:195:PHE:C	2.91	0.48
1:A:98:GLY:C	1:A:100:TYR:N	2.69	0.48
1:A:112:THR:OG1	1:A:127:HIS:CD2	2.66	0.48
1:A:141:ILE:O	1:A:174:LEU:CD2	2.62	0.48
1:B:77:TYR:C	1:B:77:TYR:CD1	2.92	0.48
1:B:150:THR:O	1:B:151:ASP:CB	2.58	0.48
1:A:65:VAL:N	1:A:73:THR:O	2.47	0.48
1:A:88:TRP:CZ3	1:B:138:LYS:HB3	2.48	0.48
1:A:115:LEU:O	1:A:116:LYS:HB3	2.13	0.48
1:A:128:PHE:CA	1:B:125:ALA:O	2.61	0.48
1:A:139:ASP:OD1	1:B:88:TRP:CH2	2.66	0.48
1:B:145:ASP:OD2	1:B:169:SER:CA	2.59	0.48
1:B:114:LYS:HG2	1:B:116:LYS:HE3	1.96	0.48
1:B:158:ARG:HB3	1:B:158:ARG:HH11	1.79	0.48
1:A:51:HIS:O	1:A:52:ILE:CD1	2.60	0.48
1:A:51:HIS:O	1:A:63:ALA:CB	2.62	0.48
1:A:65:VAL:O	1:A:72:ALA:HB1	2.14	0.48
1:A:88:TRP:CD2	1:A:182:TRP:CH2	3.02	0.48
1:A:122:GLN:CB	1:B:131:ASN:CB	2.90	0.48
1:A:182:TRP:HD1	1:A:183:GLU:CA	2.27	0.48
1:B:88:TRP:CD2	1:B:182:TRP:CZ3	3.01	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:VAL:CA	1:B:165:PRO:HA	2.27	0.48
1:A:11:THR:CG2	1:A:209:GLY:HA2	2.34	0.47
1:A:151:ASP:OD2	1:A:153:ASN:CG	2.57	0.47
1:B:44:ASP:O	1:B:46:LYS:HE3	2.14	0.47
1:A:20:PRO:CG	1:A:24:HIS:CD2	2.97	0.47
1:A:95:ALA:CB	1:A:104:ASN:ND2	2.77	0.47
1:A:128:PHE:CZ	1:A:175:PHE:CD1	3.02	0.47
1:A:160:SER:HB2	1:A:164:SER:CB	2.44	0.47
1:B:9:LEU:CD2	1:B:25:ILE:CG2	2.88	0.47
1:B:99:LEU:O	1:B:100:TYR:CD1	2.67	0.47
1:B:104:ASN:OD1	1:B:210:ILE:CG1	2.62	0.47
1:B:179:VAL:O	1:B:180:HIS:HB2	2.14	0.47
1:B:180:HIS:HE1	1:B:183:GLU:H	1.62	0.47
1:A:143:GLN:NE2	1:A:144:GLY:CA	2.77	0.47
1:A:222:PRO:C	1:A:224:GLY:H	2.21	0.47
1:B:90:ARG:HD2	1:B:175:PHE:O	2.14	0.47
1:B:121:HIS:O	1:B:121:HIS:HD2	1.95	0.47
1:B:222:PRO:CG	1:B:232:LEU:N	2.77	0.47
1:B:222:PRO:CG	1:B:232:LEU:O	2.59	0.47
1:A:181:ILE:CG2	1:A:189:VAL:CG1	2.92	0.47
1:B:7:VAL:O	1:B:211:ALA:CA	2.63	0.47
1:B:110:SER:HB2	1:B:194:THR:HG23	1.95	0.47
1:A:118:ASN:O	1:A:119:SER:HB3	2.14	0.47
1:A:229:LEU:O	1:A:231:GLY:N	2.47	0.47
1:A:215:SER:C	1:A:216:ASN:O	2.56	0.47
1:B:137:GLN:CB	1:B:140:LEU:CD2	2.93	0.47
1:A:29:ILE:CG2	1:A:84:VAL:CG1	2.91	0.47
1:A:29:ILE:O	1:A:30:LYS:CB	2.63	0.47
1:A:56:SER:CB	1:A:188:THR:CA	2.75	0.47
1:A:101:LYS:HA	1:A:166:GLU:O	2.15	0.47
1:A:116:LYS:CB	1:A:123:THR:HA	2.40	0.47
1:A:122:GLN:HE21	1:A:122:GLN:HB2	1.58	0.47
1:A:130:PHE:HE2	1:A:140:LEU:HD22	1.78	0.47
1:A:132:GLN:O	1:A:134:SER:N	2.47	0.47
1:A:137:GLN:O	1:B:88:TRP:CZ3	2.68	0.47
1:A:137:GLN:O	1:A:139:ASP:OD1	2.33	0.47
1:B:92:GLY:HA2	1:B:109:TRP:CZ2	2.46	0.47
1:B:95:ALA:CB	1:B:210:ILE:CB	2.92	0.47
1:B:139:ASP:OD2	1:B:139:ASP:N	2.47	0.47
1:B:145:ASP:CB	1:B:158:ARG:HG3	2.42	0.47
1:A:94:SER:HA	1:A:156:LEU:HD13	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:THR:C	1:B:105:THR:N	2.62	0.47
1:B:110:SER:HB2	1:B:194:THR:O	2.15	0.47
1:B:197:PHE:CD1	1:B:197:PHE:N	2.83	0.47
1:B:226:THR:O	1:B:229:LEU:HD12	2.15	0.47
1:B:228:ARG:H	1:B:228:ARG:HG2	1.54	0.47
1:A:4:ILE:HG12	1:A:5:VAL:N	2.28	0.47
