



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 02:36 PM EDT

PDB ID : 3BLX / pdb_00003blx
Title : Yeast Isocitrate Dehydrogenase (Apo Form)
Authors : Taylor, A.B.; Hu, G.; Hart, P.J.; McAlister-Henn, L.
Deposited on : 2007-12-11
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

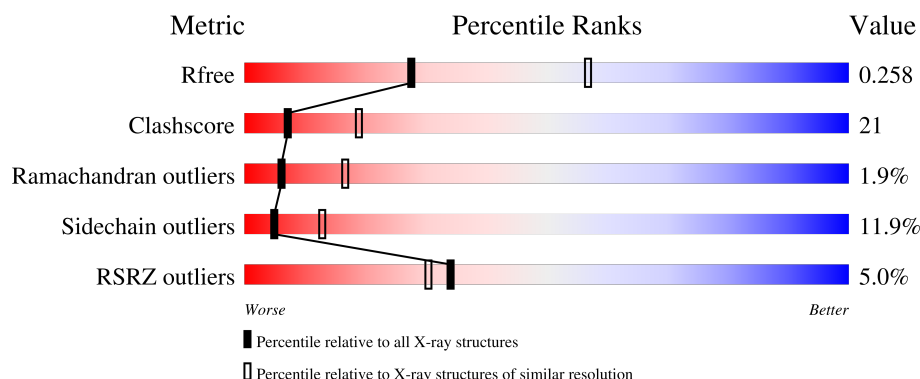
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	349	
1	C	349	
1	E	349	
1	G	349	
1	I	349	

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Mol	Chain	Length	Quality of chain
1	K	349	 % 62% 29% 6% •
1	M	349	 13% 60% 31% 6% •
1	O	349	 % 64% 26% 5% 5%
2	B	354	 6% 60% 30% 8% •
2	D	354	 7% 54% 36% 8% •
2	F	354	 5% 55% 35% 8% •
2	H	354	 3% 54% 36% 7% •
2	J	354	 16% 56% 34% 7% •
2	L	354	 4% 57% 33% 8% •
2	N	354	 11% 54% 35% 9% •
2	P	354	 4% 53% 32% 7% 8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 41336 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 Isocitrate dehydrogenase [NAD] subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	0	0
			2575	1626	451	491	7			
1	C	338	Total	C	N	O	S	0	0	0
			2605	1645	458	495	7			
1	E	341	Total	C	N	O	S	0	0	0
			2626	1659	461	499	7			
1	G	334	Total	C	N	O	S	0	0	0
			2567	1620	450	490	7			
1	I	333	Total	C	N	O	S	0	0	0
			2562	1617	448	490	7			
1	K	338	Total	C	N	O	S	0	0	0
			2605	1645	458	495	7			
1	M	337	Total	C	N	O	S	0	0	0
			2590	1638	453	492	7			
1	O	332	Total	C	N	O	S	0	0	0
			2546	1605	447	487	7			

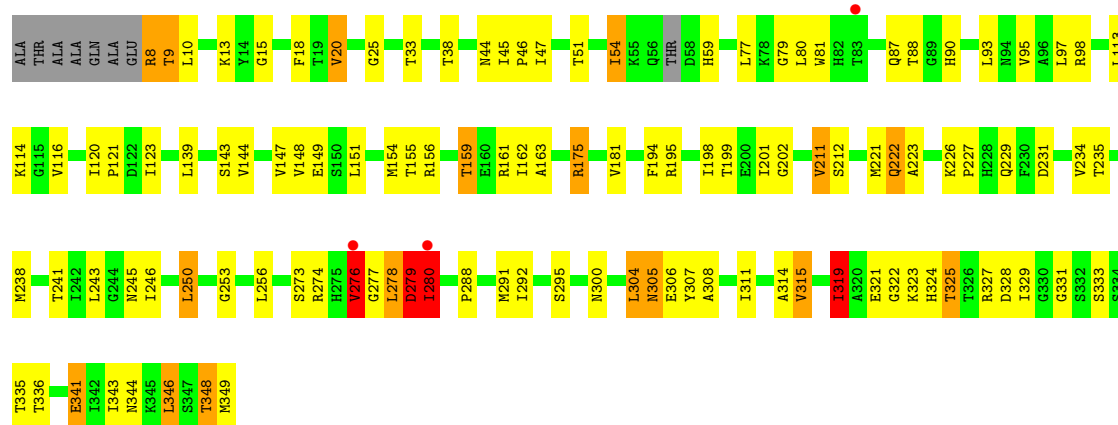
- Molecule 2 is a protein called Isocitrate dehydrogenase [NAD] subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	346	Total	C	N	O	S	0	0	0
			2608	1646	447	509	6			
2	D	345	Total	C	N	O	S	0	0	0
			2598	1640	444	508	6			
2	F	345	Total	C	N	O	S	0	0	0
			2598	1640	444	508	6			
2	H	345	Total	C	N	O	S	0	0	0
			2598	1640	444	508	6			
2	J	345	Total	C	N	O	S	0	0	0
			2598	1640	444	508	6			
2	L	346	Total	C	N	O	S	0	0	0
			2608	1646	447	509	6			

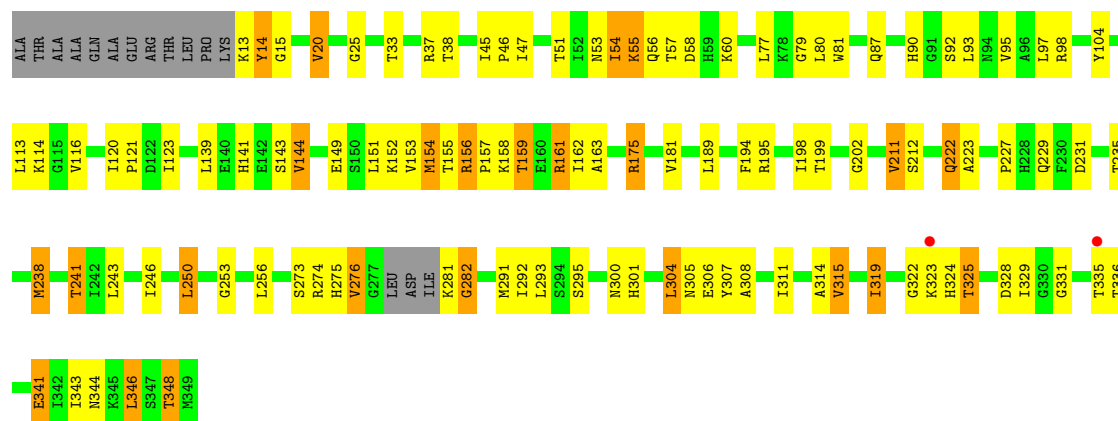
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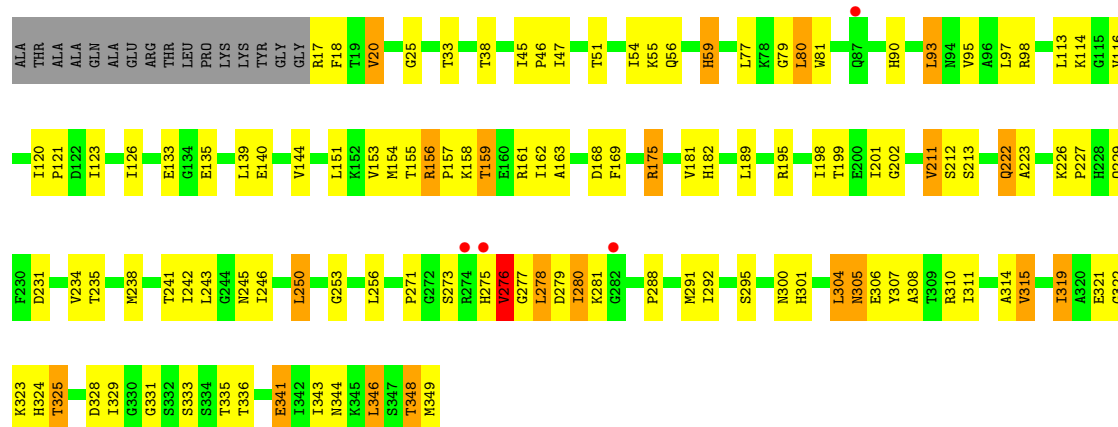
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	345	Total	C	N	O	S	0	0	0
			2598	1640	444	508	6			
2	P	326	Total	C	N	O	S	0	0	0
			2454	1549	418	481	6			



