



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:34 AM UTC

PDB ID : 1SIE / pdb_00001sie
Title : MURINE POLYOMAVIRUS COMPLEXED WITH A DISIALYLATED OLIGOSACCHARIDE
Authors : Stehle, T.; Harrison, S.C.
Deposited on : 1995-12-12
Resolution : 3.65 Å(reported)

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

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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
Mogul	:	2022.3.0, CSD as543be (2022)
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

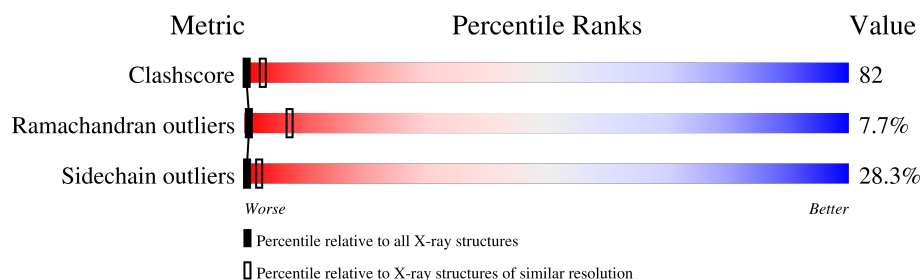
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.65 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	1009 (3.76-3.56)
Ramachandran outliers	187476	1054 (3.78-3.54)
Sidechain outliers	187428	1052 (3.78-3.54)

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	383	
1	B	383	
1	C	383	
1	D	383	
1	E	383	
1	F	383	
2	G	4	
2	H	4	

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Mol	Chain	Length	Quality of chain
2	I	4	100%
2	J	4	75%25%
2	K	4	50%50%
2	L	4	50%50%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 17141 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.

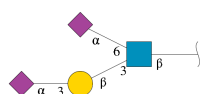
- Molecule 1 is a protein called POLYOMAVIRUS COAT PROTEIN VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total	C	N	O	S	0	0	0
			2849	1804	479	550	16			
1	B	367	Total	C	N	O	S	0	0	0
			2857	1808	481	552	16			
1	C	357	Total	C	N	O	S	0	0	0
			2784	1761	468	539	16			
1	D	340	Total	C	N	O	S	0	0	0
			2645	1674	445	511	15			
1	E	367	Total	C	N	O	S	0	0	0
			2857	1808	481	552	16			
1	F	354	Total	C	N	O	S	0	0	0
			2753	1740	461	536	16			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	6	ALA	SER	conflict	UNP P49302
B	6	ALA	SER	conflict	UNP P49302
C	6	ALA	SER	conflict	UNP P49302
D	6	ALA	SER	conflict	UNP P49302
E	6	ALA	SER	conflict	UNP P49302
F	6	ALA	SER	conflict	UNP P49302

- Molecule 2 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



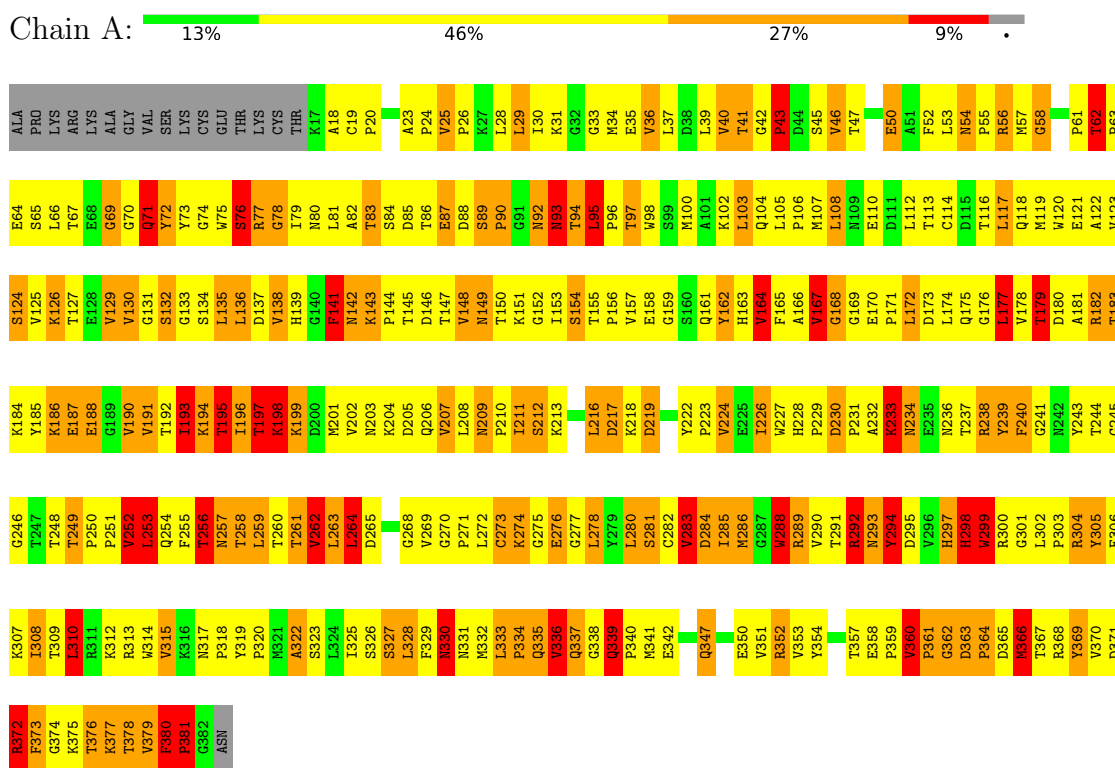
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	4	Total 66	C 36	N 3	O 27	0	0	0
2	H	4	Total 66	C 36	N 3	O 27	0	0	0
2	I	4	Total 66	C 36	N 3	O 27	0	0	0
2	J	4	Total 66	C 36	N 3	O 27	0	0	0
2	K	4	Total 66	C 36	N 3	O 27	0	0	0
2	L	4	Total 66	C 36	N 3	O 27	0	0	0

3 Residue-property plots

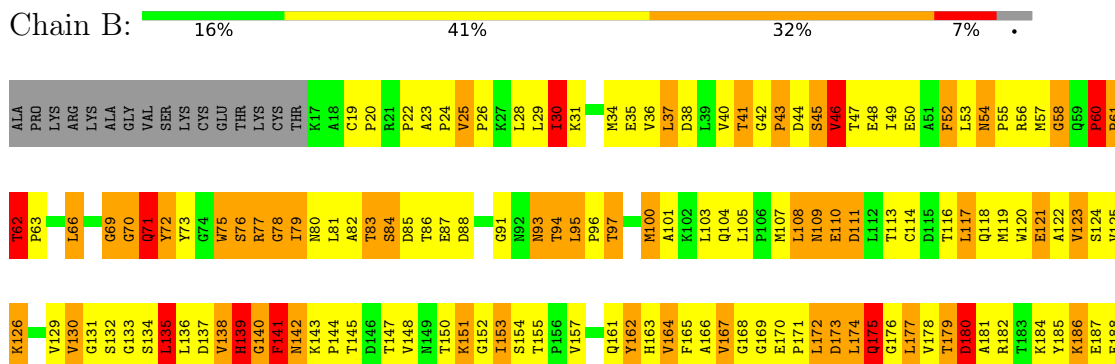
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

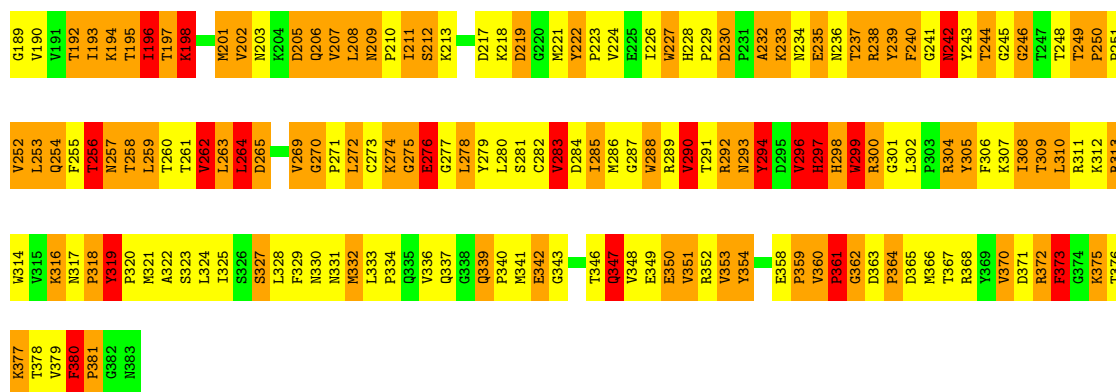
Note EDS was not executed.

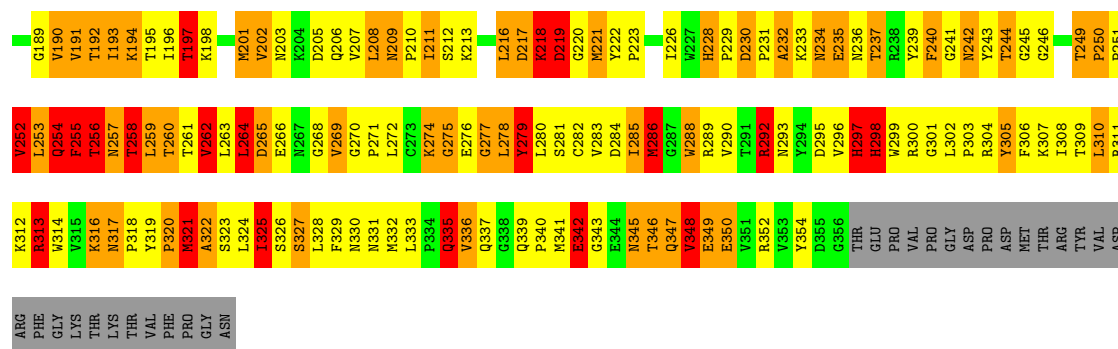
• Molecule 1: POLYOMAVIRUS COAT PROTEIN VP1



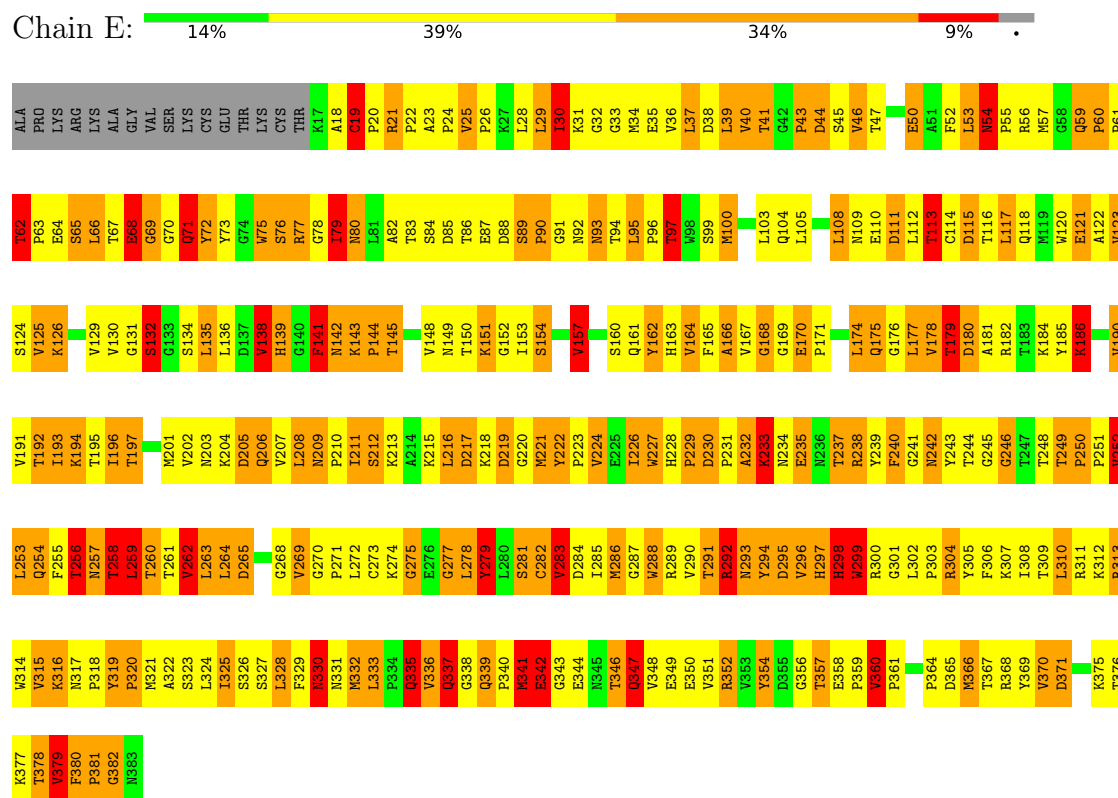
• Molecule 1: POLYOMAVIRUS COAT PROTEIN VP1



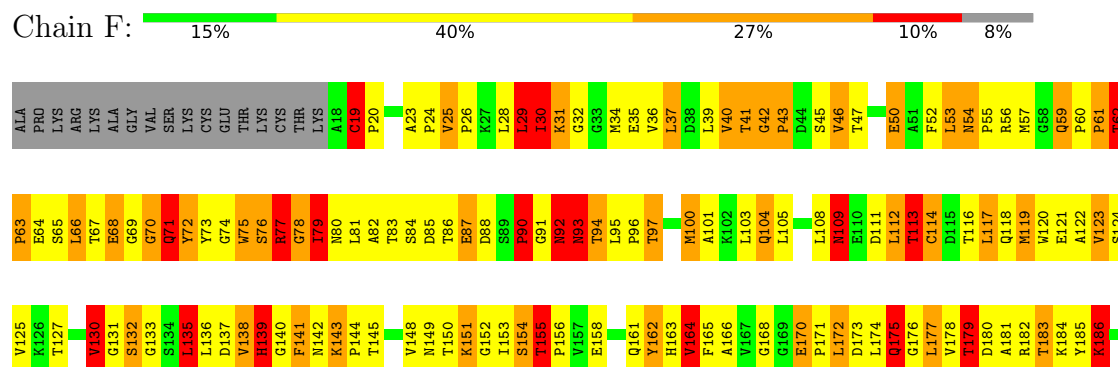


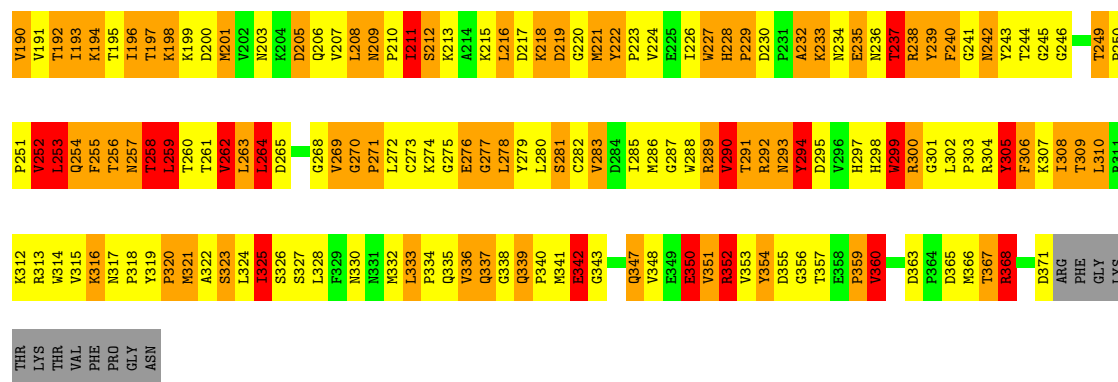


• Molecule 1: POLYOMAVIRUS COAT PROTEIN VP1



• Molecule 1: POLYOMAVIRUS COAT PROTEIN VP1





- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  50%

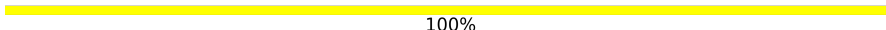


- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  50%

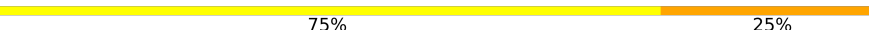


- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  100%



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  75%



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  50%



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:



MAG1
GAL2
STIA3
STIA4

4 Data and refinement statistics

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

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	570.00Å 570.00Å 570.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 3.65	Depositor
% Data completeness (in resolution range)	74.0 (12.00-3.65)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.244 , 0.264	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	17141	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, SIA, GAL

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	1.33	20/2920 (0.7%)	1.83	110/3981 (2.8%)
1	B	1.34	19/2927 (0.6%)	1.83	98/3989 (2.5%)
1	C	1.31	16/2852 (0.6%)	1.83	114/3888 (2.9%)
1	D	1.33	14/2708 (0.5%)	1.87	93/3690 (2.5%)
1	E	1.30	12/2928 (0.4%)	1.87	112/3992 (2.8%)
1	F	1.33	18/2820 (0.6%)	1.85	102/3847 (2.7%)
All	All	1.32	99/17155 (0.6%)	1.85	629/23387 (2.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	3
1	C	0	2
1	D	0	4
1	E	0	2
1	F	0	2
All	All	0	18

All (99) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	336	VAL	C-N	-10.20	1.19	1.33
1	A	262	VAL	CA-CB	-10.04	1.42	1.54
1	B	130	VAL	CA-C	-8.19	1.43	1.52
1	F	262	VAL	CA-CB	-8.14	1.44	1.54
1	E	262	VAL	CA-CB	-7.90	1.44	1.53
1	C	262	VAL	CA-CB	-7.73	1.45	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	262	VAL	CA-CB	-7.73	1.44	1.53
1	E	252	VAL	CA-CB	-7.61	1.47	1.55
1	A	360	VAL	CA-C	-7.21	1.45	1.52
1	E	166	ALA	CA-C	-7.16	1.44	1.52
1	D	46	VAL	CA-CB	-7.15	1.45	1.54
1	B	30	ILE	CA-CB	-7.14	1.50	1.55
1	D	40	VAL	CA-CB	-7.02	1.45	1.54
1	B	239	TYR	CA-C	-7.01	1.43	1.52
1	F	177	LEU	CA-C	-6.98	1.43	1.52
1	B	177	LEU	CA-C	-6.89	1.44	1.52
1	C	157	VAL	CA-CB	-6.84	1.46	1.54
1	F	360	VAL	CA-C	-6.76	1.45	1.52
1	F	50	GLU	CA-C	-6.68	1.44	1.52
1	B	353	VAL	CA-CB	-6.66	1.47	1.55
1	F	130	VAL	CA-C	-6.61	1.44	1.52
1	C	360	VAL	CA-CB	-6.54	1.44	1.54
1	A	129	VAL	CA-CB	-6.45	1.46	1.54
1	F	252	VAL	CA-CB	-6.39	1.45	1.54
1	B	130	VAL	CA-CB	-6.26	1.46	1.54
1	D	286	MET	SD-CE	6.19	1.95	1.79
1	F	360	VAL	CA-CB	-6.16	1.46	1.54
1	C	283	VAL	CA-CB	-6.10	1.48	1.55
1	C	46	VAL	CA-CB	-6.09	1.46	1.54
1	F	271	PRO	CA-C	-6.07	1.47	1.53
1	E	341	MET	SD-CE	-6.07	1.64	1.79
1	A	46	VAL	CA-CB	-6.02	1.46	1.55
1	A	325	ILE	CA-CB	6.01	1.62	1.54
1	A	40	VAL	CA-CB	-5.99	1.46	1.54
1	E	164	VAL	CA-C	-5.94	1.45	1.52
1	D	262	VAL	CA-CB	-5.93	1.47	1.54
1	F	228	HIS	CA-C	-5.92	1.46	1.52
1	E	238	ARG	CA-C	-5.90	1.45	1.52
1	C	360	VAL	CA-C	-5.89	1.45	1.52
1	D	252	VAL	CA-CB	-5.88	1.46	1.55
1	A	336	VAL	C-N	5.88	1.42	1.33
1	A	238	ARG	CA-C	-5.86	1.45	1.52
1	B	294	TYR	CA-C	-5.82	1.46	1.53
1	A	259	LEU	CB-CG	5.82	1.65	1.53
1	B	40	VAL	CA-CB	-5.79	1.47	1.54
1	C	40	VAL	CA-CB	-5.79	1.46	1.54
1	B	252	VAL	CA-CB	-5.75	1.47	1.54
1	F	305	TYR	CA-C	-5.74	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	207	VAL	CA-CB	-5.72	1.46	1.54
1	F	30	ILE	CA-CB	-5.69	1.46	1.54
1	C	176	GLY	C-O	5.66	1.31	1.23
1	C	315	VAL	CA-CB	-5.65	1.47	1.55
1	A	360	VAL	CA-CB	-5.64	1.46	1.54
1	C	353	VAL	CA-C	-5.59	1.45	1.52
1	D	250	PRO	CA-C	-5.59	1.47	1.52
1	C	258	THR	CA-CB	-5.57	1.45	1.53
1	D	59	GLN	CA-C	-5.56	1.46	1.52
1	A	239	TYR	CA-C	-5.55	1.45	1.52
1	E	138	VAL	CA-CB	-5.54	1.47	1.54
1	B	52	PHE	CA-C	-5.53	1.45	1.52
1	C	167	VAL	CA-CB	-5.53	1.47	1.54
1	C	250	PRO	CA-C	-5.52	1.47	1.52
1	E	29	LEU	CA-C	-5.49	1.45	1.52
1	D	79	ILE	CA-CB	-5.46	1.47	1.53
1	B	360	VAL	CA-CB	-5.45	1.47	1.54
1	F	25	VAL	N-CA	-5.44	1.41	1.46
1	D	332	MET	SD-CE	5.43	1.93	1.79
1	A	252	VAL	CA-CB	-5.42	1.49	1.55
1	A	283	VAL	CA-CB	-5.42	1.47	1.54
1	A	29	LEU	CA-C	-5.39	1.45	1.52
1	E	224	VAL	CA-CB	-5.39	1.47	1.54
1	E	208	LEU	CA-C	-5.38	1.47	1.53
1	F	239	TYR	CA-C	-5.38	1.46	1.52
1	B	25	VAL	CA-CB	-5.37	1.50	1.55
1	F	197	THR	CA-CB	5.36	1.59	1.52
1	F	208	LEU	CA-C	-5.33	1.45	1.52
1	C	29	LEU	CA-C	-5.32	1.45	1.52
1	B	208	LEU	CA-C	-5.32	1.45	1.52
1	E	123	VAL	CA-CB	-5.29	1.47	1.54
1	B	129	VAL	CA-C	-5.28	1.46	1.52
1	D	285	ILE	CA-C	-5.26	1.46	1.52
1	D	95	LEU	CA-C	-5.26	1.46	1.52
1	D	255	PHE	N-CA	-5.25	1.39	1.46
1	A	353	VAL	CA-C	-5.25	1.46	1.52
1	F	352	ARG	CA-C	-5.24	1.46	1.52
1	C	110	GLU	CA-C	5.22	1.59	1.52
1	F	130	VAL	CA-CB	-5.19	1.47	1.55
1	B	157	VAL	CA-CB	-5.17	1.48	1.54
1	B	164	VAL	CA-C	-5.16	1.46	1.52
1	A	25	VAL	N-CA	-5.15	1.42	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	261	THR	CA-C	-5.13	1.46	1.52
1	C	25	VAL	N-CA	-5.13	1.42	1.46
1	D	119	MET	SD-CE	5.10	1.92	1.79
1	D	253	LEU	CA-C	-5.09	1.46	1.52
1	F	29	LEU	CA-C	-5.08	1.46	1.53
1	B	370	VAL	CA-C	-5.07	1.46	1.52
1	A	250	PRO	CA-C	-5.05	1.47	1.52
1	A	253	LEU	CA-C	-5.03	1.46	1.52
1	A	129	VAL	CA-C	-5.02	1.46	1.52