1:A:44:ASP:O	1:A:46:LYS:N	2.48	0.47
1:A:52:ILE:CG2	1:A:61:LEU:CD1	2.92	0.47
1:A:116:LYS:O	1:A:117:SER:HB2	2.14	0.47
1:A:201:SER:HA	1:A:202:PRO:HD2	1.54	0.47
1:A:231:GLY:C	1:A:232:LEU:CD2	2.82	0.47
1:A:210:ILE:HG22	1:A:211:ALA:H	1.80	0.47
1:B:48:GLY:C	1:B:197:PHE:CZ	2.92	0.47
1:B:101:LYS:HA	1:B:166:GLU:O	2.15	0.47
1:B:106:ILE:HG13	1:B:154:LEU:HD13	1.96	0.47
1:B:133:PHE:CB	1:B:153:ASN:O	2.63	0.47
1:A:39:LYS:O	1:A:73:THR:HG21	2.14	0.46
1:B:181:ILE:CG2	1:B:189:VAL:HG22	2.46	0.46
1:A:17:ILE:C	1:A:19:ASP:N	2.69	0.46
1:A:88:TRP:CH2	1:A:182:TRP:CZ2	3.03	0.46
1:B:90:ARG:CB	1:B:217:ILE:HG13	2.46	0.46
1:B:103:THR:H	1:B:199:ILE:CG2	2.26	0.46
1:A:35:LYS:N	1:A:35:LYS:CD	2.79	0.46
1:A:225:SER:N	1:A:229:LEU:HD23	2.29	0.46
1:B:51:HIS:O	1:B:52:ILE:HD13	2.16	0.46
1:B:219:SER:O	1:B:219:SER:OG	2.33	0.46
1:A:4:ILE:CD1	1:A:232:LEU:HB2	2.44	0.46
1:A:44:ASP:C	1:A:46:LYS:H	2.23	0.46
1:A:80:ASP:OD2	1:A:82:ASN:ND2	2.49	0.46
1:A:139:ASP:OD1	1:B:88:TRP:CZ3	2.69	0.46
1:B:12:TYR:HD2	1:B:13:PRO:N	2.13	0.46
1:B:94:SER:HB3	1:B:213:PHE:HE1	1.81	0.46
1:A:80:ASP:C	1:A:82:ASN:H	2.24	0.46
1:B:62:SER:HA	1:B:76:SER:HA	1.97	0.46
1:B:159:VAL:HB	1:B:165:PRO:HB3	1.98	0.46
1:A:32:VAL:CG2	1:A:233:PHE:HD2	2.28	0.46
1:A:137:GLN:CB	1:A:140:LEU:CB	2.91	0.46
1:B:116:LYS:O	1:B:117:SER:CB	2.63	0.46
1:B:137:GLN:HB2	1:B:140:LEU:HD23	1.98	0.46
1:A:4:ILE:HB	1:A:215:SER:HB3	1.97	0.46
1:A:17:ILE:HG12	1:A:19:ASP:CG	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:LYS:HB3	1:A:123:THR:OG1	2.15	0.46
1:A:221:ILE:HA	1:A:222:PRO:HD2	1.64	0.46
1:B:112:THR:O	1:B:191:PHE:HA	2.16	0.46
1:B:181:ILE:HG22	1:B:189:VAL:HG13	1.92	0.46
1:B:226:THR:O	1:B:227:GLY:C	2.58	0.46
1:A:117:SER:CB	1:A:186:ALA:HA	2.45	0.46
1:A:143:GLN:O	1:A:171:GLY:CA	2.62	0.46
1:B:3:THR:O	1:B:4:ILE:HG22	2.15	0.46
1:B:29:ILE:O	1:B:30:LYS:CB	2.63	0.46
1:B:160:SER:HB3	1:B:164:SER:CB	2.45	0.46
1:B:180:HIS:CE1	1:B:182:TRP:CE2	3.03	0.46
1:A:50:ALA:N	1:A:195:PHE:O	2.48	0.46
1:A:56:SER:OG	1:A:189:VAL:N	2.49	0.46
1:A:89:VAL:CG2	1:A:215:SER:O	2.64	0.46
1:A:225:SER:H	1:A:229:LEU:HD23	1.81	0.46
1:B:74:SER:O	1:B:75:VAL:CG2	2.64	0.46
1:B:235:ASP:OD2	1:B:236:ALA:CB	2.64	0.46
1:A:66:SER:HA	1:A:72:ALA:CA	2.46	0.46
1:A:119:SER:O	1:A:121:HIS:N	2.49	0.46
1:A:158:ARG:O	1:A:159:VAL:CB	2.64	0.46
1:A:222:PRO:C	1:A:224:GLY:N	2.74	0.46
1:B:95:ALA:CB	1:B:210:ILE:HG23	2.27	0.46
1:B:106:ILE:N	1:B:154:LEU:O	2.38	0.46
1:B:115:LEU:CD1	1:B:180:HIS:CE1	2.99	0.46
1:B:116:LYS:HB2	1:B:188:THR:HG23	1.98	0.46
1:A:18:GLY:N	1:A:33:ARG:NH1	2.64	0.45
1:A:40:TRP:HA	1:A:73:THR:CG2	2.42	0.45
1:A:117:SER:CB	1:A:186:ALA:CA	2.94	0.45
1:A:154:LEU:HD22	1:A:156:LEU:HD23	1.98	0.45
1:A:158:ARG:HB2	1:A:166:GLU:OE2	2.16	0.45
1:A:225:SER:HA	1:A:229:LEU:C	2.42	0.45
1:B:157:THR:HG23	1:B:158:ARG:O	2.16	0.45
1:A:45:GLY:HA3	1:A:200:LYS:HE2	1.97	0.45
1:A:154:LEU:HD22	1:A:156:LEU:CD2	2.46	0.45