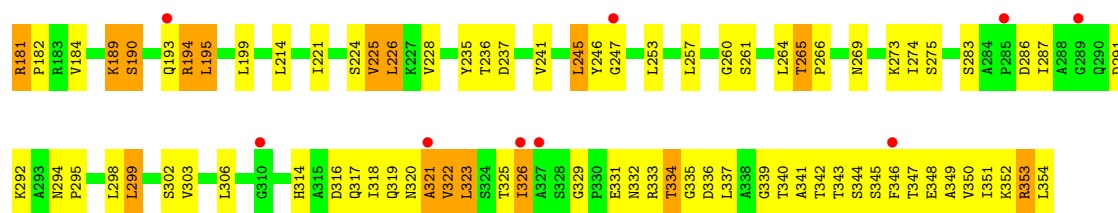
• Molecule 1: Isocitrate dehydrogenase [NAD] subunit 1



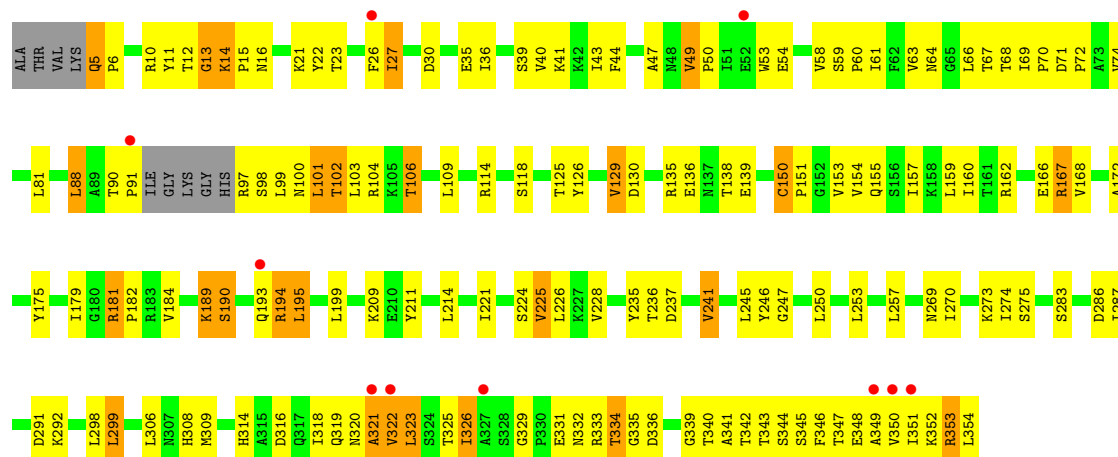
• Molecule 1: Isocitrate dehydrogenase [NAD] subunit 1



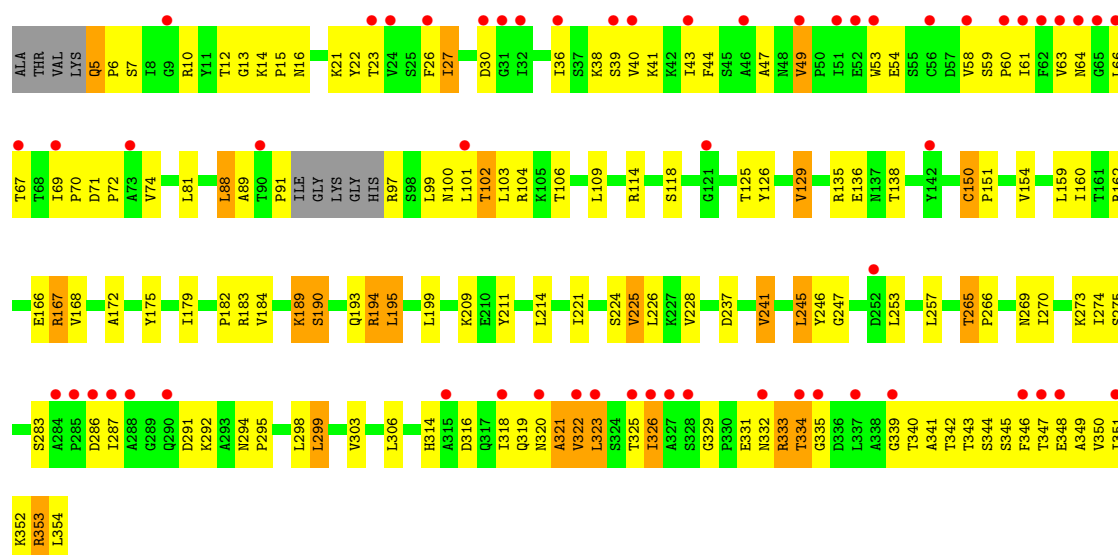
• Molecule 1: Isocitrate dehydrogenase [NAD] subunit 1