All (629) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	336	VAL	O-C-N	-23.37	93.36	122.57
1	A	258	THR	N-CA-C	16.91	133.05	111.24
1	E	336	VAL	O-C-N	14.84	139.51	123.03
1	E	256	THR	N-CA-C	14.63	130.56	108.46
1	F	254	GLN	N-CA-C	14.62	129.16	108.54
1	E	259	LEU	N-CA-C	13.70	130.21	109.25
1	F	143	LYS	CA-C-N	-13.66	106.10	120.85
1	F	143	LYS	C-N-CA	-13.66	106.10	120.85
1	C	275	GLY	N-CA-C	-13.46	88.31	111.47
1	C	327	SER	N-CA-C	-13.44	96.72	111.36
1	D	256	THR	N-CA-C	13.02	131.19	109.06
1	B	72	TYR	N-CA-C	-12.79	98.12	112.57
1	F	270	GLY	CA-C-N	-12.72	107.12	120.85
1	F	270	GLY	C-N-CA	-12.72	107.12	120.85
1	D	170	GLU	N-CA-C	-12.63	96.76	108.13
1	B	256	THR	N-CA-C	12.56	128.92	108.32
1	E	246	GLY	N-CA-C	12.38	124.67	112.04
1	C	256	THR	N-CA-C	12.27	126.99	108.46
1	D	254	GLN	N-CA-C	12.02	129.27	107.99
1	D	81	LEU	N-CA-C	12.01	118.63	108.78
1	D	89	SER	CA-C-N	11.81	134.60	119.84
1	D	89	SER	C-N-CA	11.81	134.60	119.84
1	F	256	THR	N-CA-C	11.81	127.68	108.32
1	D	259	LEU	N-CA-C	11.70	128.56	109.95
1	B	350	GLU	N-CA-C	11.21	125.56	108.52
1	D	60	PRO	CA-C-N	11.19	130.88	119.24
1	D	60	PRO	C-N-CA	11.19	130.88	119.24
1	E	220	GLY	N-CA-C	-11.19	97.21	114.10
1	E	143	LYS	CA-C-N	-11.15	105.90	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	143	LYS	C-N-CA	-11.15	105.90	119.84
1	D	297	HIS	N-CA-C	11.14	127.86	114.04
1	F	262	VAL	N-CA-C	10.93	123.95	107.99
1	C	109	ASN	N-CA-C	10.90	126.72	109.50
1	F	170	GLU	N-CA-C	-10.80	98.41	108.13
1	E	319	TYR	N-CA-C	10.75	125.77	110.07
1	E	76	SER	N-CA-C	-10.74	95.36	110.50
1	B	94	THR	N-CA-C	-10.72	96.76	111.87
1	B	298	HIS	N-CA-C	10.69	125.99	109.96
1	B	262	VAL	N-CA-C	10.63	123.42	107.15
1	B	339	GLN	CA-C-N	10.52	132.99	119.84
1	B	339	GLN	C-N-CA	10.52	132.99	119.84
1	A	256	THR	N-CA-C	10.50	126.71	108.75
1	D	258	THR	N-CA-C	10.48	122.29	111.07
1	B	275	GLY	N-CA-C	-10.45	88.41	113.18
1	B	259	LEU	N-CA-C	10.41	126.21	109.24
1	A	72	TYR	N-CA-C	-10.38	100.61	113.38
1	F	275	GLY	N-CA-C	-10.37	93.63	111.47
1	F	197	THR	N-CA-C	-10.29	92.17	108.63
1	D	141	PHE	N-CA-C	10.28	124.21	109.71
1	D	143	LYS	CA-C-N	-10.28	106.99	119.84
1	D	143	LYS	C-N-CA	-10.28	106.99	119.84
1	D	250	PRO	CA-C-N	10.26	130.21	119.85
1	D	250	PRO	C-N-CA	10.26	130.21	119.85
1	C	332	MET	N-CA-C	-10.21	100.31	113.17
1	E	339	GLN	CA-C-N	10.18	132.56	119.84
1	E	339	GLN	C-N-CA	10.18	132.56	119.84
1	A	94	THR	N-CA-C	-10.16	97.54	111.56
1	F	59	GLN	CA-C-N	10.10	130.79	120.38
1	F	59	GLN	C-N-CA	10.10	130.79	120.38
1	F	259	LEU	N-CA-C	10.05	126.36	110.17
1	E	89	SER	CA-C-N	10.03	132.38	119.84
1	E	89	SER	C-N-CA	10.03	132.38	119.84
1	D	296	VAL	N-CA-C	-10.01	96.79	109.30
1	E	72	TYR	N-CA-C	-9.92	101.18	113.38
1	C	211	ILE	N-CA-C	-9.87	102.30	111.67
1	D	350	GLU	N-CA-C	9.87	123.84	109.14
1	B	232	ALA	N-CA-C	-9.84	96.97	110.35
1	B	319	TYR	CA-C-N	9.83	132.13	119.84
1	B	319	TYR	C-N-CA	9.83	132.13	119.84
1	E	250	PRO	CA-C-N	9.79	129.72	120.03
1	E	250	PRO	C-N-CA	9.79	129.72	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	187	GLU	N-CA-C	-9.77	101.36	113.18
1	B	269	VAL	N-CA-C	9.71	120.28	112.12
1	C	226	ILE	CB-CA-C	-9.67	102.44	111.05
1	F	299	TRP	N-CA-C	9.63	124.78	110.52
1	E	288	TRP	N-CA-C	9.59	125.20	109.95
1	E	262	VAL	N-CA-C	9.58	121.79	107.51
1	C	209	ASN	CA-C-N	9.58	129.21	119.82
1	C	209	ASN	C-N-CA	9.58	129.21	119.82
1	E	254	GLN	N-CA-C	9.53	126.39	107.62
1	E	370	VAL	N-CA-C	-9.49	96.05	106.21
1	F	130	VAL	N-CA-C	9.49	123.47	108.85
1	A	376	THR	N-CA-C	9.39	124.81	108.75
1	C	94	THR	N-CA-C	-9.38	101.53	113.16
1	D	226	ILE	N-CA-C	9.36	120.28	111.48
1	A	143	LYS	CA-C-N	-9.35	108.15	119.84
1	A	143	LYS	C-N-CA	-9.35	108.15	119.84
1	E	274	LYS	N-CA-C	-9.23	95.86	109.15
1	D	197	THR	N-CA-C	-9.17	96.20	109.96
1	B	299	TRP	CA-CB-CG	9.17	131.02	113.60
1	C	78	GLY	N-CA-C	-9.14	100.05	112.57
1	B	327	SER	N-CA-C	-9.13	100.73	112.23
1	E	299	TRP	CA-CB-CG	9.12	130.92	113.60
1	F	323	SER	N-CA-C	-9.09	101.30	112.38
1	C	95	LEU	N-CA-C	9.08	128.44	109.11
1	D	94	THR	N-CA-C	-9.00	101.85	112.92
1	F	226	ILE	N-CA-C	9.00	119.68	112.12
1	F	333	LEU	CA-C-N	9.00	131.09	119.84
1	F	333	LEU	C-N-CA	9.00	131.09	119.84
1	B	377	LYS	N-CA-C	-8.99	94.25	108.63
1	D	274	LYS	N-CA-C	-8.96	96.52	109.96
1	F	253	LEU	N-CA-C	8.96	121.10	108.74
1	E	209	ASN	CA-C-N	8.93	128.57	119.56
1	E	209	ASN	C-N-CA	8.93	128.57	119.56
1	E	21	ARG	CA-C-N	8.88	130.94	119.84
1	E	21	ARG	C-N-CA	8.88	130.94	119.84
1	D	54	ASN	CA-C-N	8.87	130.93	119.84
1	D	54	ASN	C-N-CA	8.87	130.93	119.84
1	E	297	HIS	N-CA-C	8.87	124.41	113.50
1	B	376	THR	N-CA-C	8.86	123.90	109.72
1	E	292	ARG	N-CA-C	-8.82	92.02	110.80
1	C	143	LYS	CA-C-N	-8.77	108.88	119.84
1	C	143	LYS	C-N-CA	-8.77	108.88	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	76	SER	N-CA-C	-8.74	96.85	109.96
1	F	258	THR	N-CA-C	8.71	129.36	110.80
1	C	226	ILE	N-CA-C	8.70	118.49	111.62
1	C	262	VAL	N-CA-C	8.69	120.68	107.99
1	B	299	TRP	N-CA-C	8.68	123.33	110.48
1	C	339	GLN	CA-C-N	8.66	130.67	119.84
1	C	339	GLN	C-N-CA	8.66	130.67	119.84
1	C	76	SER	N-CA-C	-8.66	96.97	109.96
1	A	299	TRP	CA-CB-CG	8.65	130.03	113.60
1	B	58	GLY	N-CA-C	8.63	119.61	111.67
1	A	54	ASN	CA-C-N	8.61	130.61	119.84
1	A	54	ASN	C-N-CA	8.61	130.61	119.84
1	F	94	THR	N-CA-C	-8.58	100.75	113.61
1	C	141	PHE	N-CA-C	8.55	123.65	107.75
1	F	78	GLY	N-CA-C	-8.54	101.02	112.81
1	B	246	GLY	N-CA-C	8.54	120.06	111.95
1	C	292	ARG	N-CA-C	-8.53	92.98	107.99
1	B	274	LYS	N-CA-C	-8.47	96.29	109.25
1	C	370	VAL	N-CA-C	8.46	119.25	110.62
1	F	356	GLY	N-CA-C	8.41	124.66	112.55
1	D	76	SER	N-CA-C	-8.38	99.47	110.53
1	D	31	LYS	N-CA-C	-8.38	97.16	110.14
1	F	132	SER	N-CA-C	-8.35	102.10	111.71
1	D	298	HIS	N-CA-C	8.34	128.56	110.80
1	F	339	GLN	CA-C-N	8.31	130.22	119.84
1	F	339	GLN	C-N-CA	8.31	130.22	119.84
1	B	222	TYR	N-CA-C	-8.29	99.35	109.72
1	A	379	VAL	N-CA-C	-8.27	98.21	109.37
1	F	276	GLU	N-CA-C	-8.26	100.31	110.88
1	E	258	THR	N-CA-C	8.26	128.38	110.80
1	A	188	GLU	N-CA-C	8.21	122.12	108.73
1	C	29	LEU	CA-CB-CG	-8.21	87.55	116.30
1	C	360	VAL	CA-C-N	8.21	128.65	120.52
1	C	360	VAL	C-N-CA	8.21	128.65	120.52
1	F	289	ARG	N-CA-C	-8.18	95.90	109.07
1	B	130	VAL	N-CA-C	8.10	120.15	108.48
1	B	155	THR	CA-C-N	8.09	129.96	119.84
1	B	155	THR	C-N-CA	8.09	129.96	119.84
1	B	254	GLN	N-CA-C	8.09	123.94	107.69
1	E	291	THR	N-CA-C	8.08	122.08	109.96
1	A	233	LYS	N-CA-C	-8.03	102.60	111.36
1	A	333	LEU	CA-C-N	8.02	129.87	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	333	LEU	C-N-CA	8.02	129.87	119.84
1	C	249	THR	CA-C-N	8.02	128.64	120.38
1	C	249	THR	C-N-CA	8.02	128.64	120.38
1	E	221	MET	N-CA-C	8.02	122.98	112.72
1	D	142	ASN	N-CA-C	-7.96	98.67	110.46
1	E	141	PHE	N-CA-C	7.95	120.92	109.71
1	F	355	ASP	N-CA-C	-7.95	105.56	114.62
1	E	263	LEU	N-CA-C	-7.94	102.85	112.54
1	D	262	VAL	N-CA-C	7.92	119.55	107.99
1	A	292	ARG	N-CA-C	-7.91	95.97	108.63
1	E	69	GLY	N-CA-C	-7.88	103.38	115.66
1	E	178	VAL	CB-CA-C	-7.87	100.41	111.19
1	A	254	GLN	N-CA-C	7.82	123.03	107.62
1	D	277	GLY	N-CA-C	7.80	124.60	110.71
1	B	141	PHE	N-CA-C	7.79	122.69	107.57
1	C	360	VAL	CB-CA-C	-7.77	101.75	110.68
1	A	358	GLU	CA-C-N	-7.71	111.66	119.99
1	A	358	GLU	C-N-CA	-7.71	111.66	119.99
1	B	289	ARG	N-CA-C	-7.69	98.09	110.32
1	A	123	VAL	N-CA-C	7.64	118.66	111.48
1	D	232	ALA	N-CA-C	-7.64	99.96	110.35
1	F	335	GLN	N-CA-C	7.64	121.18	108.73
1	B	19	CYS	N-CA-C	-7.63	95.63	109.44
1	E	296	VAL	N-CA-C	-7.63	98.82	108.89
1	E	232	ALA	N-CA-C	-7.62	96.43	108.63
1	C	344	GLU	N-CA-C	-7.61	103.11	113.30
1	F	274	LYS	N-CA-C	-7.57	99.83	110.50
1	A	336	VAL	CA-C-N	7.57	135.99	121.54
1	A	336	VAL	C-N-CA	7.57	135.99	121.54
1	B	44	ASP	N-CA-C	-7.55	104.21	113.50
1	F	114	CYS	N-CA-C	-7.54	95.41	108.52
1	F	263	LEU	N-CA-C	-7.52	103.36	112.54
1	A	211	ILE	N-CA-C	-7.49	105.37	111.81
1	F	290	VAL	N-CA-C	7.49	118.66	107.80
1	B	129	VAL	CA-C-N	-7.46	112.77	123.06
1	B	129	VAL	C-N-CA	-7.46	112.77	123.06
1	E	19	CYS	CA-C-N	7.44	129.14	119.84
1	E	19	CYS	C-N-CA	7.44	129.14	119.84
1	C	348	VAL	N-CA-C	-7.43	96.44	107.51
1	D	72	TYR	N-CA-C	-7.40	103.84	113.17
1	B	25	VAL	N-CA-CB	-7.39	106.73	111.83
1	F	264	LEU	CA-CB-CG	-7.37	90.49	116.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	109	ASN	N-CA-C	7.33	121.21	110.59
1	E	298	HIS	N-CA-C	7.30	126.36	110.80
1	C	276	GLU	N-CA-C	-7.30	101.49	111.56
1	E	40	VAL	CB-CA-C	-7.28	99.35	111.29
1	C	62	THR	CA-C-N	-7.27	110.75	119.84
1	C	62	THR	C-N-CA	-7.27	110.75	119.84
1	F	292	ARG	N-CA-C	-7.23	95.39	110.80
1	F	42	GLY	N-CA-C	-7.21	97.64	112.34
1	C	155	THR	CA-C-N	7.20	128.84	119.84
1	C	155	THR	C-N-CA	7.20	128.84	119.84
1	D	62	THR	CA-C-N	-7.18	110.86	119.84
1	D	62	THR	C-N-CA	-7.18	110.86	119.84
1	D	325	ILE	N-CA-C	-7.18	103.67	110.42
1	F	220	GLY	N-CA-C	-7.17	103.93	114.61
1	F	282	CYS	N-CA-C	7.15	117.31	107.73
1	B	60	PRO	CA-C-N	7.15	128.77	119.84
1	B	60	PRO	C-N-CA	7.15	128.77	119.84
1	F	226	ILE	CB-CA-C	-7.14	103.91	110.91
1	C	274	LYS	N-CA-C	-7.14	99.92	110.48
1	E	335	GLN	N-CA-C	7.13	121.29	109.46
1	B	263	LEU	N-CA-C	-7.12	104.72	113.19
1	C	44	ASP	N-CA-C	-7.09	104.64	112.72
1	C	25	VAL	N-CA-CB	-7.09	104.08	111.87
1	D	40	VAL	N-CA-C	7.09	124.08	109.34
1	A	155	THR	CA-C-N	7.08	128.70	119.84
1	A	155	THR	C-N-CA	7.08	128.70	119.84
1	E	54	ASN	N-CA-C	-7.08	99.90	110.24
1	B	284	ASP	N-CA-C	7.07	122.59	107.67
1	A	262	VAL	N-CA-C	7.05	119.01	108.23
1	A	282	CYS	N-CA-C	7.01	119.02	107.73
1	D	209	ASN	CA-C-N	7.01	126.69	119.82
1	D	209	ASN	C-N-CA	7.01	126.69	119.82
1	E	311	ARG	N-CA-C	7.00	120.05	109.41
1	B	126	LYS	N-CA-C	-7.00	99.20	110.32
1	A	226	ILE	N-CA-C	6.97	117.98	112.12
1	F	76	SER	N-CA-C	-6.96	99.52	109.96
1	A	205	ASP	N-CA-C	-6.95	104.28	112.89
1	D	69	GLY	N-CA-C	-6.94	104.14	115.46
1	A	290	VAL	N-CA-C	6.93	117.85	107.80
1	A	339	GLN	CA-C-N	6.92	128.50	119.84
1	A	339	GLN	C-N-CA	6.92	128.50	119.84
1	B	139	HIS	N-CA-C	-6.90	99.34	109.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	289	ARG	N-CA-C	-6.89	98.38	109.96
1	A	291	THR	N-CA-C	6.89	120.37	110.24
1	A	283	VAL	CB-CA-C	-6.87	100.03	111.29
1	E	282	CYS	N-CA-C	6.87	117.56	107.88
1	E	151	LYS	N-CA-C	6.84	118.90	109.18
1	C	347	GLN	N-CA-C	-6.84	104.84	112.57
1	C	137	ASP	N-CA-C	-6.83	99.71	109.96
1	D	292	ARG	N-CA-C	-6.83	97.70	108.63
1	F	326	SER	N-CA-C	-6.83	103.92	111.36
1	F	139	HIS	N-CA-C	-6.83	103.18	108.78
1	F	29	LEU	CA-CB-CG	-6.82	92.42	116.30
1	F	325	ILE	N-CA-C	-6.82	103.83	110.72
1	D	264	LEU	N-CA-C	6.82	120.27	110.24
1	B	180	ASP	N-CA-C	6.80	120.03	107.99
1	E	50	GLU	N-CA-C	-6.79	99.52	110.32
1	A	119	MET	N-CA-C	6.78	119.25	109.14
1	F	151	LYS	N-CA-C	6.77	118.80	109.18
1	C	31	LYS	N-CA-C	-6.77	98.80	109.50
1	F	238	ARG	N-CA-C	-6.77	97.94	109.24
1	B	292	ARG	N-CA-C	-6.76	103.93	111.71
1	D	78	GLY	N-CA-C	-6.75	97.19	113.18
1	E	29	LEU	CA-CB-CG	-6.75	92.69	116.30
1	C	363	ASP	CA-C-N	6.74	126.88	119.87
1	C	363	ASP	C-N-CA	6.74	126.88	119.87
1	C	205	ASP	N-CA-C	-6.74	104.32	112.54
1	C	220	GLY	N-CA-C	-6.72	101.67	113.76
1	C	277	GLY	N-CA-C	6.71	122.18	111.64
1	B	362	GLY	N-CA-C	-6.71	97.28	113.18
1	C	170	GLU	N-CA-C	-6.71	100.42	108.14
1	F	277	GLY	N-CA-C	6.70	124.36	111.31
1	E	180	ASP	N-CA-C	6.68	119.81	107.99
1	B	238	ARG	N-CA-C	-6.66	97.50	108.76
1	A	29	LEU	N-CA-C	-6.65	105.70	113.88
1	A	288	TRP	N-CA-C	6.65	120.72	110.42
1	F	300	ARG	N-CA-C	6.64	120.86	110.17
1	D	59	GLN	CA-C-N	6.62	127.19	120.38
1	D	59	GLN	C-N-CA	6.62	127.19	120.38
1	C	54	ASN	CA-C-N	6.60	128.09	119.84
1	C	54	ASN	C-N-CA	6.60	128.09	119.84
1	E	142	ASN	N-CA-C	-6.59	100.46	110.14
1	E	227	TRP	N-CA-C	6.58	120.39	109.46
1	E	139	HIS	N-CA-C	-6.58	96.79	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	297	HIS	N-CA-C	6.58	122.21	112.94
1	D	191	VAL	CB-CA-C	-6.57	102.61	111.15
1	C	153	ILE	CB-CA-C	-6.56	98.97	110.71
1	A	54	ASN	N-CA-C	-6.56	101.81	110.07
1	A	257	ASN	N-CA-CB	-6.54	99.74	110.40
1	A	264	LEU	CA-CB-CG	-6.54	93.41	116.30
1	E	41	THR	N-CA-C	-6.53	101.56	111.56
1	F	350	GLU	N-CA-C	6.53	118.13	108.60
1	F	19	CYS	CA-C-N	-6.52	113.95	120.21
1	F	19	CYS	C-N-CA	-6.52	113.95	120.21
1	B	100	MET	N-CA-C	6.52	117.18	108.38
1	C	132	SER	N-CA-C	-6.50	104.45	112.38
1	B	360	VAL	CB-CA-C	-6.50	99.53	111.36
1	D	38	ASP	N-CA-C	6.50	119.19	111.33
1	B	290	VAL	N-CA-C	6.47	118.11	107.24
1	B	69	GLY	N-CA-C	-6.46	104.55	115.80
1	B	250	PRO	CA-C-N	6.45	126.36	119.85
1	B	250	PRO	C-N-CA	6.45	126.36	119.85
1	A	363	ASP	CA-C-N	6.44	127.89	119.84
1	A	363	ASP	C-N-CA	6.44	127.89	119.84
1	C	114	CYS	N-CA-C	-6.44	99.95	109.81
1	C	264	LEU	CA-CB-CG	-6.44	93.76	116.30
1	C	92	ASN	N-CA-C	6.43	118.86	111.02
1	C	177	LEU	N-CA-C	-6.42	98.91	108.99
1	D	64	GLU	N-CA-C	6.42	119.09	111.71
1	A	141	PHE	N-CA-C	6.42	121.11	107.70
1	B	175	GLN	CA-C-N	-6.41	116.38	122.66
1	B	175	GLN	C-N-CA	-6.41	116.38	122.66
1	A	195	THR	N-CA-C	-6.40	103.56	111.75
1	A	89	SER	CA-C-N	6.39	127.83	119.84
1	A	89	SER	C-N-CA	6.39	127.83	119.84
1	C	287	GLY	N-CA-C	-6.37	103.17	111.52
1	D	275	GLY	N-CA-C	-6.37	98.08	113.18
1	E	333	LEU	CA-C-N	6.37	126.74	119.92
1	E	333	LEU	C-N-CA	6.37	126.74	119.92
1	F	54	ASN	N-CA-C	-6.37	102.11	110.39
1	A	62	THR	CA-C-N	-6.36	111.89	119.84
1	A	62	THR	C-N-CA	-6.36	111.89	119.84
1	E	129	VAL	N-CA-C	-6.36	99.42	108.58
1	E	378	THR	N-CA-C	6.36	119.87	109.24
1	A	304	ARG	N-CA-C	6.36	119.94	108.69
1	C	40	VAL	CB-CA-C	-6.35	100.87	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	179	THR	N-CA-C	-6.35	103.98	111.03
1	E	279	TYR	N-CA-C	6.32	119.09	108.02
1	F	109	ASN	N-CA-C	6.32	118.87	110.53
1	A	310	LEU	N-CA-C	6.32	119.02	109.23
1	F	291	THR	N-CA-C	6.30	119.51	110.24
1	F	316	LYS	N-CA-C	-6.30	98.97	109.24
1	F	72	TYR	N-CA-C	-6.28	105.20	112.92
1	F	164	VAL	N-CA-C	-6.28	99.22	107.88
1	E	97	THR	N-CA-C	6.28	119.42	109.50
1	B	242	ASN	N-CA-C	6.27	118.38	108.79
1	A	238	ARG	N-CA-C	-6.25	98.71	108.90
1	F	205	ASP	N-CA-C	-6.24	104.48	111.28
1	C	232	ALA	N-CA-C	-6.23	97.52	110.80
1	C	72	TYR	N-CA-C	-6.23	104.84	112.88
1	F	209	ASN	CA-C-N	6.22	125.92	119.82
1	F	209	ASN	C-N-CA	6.22	125.92	119.82
1	C	139	HIS	N-CA-C	-6.21	100.38	109.63
1	E	44	ASP	N-CA-C	-6.20	102.26	111.81
1	D	317	ASN	N-CA-C	-6.20	100.25	109.42
1	D	249	THR	CA-C-N	6.19	126.76	120.38
1	D	249	THR	C-N-CA	6.19	126.76	120.38
1	B	205	ASP	N-CA-C	-6.19	104.45	111.07
1	E	211	ILE	N-CA-C	-6.19	105.11	110.74
1	A	62	THR	N-CA-C	6.18	123.48	109.81
1	C	283	VAL	CB-CA-C	-6.18	102.28	111.80
1	C	362	GLY	N-CA-C	-6.17	98.54	113.18
1	F	155	THR	CA-C-N	6.17	127.03	120.11
1	F	155	THR	C-N-CA	6.17	127.03	120.11
1	A	167	VAL	CB-CA-C	-6.17	101.17	111.29
1	A	322	ALA	N-CA-C	6.17	123.93	110.80
1	D	62	THR	N-CA-C	6.16	121.90	113.77
1	E	60	PRO	CA-C-N	6.15	127.53	119.84
1	E	60	PRO	C-N-CA	6.15	127.53	119.84
1	F	175	GLN	N-CA-C	-6.15	97.40	108.48
1	D	216	LEU	N-CA-C	6.15	119.98	112.23
1	C	71	GLN	N-CA-C	6.14	123.89	110.80
1	E	304	ARG	N-CA-C	6.14	119.49	109.06
1	E	380	PHE	CA-C-N	6.13	127.50	119.84
1	E	380	PHE	C-N-CA	6.13	127.50	119.84
1	B	285	ILE	CB-CA-C	-6.12	103.32	110.91
1	C	56	ARG	N-CA-C	6.12	118.75	107.73
1	C	257	ASN	CA-C-N	-6.12	112.93	122.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	257	ASN	C-N-CA	-6.12	112.93	122.42
1	C	69	GLY	N-CA-C	-6.11	104.98	115.61
1	B	62	THR	N-CA-C	6.09	123.27	109.81
1	A	256	THR	CA-C-N	6.07	131.75	121.14
1	A	256	THR	C-N-CA	6.07	131.75	121.14
1	C	263	LEU	N-CA-C	-6.06	105.93	113.15
1	C	291	THR	N-CA-C	6.06	118.12	110.24
1	F	62	THR	CA-C-N	-6.05	112.27	119.84
1	F	62	THR	C-N-CA	-6.05	112.27	119.84
1	C	154	SER	N-CA-C	-6.05	97.83	108.23
1	B	380	PHE	CA-C-N	6.04	127.40	119.84
1	B	380	PHE	C-N-CA	6.04	127.40	119.84
1	B	270	GLY	CA-C-N	-6.02	114.56	120.52
1	B	270	GLY	C-N-CA	-6.02	114.56	120.52
1	C	313	ARG	N-CA-C	6.02	119.29	109.24
1	A	137	ASP	N-CA-C	-6.01	100.75	109.59
1	B	283	VAL	CB-CA-C	-6.01	101.43	111.29
1	F	229	PRO	N-CA-C	-6.00	101.24	110.95
1	A	361	PRO	N-CA-C	-5.99	102.42	111.41
1	C	294	TYR	N-CA-C	-5.99	100.50	109.96
1	E	65	SER	N-CA-C	5.99	119.58	109.76
1	B	78	GLY	N-CA-C	-5.98	99.00	113.18
1	A	197	THR	N-CA-C	5.98	119.85	111.30
1	C	164	VAL	CB-CA-C	-5.97	102.99	111.40
1	D	136	LEU	N-CA-C	5.96	120.56	113.16
1	C	317	ASN	CA-C-N	5.96	127.28	119.84
1	C	317	ASN	C-N-CA	5.96	127.28	119.84
1	E	229	PRO	N-CA-C	-5.96	101.30	110.95
1	B	188	GLU	N-CA-C	5.95	119.52	109.76
1	A	378	THR	CB-CA-C	-5.95	99.48	109.65
1	F	137	ASP	N-CA-C	-5.95	99.46	108.67
1	D	126	LYS	N-CA-C	-5.93	99.57	109.24
1	D	29	LEU	CA-CB-CG	-5.93	95.55	116.30
1	D	92	ASN	N-CA-C	5.93	123.42	110.80
1	E	315	VAL	CB-CA-C	-5.92	101.59	111.29
1	C	42	GLY	N-CA-C	-5.91	100.28	112.34
1	E	205	ASP	N-CA-C	-5.90	105.34	112.54
1	E	365	ASP	N-CA-C	-5.88	106.74	112.97
1	D	127	THR	N-CA-C	-5.87	100.42	109.52
1	E	95	LEU	N-CA-C	5.86	118.94	109.15
1	E	164	VAL	CB-CA-C	-5.86	101.69	111.29
1	D	56	ARG	N-CA-C	5.85	118.97	107.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	348	VAL	N-CA-C	-5.85	99.45	107.99
1	A	294	TYR	CA-C-N	-5.85	113.70	122.24
1	A	294	TYR	C-N-CA	-5.85	113.70	122.24
1	E	382	GLY	N-CA-C	-5.83	99.37	113.18
1	E	115	ASP	N-CA-C	-5.82	104.22	111.90
1	C	248	THR	CB-CA-C	-5.82	102.11	111.18
1	E	168	GLY	N-CA-C	5.81	121.92	110.83
1	E	132	SER	N-CA-C	-5.81	105.29	112.38
1	C	290	VAL	N-CA-C	5.80	116.50	107.28
1	D	155	THR	CA-C-N	5.80	127.09	119.84
1	D	155	THR	C-N-CA	5.80	127.09	119.84
1	C	278	LEU	N-CA-C	-5.80	98.96	108.41
1	D	313	ARG	N-CA-C	5.79	118.91	109.59
1	A	209	ASN	CA-C-N	5.78	126.54	120.12
1	A	209	ASN	C-N-CA	5.78	126.54	120.12
1	A	76	SER	N-CA-C	-5.77	101.48	110.42
1	A	126	LYS	N-CA-C	-5.77	100.88	110.17
1	B	297	HIS	N-CA-C	5.76	120.55	112.72
1	A	149	ASN	N-CA-C	-5.75	106.11	113.01
1	E	357	THR	CB-CA-C	-5.75	104.17	111.70
1	F	175	GLN	CA-C-N	-5.75	117.03	122.66
1	F	175	GLN	C-N-CA	-5.75	117.03	122.66
1	F	25	VAL	N-CA-CB	-5.74	106.79	111.67
1	F	365	ASP	N-CA-C	5.74	117.80	109.71
1	E	45	SER	N-CA-C	-5.74	103.08	110.19
1	A	168	GLY	N-CA-C	5.73	121.62	110.73
1	A	54	ASN	CB-CA-C	5.73	116.95	108.87
1	D	23	ALA	CA-C-N	5.72	126.99	119.84
1	D	23	ALA	C-N-CA	5.72	126.99	119.84
1	D	42	GLY	N-CA-C	-5.72	100.66	112.34
1	B	353	VAL	CB-CA-C	-5.71	103.00	111.80
1	C	79	ILE	CB-CA-C	5.71	117.00	111.23
1	C	186	LYS	N-CA-C	-5.71	101.19	109.59
1	F	221	MET	CA-C-N	-5.70	113.22	121.20
1	F	221	MET	C-N-CA	-5.70	113.22	121.20
1	B	137	ASP	N-CA-C	-5.70	100.53	109.25
1	A	102	LYS	N-CA-C	5.70	118.16	108.02
1	D	87	GLU	N-CA-C	5.69	118.72	108.48
1	E	59	GLN	N-CA-C	5.69	116.82	109.65
1	E	62	THR	N-CA-C	5.69	122.38	109.81
1	B	40	VAL	CB-CA-C	-5.69	102.32	111.59
1	C	235	GLU	N-CA-C	5.69	117.77	108.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	177	LEU	N-CA-CB	5.68	120.14	110.71
1	D	260	THR	N-CA-C	5.68	119.32	110.17
1	C	180	ASP	N-CA-C	5.67	117.77	108.52
1	E	89	SER	N-CA-C	-5.67	102.49	110.31
1	A	142	ASN	N-CA-C	-5.66	100.71	109.14
1	E	68	GLU	N-CA-C	-5.66	106.51	113.41
1	E	283	VAL	CB-CA-C	-5.63	103.12	111.80
1	C	351	VAL	N-CA-C	5.63	116.39	108.17
1	E	126	LYS	N-CA-C	-5.63	101.00	109.95
1	F	62	THR	N-CA-C	5.63	122.24	109.81
1	A	159	GLY	N-CA-C	5.62	121.16	112.45
1	B	189	GLY	N-CA-C	5.61	122.97	114.61
1	D	347	GLN	N-CA-C	-5.61	106.76	113.21
1	D	311	ARG	N-CA-C	5.60	117.92	109.41
1	E	275	GLY	N-CA-C	-5.59	99.92	113.18
1	A	130	VAL	N-CA-C	5.59	116.64	108.53
1	C	238	ARG	N-CA-C	-5.59	98.98	108.26
1	F	222	TYR	N-CA-C	-5.58	101.16	109.42
1	F	257	ASN	N-CA-CB	-5.57	101.08	110.49
1	B	296	VAL	N-CA-C	-5.57	99.47	107.37
1	A	177	LEU	N-CA-CB	5.55	120.33	111.56
1	B	347	GLN	N-CA-C	-5.55	106.83	113.21
1	F	215	LYS	N-CA-C	-5.55	100.92	109.52
1	C	87	GLU	N-CA-C	5.54	117.72	108.02
1	C	158	GLU	N-CA-C	-5.54	101.09	108.74
1	A	284	ASP	N-CA-C	5.53	119.22	107.67
1	F	237	THR	N-CA-C	-5.52	101.13	109.85
1	B	349	GLU	N-CA-C	-5.51	106.14	112.92
1	E	347	GLN	N-CA-C	-5.49	106.61	113.15
1	F	186	LYS	N-CA-C	-5.49	101.73	109.96
1	C	140	GLY	CA-C-N	-5.48	115.23	122.85
1	C	140	GLY	C-N-CA	-5.48	115.23	122.85
1	F	93	ASN	N-CA-C	-5.47	104.86	113.02
1	A	177	LEU	CD1-CG-CD2	5.47	122.83	110.80
1	E	186	LYS	N-CA-C	-5.47	101.56	110.20
1	A	87	GLU	N-CA-C	5.46	117.86	109.07
1	C	253	LEU	N-CA-C	5.46	115.75	108.38
1	E	38	ASP	N-CA-C	5.46	117.93	111.33
1	E	197	THR	N-CA-C	-5.46	100.29	108.96
1	A	263	LEU	N-CA-C	-5.45	106.59	113.18
1	C	293	ASN	N-CA-C	-5.45	99.19	110.80
1	F	218	LYS	N-CA-C	5.45	122.41	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	380	PHE	CA-C-N	5.45	126.65	119.84
1	A	380	PHE	C-N-CA	5.45	126.65	119.84
1	C	103	LEU	N-CA-C	-5.43	101.13	109.76
1	C	60	PRO	CA-C-N	5.43	126.62	119.84
1	C	60	PRO	C-N-CA	5.43	126.62	119.84
1	C	91	GLY	N-CA-C	-5.43	100.32	113.18
1	E	175	GLN	N-CA-C	-5.42	99.84	109.06
1	B	194	LYS	N-CA-C	-5.42	104.78	111.40
1	A	56	ARG	CB-CA-C	5.42	120.25	112.12
1	B	78	GLY	CA-C-N	-5.41	115.75	123.10
1	B	78	GLY	C-N-CA	-5.41	115.75	123.10
1	D	339	GLN	N-CA-C	-5.41	102.33	109.84
1	E	157	VAL	CB-CA-C	-5.39	103.85	111.28
1	F	31	LYS	N-CA-C	-5.39	101.17	109.52
1	E	208	LEU	CA-C-N	-5.38	114.63	121.74
1	E	208	LEU	C-N-CA	-5.38	114.63	121.74
1	D	264	LEU	CA-CB-CG	-5.37	97.49	116.30
1	F	123	VAL	N-CA-C	5.37	120.50	109.34
1	A	226	ILE	CB-CA-C	-5.36	105.65	110.91
1	B	42	GLY	N-CA-C	-5.36	101.40	112.34
1	F	87	GLU	N-CA-C	5.36	117.26	108.52
1	A	136	LEU	CA-CB-CG	-5.36	97.55	116.30
1	E	263	LEU	CA-CB-CG	-5.36	97.56	116.30
1	B	209	ASN	CA-C-N	5.35	126.53	119.84
1	B	209	ASN	C-N-CA	5.35	126.53	119.84
1	F	53	LEU	N-CA-C	-5.35	101.05	109.50
1	D	96	PRO	N-CA-C	-5.35	102.79	111.19
1	F	79	ILE	CB-CA-C	5.35	120.06	111.29
1	E	235	GLU	N-CA-C	5.35	117.21	108.76
1	D	327	SER	N-CA-C	-5.34	104.51	111.02
1	B	359	PRO	N-CA-C	-5.34	103.46	111.57
1	A	164	VAL	CB-CA-C	-5.32	102.56	111.29
1	B	25	VAL	N-CA-C	-5.32	101.93	107.84
1	B	95	LEU	N-CA-C	5.32	120.68	108.81
1	E	379	VAL	N-CA-C	-5.32	98.27	109.34
1	A	25	VAL	N-CA-CB	-5.32	106.02	111.87
1	D	95	LEU	N-CA-C	5.32	120.22	108.73
1	A	69	GLY	N-CA-C	-5.31	106.56	115.80
1	E	100	MET	N-CA-C	5.30	115.54	108.38
1	D	132	SER	N-CA-C	-5.30	104.92	111.33
1	E	277	GLY	N-CA-C	5.30	122.03	112.54
1	A	289	ARG	N-CA-C	-5.29	99.89	108.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	299	TRP	CA-CB-CG	5.29	123.66	113.60
1	A	58	GLY	N-CA-C	5.29	117.70	111.35
1	A	360	VAL	CB-CA-C	-5.29	101.73	111.36
1	D	335	GLN	N-CA-C	-5.29	101.08	109.76
1	A	19	CYS	CA-C-N	5.29	126.45	119.84
1	A	19	CYS	C-N-CA	5.29	126.45	119.84
1	A	93	ASN	N-CA-C	-5.28	105.54	112.41
1	C	341	MET	N-CA-C	-5.28	103.75	111.30
1	F	211	ILE	N-CA-C	-5.28	106.54	111.45
1	E	299	TRP	N-CA-C	5.27	118.81	109.96
1	E	175	GLN	CA-C-N	-5.26	117.00	122.69
1	E	175	GLN	C-N-CA	-5.26	117.00	122.69
1	F	283	VAL	CB-CA-C	-5.26	102.67	111.29
1	E	46	VAL	N-CA-C	5.25	117.42	108.86
1	E	238	ARG	N-CA-C	-5.25	99.84	108.41
1	B	313	ARG	N-CA-C	5.25	117.46	108.90
1	D	54	ASN	N-CA-C	-5.25	103.16	109.72
1	B	140	GLY	CA-C-N	-5.24	115.01	122.77
1	B	140	GLY	C-N-CA	-5.24	115.01	122.77
1	F	92	ASN	N-CA-C	5.23	121.95	110.80
1	B	264	LEU	CA-CB-CG	-5.22	98.03	116.30
1	A	256	THR	CA-C-O	5.22	126.96	120.54
1	C	294	TYR	CA-C-N	-5.22	115.06	122.41
1	C	294	TYR	C-N-CA	-5.22	115.06	122.41
1	A	330	ASN	N-CA-C	5.21	121.89	110.80
1	E	196	ILE	CA-C-N	-5.20	115.28	122.30
1	E	196	ILE	C-N-CA	-5.20	115.28	122.30
1	C	110	GLU	N-CA-C	5.19	120.26	112.94
1	B	142	ASN	N-CA-C	-5.18	101.88	109.81
1	A	19	CYS	N-CA-C	5.18	117.57	108.82
1	C	78	GLY	CA-C-N	-5.17	118.05	122.96
1	C	78	GLY	C-N-CA	-5.17	118.05	122.96
1	D	221	MET	CA-C-N	-5.17	114.91	121.74
1	D	221	MET	C-N-CA	-5.17	114.91	121.74
1	D	348	VAL	CB-CA-C	-5.17	103.89	110.98
1	A	187	GLU	N-CA-C	-5.16	106.81	113.01
1	F	227	TRP	N-CA-C	5.16	118.63	109.96
1	C	131	GLY	CA-C-O	5.16	124.53	118.96
1	A	95	LEU	CA-CB-CG	-5.16	98.25	116.30
1	A	298	HIS	N-CA-C	5.16	121.78	110.80
1	C	297	HIS	N-CA-C	-5.15	102.37	110.36
1	A	274	LYS	N-CA-C	-5.15	102.23	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	351	VAL	N-CA-C	5.15	120.05	109.34
1	C	108	LEU	CA-C-N	-5.14	114.59	122.62
1	C	108	LEU	C-N-CA	-5.14	114.59	122.62
1	F	200	ASP	N-CA-C	5.14	117.36	109.95
1	F	294	TYR	CB-CA-C	-5.14	109.03	116.54
1	B	227	TRP	N-CA-C	5.13	117.92	109.76
1	C	242	ASN	N-CA-C	5.13	117.05	108.99
1	B	79	ILE	N-CA-C	5.13	114.88	106.72
1	F	119	MET	N-CA-C	5.13	116.78	109.14
1	C	227	TRP	N-CA-C	5.12	118.55	109.96
1	D	279	TYR	N-CA-C	5.12	117.24	108.90
1	C	284	ASP	N-CA-C	5.11	118.46	107.67
1	D	81	LEU	CA-C-O	5.11	120.91	117.94
1	D	140	GLY	CA-C-N	-5.11	114.95	122.06
1	D	140	GLY	C-N-CA	-5.11	114.95	122.06
1	F	25	VAL	N-CA-C	-5.11	102.31	108.45
1	D	37	LEU	CA-C-N	5.11	127.38	120.38
1	D	37	LEU	C-N-CA	5.11	127.38	120.38
1	C	169	GLY	N-CA-C	5.11	120.99	114.66
1	D	260	THR	CB-CA-C	-5.10	100.88	109.50
1	E	356	GLY	N-CA-C	5.10	121.65	112.77
1	A	217	ASP	N-CA-C	-5.10	106.14	112.93
1	E	206	GLN	N-CA-C	-5.10	105.90	111.82
1	E	295	ASP	CB-CA-C	5.10	117.98	111.40
1	B	123	VAL	N-CA-C	5.10	119.94	109.34
1	A	95	LEU	N-CA-C	5.09	120.17	108.81
1	A	258	THR	CA-C-N	-5.09	113.99	122.64
1	A	258	THR	C-N-CA	-5.09	113.99	122.64
1	A	378	THR	N-CA-C	-5.09	102.75	110.28
1	E	179	THR	N-CA-C	-5.07	100.01	110.80
1	F	232	ALA	N-CA-C	-5.07	103.46	110.35
1	B	46	VAL	N-CA-C	5.06	117.05	109.20
1	B	153	ILE	CB-CA-C	-5.05	102.61	110.69
1	C	55	PRO	CA-C-N	-5.05	115.45	123.12
1	C	55	PRO	C-N-CA	-5.05	115.45	123.12
1	A	377	LYS	N-CA-C	-5.05	101.73	109.76
1	B	300	ARG	N-CA-C	5.04	117.79	109.72
1	D	284	ASP	N-CA-C	5.04	118.31	107.67
1	D	348	VAL	N-CA-C	-5.04	100.63	107.99
1	D	164	VAL	N-CA-C	-5.04	100.63	108.44
1	F	342	GLU	N-CA-C	-5.04	100.08	110.80
1	D	235	GLU	N-CA-C	5.03	117.35	108.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	348	VAL	CB-CA-C	-5.03	104.27	111.31
1	C	290	VAL	CB-CA-C	-5.02	104.46	110.99
1	F	309	THR	N-CA-C	-5.02	100.33	108.52
1	F	158	GLU	N-CA-C	-5.02	101.27	108.60
1	A	50	GLU	N-CA-C	-5.02	101.51	109.59
1	A	78	GLY	N-CA-C	-5.02	104.53	112.66
1	B	196	ILE	CA-C-N	-5.02	115.55	123.13
1	B	196	ILE	C-N-CA	-5.02	115.55	123.13
1	E	170	GLU	N-CA-C	-5.02	98.72	109.81
1	E	226	ILE	N-CA-C	5.01	119.75	109.34
1	D	78	GLY	CA-C-N	-5.00	114.27	122.33
1	D	78	GLY	C-N-CA	-5.00	114.27	122.33

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	162	TYR	Sidechain
1	A	305	TYR	Sidechain
1	A	336	VAL	Peptide,Mainchain
1	A	71	GLN	Mainchain
1	B	162	TYR	Sidechain
1	B	305	TYR	Sidechain
1	B	319	TYR	Sidechain
1	C	162	TYR	Sidechain
1	C	305	TYR	Sidechain
1	D	162	TYR	Sidechain
1	D	305	TYR	Sidechain
1	D	354	TYR	Sidechain
1	D	71	GLN	Mainchain
1	E	162	TYR	Sidechain
1	E	71	GLN	Mainchain
1	F	162	TYR	Sidechain
1	F	305	TYR	Sidechain

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	2849	0	2815	557	1
1	B	2857	0	2820	527	0
1	C	2784	0	2743	454	0
1	D	2645	0	2616	460	0
1	E	2857	0	2821	545	0
1	F	2753	0	2710	477	0
2	G	66	0	56	2	0
2	H	66	0	56	2	0
2	I	66	0	56	0	0
2	J	66	0	56	1	0
2	K	66	0	56	3	0
2	L	66	0	56	5	0
All	All	17141	0	16861	2797	1

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 82.