1:B:50:ALA:N	1:B:197:PHE:HE1	2.13	0.45
1:B:141:ILE:O	1:B:141:ILE:HG22	2.16	0.45
1:A:80:ASP:CG	1:A:82:ASN:HD21	2.25	0.45
1:A:125:ALA:O	1:B:128:PHE:HA	2.16	0.45
1:A:140:LEU:HD12	1:A:174:LEU:C	2.41	0.45
1:A:229:LEU:CD2	1:A:235:ASP:CA	2.80	0.45
1:B:53:ILE:HD12	1:B:53:ILE:C	2.39	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:GLN:CB	1:B:140:LEU:HD22	2.45	0.45
1:A:17:ILE:CG2	1:A:228:ARG:CD	2.89	0.45
1:A:52:ILE:HG22	1:A:61:LEU:CD1	2.46	0.45
1:A:101:LYS:O	1:A:102:GLU:CG	2.64	0.45
1:A:143:GLN:CD	1:A:144:GLY:N	2.75	0.45
1:A:225:SER:CB	1:A:231:GLY:H	2.29	0.45
1:A:233:PHE:C	1:A:235:ASP:N	2.73	0.45
1:B:224:GLY:C	1:B:229:LEU:HD22	2.42	0.45
1:A:94:SER:OG	1:A:232:LEU:HD21	2.17	0.45
1:A:101:LYS:HE3	1:A:101:LYS:HB3	1.45	0.45
1:B:157:THR:CG2	1:B:158:ARG:O	2.65	0.45
1:A:35:LYS:HG3	1:A:77:TYR:OH	2.17	0.45
1:A:52:ILE:O	1:A:53:ILE:CG2	2.65	0.45
1:A:116:LYS:O	1:A:117:SER:C	2.58	0.45
1:A:128:PHE:HA	1:B:125:ALA:O	2.17	0.45
1:A:218:ASP:OD2	1:A:218:ASP:N	2.49	0.45
1:B:45:GLY:C	1:B:46:LYS:CE	2.89	0.45
1:B:166:GLU:CG	1:B:167:GLY:N	2.63	0.45
1:B:187:ALA:O	1:B:188:THR:CG2	2.63	0.45
1:A:43:GLN:OE1	1:A:46:LYS:HG2	2.17	0.45
1:A:87:GLU:CG	1:A:182:TRP:HB2	2.42	0.45
1:A:115:LEU:HD11	1:A:189:VAL:CG2	2.45	0.45
1:B:12:TYR:CD2	1:B:13:PRO:O	2.69	0.45
1:A:136:ASP:OD1	1:A:136:ASP:O	2.35	0.45
1:B:130:PHE:CZ	1:B:139:ASP:OD1	2.70	0.45
1:B:133:PHE:CG	1:B:154:LEU:HB2	2.52	0.45
1:B:225:SER:CA	1:B:229:LEU:CB	2.92	0.45
1:A:42:MET:HE2	1:A:42:MET:HB3	1.66	0.45
1:A:180:HIS:HD2	1:A:182:TRP:CE2	2.28	0.45
1:A:185:SER:O	1:A:186:ALA:O	2.34	0.45
1:A:204:SER:O	1:A:206:PRO:HD2	2.16	0.45
1:B:53:ILE:HD12	1:B:62:SER:O	2.17	0.45
1:B:67:TYR:HB3	1:B:68:PRO:HD2	1.99	0.45
1:A:12:TYR:O	1:A:14:ASN:ND2	2.51	0.44
1:A:22:TYR:CE1	1:A:39:LYS:CA	2.85	0.44
1:A:214:ILE:O	1:A:215:SER:CB	2.60	0.44
1:B:56:SER:CB	1:B:188:THR:C	2.89	0.44
1:A:158:ARG:H	1:A:169:SER:CB	2.29	0.44
1:B:54:TYR:HD2	1:B:61:LEU:HD13	1.81	0.44
1:B:54:TYR:CZ	1:B:81:LEU:HB3	2.51	0.44
1:B:226:THR:O	1:B:228:ARG:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:ILE:CD1	1:A:35:LYS:HE3	2.45	0.44
1:A:29:ILE:C	1:A:30:LYS:CG	2.87	0.44
1:A:61:LEU:HD12	1:A:61:LEU:C	2.43	0.44
1:B:53:ILE:CD1	1:B:53:ILE:C	2.89	0.44
1:B:156:LEU:HB3	1:B:171:GLY:O	2.17	0.44
1:A:68:PRO:C	1:A:69:ASN:ND2	2.76	0.44
1:A:113:SER:C	1:A:114:LYS:CG	2.91	0.44
1:B:118:ASN:O	1:B:119:SER:HB2	2.17	0.44
1:B:226:THR:H	1:B:229:LEU:CB	2.28	0.44
1:A:56:SER:CB	1:A:189:VAL:H	2.29	0.44
1:A:88:TRP:CH2	1:A:182:TRP:HH2	2.22	0.44
1:A:195:PHE:O	1:A:195:PHE:HD1	2.01	0.44
1:B:112:THR:CG2	1:B:127:HIS:HB2	2.33	0.44
1:B:200:LYS:O	1:B:201:SER:CB	2.53	0.44
1:B:228:ARG:O	1:B:230:LEU:CA	2.65	0.44
1:A:117:SER:HB2	1:A:118:ASN:H	1.26	0.44
1:A:126:LEU:HD23	1:A:179:VAL:HG13	2.00	0.44
1:B:231:GLY:O	1:B:232:LEU:CG	2.62	0.44
1:A:91:VAL:CG1	1:A:212:PHE:HZ	2.30	0.44