• Molecule 2: Isocitrate dehydrogenase [NAD] subunit 2

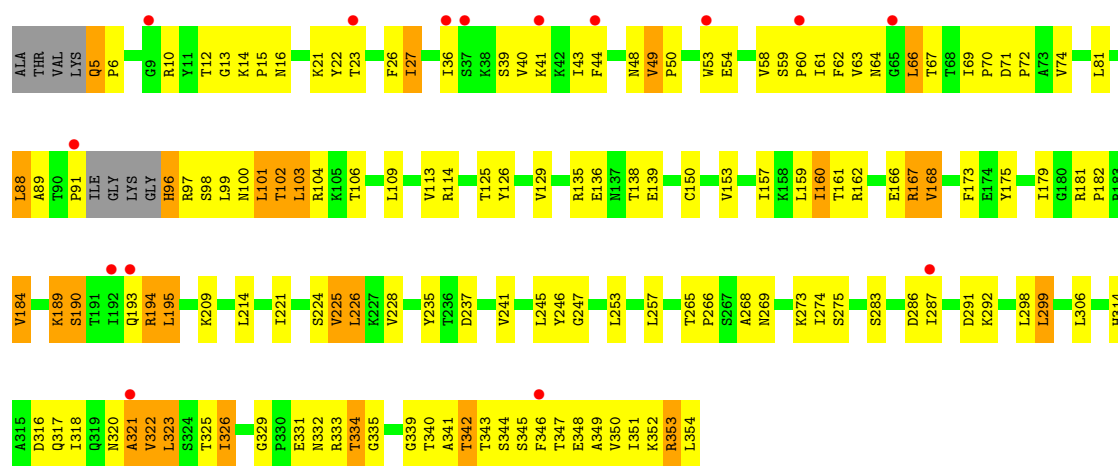


• Molecule 2: Isocitrate dehydrogenase [NAD] subunit 2

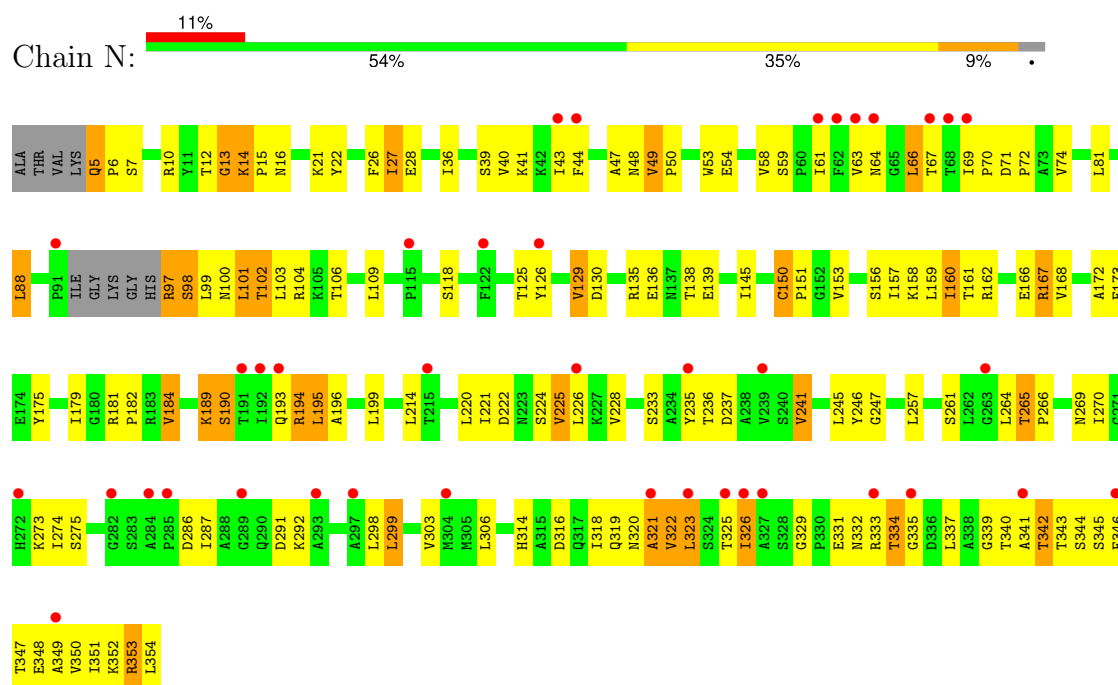


• Molecule 2: Isocitrate dehydrogenase [NAD] subunit 2

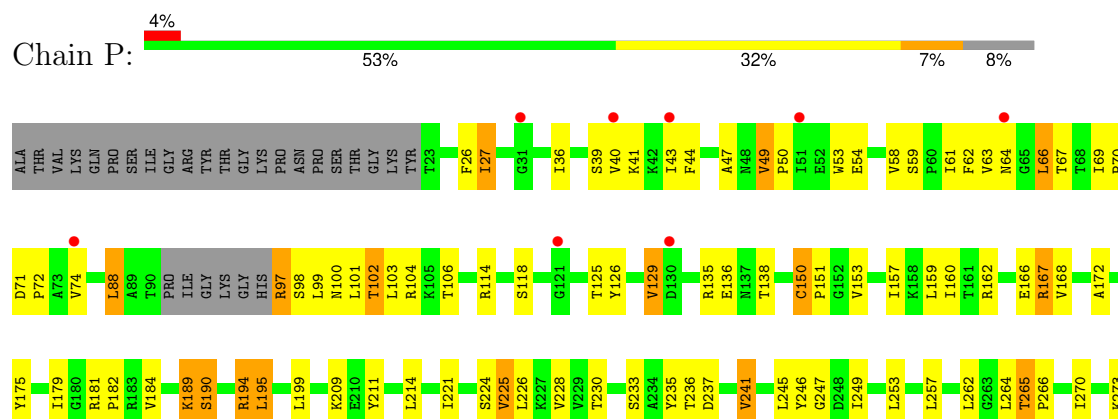


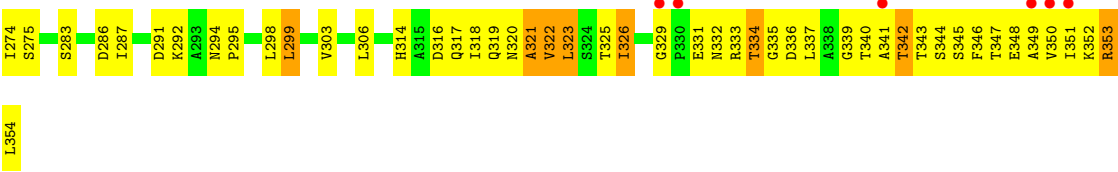


• Molecule 2: Isocitrate dehydrogenase [NAD] subunit 2



• Molecule 2: Isocitrate dehydrogenase [NAD] subunit 2





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	112.44Å 115.21Å 159.25Å 111.03° 96.08° 107.13°	Depositor
Resolution (Å)	35.74 – 2.70 35.74 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.5 (35.74-2.70) 96.5 (35.74-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 2.68Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.239 , 0.264 0.231 , 0.258	Depositor DCC
R_{free} test set	9220 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	71.3	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 36.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.005 for k,h,-h-k-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	41336	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.80	1/2619 (0.0%)	1.02	6/3538 (0.2%)
1	C	0.80	0/2650	0.99	6/3580 (0.2%)
1	E	0.71	1/2671 (0.0%)	1.01	6/3608 (0.2%)
1	G	0.75	0/2611	0.98	5/3527 (0.1%)
1	I	0.78	0/2606	0.99	5/3524 (0.1%)
1	K	0.74	0/2650	1.00	6/3580 (0.2%)
1	M	0.79	0/2634	1.02	3/3559 (0.1%)
1	O	0.69	0/2589	0.97	6/3498 (0.2%)
2	B	0.68	0/2654	1.00	11/3610 (0.3%)
2	D	0.64	0/2643	1.00	10/3595 (0.3%)
2	F	0.61	0/2643	1.01	11/3595 (0.3%)
2	H	0.60	0/2643	0.98	10/3595 (0.3%)
2	J	0.59	0/2643	0.96	12/3595 (0.3%)
2	L	0.59	0/2654	0.96	4/3610 (0.1%)
2	N	0.65	0/2643	1.02	8/3595 (0.2%)
2	P	0.60	0/2493	0.97	9/3390 (0.3%)
All	All	0.69	2/42046 (0.0%)	0.99	118/56999 (0.2%)

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	M	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	319	ILE	CA-CB	5.38	1.61	1.54
1	E	319	ILE	CA-CB	5.25	1.60	1.54