All (2797) 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:336:VAL:CG2	1:A:337:GLN:HA	1.27	1.61
1:A:328:LEU:CD2	1:A:333:LEU:HD21	1.37	1.54
1:A:328:LEU:HD12	1:A:332:MET:CE	1.44	1.44
1:A:336:VAL:HG23	1:A:337:GLN:CA	0.98	1.44
1:A:328:LEU:CD1	1:A:332:MET:HE1	1.42	1.43
1:A:328:LEU:HD21	1:A:333:LEU:CD2	1.51	1.40
1:A:328:LEU:CD1	1:A:332:MET:CE	2.00	1.34
1:A:328:LEU:HD11	1:A:333:LEU:CD2	1.58	1.33
1:A:336:VAL:CG2	1:A:337:GLN:CA	1.90	1.29
1:A:336:VAL:HG23	1:A:337:GLN:N	1.30	1.27
1:A:328:LEU:CG	1:A:332:MET:HE2	1.75	1.16
1:A:328:LEU:O	1:A:328:LEU:HD23	1.46	1.15
1:A:203:ASN:HB3	1:E:71:GLN:HG3	1.18	1.15
1:E:177:LEU:HD21	1:E:206:GLN:O	1.45	1.11
1:D:71:GLN:HG3	1:E:203:ASN:HB3	1.34	1.10
1:A:84:SER:HB3	1:A:86:THR:HG22	1.32	1.10
1:B:336:VAL:HA	1:B:337:GLN:N	1.66	1.10
1:E:193:ILE:HG12	1:E:201:MET:HE3	1.29	1.10
1:C:71:GLN:HG3	1:D:203:ASN:HB3	1.33	1.09
1:B:175:GLN:HB2	1:B:230:ASP:HB2	1.35	1.08
1:C:341:MET:HE1	1:C:347:GLN:HB2	1.31	1.08
1:A:71:GLN:HG3	1:B:203:ASN:HB3	1.36	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:168:GLY:HA3	1:F:237:THR:HG23	1.38	1.06
1:F:175:GLN:HB2	1:F:230:ASP:HB2	1.33	1.05
1:F:341:MET:HE1	1:F:347:GLN:HB2	1.38	1.05
1:A:328:LEU:CD1	1:A:333:LEU:CD2	2.34	1.05
1:A:328:LEU:HG	1:A:332:MET:HE2	1.35	1.04
1:A:336:VAL:CG2	1:A:337:GLN:N	1.95	1.04
1:D:336:VAL:CA	1:D:337:GLN:OE1	2.05	1.04
1:E:121:GLU:HG3	1:E:313:ARG:HD3	1.40	1.04
1:A:336:VAL:HG21	1:A:337:GLN:HA	1.34	1.03
1:A:328:LEU:CD1	1:A:333:LEU:HD23	1.87	1.03
1:D:336:VAL:C	1:D:337:GLN:OE1	2.01	1.03
1:B:177:LEU:HD13	1:B:207:VAL:O	1.57	1.01
1:C:168:GLY:HA3	1:C:237:THR:HG23	1.40	1.00
1:B:54:ASN:HD21	1:C:208:LEU:H	1.08	1.00
1:C:350:GLU:HG3	1:F:233:LYS:HG2	1.43	1.00
1:A:208:LEU:H	1:E:54:ASN:HD21	1.09	0.98
1:B:257:ASN:HD22	1:B:257:ASN:H	1.02	0.98
1:B:71:GLN:HG3	1:C:203:ASN:HB3	1.45	0.97
1:D:336:VAL:HA	1:D:337:GLN:OE1	1.63	0.96
1:A:328:LEU:HD11	1:A:333:LEU:HD23	0.95	0.95
1:F:205:ASP:HA	1:F:209:ASN:HB2	1.48	0.95
1:A:176:GLY:O	1:A:177:LEU:HD23	1.66	0.95
1:D:114:CYS:HB2	1:D:116:THR:HG22	1.49	0.94
1:D:192:THR:HB	1:D:194:LYS:HD3	1.50	0.94
1:D:346:THR:HG22	1:D:348:VAL:HB	1.47	0.94
1:A:251:PRO:HG2	1:B:245:GLY:HA3	1.50	0.94
1:E:305:TYR:HE1	1:E:307:LYS:HB2	1.34	0.93
1:F:192:THR:HB	1:F:194:LYS:HD3	1.49	0.93
1:A:69:GLY:HA3	1:A:71:GLN:HE22	1.35	0.92
1:B:30:ILE:HD13	1:B:36:VAL:HG13	1.48	0.92
1:A:372:ARG:HH11	1:A:372:ARG:HB2	1.33	0.92
1:A:341:MET:HE1	1:A:347:GLN:HB2	1.50	0.92
1:B:336:VAL:O	1:B:337:GLN:HA	1.70	0.91
1:A:328:LEU:CG	1:A:333:LEU:HD21	1.99	0.91
1:F:175:GLN:HG2	1:F:213:LYS:HD3	1.49	0.91
1:B:346:THR:CG2	1:B:348:VAL:HG12	2.01	0.91
1:A:328:LEU:CG	1:A:332:MET:CE	2.38	0.90
1:B:346:THR:HG21	1:B:348:VAL:HG12	1.50	0.90
1:F:122:ALA:HB3	1:F:271:PRO:HD2	1.50	0.90
1:D:138:VAL:HB	1:D:153:ILE:HD12	1.54	0.90
1:A:308:ILE:HG22	1:A:310:LEU:HD12	1.52	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:PRO:HB2	1:F:360:VAL:HG23	1.52	0.89
1:B:79:ILE:HD11	1:B:298:HIS:HA	1.52	0.89
1:B:192:THR:HB	1:B:194:LYS:HG2	1.55	0.89
1:E:258:THR:HB	1:E:259:LEU:HD22	1.55	0.89
1:F:177:LEU:HD13	1:F:207:VAL:O	1.73	0.89
1:F:258:THR:HB	1:F:259:LEU:HD13	1.52	0.89
1:F:262:VAL:HG12	1:F:264:LEU:H	1.37	0.89
1:B:262:VAL:HG12	1:B:264:LEU:H	1.38	0.88
1:D:168:GLY:HA3	1:D:237:THR:HG23	1.54	0.88
1:C:138:VAL:HB	1:C:153:ILE:HG23	1.51	0.88
1:B:177:LEU:HD21	1:B:208:LEU:HA	1.54	0.88
1:C:50:GLU:CD	1:D:233:LYS:HA	1.98	0.88
1:D:19:CYS:SG	1:E:112:LEU:HD22	2.14	0.88
1:A:328:LEU:HG	1:A:332:MET:CE	2.02	0.88
1:B:233:LYS:HG2	1:B:234:ASN:N	1.89	0.87
1:C:62:THR:OG1	1:C:63:PRO:HD3	1.73	0.87
1:E:342:GLU:N	1:E:346:THR:HG23	1.89	0.87
1:A:328:LEU:HD21	1:A:333:LEU:CG	2.04	0.87
1:F:104:GLN:HE22	1:F:276:GLU:HB2	1.37	0.87
1:A:141:PHE:CE1	1:A:292:ARG:HG3	2.10	0.87
1:F:90:PRO:HB3	1:F:95:LEU:HD11	1.56	0.87
1:D:218:LYS:O	1:D:219:ASP:HB3	1.73	0.86
1:F:30:ILE:HD13	1:F:36:VAL:HG13	1.57	0.86
1:A:328:LEU:CD2	1:A:328:LEU:O	2.24	0.86
1:C:172:LEU:HD22	1:C:173:ASP:N	1.91	0.86
1:C:350:GLU:HB3	1:F:233:LYS:HB3	1.55	0.86
1:B:141:PHE:HE1	1:B:144:PRO:HG3	1.40	0.86
1:E:62:THR:OG1	1:E:63:PRO:HD3	1.76	0.85
1:A:83:THR:HB	1:A:87:GLU:HB3	1.56	0.85
1:C:191:VAL:HG21	1:C:222:TYR:CD2	2.10	0.85
1:A:340:PRO:HG2	1:A:347:GLN:HE22	1.42	0.85
1:E:112:LEU:HB3	1:E:116:THR:HG23	1.55	0.85
1:A:328:LEU:CD1	1:A:333:LEU:HD21	2.04	0.85
1:F:288:TRP:HZ3	1:F:299:TRP:CE2	1.95	0.84
1:A:192:THR:HG22	1:A:193:ILE:CD1	2.07	0.84
1:C:97:THR:HA	1:C:223:PRO:HA	1.59	0.84
1:B:97:THR:HA	1:B:223:PRO:HA	1.59	0.84
1:A:163:HIS:HA	1:A:283:VAL:O	1.75	0.84
1:A:233:LYS:HA	1:E:50:GLU:HG2	1.57	0.84
1:B:117:LEU:HD12	1:B:117:LEU:H	1.40	0.84
1:D:57:MET:HE3	1:D:96:PRO:HB3	1.57	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:111:ASP:HB3	1:F:116:THR:HG22	1.59	0.84
1:F:172:LEU:HD22	1:F:173:ASP:N	1.93	0.84
1:F:233:LYS:HE2	1:F:234:ASN:ND2	1.93	0.84
1:E:117:LEU:HD13	1:E:118:GLN:H	1.42	0.84
1:D:292:ARG:HH11	1:D:292:ARG:HB3	1.41	0.83
1:F:286:MET:HA	1:F:286:MET:HE3	1.60	0.83
1:C:192:THR:HB	1:C:194:LYS:HD3	1.58	0.83
1:E:141:PHE:CE1	1:E:292:ARG:HG3	2.12	0.83
1:E:253:LEU:HD23	1:E:254:GLN:H	1.42	0.83
1:E:286:MET:HA	1:E:286:MET:HE3	1.60	0.83
1:A:103:LEU:HB2	1:A:278:LEU:HB3	1.60	0.83
1:E:122:ALA:HB3	1:E:271:PRO:HD2	1.59	0.83
1:B:308:ILE:N	1:B:308:ILE:HD12	1.94	0.83
1:A:192:THR:HG22	1:A:193:ILE:HD12	1.60	0.83
1:E:83:THR:HB	1:E:87:GLU:HB3	1.59	0.83
1:C:193:ILE:HG12	1:C:201:MET:HE3	1.60	0.83
1:E:175:GLN:HG3	1:E:213:LYS:HG2	1.60	0.83
1:E:288:TRP:HB3	1:E:299:TRP:HB3	1.57	0.83
1:E:222:TYR:HB3	1:E:227:TRP:CD1	2.14	0.83
1:F:97:THR:HA	1:F:223:PRO:HA	1.61	0.83
1:B:328:LEU:O	1:B:332:MET:SD	2.37	0.82
1:C:308:ILE:H	1:C:308:ILE:HD12	1.44	0.82
1:E:91:GLY:H	1:E:186:LYS:HE3	1.43	0.82
1:E:142:ASN:O	1:E:292:ARG:HG2	1.78	0.82
1:A:262:VAL:HG12	1:A:264:LEU:H	1.42	0.82
1:D:286:MET:HA	1:D:286:MET:CE	2.10	0.82
1:E:163:HIS:HA	1:E:283:VAL:O	1.79	0.82
1:B:177:LEU:CD1	1:B:207:VAL:O	2.27	0.82
1:C:233:LYS:NZ	1:F:350:GLU:HG2	1.95	0.82
1:D:257:ASN:HB3	1:E:239:TYR:CE2	2.14	0.82
1:A:336:VAL:HG23	1:A:337:GLN:CB	2.09	0.82
1:B:71:GLN:HE21	1:B:73:TYR:HB2	1.44	0.81
1:F:65:SER:HB3	1:F:68:GLU:HG2	1.62	0.81
1:A:138:VAL:HB	1:A:153:ILE:HG23	1.63	0.81
1:B:258:THR:HB	1:B:259:LEU:HD22	1.60	0.81
1:C:208:LEU:O	1:C:210:PRO:HD3	1.81	0.81
1:D:114:CYS:HB2	1:D:116:THR:CG2	2.09	0.81
1:B:286:MET:HA	1:B:286:MET:HE3	1.63	0.81
1:F:138:VAL:HB	1:F:153:ILE:HG23	1.59	0.81
1:A:122:ALA:HA	1:A:310:LEU:HB3	1.62	0.81
1:B:186:LYS:H	1:B:186:LYS:HE2	1.45	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:161:GLN:HE22	1:F:251:PRO:HA	1.45	0.81
1:B:193:ILE:HG12	1:B:201:MET:HE3	1.62	0.81
1:C:144:PRO:HD3	1:C:292:ARG:HG2	1.63	0.81
1:B:22:PRO:HG2	1:F:359:PRO:HB3	1.62	0.81
1:B:54:ASN:ND2	1:C:207:VAL:HB	1.95	0.81
1:E:168:GLY:HA3	1:E:237:THR:HG23	1.60	0.81
1:F:30:ILE:HG12	1:F:31:LYS:N	1.94	0.80
1:F:57:MET:HB2	1:F:96:PRO:HB3	1.63	0.80
1:F:178:VAL:HG22	1:F:179:THR:H	1.47	0.80
1:E:82:ALA:HB1	1:E:88:ASP:HA	1.62	0.80
1:E:103:LEU:HB2	1:E:278:LEU:HB3	1.63	0.80
1:F:203:ASN:O	1:F:206:GLN:HB3	1.81	0.80
1:A:125:VAL:HG12	1:A:263:LEU:HD21	1.63	0.80
1:C:233:LYS:HD3	1:C:234:ASN:N	1.95	0.80
1:B:125:VAL:HB	1:B:263:LEU:HD11	1.63	0.80
1:C:336:VAL:O	1:C:337:GLN:HA	1.81	0.80
1:E:233:LYS:HD2	1:E:234:ASN:H	1.46	0.80
1:E:115:ASP:O	1:E:316:LYS:HA	1.82	0.80
1:C:175:GLN:HE21	1:C:176:GLY:N	1.80	0.80
1:B:304:ARG:HD3	1:B:306:PHE:CZ	2.17	0.80
1:B:276:GLU:HG2	1:C:370:VAL:HG21	1.64	0.79
1:A:90:PRO:HG2	1:A:185:TYR:HA	1.64	0.79
1:B:276:GLU:HG2	1:C:370:VAL:CG2	2.13	0.79
1:D:257:ASN:ND2	1:E:239:TYR:H	1.81	0.79
1:C:336:VAL:C	1:C:337:GLN:HA	2.07	0.79
1:E:75:TRP:CZ2	1:E:300:ARG:HD2	2.17	0.79
1:F:317:ASN:HD22	1:F:318:PRO:HD2	1.43	0.79
1:D:175:GLN:HB2	1:D:230:ASP:HB2	1.62	0.79
1:F:177:LEU:HD21	1:F:208:LEU:HA	1.64	0.79
1:B:296:VAL:HG11	2:H:3:SIA:H32	1.64	0.79
1:B:138:VAL:HB	1:B:153:ILE:HG23	1.63	0.79
1:E:265:ASP:H	1:E:270:GLY:H	1.27	0.79
1:D:186:LYS:H	1:D:186:LYS:HD2	1.47	0.79
1:F:76:SER:O	1:F:298:HIS:HB2	1.83	0.79
1:F:308:ILE:HD12	1:F:308:ILE:N	1.98	0.79
1:B:34:MET:O	1:B:37:LEU:HB2	1.83	0.79
1:C:126:LYS:HG3	1:C:260:THR:HG23	1.62	0.79
1:C:163:HIS:HA	1:C:283:VAL:O	1.81	0.79
1:A:135:LEU:HD12	1:A:135:LEU:N	1.97	0.78
1:A:193:ILE:HG12	1:A:201:MET:HE3	1.62	0.78
1:D:153:ILE:HG12	1:E:297:HIS:ND1	1.99	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:55:PRO:O	1:E:56:ARG:HG3	1.83	0.78
1:E:350:GLU:HG2	1:E:351:VAL:N	1.97	0.78
1:D:262:VAL:HG12	1:D:264:LEU:H	1.48	0.78
1:E:259:LEU:HD22	1:E:259:LEU:N	1.98	0.78
1:B:77:ARG:HB2	1:B:93:ASN:HB2	1.66	0.78
1:D:71:GLN:HG3	1:E:203:ASN:CB	2.13	0.78
1:F:144:PRO:HD3	1:F:292:ARG:HG2	1.64	0.78
1:B:257:ASN:H	1:B:257:ASN:ND2	1.76	0.78
1:D:346:THR:CG2	1:D:348:VAL:HB	2.14	0.78
1:B:251:PRO:HD2	1:C:245:GLY:HA3	1.65	0.78
1:D:168:GLY:CA	1:D:237:THR:HG23	2.12	0.78
1:D:342:GLU:N	1:D:346:THR:HG23	1.99	0.78
1:A:41:THR:O	1:A:45:SER:HB3	1.83	0.78
1:A:52:PHE:CE2	1:B:208:LEU:HD22	2.19	0.78
1:D:180:ASP:OD2	1:D:182:ARG:HD3	1.83	0.78
1:A:180:ASP:HA	1:A:206:GLN:HE21	1.46	0.78
1:A:203:ASN:CB	1:E:71:GLN:HG3	2.07	0.78
1:D:96:PRO:HD3	1:D:299:TRP:CZ3	2.19	0.78
1:F:34:MET:O	1:F:37:LEU:HB2	1.83	0.78
1:D:71:GLN:CG	1:E:203:ASN:HB3	2.12	0.77
1:B:332:MET:SD	1:B:332:MET:N	2.57	0.77
1:D:304:ARG:HD3	1:D:306:PHE:CZ	2.19	0.77
1:A:198:LYS:N	1:A:198:LYS:HE2	1.99	0.77
1:B:186:LYS:HE2	1:B:186:LYS:N	1.99	0.77
1:C:308:ILE:HD12	1:C:308:ILE:N	2.00	0.77
1:B:103:LEU:HD22	1:F:341:MET:HG3	1.67	0.77
1:A:328:LEU:HD11	1:A:332:MET:HE1	1.62	0.77
1:C:350:GLU:CB	1:F:233:LYS:HB3	2.13	0.77
1:D:122:ALA:HB3	1:D:271:PRO:HD2	1.64	0.77
1:E:233:LYS:HD3	1:E:234:ASN:ND2	1.99	0.77
1:F:81:LEU:HG	1:F:82:ALA:H	1.50	0.77
1:C:256:THR:HA	1:D:239:TYR:CE1	2.20	0.77
1:B:203:ASN:O	1:B:206:GLN:HB3	1.83	0.77
1:F:288:TRP:HZ3	1:F:299:TRP:CD2	2.02	0.77
1:A:350:GLU:HG2	1:A:351:VAL:N	2.00	0.76
1:B:208:LEU:O	1:B:210:PRO:HD3	1.86	0.76
1:A:76:SER:O	1:A:298:HIS:HB3	1.85	0.76
1:E:90:PRO:HD2	1:E:186:LYS:NZ	2.01	0.76
1:C:142:ASN:HD21	1:C:289:ARG:HG3	1.51	0.76
1:A:239:TYR:CD1	1:E:257:ASN:HB2	2.20	0.76
1:F:182:ARG:HG3	1:F:183:THR:H	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:259:LEU:HD22	1:F:259:LEU:H	1.50	0.76
1:A:336:VAL:HG23	1:A:337:GLN:HA	0.80	0.76
1:F:208:LEU:O	1:F:210:PRO:HD3	1.85	0.76
1:C:304:ARG:HD3	1:C:306:PHE:CZ	2.21	0.76
1:A:257:ASN:ND2	1:B:238:ARG:HA	2.00	0.76
1:A:87:GLU:HA	1:A:184:LYS:NZ	1.99	0.76
1:A:170:GLU:HB2	1:A:171:PRO:HD2	1.67	0.76
1:B:117:LEU:HD12	1:B:117:LEU:N	2.00	0.76
1:B:194:LYS:HG3	1:B:195:THR:H	1.50	0.76
1:D:62:THR:OG1	1:D:63:PRO:HD3	1.86	0.76
1:E:255:PHE:O	1:E:256:THR:HB	1.86	0.76
1:A:233:LYS:HG3	1:A:234:ASN:N	2.01	0.76
1:E:186:LYS:HE2	1:E:186:LYS:N	2.01	0.76
1:C:175:GLN:HE21	1:C:176:GLY:H	1.34	0.75
1:B:192:THR:HB	1:B:194:LYS:CG	2.15	0.75
1:C:256:THR:HA	1:D:239:TYR:HE1	1.51	0.75
1:E:233:LYS:HD2	1:E:234:ASN:N	2.01	0.75
1:C:125:VAL:HB	1:C:263:LEU:HD11	1.69	0.75
1:C:197:THR:O	1:C:199:LYS:HE3	1.86	0.75
1:C:175:GLN:OE1	1:C:208:LEU:HD11	1.86	0.75
1:D:143:LYS:HA	1:D:292:ARG:HG2	1.67	0.75
1:D:164:VAL:CG2	1:D:241:GLY:HA3	2.17	0.75
1:F:122:ALA:HA	1:F:310:LEU:HB3	1.68	0.75
1:E:177:LEU:CD2	1:E:206:GLN:O	2.32	0.75
1:F:150:THR:O	1:F:150:THR:HG22	1.85	0.75
1:C:175:GLN:HB2	1:C:230:ASP:HB2	1.68	0.75
1:F:238:ARG:NH2	1:F:265:ASP:HB3	2.01	0.75
1:A:328:LEU:HD21	1:A:333:LEU:HD21	0.76	0.75
1:C:181:ALA:H	1:C:206:GLN:NE2	1.85	0.75
1:C:257:ASN:H	1:C:257:ASN:HD22	1.32	0.75
1:E:243:TYR:CZ	1:E:245:GLY:HA2	2.22	0.75
1:A:313:ARG:HD3	1:E:23:ALA:HB2	1.68	0.74
1:B:192:THR:HG22	1:B:193:ILE:CD1	2.16	0.74
1:D:211:ILE:HD12	1:D:211:ILE:N	2.01	0.74
1:F:130:VAL:HG23	1:F:303:PRO:HG2	1.68	0.74
1:B:25:VAL:HG21	1:F:360:VAL:HG13	1.69	0.74
1:B:198:LYS:H	1:B:198:LYS:CE	2.01	0.74
1:C:257:ASN:HD21	1:D:239:TYR:H	1.35	0.74
1:C:103:LEU:HB2	1:C:278:LEU:HB3	1.68	0.74
1:F:108:LEU:HB3	1:F:118:GLN:HE21	1.52	0.74
1:F:269:VAL:HG12	1:F:270:GLY:O	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:LEU:HD22	1:B:259:LEU:N	2.02	0.74
1:B:104:GLN:HE22	1:B:276:GLU:HB2	1.52	0.74
1:A:71:GLN:HG3	1:B:203:ASN:CB	2.16	0.74
1:A:71:GLN:CG	1:B:203:ASN:HB3	2.16	0.74
1:A:336:VAL:CG2	1:A:337:GLN:H	2.00	0.74
1:F:125:VAL:CG1	1:F:263:LEU:HD21	2.18	0.74
1:C:142:ASN:C	1:C:292:ARG:HB2	2.13	0.74
1:D:164:VAL:HG22	1:D:241:GLY:HA3	1.69	0.74
1:A:84:SER:HB3	1:A:86:THR:CG2	2.17	0.73
1:A:298:HIS:CD2	1:A:298:HIS:H	2.03	0.73
1:F:321:MET:O	1:F:324:LEU:HG	1.89	0.73
1:A:175:GLN:HG2	1:A:212:SER:O	1.89	0.73
1:A:328:LEU:HD23	1:A:328:LEU:C	2.13	0.73
1:A:50:GLU:HG2	1:B:233:LYS:HA	1.70	0.73
1:D:178:VAL:HG22	1:D:179:THR:N	2.02	0.73
1:D:265:ASP:H	1:D:270:GLY:H	1.36	0.73
1:F:238:ARG:HH21	1:F:265:ASP:HB3	1.54	0.73
1:B:272:LEU:N	1:B:272:LEU:HD12	2.02	0.73
1:C:138:VAL:HB	1:C:153:ILE:CG2	2.19	0.73
1:E:335:GLN:OE1	1:E:335:GLN:HA	1.87	0.73
1:F:62:THR:OG1	1:F:63:PRO:HD3	1.88	0.73
1:A:278:LEU:HD22	1:A:280:LEU:CD2	2.18	0.73
1:A:328:LEU:HD12	1:A:332:MET:HE1	0.73	0.73
1:B:162:TYR:HB3	1:B:285:ILE:HD13	1.69	0.73
1:C:28:LEU:HD23	1:C:29:LEU:N	2.03	0.73
1:C:352:ARG:NH2	1:F:233:LYS:O	2.22	0.73
1:E:135:LEU:HD12	1:E:157:VAL:HG21	1.71	0.73
1:A:257:ASN:HD22	1:B:239:TYR:H	1.34	0.72
1:C:100:MET:SD	1:C:100:MET:C	2.72	0.72
1:A:175:GLN:CB	1:A:230:ASP:HB2	2.19	0.72
1:A:306:PHE:HB3	1:A:308:ILE:HD11	1.71	0.72
1:D:141:PHE:CE1	1:D:292:ARG:HG3	2.24	0.72
1:E:313:ARG:HH11	1:E:313:ARG:CG	2.02	0.72
1:A:192:THR:HB	1:A:194:LYS:HE2	1.70	0.72
1:B:75:TRP:NE1	1:B:300:ARG:HB2	2.03	0.72
1:E:209:ASN:OD1	1:E:211:ILE:HD13	1.90	0.72
1:F:163:HIS:HA	1:F:283:VAL:O	1.88	0.72
1:A:57:MET:SD	1:A:301:GLY:HA3	2.29	0.72
1:C:50:GLU:OE2	1:D:233:LYS:HA	1.90	0.72
1:A:304:ARG:HD3	1:A:306:PHE:CZ	2.25	0.71
1:E:121:GLU:HG3	1:E:313:ARG:CD	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:144:PRO:HD3	1:E:292:ARG:HD3	1.71	0.71
1:B:125:VAL:HG12	1:B:263:LEU:HD21	1.72	0.71
1:E:228:HIS:HB3	1:E:229:PRO:HD2	1.72	0.71
1:F:288:TRP:HE3	1:F:299:TRP:HB3	1.55	0.71
1:B:50:GLU:HG2	1:C:233:LYS:HA	1.72	0.71
1:C:141:PHE:CE1	1:C:292:ARG:HG3	2.25	0.71
1:D:72:TYR:HE2	1:D:77:ARG:HH21	1.38	0.71
1:F:161:GLN:HE22	1:F:251:PRO:CA	2.03	0.71
1:A:240:PHE:N	1:A:240:PHE:CD1	2.57	0.71
1:D:240:PHE:CD1	1:D:240:PHE:N	2.57	0.71
1:E:177:LEU:HD23	1:E:178:VAL:N	2.05	0.71
1:B:265:ASP:H	1:B:270:GLY:H	1.37	0.71
1:A:62:THR:OG1	1:A:63:PRO:HD3	1.89	0.71
1:A:327:SER:O	1:A:329:PHE:N	2.24	0.71
1:B:30:ILE:HG12	1:B:31:LYS:N	2.06	0.71
1:B:217:ASP:O	1:F:336:VAL:HG13	1.91	0.71
1:C:55:PRO:HD3	1:C:303:PRO:CA	2.21	0.71
1:A:308:ILE:HD12	1:A:308:ILE:N	2.05	0.71
1:B:341:MET:C	1:B:346:THR:HG23	2.16	0.71
1:E:240:PHE:N	1:E:240:PHE:CD1	2.59	0.71
1:B:161:GLN:HE22	1:B:251:PRO:HA	1.56	0.70
1:A:265:ASP:H	1:A:270:GLY:H	1.37	0.70
1:E:317:ASN:HD22	1:E:318:PRO:HD2	1.54	0.70
1:F:287:GLY:O	1:F:299:TRP:HB2	1.91	0.70
1:B:141:PHE:CE1	1:B:292:ARG:HG3	2.27	0.70
1:B:222:TYR:HB3	1:B:227:TRP:CD1	2.26	0.70
1:C:108:LEU:HD11	1:C:120:TRP:CE2	2.27	0.70
1:F:209:ASN:ND2	1:F:211:ILE:HB	2.06	0.70
1:B:256:THR:HG23	1:B:258:THR:H	1.56	0.70
1:C:53:LEU:HD21	1:C:306:PHE:CE1	2.26	0.70
1:D:100:MET:HG3	1:D:219:ASP:HB2	1.73	0.70
1:D:209:ASN:OD1	1:D:211:ILE:HD13	1.92	0.70
1:A:39:LEU:HD12	1:A:40:VAL:H	1.56	0.70
1:B:275:GLY:C	1:B:277:GLY:H	1.99	0.70
1:F:83:THR:HB	1:F:87:GLU:HB3	1.73	0.70
1:A:84:SER:HA	1:E:141:PHE:CD2	2.27	0.70
1:D:269:VAL:HG12	1:D:270:GLY:O	1.91	0.70
1:A:124:SER:HA	1:A:263:LEU:HG	1.73	0.69
1:B:163:HIS:HA	1:B:283:VAL:O	1.92	0.69
1:D:28:LEU:HG	1:D:29:LEU:N	2.06	0.69
1:D:205:ASP:HA	1:D:209:ASN:HB2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:GLU:HG2	1:C:271:PRO:O	1.92	0.69
1:C:180:ASP:OD2	1:C:182:ARG:HD3	1.92	0.69
1:C:288:TRP:HA	1:C:299:TRP:HA	1.73	0.69
1:B:380:PHE:HD1	1:B:380:PHE:H	1.39	0.69
1:C:79:ILE:HB	1:C:297:HIS:O	1.92	0.69
1:E:88:ASP:H	1:E:184:LYS:HD3	1.57	0.69
1:E:208:LEU:O	1:E:208:LEU:HD23	1.92	0.69
1:B:324:LEU:H	1:B:324:LEU:HD22	1.57	0.69
1:C:52:PHE:CE2	1:D:208:LEU:HD22	2.27	0.69
1:C:55:PRO:HD3	1:C:303:PRO:HA	1.74	0.69
1:C:265:ASP:HB3	1:C:270:GLY:H	1.56	0.69
1:F:288:TRP:HA	1:F:299:TRP:HB3	1.73	0.69
1:F:320:PRO:O	1:F:323:SER:HB3	1.92	0.69
1:A:82:ALA:HB1	1:A:87:GLU:O	1.92	0.69
1:B:192:THR:HG22	1:B:193:ILE:HD12	1.74	0.69
1:E:178:VAL:HG22	1:E:179:THR:N	2.06	0.69
1:B:168:GLY:HA3	1:B:237:THR:HG23	1.74	0.69
1:B:232:ALA:HB3	1:B:234:ASN:O	1.91	0.69
1:B:342:GLU:HG2	1:B:343:GLY:N	2.06	0.69
1:B:371:ASP:C	1:B:373:PHE:H	1.99	0.69
1:C:76:SER:HG	1:C:299:TRP:HE3	1.40	0.69
1:C:104:GLN:HE22	1:C:276:GLU:HB2	1.58	0.69
1:C:174:LEU:N	1:C:174:LEU:HD12	2.07	0.69
1:C:191:VAL:HG21	1:C:222:TYR:CG	2.28	0.69
1:C:273:CYS:HB3	1:C:277:GLY:O	1.92	0.69
1:D:39:LEU:HD12	1:D:40:VAL:N	2.08	0.69
1:E:88:ASP:O	1:E:184:LYS:HB2	1.93	0.69
1:E:145:THR:HB	1:E:152:GLY:HA3	1.73	0.69
1:E:245:GLY:O	1:E:249:THR:HG21	1.93	0.69
1:E:285:ILE:N	1:E:285:ILE:HD12	2.08	0.69
1:F:168:GLY:CA	1:F:237:THR:HG23	2.20	0.69
1:A:298:HIS:CD2	1:A:298:HIS:N	2.61	0.69
1:C:174:LEU:HD23	1:C:227:TRP:HB3	1.73	0.69
1:D:208:LEU:O	1:D:208:LEU:HD23	1.93	0.69
1:A:336:VAL:CB	1:A:337:GLN:CA	2.71	0.69
1:B:105:LEU:HB2	1:B:276:GLU:O	1.92	0.69
1:C:100:MET:SD	1:C:101:ALA:N	2.66	0.69
1:C:108:LEU:HD11	1:C:120:TRP:NE1	2.08	0.69
1:D:192:THR:HG21	1:D:194:LYS:HE2	1.75	0.69
1:E:272:LEU:N	1:E:272:LEU:HD12	2.07	0.69
1:F:265:ASP:OD1	1:F:269:VAL:HB	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:317:ASN:ND2	1:F:318:PRO:HD2	2.08	0.69
1:A:79:ILE:HD11	1:A:298:HIS:HA	1.74	0.68
1:A:126:LYS:HG2	1:A:260:THR:HA	1.74	0.68
1:A:297:HIS:HE1	1:E:145:THR:HG21	1.58	0.68
1:A:328:LEU:CG	1:A:333:LEU:CD2	2.64	0.68
1:D:106:PRO:HD2	1:D:120:TRP:HE1	1.58	0.68
1:E:150:THR:O	1:E:150:THR:HG22	1.93	0.68
1:F:161:GLN:NE2	1:F:251:PRO:HA	2.06	0.68
1:C:209:ASN:OD1	1:C:211:ILE:HD13	1.92	0.68
1:D:112:LEU:H	1:D:112:LEU:HD12	1.57	0.68
1:E:125:VAL:HA	1:E:307:LYS:O	1.93	0.68
1:F:104:GLN:HE21	1:F:105:LEU:N	1.91	0.68
1:F:180:ASP:HB3	1:F:182:ARG:CG	2.23	0.68
1:A:197:THR:C	1:A:198:LYS:HG2	2.19	0.68
1:B:177:LEU:HD21	1:B:208:LEU:CA	2.23	0.68
1:D:83:THR:O	1:D:84:SER:HB2	1.92	0.68
1:D:340:PRO:HG2	1:D:347:GLN:HG3	1.75	0.68
1:B:161:GLN:OE1	1:B:251:PRO:HA	1.94	0.68
1:E:77:ARG:O	1:E:298:HIS:HB3	1.93	0.68
1:F:19:CYS:HB3	1:F:20:PRO:HD2	1.76	0.68
1:F:185:TYR:HB2	1:F:194:LYS:HE2	1.74	0.68
1:A:204:LYS:O	1:A:209:ASN:HB2	1.94	0.68
1:B:25:VAL:CG2	1:F:360:VAL:HG13	2.24	0.68
1:B:291:THR:HB	1:B:293:ASN:HB3	1.76	0.68
1:D:108:LEU:HB3	1:D:118:GLN:HE21	1.59	0.68
1:D:251:PRO:HD2	1:E:245:GLY:HA3	1.75	0.68
1:C:115:ASP:O	1:C:317:ASN:HB2	1.94	0.68
1:D:193:ILE:N	1:D:193:ILE:HD12	2.08	0.68
1:E:105:LEU:N	1:E:105:LEU:HD12	2.09	0.68
1:A:50:GLU:HA	1:A:306:PHE:O	1.94	0.68
1:A:105:LEU:HB3	1:A:120:TRP:NE1	2.08	0.68
1:A:184:LYS:N	1:A:184:LYS:HD2	2.08	0.68
1:C:360:VAL:HG12	1:C:361:PRO:HD2	1.76	0.68
1:D:54:ASN:HD21	1:E:208:LEU:CB	2.07	0.68
1:E:71:GLN:NE2	1:E:73:TYR:HB2	2.08	0.68
1:F:308:ILE:HD12	1:F:308:ILE:H	1.57	0.68
1:F:259:LEU:HD13	1:F:259:LEU:N	2.08	0.68
1:D:97:THR:HG22	1:D:222:TYR:C	2.18	0.68
1:E:305:TYR:CE1	1:E:307:LYS:HB2	2.23	0.68
1:C:105:LEU:N	1:C:105:LEU:HD12	2.09	0.67
1:C:313:ARG:HG2	1:C:314:TRP:N	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:ASN:O	1:D:151:LYS:HE2	1.92	0.67
1:D:177:LEU:HD23	1:D:178:VAL:N	2.09	0.67
1:F:240:PHE:N	1:F:240:PHE:CD1	2.56	0.67
1:A:56:ARG:NH1	1:A:56:ARG:HB2	2.09	0.67
1:A:328:LEU:CD1	1:A:332:MET:HE2	1.97	0.67
1:A:369:TYR:N	1:A:369:TYR:CD1	2.62	0.67
1:B:76:SER:OG	1:B:299:TRP:CE3	2.44	0.67
1:D:185:TYR:HB2	1:D:194:LYS:HE2	1.76	0.67
1:F:178:VAL:HG22	1:F:179:THR:N	2.07	0.67
1:D:193:ILE:HD11	1:D:201:MET:SD	2.34	0.67
1:A:52:PHE:CZ	1:B:208:LEU:HD22	2.29	0.67
1:E:194:LYS:H	1:E:194:LYS:HD2	1.60	0.67
1:A:39:LEU:HD12	1:A:40:VAL:N	2.10	0.67
1:B:257:ASN:HD22	1:B:257:ASN:N	1.84	0.67
1:B:275:GLY:O	1:B:277:GLY:N	2.28	0.67
1:C:263:LEU:O	1:C:270:GLY:HA2	1.95	0.67
1:E:117:LEU:HD13	1:E:118:GLN:N	2.10	0.67
1:A:141:PHE:CD2	1:B:84:SER:HA	2.30	0.67
1:D:30:ILE:CD1	1:D:36:VAL:HG13	2.25	0.67
1:D:76:SER:OG	1:D:299:TRP:HB2	1.94	0.67
1:E:194:LYS:HD3	1:E:195:THR:H	1.60	0.67
1:B:178:VAL:HG22	1:B:179:THR:N	2.09	0.67
1:C:240:PHE:N	1:C:240:PHE:CD1	2.61	0.67
1:C:300:ARG:HH21	1:D:177:LEU:HD21	1.58	0.67
1:E:109:ASN:HD22	1:E:110:GLU:H	1.43	0.67
1:A:243:TYR:HE2	1:E:251:PRO:HB2	1.60	0.67
1:C:191:VAL:CG2	1:C:222:TYR:HA	2.24	0.67
1:D:193:ILE:CD1	1:D:201:MET:SD	2.83	0.67
1:D:285:ILE:HD12	1:D:285:ILE:N	2.10	0.67
1:E:90:PRO:HB3	1:E:95:LEU:HD11	1.75	0.67
1:E:320:PRO:HG2	1:E:323:SER:CB	2.25	0.67
1:A:69:GLY:CA	1:A:71:GLN:HE22	2.05	0.67
1:A:328:LEU:CD2	1:A:333:LEU:CD2	2.30	0.67
1:D:30:ILE:HD13	1:D:36:VAL:HG13	1.76	0.67
1:A:203:ASN:HB3	1:E:71:GLN:CG	2.11	0.66
1:E:138:VAL:HB	1:E:153:ILE:HG23	1.75	0.66
1:E:169:GLY:HA3	1:E:272:LEU:O	1.95	0.66
1:E:194:LYS:HA	1:E:197:THR:O	1.95	0.66
1:F:288:TRP:CZ3	1:F:299:TRP:CD2	2.82	0.66
1:B:30:ILE:CD1	1:B:36:VAL:HG13	2.23	0.66
1:B:71:GLN:HG3	1:C:203:ASN:CB	2.23	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:SER:HA	1:B:261:THR:O	1.95	0.66
1:B:269:VAL:HA	1:B:313:ARG:NH2	2.11	0.66
1:D:318:PRO:HG2	1:D:319:TYR:CD2	2.30	0.66
1:B:105:LEU:HB3	1:B:120:TRP:CD1	2.31	0.66
1:E:109:ASN:OD1	1:E:117:LEU:HA	1.96	0.66
1:E:191:VAL:HG23	1:E:221:MET:HG3	1.77	0.66
1:B:265:ASP:HB3	1:B:270:GLY:H	1.60	0.66
1:C:316:LYS:NZ	1:F:359:PRO:HD2	2.10	0.66
1:D:177:LEU:HD23	1:D:177:LEU:C	2.19	0.66
1:F:81:LEU:HG	1:F:82:ALA:N	2.10	0.66
1:C:105:LEU:HB3	1:C:120:TRP:CD1	2.29	0.66
1:B:161:GLN:NE2	1:B:251:PRO:HA	2.11	0.66
1:B:192:THR:HG23	1:B:226:ILE:HD13	1.77	0.66
1:D:192:THR:H	1:D:195:THR:CB	2.08	0.66
1:E:180:ASP:OD1	1:E:182:ARG:HG2	1.95	0.66
1:B:161:GLN:HE22	1:B:251:PRO:CA	2.08	0.66
1:B:177:LEU:HD22	1:B:207:VAL:C	2.20	0.66
1:C:82:ALA:HB1	1:C:88:ASP:HA	1.76	0.66
1:D:132:SER:O	1:D:135:LEU:HD23	1.96	0.66
1:F:150:THR:CG2	1:F:292:ARG:HH21	2.09	0.66
1:A:35:GLU:HG2	1:A:36:VAL:N	2.11	0.66
1:A:37:LEU:HD23	1:A:106:PRO:HD3	1.78	0.66
1:A:264:LEU:HD23	1:A:268:GLY:HA2	1.78	0.66
1:B:318:PRO:HG2	1:B:319:TYR:H	1.60	0.66
1:C:112:LEU:HD22	1:C:112:LEU:H	1.61	0.66
1:E:66:LEU:HD23	1:E:66:LEU:H	1.58	0.66
1:F:75:TRP:NE1	1:F:300:ARG:HB2	2.11	0.66
1:A:340:PRO:HG2	1:A:347:GLN:NE2	2.09	0.66
1:A:350:GLU:CG	1:A:351:VAL:N	2.58	0.66
1:B:164:VAL:HA	1:B:241:GLY:HA3	1.78	0.66
1:B:263:LEU:O	1:B:270:GLY:HA2	1.96	0.66
1:B:321:MET:HE1	1:F:324:LEU:HD11	1.78	0.66
1:A:97:THR:HA	1:A:223:PRO:HA	1.76	0.66
1:A:217:ASP:OD1	1:A:218:LYS:HD3	1.96	0.66
1:E:367:THR:HG22	1:E:368:ARG:N	2.09	0.66
1:F:92:ASN:OD1	1:F:186:LYS:HD2	1.96	0.66
1:A:57:MET:HB2	1:A:96:PRO:HB3	1.78	0.65
1:C:54:ASN:HD21	1:D:208:LEU:HB3	1.61	0.65
1:D:72:TYR:HE2	1:D:77:ARG:NH2	1.94	0.65
1:E:378:THR:HG22	1:E:379:VAL:O	1.94	0.65
1:F:30:ILE:HG23	1:F:36:VAL:HG13	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:ILE:HG13	1:A:297:HIS:HB2	1.79	0.65
1:A:208:LEU:N	1:E:54:ASN:HD21	1.89	0.65
1:C:172:LEU:HD22	1:C:173:ASP:H	1.61	0.65
1:E:118:GLN:HB2	1:E:314:TRP:CZ3	2.30	0.65
1:F:103:LEU:HB2	1:F:278:LEU:HB3	1.76	0.65
1:A:269:VAL:HG12	1:A:270:GLY:O	1.97	0.65
1:B:177:LEU:CD2	1:B:208:LEU:HA	2.24	0.65
1:B:273:CYS:HB3	1:B:277:GLY:O	1.96	0.65
1:E:112:LEU:O	1:E:116:THR:HG22	1.96	0.65
1:E:218:LYS:HD2	1:E:218:LYS:N	2.10	0.65
1:A:328:LEU:HD21	1:A:333:LEU:CD1	2.27	0.65
1:A:371:ASP:O	1:A:373:PHE:N	2.29	0.65
1:B:83:THR:HB	1:B:87:GLU:HB3	1.79	0.65
1:D:239:TYR:C	1:D:240:PHE:CD1	2.75	0.65
1:F:108:LEU:HD11	1:F:120:TRP:CZ2	2.32	0.65
1:A:30:ILE:HG12	1:A:36:VAL:HG13	1.79	0.65
1:A:175:GLN:HB3	1:A:230:ASP:HB2	1.78	0.65
1:D:172:LEU:HD22	1:D:173:ASP:N	2.10	0.65
1:E:82:ALA:CB	1:E:88:ASP:HA	2.26	0.65
1:F:177:LEU:CD2	1:F:208:LEU:HA	2.25	0.65
1:F:324:LEU:HD12	1:F:325:ILE:N	2.11	0.65
1:B:84:SER:O	1:B:86:THR:N	2.29	0.65
1:D:105:LEU:HB2	1:D:276:GLU:O	1.96	0.65
1:D:105:LEU:HD23	1:D:120:TRP:CG	2.32	0.65
1:F:177:LEU:HD22	1:F:205:ASP:O	1.97	0.65
1:A:88:ASP:H	1:A:184:LYS:HD3	1.62	0.65
1:A:135:LEU:N	1:A:135:LEU:CD1	2.58	0.65
1:B:50:GLU:CD	1:C:233:LYS:HB2	2.22	0.65
1:F:233:LYS:HE2	1:F:234:ASN:CG	2.21	0.65
1:A:239:TYR:CE1	1:E:257:ASN:HB2	2.31	0.65
1:D:216:LEU:O	1:D:218:LYS:N	2.29	0.65
1:F:72:TYR:O	1:F:75:TRP:HB2	1.97	0.65
1:F:318:PRO:HG2	1:F:319:TYR:CD2	2.32	0.65
1:A:108:LEU:HD11	1:A:120:TRP:CE2	2.31	0.65
1:A:369:TYR:N	1:A:369:TYR:HD1	1.94	0.65
1:C:126:LYS:HG3	1:C:260:THR:CG2	2.27	0.65
1:F:19:CYS:HB3	1:F:20:PRO:CD	2.27	0.65
1:F:233:LYS:HD3	1:F:234:ASN:N	2.12	0.65
1:B:209:ASN:OD1	1:B:211:ILE:HD13	1.98	0.64
1:B:255:PHE:O	1:B:256:THR:HB	1.95	0.64
1:B:308:ILE:HD12	1:B:308:ILE:H	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:ILE:HG12	1:C:201:MET:CE	2.27	0.64
1:E:175:GLN:HG2	1:E:212:SER:O	1.97	0.64
1:E:191:VAL:HA	1:E:195:THR:HG21	1.80	0.64
2:L:2:GAL:H3	2:L:3:SIA:O1B	1.96	0.64
1:A:194:LYS:HD3	1:A:195:THR:H	1.62	0.64
1:B:192:THR:HG23	1:B:226:ILE:CD1	2.27	0.64
1:D:32:GLY:HA3	1:D:36:VAL:CG2	2.27	0.64
1:E:217:ASP:C	1:E:218:LYS:HD2	2.22	0.64
1:F:90:PRO:HD2	1:F:184:LYS:O	1.97	0.64
1:F:288:TRP:HA	1:F:299:TRP:CB	2.27	0.64
1:B:278:LEU:HD23	1:B:279:TYR:N	2.12	0.64
1:D:265:ASP:CG	1:D:269:VAL:HB	2.22	0.64
1:B:194:LYS:HG3	1:B:195:THR:N	2.13	0.64
1:C:135:LEU:HD22	1:C:135:LEU:N	2.13	0.64
1:D:111:ASP:HB3	1:D:116:THR:HG23	1.78	0.64
1:D:327:SER:OG	1:D:328:LEU:N	2.30	0.64
1:A:174:LEU:HD13	1:A:227:TRP:HB3	1.80	0.64
1:A:231:PRO:HB2	1:E:305:TYR:CE2	2.33	0.64
1:C:233:LYS:HE2	1:F:352:ARG:NH1	2.13	0.64
1:E:317:ASN:ND2	1:E:318:PRO:HD2	2.12	0.64
1:F:306:PHE:N	1:F:306:PHE:CD1	2.63	0.64
1:A:117:LEU:HD22	1:A:317:ASN:HA	1.79	0.64
1:A:176:GLY:C	1:A:177:LEU:HD23	2.23	0.64
1:B:193:ILE:HG22	1:B:212:SER:HB3	1.80	0.64
1:D:322:ALA:O	1:D:325:ILE:HB	1.98	0.64
1:E:164:VAL:HA	1:E:241:GLY:HA3	1.80	0.64
1:E:304:ARG:HD3	1:E:306:PHE:CZ	2.33	0.64
1:A:319:TYR:N	1:A:320:PRO:HD2	2.12	0.64
1:B:76:SER:HG	1:B:299:TRP:HE3	1.40	0.64
1:B:211:ILE:HD12	1:B:211:ILE:N	2.13	0.64
1:F:108:LEU:HD11	1:F:120:TRP:CE2	2.33	0.64
1:F:218:LYS:HB2	1:F:222:TYR:CE1	2.33	0.64
1:B:29:LEU:HB3	1:B:30:ILE:HG22	1.80	0.64
1:C:211:ILE:N	1:C:211:ILE:HD12	2.12	0.64
1:D:97:THR:HA	1:D:223:PRO:HA	1.80	0.64
1:A:233:LYS:HG3	1:A:234:ASN:H	1.61	0.64
1:B:104:GLN:NE2	1:B:276:GLU:HB2	2.13	0.64
1:B:180:ASP:HB3	1:B:182:ARG:HG2	1.79	0.64
1:D:75:TRP:CE2	1:D:300:ARG:HD2	2.33	0.64
1:D:292:ARG:HB3	1:D:292:ARG:NH1	2.13	0.64
1:E:317:ASN:HD21	1:E:319:TYR:HB2	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:THR:O	1:A:198:LYS:HG2	1.99	0.63
1:B:240:PHE:N	1:B:240:PHE:CD1	2.65	0.63
1:C:84:SER:O	1:C:86:THR:N	2.31	0.63
1:C:71:GLN:NE2	1:C:71:GLN:HA	2.00	0.63
1:C:79:ILE:HD13	1:C:94:THR:HG23	1.79	0.63
1:C:194:LYS:O	1:C:198:LYS:N	2.30	0.63
1:F:111:ASP:HB3	1:F:116:THR:CG2	2.29	0.63
1:F:150:THR:HG21	1:F:292:ARG:NH2	2.13	0.63
1:A:232:ALA:HB3	1:A:234:ASN:O	1.97	0.63
1:A:328:LEU:CB	1:A:332:MET:HE2	2.28	0.63
1:B:54:ASN:HD21	1:C:207:VAL:HB	1.62	0.63
1:A:82:ALA:HB1	1:A:88:ASP:HA	1.81	0.63
1:A:265:ASP:CG	1:A:269:VAL:HB	2.23	0.63
1:A:380:PHE:CG	1:A:381:PRO:HD2	2.33	0.63
1:D:233:LYS:HG3	1:D:234:ASN:HD22	1.64	0.63
1:F:125:VAL:HG11	1:F:263:LEU:HD21	1.79	0.63
1:F:135:LEU:HD22	1:F:135:LEU:H	1.64	0.63
1:B:23:ALA:O	1:F:359:PRO:HA	1.98	0.63
1:C:256:THR:HB	1:D:240:PHE:HA	1.80	0.63
1:D:35:GLU:HG2	1:D:36:VAL:N	2.13	0.63
1:D:341:MET:SD	1:D:348:VAL:HG23	2.39	0.63
1:F:112:LEU:HD12	1:F:112:LEU:N	2.14	0.63
1:F:177:LEU:CD1	1:F:207:VAL:O	2.47	0.63
1:C:71:GLN:HE21	1:C:73:TYR:H	1.44	0.63
1:C:153:ILE:HD11	1:D:297:HIS:CG	2.34	0.63
1:D:103:LEU:N	1:D:103:LEU:HD22	2.13	0.63
1:F:272:LEU:HD12	1:F:272:LEU:N	2.13	0.63
1:F:288:TRP:CZ3	1:F:299:TRP:CE2	2.83	0.63
1:A:174:LEU:CD1	1:A:227:TRP:HB3	2.28	0.63
1:A:271:PRO:C	1:A:272:LEU:HD12	2.24	0.63
1:D:32:GLY:HA3	1:D:36:VAL:HG21	1.80	0.63
1:E:113:THR:C	1:E:115:ASP:H	2.07	0.63
1:F:79:ILE:HD13	1:F:94:THR:HG23	1.81	0.63
1:C:141:PHE:CD1	1:C:292:ARG:HG3	2.34	0.63
1:E:150:THR:CG2	1:E:292:ARG:HH21	2.12	0.63
1:F:62:THR:O	1:F:64:GLU:N	2.31	0.63
1:F:269:VAL:HA	1:F:313:ARG:HH21	1.64	0.63
1:C:39:LEU:HD12	1:C:40:VAL:H	1.63	0.63
1:D:257:ASN:HD22	1:E:239:TYR:H	1.44	0.63
1:E:166:ALA:HA	1:E:238:ARG:O	1.98	0.63
1:E:192:THR:HG22	1:E:193:ILE:HD12	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:228:HIS:HB3	1:F:229:PRO:HD2	1.79	0.63
1:C:265:ASP:CG	1:C:269:VAL:HB	2.23	0.62
1:A:34:MET:O	1:A:37:LEU:HD13	1.99	0.62
1:A:79:ILE:HA	1:A:94:THR:HG23	1.81	0.62
1:B:46:VAL:O	1:F:353:VAL:HA	1.98	0.62
1:B:71:GLN:HA	1:B:71:GLN:NE2	1.98	0.62
1:B:79:ILE:HD11	1:B:298:HIS:CA	2.26	0.62
1:C:352:ARG:HG3	1:C:354:TYR:HE1	1.63	0.62
1:E:318:PRO:HG2	1:E:319:TYR:CD2	2.35	0.62
1:A:114:CYS:C	1:A:116:THR:H	2.08	0.62
1:A:178:VAL:HG22	1:A:179:THR:N	2.14	0.62
1:A:341:MET:CE	1:A:347:GLN:HB2	2.25	0.62
1:B:285:ILE:N	1:B:285:ILE:HD12	2.14	0.62
1:B:324:LEU:O	1:B:328:LEU:HD23	1.98	0.62
1:D:45:SER:OG	1:D:312:LYS:HD2	1.98	0.62
1:F:57:MET:SD	1:F:301:GLY:HA3	2.39	0.62
1:F:222:TYR:HB3	1:F:227:TRP:CD1	2.34	0.62
1:B:48:GLU:O	1:F:351:VAL:HA	1.99	0.62
1:D:55:PRO:HD3	1:D:303:PRO:CA	2.29	0.62
1:E:192:THR:HB	1:E:194:LYS:HD3	1.82	0.62
1:E:370:VAL:HG22	1:E:375:LYS:HA	1.81	0.62
1:B:257:ASN:ND2	1:C:239:TYR:O	2.33	0.62
1:D:66:LEU:N	1:D:66:LEU:HD23	2.14	0.62
1:D:349:GLU:C	1:D:350:GLU:HG2	2.24	0.62
1:E:192:THR:O	1:E:195:THR:HB	2.00	0.62
1:E:232:ALA:O	1:E:234:ASN:N	2.31	0.62
1:A:257:ASN:HB2	1:B:239:TYR:CE2	2.35	0.62
1:B:262:VAL:CG1	1:B:264:LEU:HB2	2.29	0.62
1:B:346:THR:HG21	1:B:348:VAL:CG1	2.27	0.62
1:C:50:GLU:OE1	1:D:233:LYS:HA	1.99	0.62
1:C:232:ALA:C	1:C:234:ASN:H	2.07	0.62
1:C:342:GLU:N	1:C:346:THR:HG23	2.14	0.62
1:D:278:LEU:HD23	1:D:279:TYR:N	2.15	0.62
1:D:286:MET:HA	1:D:286:MET:HE3	1.81	0.62
1:E:243:TYR:OH	1:E:245:GLY:HA2	2.00	0.62
1:F:97:THR:HG22	1:F:222:TYR:C	2.24	0.62
1:F:264:LEU:HD23	1:F:268:GLY:HA2	1.81	0.62
1:F:336:VAL:C	1:F:337:GLN:HA	2.25	0.62
1:A:164:VAL:HG23	1:A:283:VAL:HG23	1.82	0.62
1:B:28:LEU:HD12	1:F:353:VAL:O	2.00	0.62
1:B:261:THR:HG22	1:B:262:VAL:N	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:233:LYS:HD3	1:E:234:ASN:HD22	1.62	0.62
1:F:174:LEU:N	1:F:174:LEU:HD12	2.14	0.62
1:F:208:LEU:O	1:F:208:LEU:HD23	2.00	0.62
1:A:118:GLN:HB2	1:A:314:TRP:CZ3	2.34	0.62
1:B:165:PHE:CZ	1:B:240:PHE:CE1	2.87	0.62
1:B:172:LEU:HD22	1:B:173:ASP:N	2.15	0.62
1:B:243:TYR:CZ	1:B:245:GLY:HA2	2.35	0.62
1:D:71:GLN:HE21	1:D:73:TYR:HB2	1.64	0.62
1:B:262:VAL:HG12	1:B:264:LEU:HB2	1.81	0.62
1:C:192:THR:HG21	1:C:194:LYS:HE2	1.80	0.62
1:E:46:VAL:HG12	1:E:47:THR:N	2.14	0.62
1:F:233:LYS:HD3	1:F:234:ASN:H	1.65	0.62