1:A:115:LEU:HD12	1:A:189:VAL:CG1	2.46	0.44
1:A:222:PRO:CD	1:A:231:GLY:O	2.66	0.44
1:A:224:GLY:CA	1:A:229:LEU:CD2	2.92	0.44
1:A:228:ARG:C	1:A:230:LEU:H	2.24	0.44
1:B:14:ASN:O	1:B:19:ASP:HB2	2.17	0.44
1:B:14:ASN:C	1:B:16:ASP:N	2.76	0.44
1:B:25:ILE:HD13	1:B:25:ILE:N	2.33	0.44
1:B:89:VAL:HG13	1:B:215:SER:C	2.38	0.44
1:A:141:ILE:HG22	1:A:174:LEU:HD21	1.96	0.44
1:B:41:ASN:HD22	1:B:41:ASN:HA	1.26	0.44
1:B:154:LEU:CD1	1:B:156:LEU:HD21	2.48	0.44
1:B:230:LEU:HD22	1:B:230:LEU:HA	1.86	0.44
1:B:236:ALA:C	1:B:237:ASN:HD22	2.25	0.44
1:A:13:PRO:CB	1:A:22:TYR:N	2.72	0.44
1:B:122:GLN:HE21	1:B:122:GLN:CA	2.31	0.44
1:B:145:ASP:OD2	1:B:158:ARG:CD	2.66	0.44
1:A:122:GLN:NE2	1:B:132:GLN:HE22	1.89	0.43
1:B:14:ASN:HB3	1:B:228:ARG:HH21	1.79	0.43
1:B:229:LEU:O	1:B:233:PHE:CD2	2.71	0.43
1:A:90:ARG:NH1	1:A:176:TYR:O	2.52	0.43
1:A:93:LEU:N	1:A:173:ALA:O	2.43	0.43
1:B:6:ALA:HB1	1:B:213:PHE:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:VAL:O	1:B:66:SER:CB	2.58	0.43
1:B:86:PRO:O	1:B:87:GLU:C	2.62	0.43
1:B:108:SER:O	1:B:195:PHE:CB	2.66	0.43
1:A:27:ILE:O	1:A:29:ILE:HD11	2.18	0.43
1:A:49:THR:CA	1:A:195:PHE:O	2.62	0.43
1:A:93:LEU:HD22	1:A:212:PHE:CE1	2.52	0.43
1:A:102:GLU:OE1	1:A:104:ASN:OD1	2.36	0.43
1:A:143:GLN:O	1:A:171:GLY:C	2.62	0.43
1:A:224:GLY:C	1:A:226:THR:N	2.73	0.43
1:A:224:GLY:O	1:A:225:SER:OG	2.33	0.43
1:B:94:SER:HB3	1:B:213:PHE:CE1	2.54	0.43
1:B:103:THR:O	1:B:105:THR:HB	2.18	0.43
1:B:141:ILE:CG2	1:B:174:LEU:N	2.63	0.43
1:A:54:TYR:HB2	1:A:191:PHE:CZ	2.53	0.43
1:A:89:VAL:CG2	1:A:215:SER:H	2.31	0.43
1:A:92:GLY:CA	1:A:174:LEU:CB	2.87	0.43
1:B:98:GLY:O	1:B:99:LEU:CD2	2.51	0.43
1:A:17:ILE:HG12	1:A:19:ASP:CB	2.48	0.43
1:B:7:VAL:HA	1:B:26:GLY:O	2.18	0.43
1:B:101:LYS:CG	1:B:165:PRO:O	2.67	0.43
1:B:233:PHE:HA	1:B:234:PRO:HD2	1.84	0.43
1:A:13:PRO:O	1:A:15:THR:HG23	2.19	0.43
1:A:111:PHE:HB3	1:A:128:PHE:CE1	2.54	0.43
1:A:122:GLN:CB	1:B:131:ASN:HB3	2.48	0.43
1:B:146:ALA:HB1	1:B:156:LEU:HA	2.00	0.43
1:A:116:LYS:N	1:A:116:LYS:CD	2.50	0.43
1:A:131:ASN:HD22	1:A:131:ASN:HA	1.68	0.43
1:B:51:HIS:O	1:B:52:ILE:HG12	2.18	0.43
1:A:49:THR:HA	1:A:196:ALA:HA	2.00	0.43
1:A:134:SER:OG	1:A:135:LYS:N	2.49	0.43
1:A:137:GLN:O	1:A:139:ASP:CG	2.62	0.43
1:A:139:ASP:C	1:A:176:TYR:HB2	2.42	0.43
1:A:237:ASN:HD22	1:A:237:ASN:HA	1.49	0.43
1:A:145:ASP:CG	1:A:158:ARG:HD2	2.41	0.43
1:B:25:ILE:HD11	1:B:75:VAL:HG21	2.01	0.43
1:B:52:ILE:HG13	1:B:212:PHE:CE2	2.52	0.43
1:B:127:HIS:ND1	1:B:128:PHE:N	2.66	0.43
1:A:99:LEU:HD13	1:A:99:LEU:HA	1.69	0.43
1:A:106:ILE:HD13	1:A:154:LEU:CD2	2.46	0.43
1:A:205:HIS:HA	1:A:206:PRO:HD2	1.70	0.43
1:B:95:ALA:HB1	1:B:210:ILE:CG1	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:SER:CB	1:A:72:ALA:HB2	2.48	0.42
1:A:106:ILE:HD12	1:A:154:LEU:CD2	2.43	0.42
1:A:111:PHE:O	1:A:127:HIS:HA	2.18	0.42
1:A:143:GLN:C	1:A:143:GLN:HE21	2.22	0.42
1:A:160:SER:OG	1:A:161:SER:N	2.52	0.42