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	9	THR	N-CA-C	-10.12	100.48	112.92
2	N	5	GLN	CA-C-N	8.85	130.90	119.84
2	N	5	GLN	C-N-CA	8.85	130.90	119.84
1	A	306	GLU	N-CA-C	-8.67	101.80	111.07
2	N	329	GLY	CA-C-N	8.59	128.32	119.56
2	N	329	GLY	C-N-CA	8.59	128.32	119.56
1	E	9	THR	N-CA-C	-8.34	103.01	113.02
1	E	306	GLU	N-CA-C	-8.33	102.14	111.14
1	G	306	GLU	N-CA-C	-8.33	102.14	111.14
1	K	306	GLU	N-CA-C	-8.33	102.14	111.14
1	C	306	GLU	N-CA-C	-8.18	102.31	111.14
1	M	306	GLU	N-CA-C	-8.15	102.34	111.14
2	H	5	GLN	CA-C-N	7.99	129.82	119.84
2	H	5	GLN	C-N-CA	7.99	129.82	119.84
1	M	253	GLY	CA-C-N	7.91	127.98	119.28
1	M	253	GLY	C-N-CA	7.91	127.98	119.28
2	F	329	GLY	CA-C-N	7.64	127.35	119.56
2	F	329	GLY	C-N-CA	7.64	127.35	119.56
1	E	253	GLY	CA-C-N	7.49	127.52	119.28
1	E	253	GLY	C-N-CA	7.49	127.52	119.28
1	K	253	GLY	CA-C-N	7.40	127.42	119.28
1	K	253	GLY	C-N-CA	7.40	127.42	119.28
2	P	329	GLY	CA-C-N	7.36	128.00	119.47
2	P	329	GLY	C-N-CA	7.36	128.00	119.47
1	O	306	GLU	N-CA-C	-7.26	103.30	111.14
2	L	49	VAL	CA-C-N	7.09	128.71	119.84
2	L	49	VAL	C-N-CA	7.09	128.71	119.84
2	P	49	VAL	CA-C-N	7.09	128.71	119.84
2	P	49	VAL	C-N-CA	7.09	128.71	119.84
2	N	49	VAL	CA-C-N	7.03	128.63	119.84
2	N	49	VAL	C-N-CA	7.03	128.63	119.84
2	F	49	VAL	CA-C-N	6.91	128.47	119.84
2	F	49	VAL	C-N-CA	6.91	128.47	119.84
2	L	329	GLY	CA-C-N	6.90	127.47	119.47
2	L	329	GLY	C-N-CA	6.90	127.47	119.47
2	D	49	VAL	CA-C-N	6.86	128.41	119.84
2	D	49	VAL	C-N-CA	6.86	128.41	119.84
2	J	49	VAL	CA-C-N	6.79	128.32	119.84
2	J	49	VAL	C-N-CA	6.79	128.32	119.84
2	F	265	THR	CA-C-N	6.76	127.31	120.14
2	F	265	THR	C-N-CA	6.76	127.31	120.14
2	J	5	GLN	CA-C-N	6.64	128.15	119.84
2	J	5	GLN	C-N-CA	6.64	128.15	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	181	ARG	CA-C-N	6.63	125.86	118.97
2	H	181	ARG	C-N-CA	6.63	125.86	118.97
1	O	253	GLY	CA-C-N	6.62	126.56	119.28
1	O	253	GLY	C-N-CA	6.62	126.56	119.28
1	I	306	GLU	N-CA-C	-6.58	104.04	111.14
1	G	253	GLY	CA-C-N	6.57	126.50	119.28
1	G	253	GLY	C-N-CA	6.57	126.50	119.28
2	H	329	GLY	CA-C-N	6.51	127.98	119.84
2	H	329	GLY	C-N-CA	6.51	127.98	119.84
1	C	253	GLY	CA-C-N	6.43	126.36	119.28
1	C	253	GLY	C-N-CA	6.43	126.36	119.28
2	N	265	THR	CA-C-N	6.41	127.65	120.66
2	N	265	THR	C-N-CA	6.41	127.65	120.66
2	B	49	VAL	CA-C-N	6.38	127.82	119.84
2	B	49	VAL	C-N-CA	6.38	127.82	119.84
2	D	329	GLY	CA-C-N	6.37	127.80	119.84
2	D	329	GLY	C-N-CA	6.37	127.80	119.84
1	I	253	GLY	CA-C-N	6.33	126.25	119.28
1	I	253	GLY	C-N-CA	6.33	126.25	119.28
2	J	265	THR	CA-C-N	6.31	127.54	120.66
2	J	265	THR	C-N-CA	6.31	127.54	120.66
2	D	178	ALA	N-CA-C	6.23	119.98	112.38
2	H	49	VAL	CA-C-N	6.23	127.62	119.84
2	H	49	VAL	C-N-CA	6.23	127.62	119.84
2	J	329	GLY	CA-C-N	6.17	127.56	119.84
2	J	329	GLY	C-N-CA	6.17	127.56	119.84
2	B	265	THR	CA-C-N	6.04	127.25	120.66
2	B	265	THR	C-N-CA	6.04	127.25	120.66
2	H	211	TYR	CA-C-N	5.98	125.53	119.19
2	H	211	TYR	C-N-CA	5.98	125.53	119.19
1	G	282	GLY	N-CA-C	-5.89	102.15	110.75
1	I	226	LYS	CA-C-N	5.89	125.57	119.56
1	I	226	LYS	C-N-CA	5.89	125.57	119.56
1	A	226	LYS	CA-C-N	5.88	125.56	119.56
1	A	226	LYS	C-N-CA	5.88	125.56	119.56
2	F	86	GLY	CA-C-N	5.79	126.12	119.92
2	F	86	GLY	C-N-CA	5.79	126.12	119.92
2	B	329	GLY	CA-C-N	5.79	127.08	119.84
2	B	329	GLY	C-N-CA	5.79	127.08	119.84
1	A	253	GLY	CA-C-N	5.78	125.64	119.28
1	A	253	GLY	C-N-CA	5.78	125.64	119.28
1	E	226	LYS	CA-C-N	5.62	125.29	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	226	LYS	C-N-CA	5.62	125.29	119.56
2	P	249	ILE	N-CA-C	5.60	115.80	110.42
2	P	265	THR	CA-C-N	5.58	127.54	120.51
2	P	265	THR	C-N-CA	5.58	127.54	120.51
1	A	251	ILE	N-CA-C	5.47	117.44	112.29
2	D	211	TYR	CA-C-N	5.42	125.03	119.56
2	D	211	TYR	C-N-CA	5.42	125.03	119.56
2	B	86	GLY	CA-C-N	5.36	125.66	119.92
2	B	86	GLY	C-N-CA	5.36	125.66	119.92
2	B	245	LEU	N-CA-C	5.33	117.51	111.11
1	G	238	MET	N-CA-C	5.30	117.97	111.82
2	F	245	LEU	N-CA-C	5.28	117.44	111.11
2	J	245	LEU	N-CA-C	5.26	117.43	111.11
2	F	181	ARG	CA-C-N	5.25	126.41	119.84
2	F	181	ARG	C-N-CA	5.25	126.41	119.84
2	B	168	VAL	CB-CA-C	-5.24	103.77	112.26
1	C	226	LYS	CA-C-N	5.22	124.88	119.56
1	C	226	LYS	C-N-CA	5.22	124.88	119.56
1	C	250	LEU	N-CA-C	5.18	117.59	111.33
1	O	226	LYS	CA-C-N	5.18	124.84	119.56
1	O	226	LYS	C-N-CA	5.18	124.84	119.56
2	B	333	ARG	CB-CA-C	-5.11	109.18	116.34
2	P	211	TYR	CA-C-N	5.09	124.59	119.19
2	P	211	TYR	C-N-CA	5.09	124.59	119.19
2	D	333	ARG	CB-CA-C	-5.08	109.18	115.89
1	O	92	SER	N-CA-C	5.07	117.46	111.33
2	D	265	THR	CA-C-N	5.01	126.83	120.51
2	D	265	THR	C-N-CA	5.01	126.83	120.51
1	K	226	LYS	CA-C-N	5.01	124.67	119.56
1	K	226	LYS	C-N-CA	5.01	124.67	119.56
2	J	333	ARG	CB-CA-C	-5.01	109.27	115.89
2	J	211	TYR	CA-C-N	5.01	124.50	119.19
2	J	211	TYR	C-N-CA	5.01	124.50	119.19