1:A:57:MET:SD	1:A:301:GLY:CA	2.88	0.61
1:B:56:ARG:NH2	1:F:339:GLN:HG3	2.14	0.61
1:D:335:GLN:HA	1:D:335:GLN:NE2	2.14	0.61
1:E:78:GLY:HA3	2:K:2:GAL:O4	2.01	0.61
1:E:305:TYR:CD1	1:E:306:PHE:N	2.68	0.61
1:F:142:ASN:N	1:F:292:ARG:HB2	2.15	0.61
1:A:86:THR:HG23	1:A:87:GLU:N	2.15	0.61
1:A:288:TRP:HB3	1:A:297:HIS:O	2.00	0.61
1:B:29:LEU:HB2	1:F:353:VAL:HG23	1.81	0.61
1:C:152:GLY:HA2	1:D:295:ASP:HB3	1.82	0.61
1:E:180:ASP:HA	1:E:206:GLN:HE21	1.65	0.61
1:A:257:ASN:HD22	1:B:239:TYR:N	1.99	0.61
1:B:380:PHE:N	1:B:380:PHE:CD1	2.68	0.61
1:C:57:MET:HB3	1:C:96:PRO:HB3	1.82	0.61
1:C:228:HIS:HB3	1:C:229:PRO:HD2	1.81	0.61
1:E:177:LEU:HD23	1:E:178:VAL:H	1.65	0.61
1:A:222:TYR:HB3	1:A:227:TRP:CD1	2.35	0.61
1:A:297:HIS:CE1	1:E:145:THR:HG21	2.35	0.61
1:B:164:VAL:HG12	1:B:165:PHE:N	2.15	0.61
1:B:177:LEU:HD22	1:B:208:LEU:N	2.16	0.61
1:C:269:VAL:HG12	1:C:270:GLY:O	2.01	0.61
1:E:320:PRO:HG2	1:E:323:SER:HB3	1.82	0.61
1:A:104:GLN:HE22	1:A:276:GLU:HB2	1.65	0.61
1:C:105:LEU:HB3	1:C:120:TRP:NE1	2.16	0.61
1:C:335:GLN:OE1	1:C:335:GLN:HA	2.01	0.61
1:E:28:LEU:HG	1:E:29:LEU:N	2.09	0.61
1:F:192:THR:H	1:F:195:THR:CB	2.12	0.61
1:F:287:GLY:C	1:F:299:TRP:HB2	2.25	0.61
1:A:238:ARG:NH2	1:A:265:ASP:HB3	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:MET:SD	1:B:101:ALA:N	2.73	0.61
1:C:82:ALA:HB2	1:C:88:ASP:OD1	2.00	0.61
1:E:166:ALA:HB2	1:E:239:TYR:HB3	1.82	0.61
1:A:370:VAL:HG13	1:A:374:GLY:O	2.00	0.61
1:D:278:LEU:HD23	1:D:278:LEU:C	2.25	0.61
1:D:288:TRP:HB3	1:D:299:TRP:HA	1.82	0.61
1:D:342:GLU:HG2	1:D:343:GLY:N	2.15	0.61
1:E:112:LEU:HB3	1:E:116:THR:CG2	2.31	0.61
1:E:253:LEU:HD23	1:E:254:GLN:N	2.12	0.61
1:F:104:GLN:NE2	1:F:105:LEU:N	2.49	0.61
1:F:243:TYR:CZ	1:F:245:GLY:CA	2.83	0.61
1:F:285:ILE:HD12	1:F:285:ILE:N	2.15	0.61
1:D:161:GLN:OE1	1:D:251:PRO:HA	2.01	0.61
1:D:192:THR:H	1:D:195:THR:HB	1.65	0.61
1:E:25:VAL:HG12	1:E:26:PRO:HD2	1.83	0.61
1:E:84:SER:O	1:E:86:THR:N	2.34	0.61
1:E:246:GLY:HA3	1:E:249:THR:OG1	2.01	0.61
1:A:352:ARG:HG3	1:A:354:TYR:HE1	1.66	0.60
1:B:122:ALA:HA	1:B:310:LEU:HB3	1.83	0.60
1:C:28:LEU:HD23	1:C:30:ILE:N	2.15	0.60
1:C:233:LYS:HD3	1:C:234:ASN:CB	2.31	0.60
1:D:191:VAL:HA	1:D:195:THR:HG21	1.83	0.60
1:E:66:LEU:HD23	1:E:66:LEU:N	2.16	0.60
1:E:79:ILE:O	1:E:79:ILE:HG22	2.01	0.60
1:E:177:LEU:CD2	1:E:178:VAL:N	2.64	0.60
1:F:177:LEU:CD2	1:F:205:ASP:O	2.49	0.60
1:B:193:ILE:HD11	1:B:201:MET:SD	2.41	0.60
1:C:153:ILE:HG22	1:C:154:SER:N	2.15	0.60
1:E:308:ILE:N	1:E:308:ILE:HD12	2.16	0.60
1:A:208:LEU:HD23	1:A:208:LEU:C	2.27	0.60
1:A:300:ARG:HG3	1:A:300:ARG:HH11	1.66	0.60
1:A:308:ILE:CG2	1:A:310:LEU:HD12	2.28	0.60
1:B:103:LEU:CD2	1:F:341:MET:HG3	2.31	0.60
1:B:110:GLU:CD	1:F:322:ALA:H	2.10	0.60
1:D:104:GLN:HE21	1:D:105:LEU:N	1.99	0.60
1:E:346:THR:HG22	1:E:348:VAL:HG23	1.82	0.60
1:F:125:VAL:HG12	1:F:263:LEU:HD21	1.82	0.60
1:B:125:VAL:CG1	1:B:263:LEU:HD21	2.31	0.60
1:B:341:MET:CE	1:B:348:VAL:HB	2.31	0.60
1:D:55:PRO:HD3	1:D:303:PRO:HA	1.82	0.60
1:D:342:GLU:HG2	1:D:343:GLY:H	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:346:THR:C	1:D:348:VAL:H	2.10	0.60
1:B:198:LYS:H	1:B:198:LYS:HE3	1.66	0.60
1:B:258:THR:HB	1:B:259:LEU:CD2	2.31	0.60
1:F:211:ILE:N	1:F:211:ILE:HD12	2.16	0.60
1:A:25:VAL:HG13	1:A:26:PRO:HD2	1.83	0.60
1:C:50:GLU:HG3	1:C:307:LYS:HG3	1.82	0.60
1:C:53:LEU:CD2	1:C:306:PHE:HE1	2.15	0.60
1:E:94:THR:C	1:E:95:LEU:HD23	2.26	0.60
1:F:193:ILE:HG12	1:F:201:MET:CE	2.31	0.60
1:F:305:TYR:C	1:F:306:PHE:CD1	2.80	0.60
1:B:111:ASP:OD2	1:B:114:CYS:SG	2.60	0.60
1:B:262:VAL:HG12	1:B:264:LEU:N	2.13	0.60
1:B:323:SER:O	1:B:327:SER:N	2.33	0.60
1:C:62:THR:HG1	1:C:63:PRO:HD3	1.65	0.60
1:C:82:ALA:CB	1:C:88:ASP:HA	2.31	0.60
1:F:150:THR:HG21	1:F:292:ARG:HH21	1.65	0.60
1:A:192:THR:CB	1:A:194:LYS:HE2	2.30	0.60
1:B:192:THR:O	1:B:196:ILE:HG22	2.02	0.60
1:B:336:VAL:C	1:B:337:GLN:HA	2.25	0.60
1:C:174:LEU:HA	1:C:228:HIS:O	2.02	0.60
1:D:192:THR:CB	1:D:194:LYS:HD3	2.29	0.60
1:D:278:LEU:HD12	1:D:310:LEU:HD21	1.82	0.60
1:A:174:LEU:HA	1:A:230:ASP:H	1.65	0.60
1:A:228:HIS:HB3	1:A:229:PRO:HD2	1.84	0.60
1:A:339:GLN:HG3	1:A:340:PRO:HD2	1.84	0.60
1:B:25:VAL:HG12	1:B:26:PRO:HD2	1.83	0.60
1:C:76:SER:OG	1:C:299:TRP:HE3	1.84	0.60
1:C:313:ARG:HG2	1:C:314:TRP:H	1.65	0.60
1:A:328:LEU:HD21	1:A:333:LEU:HD11	1.84	0.60
1:B:121:GLU:HG2	1:B:271:PRO:O	2.01	0.60
1:B:339:GLN:NE2	1:B:347:GLN:NE2	2.50	0.60
1:C:67:THR:OG1	1:C:68:GLU:HG3	2.01	0.60
1:C:69:GLY:O	1:C:71:GLN:N	2.35	0.60
1:E:136:LEU:O	1:E:138:VAL:HG22	2.02	0.60
1:E:192:THR:HG22	1:E:193:ILE:CD1	2.32	0.60
1:E:298:HIS:CD2	1:E:298:HIS:N	2.70	0.60
1:A:75:TRP:NE1	1:A:300:ARG:HB2	2.17	0.59
1:C:233:LYS:HZ2	1:F:350:GLU:HG2	1.65	0.59
1:C:285:ILE:HD12	1:C:285:ILE:N	2.16	0.59
1:D:308:ILE:HD12	1:D:308:ILE:N	2.17	0.59
1:D:317:ASN:HD22	1:D:318:PRO:HD2	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:THR:HB	1:A:194:LYS:HD3	1.83	0.59
1:A:233:LYS:HA	1:E:50:GLU:CG	2.32	0.59
1:C:175:GLN:HG2	1:C:213:LYS:HG2	1.83	0.59
1:C:232:ALA:C	1:C:234:ASN:N	2.55	0.59
1:D:30:ILE:HG21	1:D:39:LEU:HD23	1.84	0.59
1:F:259:LEU:HD22	1:F:259:LEU:N	2.16	0.59
1:A:164:VAL:HG13	1:A:241:GLY:HA3	1.84	0.59
1:A:175:GLN:HB2	1:A:213:LYS:HD3	1.83	0.59
1:A:285:ILE:HD12	1:A:285:ILE:N	2.17	0.59
1:C:233:LYS:CE	1:F:350:GLU:HG2	2.32	0.59
1:C:304:ARG:HG2	1:C:306:PHE:CE1	2.37	0.59
1:B:175:GLN:HE21	1:B:176:GLY:N	2.00	0.59
1:C:77:ARG:HB2	1:C:93:ASN:HB2	1.84	0.59
1:C:236:ASN:OD1	1:C:272:LEU:HD12	2.02	0.59
1:C:286:MET:HA	1:C:286:MET:CE	2.32	0.59
1:D:232:ALA:HB3	1:D:235:GLU:OE1	2.02	0.59
1:E:333:LEU:HD22	1:E:333:LEU:H	1.67	0.59
1:A:86:THR:HG23	1:A:87:GLU:H	1.67	0.59
1:B:145:THR:HB	1:B:152:GLY:HA3	1.85	0.59
1:C:186:LYS:H	1:C:186:LYS:CD	2.15	0.59
1:F:19:CYS:CB	1:F:20:PRO:HD2	2.32	0.59
1:F:293:ASN:OD1	1:F:294:TYR:HB2	2.02	0.59
1:E:342:GLU:H	1:E:346:THR:HG23	1.66	0.59
1:A:164:VAL:HA	1:A:241:GLY:HA3	1.84	0.59
1:B:233:LYS:HG2	1:B:234:ASN:H	1.65	0.59
1:B:370:VAL:HA	1:B:375:LYS:HA	1.84	0.59
1:C:233:LYS:HG2	1:F:350:GLU:HB2	1.84	0.59
1:A:328:LEU:HD11	1:A:332:MET:CE	2.19	0.59
1:B:175:GLN:CB	1:B:230:ASP:HB2	2.22	0.59
1:B:288:TRP:CZ3	1:B:299:TRP:CD1	2.90	0.59
1:D:142:ASN:ND2	1:D:289:ARG:HG3	2.17	0.59
1:D:144:PRO:HA	1:D:153:ILE:O	2.03	0.59
1:D:179:THR:O	1:D:206:GLN:HG3	2.03	0.59
1:E:264:LEU:HD12	1:E:270:GLY:HA3	1.83	0.59
1:F:71:GLN:NE2	1:F:71:GLN:HA	2.09	0.59
1:F:263:LEU:O	1:F:270:GLY:HA2	2.02	0.59
1:B:25:VAL:HG21	1:F:360:VAL:HA	1.84	0.59
1:B:161:GLN:CD	1:B:251:PRO:HA	2.28	0.59
1:B:207:VAL:HG23	1:B:208:LEU:N	2.18	0.59
1:D:191:VAL:HG21	1:D:222:TYR:CE1	2.37	0.59
1:E:122:ALA:HA	1:E:310:LEU:HB3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:177:LEU:HD23	1:E:205:ASP:O	2.02	0.59
1:B:75:TRP:CZ2	1:B:300:ARG:HD2	2.38	0.59
1:B:313:ARG:HG2	1:B:314:TRP:N	2.17	0.59
1:B:328:LEU:O	1:B:330:ASN:N	2.36	0.59
1:C:111:ASP:CG	1:C:114:CYS:HB3	2.28	0.59
1:C:123:VAL:HG13	1:C:264:LEU:HD13	1.84	0.59
1:D:141:PHE:CD1	1:D:292:ARG:HG3	2.38	0.59
1:F:181:ALA:HB1	1:F:201:MET:HB3	1.84	0.59
1:A:272:LEU:HD12	1:A:272:LEU:N	2.18	0.58
1:D:72:TYR:O	1:D:75:TRP:HB2	2.02	0.58
1:E:335:GLN:OE1	1:E:336:VAL:HG22	2.03	0.58
1:E:366:MET:HG2	1:E:367:THR:N	2.18	0.58
1:A:192:THR:HB	1:A:194:LYS:CD	2.33	0.58
1:A:198:LYS:HE2	1:A:198:LYS:H	1.66	0.58
1:B:166:ALA:HB2	1:B:239:TYR:HB3	1.86	0.58
1:C:117:LEU:HD13	1:C:118:GLN:N	2.18	0.58
1:C:300:ARG:HH11	1:C:300:ARG:HG3	1.66	0.58
1:E:54:ASN:HD22	1:E:303:PRO:HB3	1.68	0.58
1:B:360:VAL:HG12	1:B:361:PRO:HD2	1.85	0.58
1:C:142:ASN:ND2	1:C:289:ARG:HG3	2.16	0.58
1:D:72:TYR:CE2	1:D:77:ARG:NH2	2.71	0.58
1:E:320:PRO:C	1:E:324:LEU:HD12	2.27	0.58
1:F:196:ILE:HD12	1:F:196:ILE:O	2.03	0.58
1:B:211:ILE:O	1:B:213:LYS:N	2.37	0.58
1:F:218:LYS:O	1:F:219:ASP:HB2	2.03	0.58
1:C:271:PRO:C	1:C:272:LEU:HG	2.28	0.58
1:D:133:GLY:CA	1:E:228:HIS:HE1	2.17	0.58
1:D:203:ASN:O	1:D:206:GLN:HB3	2.03	0.58
1:F:184:LYS:N	1:F:184:LYS:HD2	2.18	0.58
1:B:379:VAL:HG12	1:B:380:PHE:O	2.03	0.58
1:D:83:THR:HB	1:D:87:GLU:HB3	1.86	0.58
1:F:108:LEU:HB3	1:F:118:GLN:NE2	2.18	0.58
1:A:246:GLY:HA3	1:A:249:THR:OG1	2.03	0.58
1:B:165:PHE:CE1	1:B:240:PHE:HE1	2.22	0.58
1:B:170:GLU:HB2	1:B:171:PRO:HD2	1.85	0.58
1:B:205:ASP:HA	1:B:209:ASN:HB2	1.86	0.58
1:B:233:LYS:C	1:B:234:ASN:HD22	2.11	0.58
1:C:30:ILE:HD13	1:C:36:VAL:HG13	1.85	0.58
1:D:90:PRO:HB3	1:D:95:LEU:HD11	1.86	0.58
1:D:178:VAL:CG2	1:D:179:THR:N	2.66	0.58
1:A:87:GLU:HA	1:A:184:LYS:HZ1	1.65	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:THR:OG1	1:B:63:PRO:HD3	2.03	0.58
1:C:69:GLY:C	1:C:71:GLN:N	2.60	0.58
1:C:116:THR:HG23	1:C:314:TRP:CE3	2.38	0.58
1:D:175:GLN:CG	1:D:213:LYS:HG2	2.33	0.58
1:D:337:GLN:OE1	1:D:337:GLN:HA	2.02	0.58
1:E:135:LEU:HD22	1:E:135:LEU:H	1.68	0.58
1:E:181:ALA:H	1:E:206:GLN:NE2	2.02	0.58
1:E:354:TYR:CD1	1:E:354:TYR:N	2.70	0.58
1:A:192:THR:HB	1:A:194:LYS:CE	2.34	0.58
1:F:186:LYS:H	1:F:186:LYS:HE2	1.68	0.58
1:F:192:THR:H	1:F:195:THR:HB	1.68	0.58
1:F:239:TYR:C	1:F:240:PHE:CD1	2.81	0.58
1:F:265:ASP:H	1:F:270:GLY:H	1.49	0.58
1:A:100:MET:SD	1:A:219:ASP:HB2	2.44	0.58
1:A:185:TYR:CZ	1:A:226:ILE:HD11	2.39	0.58
1:B:97:THR:HG22	1:B:222:TYR:O	2.03	0.58
1:E:170:GLU:HB2	1:E:171:PRO:HD2	1.86	0.58
1:A:69:GLY:O	1:A:71:GLN:N	2.37	0.57
1:A:181:ALA:H	1:A:206:GLN:NE2	2.02	0.57
1:B:52:PHE:CE2	1:C:208:LEU:HD23	2.39	0.57
1:C:34:MET:O	1:C:37:LEU:HB2	2.04	0.57
1:D:71:GLN:HE21	1:D:73:TYR:H	1.50	0.57
1:E:109:ASN:OD1	1:E:118:GLN:N	2.37	0.57
1:F:50:GLU:HA	1:F:306:PHE:O	2.04	0.57
1:F:192:THR:HG22	1:F:193:ILE:CD1	2.34	0.57
1:A:138:VAL:O	1:A:153:ILE:HG23	2.03	0.57
1:B:46:VAL:HG12	1:B:47:THR:H	1.67	0.57
1:B:76:SER:OG	1:B:299:TRP:HE3	1.85	0.57
1:C:192:THR:HB	1:C:194:LYS:CD	2.32	0.57
1:C:321:MET:HA	1:C:324:LEU:HD12	1.85	0.57
1:D:257:ASN:CB	1:E:239:TYR:CE2	2.86	0.57
1:E:90:PRO:HG2	1:E:185:TYR:HA	1.86	0.57
1:E:193:ILE:HD12	1:E:193:ILE:H	1.69	0.57
1:E:307:LYS:C	1:E:308:ILE:HD12	2.29	0.57
1:F:125:VAL:HB	1:F:263:LEU:HD11	1.86	0.57
1:A:161:GLN:OE1	1:A:251:PRO:HA	2.03	0.57
1:B:165:PHE:CD1	1:B:165:PHE:C	2.81	0.57
1:A:129:VAL:HB	1:A:253:LEU:HD21	1.86	0.57
1:B:366:MET:HE1	1:B:377:LYS:HG2	1.85	0.57
1:C:153:ILE:HD11	1:D:297:HIS:CB	2.35	0.57
1:D:98:TRP:HH2	1:D:164:VAL:CG1	2.16	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:232:ALA:C	1:E:234:ASN:H	2.12	0.57
1:E:233:LYS:C	1:E:234:ASN:HD22	2.13	0.57
1:F:30:ILE:CD1	1:F:36:VAL:HG22	2.35	0.57
1:A:46:VAL:HG12	1:A:47:THR:N	2.19	0.57
1:A:124:SER:CA	1:A:263:LEU:HG	2.35	0.57
1:B:50:GLU:CD	1:C:233:LYS:CB	2.77	0.57
1:B:342:GLU:HG2	1:B:343:GLY:H	1.69	0.57
1:C:152:GLY:O	1:C:153:ILE:HD13	2.04	0.57
1:C:310:LEU:HD12	1:C:310:LEU:N	2.19	0.57
1:D:254:GLN:OE1	1:D:254:GLN:HA	2.00	0.57
1:F:142:ASN:C	1:F:292:ARG:HB2	2.29	0.57
1:A:298:HIS:H	1:A:298:HIS:HD2	1.53	0.57
1:B:77:ARG:CB	1:B:93:ASN:HB2	2.33	0.57
1:B:193:ILE:CG2	1:B:212:SER:HB3	2.35	0.57
1:C:111:ASP:OD2	1:C:114:CYS:HB3	2.04	0.57
1:C:142:ASN:N	1:C:154:SER:OG	2.36	0.57
1:C:341:MET:C	1:C:346:THR:HG23	2.30	0.57
1:C:362:GLY:O	1:C:364:PRO:HD3	2.05	0.57
1:D:313:ARG:HG2	1:D:314:TRP:N	2.20	0.57
1:E:135:LEU:HD13	1:E:135:LEU:N	2.19	0.57
1:E:233:LYS:CD	1:E:234:ASN:N	2.66	0.57
1:A:288:TRP:CZ3	1:A:299:TRP:CD1	2.93	0.57
1:B:239:TYR:C	1:B:240:PHE:CG	2.83	0.57
1:C:178:VAL:HG22	1:C:179:THR:N	2.20	0.57
1:D:76:SER:HG	1:D:299:TRP:HB2	1.69	0.57
1:A:35:GLU:HG2	1:A:36:VAL:H	1.68	0.57
1:D:172:LEU:HD22	1:D:173:ASP:O	2.05	0.57
1:E:125:VAL:HG11	1:E:263:LEU:HD21	1.87	0.57
1:A:295:ASP:O	1:E:152:GLY:HA2	2.05	0.57
1:A:328:LEU:HD12	1:A:332:MET:HE2	1.62	0.57
1:A:366:MET:HA	1:A:380:PHE:CE1	2.40	0.57
1:B:228:HIS:HB3	1:B:229:PRO:HD2	1.86	0.57
1:C:109:ASN:HB3	1:C:117:LEU:HD21	1.87	0.57
1:C:125:VAL:HA	1:C:307:LYS:O	2.05	0.57
1:F:94:THR:O	1:F:95:LEU:HD23	2.03	0.57
1:F:367:THR:HG22	1:F:368:ARG:H	1.69	0.57
1:C:75:TRP:NE1	1:C:300:ARG:HB2	2.19	0.57
1:E:122:ALA:O	1:E:271:PRO:HD2	2.05	0.57
1:F:28:LEU:HD23	1:F:29:LEU:N	2.20	0.57
1:A:105:LEU:HB3	1:A:106:PRO:HD2	1.86	0.56
1:A:192:THR:HG23	1:A:226:ILE:HD13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:PHE:CE1	1:B:144:PRO:HG3	2.31	0.56
1:B:166:ALA:HB2	1:B:239:TYR:CB	2.34	0.56
1:B:360:VAL:CG1	1:B:361:PRO:HD2	2.34	0.56
1:C:186:LYS:N	1:C:186:LYS:HE2	2.19	0.56
1:E:124:SER:HA	1:E:261:THR:O	2.05	0.56
1:E:130:VAL:O	1:E:302:LEU:HD22	2.05	0.56
1:E:265:ASP:OD1	1:E:269:VAL:HB	2.05	0.56
1:E:313:ARG:HH11	1:E:313:ARG:HG3	1.67	0.56
1:E:367:THR:CG2	1:E:368:ARG:N	2.68	0.56
1:F:66:LEU:HD23	1:F:66:LEU:H	1.69	0.56
1:F:259:LEU:HD13	1:F:259:LEU:H	1.67	0.56
1:B:55:PRO:HB3	1:B:302:LEU:O	2.05	0.56
1:B:69:GLY:C	1:B:71:GLN:N	2.61	0.56
1:D:60:PRO:CB	1:D:61:PRO:HD2	2.35	0.56
1:D:304:ARG:HG2	1:D:306:PHE:CE1	2.40	0.56
1:E:114:CYS:C	1:E:116:THR:N	2.61	0.56
1:A:263:LEU:N	1:A:263:LEU:HD23	2.20	0.56
1:A:380:PHE:CD1	1:A:381:PRO:HD2	2.41	0.56
1:B:107:MET:C	1:B:108:LEU:HD12	2.30	0.56
1:B:185:TYR:CD2	1:B:192:THR:HG21	2.40	0.56
1:D:190:VAL:HA	1:D:221:MET:HG3	1.86	0.56
1:D:265:ASP:OD1	1:D:269:VAL:HB	2.04	0.56
1:F:55:PRO:HD3	1:F:303:PRO:CA	2.36	0.56
1:F:121:GLU:HG2	1:F:271:PRO:O	2.04	0.56
1:F:177:LEU:HD21	1:F:209:ASN:H	1.68	0.56
1:F:269:VAL:CG1	1:F:272:LEU:HD11	2.35	0.56
1:A:286:MET:HA	1:A:286:MET:CE	2.35	0.56
1:A:326:SER:O	1:A:327:SER:O	2.22	0.56
1:C:132:SER:O	1:C:135:LEU:HD23	2.06	0.56
1:D:211:ILE:N	1:D:211:ILE:CD1	2.67	0.56
1:E:71:GLN:HE21	1:E:73:TYR:HB2	1.71	0.56
1:A:28:LEU:HD12	1:A:29:LEU:H	1.70	0.56
1:A:174:LEU:HD11	1:A:227:TRP:CE3	2.41	0.56
1:B:105:LEU:HD23	1:B:120:TRP:CD1	2.39	0.56
1:B:269:VAL:HG12	1:B:270:GLY:O	2.05	0.56
1:C:190:VAL:HG22	1:C:191:VAL:O	2.06	0.56
1:D:91:GLY:H	1:D:186:LYS:CE	2.17	0.56
1:D:286:MET:HA	1:D:286:MET:HE2	1.85	0.56
1:F:279:TYR:C	1:F:280:LEU:HD23	2.30	0.56
1:A:28:LEU:HD21	1:A:31:LYS:HB3	1.87	0.56
1:A:239:TYR:C	1:A:240:PHE:CD1	2.84	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:TYR:HE1	1:A:307:LYS:HB2	1.71	0.56
1:C:211:ILE:O	1:C:213:LYS:N	2.39	0.56
1:D:25:VAL:HG23	1:D:26:PRO:CD	2.36	0.56
1:E:207:VAL:HG23	1:E:208:LEU:N	2.20	0.56
1:A:197:THR:O	1:A:197:THR:HG23	2.06	0.56
1:A:372:ARG:O	1:A:373:PHE:CD1	2.58	0.56
1:C:316:LYS:HZ2	1:F:359:PRO:HD2	1.69	0.56
1:C:346:THR:HG22	1:C:348:VAL:HG23	1.87	0.56
1:E:197:THR:O	1:E:197:THR:HG23	2.06	0.56
1:F:65:SER:HB3	1:F:68:GLU:CG	2.33	0.56
1:F:263:LEU:HB3	1:F:271:PRO:HD3	1.88	0.56
1:A:275:GLY:O	1:A:277:GLY:N	2.39	0.56
1:B:78:GLY:O	1:B:79:ILE:HD13	2.05	0.56
1:B:278:LEU:HD23	1:B:279:TYR:H	1.71	0.56
1:C:43:PRO:HD2	1:C:44:ASP:H	1.71	0.56
1:D:112:LEU:HD12	1:D:112:LEU:N	2.20	0.56
1:E:75:TRP:NE1	1:E:300:ARG:HB2	2.20	0.56
1:E:141:PHE:CZ	1:E:292:ARG:HG3	2.41	0.56
1:E:223:PRO:HG3	1:E:226:ILE:HD12	1.88	0.56
1:E:243:TYR:CZ	1:E:245:GLY:CA	2.89	0.56
1:E:341:MET:HE3	1:E:348:VAL:CG2	2.36	0.56
1:F:66:LEU:HD23	1:F:66:LEU:N	2.21	0.56
1:F:313:ARG:HG2	1:F:314:TRP:N	2.21	0.56
2:H:2:GAL:H3	2:H:3:SIA:O1B	2.05	0.56
1:B:94:THR:O	1:B:95:LEU:HG	2.05	0.56
1:B:100:MET:SD	1:B:100:MET:C	2.89	0.56
1:C:28:LEU:CD2	1:C:30:ILE:N	2.68	0.56
1:C:352:ARG:HG3	1:C:354:TYR:CE1	2.41	0.56
1:D:57:MET:HB2	1:D:96:PRO:HB3	1.88	0.56
1:D:186:LYS:HD2	1:D:186:LYS:N	2.17	0.56
1:A:130:VAL:O	1:A:302:LEU:HD22	2.05	0.56
1:A:372:ARG:C	1:A:373:PHE:CD1	2.84	0.56
1:B:69:GLY:HA3	1:B:71:GLN:OE1	2.06	0.56
1:B:135:LEU:HD13	1:B:135:LEU:N	2.21	0.56
1:D:71:GLN:NE2	1:D:73:TYR:H	2.04	0.56
1:D:243:TYR:CZ	1:D:245:GLY:CA	2.89	0.56
1:F:192:THR:HG22	1:F:193:ILE:HD12	1.87	0.56
1:B:142:ASN:O	1:B:292:ARG:HB2	2.05	0.55
1:B:172:LEU:HD22	1:B:173:ASP:O	2.06	0.55
1:B:258:THR:C	1:B:259:LEU:HD22	2.30	0.55
1:D:342:GLU:CA	1:D:346:THR:HG23	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:75:TRP:CH2	1:E:300:ARG:HD2	2.40	0.55
1:E:318:PRO:HG2	1:E:319:TYR:CG	2.41	0.55
1:F:86:THR:HG23	1:F:87:GLU:N	2.21	0.55
1:A:224:VAL:HG11	1:A:283:VAL:HG11	1.88	0.55
1:C:76:SER:OG	1:C:299:TRP:HB2	2.06	0.55
1:C:192:THR:O	1:C:193:ILE:C	2.48	0.55
1:C:239:TYR:C	1:C:239:TYR:CD1	2.83	0.55
1:F:42:GLY:O	1:F:312:LYS:NZ	2.31	0.55
1:F:59:GLN:HE21	1:F:71:GLN:HE22	1.54	0.55
1:A:50:GLU:HG2	1:A:305:TYR:OH	2.06	0.55
1:A:238:ARG:HH21	1:A:265:ASP:HB3	1.71	0.55
1:A:305:TYR:CE1	1:A:307:LYS:HB2	2.41	0.55
1:B:219:ASP:HB3	1:F:338:GLY:H	1.71	0.55
1:C:173:ASP:C	1:C:174:LEU:HD12	2.32	0.55
1:C:316:LYS:HE3	1:F:359:PRO:HB2	1.88	0.55
1:D:145:THR:HG21	1:E:297:HIS:HE1	1.70	0.55
1:E:62:THR:O	1:E:64:GLU:N	2.39	0.55
1:F:201:MET:HA	1:F:201:MET:HE3	1.87	0.55
1:B:48:GLU:HG2	1:B:309:THR:HG23	1.87	0.55
1:B:264:LEU:HD12	1:B:270:GLY:HA3	1.88	0.55
1:E:82:ALA:HB2	1:E:88:ASP:OD1	2.05	0.55
1:E:175:GLN:NE2	1:E:176:GLY:O	2.39	0.55
1:A:138:VAL:HB	1:A:153:ILE:CG2	2.34	0.55
1:B:111:ASP:OD2	1:B:113:THR:HB	2.07	0.55
1:B:177:LEU:CD2	1:B:208:LEU:CA	2.84	0.55
1:C:232:ALA:O	1:C:234:ASN:N	2.39	0.55
1:E:193:ILE:O	1:E:196:ILE:HG23	2.06	0.55
1:E:288:TRP:HE3	1:E:299:TRP:CG	2.24	0.55
1:F:72:TYR:HE2	1:F:77:ARG:NH2	2.04	0.55
1:F:232:ALA:HB3	1:F:235:GLU:OE1	2.06	0.55
1:A:278:LEU:HD22	1:A:280:LEU:HD22	1.87	0.55
1:B:328:LEU:C	1:B:332:MET:SD	2.90	0.55
1:C:164:VAL:HG22	1:C:241:GLY:HA3	1.88	0.55
1:C:239:TYR:C	1:C:240:PHE:CD1	2.85	0.55
1:E:341:MET:HE3	1:E:348:VAL:HG23	1.89	0.55
1:E:368:ARG:HA	1:E:376:THR:O	2.06	0.55
1:B:43:PRO:HA	1:B:312:LYS:HD2	1.89	0.55
1:B:193:ILE:HG12	1:B:201:MET:CE	2.36	0.55
1:B:265:ASP:N	1:B:270:GLY:H	2.04	0.55
1:B:265:ASP:OD1	1:B:269:VAL:HB	2.06	0.55
1:E:139:HIS:O	1:E:154:SER:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:354:TYR:N	1:E:354:TYR:HD1	2.03	0.55
1:A:106:PRO:HD2	1:A:120:TRP:HE1	1.71	0.55
1:B:75:TRP:HE1	1:B:300:ARG:HB2	1.72	0.55
1:B:177:LEU:CD2	1:B:205:ASP:O	2.55	0.55
1:D:135:LEU:H	1:D:135:LEU:HD22	1.72	0.55
1:E:54:ASN:ND2	1:E:303:PRO:HB3	2.21	0.55
1:E:76:SER:OG	1:E:299:TRP:CE3	2.56	0.55
1:E:186:LYS:HE2	1:E:186:LYS:H	1.71	0.55
1:E:192:THR:HB	1:E:194:LYS:CD	2.36	0.55
1:E:342:GLU:HG2	1:E:343:GLY:N	2.21	0.55
1:A:178:VAL:HG22	1:A:180:ASP:N	2.22	0.55
1:A:211:ILE:O	1:A:213:LYS:N	2.39	0.55
1:A:251:PRO:CG	1:B:245:GLY:HA3	2.32	0.55
1:A:372:ARG:O	1:A:373:PHE:HD1	1.90	0.55
1:B:66:LEU:O	1:B:70:GLY:HA2	2.05	0.55
1:B:104:GLN:HE21	1:B:105:LEU:N	2.04	0.55
1:B:114:CYS:HB2	1:B:116:THR:HG22	1.88	0.55
1:B:165:PHE:CZ	1:B:240:PHE:HE1	2.23	0.55
1:C:82:ALA:HB1	1:C:87:GLU:O	2.07	0.55
1:E:33:GLY:O	1:E:36:VAL:HG23	2.07	0.55
1:F:90:PRO:HB2	1:F:186:LYS:HE3	1.89	0.55
1:B:193:ILE:HD12	1:B:193:ILE:N	2.21	0.55
1:C:164:VAL:HG12	1:C:165:PHE:N	2.21	0.55
1:D:193:ILE:HD12	1:D:193:ILE:H	1.71	0.55
1:D:290:VAL:HG22	1:D:297:HIS:CD2	2.41	0.55
1:E:117:LEU:O	1:E:314:TRP:HE3	1.90	0.55
1:E:179:THR:O	1:E:206:GLN:HG3	2.07	0.55
1:E:192:THR:H	1:E:195:THR:CB	2.19	0.55
1:F:193:ILE:CD1	1:F:201:MET:SD	2.95	0.55
1:A:84:SER:C	1:A:86:THR:N	2.63	0.54
1:A:130:VAL:CG2	1:A:303:PRO:HG2	2.38	0.54
1:A:241:GLY:O	1:E:255:PHE:HB2	2.07	0.54
1:B:103:LEU:HB2	1:B:278:LEU:HB3	1.89	0.54
1:B:305:TYR:C	1:B:306:PHE:CD1	2.85	0.54
1:C:53:LEU:HD21	1:C:306:PHE:HE1	1.69	0.54
1:C:145:THR:HG21	1:D:297:HIS:HE1	1.72	0.54
1:C:193:ILE:O	1:C:197:THR:N	2.40	0.54
1:D:32:GLY:CA	1:D:36:VAL:HG21	2.37	0.54
1:D:272:LEU:HD12	1:D:272:LEU:N	2.21	0.54
1:E:208:LEU:O	1:E:210:PRO:HD3	2.07	0.54
1:F:104:GLN:NE2	1:F:105:LEU:O	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:174:LEU:HD23	1:F:227:TRP:HB3	1.89	0.54
1:F:209:ASN:OD1	1:F:211:ILE:HD13	2.06	0.54
1:A:82:ALA:CB	1:A:88:ASP:HA	2.37	0.54
1:A:106:PRO:HD2	1:A:120:TRP:NE1	2.22	0.54
1:B:152:GLY:O	1:B:153:ILE:HD13	2.06	0.54
1:D:98:TRP:HH2	1:D:164:VAL:HG11	1.72	0.54
1:E:291:THR:HB	1:E:293:ASN:HB3	1.88	0.54
1:E:320:PRO:HG2	1:E:323:SER:HB2	1.89	0.54
1:E:321:MET:O	1:E:324:LEU:HB2	2.07	0.54
1:F:185:TYR:HB2	1:F:194:LYS:CE	2.38	0.54
1:F:239:TYR:C	1:F:240:PHE:CG	2.84	0.54
1:D:125:VAL:HG12	1:D:263:LEU:HD21	1.89	0.54
1:F:186:LYS:HE2	1:F:186:LYS:N	2.21	0.54
1:A:71:GLN:OE1	1:A:71:GLN:HA	2.02	0.54
1:B:72:TYR:O	1:B:75:TRP:HB2	2.07	0.54
1:F:124:SER:HA	1:F:261:THR:O	2.08	0.54
1:A:54:ASN:ND2	1:B:207:VAL:HB	2.22	0.54
1:A:174:LEU:HD12	1:A:175:GLN:N	2.21	0.54
1:A:231:PRO:HG2	1:E:305:TYR:HD2	1.71	0.54
1:B:290:VAL:HG22	1:B:297:HIS:CD2	2.43	0.54
1:B:346:THR:HG22	1:B:348:VAL:H	1.73	0.54
1:C:39:LEU:HD12	1:C:40:VAL:N	2.21	0.54
1:D:269:VAL:HA	1:D:313:ARG:HH21	1.73	0.54
1:E:321:MET:O	1:E:325:ILE:HD12	2.07	0.54
1:F:288:TRP:CE3	1:F:299:TRP:HB3	2.41	0.54
1:A:74:GLY:O	1:A:300:ARG:NH1	2.41	0.54
1:A:83:THR:O	1:A:84:SER:HB2	2.06	0.54
1:A:166:ALA:HB1	1:A:237:THR:HG22	1.88	0.54
1:A:243:TYR:CZ	1:A:245:GLY:CA	2.91	0.54
1:C:131:GLY:H	1:C:255:PHE:HZ	1.56	0.54
1:E:193:ILE:HD12	1:E:193:ILE:N	2.23	0.54
1:F:197:THR:O	1:F:197:THR:HG23	2.07	0.54
1:A:80:ASN:HB3	1:A:90:PRO:O	2.07	0.54
1:A:336:VAL:HG23	1:A:337:GLN:H	1.50	0.54
1:C:253:LEU:O	1:D:242:ASN:HB2	2.08	0.54
1:E:115:ASP:OD1	1:E:317:ASN:HB3	2.08	0.54
1:F:39:LEU:O	1:F:41:THR:N	2.40	0.54
1:A:76:SER:OG	1:A:299:TRP:CE3	2.61	0.54
1:A:108:LEU:HD11	1:A:120:TRP:CZ2	2.43	0.54
1:D:181:ALA:HA	1:D:201:MET:HE2	1.90	0.54
1:E:164:VAL:HA	1:E:241:GLY:CA	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:288:TRP:CE3	1:E:299:TRP:CG	2.96	0.54
1:E:306:PHE:HB3	1:E:308:ILE:CD1	2.38	0.54
1:F:100:MET:SD	1:F:100:MET:C	2.91	0.54
1:F:175:GLN:HG3	1:F:213:LYS:NZ	2.23	0.54
1:F:194:LYS:C	1:F:196:ILE:H	2.14	0.54
1:F:201:MET:CE	1:F:201:MET:HA	2.38	0.54
1:B:378:THR:HG22	1:B:379:VAL:N	2.22	0.54
1:C:72:TYR:O	1:C:75:TRP:HB2	2.08	0.54
1:D:28:LEU:HD11	1:D:30:ILE:O	2.07	0.54
1:F:304:ARG:HG2	1:F:305:TYR:N	2.23	0.54
1:A:139:HIS:O	1:A:154:SER:HB2	2.08	0.54
1:B:175:GLN:NE2	1:B:176:GLY:O	2.40	0.54
1:C:25:VAL:HG13	1:C:26:PRO:HD2	1.89	0.54
1:C:360:VAL:CG1	1:C:361:PRO:HD2	2.37	0.54
1:D:135:LEU:HD22	1:D:135:LEU:N	2.22	0.54
1:E:370:VAL:HG22	1:E:375:LYS:CB	2.37	0.54
1:F:28:LEU:HD23	1:F:28:LEU:C	2.33	0.54
1:B:97:THR:HG22	1:B:222:TYR:C	2.33	0.53
1:C:76:SER:CB	1:C:299:TRP:HE3	2.22	0.53
1:C:341:MET:HE1	1:C:347:GLN:CB	2.23	0.53
1:D:139:HIS:HD2	1:E:88:ASP:OD1	1.91	0.53
1:D:288:TRP:CE3	1:D:299:TRP:CD1	2.95	0.53
1:E:50:GLU:HG3	1:E:307:LYS:HG3	1.90	0.53
1:E:161:GLN:NE2	1:E:251:PRO:HA	2.23	0.53
1:E:166:ALA:HB2	1:E:239:TYR:CB	2.38	0.53
1:E:190:VAL:HG23	1:E:223:PRO:HD3	1.90	0.53
1:E:317:ASN:ND2	1:E:319:TYR:H	2.06	0.53
1:E:328:LEU:HG	1:E:329:PHE:N	2.23	0.53
1:E:370:VAL:HA	1:E:375:LYS:HA	1.90	0.53
1:F:40:VAL:HG23	1:F:40:VAL:O	2.08	0.53
1:A:293:ASN:CG	1:A:294:TYR:H	2.15	0.53
1:B:78:GLY:HA2	1:B:298:HIS:CD2	2.43	0.53
1:B:251:PRO:HD2	1:C:245:GLY:CA	2.38	0.53
1:B:261:THR:CG2	1:B:262:VAL:N	2.71	0.53
1:C:97:THR:HG22	1:C:222:TYR:C	2.33	0.53
1:C:190:VAL:HG23	1:C:221:MET:O	2.08	0.53
1:C:352:ARG:HD2	1:F:234:ASN:HD21	1.72	0.53
1:E:222:TYR:N	1:E:222:TYR:CD1	2.75	0.53
1:F:194:LYS:HA	1:F:197:THR:O	2.08	0.53
1:A:54:ASN:OD1	1:B:208:LEU:HB3	2.08	0.53
1:A:172:LEU:C	1:A:172:LEU:HD22	2.33	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:LEU:HD22	1:C:53:LEU:N	2.24	0.53
1:C:56:ARG:HH22	1:C:219:ASP:CG	2.16	0.53
1:C:76:SER:O	1:C:298:HIS:HB2	2.08	0.53
1:D:62:THR:O	1:D:64:GLU:N	2.41	0.53
1:D:180:ASP:HA	1:D:206:GLN:HE21	1.74	0.53
1:D:192:THR:HB	1:D:194:LYS:CD	2.33	0.53
1:A:280:LEU:HD12	1:A:306:PHE:CD2	2.42	0.53
1:B:341:MET:HA	1:B:346:THR:HG23	1.91	0.53
1:C:97:THR:HG22	1:C:223:PRO:N	2.23	0.53
1:C:162:TYR:HB3	1:C:285:ILE:HD13	1.89	0.53
1:E:208:LEU:HD23	1:E:208:LEU:C	2.34	0.53
1:F:286:MET:HA	1:F:286:MET:CE	2.37	0.53
1:A:90:PRO:HG2	1:A:185:TYR:CA	2.38	0.53
1:A:121:GLU:O	1:A:310:LEU:HB2	2.08	0.53
1:A:238:ARG:HA	1:E:257:ASN:HD22	1.74	0.53
1:B:166:ALA:HA	1:B:238:ARG:O	2.08	0.53
1:C:152:GLY:HA2	1:D:295:ASP:CB	2.38	0.53
1:E:177:LEU:HG	1:E:207:VAL:O	2.08	0.53
1:A:278:LEU:HD22	1:A:280:LEU:HD21	1.89	0.53
1:B:122:ALA:HB3	1:B:271:PRO:HD2	1.90	0.53
1:B:202:VAL:HG12	1:B:203:ASN:H	1.73	0.53
1:B:293:ASN:OD1	1:B:294:TYR:HB2	2.09	0.53
1:B:341:MET:CA	1:B:346:THR:HG23	2.39	0.53
1:C:131:GLY:HA2	1:D:228:HIS:CE1	2.43	0.53
1:D:76:SER:O	1:D:298:HIS:HB2	2.07	0.53
1:D:229:PRO:HB2	1:D:239:TYR:CE2	2.43	0.53
1:D:268:GLY:O	1:D:313:ARG:NH2	2.41	0.53
1:E:94:THR:HG22	1:E:94:THR:O	2.08	0.53
1:E:145:THR:OG1	1:E:153:ILE:HB	2.08	0.53
1:F:28:LEU:HD23	1:F:30:ILE:N	2.23	0.53
1:A:62:THR:O	1:A:64:GLU:N	2.41	0.53
1:A:165:PHE:HB2	1:A:281:SER:O	2.09	0.53
1:B:176:GLY:O	1:B:177:LEU:HD23	2.09	0.53
1:B:192:THR:H	1:B:195:THR:CB	2.21	0.53
1:C:123:VAL:HG13	1:C:264:LEU:CD1	2.39	0.53
1:D:219:ASP:C	1:D:221:MET:N	2.64	0.53
1:D:305:TYR:CE2	1:E:231:PRO:HB2	2.44	0.53
1:D:320:PRO:O	1:D:321:MET:C	2.51	0.53
1:A:122:ALA:HB3	1:A:271:PRO:HD2	1.90	0.53
1:A:178:VAL:HG22	1:A:180:ASP:H	1.73	0.53
1:B:317:ASN:OD1	1:B:318:PRO:HD2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:HIS:HD2	1:D:88:ASP:OD2	1.92	0.53
1:D:207:VAL:O	1:D:208:LEU:HB2	2.09	0.53
1:E:115:ASP:HB3	1:E:317:ASN:H	1.73	0.53
1:A:131:GLY:O	1:A:134:SER:HB3	2.09	0.53
1:A:372:ARG:HB2	1:A:372:ARG:NH1	2.14	0.53
1:B:285:ILE:HD12	1:B:285:ILE:H	1.73	0.53
1:B:286:MET:HA	1:B:286:MET:CE	2.38	0.53
1:B:325:ILE:O	1:B:328:LEU:HB2	2.09	0.53
1:C:104:GLN:NE2	1:C:276:GLU:HB2	2.22	0.53
1:C:288:TRP:HB2	1:C:297:HIS:HB3	1.90	0.53
1:C:318:PRO:HB3	1:F:363:ASP:H	1.74	0.53
1:C:321:MET:O	1:C:324:LEU:HB2	2.08	0.53
1:D:54:ASN:HD22	1:D:303:PRO:HB3	1.73	0.53
1:D:218:LYS:O	1:D:219:ASP:CB	2.52	0.53
1:D:325:ILE:O	1:D:328:LEU:HB3	2.08	0.53
1:E:150:THR:HG21	1:E:292:ARG:HH21	1.73	0.53
1:A:88:ASP:OD1	1:E:139:HIS:HD2	1.91	0.53
1:C:54:ASN:ND2	1:D:207:VAL:HG23	2.24	0.53
1:D:125:VAL:HA	1:D:307:LYS:O	2.09	0.53
1:F:145:THR:HB	1:F:152:GLY:HA3	1.91	0.53
1:F:324:LEU:O	1:F:327:SER:HB2	2.08	0.53
1:B:46:VAL:HG12	1:B:47:THR:N	2.24	0.52
1:C:339:GLN:NE2	1:C:347:GLN:HE22	2.07	0.52
1:D:41:THR:HB	1:D:45:SER:OG	2.09	0.52
1:D:144:PRO:HD3	1:D:292:ARG:HG2	1.90	0.52
1:D:185:TYR:HB2	1:D:194:LYS:CE	2.39	0.52
1:F:178:VAL:CG2	1:F:179:THR:H	2.21	0.52
1:A:104:GLN:NE2	1:A:105:LEU:N	2.56	0.52
1:A:181:ALA:O	1:A:201:MET:HB2	2.10	0.52
1:A:305:TYR:CG	1:A:306:PHE:N	2.76	0.52
1:C:52:PHE:C	1:C:53:LEU:HD13	2.33	0.52
1:D:175:GLN:HG2	1:D:213:LYS:HG2	1.90	0.52
1:E:77:ARG:O	1:E:298:HIS:CG	2.61	0.52
1:E:258:THR:HB	1:E:259:LEU:CD2	2.35	0.52
1:F:161:GLN:OE1	1:F:251:PRO:HA	2.09	0.52
1:F:175:GLN:HG3	1:F:213:LYS:HZ2	1.73	0.52
1:A:76:SER:OG	1:A:299:TRP:HE3	1.93	0.52
1:A:88:ASP:OD2	1:A:183:THR:HG23	2.08	0.52
1:A:166:ALA:HA	1:A:238:ARG:O	2.09	0.52
1:B:308:ILE:N	1:B:308:ILE:CD1	2.67	0.52
1:D:54:ASN:HD22	1:D:55:PRO:HD2	1.72	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:165:PHE:HB2	1:D:282:CYS:HB3	1.91	0.52
1:F:84:SER:O	1:F:87:GLU:N	2.42	0.52
1:F:164:VAL:HA	1:F:240:PHE:O	2.09	0.52
1:F:176:GLY:O	1:F:177:LEU:HD23	2.09	0.52
1:A:178:VAL:HG11	1:A:201:MET:HE1	1.90	0.52
1:A:231:PRO:HG2	1:E:305:TYR:CD2	2.44	0.52
1:B:177:LEU:HD22	1:B:205:ASP:O	2.10	0.52
1:B:193:ILE:CD1	1:B:201:MET:SD	2.98	0.52
1:C:234:ASN:OD1	1:F:352:ARG:NH2	2.42	0.52
1:D:43:PRO:O	1:D:312:LYS:HB2	2.09	0.52
1:E:256:THR:OG1	1:E:257:ASN:N	2.43	0.52
1:E:368:ARG:CZ	1:E:377:LYS:HE3	2.40	0.52
1:F:166:ALA:HB2	1:F:239:TYR:CB	2.40	0.52
1:F:182:ARG:HG3	1:F:183:THR:N	2.20	0.52
1:F:193:ILE:C	1:F:197:THR:HG22	2.35	0.52
1:F:256:THR:OG1	1:F:257:ASN:N	2.41	0.52
1:A:75:TRP:CE2	1:A:300:ARG:HD2	2.45	0.52
1:A:133:GLY:HA3	1:B:228:HIS:HE1	1.74	0.52
1:A:150:THR:HG22	1:A:150:THR:O	2.09	0.52
1:A:196:ILE:HD12	1:A:196:ILE:O	2.10	0.52
1:A:234:ASN:N	1:A:234:ASN:HD22	2.08	0.52
1:C:43:PRO:CD	1:C:44:ASP:H	2.22	0.52
1:D:175:GLN:NE2	1:D:176:GLY:O	2.43	0.52
1:D:255:PHE:O	1:E:240:PHE:HA	2.10	0.52
1:E:232:ALA:C	1:E:234:ASN:N	2.68	0.52
1:F:103:LEU:HD22	1:F:103:LEU:N	2.25	0.52
1:F:350:GLU:HG3	1:F:351:VAL:H	1.74	0.52
1:A:30:ILE:CG1	1:A:36:VAL:HG13	2.40	0.52
1:A:69:GLY:C	1:A:71:GLN:N	2.66	0.52
1:A:141:PHE:HD2	1:B:84:SER:HA	1.71	0.52
1:B:339:GLN:HG2	1:B:340:PRO:HD2	1.91	0.52
1:C:193:ILE:HD12	1:C:193:ILE:N	2.24	0.52
1:D:124:SER:HA	1:D:261:THR:O	2.09	0.52
1:D:255:PHE:HB2	1:E:241:GLY:O	2.10	0.52
1:D:321:MET:O	1:D:322:ALA:C	2.53	0.52
1:E:265:ASP:H	1:E:270:GLY:N	2.03	0.52
1:E:304:ARG:HD3	1:E:306:PHE:CE1	2.45	0.52
1:F:35:GLU:O	1:F:36:VAL:C	2.53	0.52
1:F:321:MET:C	1:F:323:SER:H	2.18	0.52
1:A:35:GLU:O	1:A:36:VAL:C	2.52	0.52
1:A:104:GLN:HE21	1:A:105:LEU:N	2.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:LEU:HD22	1:A:173:ASP:O	2.10	0.52
1:B:71:GLN:NE2	1:B:73:TYR:HB2	2.19	0.52
1:B:135:LEU:N	1:B:135:LEU:CD1	2.72	0.52
1:B:275:GLY:C	1:B:277:GLY:N	2.66	0.52
1:B:371:ASP:C	1:B:373:PHE:N	2.68	0.52
1:C:71:GLN:NE2	1:C:73:TYR:H	2.07	0.52
1:C:94:THR:O	1:C:94:THR:HG22	2.09	0.52
1:C:132:SER:C	1:C:135:LEU:HD23	2.35	0.52
1:C:145:THR:OG1	1:C:153:ILE:N	2.43	0.52
1:C:366:MET:SD	1:F:319:TYR:CE1	3.03	0.52
1:D:306:PHE:HB3	1:D:308:ILE:HD11	1.92	0.52
1:E:239:TYR:CD1	1:E:239:TYR:C	2.85	0.52
1:F:265:ASP:CG	1:F:269:VAL:HB	2.34	0.52
1:A:54:ASN:HD22	1:A:55:PRO:HD2	1.74	0.52
1:B:211:ILE:N	1:B:211:ILE:CD1	2.73	0.52
1:C:28:LEU:HD23	1:C:28:LEU:C	2.35	0.52
1:D:105:LEU:HB3	1:D:120:TRP:CD1	2.45	0.52
1:E:165:PHE:HB2	1:E:281:SER:O	2.10	0.52
1:E:329:PHE:O	1:E:332:MET:HB2	2.09	0.52
1:E:350:GLU:CG	1:E:351:VAL:N	2.72	0.52
1:A:138:VAL:CB	1:A:153:ILE:HG23	2.38	0.52
1:B:108:LEU:HB3	1:B:118:GLN:HG3	1.90	0.52
1:C:52:PHE:C	1:C:52:PHE:CD2	2.88	0.52
1:E:141:PHE:C	1:E:292:ARG:HB2	2.35	0.52
1:F:57:MET:CB	1:F:96:PRO:HB3	2.35	0.52
1:F:125:VAL:HG13	1:F:125:VAL:O	2.09	0.52
1:F:172:LEU:HD22	1:F:173:ASP:H	1.69	0.52
1:A:63:PRO:HB2	1:A:69:GLY:HA3	1.91	0.52
1:D:30:ILE:CG1	1:D:36:VAL:HG13	2.40	0.52
1:D:77:ARG:NH2	2:J:3:SIA:O1B	2.43	0.52
1:D:300:ARG:NH2	1:E:206:GLN:O	2.42	0.52
1:F:161:GLN:CD	1:F:251:PRO:HA	2.35	0.52
1:A:162:TYR:HE1	1:E:255:PHE:HE2	1.58	0.51
1:A:185:TYR:CE2	1:A:226:ILE:HD11	2.45	0.51
1:C:54:ASN:HD21	1:D:208:LEU:CB	2.23	0.51
1:C:89:SER:OG	1:C:186:LYS:NZ	2.43	0.51
1:E:284:ASP:OD1	1:E:304:ARG:NH1	2.43	0.51
1:F:194:LYS:C	1:F:196:ILE:N	2.65	0.51
1:F:232:ALA:HB3	1:F:234:ASN:O	2.09	0.51
1:A:135:LEU:CD1	1:A:135:LEU:H	2.21	0.51
1:B:30:ILE:HG23	1:F:353:VAL:CG2	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:MET:CG	1:C:370:VAL:HG22	2.40	0.51
1:B:342:GLU:N	1:B:346:THR:HG23	2.24	0.51
1:C:28:LEU:HD21	1:C:30:ILE:C	2.36	0.51
1:C:168:GLY:CA	1:C:237:THR:HG23	2.27	0.51
1:D:50:GLU:HG2	1:D:305:TYR:OH	2.11	0.51
1:E:92:ASN:C	1:E:94:THR:H	2.19	0.51
1:E:288:TRP:CB	1:E:299:TRP:HB3	2.32	0.51
1:A:177:LEU:HD22	1:A:207:VAL:O	2.11	0.51
1:A:365:ASP:HB3	1:A:380:PHE:CE2	2.45	0.51
1:A:378:THR:HG22	1:A:379:VAL:O	2.11	0.51
1:C:363:ASP:HB3	1:C:366:MET:CE	2.40	0.51
1:D:71:GLN:NE2	1:D:71:GLN:HA	2.08	0.51
1:D:130:VAL:O	1:D:302:LEU:HD22	2.10	0.51