1:A:189:VAL:O	1:A:189:VAL:HG12	2.19	0.42
1:B:36:LYS:HD3	1:B:37:THR:O	2.17	0.42
1:B:65:VAL:CG2	1:B:73:THR:HG21	2.49	0.42
1:A:65:VAL:O	1:A:72:ALA:CB	2.67	0.42
1:A:88:TRP:CH2	1:B:138:LYS:HB3	2.54	0.42
1:A:112:THR:O	1:A:191:PHE:HA	2.18	0.42
1:A:142:LEU:HD11	1:A:148:THR:HB	2.01	0.42
1:B:48:GLY:O	1:B:197:PHE:CD1	2.72	0.42
1:B:58:ASP:O	1:B:59:LYS:CE	2.66	0.42
1:B:226:THR:H	1:B:229:LEU:CG	2.30	0.42
1:A:112:THR:CB	1:A:127:HIS:HB2	2.48	0.42
1:A:185:SER:O	1:A:186:ALA:C	2.63	0.42
1:B:19:ASP:O	1:B:20:PRO:O	2.36	0.42
1:B:79:VAL:CG2	1:B:80:ASP:H	2.30	0.42
1:B:115:LEU:HG	1:B:189:VAL:HG23	2.01	0.42
1:A:197:PHE:CD2	1:A:197:PHE:C	2.97	0.42
1:B:89:VAL:O	1:B:179:VAL:CB	2.66	0.42
1:B:94:SER:O	1:B:95:ALA:CB	2.66	0.42
1:B:117:SER:HB3	1:B:187:ALA:N	2.34	0.42
1:A:23:PRO:O	1:A:40:TRP:N	2.53	0.42
1:A:45:GLY:CA	1:A:200:LYS:HG3	2.48	0.42
1:A:106:ILE:N	1:A:154:LEU:O	2.42	0.42
1:B:104:ASN:HA	1:B:210:ILE:HD11	2.00	0.42
1:B:159:VAL:HG23	1:B:160:SER:O	2.19	0.42
1:A:41:ASN:C	1:A:42:MET:O	2.62	0.42
1:A:93:LEU:O	1:A:156:LEU:HD13	2.19	0.42
1:B:7:VAL:O	1:B:211:ALA:CB	2.68	0.42
1:B:146:ALA:HB2	1:B:156:LEU:HA	1.97	0.42
1:A:17:ILE:CA	1:A:33:ARG:CZ	2.93	0.42
1:A:27:ILE:O	1:A:27:ILE:CG2	2.67	0.42
1:B:44:ASP:C	1:B:46:LYS:N	2.77	0.42
1:B:130:PHE:CE1	1:B:137:GLN:OE1	2.72	0.42
1:B:183:GLU:O	1:B:184:SER:C	2.62	0.42
1:A:18:GLY:C	1:A:19:ASP:O	2.61	0.42
1:A:122:GLN:C	1:A:123:THR:O	2.62	0.42
1:B:36:LYS:HB2	1:B:77:TYR:HD2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:LYS:CE	1:A:78:ASP:HB3	2.19	0.42
1:A:158:ARG:O	1:A:159:VAL:HB	2.20	0.42
1:A:222:PRO:HG3	1:A:232:LEU:N	2.35	0.42
1:A:235:ASP:O	1:A:236:ALA:C	2.62	0.42
1:B:12:TYR:O	1:B:14:ASN:ND2	2.53	0.42
1:B:139:ASP:O	1:B:176:TYR:CB	2.57	0.42
1:B:158:ARG:O	1:B:159:VAL:CG1	2.62	0.42
1:A:120:THR:O	1:A:120:THR:CG2	2.65	0.42
1:B:55:ASN:O	1:B:59:LYS:CA	2.67	0.42
1:B:88:TRP:CH2	1:B:180:HIS:CD2	3.06	0.42
1:B:88:TRP:HE3	1:B:179:VAL:O	2.02	0.42
1:B:116:LYS:C	1:B:117:SER:OG	2.63	0.42
1:B:207:ALA:HB1	1:B:208:ASP:CG	2.45	0.42
1:A:48:GLY:N	1:A:197:PHE:O	2.34	0.41
1:B:9:LEU:CG	1:B:40:TRP:CH2	3.03	0.41
1:B:76:SER:O	1:B:77:TYR:HB2	2.19	0.41
1:B:87:GLU:OE2	1:B:182:TRP:CZ2	2.73	0.41
1:B:102:GLU:HG3	1:B:103:THR:H	1.85	0.41
1:B:135:LYS:H	1:B:135:LYS:HG2	1.56	0.41
1:A:24:HIS:CG	1:A:25:ILE:N	2.87	0.41
1:A:29:ILE:O	1:A:30:LYS:CG	2.68	0.41
1:A:72:ALA:C	1:A:73:THR:HG23	2.45	0.41
1:A:130:PHE:HD1	1:A:130:PHE:HA	1.60	0.41
1:A:158:ARG:O	1:A:159:VAL:HG12	2.20	0.41
1:A:22:TYR:CD1	1:A:22:TYR:C	2.97	0.41
1:A:120:THR:C	1:A:121:HIS:ND1	2.77	0.41
1:A:120:THR:HG22	1:A:122:GLN:CD	2.45	0.41
1:A:182:TRP:CG	1:A:183:GLU:N	2.77	0.41
1:A:214:ILE:C	1:A:215:SER:OG	2.60	0.41
1:B:7:VAL:N	1:B:212:PHE:O	2.53	0.41
1:B:101:LYS:O	1:B:102:GLU:CB	2.67	0.41
1:B:151:ASP:C	1:B:153:ASN:N	2.78	0.41
1:A:116:LYS:HB3	1:A:123:THR:CB	2.50	0.41
1:A:137:GLN:CB	1:A:140:LEU:H	2.24	0.41