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	M	53	ASN	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2575	0	2608	87	0
1	C	2605	0	2645	86	0
1	E	2626	0	2667	97	0
1	G	2567	0	2597	91	0
1	I	2562	0	2596	91	0
1	K	2605	0	2645	83	0
1	M	2590	0	2635	120	0
1	O	2546	0	2575	85	0
2	B	2608	0	2648	127	0
2	D	2598	0	2641	141	0
2	F	2598	0	2641	156	0
2	H	2598	0	2641	152	0
2	J	2598	0	2641	136	0
2	L	2608	0	2648	141	0
2	N	2598	0	2641	172	0
2	P	2454	0	2498	127	0
All	All	41336	0	41967	1735	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

All (1735) 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)
2:N:97:ARG:NH1	2:N:102:THR:HG23	1.63	1.12
1:E:54:ILE:H	1:E:54:ILE:HD12	1.19	1.06
1:O:181:VAL:HB	1:O:235:THR:HG22	1.37	1.04
1:E:181:VAL:HB	1:E:235:THR:HG22	1.38	1.04
1:A:181:VAL:HB	1:A:235:THR:HG22	1.38	1.03
1:C:181:VAL:HB	1:C:235:THR:HG22	1.40	1.02
2:B:318:ILE:O	2:B:322:VAL:HG21	1.61	1.01
1:I:18:PHE:CZ	1:M:44:ASN:ND2	2.29	1.00
1:K:181:VAL:HB	1:K:235:THR:HG22	1.40	1.00
1:M:54:ILE:HA	1:M:62:GLY:HA3	1.43	1.00
1:I:181:VAL:HB	1:I:235:THR:HG22	1.42	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:181:VAL:HB	1:G:235:THR:HG22	1.43	0.99
1:M:147:VAL:HG22	2:N:161:THR:HG22	1.41	0.99
2:F:287:ILE:HD11	2:F:292:LYS:HD2	1.44	0.98
1:I:18:PHE:HZ	1:M:44:ASN:HD21	1.03	0.98
1:K:175:ARG:HG3	1:K:175:ARG:HH11	1.27	0.98
1:G:54:ILE:H	1:G:54:ILE:HD12	1.29	0.96
1:E:175:ARG:HH11	1:E:175:ARG:HG3	1.29	0.96
1:O:175:ARG:HH11	1:O:175:ARG:HG3	1.29	0.96
2:N:97:ARG:HH12	2:N:102:THR:HG23	1.28	0.96
2:P:135:ARG:HD3	2:P:247:GLY:HA3	1.48	0.96
1:G:175:ARG:HH11	1:G:175:ARG:HG3	1.31	0.95
1:M:175:ARG:HH11	1:M:175:ARG:HG3	1.29	0.95
2:N:287:ILE:HD11	2:N:292:LYS:HD2	1.46	0.95
2:H:194:ARG:HH21	2:H:194:ARG:HG3	1.30	0.95
1:E:280:ILE:HG22	1:E:327:ARG:HE	1.31	0.95
2:H:287:ILE:HD11	2:H:292:LYS:HD2	1.48	0.94
2:F:318:ILE:O	2:F:322:VAL:HG21	1.66	0.94
1:M:181:VAL:HB	1:M:235:THR:HG22	1.47	0.94
2:P:287:ILE:HD11	2:P:292:LYS:HD2	1.47	0.94
2:J:318:ILE:O	2:J:322:VAL:HG21	1.68	0.94
2:B:189:LYS:HD2	2:B:190:SER:H	1.29	0.94
2:L:189:LYS:HD2	2:L:190:SER:H	1.32	0.94
2:N:135:ARG:HD3	2:N:247:GLY:HA3	1.48	0.94
2:N:194:ARG:HG3	2:N:194:ARG:HH21	1.33	0.93
2:D:189:LYS:HD2	2:D:190:SER:H	1.33	0.93
2:L:135:ARG:HD3	2:L:247:GLY:HA3	1.50	0.93
1:M:148:VAL:HB	2:N:160:ILE:HG22	1.47	0.93
2:F:159:LEU:HD21	1:G:144:VAL:HG12	1.49	0.93
2:F:189:LYS:HD2	2:F:190:SER:H	1.32	0.92
2:N:97:ARG:HD2	2:N:101:LEU:HD12	1.50	0.92
1:C:175:ARG:HG3	1:C:175:ARG:HH11	1.33	0.92
2:H:47:ALA:HB2	2:H:354:LEU:HD11	1.50	0.92
1:I:175:ARG:HH11	1:I:175:ARG:HG3	1.35	0.92
2:J:135:ARG:HD3	2:J:247:GLY:HA3	1.51	0.92
2:F:135:ARG:HD3	2:F:247:GLY:HA3	1.51	0.91
2:J:189:LYS:HD2	2:J:190:SER:H	1.31	0.91
2:N:318:ILE:O	2:N:322:VAL:HG21	1.70	0.91
1:I:17:ARG:HH21	1:I:46:PRO:HA	1.34	0.91
2:D:194:ARG:HG3	2:D:194:ARG:HH21	1.35	0.91
2:P:194:ARG:HH21	2:P:194:ARG:HG3	1.36	0.91
2:H:194:ARG:HH21	2:H:194:ARG:CG	1.84	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:135:ARG:HD3	2:D:247:GLY:HA3	1.51	0.90
2:D:318:ILE:O	2:D:322:VAL:HG21	1.71	0.90
1:M:151:LEU:HD23	2:N:157:ILE:HG12	1.53	0.90
2:P:318:ILE:O	2:P:322:VAL:HG21	1.69	0.90
2:P:189:LYS:HD2	2:P:190:SER:H	1.34	0.90
2:N:189:LYS:HD2	2:N:190:SER:H	1.34	0.90
2:H:189:LYS:HD2	2:H:190:SER:H	1.35	0.90
2:H:135:ARG:HD3	2:H:247:GLY:HA3	1.54	0.90
1:E:143:SER:HB3	2:H:159:LEU:HD22	1.53	0.89
2:N:194:ARG:HH21	2:N:194:ARG:CG	1.84	0.89
2:J:287:ILE:HD11	2:J:292:LYS:HD2	1.52	0.89
2:J:194:ARG:HH21	2:J:194:ARG:HG3	1.36	0.89
2:F:194:ARG:HH21	2:F:194:ARG:HG3	1.37	0.88
2:B:135:ARG:HD3	2:B:247:GLY:HA3	1.53	0.88
2:L:194:ARG:HG3	2:L:194:ARG:HH21	1.37	0.88
2:B:194:ARG:HH21	2:B:194:ARG:HG3	1.34	0.88