1:D:300:ARG:HG3	1:D:301:GLY:N	2.25	0.51
1:E:115:ASP:HB2	1:E:316:LYS:NZ	2.25	0.51
1:E:203:ASN:O	1:E:206:GLN:HB3	2.11	0.51
1:A:130:VAL:O	1:A:130:VAL:HG23	2.11	0.51
1:A:134:SER:HB3	1:A:135:LEU:HD12	1.93	0.51
1:A:257:ASN:HD22	1:B:238:ARG:HA	1.74	0.51
1:A:292:ARG:HD2	1:A:292:ARG:C	2.34	0.51
1:B:41:THR:HB	1:B:45:SER:OG	2.10	0.51
1:C:308:ILE:H	1:C:308:ILE:CD1	2.18	0.51
1:C:354:TYR:N	1:C:354:TYR:CD1	2.77	0.51
1:D:257:ASN:HD21	1:E:238:ARG:HA	1.76	0.51
1:E:50:GLU:HG2	1:E:305:TYR:OH	2.10	0.51
1:E:313:ARG:CG	1:E:313:ARG:NH1	2.72	0.51
1:E:321:MET:HG2	1:E:325:ILE:CD1	2.41	0.51
1:A:208:LEU:HD22	1:A:210:PRO:HG3	1.93	0.51
1:B:37:LEU:HD11	1:B:47:THR:HG21	1.93	0.51
1:B:339:GLN:HE21	1:B:347:GLN:CD	2.19	0.51
1:C:67:THR:OG1	1:C:68:GLU:N	2.43	0.51
1:C:75:TRP:HD1	1:C:299:TRP:O	1.93	0.51
1:D:98:TRP:N	1:D:222:TYR:O	2.39	0.51
1:D:327:SER:O	1:D:328:LEU:C	2.52	0.51
1:E:180:ASP:HA	1:E:206:GLN:NE2	2.26	0.51
1:E:193:ILE:CD1	1:E:193:ILE:H	2.23	0.51
1:F:191:VAL:HA	1:F:195:THR:HG21	1.92	0.51
2:K:2:GAL:H3	2:K:3:SIA:O1B	2.08	0.51
1:C:177:LEU:HD23	1:C:177:LEU:C	2.36	0.51
1:D:97:THR:HG22	1:D:223:PRO:N	2.26	0.51
1:E:97:THR:HG22	1:E:222:TYR:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:285:ILE:N	1:E:285:ILE:CD1	2.73	0.51
1:F:100:MET:HG2	1:F:216:LEU:HD13	1.93	0.51
1:F:190:VAL:HA	1:F:221:MET:HG3	1.93	0.51
1:A:204:LYS:C	1:A:209:ASN:HB2	2.36	0.51
1:A:328:LEU:CD2	1:A:328:LEU:C	2.80	0.51
1:C:165:PHE:O	1:C:239:TYR:HA	2.10	0.51
1:D:192:THR:O	1:D:195:THR:HB	2.11	0.51
1:D:257:ASN:HB3	1:E:239:TYR:CZ	2.45	0.51
1:E:259:LEU:N	1:E:259:LEU:CD2	2.73	0.51
1:E:293:ASN:OD1	1:E:294:TYR:N	2.43	0.51
1:F:342:GLU:HG2	1:F:343:GLY:N	2.26	0.51
1:A:169:GLY:HA2	1:A:273:CYS:HA	1.93	0.51
1:A:180:ASP:OD1	1:A:182:ARG:HD2	2.11	0.51
1:A:256:THR:OG1	1:A:257:ASN:N	2.44	0.51
1:B:181:ALA:H	1:B:206:GLN:HE21	1.58	0.51
1:B:222:TYR:N	1:B:222:TYR:CD1	2.78	0.51
1:B:288:TRP:CZ3	1:B:299:TRP:NE1	2.78	0.51
1:D:52:PHE:HB2	1:D:304:ARG:O	2.11	0.51
1:E:83:THR:HG22	1:E:84:SER:N	2.26	0.51
1:F:37:LEU:HD11	1:F:47:THR:HG21	1.92	0.51
1:F:141:PHE:CD1	1:F:292:ARG:HG3	2.46	0.51
1:A:63:PRO:O	1:A:71:GLN:NE2	2.44	0.51
1:A:164:VAL:HG23	1:A:283:VAL:CG2	2.40	0.51
1:A:362:GLY:O	1:A:363:ASP:C	2.52	0.51
1:B:271:PRO:C	1:B:272:LEU:HD12	2.35	0.51
1:B:373:PHE:N	1:B:373:PHE:CD1	2.77	0.51
1:C:162:TYR:CE2	1:C:224:VAL:HG11	2.46	0.51
1:D:100:MET:C	1:D:100:MET:SD	2.94	0.51
1:D:145:THR:HG21	1:E:297:HIS:CE1	2.46	0.51
1:D:246:GLY:HA3	1:D:249:THR:OG1	2.11	0.51
1:E:223:PRO:CG	1:E:226:ILE:HD12	2.40	0.51
1:B:265:ASP:H	1:B:270:GLY:N	2.07	0.51
1:D:142:ASN:HA	1:D:290:VAL:O	2.11	0.51
1:E:194:LYS:C	1:E:196:ILE:N	2.68	0.51
1:E:308:ILE:N	1:E:308:ILE:CD1	2.74	0.51
1:A:40:VAL:HG12	1:A:42:GLY:H	1.75	0.50
1:A:177:LEU:HD12	1:E:131:GLY:HA3	1.92	0.50
1:A:280:LEU:CD2	1:A:280:LEU:N	2.74	0.50
1:A:340:PRO:CG	1:A:347:GLN:HE22	2.21	0.50
1:B:109:ASN:H	1:B:118:GLN:HE21	1.58	0.50
1:B:372:ARG:C	1:B:373:PHE:CD1	2.89	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:243:TYR:CZ	1:C:245:GLY:HA2	2.45	0.50
1:D:91:GLY:H	1:D:186:LYS:HE3	1.76	0.50
1:D:106:PRO:HD2	1:D:120:TRP:NE1	2.25	0.50
1:A:87:GLU:HA	1:A:184:LYS:HZ2	1.75	0.50
1:A:211:ILE:N	1:A:211:ILE:HD12	2.25	0.50
1:A:293:ASN:CG	1:A:294:TYR:N	2.69	0.50
1:B:76:SER:O	1:B:298:HIS:HB2	2.10	0.50
1:B:82:ALA:HB1	1:B:88:ASP:HA	1.93	0.50
1:B:105:LEU:HD23	1:B:120:TRP:CG	2.46	0.50
1:B:143:LYS:HA	1:B:292:ARG:HA	1.92	0.50
1:C:105:LEU:CB	1:C:120:TRP:CD1	2.94	0.50
1:E:174:LEU:HD13	1:E:227:TRP:CE3	2.46	0.50
1:F:170:GLU:HB2	1:F:171:PRO:HD2	1.92	0.50
1:F:205:ASP:CA	1:F:209:ASN:HB2	2.32	0.50
1:F:306:PHE:N	1:F:306:PHE:HD1	2.07	0.50
1:F:341:MET:CE	1:F:347:GLN:HB2	2.26	0.50
1:A:178:VAL:CG2	1:A:179:THR:N	2.74	0.50
1:A:233:LYS:HE2	1:A:234:ASN:HD21	1.76	0.50
1:A:305:TYR:CD1	1:A:306:PHE:N	2.79	0.50
1:A:306:PHE:HB3	1:A:308:ILE:CD1	2.40	0.50
1:A:367:THR:HB	1:A:378:THR:OG1	2.11	0.50
1:C:28:LEU:HD23	1:C:29:LEU:C	2.37	0.50
1:C:172:LEU:HB3	1:C:216:LEU:HD12	1.93	0.50
1:C:174:LEU:N	1:C:174:LEU:CD1	2.72	0.50
1:D:288:TRP:CD1	1:D:288:TRP:N	2.75	0.50
1:E:35:GLU:HG2	1:E:36:VAL:N	2.26	0.50
1:E:207:VAL:HG23	1:E:208:LEU:H	1.76	0.50
1:E:291:THR:OG1	1:E:296:VAL:HB	2.11	0.50
1:E:351:VAL:HG12	1:E:352:ARG:N	2.27	0.50
1:F:300:ARG:CG	1:F:301:GLY:N	2.74	0.50
1:A:194:LYS:O	1:A:198:LYS:N	2.45	0.50
1:A:350:GLU:CG	1:A:351:VAL:H	2.25	0.50
1:B:57:MET:HE1	1:B:285:ILE:HG13	1.93	0.50
1:B:139:HIS:HD2	1:C:88:ASP:OD2	1.94	0.50
1:B:318:PRO:HB2	1:B:319:TYR:CZ	2.46	0.50
1:D:28:LEU:CG	1:D:29:LEU:N	2.73	0.50
1:D:54:ASN:HD21	1:E:208:LEU:HB2	1.76	0.50
1:D:181:ALA:HA	1:D:201:MET:CE	2.41	0.50
1:E:178:VAL:CG2	1:E:179:THR:N	2.75	0.50
1:E:349:GLU:O	1:E:350:GLU:HB2	2.11	0.50
1:F:135:LEU:HD22	1:F:135:LEU:N	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:136:LEU:O	1:F:138:VAL:HG22	2.11	0.50
1:B:150:THR:O	1:B:150:THR:HG22	2.11	0.50
1:B:193:ILE:HD13	1:B:201:MET:HG2	1.94	0.50
1:B:219:ASP:C	1:B:221:MET:N	2.66	0.50
1:B:288:TRP:HA	1:B:299:TRP:HA	1.93	0.50
1:B:367:THR:HG22	1:B:368:ARG:H	1.77	0.50
1:C:288:TRP:CE3	1:C:299:TRP:CD1	3.00	0.50
1:D:263:LEU:O	1:D:270:GLY:HA2	2.12	0.50
1:D:289:ARG:O	1:D:297:HIS:O	2.30	0.50
1:D:305:TYR:CG	1:D:306:PHE:N	2.79	0.50
1:E:105:LEU:HD12	1:E:105:LEU:H	1.73	0.50
1:E:181:ALA:H	1:E:206:GLN:HE21	1.57	0.50
1:F:90:PRO:HG2	1:F:185:TYR:CD1	2.47	0.50
1:F:180:ASP:HB3	1:F:182:ARG:HG2	1.94	0.50
1:A:194:LYS:HB2	1:A:198:LYS:O	2.12	0.50
1:A:245:GLY:O	1:A:249:THR:HG21	2.12	0.50
1:A:265:ASP:H	1:A:270:GLY:N	2.09	0.50
1:B:69:GLY:O	1:B:71:GLN:N	2.44	0.50
1:B:123:VAL:HG13	1:B:264:LEU:HD13	1.92	0.50
1:C:186:LYS:H	1:C:186:LYS:CE	2.25	0.50
1:C:233:LYS:HE3	1:F:350:GLU:HB3	1.94	0.50
1:E:65:SER:HB3	1:E:68:GLU:OE2	2.12	0.50
1:E:138:VAL:O	1:E:153:ILE:HG23	2.12	0.50
1:E:346:THR:HG22	1:E:348:VAL:H	1.76	0.50
1:A:94:THR:O	1:A:94:THR:HG22	2.12	0.50
1:A:265:ASP:OD1	1:A:269:VAL:N	2.44	0.50
1:A:305:TYR:C	1:A:306:PHE:CD1	2.90	0.50
1:B:108:LEU:HD11	1:B:120:TRP:CE2	2.47	0.50
1:B:350:GLU:HG2	1:B:352:ARG:HH21	1.76	0.50
1:C:69:GLY:HA3	1:C:71:GLN:OE1	2.11	0.50
1:D:56:ARG:NH2	1:D:219:ASP:OD2	2.45	0.50
1:D:83:THR:HG22	1:D:84:SER:N	2.26	0.50
1:D:274:LYS:C	1:D:275:GLY:O	2.51	0.50
1:B:76:SER:CB	1:B:299:TRP:HE3	2.24	0.50
1:B:364:PRO:HG2	1:B:365:ASP:N	2.26	0.50
1:C:57:MET:HE1	1:C:300:ARG:CA	2.42	0.50
1:C:71:GLN:HG3	1:D:203:ASN:CB	2.23	0.50
1:C:186:LYS:H	1:C:186:LYS:HE2	1.77	0.50
1:C:320:PRO:C	1:C:322:ALA:N	2.69	0.50
1:D:69:GLY:C	1:D:71:GLN:N	2.69	0.50
1:D:180:ASP:CG	1:D:182:ARG:HD3	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:329:PHE:O	1:E:332:MET:N	2.43	0.50
1:F:19:CYS:CB	1:F:20:PRO:CD	2.89	0.50
1:A:61:PRO:HG2	1:A:62:THR:H	1.76	0.50
1:A:272:LEU:O	1:A:274:LYS:N	2.45	0.50
1:B:104:GLN:NE2	1:B:105:LEU:N	2.59	0.50
1:B:165:PHE:HA	1:B:282:CYS:HA	1.94	0.50
1:C:91:GLY:H	1:C:186:LYS:HE3	1.77	0.50
1:C:109:ASN:HB3	1:C:117:LEU:CD2	2.42	0.50
1:C:233:LYS:CD	1:C:234:ASN:N	2.73	0.50
1:D:123:VAL:O	1:D:263:LEU:N	2.44	0.50
1:E:69:GLY:O	1:E:71:GLN:N	2.45	0.50
1:F:28:LEU:HD21	1:F:30:ILE:C	2.37	0.50
1:F:243:TYR:CZ	1:F:245:GLY:HA2	2.47	0.50
1:A:207:VAL:HB	1:E:54:ASN:ND2	2.26	0.49
1:B:185:TYR:HD2	1:B:192:THR:HG21	1.76	0.49
1:C:103:LEU:HD22	1:C:103:LEU:N	2.26	0.49
1:C:129:VAL:HB	1:C:253:LEU:HD21	1.93	0.49
1:E:90:PRO:HD2	1:E:186:LYS:HZ1	1.74	0.49
1:E:325:ILE:O	1:E:326:SER:C	2.55	0.49
1:E:368:ARG:HG3	1:E:376:THR:O	2.12	0.49
1:A:79:ILE:HD11	1:A:298:HIS:N	2.27	0.49
1:B:75:TRP:CE2	1:B:300:ARG:HD2	2.47	0.49
1:B:101:ALA:HB2	1:F:339:GLN:HB2	1.94	0.49
1:B:103:LEU:O	1:B:277:GLY:HA2	2.10	0.49
1:B:111:ASP:C	1:B:113:THR:N	2.69	0.49
1:B:265:ASP:HB3	1:B:270:GLY:N	2.26	0.49
1:B:276:GLU:CD	1:B:276:GLU:N	2.69	0.49
1:C:288:TRP:CZ3	1:C:299:TRP:NE1	2.80	0.49
1:D:103:LEU:N	1:D:103:LEU:CD2	2.76	0.49
1:D:145:THR:OG1	1:D:153:ILE:N	2.44	0.49
1:D:217:ASP:OD1	1:D:218:LYS:N	2.44	0.49
1:A:116:THR:HA	1:A:315:VAL:O	2.12	0.49
1:A:147:THR:OG1	1:A:148:VAL:N	2.45	0.49
1:A:190:VAL:HG23	1:A:223:PRO:HD3	1.94	0.49
1:A:298:HIS:N	1:A:298:HIS:HD2	2.07	0.49
1:B:35:GLU:O	1:B:38:ASP:HB2	2.11	0.49
1:C:54:ASN:ND2	1:D:207:VAL:O	2.45	0.49
1:D:275:GLY:C	1:D:277:GLY:H	2.21	0.49
1:E:194:LYS:H	1:E:194:LYS:CD	2.25	0.49
1:A:75:TRP:CZ2	1:A:300:ARG:HD2	2.47	0.49
1:A:167:VAL:C	1:A:237:THR:HG23	2.36	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:ARG:HA	1:E:257:ASN:ND2	2.26	0.49
1:A:339:GLN:HG2	1:A:347:GLN:NE2	2.27	0.49
1:C:25:VAL:CG1	1:C:26:PRO:HD2	2.43	0.49
1:D:30:ILE:HG12	1:D:36:VAL:HG13	1.93	0.49
1:E:72:TYR:O	1:E:75:TRP:HB2	2.12	0.49
1:E:124:SER:HB2	1:E:260:THR:HG22	1.93	0.49
1:E:125:VAL:CG1	1:E:263:LEU:HD21	2.43	0.49
1:E:126:LYS:HG2	1:E:260:THR:HG23	1.93	0.49
1:F:25:VAL:HG12	1:F:26:PRO:HD2	1.94	0.49
1:F:150:THR:O	1:F:150:THR:CG2	2.55	0.49
1:A:58:GLY:HA3	1:A:76:SER:HA	1.94	0.49
1:A:105:LEU:N	1:A:105:LEU:HD12	2.26	0.49
1:A:253:LEU:O	1:B:242:ASN:HB2	2.13	0.49
1:C:287:GLY:O	1:C:299:TRP:HA	2.13	0.49
1:E:143:LYS:NZ	1:E:295:ASP:OD2	2.45	0.49
1:E:175:GLN:HA	1:E:213:LYS:HA	1.94	0.49
1:F:69:GLY:C	1:F:71:GLN:N	2.66	0.49
1:F:79:ILE:HG21	1:F:297:HIS:H	1.76	0.49
1:A:52:PHE:HA	1:A:304:ARG:O	2.12	0.49
1:B:54:ASN:HD22	1:B:55:PRO:HD3	1.76	0.49
1:B:60:PRO:HB2	1:B:61:PRO:HD2	1.94	0.49
1:B:178:VAL:CG2	1:B:179:THR:N	2.75	0.49
1:C:211:ILE:N	1:C:211:ILE:CD1	2.76	0.49
1:D:150:THR:HG22	1:D:150:THR:O	2.13	0.49
1:E:178:VAL:HG22	1:E:179:THR:H	1.75	0.49
1:E:258:THR:CB	1:E:259:LEU:HD22	2.36	0.49
1:E:333:LEU:HD22	1:E:333:LEU:N	2.27	0.49
1:E:370:VAL:HG22	1:E:375:LYS:CA	2.42	0.49
1:F:164:VAL:HG22	1:F:241:GLY:HA3	1.95	0.49
1:F:166:ALA:HB2	1:F:239:TYR:HB3	1.94	0.49
1:B:104:GLN:NE2	1:B:105:LEU:H	2.11	0.49
1:B:177:LEU:HD21	1:B:209:ASN:H	1.76	0.49
1:B:359:PRO:O	1:B:360:VAL:C	2.56	0.49
1:C:41:THR:HB	1:C:312:LYS:HE3	1.95	0.49
1:C:76:SER:HB2	1:C:298:HIS:HB2	1.95	0.49
1:C:264:LEU:HD23	1:C:268:GLY:HA2	1.95	0.49
1:D:69:GLY:HA3	1:D:71:GLN:OE1	2.13	0.49
1:D:145:THR:OG1	1:D:153:ILE:HB	2.12	0.49
1:D:152:GLY:HA2	1:E:295:ASP:O	2.12	0.49
1:D:305:TYR:C	1:D:306:PHE:CD1	2.91	0.49
1:E:94:THR:O	1:E:95:LEU:HD23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:125:VAL:HB	1:E:263:LEU:HD11	1.95	0.49
1:E:141:PHE:CD1	1:E:292:ARG:HG3	2.47	0.49
1:F:69:GLY:O	1:F:71:GLN:N	2.45	0.49
1:B:30:ILE:O	1:F:353:VAL:HG22	2.13	0.49
1:C:132:SER:HA	1:C:135:LEU:HD23	1.94	0.49
1:D:168:GLY:N	1:D:237:THR:HG23	2.26	0.49
1:E:261:THR:HG22	1:E:262:VAL:N	2.26	0.49
1:F:104:GLN:NE2	1:F:276:GLU:HB2	2.16	0.49
1:A:180:ASP:CG	1:A:182:ARG:HD2	2.37	0.49
1:C:180:ASP:HA	1:C:206:GLN:NE2	2.28	0.49
1:C:208:LEU:HA	1:C:208:LEU:HD12	1.35	0.49
1:C:276:GLU:OE1	1:C:276:GLU:HA	2.11	0.49
1:D:169:GLY:HA3	1:D:272:LEU:O	2.13	0.49
1:D:321:MET:HE3	1:D:324:LEU:HD11	1.94	0.49
1:E:34:MET:O	1:E:37:LEU:HD22	2.13	0.49
1:E:61:PRO:HG2	1:E:62:THR:H	1.78	0.49
1:E:305:TYR:C	1:E:306:PHE:CD1	2.91	0.49
1:F:66:LEU:HB3	1:F:71:GLN:HB2	1.95	0.49
1:F:97:THR:HG22	1:F:222:TYR:O	2.13	0.49
1:A:84:SER:O	1:A:87:GLU:N	2.45	0.49
1:A:88:ASP:C	1:A:184:LYS:HD3	2.38	0.49
1:A:144:PRO:HB2	1:A:146:ASP:O	2.13	0.49
1:A:224:VAL:CG1	1:A:283:VAL:HG11	2.42	0.49
1:C:236:ASN:OD1	1:C:271:PRO:HA	2.12	0.49
1:D:57:MET:O	1:D:57:MET:HG3	2.13	0.49
1:D:161:GLN:HE22	1:D:251:PRO:HA	1.77	0.49
1:D:181:ALA:O	1:D:201:MET:HE2	2.13	0.49
1:E:62:THR:OG1	1:E:63:PRO:CD	2.56	0.49
1:E:180:ASP:CG	1:E:182:ARG:HG2	2.38	0.49
1:E:319:TYR:HB3	1:E:320:PRO:HD2	1.94	0.49
1:F:75:TRP:CZ2	1:F:300:ARG:HD2	2.48	0.49
1:F:93:ASN:N	1:F:93:ASN:OD1	2.45	0.49
1:F:285:ILE:HD12	1:F:285:ILE:H	1.78	0.49
1:A:83:THR:HB	1:A:87:GLU:CB	2.37	0.48
1:B:105:LEU:HB3	1:B:120:TRP:NE1	2.29	0.48
1:C:54:ASN:ND2	1:D:208:LEU:HB3	2.25	0.48
1:C:205:ASP:OD1	1:C:209:ASN:ND2	2.46	0.48
1:D:103:LEU:HB2	1:D:278:LEU:HB3	1.94	0.48
1:D:288:TRP:CD1	1:D:288:TRP:H	2.30	0.48
1:E:57:MET:HA	1:E:96:PRO:HA	1.94	0.48
1:E:123:VAL:HG13	1:E:264:LEU:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:209:ASN:HB3	1:F:212:SER:OG	2.13	0.48
1:F:252:VAL:O	1:F:253:LEU:HD12	2.13	0.48
1:A:141:PHE:CZ	1:A:292:ARG:HG3	2.48	0.48
1:A:233:LYS:CE	1:A:234:ASN:ND2	2.75	0.48
1:B:50:GLU:OE2	1:C:233:LYS:HB2	2.12	0.48
1:B:350:GLU:HG3	1:B:351:VAL:N	2.27	0.48
1:B:378:THR:CG2	1:B:379:VAL:N	2.76	0.48
1:C:83:THR:HB	1:C:87:GLU:HB3	1.95	0.48
1:D:181:ALA:C	1:D:201:MET:HE2	2.38	0.48
1:E:168:GLY:HA3	1:E:237:THR:CG2	2.38	0.48
1:E:171:PRO:HG2	1:E:215:LYS:HD2	1.95	0.48
1:E:320:PRO:O	1:E:324:LEU:HD12	2.13	0.48
1:E:342:GLU:HG2	1:E:343:GLY:H	1.77	0.48
1:F:43:PRO:HA	1:F:312:LYS:HD3	1.94	0.48
1:F:141:PHE:CE1	1:F:292:ARG:HG3	2.46	0.48
1:F:192:THR:HG21	1:F:194:LYS:HE2	1.96	0.48
1:F:219:ASP:C	1:F:221:MET:N	2.68	0.48
1:B:52:PHE:CD2	1:C:208:LEU:HD23	2.48	0.48
1:C:166:ALA:HB2	1:C:239:TYR:CB	2.44	0.48
1:C:166:ALA:HA	1:C:238:ARG:O	2.13	0.48
1:C:329:PHE:HA	1:C:332:MET:HG2	1.95	0.48
1:D:142:ASN:N	1:D:154:SER:OG	2.41	0.48
1:D:264:LEU:HG	1:D:268:GLY:HA2	1.96	0.48
1:E:75:TRP:CE2	1:E:300:ARG:HB2	2.49	0.48
1:F:172:LEU:HD13	1:F:174:LEU:HG	1.95	0.48
1:F:254:GLN:OE1	1:F:254:GLN:HA	2.14	0.48
1:F:269:VAL:HA	1:F:313:ARG:NH2	2.29	0.48
1:A:105:LEU:HB3	1:A:120:TRP:CD1	2.49	0.48
1:B:165:PHE:CD1	1:B:166:ALA:N	2.81	0.48
1:C:170:GLU:HB2	1:C:171:PRO:HD2	1.95	0.48
1:D:327:SER:O	1:D:330:ASN:N	2.46	0.48
1:E:192:THR:O	1:E:196:ILE:HG22	2.14	0.48
1:F:216:LEU:HD23	1:F:216:LEU:HA	1.71	0.48
1:A:56:ARG:CB	1:A:56:ARG:HH11	2.26	0.48
1:A:142:ASN:C	1:A:292:ARG:HB2	2.39	0.48
1:A:229:PRO:O	1:A:229:PRO:HG2	2.13	0.48
1:A:269:VAL:HG22	1:A:313:ARG:HH12	1.79	0.48
1:A:280:LEU:HD11	1:A:308:ILE:HD11	1.96	0.48
1:B:35:GLU:O	1:B:36:VAL:C	2.55	0.48
1:B:239:TYR:C	1:B:239:TYR:CD1	2.92	0.48
1:C:194:LYS:O	1:C:196:ILE:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:354:TYR:N	1:C:354:TYR:HD1	2.12	0.48
1:D:182:ARG:O	1:D:183:THR:C	2.57	0.48
1:D:236:ASN:OD1	1:D:271:PRO:HA	2.13	0.48
1:D:348:VAL:O	1:D:348:VAL:HG12	2.13	0.48
1:F:111:ASP:C	1:F:113:THR:N	2.71	0.48
1:F:175:GLN:CB	1:F:230:ASP:HB2	2.24	0.48
1:F:193:ILE:HD11	1:F:201:MET:SD	2.54	0.48
1:A:174:LEU:HB2	1:A:228:HIS:O	2.12	0.48
1:A:208:LEU:O	1:A:210:PRO:HD3	2.13	0.48
1:A:303:PRO:HG3	1:B:207:VAL:O	2.13	0.48
1:B:164:VAL:HG22	1:B:241:GLY:HA3	1.94	0.48
1:B:243:TYR:CZ	1:B:245:GLY:CA	2.96	0.48
1:D:175:GLN:HG3	1:D:213:LYS:HG2	1.95	0.48
1:E:104:GLN:HA	1:E:104:GLN:NE2	2.28	0.48
1:E:286:MET:HA	1:E:286:MET:CE	2.40	0.48
1:F:55:PRO:HD3	1:F:303:PRO:HA	1.96	0.48
1:F:236:ASN:ND2	1:F:272:LEU:O	2.46	0.48
1:F:322:ALA:C	1:F:324:LEU:N	2.70	0.48
1:B:50:GLU:HG2	1:C:233:LYS:CA	2.42	0.48
1:B:60:PRO:CB	1:B:61:PRO:HD2	2.44	0.48
1:B:290:VAL:HG22	1:B:297:HIS:HD2	1.77	0.48
1:C:346:THR:HG22	1:C:348:VAL:CG2	2.43	0.48
1:D:19:CYS:SG	1:E:112:LEU:CD2	2.96	0.48
1:D:207:VAL:O	1:D:208:LEU:CB	2.61	0.48
1:D:228:HIS:HB3	1:D:229:PRO:HD2	1.95	0.48
1:E:109:ASN:OD1	1:E:117:LEU:HD22	2.13	0.48
1:E:175:GLN:CB	1:E:230:ASP:HB2	2.44	0.48
1:F:41:THR:HB	1:F:45:SER:OG	2.13	0.48
1:F:305:TYR:C	1:F:305:TYR:CD1	2.90	0.48
1:A:92:ASN:HD21	1:A:190:VAL:HG12	1.79	0.48
1:A:285:ILE:N	1:A:285:ILE:CD1	2.77	0.48
1:B:194:LYS:CG	1:B:195:THR:H	2.20	0.48
1:B:311:ARG:HH21	1:B:313:ARG:NH2	2.12	0.48
1:E:108:LEU:HD12	1:E:108:LEU:N	2.28	0.48
1:E:161:GLN:CD	1:E:251:PRO:HA	2.39	0.48
1:F:25:VAL:CG1	1:F:26:PRO:HD2	2.44	0.48
1:A:142:ASN:ND2	1:A:289:ARG:HG3	2.29	0.48
1:A:239:TYR:CE1	1:E:257:ASN:CB	2.97	0.48
1:A:261:THR:HG22	1:A:262:VAL:N	2.27	0.48
1:B:134:SER:OG	1:C:179:THR:HG23	2.13	0.48
1:D:79:ILE:HG12	1:D:298:HIS:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:300:ARG:CG	1:E:301:GLY:N	2.76	0.48
1:A:84:SER:O	1:A:86:THR:N	2.47	0.48
1:A:194:LYS:HD3	1:A:194:LYS:H	1.79	0.48
1:D:54:ASN:HD22	1:D:54:ASN:HA	1.64	0.48
1:D:133:GLY:HA3	1:E:228:HIS:CE1	2.49	0.48
1:D:257:ASN:ND2	1:E:239:TYR:N	2.58	0.48
1:E:160:SER:HA	1:E:244:THR:O	2.13	0.48
1:E:259:LEU:HA	1:E:259:LEU:HD13	1.49	0.48
1:E:322:ALA:O	1:E:323:SER:C	2.56	0.48
1:F:164:VAL:HA	1:F:241:GLY:HA3	1.94	0.48
1:B:108:LEU:N	1:B:108:LEU:CD1	2.77	0.47
1:B:164:VAL:CG1	1:B:165:PHE:N	2.77	0.47
1:B:305:TYR:CG	1:B:306:PHE:N	2.82	0.47
1:C:194:LYS:HD3	1:C:194:LYS:H	1.79	0.47
1:C:194:LYS:HA	1:C:197:THR:HG22	1.96	0.47
1:C:300:ARG:NH2	1:D:206:GLN:O	2.46	0.47
1:D:258:THR:O	1:D:259:LEU:HD22	2.13	0.47
1:D:278:LEU:C	1:D:278:LEU:CD2	2.87	0.47
1:E:115:ASP:HB2	1:E:316:LYS:HZ3	1.79	0.47
1:E:364:PRO:C	1:E:366:MET:H	2.21	0.47
1:F:30:ILE:HD11	1:F:36:VAL:HG22	1.94	0.47
1:F:109:ASN:OD1	1:F:109:ASN:N	2.47	0.47
1:F:185:TYR:CD2	1:F:192:THR:HG21	2.49	0.47
1:B:84:SER:O	1:B:87:GLU:N	2.45	0.47
1:B:209:ASN:C	1:B:211:ILE:H	2.21	0.47
1:B:217:ASP:C	1:B:218:LYS:HD2	2.38	0.47
1:B:250:PRO:HA	1:B:251:PRO:HD3	1.62	0.47
1:B:262:VAL:C	1:B:264:LEU:N	2.72	0.47
1:B:288:TRP:HZ3	1:B:299:TRP:NE1	2.11	0.47
1:C:186:LYS:H	1:C:186:LYS:HD2	1.79	0.47
1:C:194:LYS:HG2	1:C:195:THR:N	2.29	0.47
1:E:115:ASP:HB3	1:E:316:LYS:HD3	1.95	0.47
1:E:204:LYS:O	1:E:208:LEU:N	2.47	0.47
1:E:332:MET:HA	1:E:332:MET:HE3	1.96	0.47
1:A:69:GLY:CA	1:A:71:GLN:NE2	2.74	0.47
1:A:96:PRO:HD2	1:A:299:TRP:CH2	2.48	0.47
1:A:175:GLN:HB2	1:A:230:ASP:HB2	1.92	0.47
1:A:181:ALA:H	1:A:206:GLN:HE21	1.61	0.47
1:A:257:ASN:HB2	1:B:239:TYR:CD2	2.49	0.47
1:A:268:GLY:O	1:A:313:ARG:NH2	2.46	0.47
1:B:35:GLU:HG2	1:B:36:VAL:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:105:LEU:HD23	1:D:120:TRP:CD1	2.49	0.47
1:E:100:MET:HG2	1:E:216:LEU:HD13	1.96	0.47
1:E:219:ASP:C	1:E:221:MET:N	2.68	0.47
1:E:287:GLY:O	1:E:299:TRP:HB2	2.14	0.47
1:F:233:LYS:HB2	1:F:233:LYS:HE3	1.60	0.47
1:F:293:ASN:OD1	1:F:294:TYR:N	2.47	0.47
1:A:72:TYR:O	1:A:75:TRP:N	2.47	0.47
1:A:105:LEU:HB3	1:A:106:PRO:CD	2.45	0.47
1:A:135:LEU:HD12	1:A:135:LEU:H	1.78	0.47
1:B:22:PRO:HG2	1:F:359:PRO:CB	2.40	0.47
1:B:305:TYR:CE1	1:B:307:LYS:HB2	2.49	0.47
1:C:30:ILE:HD11	1:C:36:VAL:HG22	1.95	0.47
1:C:238:ARG:HH21	1:C:270:GLY:HA2	1.80	0.47
1:E:46:VAL:CG1	1:E:47:THR:N	2.77	0.47
1:F:78:GLY:HA3	2:L:2:GAL:H4	1.97	0.47
1:A:72:TYR:O	1:A:73:TYR:C	2.58	0.47
1:A:93:ASN:N	1:A:93:ASN:OD1	2.46	0.47
1:A:245:GLY:HA3	1:E:251:PRO:HD2	1.97	0.47
1:A:308:ILE:N	1:A:308:ILE:CD1	2.73	0.47
1:B:52:PHE:CZ	1:F:347:GLN:HB3	2.50	0.47
1:B:358:GLU:HG3	1:B:359:PRO:O	2.14	0.47
1:C:133:GLY:O	1:C:135:LEU:N	2.47	0.47
1:C:210:PRO:HA	1:C:213:LYS:HE2	1.96	0.47
1:C:302:LEU:HB3	1:C:303:PRO:HD2	1.96	0.47
1:D:161:GLN:NE2	1:D:251:PRO:HA	2.29	0.47
1:D:175:GLN:HG3	1:D:213:LYS:NZ	2.30	0.47
1:F:339:GLN:CB	1:F:340:PRO:HD2	2.43	0.47
1:A:56:ARG:NH1	1:A:219:ASP:OD1	2.48	0.47
1:A:90:PRO:HD2	1:A:186:LYS:HE3	1.97	0.47
1:A:100:MET:HB3	1:A:216:LEU:HD13	1.96	0.47
1:B:54:ASN:HD22	1:B:55:PRO:CD	2.27	0.47
1:C:57:MET:HE1	1:C:300:ARG:HA	1.96	0.47
1:C:111:ASP:C	1:C:113:THR:H	2.23	0.47
1:C:112:LEU:HD22	1:C:112:LEU:N	2.27	0.47
1:C:133:GLY:C	1:C:135:LEU:H	2.23	0.47
1:C:350:GLU:OE1	1:C:352:ARG:NH1	2.48	0.47
1:C:367:THR:HB	1:C:372:ARG:HB2	1.95	0.47
1:D:54:ASN:HD21	1:E:208:LEU:HB3	1.79	0.47
1:D:133:GLY:CA	1:E:228:HIS:CE1	2.98	0.47
1:E:69:GLY:C	1:E:71:GLN:N	2.72	0.47
1:E:248:THR:O	1:E:249:THR:C	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:100:MET:SD	1:F:101:ALA:N	2.87	0.47
1:F:211:ILE:N	1:F:211:ILE:CD1	2.78	0.47
1:A:145:THR:HB	1:A:152:GLY:HA3	1.97	0.47
1:A:209:ASN:ND2	1:A:212:SER:OG	2.47	0.47
1:A:233:LYS:HE2	1:E:31:LYS:HD2	1.97	0.47
1:B:63:PRO:HB2	1:B:69:GLY:HA3	1.97	0.47
1:B:134:SER:C	1:B:136:LEU:H	2.22	0.47
1:C:71:GLN:CG	1:D:203:ASN:HB3	2.24	0.47
1:C:77:ARG:O	1:C:298:HIS:CD2	2.68	0.47
1:C:105:LEU:HB3	1:C:106:PRO:HD2	1.97	0.47
1:C:133:GLY:C	1:C:135:LEU:N	2.72	0.47
1:C:194:LYS:O	1:C:195:THR:C	2.57	0.47
1:C:360:VAL:O	1:F:316:LYS:N	2.45	0.47
1:D:100:MET:HG2	1:D:216:LEU:HD13	1.96	0.47
1:D:193:ILE:CD1	1:D:193:ILE:H	2.26	0.47
1:D:279:TYR:N	1:D:279:TYR:CD1	2.82	0.47
1:E:211:ILE:HD12	1:E:211:ILE:N	2.30	0.47
1:E:239:TYR:C	1:E:240:PHE:CG	2.91	0.47
1:F:30:ILE:CG2	1:F:36:VAL:HG13	2.44	0.47
1:F:39:LEU:HG	1:F:40:VAL:N	2.25	0.47
1:F:117:LEU:C	1:F:314:TRP:CE3	2.93	0.47
1:F:265:ASP:OD1	1:F:269:VAL:N	2.48	0.47
1:A:194:LYS:O	1:A:195:THR:C	2.58	0.47
1:A:313:ARG:HG2	1:A:314:TRP:N	2.30	0.47
1:B:262:VAL:HG12	1:B:264:LEU:CB	2.44	0.47
1:B:341:MET:HE1	1:B:348:VAL:N	2.30	0.47
1:C:72:TYR:O	1:C:73:TYR:C	2.56	0.47
1:C:131:GLY:C	1:C:133:GLY:N	2.70	0.47
1:C:243:TYR:CZ	1:C:245:GLY:CA	2.98	0.47
1:D:25:VAL:HG23	1:D:26:PRO:N	2.29	0.47
1:D:120:TRP:O	1:D:272:LEU:HA	2.15	0.47
1:D:308:ILE:HG22	1:D:310:LEU:HG	1.97	0.47
1:B:152:GLY:C	1:B:153:ILE:HD13	2.40	0.47
1:B:294:TYR:HD1	1:B:294:TYR:HA	1.61	0.47
1:C:75:TRP:CE2	1:C:300:ARG:HD2	2.50	0.47
1:C:161:GLN:HE22	1:C:251:PRO:HA	1.78	0.47
1:C:265:ASP:OD1	1:C:269:VAL:HB	2.14	0.47
1:E:165:PHE:CD2	1:E:166:ALA:N	2.83	0.47
1:F:65:SER:C	1:F:67:THR:H	2.23	0.47
1:F:142:ASN:HB2	1:F:154:SER:HB3	1.97	0.47
1:F:164:VAL:CG1	1:F:165:PHE:N	2.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2:GAL:H3	2:G:3:SIA:O1B	2.15	0.47
1:A:57:MET:HA	1:A:96:PRO:HA	1.96	0.47
1:A:83:THR:CB	1:A:87:GLU:HB3	2.35	0.47
1:A:125:VAL:O	1:A:125:VAL:HG13	2.14	0.47
1:A:243:TYR:CZ	1:A:245:GLY:HA2	2.50	0.47
1:B:25:VAL:HG21	1:F:360:VAL:CG1	2.40	0.47
1:C:172:LEU:O	1:C:174:LEU:CD1	2.62	0.47
1:C:194:LYS:C	1:C:196:ILE:N	2.72	0.47
1:E:66:LEU:HB3	1:E:71:GLN:HB2	1.96	0.47
1:E:76:SER:O	1:E:298:HIS:CB	2.63	0.47
1:E:197:THR:O	1:E:197:THR:CG2	2.63	0.47
1:E:321:MET:O	1:E:322:ALA:C	2.58	0.47
1:F:141:PHE:HD1	1:F:141:PHE:HA	1.54	0.47
1:F:197:THR:C	1:F:199:LYS:N	2.72	0.47
1:A:33:GLY:O	1:A:36:VAL:HG23	2.14	0.46
1:B:306:PHE:HB3	1:B:308:ILE:HD11	1.97	0.46
1:C:53:LEU:CD2	1:C:306:PHE:CE1	2.93	0.46
1:C:66:LEU:N	1:C:66:LEU:HD23	2.30	0.46
1:C:305:TYR:CZ	1:D:231:PRO:HB2	2.50	0.46
1:D:76:SER:OG	1:D:299:TRP:N	2.48	0.46
1:D:203:ASN:N	1:D:203:ASN:OD1	2.46	0.46
1:D:254:GLN:HE22	1:E:242:ASN:HB2	1.80	0.46
1:D:316:LYS:HG3	1:D:317:ASN:O	2.14	0.46
1:E:57:MET:CB	1:E:96:PRO:HA	2.44	0.46
1:A:292:ARG:O	1:A:293:ASN:HB2	2.15	0.46
1:A:300:ARG:HG3	1:A:300:ARG:NH1	2.28	0.46
1:B:372:ARG:C	1:B:373:PHE:CG	2.94	0.46
1:B:380:PHE:HA	1:B:381:PRO:HD2	1.46	0.46
1:C:175:GLN:CB	1:C:230:ASP:HB2	2.41	0.46
1:D:109:ASN:H	1:D:118:GLN:HE21	1.63	0.46
1:E:31:LYS:HG3	1:E:32:GLY:N	2.30	0.46
1:F:127:THR:OG1	1:F:304:ARG:HD3	2.15	0.46
1:A:201:MET:HE2	1:A:201:MET:HB3	1.59	0.46
1:B:287:GLY:O	1:B:299:TRP:HB2	2.15	0.46
1:B:300:ARG:CG	1:B:301:GLY:N	2.78	0.46
1:E:77:ARG:O	1:E:298:HIS:CB	2.62	0.46
1:E:209:ASN:HA	1:E:210:PRO:HD3	1.60	0.46
1:F:78:GLY:HA3	2:L:2:GAL:C4	2.46	0.46
1:F:256:THR:OG1	1:F:258:THR:OG1	2.30	0.46
1:A:77:ARG:O	1:A:298:HIS:CG	2.69	0.46
1:A:94:THR:O	1:A:95:LEU:HG	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:TYR:HD1	1:A:294:TYR:HA	1.64	0.46
1:A:336:VAL:HB	1:A:338:GLY:H	1.79	0.46
1:B:198:LYS:CE	1:B:198:LYS:N	2.74	0.46
1:B:276:GLU:N	1:B:276:GLU:OE2	2.49	0.46
1:B:354:TYR:N	1:B:354:TYR:CD1	2.84	0.46
1:C:153:ILE:HG22	1:C:154:SER:O	2.15	0.46
1:D:54:ASN:CG	1:E:207:VAL:HG23	2.41	0.46
1:D:60:PRO:HB2	1:D:61:PRO:HD2	1.98	0.46
1:D:157:VAL:HG13	1:D:288:TRP:C	2.41	0.46
1:D:211:ILE:HD12	1:D:211:ILE:H	1.80	0.46
1:D:341:MET:C	1:D:346:THR:HG23	2.40	0.46
1:E:60:PRO:HB2	1:E:61:PRO:HD2	1.97	0.46
1:E:112:LEU:O	1:E:114:CYS:N	2.49	0.46
1:E:177:LEU:HD21	1:E:206:GLN:C	2.31	0.46
1:E:300:ARG:HH11	1:E:300:ARG:HG3	1.81	0.46
1:E:369:TYR:CD1	1:E:371:ASP:HA	2.50	0.46
1:F:273:CYS:HB3	1:F:277:GLY:O	2.16	0.46
1:F:283:VAL:O	1:F:283:VAL:HG23	2.15	0.46
1:A:43:PRO:HA	1:A:312:LYS:HD2	1.97	0.46
1:C:285:ILE:HD12	1:C:285:ILE:H	1.80	0.46
1:F:34:MET:SD	1:F:37:LEU:CD2	3.03	0.46
1:F:139:HIS:O	1:F:154:SER:HB2	2.16	0.46
1:B:125:VAL:HA	1:B:307:LYS:O	2.16	0.46
1:D:249:THR:HA	1:D:250:PRO:HD3	1.68	0.46
1:D:317:ASN:ND2	1:D:318:PRO:HD2	2.31	0.46
1:E:78:GLY:HA3	2:K:2:GAL:C4	2.45	0.46
1:E:79:ILE:HD13	1:E:79:ILE:HA	1.79	0.46
1:E:165:PHE:O	1:E:239:TYR:HA	2.16	0.46
1:E:224:VAL:C	1:E:226:ILE:N	2.73	0.46
1:F:30:ILE:HG23	1:F:36:VAL:CG1	2.45	0.46
1:F:94:THR:O	1:F:94:THR:HG22	2.15	0.46
1:F:218:LYS:HB2	1:F:222:TYR:HE1	1.79	0.46
1:A:263:LEU:O	1:A:270:GLY:HA2	2.15	0.46
1:A:335:GLN:NE2	1:A:336:VAL:HG13	2.31	0.46
1:B:76:SER:CB	1:B:299:TRP:CE3	2.98	0.46
1:C:46:VAL:HG12	1:C:47:THR:N	2.30	0.46
1:C:239:TYR:C	1:C:240:PHE:CG	2.94	0.46
1:C:284:ASP:O	1:C:301:GLY:HA2	2.15	0.46
1:D:198:LYS:HA	1:D:198:LYS:HD3	1.47	0.46
1:E:39:LEU:O	1:E:40:VAL:C	2.57	0.46
1:E:82:ALA:HB1	1:E:87:GLU:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:192:THR:CB	1:E:194:LYS:HE2	2.45	0.46
1:F:105:LEU:N	1:F:105:LEU:HD12	2.31	0.46
1:A:149:ASN:O	1:A:150:THR:HB	2.14	0.46
1:A:163:HIS:HB3	1:A:284:ASP:OD1	2.16	0.46
1:A:257:ASN:HB2	1:B:239:TYR:CZ	2.51	0.46
1:A:352:ARG:HG3	1:A:354:TYR:CE1	2.48	0.46
1:B:163:HIS:O	1:B:241:GLY:HA3	2.15	0.46
1:B:172:LEU:CD2	1:B:173:ASP:N	2.78	0.46
1:B:265:ASP:CG	1:B:269:VAL:HB	2.41	0.46
1:C:133:GLY:O	1:C:136:LEU:HG	2.16	0.46
1:C:192:THR:HB	1:C:193:ILE:HD12	1.98	0.46
1:D:69:GLY:O	1:D:71:GLN:N	2.49	0.46
1:D:164:VAL:CG1	1:D:165:PHE:N	2.77	0.46
1:D:208:LEU:HD23	1:D:208:LEU:C	2.41	0.46
1:D:239:TYR:C	1:D:240:PHE:CG	2.94	0.46
1:D:316:LYS:HA	1:D:316:LYS:HE3	1.96	0.46
1:E:175:GLN:CG	1:E:213:LYS:HG2	2.38	0.46
1:E:340:PRO:O	1:E:346:THR:HA	2.16	0.46
1:F:177:LEU:HD21	1:F:208:LEU:CA	2.40	0.46
1:F:180:ASP:HB3	1:F:182:ARG:HG3	1.96	0.46
1:F:208:LEU:CD2	1:F:210:PRO:HG3	2.46	0.46
1:F:209:ASN:C	1:F:211:ILE:H	2.23	0.46
1:F:351:VAL:CG1	1:F:352:ARG:N	2.79	0.46
1:A:194:LYS:C	1:A:196:ILE:N	2.69	0.46
1:B:253:LEU:O	1:C:242:ASN:HB2	2.16	0.46
1:B:311:ARG:NH2	1:B:313:ARG:NH2	2.63	0.46
1:C:142:ASN:O	1:C:292:ARG:HB2	2.16	0.46
1:C:207:VAL:HG23	1:C:208:LEU:N	2.31	0.46
1:C:233:LYS:HD3	1:C:234:ASN:CA	2.46	0.46
1:D:28:LEU:HD11	1:D:30:ILE:C	2.41	0.46
1:D:76:SER:OG	1:D:299:TRP:HE3	1.99	0.46
1:D:178:VAL:HG11	1:D:201:MET:HE3	1.98	0.46
1:E:93:ASN:OD1	1:E:93:ASN:N	2.47	0.46
1:E:192:THR:H	1:E:195:THR:HB	1.80	0.46
1:F:97:THR:HG22	1:F:223:PRO:N	2.31	0.46
1:F:162:TYR:CE1	1:F:283:VAL:HG21	2.51	0.46
1:F:192:THR:O	1:F:195:THR:HB	2.15	0.46
1:F:243:TYR:CZ	1:F:245:GLY:HA3	2.50	0.46
1:F:302:LEU:HB3	1:F:303:PRO:HD2	1.98	0.46
1:A:72:TYR:O	1:A:75:TRP:HB2	2.15	0.46
1:A:118:GLN:HB2	1:A:314:TRP:CE3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:LEU:HA	1:A:302:LEU:HD23	1.75	0.46
1:A:319:TYR:N	1:A:320:PRO:CD	2.79	0.46
1:B:72:TYR:CD2	1:B:77:ARG:NE	2.84	0.46
1:B:177:LEU:HA	1:B:205:ASP:O	2.16	0.46
1:C:350:GLU:CD	1:F:233:LYS:HZ1	2.23	0.46
1:E:123:VAL:O	1:E:263:LEU:N	2.49	0.46
1:E:289:ARG:O	1:E:297:HIS:O	2.34	0.46
1:E:291:THR:O	1:E:293:ASN:N	2.49	0.46
1:F:131:GLY:C	1:F:133:GLY:N	2.71	0.46
1:A:46:VAL:HG12	1:A:47:THR:H	1.80	0.45
1:A:69:GLY:C	1:A:71:GLN:NE2	2.74	0.45
1:B:58:GLY:HA2	1:B:93:ASN:HA	1.97	0.45
1:B:192:THR:CG2	1:B:193:ILE:HD12	2.45	0.45
1:C:115:ASP:CG	1:C:116:THR:H	2.23	0.45
1:C:139:HIS:HD2	1:D:88:ASP:CG	2.24	0.45
1:D:115:ASP:O	1:D:316:LYS:HE2	2.16	0.45
1:D:278:LEU:HD12	1:D:310:LEU:CD2	2.45	0.45
1:E:59:GLN:HG3	1:E:60:PRO:N	2.29	0.45
1:E:177:LEU:CD2	1:E:177:LEU:C	2.89	0.45
1:A:269:VAL:HG22	1:A:313:ARG:NH1	2.31	0.45
1:B:131:GLY:O	1:B:134:SER:HB3	2.15	0.45
1:B:256:THR:HA	1:C:239:TYR:CE1	2.51	0.45
1:B:328:LEU:HA	1:B:328:LEU:HD13	1.53	0.45
1:C:79:ILE:O	1:C:79:ILE:CG2	2.64	0.45
1:C:192:THR:O	1:C:195:THR:N	2.48	0.45
1:C:288:TRP:CD1	1:C:288:TRP:H	2.32	0.45
1:E:150:THR:HG23	1:E:292:ARG:HH21	1.82	0.45
1:E:194:LYS:O	1:E:196:ILE:N	2.49	0.45
1:F:255:PHE:O	1:F:256:THR:HB	2.16	0.45
1:A:145:THR:OG1	1:A:153:ILE:N	2.49	0.45
1:A:207:VAL:O	1:A:209:ASN:N	2.50	0.45
1:A:288:TRP:HZ3	1:A:299:TRP:CE2	2.35	0.45
1:B:125:VAL:HG22	1:B:126:LYS:O	2.16	0.45
1:B:138:VAL:CB	1:B:153:ILE:HG23	2.40	0.45
1:B:255:PHE:O	1:C:240:PHE:HA	2.15	0.45
1:B:257:ASN:HB3	1:C:239:TYR:CE2	2.51	0.45
1:B:320:PRO:O	1:B:324:LEU:HD22	2.16	0.45
1:C:108:LEU:N	1:C:108:LEU:HD12	2.32	0.45
1:C:117:LEU:HD13	1:C:118:GLN:H	1.80	0.45
1:C:164:VAL:HA	1:C:240:PHE:O	2.16	0.45
1:D:50:GLU:HA	1:D:306:PHE:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:97:THR:HG22	1:D:222:TYR:O	2.16	0.45
1:D:194:LYS:HG2	1:D:195:THR:N	2.32	0.45
1:E:29:LEU:C	1:E:30:ILE:HG22	2.41	0.45
1:E:60:PRO:CB	1:E:61:PRO:HD2	2.46	0.45
1:E:112:LEU:HD23	1:E:112:LEU:HA	1.57	0.45
1:E:136:LEU:HD23	1:E:136:LEU:HA	1.75	0.45
1:F:52:PHE:HB2	1:F:304:ARG:O	2.15	0.45
1:F:180:ASP:CG	1:F:182:ARG:HD2	2.42	0.45
1:B:45:SER:HA	1:F:354:TYR:O	2.17	0.45
1:B:117:LEU:N	1:B:117:LEU:CD1	2.71	0.45
1:B:174:LEU:HA	1:B:230:ASP:H	1.82	0.45
1:C:118:GLN:HB3	1:C:314:TRP:CE3	2.51	0.45
1:C:192:THR:CG2	1:C:194:LYS:HE2	2.44	0.45
1:D:46:VAL:HG12	1:D:47:THR:N	2.31	0.45
1:D:59:GLN:OE1	1:D:77:ARG:HD2	2.17	0.45
1:D:59:GLN:HA	1:D:60:PRO:HD2	1.81	0.45
1:D:79:ILE:HA	1:D:94:THR:HG23	1.97	0.45
1:D:105:LEU:HB3	1:D:120:TRP:NE1	2.32	0.45
1:D:132:SER:O	1:D:135:LEU:CD2	2.63	0.45
1:D:165:PHE:HA	1:D:282:CYS:HA	1.99	0.45
1:D:285:ILE:N	1:D:285:ILE:CD1	2.76	0.45
1:D:342:GLU:HA	1:D:346:THR:HG23	1.97	0.45
1:E:95:LEU:HA	1:E:96:PRO:HD3	1.80	0.45
1:E:113:THR:C	1:E:115:ASP:N	2.73	0.45
1:E:120:TRP:O	1:E:272:LEU:HA	2.15	0.45
1:F:178:VAL:CG2	1:F:179:THR:N	2.76	0.45
1:F:332:MET:O	1:F:334:PRO:HD3	2.17	0.45
1:A:288:TRP:CZ3	1:A:299:TRP:NE1	2.85	0.45
1:B:30:ILE:CG1	1:B:31:LYS:N	2.79	0.45
1:B:108:LEU:HD12	1:B:108:LEU:N	2.32	0.45
1:B:121:GLU:OE2	1:B:313:ARG:NH2	2.48	0.45
1:B:139:HIS:CD2	1:C:90:PRO:HG3	2.51	0.45
1:B:316:LYS:HD3	1:B:317:ASN:N	2.32	0.45
1:C:192:THR:CB	1:C:194:LYS:HE2	2.46	0.45
1:D:116:THR:OG1	1:D:314:TRP:CE3	2.69	0.45
1:D:209:ASN:HA	1:D:210:PRO:HD3	1.72	0.45
1:D:326:SER:O	1:D:327:SER:C	2.57	0.45
1:E:90:PRO:HD2	1:E:186:LYS:HZ2	1.80	0.45
1:E:366:MET:HE2	1:E:366:MET:HB3	1.81	0.45
1:B:319:TYR:HA	1:B:320:PRO:HD3	1.50	0.45
1:C:165:PHE:CZ	1:C:240:PHE:CD1	3.04	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:279:TYR:N	1:E:279:TYR:CD1	2.85	0.45
1:E:329:PHE:O	1:E:331:ASN:N	2.50	0.45
1:F:35:GLU:H	1:F:35:GLU:CD	2.24	0.45
1:F:192:THR:HG22	1:F:193:ILE:H	1.80	0.45
1:A:297:HIS:O	1:A:298:HIS:C	2.57	0.45
1:A:299:TRP:HE3	1:A:299:TRP:H	1.65	0.45
1:A:328:LEU:CD2	1:A:333:LEU:HD11	2.46	0.45
1:A:371:ASP:C	1:A:373:PHE:N	2.74	0.45
1:B:66:LEU:N	1:B:66:LEU:HD23	2.32	0.45
1:B:153:ILE:HG12	1:C:297:HIS:CE1	2.51	0.45
1:C:233:LYS:HD2	1:F:350:GLU:OE2	2.16	0.45
1:D:153:ILE:HD13	1:D:153:ILE:HA	1.66	0.45
1:E:56:ARG:HH12	1:E:219:ASP:CG	2.25	0.45
1:F:118:GLN:HB2	1:F:314:TRP:CZ3	2.51	0.45
1:F:218:LYS:O	1:F:219:ASP:CB	2.65	0.45
1:A:142:ASN:HD21	1:A:289:ARG:HG3	1.81	0.45
1:A:175:GLN:HA	1:A:213:LYS:HA	1.99	0.45
1:A:194:LYS:CD	1:A:194:LYS:H	2.29	0.45
1:A:231:PRO:O	1:E:305:TYR:HE2	1.99	0.45