1:B:5:VAL:O	1:B:214:ILE:HG12	2.20	0.41
1:B:14:ASN:N	1:B:19:ASP:CB	2.61	0.41
1:B:21:SER:C	1:B:22:TYR:CD2	2.98	0.41
1:B:43:GLN:OE1	1:B:46:LYS:HG3	2.20	0.41
1:B:154:LEU:HD13	1:B:156:LEU:HD21	2.03	0.41
1:B:160:SER:HB3	1:B:164:SER:CA	2.50	0.41
1:A:4:ILE:HD13	1:A:233:PHE:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:ILE:HG22	1:A:174:LEU:HG	2.03	0.41
1:B:205:HIS:H	1:B:206:PRO:CD	2.27	0.41
1:A:35:LYS:HB3	1:A:77:TYR:CE2	2.55	0.41
1:A:72:ALA:O	1:A:73:THR:HG23	2.20	0.41
1:B:3:THR:O	1:B:215:SER:HB2	2.21	0.41
1:B:88:TRP:CE3	1:B:180:HIS:HB2	2.55	0.41
1:B:91:VAL:O	1:B:174:LEU:HB3	2.20	0.41
1:A:79:VAL:CG1	1:A:81:LEU:HD12	2.51	0.41
1:A:115:LEU:CD2	1:A:183:GLU:HB2	2.51	0.41
1:B:35:LYS:HZ3	1:B:35:LYS:HG3	1.78	0.41
1:B:90:ARG:HB3	1:B:217:ILE:HG13	2.03	0.41
1:A:4:ILE:HD11	1:A:232:LEU:HB2	2.03	0.41
1:A:4:ILE:CG1	1:A:5:VAL:N	2.84	0.41
1:A:32:VAL:HG22	1:A:233:PHE:HB2	1.98	0.41
1:A:52:ILE:O	1:A:53:ILE:CB	2.69	0.41
1:A:91:VAL:HG21	1:A:179:VAL:HG21	1.94	0.41
1:A:109:TRP:CH2	1:A:174:LEU:HA	2.47	0.41
1:A:126:LEU:CD2	1:A:179:VAL:HG13	2.51	0.41
1:B:46:LYS:HD3	1:B:46:LYS:HA	1.64	0.41
1:B:51:HIS:O	1:B:52:ILE:CD1	2.69	0.41
1:B:145:ASP:CG	1:B:169:SER:HB2	2.45	0.41
1:A:17:ILE:C	1:A:33:ARG:NH1	2.78	0.41
1:A:98:GLY:C	1:A:100:TYR:H	2.28	0.41
1:A:115:LEU:CB	1:A:180:HIS:CE1	3.03	0.41
1:A:160:SER:HB3	1:A:164:SER:N	2.33	0.41
1:A:225:SER:O	1:A:230:LEU:N	2.53	0.41
1:B:117:SER:OG	1:B:188:THR:HG22	2.20	0.41
1:B:135:LYS:O	1:B:136:ASP:CG	2.64	0.41
1:B:221:ILE:HD12	1:B:221:ILE:HA	1.62	0.41
1:A:53:ILE:CD1	1:A:62:SER:O	2.69	0.40
1:B:17:ILE:O	1:B:33:ARG:CD	2.69	0.40
1:B:65:VAL:HG23	1:B:73:THR:HG21	1.98	0.40
1:B:74:SER:O	1:B:75:VAL:CB	2.69	0.40
1:B:99:LEU:HD13	1:B:99:LEU:HA	1.84	0.40
1:B:111:PHE:HE2	1:B:113:SER:OG	2.05	0.40
1:A:67:TYR:HA	1:A:68:PRO:HD2	1.79	0.40
1:A:82:ASN:OD1	1:A:82:ASN:N	2.52	0.40
1:A:117:SER:HA	1:A:187:ALA:CB	2.50	0.40
1:A:159:VAL:HG23	1:A:165:PRO:CD	2.50	0.40
1:B:53:ILE:HD12	1:B:53:ILE:H	1.86	0.40
1:B:54:TYR:CB	1:B:191:PHE:CE2	3.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:LEU:HD12	1:B:61:LEU:HA	1.83	0.40
1:B:117:SER:OG	1:B:187:ALA:C	2.64	0.40
1:A:52:ILE:C	1:A:53:ILE:CD1	2.87	0.40
1:A:52:ILE:C	1:A:53:ILE:CG1	2.94	0.40
1:A:120:THR:HG21	1:A:122:GLN:NE2	2.37	0.40
1:B:6:ALA:CB	1:B:212:PHE:O	2.45	0.40
1:A:10:ASP:CB	1:A:24:HIS:HE1	2.32	0.40
1:A:12:TYR:CB	1:A:14:ASN:HD21	2.34	0.40
1:A:33:ARG:NH2	1:A:237:ASN:OD1	2.54	0.40
1:A:42:MET:SD	1:A:43:GLN:N	2.95	0.40
1:A:116:LYS:HD3	1:A:188:THR:O	2.21	0.40
1:A:172:ARG:HG3	1:A:213:PHE:CZ	2.55	0.40
1:A:188:THR:C	1:A:189:VAL:HG23	2.47	0.40
1:B:13:PRO:O	1:B:14:ASN:ND2	2.55	0.40
1:B:122:GLN:O	1:B:123:THR:CB	2.55	0.40
1:B:225:SER:CB	1:B:231:GLY:HA2	2.52	0.40

All (23) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:ASP:O	1:B:69:ASN:CG[4_455]	1.16	1.04
1:B:16:ASP:CB	1:B:69:ASN:CA[4_455]	1.20	1.00