2:P:194:ARG:HH21	2:P:194:ARG:CG	1.86	0.88
1:I:275:HIS:ND1	1:I:278:LEU:HD12	1.88	0.88
1:A:275:HIS:ND1	1:A:278:LEU:HD12	1.87	0.88
2:D:194:ARG:HH21	2:D:194:ARG:CG	1.87	0.88
2:B:159:LEU:HD22	1:C:143:SER:HB3	1.54	0.87
2:D:287:ILE:HD11	2:D:292:LYS:HD2	1.56	0.87
2:F:194:ARG:HH21	2:F:194:ARG:CG	1.87	0.87
1:K:175:ARG:HH11	1:K:175:ARG:CG	1.87	0.87
1:A:301:HIS:HE1	1:E:15:GLY:O	1.57	0.87
1:A:175:ARG:HH11	1:A:175:ARG:HG3	1.40	0.87
2:H:318:ILE:O	2:H:322:VAL:HG21	1.74	0.86
2:B:322:VAL:O	2:B:326:ILE:HG23	1.75	0.86
2:J:194:ARG:HH21	2:J:194:ARG:CG	1.88	0.86
2:F:159:LEU:CD2	1:G:144:VAL:HG12	2.06	0.86
1:E:151:LEU:HD23	2:F:157:ILE:HG12	1.56	0.85
2:L:287:ILE:HD11	2:L:292:LYS:HD2	1.59	0.85
2:B:194:ARG:HH21	2:B:194:ARG:CG	1.89	0.84
1:A:325:THR:HG22	1:A:331:GLY:HA3	1.60	0.84
2:B:343:THR:O	2:B:347:THR:HG23	1.78	0.84
2:P:318:ILE:HA	2:P:322:VAL:HG11	1.60	0.84
1:I:310:ARG:HG2	1:I:349:MET:HE2	1.58	0.83
2:J:47:ALA:HB2	2:J:354:LEU:HD11	1.59	0.83
2:P:47:ALA:HB2	2:P:354:LEU:HD11	1.60	0.83
1:A:18:PHE:HZ	1:E:44:ASN:ND2	1.75	0.83
1:I:175:ARG:HH11	1:I:175:ARG:CG	1.90	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:175:ARG:HH11	1:E:175:ARG:CG	1.91	0.83
1:G:175:ARG:HH11	1:G:175:ARG:CG	1.91	0.83
2:H:343:THR:O	2:H:347:THR:HG23	1.78	0.83
1:O:175:ARG:HH11	1:O:175:ARG:CG	1.92	0.83
2:B:287:ILE:HD11	2:B:292:LYS:HD2	1.61	0.83
2:L:194:ARG:HH21	2:L:194:ARG:CG	1.91	0.83
2:N:318:ILE:HA	2:N:322:VAL:HG11	1.60	0.83
2:J:343:THR:O	2:J:347:THR:HG23	1.80	0.82
2:F:323:LEU:HD23	2:F:323:LEU:H	1.44	0.82
2:B:102:THR:O	2:B:106:THR:HG23	1.79	0.82
2:J:67:THR:HG21	2:J:97:ARG:N	1.95	0.82
2:L:318:ILE:HA	2:L:322:VAL:HG11	1.61	0.82
2:F:318:ILE:HA	2:F:322:VAL:HG11	1.61	0.82
1:C:175:ARG:HH11	1:C:175:ARG:CG	1.93	0.81
2:L:318:ILE:O	2:L:322:VAL:HG21	1.79	0.81
1:M:175:ARG:HH11	1:M:175:ARG:CG	1.93	0.81
2:F:343:THR:O	2:F:347:THR:HG23	1.81	0.81
2:P:343:THR:O	2:P:347:THR:HG23	1.81	0.81
2:D:322:VAL:O	2:D:326:ILE:HG23	1.81	0.80
2:N:343:THR:O	2:N:347:THR:HG23	1.80	0.80
1:E:280:ILE:CG2	1:E:327:ARG:HE	1.95	0.80
2:F:322:VAL:HB	2:F:323:LEU:HD23	1.63	0.80
2:D:318:ILE:HA	2:D:322:VAL:HG11	1.64	0.80
2:D:343:THR:O	2:D:347:THR:HG23	1.81	0.80
2:F:322:VAL:O	2:F:326:ILE:HG23	1.81	0.80
2:J:318:ILE:HA	2:J:322:VAL:HG11	1.63	0.80
1:M:82:HIS:HB3	1:M:279:ASP:HB3	1.63	0.80
1:A:38:THR:HG22	1:A:343:ILE:HD11	1.63	0.80
1:A:300:ASN:HA	1:A:305:ASN:HB3	1.64	0.80
2:J:159:LEU:HD22	1:K:143:SER:HB3	1.64	0.80
2:J:322:VAL:O	2:J:326:ILE:HG23	1.82	0.79
2:P:66:LEU:HD21	2:P:97:ARG:HH21	1.47	0.79
1:E:280:ILE:HG22	1:E:327:ARG:NE	1.98	0.78
2:L:343:THR:O	2:L:347:THR:HG23	1.81	0.78
2:L:97:ARG:HG2	2:L:98:SER:H	1.48	0.78
1:M:151:LEU:CD2	2:N:157:ILE:HG12	2.14	0.78
2:N:97:ARG:HH12	2:N:102:THR:CG2	1.96	0.78
2:N:159:LEU:HD21	1:O:144:VAL:HG12	1.65	0.78
2:H:318:ILE:HA	2:H:322:VAL:HG11	1.63	0.78
1:M:38:THR:HG22	1:M:343:ILE:HD11	1.64	0.78
1:M:88:THR:HB	2:N:189:LYS:HE3	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:151:LEU:CD2	2:F:157:ILE:HG12	2.14	0.77
2:L:322:VAL:O	2:L:326:ILE:HG23	1.84	0.77
1:M:54:ILE:HD13	1:M:81:TRP:HZ2	1.50	0.77
2:N:314:HIS:O	2:N:318:ILE:HG13	1.84	0.77
2:H:322:VAL:O	2:H:326:ILE:HG23	1.85	0.77
1:K:15:GLY:O	1:O:301:HIS:HE1	1.68	0.77
2:P:97:ARG:HG3	2:P:98:SER:H	1.49	0.77
1:E:325:THR:HG23	1:E:329:ILE:HG13	1.66	0.77
2:B:212:PRO:HG2	1:O:228:HIS:CD2	2.20	0.76
2:F:159:LEU:HD21	1:G:144:VAL:CG1	2.16	0.76
2:J:5:GLN:HG3	2:J:6:PRO:HD2	1.65	0.76
1:O:315:VAL:O	1:O:319:ILE:HG23	1.85	0.76
2:N:323:LEU:HD23	2:N:323:LEU:H	1.49	0.76
1:A:175:ARG:HH11	1:A:175:ARG:CG	1.98	0.76
1:O:38:THR:HG22	1:O:343:ILE:HD11	1.67	0.76
1:G:151:LEU:HD23	2:H:157:ILE:HG12	1.66	0.76
2:H:97:ARG:NH2	2:H:102:THR:HG23	2.00	0.75