1:A:233:LYS:CG	1:A:234:ASN:N	2.75	0.45
1:A:308:ILE:HD12	1:A:308:ILE:H	1.81	0.45
1:B:236:ASN:OD1	1:B:271:PRO:HA	2.17	0.45
1:B:243:TYR:OH	1:B:245:GLY:HA2	2.17	0.45
1:C:308:ILE:HG22	1:C:310:LEU:HG	1.99	0.45
1:D:29:LEU:HB3	1:D:30:ILE:HG22	1.98	0.45
1:D:181:ALA:CA	1:D:201:MET:HE2	2.47	0.45
1:D:243:TYR:CZ	1:D:245:GLY:HA3	2.51	0.45
1:E:138:VAL:CB	1:E:153:ILE:HG23	2.45	0.45
1:E:224:VAL:C	1:E:226:ILE:H	2.22	0.45
1:E:234:ASN:N	1:E:234:ASN:HD22	2.15	0.45
1:E:288:TRP:HZ3	1:E:299:TRP:CE2	2.35	0.45
1:F:79:ILE:HG23	1:F:79:ILE:O	2.17	0.45
1:F:209:ASN:C	1:F:211:ILE:N	2.75	0.45
1:A:162:TYR:HD2	1:A:285:ILE:HD13	1.82	0.45
1:B:321:MET:O	1:B:322:ALA:C	2.60	0.45
1:B:336:VAL:O	1:B:337:GLN:CA	2.54	0.45
1:C:135:LEU:HD12	1:C:157:VAL:HG21	1.99	0.45
1:C:209:ASN:HA	1:C:210:PRO:HD3	1.76	0.45
1:C:256:THR:OG1	1:C:257:ASN:N	2.50	0.45
1:D:33:GLY:H	1:D:36:VAL:HG23	1.81	0.45
1:D:38:ASP:O	1:D:39:LEU:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:CYS:C	1:D:116:THR:HG22	2.42	0.45
1:D:236:ASN:ND2	1:D:272:LEU:O	2.49	0.45
1:D:285:ILE:HD12	1:D:285:ILE:H	1.80	0.45
1:E:43:PRO:O	1:E:312:LYS:HB2	2.17	0.45
1:E:117:LEU:HA	1:E:117:LEU:HD22	1.50	0.45
1:E:194:LYS:CD	1:E:194:LYS:N	2.80	0.45
1:F:127:THR:HA	1:F:305:TYR:O	2.17	0.45
1:A:198:LYS:O	1:A:199:LYS:C	2.60	0.45
1:A:206:GLN:O	1:E:300:ARG:NH2	2.48	0.45
1:C:139:HIS:HD2	1:D:88:ASP:OD1	2.00	0.45
1:C:198:LYS:N	1:C:198:LYS:HD3	2.32	0.45
1:E:109:ASN:HD22	1:E:110:GLU:N	2.12	0.45
1:E:117:LEU:O	1:E:314:TRP:CE3	2.70	0.45
1:F:194:LYS:O	1:F:196:ILE:N	2.50	0.45
1:A:79:ILE:HG13	1:A:297:HIS:CB	2.47	0.44
1:A:100:MET:SD	1:A:100:MET:C	3.00	0.44
1:A:108:LEU:HD21	1:A:120:TRP:CD2	2.52	0.44
1:A:191:VAL:HG21	1:A:222:TYR:CZ	2.52	0.44
1:B:83:THR:O	1:B:84:SER:HB2	2.17	0.44
1:B:141:PHE:HE1	1:B:144:PRO:CG	2.22	0.44
1:B:177:LEU:CD2	1:B:209:ASN:H	2.30	0.44
1:B:259:LEU:HA	1:B:259:LEU:HD13	1.54	0.44
1:C:120:TRP:CE3	1:C:120:TRP:HA	2.52	0.44
1:C:150:THR:O	1:C:150:THR:HG22	2.17	0.44
1:C:181:ALA:H	1:C:206:GLN:HE21	1.61	0.44
1:D:208:LEU:O	1:D:210:PRO:HD3	2.16	0.44
1:D:288:TRP:CZ3	1:D:299:TRP:NE1	2.85	0.44
1:D:340:PRO:HG2	1:D:347:GLN:CG	2.46	0.44
1:E:72:TYR:O	1:E:73:TYR:C	2.59	0.44
1:E:144:PRO:CD	1:E:292:ARG:HD3	2.43	0.44
1:E:192:THR:CG2	1:E:193:ILE:HD12	2.46	0.44
1:F:308:ILE:HG21	1:F:310:LEU:HD23	1.98	0.44
1:C:269:VAL:HA	1:C:313:ARG:NH2	2.32	0.44
1:C:305:TYR:CD1	1:C:305:TYR:C	2.95	0.44
1:D:109:ASN:H	1:D:118:GLN:NE2	2.14	0.44
1:D:164:VAL:HA	1:D:241:GLY:HA3	1.99	0.44
1:E:125:VAL:O	1:E:125:VAL:HG13	2.17	0.44
1:E:250:PRO:HA	1:E:251:PRO:HD3	1.48	0.44
1:F:182:ARG:O	1:F:183:THR:C	2.59	0.44
1:B:209:ASN:C	1:B:211:ILE:N	2.76	0.44
1:B:262:VAL:C	1:B:264:LEU:H	2.23	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:PRO:C	1:B:366:MET:H	2.25	0.44
1:D:193:ILE:N	1:D:193:ILE:CD1	2.74	0.44
1:E:275:GLY:C	1:E:277:GLY:H	2.25	0.44
1:E:346:THR:C	1:E:348:VAL:H	2.25	0.44
1:F:268:GLY:O	1:F:313:ARG:NH2	2.50	0.44
1:A:148:VAL:C	1:A:150:THR:H	2.24	0.44
1:A:339:GLN:HA	1:A:340:PRO:HD2	1.68	0.44
1:B:48:GLU:HB2	1:F:352:ARG:HG3	2.00	0.44
1:B:71:GLN:C	1:B:73:TYR:H	2.26	0.44
1:B:133:GLY:O	1:B:134:SER:C	2.58	0.44
1:B:161:GLN:HE22	1:B:251:PRO:N	2.16	0.44
1:B:232:ALA:HB3	1:B:235:GLU:OE1	2.17	0.44
1:C:111:ASP:O	1:C:114:CYS:O	2.34	0.44
1:D:19:CYS:SG	1:E:116:THR:HG21	2.58	0.44
1:D:172:LEU:HD22	1:D:172:LEU:C	2.42	0.44
1:D:193:ILE:CG2	1:D:212:SER:HB3	2.47	0.44
1:E:50:GLU:CG	1:E:305:TYR:OH	2.65	0.44
1:E:263:LEU:O	1:E:264:LEU:C	2.58	0.44
1:E:264:LEU:HD12	1:E:264:LEU:HA	1.58	0.44
1:E:293:ASN:OD1	1:E:294:TYR:HB2	2.18	0.44
1:E:339:GLN:HA	1:E:340:PRO:HD3	1.59	0.44
1:F:285:ILE:HG23	1:F:299:TRP:CD1	2.53	0.44
1:A:61:PRO:HA	1:A:73:TYR:CD1	2.52	0.44
1:A:112:LEU:O	1:A:112:LEU:HG	2.16	0.44
1:A:176:GLY:HA3	1:A:226:ILE:O	2.17	0.44
1:A:233:LYS:HG3	1:A:234:ASN:ND2	2.32	0.44
1:A:336:VAL:HB	1:A:338:GLY:N	2.33	0.44
1:A:359:PRO:O	1:A:360:VAL:C	2.60	0.44
1:B:23:ALA:HA	1:B:24:PRO:HD3	1.71	0.44
1:B:57:MET:SD	1:B:301:GLY:HA3	2.57	0.44
1:B:179:THR:O	1:B:206:GLN:HG3	2.18	0.44
1:B:259:LEU:N	1:B:259:LEU:CD2	2.75	0.44
1:C:340:PRO:HG2	1:C:347:GLN:HG3	1.98	0.44
1:D:239:TYR:C	1:D:239:TYR:CD1	2.96	0.44
1:E:164:VAL:HG12	1:E:165:PHE:N	2.33	0.44
1:E:184:LYS:HD2	1:E:184:LYS:N	2.33	0.44
1:F:74:GLY:O	1:F:300:ARG:NH1	2.50	0.44
1:F:90:PRO:HD2	1:F:186:LYS:NZ	2.33	0.44
1:F:177:LEU:HD23	1:F:177:LEU:HA	1.74	0.44
1:F:285:ILE:N	1:F:285:ILE:CD1	2.78	0.44
1:A:148:VAL:C	1:A:150:THR:N	2.74	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:TYR:CD1	1:A:222:TYR:N	2.86	0.44
1:A:233:LYS:CE	1:A:234:ASN:HD21	2.31	0.44
1:A:304:ARG:HD3	1:A:306:PHE:CE1	2.52	0.44
1:A:341:MET:HE1	1:A:347:GLN:CB	2.35	0.44
1:B:54:ASN:H	1:F:339:GLN:HE22	1.64	0.44
1:B:285:ILE:HG22	1:B:287:GLY:N	2.32	0.44
1:B:346:THR:C	1:B:348:VAL:H	2.25	0.44
1:C:37:LEU:HG	1:C:106:PRO:HD3	1.99	0.44
1:C:178:VAL:HG22	1:C:179:THR:H	1.82	0.44
1:D:125:VAL:CG1	1:D:263:LEU:HD21	2.47	0.44
1:D:161:GLN:CD	1:D:251:PRO:HA	2.42	0.44
1:D:205:ASP:CA	1:D:209:ASN:HB2	2.46	0.44
1:D:252:VAL:HA	1:E:243:TYR:O	2.18	0.44
1:E:59:GLN:HG3	1:E:60:PRO:O	2.18	0.44
1:E:80:ASN:HB3	1:E:90:PRO:O	2.17	0.44
1:F:30:ILE:HD13	1:F:36:VAL:HG22	1.98	0.44
1:F:66:LEU:C	1:F:70:GLY:HA2	2.43	0.44
1:A:255:PHE:O	1:B:240:PHE:HA	2.17	0.44
1:B:170:GLU:HA	1:B:279:TYR:CE1	2.52	0.44
1:B:341:MET:HA	1:B:341:MET:HE3	2.00	0.44
1:C:105:LEU:N	1:C:105:LEU:CD1	2.76	0.44
1:C:337:GLN:HE21	1:C:337:GLN:HB2	1.56	0.44
1:D:23:ALA:HA	1:D:24:PRO:HD3	1.66	0.44
1:D:345:ASN:O	1:D:346:THR:C	2.61	0.44
1:E:57:MET:HB2	1:E:96:PRO:HB3	1.99	0.44
1:A:193:ILE:O	1:A:197:THR:HG22	2.17	0.44
1:A:285:ILE:CD1	1:A:285:ILE:H	2.31	0.44
1:B:35:GLU:C	1:B:37:LEU:N	2.75	0.44
1:B:323:SER:O	1:B:327:SER:HB3	2.18	0.44
1:C:249:THR:HA	1:C:250:PRO:HD3	1.55	0.44
1:D:52:PHE:CZ	1:E:208:LEU:HD22	2.53	0.44
1:D:202:VAL:HG23	1:D:205:ASP:OD1	2.18	0.44
1:E:121:GLU:O	1:E:310:LEU:CB	2.66	0.44
1:E:165:PHE:CZ	1:E:240:PHE:CE1	3.05	0.44
1:E:239:TYR:C	1:E:240:PHE:CD1	2.96	0.44
1:E:380:PHE:O	1:E:382:GLY:N	2.51	0.44
1:F:72:TYR:O	1:F:73:TYR:C	2.60	0.44
1:F:162:TYR:CD1	1:F:283:VAL:HG21	2.53	0.44
1:A:25:VAL:CG1	1:A:26:PRO:HD2	2.47	0.44
1:A:162:TYR:CE1	1:E:255:PHE:HE2	2.35	0.44
1:B:86:THR:HG23	1:B:87:GLU:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:PRO:HG2	1:B:365:ASP:H	1.83	0.44
1:C:119:MET:HE2	1:C:315:VAL:HG21	2.00	0.44
1:C:153:ILE:CG2	1:C:154:SER:N	2.81	0.44
1:D:161:GLN:HE22	1:D:251:PRO:CA	2.30	0.44
1:E:104:GLN:HE21	1:E:105:LEU:N	2.16	0.44
1:E:305:TYR:CD1	1:E:305:TYR:C	2.95	0.44
1:F:59:GLN:NE2	1:F:69:GLY:HA3	2.33	0.44
1:F:93:ASN:ND2	2:L:2:GAL:H62	2.32	0.44
1:F:139:HIS:HB2	1:F:140:GLY:H	1.56	0.44
1:A:28:LEU:HD12	1:A:29:LEU:N	2.31	0.43
1:A:81:LEU:HG	1:A:82:ALA:H	1.83	0.43
1:A:136:LEU:HA	1:A:136:LEU:HD23	1.55	0.43
1:A:248:THR:O	1:A:249:THR:C	2.61	0.43
1:C:293:ASN:OD1	1:C:294:TYR:N	2.51	0.43
1:C:300:ARG:HG3	1:C:300:ARG:NH1	2.32	0.43
1:C:320:PRO:HD3	1:F:366:MET:CE	2.47	0.43
1:D:193:ILE:HD13	1:D:201:MET:SD	2.58	0.43
1:E:105:LEU:N	1:E:105:LEU:CD1	2.77	0.43
1:E:122:ALA:O	1:E:271:PRO:CD	2.65	0.43
1:E:328:LEU:O	1:E:329:PHE:C	2.61	0.43
1:F:164:VAL:HG12	1:F:165:PHE:N	2.33	0.43
1:F:168:GLY:HA2	1:F:237:THR:HA	2.00	0.43
1:F:208:LEU:HD23	1:F:208:LEU:C	2.42	0.43
1:A:89:SER:HA	1:A:184:LYS:HB2	2.00	0.43
1:A:142:ASN:ND2	1:A:289:ARG:CG	2.81	0.43
1:A:165:PHE:CD2	1:A:166:ALA:N	2.86	0.43
1:A:172:LEU:HB3	1:A:216:LEU:HB2	1.98	0.43
1:A:192:THR:HG22	1:A:193:ILE:HD11	1.96	0.43
1:B:88:ASP:O	1:B:184:LYS:HB2	2.18	0.43
1:C:322:ALA:O	1:C:326:SER:N	2.47	0.43
1:D:29:LEU:CB	1:D:30:ILE:HG22	2.48	0.43
1:D:131:GLY:O	1:D:134:SER:HB3	2.18	0.43
1:D:193:ILE:HD12	1:D:194:LYS:HD3	2.00	0.43
1:E:211:ILE:O	1:E:213:LYS:N	2.52	0.43
1:E:229:PRO:HG2	1:E:229:PRO:O	2.18	0.43
1:E:326:SER:O	1:E:330:ASN:N	2.41	0.43
1:F:60:PRO:HB2	1:F:61:PRO:HD2	2.00	0.43
1:F:138:VAL:CB	1:F:153:ILE:HG23	2.38	0.43
1:F:262:VAL:CG1	1:F:264:LEU:HB2	2.47	0.43
1:F:290:VAL:HG13	1:F:297:HIS:HA	2.00	0.43
1:F:308:ILE:N	1:F:308:ILE:CD1	2.70	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:GLY:HA3	1:A:236:ASN:ND2	2.33	0.43
1:A:209:ASN:OD1	1:A:211:ILE:HD13	2.17	0.43
1:B:50:GLU:HA	1:B:306:PHE:O	2.18	0.43
1:B:56:ARG:HE	1:F:339:GLN:NE2	2.14	0.43
1:B:181:ALA:H	1:B:206:GLN:NE2	2.15	0.43
1:C:320:PRO:HD3	1:F:366:MET:HE1	2.00	0.43
1:C:322:ALA:O	1:C:323:SER:C	2.62	0.43
1:D:37:LEU:HD23	1:D:106:PRO:HD3	2.00	0.43
1:D:47:THR:O	1:D:310:LEU:HD12	2.19	0.43
1:D:117:LEU:O	1:D:314:TRP:HE3	2.01	0.43
1:D:194:LYS:C	1:D:196:ILE:N	2.75	0.43
1:D:328:LEU:HA	1:D:331:ASN:HD22	1.83	0.43
1:E:91:GLY:H	1:E:186:LYS:CE	2.23	0.43
1:E:121:GLU:CD	1:E:269:VAL:O	2.61	0.43
1:E:162:TYR:CE1	1:E:283:VAL:HG21	2.53	0.43
1:E:205:ASP:HA	1:E:209:ASN:HB2	1.99	0.43
1:E:269:VAL:HG12	1:E:270:GLY:O	2.17	0.43
1:F:124:SER:HB2	1:F:260:THR:HG22	2.01	0.43
1:F:184:LYS:N	1:F:184:LYS:CD	2.81	0.43
1:A:168:GLY:N	1:A:237:THR:HG23	2.33	0.43
1:B:136:LEU:O	1:B:138:VAL:HG22	2.18	0.43
1:B:178:VAL:HG22	1:B:179:THR:H	1.81	0.43
1:B:232:ALA:C	1:B:234:ASN:N	2.73	0.43
1:B:304:ARG:HG2	1:B:305:TYR:N	2.33	0.43
1:C:43:PRO:HA	1:C:312:LYS:HD2	1.99	0.43
1:C:164:VAL:HA	1:C:241:GLY:HA3	2.01	0.43
1:D:138:VAL:HG12	1:D:153:ILE:HG23	2.00	0.43
1:D:174:LEU:HD12	1:D:174:LEU:O	2.18	0.43
1:D:197:THR:HG23	1:D:197:THR:O	2.18	0.43
1:D:228:HIS:CD2	1:D:228:HIS:N	2.87	0.43
1:D:288:TRP:HB2	1:D:297:HIS:O	2.18	0.43
1:E:145:THR:OG1	1:E:153:ILE:N	2.49	0.43
1:E:286:MET:SD	1:E:302:LEU:HD12	2.58	0.43
1:F:39:LEU:HD12	1:F:39:LEU:HA	1.77	0.43
1:F:254:GLN:O	1:F:256:THR:N	2.51	0.43
1:F:291:THR:HB	1:F:293:ASN:HB3	1.99	0.43
1:A:125:VAL:HA	1:A:307:LYS:O	2.18	0.43
1:A:208:LEU:C	1:A:208:LEU:CD2	2.92	0.43
1:B:78:GLY:C	1:B:79:ILE:HD13	2.44	0.43
1:B:164:VAL:HB	1:B:283:VAL:CG2	2.48	0.43
1:C:75:TRP:CZ2	1:C:300:ARG:HD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:VAL:HG12	1:C:130:VAL:N	2.34	0.43
1:C:155:THR:HA	1:C:156:PRO:HD2	1.80	0.43
1:C:170:GLU:HA	1:C:279:TYR:CE1	2.53	0.43
1:C:177:LEU:HD23	1:C:178:VAL:N	2.33	0.43
1:C:254:GLN:O	1:C:256:THR:N	2.51	0.43
1:C:350:GLU:CG	1:F:233:LYS:HG2	2.31	0.43
1:E:18:ALA:O	1:E:19:CYS:C	2.61	0.43
1:E:149:ASN:O	1:E:150:THR:HB	2.18	0.43
1:E:268:GLY:O	1:E:313:ARG:NH2	2.47	0.43
1:E:306:PHE:HB3	1:E:308:ILE:HD11	2.01	0.43
1:F:103:LEU:HA	1:F:103:LEU:HD13	1.76	0.43
1:F:105:LEU:HB2	1:F:276:GLU:O	2.18	0.43
1:F:123:VAL:O	1:F:263:LEU:N	2.50	0.43
1:F:149:ASN:O	1:F:150:THR:HB	2.18	0.43
1:F:285:ILE:H	1:F:285:ILE:CD1	2.31	0.43
1:B:139:HIS:HD2	1:C:88:ASP:CG	2.27	0.43
1:C:124:SER:HA	1:C:261:THR:O	2.19	0.43
1:C:181:ALA:N	1:C:206:GLN:HE21	2.16	0.43
1:D:28:LEU:HD12	1:D:29:LEU:H	1.83	0.43
1:D:180:ASP:HA	1:D:206:GLN:NE2	2.32	0.43
1:E:108:LEU:HD12	1:E:108:LEU:H	1.82	0.43
1:E:288:TRP:HB2	1:E:297:HIS:O	2.18	0.43
1:F:113:THR:HB	1:F:114:CYS:H	1.58	0.43
1:F:125:VAL:HA	1:F:307:LYS:O	2.18	0.43
1:F:141:PHE:CZ	1:F:292:ARG:CZ	3.01	0.43
1:A:265:ASP:N	1:A:270:GLY:H	2.12	0.43
1:A:318:PRO:C	1:A:320:PRO:HD2	2.43	0.43
1:B:69:GLY:C	1:B:71:GLN:H	2.25	0.43
1:B:324:LEU:HA	1:B:327:SER:OG	2.19	0.43
1:C:190:VAL:CG2	1:C:223:PRO:HD3	2.48	0.43
1:C:257:ASN:H	1:C:257:ASN:ND2	2.06	0.43
1:D:229:PRO:O	1:D:229:PRO:HG2	2.18	0.43
1:D:233:LYS:HG3	1:D:234:ASN:ND2	2.32	0.43
1:E:216:LEU:HA	1:E:216:LEU:HD23	1.52	0.43
1:F:46:VAL:HG12	1:F:47:THR:N	2.34	0.43
1:F:82:ALA:HB1	1:F:87:GLU:O	2.19	0.43
1:F:105:LEU:N	1:F:105:LEU:CD1	2.81	0.43
1:F:294:TYR:HB3	1:F:295:ASP:H	1.40	0.43
1:A:88:ASP:N	1:A:184:LYS:HD3	2.31	0.43
1:A:197:THR:O	1:A:199:LYS:N	2.51	0.43
1:A:217:ASP:OD1	1:A:218:LYS:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:TRP:CE3	1:A:299:TRP:CG	3.06	0.43
1:A:375:LYS:HB2	1:A:375:LYS:HE3	1.62	0.43
1:A:376:THR:HG22	1:A:377:LYS:O	2.18	0.43
1:B:56:ARG:HH21	1:F:339:GLN:CD	2.27	0.43
1:B:274:LYS:C	1:B:275:GLY:O	2.55	0.43
1:B:324:LEU:O	1:B:325:ILE:C	2.62	0.43
1:C:286:MET:HA	1:C:286:MET:HE3	2.00	0.43
1:D:29:LEU:HD23	1:D:29:LEU:HA	1.55	0.43
1:D:318:PRO:HG2	1:D:319:TYR:CE2	2.54	0.43
1:E:96:PRO:HG2	1:E:299:TRP:CE2	2.53	0.43
1:E:150:THR:O	1:E:150:THR:CG2	2.64	0.43
1:E:203:ASN:O	1:E:206:GLN:CB	2.67	0.43
1:E:226:ILE:HG22	1:E:227:TRP:CD1	2.54	0.43
1:E:263:LEU:HD23	1:E:263:LEU:HA	1.65	0.43
1:F:197:THR:O	1:F:197:THR:CG2	2.66	0.43
1:F:242:ASN:HD22	1:F:242:ASN:N	2.17	0.43
1:A:142:ASN:C	1:A:143:LYS:O	2.61	0.43
1:A:172:LEU:HD22	1:A:173:ASP:N	2.34	0.43
1:A:238:ARG:HH21	1:A:270:GLY:HA2	1.83	0.43
1:A:333:LEU:HA	1:A:334:PRO:HD3	1.65	0.43
1:B:185:TYR:HB2	1:B:194:LYS:HE3	2.00	0.43
1:C:71:GLN:HE21	1:C:73:TYR:HB2	1.84	0.43
1:C:310:LEU:HD12	1:C:310:LEU:H	1.84	0.43
1:D:52:PHE:CD1	1:D:52:PHE:C	2.95	0.43
1:D:84:SER:O	1:D:86:THR:N	2.51	0.43
1:D:94:THR:C	1:D:95:LEU:HG	2.43	0.43
1:D:149:ASN:O	1:D:150:THR:C	2.61	0.43
1:E:297:HIS:O	1:E:298:HIS:C	2.61	0.43
1:F:80:ASN:OD1	1:F:90:PRO:O	2.36	0.43
1:F:254:GLN:OE1	1:F:254:GLN:CA	2.67	0.43
1:A:23:ALA:HA	1:A:24:PRO:HD3	1.71	0.43
1:A:50:GLU:CD	1:B:233:LYS:HB2	2.44	0.43
1:A:192:THR:CG2	1:A:193:ILE:HD12	2.42	0.43
1:A:239:TYR:C	1:A:240:PHE:CG	2.96	0.43
1:C:193:ILE:N	1:C:193:ILE:CD1	2.82	0.43
1:D:95:LEU:HA	1:D:96:PRO:HD2	1.85	0.43
1:D:100:MET:HB2	1:D:280:LEU:O	2.19	0.43
1:D:219:ASP:O	1:D:221:MET:HB2	2.19	0.43
1:E:164:VAL:HG13	1:E:240:PHE:C	2.43	0.43
1:F:35:GLU:OE2	1:F:36:VAL:HG23	2.18	0.43
1:F:77:ARG:HB2	1:F:93:ASN:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:THR:CG2	1:A:262:VAL:N	2.82	0.42
1:A:288:TRP:HA	1:A:299:TRP:HA	2.00	0.42
1:B:379:VAL:O	1:B:380:PHE:C	2.61	0.42
1:C:135:LEU:N	1:C:135:LEU:CD2	2.81	0.42
1:C:142:ASN:O	1:C:143:LYS:C	2.62	0.42
1:C:192:THR:HG22	1:C:193:ILE:CD1	2.48	0.42
1:D:94:THR:O	1:D:299:TRP:HZ3	2.02	0.42
1:D:164:VAL:HG23	1:D:241:GLY:HA3	2.00	0.42
1:D:192:THR:HG22	1:D:193:ILE:HD12	2.01	0.42
1:D:256:THR:OG1	1:D:257:ASN:N	2.52	0.42
1:E:164:VAL:HG22	1:E:241:GLY:HA3	2.01	0.42
1:E:207:VAL:CG2	1:E:208:LEU:N	2.81	0.42
1:E:335:GLN:CD	1:E:336:VAL:H	2.27	0.42
1:F:117:LEU:O	1:F:315:VAL:HG22	2.19	0.42
1:F:155:THR:HA	1:F:156:PRO:HD2	1.73	0.42
1:F:285:ILE:HG23	1:F:299:TRP:HD1	1.83	0.42
1:F:320:PRO:HG2	1:F:323:SER:HB3	2.01	0.42
1:A:56:ARG:NH1	1:A:56:ARG:CB	2.79	0.42
1:A:184:LYS:N	1:A:184:LYS:CD	2.79	0.42
1:A:338:GLY:O	1:A:339:GLN:O	2.37	0.42
1:B:217:ASP:O	1:F:336:VAL:CG1	2.64	0.42
1:C:77:ARG:CB	1:C:93:ASN:HB2	2.49	0.42
1:C:100:MET:SD	1:C:101:ALA:HA	2.59	0.42
1:D:174:LEU:HA	1:D:230:ASP:H	1.85	0.42
1:E:57:MET:CB	1:E:96:PRO:HB3	2.49	0.42
1:E:57:MET:HG3	1:E:57:MET:O	2.19	0.42
1:F:32:GLY:N	1:F:36:VAL:HG21	2.34	0.42
1:F:321:MET:C	1:F:323:SER:N	2.77	0.42
1:A:78:GLY:O	1:A:79:ILE:HD13	2.19	0.42
1:B:234:ASN:N	1:B:234:ASN:HD22	2.17	0.42
1:B:288:TRP:CE3	1:B:299:TRP:CD1	3.06	0.42
1:B:322:ALA:O	1:B:323:SER:C	2.63	0.42
1:C:48:GLU:HG2	1:C:309:THR:HG23	2.01	0.42
1:C:100:MET:SD	1:C:101:ALA:CA	3.07	0.42
1:D:172:LEU:CD2	1:D:173:ASP:N	2.78	0.42
1:D:265:ASP:HB3	1:D:270:GLY:H	1.83	0.42
1:E:89:SER:HA	1:E:90:PRO:HD3	1.61	0.42
1:E:143:LYS:HA	1:E:292:ARG:HA	2.01	0.42
1:F:142:ASN:O	1:F:143:LYS:C	2.60	0.42
1:F:286:MET:HE3	1:F:286:MET:CA	2.34	0.42
1:A:84:SER:O	1:A:85:ASP:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:LEU:CD1	1:A:227:TRP:CE3	3.02	0.42
1:B:288:TRP:CE3	1:B:299:TRP:CG	3.07	0.42
1:C:62:THR:CB	1:C:63:PRO:HD3	2.48	0.42
1:C:73:TYR:CE2	1:D:207:VAL:HG21	2.54	0.42
1:C:165:PHE:HA	1:C:282:CYS:HA	2.01	0.42
1:D:91:GLY:N	1:D:186:LYS:HZ1	2.17	0.42
1:D:96:PRO:CD	1:D:299:TRP:CZ3	2.98	0.42
1:D:177:LEU:C	1:D:177:LEU:CD2	2.88	0.42
1:D:209:ASN:HB3	1:D:212:SER:OG	2.20	0.42
1:E:194:LYS:O	1:E:195:THR:C	2.62	0.42
1:F:124:SER:HB2	1:F:260:THR:CG2	2.50	0.42
1:A:203:ASN:N	1:A:203:ASN:OD1	2.52	0.42
1:B:142:ASN:O	1:B:143:LYS:C	2.63	0.42
1:B:164:VAL:HB	1:B:283:VAL:HG23	2.01	0.42
1:B:173:ASP:N	1:B:173:ASP:OD1	2.52	0.42
1:B:178:VAL:HG11	1:B:201:MET:HE1	2.02	0.42
1:B:239:TYR:C	1:B:240:PHE:CD1	2.98	0.42
1:B:346:THR:HG22	1:B:348:VAL:N	2.35	0.42
1:D:29:LEU:C	1:D:30:ILE:HG22	2.45	0.42
1:D:229:PRO:HB2	1:D:239:TYR:CD2	2.54	0.42
1:E:97:THR:HA	1:E:223:PRO:HA	2.01	0.42
1:E:321:MET:HG2	1:E:325:ILE:HD11	2.02	0.42
1:E:342:GLU:CA	1:E:346:THR:HG23	2.49	0.42
1:F:84:SER:O	1:F:85:ASP:C	2.63	0.42
1:F:111:ASP:OD1	1:F:114:CYS:HB3	2.19	0.42
1:F:182:ARG:CG	1:F:183:THR:H	2.27	0.42
1:A:192:THR:HG23	1:A:226:ILE:CD1	2.49	0.42
1:B:134:SER:O	1:B:136:LEU:N	2.52	0.42
1:B:193:ILE:HD12	1:B:194:LYS:H	1.83	0.42
1:B:255:PHE:O	1:B:256:THR:CB	2.61	0.42
1:B:379:VAL:O	1:B:381:PRO:N	2.53	0.42
1:C:76:SER:O	1:C:77:ARG:O	2.37	0.42
1:C:233:LYS:HB2	1:C:233:LYS:HE3	1.72	0.42
1:C:253:LEU:HD23	1:C:254:GLN:H	1.84	0.42
1:C:303:PRO:HG3	1:D:208:LEU:HB2	2.02	0.42
1:C:346:THR:C	1:C:348:VAL:H	2.27	0.42
1:E:368:ARG:HE	1:E:368:ARG:HB2	1.62	0.42
1:F:121:GLU:CD	1:F:269:VAL:O	2.63	0.42
1:A:203:ASN:O	1:A:206:GLN:HB2	2.19	0.42
1:B:152:GLY:HA2	1:C:295:ASP:O	2.18	0.42
1:C:168:GLY:HA3	1:C:237:THR:CG2	2.29	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:LEU:O	1:C:174:LEU:HD12	2.20	0.42
1:C:314:TRP:CE3	1:C:314:TRP:HA	2.55	0.42
1:C:352:ARG:HD3	1:F:233:LYS:NZ	2.34	0.42
1:D:55:PRO:HD3	1:D:303:PRO:HB3	2.02	0.42
1:D:77:ARG:O	1:D:298:HIS:CG	2.73	0.42
1:E:25:VAL:CG1	1:E:26:PRO:HD2	2.49	0.42
1:E:36:VAL:O	1:E:37:LEU:C	2.62	0.42
1:E:57:MET:CA	1:E:96:PRO:HA	2.49	0.42
1:E:132:SER:O	1:E:135:LEU:CD2	2.68	0.42
1:F:97:THR:HG22	1:F:223:PRO:CA	2.50	0.42
1:F:150:THR:CG2	1:F:292:ARG:NH2	2.75	0.42
1:A:56:ARG:HB2	1:A:56:ARG:HH11	1.77	0.42
1:A:79:ILE:HG12	1:A:297:HIS:H	1.85	0.42
1:A:86:THR:CG2	1:A:87:GLU:N	2.83	0.42
1:A:133:GLY:CA	1:B:228:HIS:HE1	2.33	0.42
1:A:216:LEU:HD23	1:A:216:LEU:HA	1.85	0.42
1:A:233:LYS:HB2	1:A:233:LYS:HE3	1.39	0.42
1:B:233:LYS:HG3	1:B:234:ASN:ND2	2.35	0.42
1:B:358:GLU:OE2	1:B:368:ARG:NH2	2.53	0.42
1:C:103:LEU:N	1:C:103:LEU:CD2	2.83	0.42
1:C:104:GLN:HE21	1:C:105:LEU:N	2.18	0.42
1:C:115:ASP:CG	1:C:116:THR:N	2.78	0.42
1:C:192:THR:N	1:C:195:THR:OG1	2.51	0.42
1:C:216:LEU:HA	1:C:216:LEU:HD23	1.47	0.42
1:E:153:ILE:HG22	1:E:154:SER:N	2.35	0.42
1:F:37:LEU:HD12	1:F:37:LEU:HA	1.73	0.42
1:F:56:ARG:NH1	1:F:219:ASP:OD2	2.52	0.42
1:F:174:LEU:HA	1:F:228:HIS:O	2.20	0.42
1:F:222:TYR:N	1:F:222:TYR:CD1	2.87	0.42
1:A:84:SER:C	1:A:86:THR:H	2.28	0.42
1:A:133:GLY:HA3	1:B:228:HIS:CE1	2.53	0.42
1:A:197:THR:O	1:A:199:LYS:HG3	2.20	0.42
1:B:96:PRO:O	1:B:224:VAL:HG23	2.20	0.42
1:B:217:ASP:C	1:F:336:VAL:HG13	2.45	0.42
1:B:264:LEU:HD12	1:B:264:LEU:HA	1.47	0.42
1:B:328:LEU:O	1:B:331:ASN:N	2.50	0.42
1:B:333:LEU:CD1	1:B:334:PRO:HD3	2.50	0.42
1:B:362:GLY:O	1:B:363:ASP:C	2.63	0.42
1:C:285:ILE:N	1:C:285:ILE:CD1	2.83	0.42
1:C:346:THR:CG2	1:C:348:VAL:HB	2.49	0.42
1:D:21:ARG:H	1:D:21:ARG:NE	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:72:TYR:O	1:D:73:TYR:C	2.61	0.42
1:D:98:TRP:CH2	1:D:164:VAL:CG1	3.01	0.42
1:D:114:CYS:HB2	1:D:116:THR:HG21	2.00	0.42
1:E:37:LEU:H	1:E:37:LEU:HD13	1.84	0.42
1:E:193:ILE:HD13	1:E:201:MET:HG2	2.02	0.42
1:E:205:ASP:OD1	1:E:205:ASP:N	2.52	0.42
1:E:347:GLN:H	1:E:347:GLN:HG2	1.58	0.42
1:F:111:ASP:C	1:F:113:THR:H	2.27	0.42
1:F:121:GLU:OE2	1:F:313:ARG:NH2	2.53	0.42
1:F:180:ASP:O	1:F:181:ALA:C	2.62	0.42
1:F:246:GLY:HA3	1:F:249:THR:OG1	2.20	0.42
1:A:165:PHE:O	1:A:239:TYR:HA	2.20	0.42
1:A:174:LEU:HD11	1:A:227:TRP:HB3	1.99	0.42
1:A:255:PHE:HD1	1:A:255:PHE:HA	1.72	0.42
1:A:286:MET:HA	1:A:286:MET:HE3	2.02	0.42
1:B:177:LEU:CD2	1:B:208:LEU:N	2.82	0.42
1:B:222:TYR:HD1	1:B:222:TYR:H	1.65	0.42
1:C:30:ILE:CD1	1:C:36:VAL:HG22	2.50	0.42
1:C:50:GLU:OE2	1:D:233:LYS:CA	2.65	0.42
1:C:192:THR:HB	1:C:194:LYS:CE	2.50	0.42
1:C:209:ASN:HB3	1:C:212:SER:HB2	2.01	0.42
1:D:71:GLN:HE21	1:D:73:TYR:N	2.16	0.42
1:D:306:PHE:HB3	1:D:308:ILE:CD1	2.49	0.42
1:E:298:HIS:N	1:E:298:HIS:HD2	2.15	0.42
1:F:75:TRP:HE1	1:F:300:ARG:HB2	1.83	0.42
1:A:97:THR:HB	1:A:222:TYR:O	2.20	0.41
1:A:142:ASN:HD21	1:A:289:ARG:CG	2.32	0.41
1:A:252:VAL:HG12	1:B:244:THR:HA	2.01	0.41
1:B:142:ASN:C	1:B:292:ARG:HB2	2.45	0.41
1:B:246:GLY:HA3	1:B:249:THR:OG1	2.20	0.41
1:B:254:GLN:HA	1:B:254:GLN:OE1	2.20	0.41
1:B:280:LEU:HD13	1:B:306:PHE:CD2	2.55	0.41
1:C:59:GLN:OE1	1:C:60:PRO:HD2	2.20	0.41
1:C:193:ILE:O	1:C:196:ILE:HG23	2.20	0.41
1:C:218:LYS:HB3	1:C:219:ASP:H	1.78	0.41
1:D:302:LEU:HD23	1:D:302:LEU:HA	1.79	0.41
1:E:142:ASN:O	1:E:292:ARG:CG	2.60	0.41
1:E:175:GLN:HB2	1:E:230:ASP:HB2	2.02	0.41
1:E:204:LYS:NZ	1:E:204:LYS:HB3	2.35	0.41
1:F:210:PRO:HA	1:F:213:LYS:HE2	2.00	0.41
1:A:79:ILE:HA	1:A:94:THR:CG2	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:PRO:CD	1:A:299:TRP:CH2	3.03	0.41
1:A:203:ASN:HD22	1:E:71:GLN:HE21	1.68	0.41
1:A:222:TYR:H	1:A:222:TYR:HD1	1.68	0.41
1:A:233:LYS:HB2	1:E:50:GLU:OE2	2.20	0.41
1:A:252:VAL:CG1	1:B:244:THR:HA	2.51	0.41
1:B:77:ARG:HD2	1:B:77:ARG:HA	1.95	0.41
1:B:167:VAL:HG11	1:B:263:LEU:HD13	2.02	0.41
1:C:233:LYS:HE3	1:F:350:GLU:HG2	2.01	0.41
1:C:325:ILE:O	1:C:328:LEU:HB2	2.20	0.41
1:D:25:VAL:HG23	1:D:26:PRO:HD2	2.01	0.41
1:D:104:GLN:NE2	1:D:105:LEU:N	2.68	0.41
1:D:111:ASP:OD1	1:D:113:THR:HB	2.20	0.41
1:D:265:ASP:H	1:D:270:GLY:N	2.11	0.41
1:E:23:ALA:HA	1:E:24:PRO:HD3	1.75	0.41
1:E:105:LEU:HB3	1:E:120:TRP:NE1	2.35	0.41
1:E:273:CYS:HB3	1:E:277:GLY:O	2.20	0.41
1:E:337:GLN:HB3	1:E:338:GLY:H	1.50	0.41
1:E:378:THR:C	1:E:379:VAL:O	2.63	0.41
1:F:77:ARG:HH21	2:L:3:SIA:C1	2.33	0.41
1:F:94:THR:C	1:F:95:LEU:HD23	2.44	0.41
1:F:194:LYS:CD	1:F:194:LYS:H	2.33	0.41
1:F:218:LYS:H	1:F:222:TYR:HE1	1.66	0.41
1:A:218:LYS:HD3	1:A:218:LYS:N	2.35	0.41
1:C:118:GLN:HA	1:C:313:ARG:O	2.19	0.41
1:C:209:ASN:C	1:C:211:ILE:H	2.29	0.41
1:D:138:VAL:HG12	1:D:153:ILE:CG2	2.51	0.41
1:D:202:VAL:O	1:D:203:ASN:C	2.64	0.41
1:F:77:ARG:O	1:F:298:HIS:CG	2.73	0.41
1:F:291:THR:O	1:F:293:ASN:N	2.54	0.41
1:A:132:SER:O	1:A:135:LEU:HD13	2.20	0.41
1:A:172:LEU:C	1:A:172:LEU:CD2	2.93	0.41
1:A:182:ARG:HG3	1:E:66:LEU:HD12	2.01	0.41
1:A:293:ASN:OD1	1:A:294:TYR:HB2	2.21	0.41
1:B:217:ASP:CG	1:B:222:TYR:OH	2.63	0.41
1:B:300:ARG:HG3	1:B:301:GLY:N	2.36	0.41
1:B:350:GLU:CG	1:B:351:VAL:N	2.82	0.41
1:C:166:ALA:HB2	1:C:239:TYR:HB3	2.02	0.41
1:C:263:LEU:HA	1:C:263:LEU:HD23	1.84	0.41
1:C:350:GLU:CD	1:C:351:VAL:N	2.79	0.41
1:D:21:ARG:O	1:D:21:ARG:HG2	2.21	0.41
1:D:104:GLN:NE2	1:D:105:LEU:O	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:36:VAL:O	1:E:39:LEU:HG	2.20	0.41
1:E:177:LEU:CD2	1:E:206:GLN:C	2.89	0.41
1:E:192:THR:HG23	1:E:226:ILE:CD1	2.50	0.41
1:E:254:GLN:OE1	1:E:254:GLN:HA	2.20	0.41
1:F:92:ASN:HD21	1:F:190:VAL:HG12	1.85	0.41
1:A:158:GLU:HB3	1:A:248:THR:O	2.20	0.41
1:A:364:PRO:HG2	1:A:365:ASP:N	2.34	0.41
1:B:35:GLU:H	1:B:35:GLU:CD	2.29	0.41
1:B:141:PHE:CD1	1:B:292:ARG:HB2	2.55	0.41
1:B:198:LYS:HE2	1:B:198:LYS:CA	2.51	0.41
1:C:132:SER:CA	1:C:135:LEU:HD23	2.50	0.41
1:C:165:PHE:CZ	1:C:240:PHE:CE1	3.08	0.41
1:C:196:ILE:HD12	1:C:196:ILE:O	2.20	0.41
1:D:159:GLY:HA3	1:D:288:TRP:NE1	2.36	0.41
1:D:263:LEU:H	1:D:263:LEU:HG	1.58	0.41
1:D:318:PRO:O	1:D:319:TYR:CD1	2.74	0.41
1:E:76:SER:O	1:E:298:HIS:HB3	2.21	0.41
1:E:166:ALA:C	1:E:167:VAL:HG23	2.46	0.41
1:E:193:ILE:HG12	1:E:201:MET:CE	2.22	0.41
1:F:91:GLY:O	1:F:93:ASN:N	2.54	0.41
1:A:98:TRP:HB3	1:A:216:LEU:HD11	2.03	0.41
1:B:194:LYS:HA	1:B:197:THR:O	2.21	0.41
1:C:54:ASN:ND2	1:D:207:VAL:CG2	2.84	0.41
1:D:33:GLY:O	1:D:36:VAL:N	2.53	0.41
1:D:139:HIS:O	1:D:154:SER:CB	2.69	0.41
1:D:346:THR:C	1:D:348:VAL:N	2.77	0.41
1:E:80:ASN:OD1	1:E:90:PRO:C	2.64	0.41
1:E:360:VAL:HA	1:E:361:PRO:HD2	1.66	0.41
1:F:79:ILE:HD13	1:F:79:ILE:HA	1.57	0.41
1:F:164:VAL:CG2	1:F:241:GLY:HA3	2.49	0.41
1:F:165:PHE:CD2	1:F:166:ALA:N	2.88	0.41
1:F:264:LEU:N	1:F:264:LEU:HD12	2.35	0.41
1:A:192:THR:O	1:A:195:THR:N	2.54	0.41
1:A:330:ASN:HB3	1:A:331:ASN:H	1.62	0.41
1:B:111:ASP:C	1:B:113:THR:H	2.27	0.41
1:B:218:LYS:HA	1:F:337:GLN:N	2.36	0.41
1:D:55:PRO:HD3	1:D:303:PRO:CB	2.51	0.41
1:D:68:GLU:H	1:D:68:GLU:HG2	1.60	0.41
1:D:151:LYS:HD3	1:D:151:LYS:HA	1.78	0.41
1:D:321:MET:C	1:D:325:ILE:HD12	2.46	0.41
1:E:52:PHE:C	1:E:53:LEU:HD13	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:25:VAL:HG12	1:F:26:PRO:CD	2.51	0.41
1:A:184:LYS:HD2	1:A:184:LYS:H	1.84	0.41
1:A:231:PRO:CG	1:E:305:TYR:CD2	3.04	0.41
1:A:371:ASP:O	1:A:372:ARG:C	2.63	0.41
1:B:80:ASN:HB3	1:B:91:GLY:H	1.85	0.41
1:D:34:MET:O	1:D:37:LEU:HB2	2.21	0.41
1:D:189:GLY:O	1:D:190:VAL:HB	2.21	0.41
1:D:219:ASP:O	1:D:220:GLY:C	2.63	0.41
1:D:328:LEU:O	1:D:329:PHE:C	2.62	0.41
1:F:175:GLN:HG2	1:F:213:LYS:CD	2.33	0.41
1:F:192:THR:CG2	1:F:193:ILE:HD12	2.51	0.41
1:A:69:GLY:HA3	1:A:71:GLN:NE2	2.17	0.41
1:A:90:PRO:HD3	1:A:184:LYS:HB2	2.02	0.41
1:A:170:GLU:HB2	1:A:171:PRO:CD	2.46	0.41
1:A:175:GLN:HE22	1:A:177:LEU:HD21	1.86	0.41
1:B:48:GLU:HB2	1:F:352:ARG:CG	2.50	0.41
1:B:141:PHE:CZ	1:B:292:ARG:HG3	2.55	0.41
1:B:288:TRP:HZ3	1:B:299:TRP:CE2	2.37	0.41
1:B:317:ASN:HD21	1:B:319:TYR:C	2.28	0.41
1:B:360:VAL:HG12	1:B:361:PRO:CD	2.49	0.41
1:C:116:THR:HG23	1:C:314:TRP:CZ3	2.56	0.41
1:C:132:SER:HB2	1:C:255:PHE:CE2	2.56	0.41
1:C:142:ASN:O	1:C:144:PRO:HG3	2.21	0.41
1:C:164:VAL:O	1:C:282:CYS:HB2	2.20	0.41
1:C:273:CYS:CB	1:C:277:GLY:O	2.66	0.41
1:C:319:TYR:HA	1:C:320:PRO:HD3	1.98	0.41
1:D:264:LEU:HD12	1:D:264:LEU:HA	1.43	0.41
1:D:302:LEU:HD23	1:D:303:PRO:HD3	2.03	0.41
1:E:68:GLU:CD	1:E:68:GLU:H	2.29	0.41
1:E:114:CYS:C	1:E:116:THR:H	2.29	0.41
1:E:207:VAL:CG2	1:E:208:LEU:H	2.34	0.41
1:E:251:PRO:O	1:E:252:VAL:HG13	2.21	0.41
1:E:265:ASP:OD1	1:E:269:VAL:N	2.54	0.41
1:E:351:VAL:CG1	1:E:352:ARG:N	2.83	0.41
1:F:77:ARG:O	1:F:298:HIS:CB	2.69	0.41
1:F:79:ILE:O	1:F:79:ILE:CG2	2.69	0.41
1:F:88:ASP:O	1:F:90:PRO:HD3	2.20	0.41
1:F:289:ARG:HB3	1:F:298:HIS:O	2.21	0.41
1:A:20:PRO:HG2	1:B:116:THR:HG21	2.03	0.41
1:A:41:THR:O	1:A:42:GLY:C	2.63	0.41
1:A:65:SER:C	1:A:67:THR:H	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:ASN:O	1:A:292:ARG:HG2	2.21	0.41
1:A:260:THR:HG22	1:A:261:THR:N	2.36	0.41
1:A:327:SER:C	1:A:329:PHE:N	2.78	0.41
1:B:49:ILE:HG12	1:F:351:VAL:HG22	2.01	0.41
1:B:95:LEU:HA	1:B:96:PRO:HD2	1.76	0.41
1:B:151:LYS:HA	1:B:151:LYS:HD3	1.86	0.41
1:B:194:LYS:O	1:B:197:THR:N	2.54	0.41
1:B:318:PRO:HB2	1:B:319:TYR:CE1	2.56	0.41
1:C:127:THR:HA	1:C:305:TYR:O	2.21	0.41
1:D:35:GLU:O	1:D:36:VAL:C	2.63	0.41
1:D:264:LEU:HD12	1:D:270:GLY:HA3	2.03	0.41
1:D:275:GLY:O	1:D:277:GLY:N	2.54	0.41
1:E:90:PRO:HD2	1:E:186:LYS:CE	2.50	0.41
1:E:134:SER:C	1:E:136:LEU:H	2.29	0.41
1:E:194:LYS:HD3	1:E:195:THR:N	2.31	0.41
1:F:116:THR:HG23	1:F:314:TRP:CZ3	2.56	0.41
1:F:142:ASN:CA	1:F:292:ARG:HB2	2.51	0.41
1:F:259:LEU:H	1:F:259:LEU:CD1	2.30	0.41
1:F:280:LEU:HD13	1:F:306:PHE:CD2	2.56	0.41
1:F:354:TYR:CD1	1:F:354:TYR:N	2.89	0.41
1:A:125:VAL:CG1	1:A:263:LEU:HD21	2.40	0.40
1:A:231:PRO:HB2	1:E:305:TYR:CD2	2.55	0.40
1:A:233:LYS:CE	1:E:31:LYS:HD2	2.51	0.40
1:A:263:LEU:N	1:A:263:LEU:CD2	2.82	0.40
1:B:52:PHE:CZ	1:C:208:LEU:HD23	2.56	0.40
1:B:153:ILE:HD11	1:C:297:HIS:CG	2.56	0.40
1:B:176:GLY:HA2	1:B:226:ILE:O	2.21	0.40
1:C:65:SER:C	1:C:67:THR:H	2.29	0.40
1:C:175:GLN:NE2	1:C:176:GLY:N	2.60	0.40
1:D:50:GLU:CD	1:E:233:LYS:CB	2.94	0.40
1:D:165:PHE:CB	1:D:282:CYS:HB3	2.51	0.40
1:E:92:ASN:C	1:E:94:THR:N	2.78	0.40
1:F:165:PHE:HA	1:F:281:SER:O	2.20	0.40
1:F:280:LEU:HD23	1:F:280:LEU:N	2.35	0.40
1:F:302:LEU:HA	1:F:302:LEU:HD23	1.77	0.40
1:A:105:LEU:HD23	1:A:120:TRP:CE2	2.56	0.40
1:A:176:GLY:CA	1:A:226:ILE:O	2.70	0.40
1:A:192:THR:H	1:A:195:THR:HB	1.87	0.40
1:B:263:LEU:H	1:B:263:LEU:HG	1.61	0.40
1:B:306:PHE:CD1	1:B:306:PHE:N	2.89	0.40
1:C:55:PRO:HB3	1:C:302:LEU:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:VAL:HG13	1:D:244:THR:HG23	2.01	0.40
1:C:329:PHE:C	1:C:331:ASN:H	2.29	0.40
1:D:54:ASN:ND2	1:E:207:VAL:HG23	2.35	0.40
1:E:166:ALA:CA	1:E:238:ARG:O	2.67	0.40
1:E:209:ASN:OD1	1:E:210:PRO:HD2	2.21	0.40
1:E:217:ASP:CG	1:E:222:TYR:OH	2.64	0.40
1:E:222:TYR:H	1:E:222:TYR:HD1	1.68	0.40
1:E:283:VAL:C	1:E:284:ASP:CG	2.90	0.40
1:E:288:TRP:CE3	1:E:299:TRP:HB3	2.56	0.40
1:E:300:ARG:HG3	1:E:301:GLY:N	2.37	0.40
1:F:175:GLN:HE21	1:F:176:GLY:N	2.19	0.40
1:F:250:PRO:HA	1:F:251:PRO:HD3	1.73	0.40
1:F:308:ILE:H	1:F:308:ILE:CD1	2.29	0.40
1:A:71:GLN:CB	1:B:203:ASN:HB3	2.52	0.40
1:A:93:ASN:ND2	2:G:2:GAL:H62	2.36	0.40
1:A:182:ARG:O	1:A:183:THR:O	2.40	0.40
1:B:175:GLN:HG2	1:B:213:LYS:HG2	2.04	0.40
1:B:209:ASN:HA	1:B:210:PRO:HD3	1.68	0.40
1:B:305:TYR:C	1:B:305:TYR:CD1	3.00	0.40
1:C:28:LEU:HD21	1:C:30:ILE:CA	2.51	0.40
1:C:151:LYS:HD3	1:C:151:LYS:HA	1.83	0.40
1:D:50:GLU:OE2	1:E:233:LYS:O	2.39	0.40
1:D:59:GLN:NE2	1:D:72:TYR:HB2	2.36	0.40
1:D:192:THR:O	1:D:196:ILE:HG22	2.21	0.40
1:D:211:ILE:CD1	1:D:211:ILE:H	2.33	0.40
1:E:109:ASN:ND2	1:E:110:GLU:H	2.15	0.40
1:E:162:TYR:CE1	1:E:164:VAL:HG23	2.56	0.40
1:E:285:ILE:CG2	1:E:299:TRP:HD1	2.34	0.40
1:E:287:GLY:C	1:E:299:TRP:HB2	2.47	0.40
1:E:320:PRO:O	1:E:321:MET:C	2.63	0.40
1:E:326:SER:O	1:E:327:SER:C	2.65	0.40
1:F:23:ALA:HA	1:F:24:PRO:HD3	1.70	0.40
1:F:103:LEU:N	1:F:103:LEU:CD2	2.84	0.40
1:F:105:LEU:HB3	1:F:120:TRP:NE1	2.36	0.40
1:F:192:THR:HB	1:F:194:LYS:CD	2.36	0.40
1:A:175:GLN:NE2	1:A:177:LEU:HD21	2.36	0.40
1:A:208:LEU:CD2	1:A:210:PRO:HG3	2.51	0.40
1:A:233:LYS:C	1:A:234:ASN:HD22	2.28	0.40
1:B:23:ALA:O	1:F:360:VAL:HG22	2.20	0.40
1:B:209:ASN:O	1:B:211:ILE:N	2.55	0.40
1:C:76:SER:OG	1:C:299:TRP:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:140:GLY:O	1:D:154:SER:OG	2.39	0.40
1:D:250:PRO:HA	1:D:251:PRO:HD3	1.43	0.40
1:D:298:HIS:N	1:D:298:HIS:CD2	2.89	0.40
1:E:165:PHE:HB2	1:E:282:CYS:HB3	2.03	0.40
1:E:191:VAL:HG11	1:E:222:TYR:CE2	2.57	0.40
1:E:302:LEU:HD23	1:E:302:LEU:HA	1.90	0.40
1:E:316:LYS:HE2	1:E:316:LYS:HB2	1.95	0.40
1:F:174:LEU:CD2	1:F:227:TRP:HB3	2.51	0.40
1:A:29:LEU:HB2	1:A:30:ILE:HG22	2.03	0.40
1:A:57:MET:HG3	1:A:57:MET:O	2.22	0.40
1:A:79:ILE:HG23	1:A:79:ILE:HD12	1.82	0.40
1:A:79:ILE:CG1	1:A:297:HIS:H	2.34	0.40
1:A:134:SER:OG	1:B:179:THR:HG23	2.22	0.40
1:A:184:LYS:O	1:A:185:TYR:C	2.62	0.40
1:B:139:HIS:HB2	1:B:140:GLY:H	1.80	0.40
1:B:144:PRO:HD3	1:B:292:ARG:CG	2.52	0.40
1:B:169:GLY:HA3	1:B:272:LEU:O	2.22	0.40
1:B:180:ASP:O	1:B:182:ARG:N	2.55	0.40
1:B:324:LEU:HD22	1:B:324:LEU:N	2.32	0.40
1:C:79:ILE:HD13	1:C:94:THR:CG2	2.48	0.40
1:D:108:LEU:HG	1:D:312:LYS:HE2	2.04	0.40
1:D:122:ALA:HA	1:D:310:LEU:HB3	2.03	0.40
1:D:164:VAL:HA	1:D:240:PHE:O	2.20	0.40
1:D:283:VAL:HG23	1:D:283:VAL:O	2.20	0.40
1:E:300:ARG:HG3	1:E:301:GLY:H	1.87	0.40
1:F:46:VAL:HG12	1:F:47:THR:H	1.87	0.40
1:F:192:THR:N	1:F:195:THR:HB	2.36	0.40
1:F:197:THR:O	1:F:198:LYS:C	2.61	0.40