1:B:16:ASP:O	1:B:69:ASN:ND2[4_455]	1.30	0.90
1:B:16:ASP:O	1:B:69:ASN:CB[4_455]	1.36	0.84
1:B:16:ASP:C	1:B:69:ASN:CB[4_455]	1.42	0.78
1:A:204:SER:OG	1:B:82:ASN:O[3_565]	1.45	0.75
1:B:70:ALA:CA	1:B:228:ARG:NH1[4_454]	1.48	0.72
1:B:16:ASP:CG	1:B:69:ASN:N[4_455]	1.71	0.49
1:B:16:ASP:OD2	1:B:69:ASN:N[4_455]	1.71	0.49
1:A:12:TYR:OH	1:B:184:SER:CA[3_565]	1.73	0.47
1:B:70:ALA:N	1:B:228:ARG:NH1[4_454]	1.77	0.43
1:B:16:ASP:CB	1:B:69:ASN:N[4_455]	1.83	0.37
1:A:12:TYR:OH	1:B:184:SER:CB[3_565]	1.93	0.27
1:B:16:ASP:CA	1:B:69:ASN:CA[4_455]	1.94	0.26
1:B:16:ASP:CB	1:B:69:ASN:C[4_455]	1.94	0.26
1:B:69:ASN:O	1:B:228:ARG:NH1[4_454]	1.95	0.25
1:B:16:ASP:OD2	1:B:68:PRO:C[4_455]	1.97	0.23
1:A:12:TYR:OH	1:B:184:SER:C[3_565]	2.03	0.17
1:B:16:ASP:C	1:B:69:ASN:CA[4_455]	2.06	0.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:ASN:C	1:B:228:ARG:NH1[4_454]	2.08	0.12
1:B:17:ILE:N	1:B:69:ASN:CB[4_455]	2.10	0.10
1:A:68:PRO:CA	1:B:119:SER:OG[2_555]	2.14	0.06
1:B:69:ASN:O	1:B:228:ARG:CZ[4_454]	2.17	0.03

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	235/237 (99%)	141 (60%)	52 (22%)	42 (18%)	0	0
1	B	235/237 (99%)	131 (56%)	48 (20%)	56 (24%)	0	0
All	All	470/474 (99%)	272 (58%)	100 (21%)	98 (21%)	0	0

All (98) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	13	PRO
1	A	17	ILE
1	A	25	ILE
1	A	42	MET
1	A	53	ILE
1	A	102	GLU
1	A	116	LYS
1	A	118	ASN
1	A	133	PHE
1	A	159	VAL
1	A	170	VAL
1	A	181	ILE
1	A	184	SER
1	A	185	SER
1	A	186	ALA
1	A	216	ASN

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Mol	Chain	Res	Type
1	A	235	ASP
1	B	19	ASP
1	B	21	SER
1	B	22	TYR
1	B	31	SER
1	B	57	VAL
1	B	58	ASP
1	B	75	VAL
1	B	82	ASN
1	B	87	GLU
1	B	102	GLU
1	B	119	SER
1	B	121	HIS
1	B	136	ASP
1	B	151	ASP
1	B	161	SER
1	B	183	GLU
1	B	187	ALA
1	B	188	THR
1	B	194	THR
1	B	216	ASN
1	B	229	LEU
1	B	230	LEU
1	A	15	THR
1	A	18	GLY
1	A	32	VAL
1	A	69	ASN
1	A	123	THR
1	A	151	ASP
1	A	163	GLY
1	A	168	SER
1	A	183	GLU
1	A	215	SER
1	A	225	SER
1	B	30	LYS
1	B	39	LYS
1	B	45	GLY
1	B	95	ALA
1	B	118	ASN
1	B	122	GLN
1	B	138	LYS
1	B	140	LEU

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Mol	Chain	Res	Type
1	B	149	GLY
1	B	185	SER
1	B	203	ASP
1	B	215	SER
1	B	227	GLY
1	B	228	ARG
1	B	232	LEU
1	B	235	ASP
1	A	22	TYR
1	A	34	SER
1	A	120	THR
1	A	172	ARG
1	B	69	ASN
1	B	98	GLY
1	B	182	TRP
1	B	211	ALA
1	B	223	SER
1	A	19	ASP
1	A	45	GLY
1	A	59	LYS
1	A	75	VAL
1	A	194	THR
1	A	230	LEU
1	B	20	PRO
1	B	77	TYR
1	B	99	LEU
1	B	104	ASN
1	B	117	SER
1	B	180	HIS
1	B	201	SER
1	A	60	ARG
1	B	15	THR
1	B	198	LEU
1	A	10	ASP
1	B	123	THR
1	A	189	VAL
1	B	205	HIS
1	B	179	VAL
1	A	179	VAL
1	B	210	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	202/202 (100%)	113 (56%)	89 (44%)	0	0
1	B	202/202 (100%)	116 (57%)	86 (43%)	0	0
All	All	404/404 (100%)	229 (57%)	175 (43%)	0	0

All (175) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	4	ILE