2:N:322:VAL:O	2:N:326:ILE:HG23	1.84	0.75
2:B:318:ILE:HA	2:B:322:VAL:HG11	1.66	0.75
1:G:38:THR:HG22	1:G:343:ILE:HD11	1.66	0.75
1:I:315:VAL:O	1:I:319:ILE:HG23	1.86	0.75
1:E:38:THR:HG22	1:E:343:ILE:HD11	1.69	0.75
1:G:56:GLN:C	1:G:58:ASP:H	1.94	0.74
1:I:17:ARG:NH2	1:I:46:PRO:HA	2.01	0.74
1:C:17:ARG:NH1	1:C:48:ASP:OD1	2.21	0.73
2:H:323:LEU:HD23	2:H:323:LEU:H	1.52	0.73
1:M:17:ARG:NH1	1:M:48:ASP:OD1	2.20	0.73
1:M:325:THR:HG23	1:M:329:ILE:HG13	1.71	0.73
1:C:211:VAL:O	2:J:38:LYS:HE3	1.87	0.73
1:C:15:GLY:O	1:G:301:HIS:HE1	1.71	0.73
2:F:69:ILE:HD12	2:F:70:PRO:HD2	1.69	0.73
2:H:97:ARG:HG2	2:H:98:SER:H	1.54	0.73
2:N:47:ALA:HB2	2:N:354:LEU:HD21	1.71	0.73
2:B:36:ILE:HG22	2:B:298:LEU:HD23	1.70	0.72
2:F:97:ARG:NH2	2:F:102:THR:HG23	2.04	0.72
1:I:325:THR:HG23	1:I:329:ILE:HG13	1.71	0.72
1:M:315:VAL:O	1:M:319:ILE:HG23	1.89	0.72
1:C:38:THR:HG22	1:C:343:ILE:HD11	1.71	0.72
2:H:273:LYS:HG3	2:H:274:ILE:HD12	1.71	0.72
2:L:323:LEU:HD23	2:L:323:LEU:H	1.54	0.72
2:L:342:THR:CG2	2:L:345:SER:H	2.02	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:323:LEU:HD23	2:P:323:LEU:H	1.54	0.72
2:N:322:VAL:HB	2:N:323:LEU:HD23	1.72	0.72
2:P:322:VAL:O	2:P:326:ILE:HG23	1.89	0.71
2:L:342:THR:HG22	2:L:345:SER:H	1.53	0.71
2:F:349:ALA:O	2:F:353:ARG:HD3	1.91	0.71
2:B:342:THR:CG2	2:B:345:SER:H	2.04	0.71
1:C:325:THR:HG23	1:C:329:ILE:HG13	1.71	0.71
1:G:281:LYS:HG2	1:G:282:GLY:H	1.55	0.71
1:I:38:THR:HG22	1:I:343:ILE:HD11	1.72	0.71
2:N:159:LEU:CD2	1:O:144:VAL:HG12	2.20	0.71
1:G:315:VAL:O	1:G:319:ILE:HG23	1.91	0.71
2:P:318:ILE:C	2:P:322:VAL:HG21	2.15	0.71
2:H:314:HIS:O	2:H:318:ILE:HG13	1.90	0.71
1:M:113:LEU:HD13	1:M:256:LEU:HD22	1.71	0.71
2:D:89:ALA:O	2:D:91:PRO:HD3	1.91	0.70
2:F:287:ILE:HD11	2:F:292:LYS:CD	2.21	0.70
1:K:315:VAL:O	1:K:319:ILE:HG23	1.91	0.70
2:J:323:LEU:H	2:J:323:LEU:HD23	1.55	0.70
2:P:314:HIS:O	2:P:318:ILE:HG13	1.90	0.70
1:A:79:GLY:HA2	1:A:291:MET:HE1	1.72	0.70
1:A:181:VAL:HB	1:A:235:THR:CG2	2.19	0.70
2:D:342:THR:CG2	2:D:345:SER:H	2.05	0.70
2:D:342:THR:HG22	2:D:345:SER:H	1.55	0.70
1:O:325:THR:HG23	1:O:329:ILE:HG13	1.72	0.70
2:P:194:ARG:HH21	2:P:194:ARG:CB	2.05	0.70
2:D:323:LEU:HD23	2:D:323:LEU:H	1.56	0.70
2:B:323:LEU:H	2:B:323:LEU:HD23	1.55	0.70
2:D:322:VAL:HB	2:D:323:LEU:HD23	1.74	0.70
2:F:189:LYS:HD2	2:F:190:SER:N	2.05	0.70
1:M:147:VAL:HG22	2:N:161:THR:CG2	2.21	0.70
2:J:342:THR:CG2	2:J:345:SER:H	2.05	0.69
1:M:90:HIS:CB	2:N:193:GLN:HG3	2.22	0.69
1:O:55:LYS:HD3	1:O:59:HIS:CD2	2.27	0.69
2:F:194:ARG:HG3	2:F:194:ARG:NH2	2.07	0.69
1:K:38:THR:HG22	1:K:343:ILE:HD11	1.75	0.69
1:A:325:THR:HG23	1:A:329:ILE:HG13	1.74	0.69
2:J:102:THR:O	2:J:106:THR:HG23	1.92	0.69
2:B:322:VAL:HG23	2:B:323:LEU:N	2.07	0.69
2:F:322:VAL:C	2:F:326:ILE:HG23	2.18	0.69
1:K:325:THR:HG23	1:K:329:ILE:HG13	1.74	0.69
2:N:287:ILE:HD11	2:N:292:LYS:CD	2.21	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:314:HIS:O	2:F:318:ILE:HG13	1.93	0.69
1:O:325:THR:HG22	1:O:331:GLY:HA3	1.75	0.69
2:P:189:LYS:HD2	2:P:190:SER:N	2.08	0.69
2:B:189:LYS:HD2	2:B:190:SER:N	2.06	0.68
2:F:273:LYS:HG3	2:F:274:ILE:HD12	1.75	0.68
2:L:66:LEU:CD2	2:L:97:ARG:HH21	2.06	0.68
2:P:194:ARG:HG3	2:P:194:ARG:NH2	2.05	0.68
2:H:342:THR:CG2	2:H:345:SER:H	2.05	0.68
2:J:342:THR:HG22	2:J:345:SER:H	1.58	0.68
2:P:102:THR:O	2:P:106:THR:HG23	1.93	0.68
1:E:147:VAL:HG22	2:F:161:THR:HG22	1.74	0.68
2:H:102:THR:O	2:H:106:THR:HG23	1.93	0.68
2:N:318:ILE:C	2:N:322:VAL:HG21	2.19	0.68
2:N:194:ARG:HH21	2:N:194:ARG:CB	2.06	0.68
2:B:89:ALA:O	2:B:91:PRO:HD3	1.92	0.68
2:F:97:ARG:HH11	2:F:101:LEU:HD12	1.59	0.68
2:F:318:ILE:C	2:F:322:VAL:HG21	2.17	0.68
1:G:325:THR:HG23	1:G:329:ILE:HG13	1.73	0.68
1:A:113:LEU:HD13	1:A:256:LEU:HD22	1.76	0.68