All (1) 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:A:274:LYS:CD	1:A:328:LEU:O[2_555]	1.11	1.09

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	364/383 (95%)	254 (70%)	75 (21%)	35 (10%)	0	5
1	B	363/383 (95%)	278 (77%)	62 (17%)	23 (6%)	1	11
1	C	353/383 (92%)	279 (79%)	55 (16%)	19 (5%)	1	13
1	D	336/383 (88%)	257 (76%)	56 (17%)	23 (7%)	1	10
1	E	365/383 (95%)	264 (72%)	67 (18%)	34 (9%)	0	5
1	F	350/383 (91%)	263 (75%)	57 (16%)	30 (9%)	0	6
All	All	2131/2298 (93%)	1595 (75%)	372 (18%)	164 (8%)	1	7

All (164) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	PRO
1	A	148	VAL
1	A	183	THR
1	A	276	GLU
1	A	293	ASN
1	A	323	SER
1	A	327	SER
1	A	334	PRO
1	A	339	GLN
1	A	372	ARG
1	A	381	PRO
1	B	43	PRO
1	B	85	ASP
1	B	148	VAL
1	B	212	SER
1	B	329	PHE
1	C	43	PRO
1	C	62	THR
1	C	77	ARG
1	C	85	ASP

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Mol	Chain	Res	Type
1	C	193	ILE
1	C	233	LYS
1	C	293	ASN
1	C	299	TRP
1	D	43	PRO
1	D	84	SER
1	D	85	ASP
1	D	208	LEU
1	D	217	ASP
1	D	219	ASP
1	D	293	ASN
1	D	298	HIS
1	D	320	PRO
1	D	321	MET
1	E	22	PRO
1	E	43	PRO
1	E	77	ARG
1	E	85	ASP
1	E	113	THR
1	E	212	SER
1	E	233	LYS
1	E	257	ASN
1	E	258	THR
1	E	293	ASN
1	E	337	GLN
1	E	342	GLU
1	E	381	PRO
1	F	19	CYS
1	F	40	VAL
1	F	41	THR
1	F	61	PRO
1	F	62	THR
1	F	77	ARG
1	F	92	ASN
1	F	183	THR
1	F	293	ASN
1	F	320	PRO
1	A	70	GLY
1	A	71	GLN
1	A	92	ASN
1	A	110	GLU
1	A	198	LYS

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Mol	Chain	Res	Type
1	A	212	SER
1	A	273	CYS
1	A	322	ALA
1	A	328	LEU
1	A	336	VAL
1	A	337	GLN
1	A	362	GLY
1	A	366	MET
1	B	62	THR
1	B	198	LYS
1	B	276	GLU
1	B	318	PRO
1	B	373	PHE
1	B	381	PRO
1	C	70	GLY
1	C	71	GLN
1	C	148	VAL
1	C	207	VAL
1	C	298	HIS
1	D	71	GLN
1	D	183	THR
1	D	322	ALA
1	D	342	GLU
1	E	20	PRO
1	E	30	ILE
1	E	71	GLN
1	E	80	ASN
1	E	111	ASP
1	E	148	VAL
1	E	298	HIS
1	F	43	PRO
1	F	179	THR
1	F	212	SER
1	F	219	ASP
1	F	255	PHE
1	F	258	THR
1	F	342	GLU
1	F	368	ARG
1	A	18	ALA
1	A	90	PRO
1	A	249	THR
1	A	342	GLU

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Mol	Chain	Res	Type
1	B	77	ARG
1	C	212	SER
1	D	55	PRO
1	D	92	ASN
1	E	70	GLY
1	E	90	PRO
1	E	371	ASP
1	E	379	VAL
1	F	71	GLN
1	F	90	PRO
1	F	113	THR
1	F	148	VAL
1	A	77	ARG
1	A	156	PRO
1	A	330	ASN
1	B	20	PRO
1	B	111	ASP
1	B	135	LEU
1	B	249	THR
1	B	372	ARG
1	C	61	PRO
1	C	255	PHE
1	C	342	GLU
1	D	144	PRO
1	D	179	THR
1	D	190	VAL
1	E	93	ASN
1	E	144	PRO
1	E	330	ASN
1	F	198	LYS
1	B	71	GLN
1	B	361	PRO
1	D	41	THR
1	D	218	LYS
1	E	62	THR
1	F	135	LEU
1	F	190	VAL
1	A	62	THR
1	B	84	SER
1	B	206	GLN
1	D	70	GLY
1	E	145	THR

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Mol	Chain	Res	Type
1	E	249	THR
1	F	70	GLY
1	F	155	THR
1	A	36	VAL
1	E	79	ILE
1	F	269	VAL
1	A	193	ILE
1	A	207	VAL
1	B	70	GLY
1	C	90	PRO
1	E	320	PRO
1	C	320	PRO
1	F	63	PRO
1	B	61	PRO
1	D	90	PRO
1	E	190	VAL
1	E	360	VAL
1	F	249	THR

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	321/335 (96%)	235 (73%)	86 (27%)	0	3
1	B	322/335 (96%)	230 (71%)	92 (29%)	0	2
1	C	314/335 (94%)	231 (74%)	83 (26%)	0	3
1	D	298/335 (89%)	199 (67%)	99 (33%)	0	1
1	E	322/335 (96%)	230 (71%)	92 (29%)	0	2
1	F	311/335 (93%)	228 (73%)	83 (27%)	0	3
All	All	1888/2010 (94%)	1353 (72%)	535 (28%)	0	2

All (535) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	A	43	PRO
1	A	53	LEU
1	A	66	LEU
1	A	76	SER
1	A	83	THR
1	A	93	ASN
1	A	95	LEU
1	A	97	THR
1	A	103	LEU
1	A	107	MET
1	A	108	LEU
1	A	113	THR
1	A	117	LEU
1	A	124	SER
1	A	127	THR
1	A	132	SER
1	A	135	LEU
1	A	138	VAL
1	A	141	PHE
1	A	151	LYS
1	A	154	SER
1	A	157	VAL
1	A	164	VAL
1	A	167	VAL
1	A	172	LEU
1	A	177	LEU
1	A	179	THR
1	A	182	ARG
1	A	186	LYS
1	A	187	GLU
1	A	188	GLU
1	A	190	VAL
1	A	191	VAL
1	A	193	ILE
1	A	194	LYS
1	A	195	THR
1	A	196	ILE
1	A	197	THR
1	A	198	LYS
1	A	199	LYS
1	A	202	VAL
1	A	216	LEU

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Mol	Chain	Res	Type
1	A	219	ASP
1	A	224	VAL
1	A	230	ASP
1	A	233	LYS
1	A	234	ASN
1	A	240	PHE
1	A	244	THR
1	A	252	VAL
1	A	253	LEU
1	A	256	THR
1	A	258	THR
1	A	259	LEU
1	A	262	VAL
1	A	264	LEU
1	A	278	LEU
1	A	280	LEU
1	A	281	SER
1	A	283	VAL
1	A	285	ILE
1	A	286	MET
1	A	288	TRP
1	A	292	ARG
1	A	294	TYR
1	A	298	HIS
1	A	299	TRP
1	A	308	ILE
1	A	309	THR
1	A	310	LEU
1	A	315	VAL
1	A	335	GLN
1	A	347	GLN
1	A	352	ARG
1	A	357	THR
1	A	360	VAL
1	A	361	PRO
1	A	364	PRO
1	A	366	MET
1	A	368	ARG
1	A	369	TYR
1	A	372	ARG
1	A	373	PHE
1	A	380	PHE

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Mol	Chain	Res	Type
1	A	381	PRO
1	B	30	ILE
1	B	37	LEU
1	B	41	THR
1	B	45	SER
1	B	46	VAL
1	B	53	LEU
1	B	54	ASN
1	B	60	PRO
1	B	66	LEU
1	B	71	GLN
1	B	75	TRP
1	B	81	LEU
1	B	83	THR
1	B	93	ASN
1	B	97	THR
1	B	108	LEU
1	B	110	GLU
1	B	117	LEU
1	B	119	MET
1	B	121	GLU
1	B	130	VAL
1	B	132	SER
1	B	135	LEU
1	B	138	VAL
1	B	139	HIS
1	B	141	PHE
1	B	147	THR
1	B	151	LYS
1	B	154	SER
1	B	167	VAL
1	B	172	LEU
1	B	173	ASP
1	B	174	LEU
1	B	175	GLN
1	B	179	THR
1	B	180	ASP
1	B	186	LYS
1	B	190	VAL
1	B	192	THR
1	B	193	ILE
1	B	195	THR

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Mol	Chain	Res	Type
1	B	196	ILE
1	B	197	THR
1	B	198	LYS
1	B	201	MET
1	B	202	VAL
1	B	211	ILE
1	B	219	ASP
1	B	230	ASP
1	B	233	LYS
1	B	235	GLU
1	B	237	THR
1	B	240	PHE
1	B	242	ASN
1	B	244	THR
1	B	248	THR
1	B	252	VAL
1	B	253	LEU
1	B	256	THR
1	B	257	ASN
1	B	258	THR
1	B	260	THR
1	B	262	VAL
1	B	264	LEU
1	B	265	ASP
1	B	272	LEU
1	B	276	GLU
1	B	278	LEU
1	B	281	SER
1	B	283	VAL
1	B	288	TRP
1	B	290	VAL
1	B	293	ASN
1	B	294	TYR
1	B	296	VAL
1	B	297	HIS
1	B	299	TRP
1	B	304	ARG
1	B	308	ILE
1	B	309	THR
1	B	310	LEU
1	B	316	LYS
1	B	332	MET

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Mol	Chain	Res	Type
1	B	342	GLU
1	B	347	GLN
1	B	353	VAL
1	B	354	TYR
1	B	361	PRO
1	B	364	PRO
1	B	373	PHE
1	B	375	LYS
1	B	380	PHE
1	C	29	LEU
1	C	30	ILE
1	C	31	LYS
1	C	37	LEU
1	C	41	THR
1	C	43	PRO
1	C	45	SER
1	C	53	LEU
1	C	57	MET
1	C	66	LEU
1	C	71	GLN
1	C	75	TRP
1	C	76	SER
1	C	79	ILE
1	C	81	LEU
1	C	97	THR
1	C	99	SER
1	C	100	MET
1	C	109	ASN
1	C	112	LEU
1	C	116	THR
1	C	117	LEU
1	C	121	GLU
1	C	132	SER
1	C	138	VAL
1	C	139	HIS
1	C	141	PHE
1	C	151	LYS
1	C	154	SER
1	C	170	GLU
1	C	172	LEU
1	C	174	LEU
1	C	175	GLN

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Mol	Chain	Res	Type
1	C	179	THR
1	C	182	ARG
1	C	186	LYS
1	C	192	THR
1	C	193	ILE
1	C	194	LYS
1	C	196	ILE
1	C	197	THR
1	C	201	MET
1	C	202	VAL
1	C	211	ILE
1	C	217	ASP
1	C	219	ASP
1	C	224	VAL
1	C	233	LYS
1	C	235	GLU
1	C	237	THR
1	C	240	PHE
1	C	244	THR
1	C	252	VAL
1	C	253	LEU
1	C	255	PHE
1	C	257	ASN
1	C	258	THR
1	C	260	THR
1	C	262	VAL
1	C	264	LEU
1	C	265	ASP
1	C	272	LEU
1	C	278	LEU
1	C	281	SER
1	C	283	VAL
1	C	286	MET
1	C	288	TRP
1	C	290	VAL
1	C	291	THR
1	C	292	ARG
1	C	296	VAL
1	C	305	TYR
1	C	308	ILE
1	C	309	THR
1	C	310	LEU

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Mol	Chain	Res	Type
1	C	329	PHE
1	C	330	ASN
1	C	336	VAL
1	C	337	GLN
1	C	354	TYR
1	C	359	PRO
1	C	360	VAL
1	C	370	VAL
1	D	21	ARG
1	D	25	VAL
1	D	30	ILE
1	D	39	LEU
1	D	41	THR
1	D	45	SER
1	D	53	LEU
1	D	54	ASN
1	D	59	GLN
1	D	66	LEU
1	D	68	GLU
1	D	71	GLN
1	D	76	SER
1	D	80	ASN
1	D	81	LEU
1	D	83	THR
1	D	84	SER
1	D	85	ASP
1	D	93	ASN
1	D	97	THR
1	D	99	SER
1	D	100	MET
1	D	108	LEU
1	D	112	LEU
1	D	113	THR
1	D	116	THR
1	D	117	LEU
1	D	118	GLN
1	D	119	MET
1	D	124	SER
1	D	132	SER
1	D	138	VAL
1	D	139	HIS
1	D	141	PHE