1	A	5	VAL
1	A	8	GLU
1	A	12	TYR
1	A	17	ILE
1	A	25	ILE
1	A	27	ILE
1	A	29	ILE
1	A	32	VAL
1	A	35	LYS
1	A	37	THR
1	A	42	MET
1	A	44	ASP
1	A	46	LYS
1	A	51	HIS
1	A	52	ILE
1	A	53	ILE
1	A	58	ASP
1	A	60	ARG
1	A	64	VAL
1	A	65	VAL
1	A	69	ASN
1	A	75	VAL
1	A	76	SER
1	A	79	VAL
1	A	81	LEU

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Mol	Chain	Res	Type
1	A	82	ASN
1	A	93	LEU
1	A	99	LEU
1	A	100	TYR
1	A	101	LYS
1	A	106	ILE
1	A	110	SER
1	A	114	LYS
1	A	116	LYS
1	A	117	SER
1	A	121	HIS
1	A	122	GLN
1	A	123	THR
1	A	127	HIS
1	A	128	PHE
1	A	129	MET
1	A	135	LYS
1	A	137	GLN
1	A	138	LYS
1	A	140	LEU
1	A	141	ILE
1	A	142	LEU
1	A	143	GLN
1	A	148	THR
1	A	151	ASP
1	A	154	LEU
1	A	157	THR
1	A	158	ARG
1	A	159	VAL
1	A	164	SER
1	A	166	GLU
1	A	168	SER
1	A	169	SER
1	A	172	ARG
1	A	174	LEU
1	A	179	VAL
1	A	180	HIS
1	A	181	ILE
1	A	184	SER
1	A	185	SER
1	A	188	THR
1	A	190	SER

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Mol	Chain	Res	Type
1	A	192	GLU
1	A	194	THR
1	A	198	LEU
1	A	199	ILE
1	A	200	LYS
1	A	201	SER
1	A	204	SER
1	A	210	ILE
1	A	214	ILE
1	A	215	SER
1	A	217	ILE
1	A	218	ASP
1	A	219	SER
1	A	220	SER
1	A	221	ILE
1	A	223	SER
1	A	226	THR
1	A	228	ARG
1	A	230	LEU
1	A	237	ASN
1	B	3	THR
1	B	4	ILE
1	B	8	GLU
1	B	10	ASP
1	B	16	ASP
1	B	17	ILE
1	B	19	ASP
1	B	21	SER
1	B	22	TYR
1	B	25	ILE
1	B	29	ILE
1	B	35	LYS
1	B	41	ASN
1	B	42	MET
1	B	46	LYS
1	B	49	THR
1	B	52	ILE
1	B	53	ILE
1	B	58	ASP
1	B	59	LYS
1	B	61	LEU
1	B	64	VAL

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Mol	Chain	Res	Type
1	B	69	ASN
1	B	71	ASP
1	B	73	THR
1	B	76	SER
1	B	79	VAL
1	B	81	LEU
1	B	82	ASN
1	B	90	ARG
1	B	99	LEU
1	B	101	LYS
1	B	102	GLU
1	B	105	THR
1	B	106	ILE
1	B	110	SER
1	B	112	THR
1	B	113	SER
1	B	114	LYS
1	B	117	SER
1	B	118	ASN
1	B	119	SER
1	B	120	THR
1	B	122	GLN
1	B	123	THR
1	B	126	LEU
1	B	127	HIS
1	B	129	MET
1	B	132	GLN
1	B	134	SER
1	B	135	LYS
1	B	137	GLN
1	B	138	LYS
1	B	139	ASP
1	B	140	LEU
1	B	141	ILE
1	B	143	GLN
1	B	147	THR
1	B	148	THR
1	B	151	ASP
1	B	154	LEU
1	B	156	LEU
1	B	157	THR
1	B	158	ARG

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Mol	Chain	Res	Type
1	B	159	VAL
1	B	160	SER
1	B	169	SER
1	B	172	ARG
1	B	174	LEU
1	B	180	HIS
1	B	181	ILE
1	B	184	SER
1	B	185	SER
1	B	189	VAL
1	B	190	SER
1	B	199	ILE
1	B	200	LYS
1	B	208	ASP
1	B	214	ILE
1	B	216	ASN
1	B	217	ILE
1	B	220	SER
1	B	221	ILE
1	B	226	THR
1	B	228	ARG
1	B	230	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	41	ASN
1	A	55	ASN
1	A	69	ASN
1	A	104	ASN
1	A	122	GLN
1	A	131	ASN
1	A	143	GLN
1	A	180	HIS
1	B	14	ASN
1	B	41	ASN
1	B	121	HIS
1	B	122	GLN
1	B	137	GLN
1	B	143	GLN
1	B	153	ASN

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Mol	Chain	Res	Type
1	B	162	ASN
1	B	180	HIS

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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.