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Mol	Chain	Res	Type
1	D	151	LYS
1	D	153	ILE
1	D	154	SER
1	D	161	GLN
1	D	164	VAL
1	D	172	LEU
1	D	174	LEU
1	D	175	GLN
1	D	179	THR
1	D	182	ARG
1	D	184	LYS
1	D	186	LYS
1	D	192	THR
1	D	193	ILE
1	D	194	LYS
1	D	197	THR
1	D	201	MET
1	D	202	VAL
1	D	211	ILE
1	D	218	LYS
1	D	219	ASP
1	D	228	HIS
1	D	230	ASP
1	D	234	ASN
1	D	237	THR
1	D	240	PHE
1	D	242	ASN
1	D	244	THR
1	D	252	VAL
1	D	253	LEU
1	D	254	GLN
1	D	255	PHE
1	D	256	THR
1	D	257	ASN
1	D	258	THR
1	D	260	THR
1	D	262	VAL
1	D	264	LEU
1	D	265	ASP
1	D	266	GLU
1	D	269	VAL
1	D	278	LEU

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Mol	Chain	Res	Type
1	D	279	TYR
1	D	281	SER
1	D	286	MET
1	D	288	TRP
1	D	292	ARG
1	D	297	HIS
1	D	298	HIS
1	D	309	THR
1	D	310	LEU
1	D	313	ARG
1	D	316	LYS
1	D	321	MET
1	D	323	SER
1	D	325	ILE
1	D	333	LEU
1	D	335	GLN
1	D	336	VAL
1	D	342	GLU
1	D	345	ASN
1	D	346	THR
1	D	348	VAL
1	D	349	GLU
1	D	352	ARG
1	E	19	CYS
1	E	21	ARG
1	E	25	VAL
1	E	30	ILE
1	E	37	LEU
1	E	39	LEU
1	E	41	THR
1	E	44	ASP
1	E	53	LEU
1	E	54	ASN
1	E	66	LEU
1	E	67	THR
1	E	68	GLU
1	E	75	TRP
1	E	79	ILE
1	E	97	THR
1	E	99	SER
1	E	108	LEU
1	E	111	ASP

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Mol	Chain	Res	Type
1	E	113	THR
1	E	117	LEU
1	E	121	GLU
1	E	125	VAL
1	E	132	SER
1	E	135	LEU
1	E	138	VAL
1	E	141	PHE
1	E	151	LYS
1	E	154	SER
1	E	157	VAL
1	E	174	LEU
1	E	177	LEU
1	E	179	THR
1	E	186	LYS
1	E	192	THR
1	E	193	ILE
1	E	194	LYS
1	E	202	VAL
1	E	216	LEU
1	E	217	ASP
1	E	219	ASP
1	E	222	TYR
1	E	230	ASP
1	E	233	LYS
1	E	235	GLU
1	E	237	THR
1	E	240	PHE
1	E	242	ASN
1	E	252	VAL
1	E	253	LEU
1	E	256	THR
1	E	258	THR
1	E	259	LEU
1	E	260	THR
1	E	262	VAL
1	E	264	LEU
1	E	265	ASP
1	E	269	VAL
1	E	278	LEU
1	E	279	TYR
1	E	281	SER

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Mol	Chain	Res	Type
1	E	283	VAL
1	E	286	MET
1	E	290	VAL
1	E	292	ARG
1	E	294	TYR
1	E	298	HIS
1	E	299	TRP
1	E	309	THR
1	E	310	LEU
1	E	313	ARG
1	E	315	VAL
1	E	316	LYS
1	E	325	ILE
1	E	328	LEU
1	E	330	ASN
1	E	332	MET
1	E	335	GLN
1	E	337	GLN
1	E	341	MET
1	E	342	GLU
1	E	344	GLU
1	E	346	THR
1	E	347	GLN
1	E	352	ARG
1	E	354	TYR
1	E	357	THR
1	E	358	GLU
1	E	359	PRO
1	E	360	VAL
1	E	366	MET
1	E	381	PRO
1	F	29	LEU
1	F	30	ILE
1	F	37	LEU
1	F	46	VAL
1	F	53	LEU
1	F	54	ASN
1	F	66	LEU
1	F	68	GLU
1	F	71	GLN
1	F	75	TRP
1	F	77	ARG

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Mol	Chain	Res	Type
1	F	79	ILE
1	F	90	PRO
1	F	93	ASN
1	F	97	THR
1	F	100	MET
1	F	104	GLN
1	F	109	ASN
1	F	112	LEU
1	F	113	THR
1	F	117	LEU
1	F	119	MET
1	F	130	VAL
1	F	132	SER
1	F	135	LEU
1	F	138	VAL
1	F	139	HIS
1	F	141	PHE
1	F	151	LYS
1	F	154	SER
1	F	164	VAL
1	F	172	LEU
1	F	175	GLN
1	F	179	THR
1	F	186	LYS
1	F	192	THR
1	F	193	ILE
1	F	194	LYS
1	F	196	ILE
1	F	201	MET
1	F	211	ILE
1	F	216	LEU
1	F	217	ASP
1	F	224	VAL
1	F	233	LYS
1	F	235	GLU
1	F	237	THR
1	F	240	PHE
1	F	242	ASN
1	F	244	THR
1	F	252	VAL
1	F	253	LEU
1	F	258	THR

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Mol	Chain	Res	Type
1	F	259	LEU
1	F	262	VAL
1	F	264	LEU
1	F	278	LEU
1	F	281	SER
1	F	290	VAL
1	F	294	TYR
1	F	299	TRP
1	F	306	PHE
1	F	308	ILE
1	F	309	THR
1	F	310	LEU
1	F	321	MET
1	F	325	ILE
1	F	328	LEU
1	F	330	ASN
1	F	333	LEU
1	F	336	VAL
1	F	337	GLN
1	F	347	GLN
1	F	350	GLU
1	F	351	VAL
1	F	352	ARG
1	F	354	TYR
1	F	357	THR
1	F	359	PRO
1	F	360	VAL
1	F	367	THR
1	F	368	ARG
1	F	371	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	71	GLN
1	A	92	ASN
1	A	104	GLN
1	A	139	HIS
1	A	175	GLN
1	A	206	GLN
1	A	228	HIS

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Mol	Chain	Res	Type
1	A	234	ASN
1	A	257	ASN
1	A	297	HIS
1	A	298	HIS
1	A	331	ASN
1	A	335	GLN
1	A	347	GLN
1	B	54	ASN
1	B	93	ASN
1	B	104	GLN
1	B	118	GLN
1	B	175	GLN
1	B	206	GLN
1	B	228	HIS
1	B	234	ASN
1	B	257	ASN
1	B	339	GLN
1	B	345	ASN
1	B	347	GLN
1	C	54	ASN
1	C	71	GLN
1	C	104	GLN
1	C	139	HIS
1	C	142	ASN
1	C	175	GLN
1	C	206	GLN
1	C	228	HIS
1	C	257	ASN
1	C	331	ASN
1	C	337	GLN
1	C	347	GLN
1	D	54	ASN
1	D	59	GLN
1	D	71	GLN
1	D	93	ASN
1	D	104	GLN
1	D	109	ASN
1	D	118	GLN
1	D	206	GLN
1	D	228	HIS
1	D	234	ASN
1	D	257	ASN

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Mol	Chain	Res	Type
1	D	297	HIS
1	D	317	ASN
1	D	331	ASN
1	D	335	GLN
1	D	347	GLN
1	E	54	ASN
1	E	104	GLN
1	E	139	HIS
1	E	161	GLN
1	E	206	GLN
1	E	228	HIS
1	E	234	ASN
1	E	297	HIS
1	E	317	ASN
1	E	331	ASN
1	E	339	GLN
1	E	347	GLN
1	F	54	ASN
1	F	59	GLN
1	F	104	GLN
1	F	118	GLN
1	F	142	ASN
1	F	175	GLN
1	F	242	ASN
1	F	317	ASN
1	F	331	ASN
1	F	335	GLN
1	F	337	GLN
1	F	339	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

24 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	G	1	2	15,15,15	1.35	1 (6%)	21,21,21	1.52	4 (19%)
2	GAL	G	2	2	11,11,12	0.47	0	15,15,17	1.30	1 (6%)
2	SIA	G	3	2	20,20,21	1.19	2 (10%)	21,28,31	0.92	1 (4%)
2	SIA	G	4	2	20,20,21	1.65	4 (20%)	21,28,31	1.06	1 (4%)
2	NAG	H	1	2	15,15,15	1.65	2 (13%)	21,21,21	2.15	5 (23%)
2	GAL	H	2	2	11,11,12	0.45	0	15,15,17	1.48	1 (6%)
2	SIA	H	3	2	20,20,21	1.02	2 (10%)	21,28,31	1.10	2 (9%)
2	SIA	H	4	2	20,20,21	1.85	5 (25%)	21,28,31	0.97	1 (4%)
2	NAG	I	1	2	15,15,15	1.49	1 (6%)	21,21,21	1.90	5 (23%)
2	GAL	I	2	2	11,11,12	0.39	0	15,15,17	1.18	1 (6%)
2	SIA	I	3	2	20,20,21	0.76	0	21,28,31	1.00	2 (9%)
2	SIA	I	4	2	20,20,21	1.72	4 (20%)	21,28,31	1.00	1 (4%)
2	NAG	J	1	2	15,15,15	0.87	1 (6%)	21,21,21	0.90	1 (4%)
2	GAL	J	2	2	11,11,12	0.48	0	15,15,17	1.20	1 (6%)
2	SIA	J	3	2	20,20,21	1.28	3 (15%)	21,28,31	1.15	3 (14%)
2	SIA	J	4	2	20,20,21	1.73	5 (25%)	21,28,31	0.84	1 (4%)
2	NAG	K	1	2	15,15,15	1.78	1 (6%)	21,21,21	2.37	5 (23%)
2	GAL	K	2	2	11,11,12	0.30	0	15,15,17	1.47	1 (6%)
2	SIA	K	3	2	20,20,21	0.75	0	21,28,31	1.11	1 (4%)
2	SIA	K	4	2	20,20,21	1.88	5 (25%)	21,28,31	0.87	1 (4%)
2	NAG	L	1	2	15,15,15	1.52	2 (13%)	21,21,21	1.79	4 (19%)
2	GAL	L	2	2	11,11,12	0.40	0	15,15,17	1.68	1 (6%)
2	SIA	L	3	2	20,20,21	0.97	2 (10%)	21,28,31	1.00	1 (4%)
2	SIA	L	4	2	20,20,21	1.79	4 (20%)	21,28,31	0.95	1 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	G	1	2	-	2/6/26/26	0/1/1/1
2	GAL	G	2	2	-	0/2/19/22	0/1/1/1
2	SIA	G	3	2	-	5/18/34/38	0/1/1/1
2	SIA	G	4	2	-	1/18/34/38	0/1/1/1
2	NAG	H	1	2	-	2/6/26/26	0/1/1/1
2	GAL	H	2	2	-	0/2/19/22	0/1/1/1
2	SIA	H	3	2	-	6/18/34/38	0/1/1/1
2	SIA	H	4	2	-	2/18/34/38	0/1/1/1
2	NAG	I	1	2	-	2/6/26/26	0/1/1/1
2	GAL	I	2	2	-	0/2/19/22	0/1/1/1
2	SIA	I	3	2	-	1/18/34/38	0/1/1/1
2	SIA	I	4	2	-	1/18/34/38	0/1/1/1
2	NAG	J	1	2	-	4/6/26/26	0/1/1/1
2	GAL	J	2	2	-	0/2/19/22	0/1/1/1
2	SIA	J	3	2	-	4/18/34/38	0/1/1/1
2	SIA	J	4	2	-	1/18/34/38	0/1/1/1
2	NAG	K	1	2	-	2/6/26/26	0/1/1/1
2	GAL	K	2	2	-	0/2/19/22	0/1/1/1
2	SIA	K	3	2	-	5/18/34/38	0/1/1/1
2	SIA	K	4	2	-	3/18/34/38	0/1/1/1
2	NAG	L	1	2	-	2/6/26/26	0/1/1/1
2	GAL	L	2	2	-	0/2/19/22	0/1/1/1
2	SIA	L	3	2	-	5/18/34/38	0/1/1/1
2	SIA	L	4	2	-	0/18/34/38	0/1/1/1

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	1	NAG	C1-C2	6.03	1.60	1.52
2	H	1	NAG	C1-C2	5.33	1.59	1.52
2	I	1	NAG	C1-C2	5.01	1.58	1.52
2	L	1	NAG	C1-C2	4.97	1.58	1.52
2	I	4	SIA	C2-C1	4.50	1.57	1.52
2	G	1	NAG	C1-C2	4.43	1.58	1.52
2	H	4	SIA	C2-C1	4.17	1.57	1.52
2	J	4	SIA	C2-C1	4.02	1.57	1.52
2	G	4	SIA	C2-C1	3.90	1.57	1.52
2	G	3	SIA	C4-C5	-3.75	1.49	1.53
2	H	4	SIA	C7-C6	3.74	1.57	1.52
2	J	3	SIA	C4-C5	-3.74	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	4	SIA	C2-C1	3.71	1.56	1.52
2	K	4	SIA	C2-C1	3.70	1.56	1.52
2	K	4	SIA	C7-C6	3.64	1.57	1.52
2	K	4	SIA	C4-C5	3.64	1.56	1.53
2	K	4	SIA	C6-C5	3.60	1.58	1.53
2	L	4	SIA	C7-C6	3.58	1.57	1.52
2	J	4	SIA	C7-C6	3.54	1.57	1.52
2	L	4	SIA	C6-C5	3.41	1.58	1.53
2	L	4	SIA	C4-C5	3.15	1.56	1.53
2	G	4	SIA	C3-C2	3.03	1.57	1.52
2	I	4	SIA	C7-C6	2.84	1.56	1.52
2	H	4	SIA	C6-C5	2.76	1.57	1.53
2	G	4	SIA	C7-C6	2.65	1.56	1.52
2	H	4	SIA	C3-C2	2.64	1.56	1.52
2	J	4	SIA	C4-C5	2.52	1.55	1.53
2	G	4	SIA	C6-C5	2.49	1.57	1.53
2	J	4	SIA	C6-C5	2.47	1.57	1.53
2	J	4	SIA	C3-C2	2.43	1.56	1.52
2	H	4	SIA	C8-C7	2.40	1.57	1.53
2	J	1	NAG	C1-C2	2.38	1.55	1.52
2	I	4	SIA	C3-C2	2.35	1.56	1.52
2	I	4	SIA	C4-C5	2.35	1.55	1.53
2	H	3	SIA	C7-C6	-2.34	1.50	1.52
2	J	3	SIA	C6-C5	-2.32	1.49	1.53
2	L	3	SIA	C4-C5	-2.29	1.51	1.53
2	L	3	SIA	C3-C2	2.17	1.55	1.52
2	H	1	NAG	C3-C2	2.16	1.57	1.53
2	J	3	SIA	O1B-C1	-2.11	1.23	1.30
2	K	4	SIA	C8-C7	2.11	1.57	1.53
2	H	3	SIA	C4-C5	-2.08	1.51	1.53
2	G	3	SIA	O1B-C1	-2.07	1.24	1.30
2	L	1	NAG	C3-C2	2.05	1.56	1.53

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	1	NAG	O5-C1-C2	6.79	116.34	109.52
2	H	1	NAG	O5-C1-C2	5.82	115.36	109.52
2	L	2	GAL	C1-C2-C3	-5.68	101.38	109.64
2	K	1	NAG	C3-C4-C5	-5.57	100.13	110.23
2	H	2	GAL	C1-C2-C3	-5.25	102.00	109.64
2	I	1	NAG	O5-C1-C2	5.20	114.75	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	2	GAL	C1-C2-C3	-5.01	102.34	109.64
2	L	1	NAG	O5-C1-C2	4.42	113.95	109.52
2	G	2	GAL	C1-C2-C3	-4.33	103.34	109.64
2	J	2	GAL	C1-C2-C3	-4.22	103.50	109.64
2	I	1	NAG	C1-C2-C3	4.16	116.22	110.54
2	L	1	NAG	C3-C4-C5	-4.10	102.80	110.23
2	H	1	NAG	C3-C4-C5	-3.96	103.06	110.23
2	G	1	NAG	O5-C1-C2	3.84	113.37	109.52
2	I	2	GAL	C1-C2-C3	-3.82	104.08	109.64
2	H	1	NAG	C1-C2-N2	-3.58	106.58	110.73
2	G	1	NAG	C3-C4-C5	-3.52	103.84	110.23
2	K	1	NAG	C1-C2-C3	3.17	114.86	110.54
2	H	1	NAG	C1-C2-C3	3.13	114.81	110.54
2	J	3	SIA	C8-C7-C6	-3.12	107.19	113.05
2	K	1	NAG	O3-C3-C2	3.08	115.72	109.58
2	I	1	NAG	C3-C4-C5	-2.97	104.85	110.23
2	H	1	NAG	C4-C3-C2	2.94	114.69	110.40
2	K	1	NAG	C1-C2-N2	-2.90	107.37	110.73
2	H	3	SIA	C8-C7-C6	-2.77	107.84	113.05
2	G	1	NAG	C1-C2-N2	-2.75	107.54	110.73
2	L	1	NAG	C1-C2-N2	-2.72	107.58	110.73
2	L	1	NAG	C1-C2-C3	2.69	114.21	110.54
2	L	4	SIA	O1B-C1-C2	2.66	119.64	112.71
2	K	3	SIA	O1B-C1-C2	2.64	119.58	112.71
2	H	4	SIA	O1B-C1-C2	2.64	119.57	112.71
2	I	4	SIA	O1B-C1-C2	2.63	119.55	112.71
2	G	4	SIA	O1B-C1-C2	2.61	119.49	112.71
2	I	1	NAG	C1-C2-N2	-2.52	107.81	110.73
2	I	3	SIA	O1B-C1-C2	2.52	119.26	112.71
2	H	3	SIA	O1B-C1-C2	2.50	119.21	112.71
2	G	3	SIA	O1B-C1-C2	2.48	119.16	112.71
2	L	3	SIA	O1B-C1-C2	2.47	119.13	112.71
2	J	4	SIA	O1B-C1-C2	2.44	119.07	112.71
2	K	4	SIA	O1B-C1-C2	2.44	119.06	112.71
2	I	1	NAG	C3-C2-N2	-2.38	106.23	110.62
2	J	1	NAG	C1-C2-N2	-2.36	108.00	110.73
2	G	1	NAG	O3-C3-C2	2.30	114.16	109.58
2	J	3	SIA	O1B-C1-C2	2.19	118.41	112.71
2	I	3	SIA	C8-C7-C6	-2.07	109.17	113.05
2	J	3	SIA	C5-N5-C10	-2.05	118.31	123.11

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	3	SIA	O7-C7-C8-C9
2	H	3	SIA	C5-C6-C7-O7
2	H	3	SIA	O6-C6-C7-O7
2	H	4	SIA	C7-C8-C9-O9
2	H	4	SIA	O8-C8-C9-O9
2	J	1	NAG	C1-C2-N2-C7
2	J	3	SIA	C5-C6-C7-C8
2	J	3	SIA	C5-C6-C7-O7
2	J	3	SIA	O6-C6-C7-C8
2	J	3	SIA	O6-C6-C7-O7
2	K	3	SIA	O7-C7-C8-C9
2	L	3	SIA	C5-C6-C7-O7
2	L	3	SIA	O6-C6-C7-O7
2	G	1	NAG	O5-C5-C6-O6
2	G	3	SIA	C6-C7-C8-O8
2	G	3	SIA	C6-C7-C8-C9
2	K	3	SIA	C6-C7-C8-C9
2	L	1	NAG	C4-C5-C6-O6
2	J	1	NAG	O5-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6
2	H	1	NAG	C4-C5-C6-O6
2	I	1	NAG	C4-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6
2	L	1	NAG	O5-C5-C6-O6
2	J	1	NAG	C4-C5-C6-O6
2	G	3	SIA	O7-C7-C8-O8
2	K	3	SIA	O7-C7-C8-O8
2	K	3	SIA	C6-C7-C8-O8
2	K	1	NAG	C4-C5-C6-O6
2	H	3	SIA	C7-C8-C9-O9
2	K	1	NAG	O5-C5-C6-O6
2	H	3	SIA	O8-C8-C9-O9
2	K	4	SIA	O8-C8-C9-O9
2	K	3	SIA	O6-C6-C7-O7
2	H	3	SIA	C5-C6-C7-C8
2	L	3	SIA	C5-C6-C7-C8
2	G	4	SIA	O8-C8-C9-O9
2	I	4	SIA	O8-C8-C9-O9
2	I	3	SIA	C7-C8-C9-O9
2	G	3	SIA	O1A-C1-C2-O6
2	H	3	SIA	O1A-C1-C2-O6

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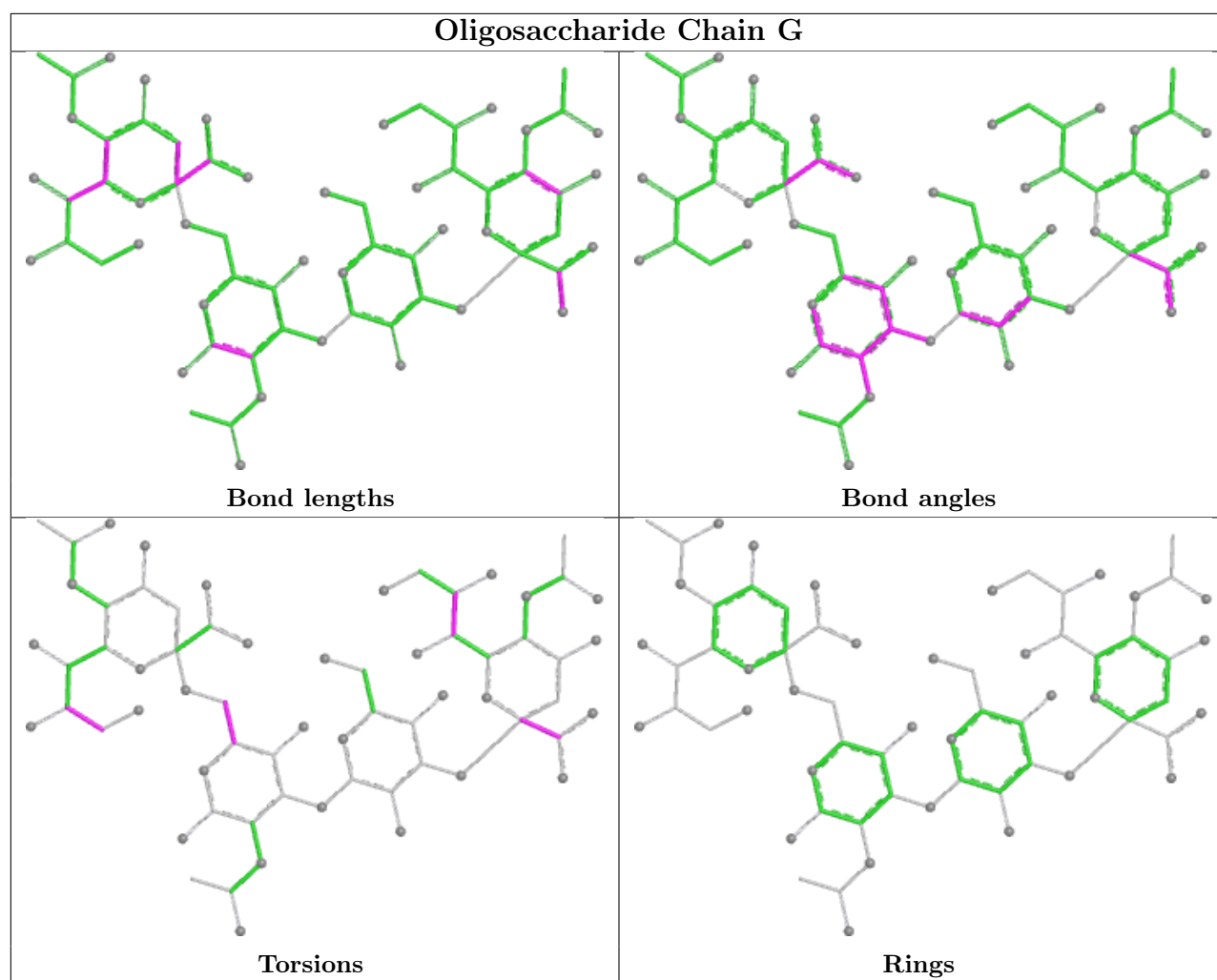
Mol	Chain	Res	Type	Atoms
2	J	4	SIA	O1A-C1-C2-O6
2	L	3	SIA	O1A-C1-C2-O6
2	K	4	SIA	C7-C8-C9-O9
2	J	1	NAG	C3-C2-N2-C7
2	K	4	SIA	C4-C5-N5-C10
2	L	3	SIA	O6-C6-C7-C8

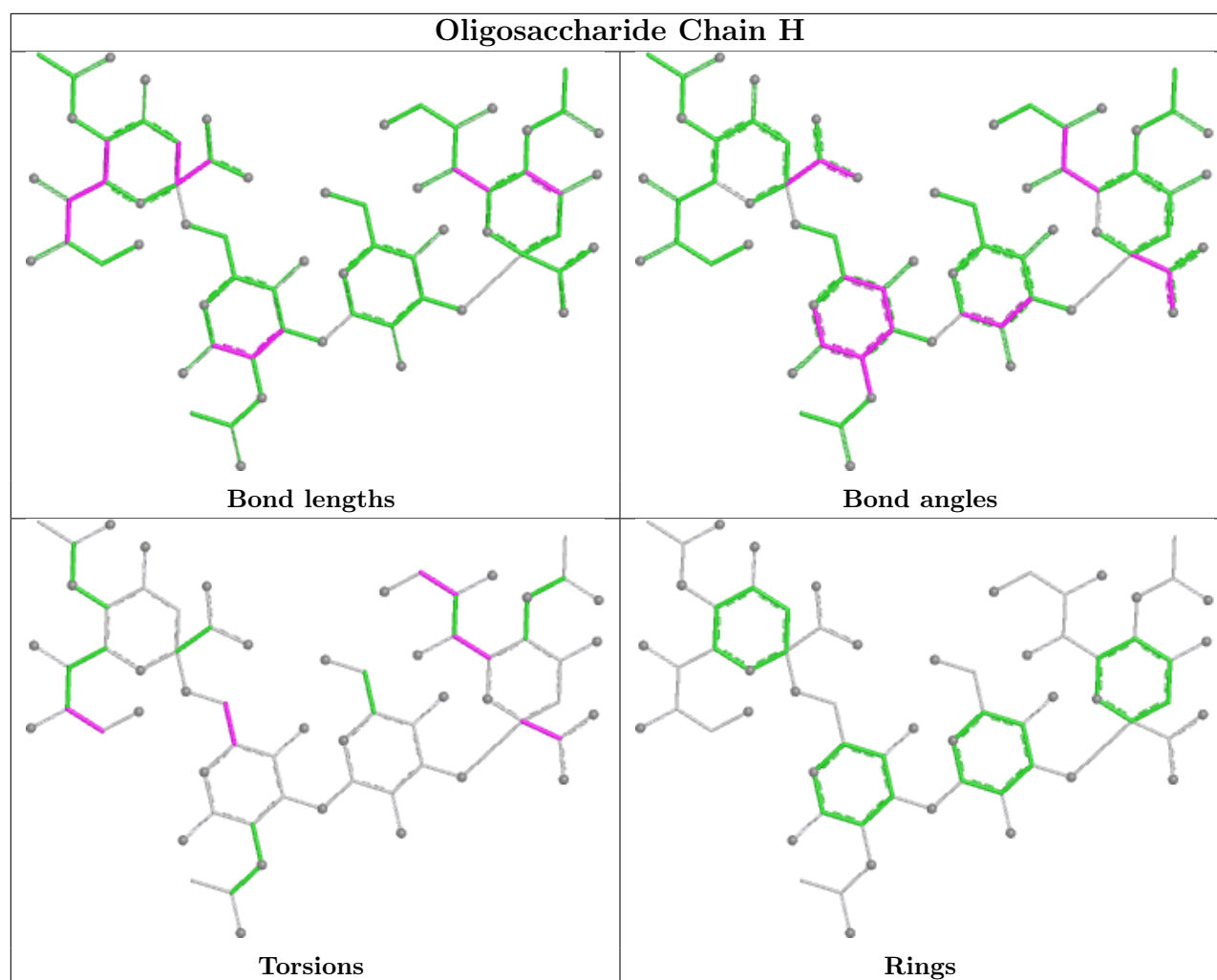
There are no ring outliers.

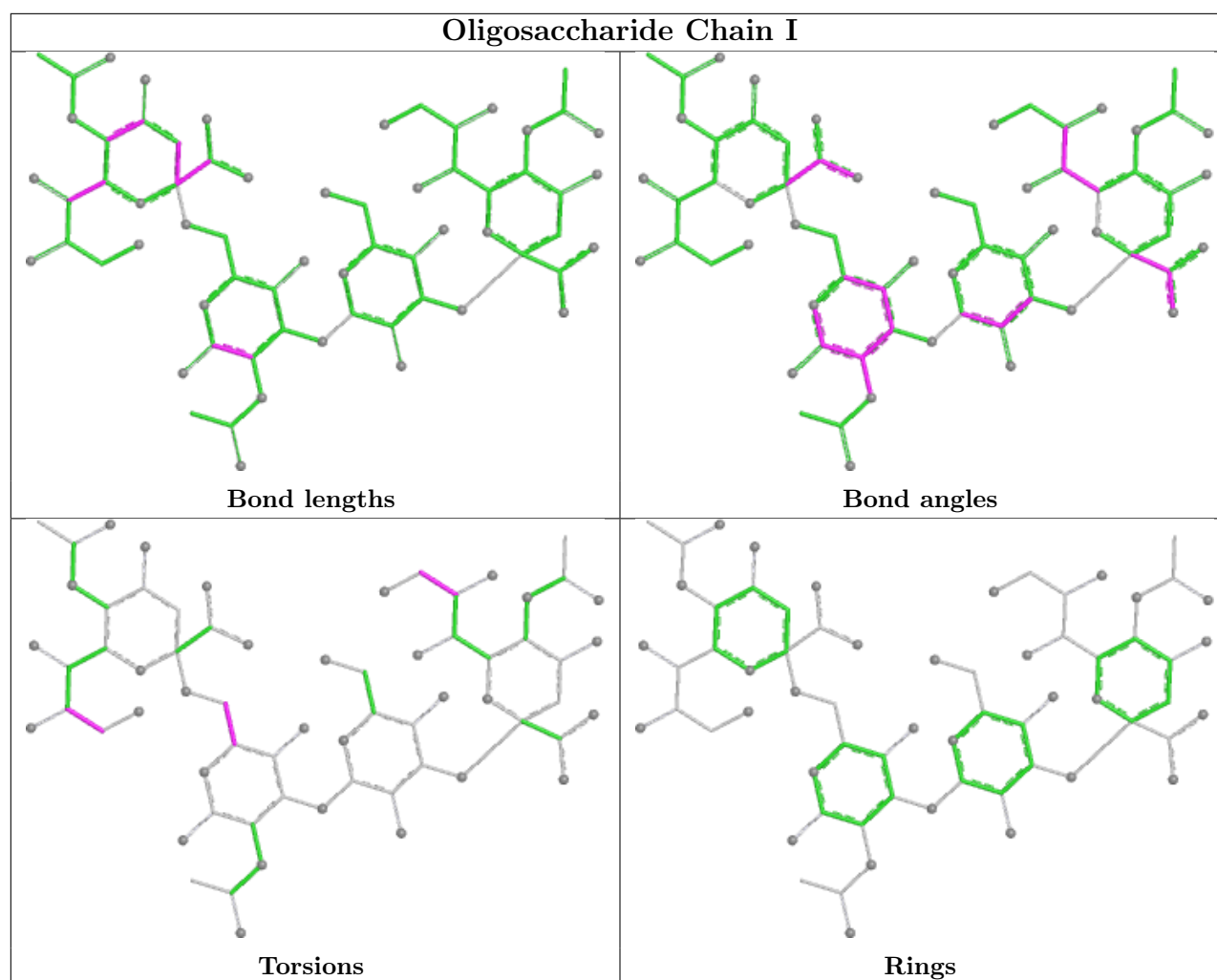
9 monomers are involved in 13 short contacts:

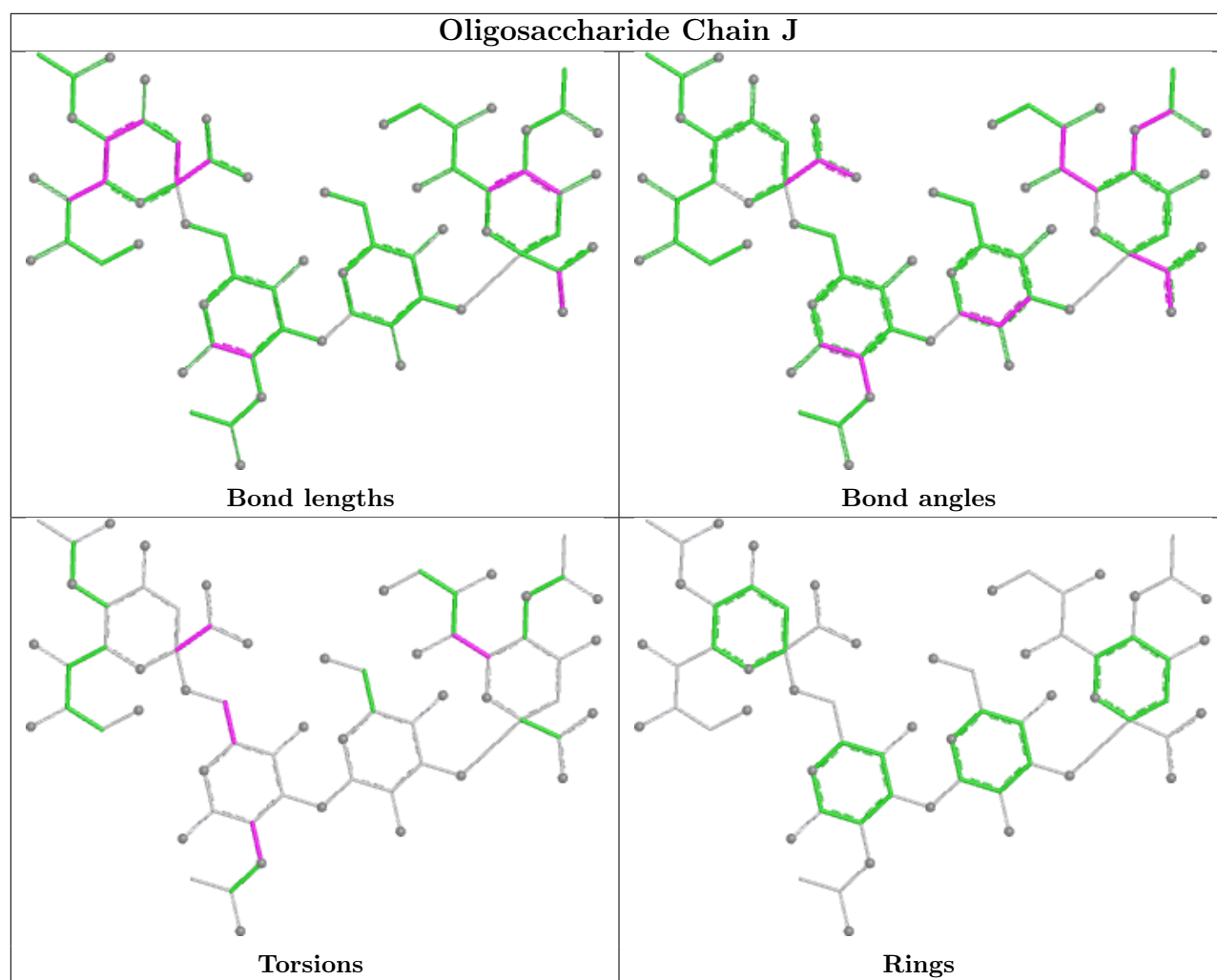
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	3	SIA	2	0
2	K	2	GAL	3	0
2	J	3	SIA	1	0
2	G	2	GAL	2	0
2	L	2	GAL	4	0
2	K	3	SIA	1	0
2	H	2	GAL	1	0
2	G	3	SIA	1	0
2	L	3	SIA	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

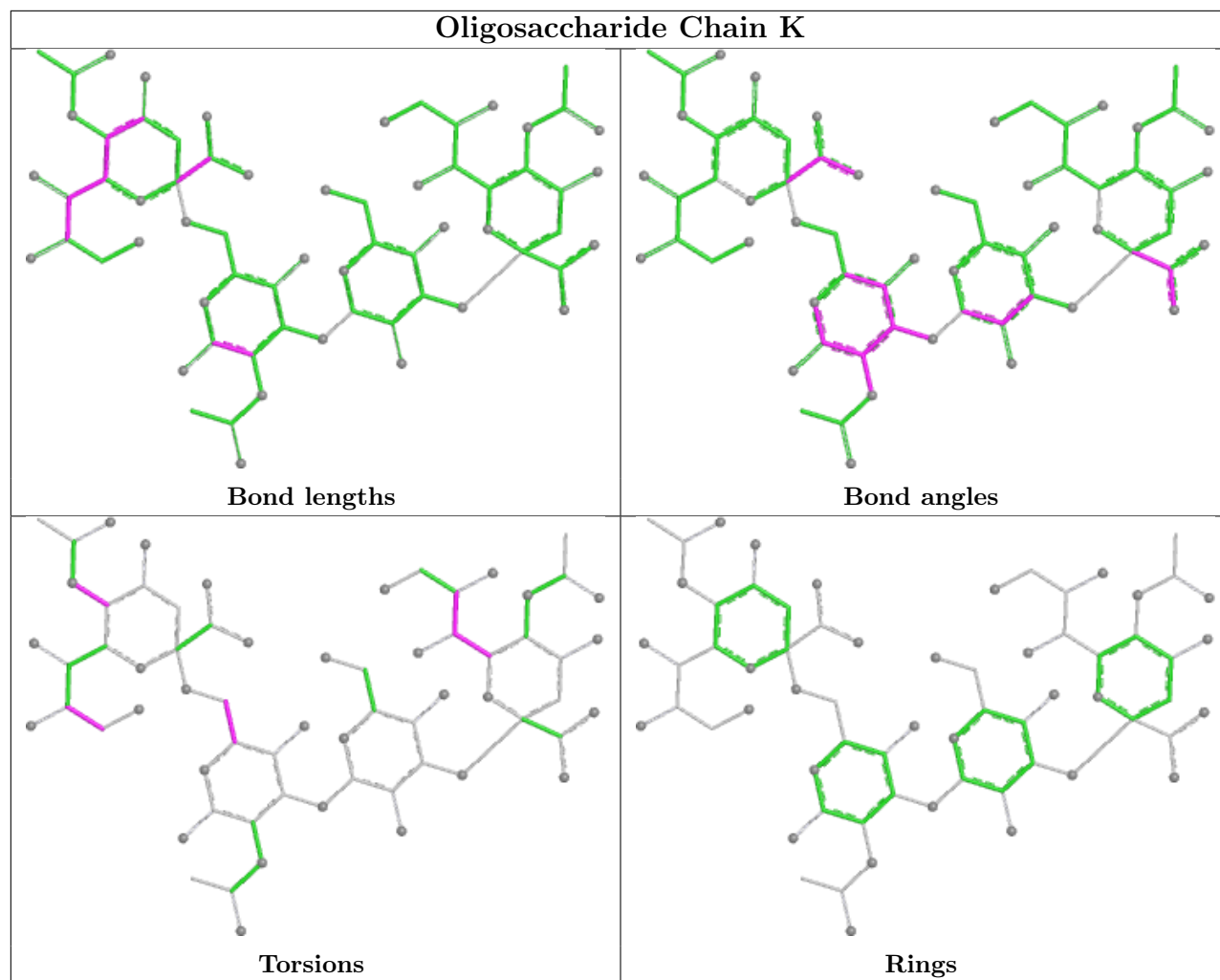


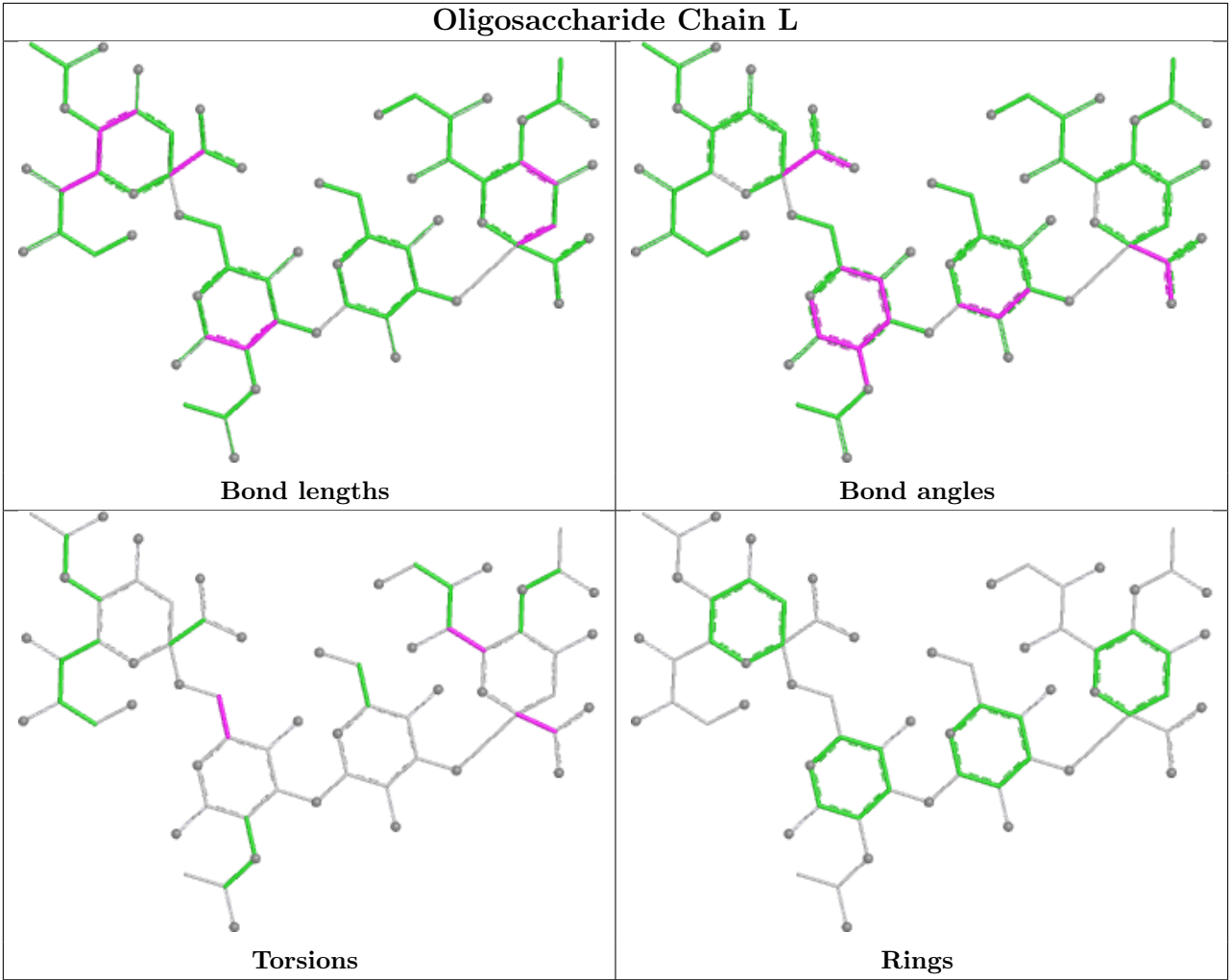






Oligosaccharide Chain K





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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	1
1	F	1
1	C	1

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Mol	Chain	Number of breaks
1	B	1
1	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	336:VAL	C	337:GLN	N	4.77
1	F	336:VAL	C	337:GLN	N	4.21
1	C	336:VAL	C	337:GLN	N	3.33
1	B	336:VAL	C	337:GLN	N	3.13
1	E	336:VAL	C	337:GLN	N	1.19

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.