2:H:189:LYS:HD2	2:H:190:SER:N	2.09	0.68
2:L:36:ILE:HG22	2:L:298:LEU:HD23	1.76	0.68
2:D:97:ARG:HH21	2:D:102:THR:HG23	1.58	0.68
2:P:342:THR:CG2	2:P:345:SER:H	2.07	0.68
2:J:314:HIS:O	2:J:318:ILE:HG13	1.94	0.68
2:L:314:HIS:O	2:L:318:ILE:HG13	1.93	0.68
2:B:322:VAL:C	2:B:326:ILE:HG23	2.18	0.68
2:J:194:ARG:HG3	2:J:194:ARG:NH2	2.08	0.68
2:L:273:LYS:HG3	2:L:274:ILE:HD12	1.76	0.68
2:N:349:ALA:O	2:N:353:ARG:HD3	1.93	0.67
2:P:273:LYS:HG3	2:P:274:ILE:HD12	1.76	0.67
2:F:194:ARG:HH21	2:F:194:ARG:CB	2.06	0.67
1:C:79:GLY:HA2	1:C:291:MET:HE1	1.74	0.67
1:M:90:HIS:HB3	2:N:193:GLN:HG3	1.76	0.67
2:D:273:LYS:HG3	2:D:274:ILE:HD12	1.75	0.67
1:G:175:ARG:HG3	1:G:175:ARG:NH1	2.09	0.67
2:L:189:LYS:HD2	2:L:190:SER:N	2.05	0.67
2:F:36:ILE:HG22	2:F:298:LEU:HD23	1.77	0.67
2:H:318:ILE:C	2:H:322:VAL:HG21	2.19	0.67
2:J:318:ILE:C	2:J:322:VAL:HG21	2.18	0.67
2:L:333:ARG:HB2	2:L:339:GLY:HA3	1.77	0.67
2:B:318:ILE:C	2:B:322:VAL:HG21	2.19	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:97:ARG:NH2	2:H:102:THR:CG2	2.57	0.67
2:D:349:ALA:O	2:D:353:ARG:HD3	1.94	0.67
1:E:90:HIS:CB	2:F:193:GLN:HG3	2.25	0.67
1:A:58:ASP:HA	1:A:92:SER:HB2	1.77	0.66
1:A:315:VAL:O	1:A:319:ILE:HG23	1.95	0.66
2:D:314:HIS:O	2:D:318:ILE:HG13	1.95	0.66
2:F:342:THR:CG2	2:F:345:SER:H	2.09	0.66
1:G:151:LEU:CD2	2:H:157:ILE:HG12	2.26	0.66
1:G:281:LYS:CG	1:G:282:GLY:H	2.08	0.66
2:H:342:THR:HG22	2:H:345:SER:H	1.60	0.66
2:P:342:THR:HG22	2:P:345:SER:H	1.58	0.66
2:H:194:ARG:HG3	2:H:194:ARG:NH2	2.03	0.66
1:I:140:GLU:OE2	2:J:194:ARG:HA	1.95	0.66
1:O:300:ASN:HA	1:O:305:ASN:HB3	1.77	0.66
1:A:163:ALA:HB2	1:A:198:ILE:HD13	1.76	0.66
2:N:273:LYS:HG3	2:N:274:ILE:HD12	1.76	0.66
1:A:300:ASN:OD1	1:A:305:ASN:HB2	1.96	0.66
2:B:314:HIS:O	2:B:318:ILE:HG13	1.95	0.66
1:G:300:ASN:HA	1:G:305:ASN:HB3	1.78	0.66
2:H:69:ILE:HD12	2:H:70:PRO:HD2	1.77	0.66
1:M:149:GLU:HG3	2:N:159:LEU:CD1	2.25	0.66
2:P:273:LYS:HE3	2:P:274:ILE:HD11	1.78	0.66
2:J:273:LYS:HG3	2:J:274:ILE:HD12	1.76	0.66
1:C:315:VAL:O	1:C:319:ILE:HG23	1.96	0.66
2:D:322:VAL:C	2:D:326:ILE:HG23	2.21	0.66
2:P:97:ARG:CG	2:P:98:SER:H	2.07	0.66
2:D:194:ARG:HH21	2:D:194:ARG:CB	2.09	0.66
2:F:97:ARG:NH1	2:F:101:LEU:HD12	2.11	0.66
1:M:79:GLY:HA2	1:M:291:MET:HE1	1.78	0.66
2:D:102:THR:O	2:D:106:THR:HG23	1.96	0.65
2:L:349:ALA:O	2:L:353:ARG:HD3	1.96	0.65
2:N:189:LYS:HD2	2:N:190:SER:N	2.07	0.65
2:P:287:ILE:HD11	2:P:292:LYS:CD	2.24	0.65
2:D:291:ASP:O	2:D:343:THR:HG22	1.95	0.65
2:N:69:ILE:HD12	2:N:70:PRO:HD2	1.78	0.65
2:D:318:ILE:C	2:D:322:VAL:HG21	2.21	0.65
1:K:79:GLY:HA2	1:K:291:MET:HE1	1.78	0.65
1:O:151:LEU:HD23	2:P:157:ILE:HG12	1.78	0.65
1:I:245:ASN:OD1	1:I:276:VAL:HG21	1.97	0.65
1:A:301:HIS:CE1	1:E:15:GLY:O	2.45	0.65
2:F:326:ILE:HD11	2:F:346:PHE:CE1	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:325:THR:HG22	1:G:331:GLY:HA3	1.78	0.65
2:J:189:LYS:HD2	2:J:190:SER:N	2.06	0.65
1:C:325:THR:HG22	1:C:331:GLY:HA3	1.79	0.65
2:H:333:ARG:HB2	2:H:339:GLY:HA3	1.77	0.65
2:P:69:ILE:HD12	2:P:70:PRO:HD2	1.79	0.65
2:P:347:THR:O	2:P:351:ILE:HG13	1.97	0.65
2:B:322:VAL:HB	2:B:323:LEU:HD23	1.79	0.65
2:J:322:VAL:C	2:J:326:ILE:HG23	2.22	0.65
2:N:326:ILE:HG21	2:N:350:VAL:HA	1.79	0.65
1:I:310:ARG:HA	1:I:349:MET:HE1	1.78	0.65
2:N:342:THR:CG2	2:N:345:SER:H	2.10	0.65
1:A:305:ASN:HA	1:A:308:ALA:HB3	1.79	0.64
2:D:286:ASP:OD2	2:J:287:ILE:HG12	1.98	0.64
2:L:273:LYS:HE3	2:L:274:ILE:HD11	1.78	0.64
2:L:322:VAL:C	2:L:326:ILE:HG23	2.22	0.64
2:P:326:ILE:HG21	2:P:350:VAL:HA	1.80	0.64
1:A:325:THR:HG22	1:A:331:GLY:CA	2.25	0.64
1:C:300:ASN:HA	1:C:305:ASN:HB3	1.77	0.64
1:E:315:VAL:O	1:E:319:ILE:HG23	1.97	0.64
2:F:342:THR:HG22	2:F:345:SER:H	1.63	0.64
2:H:273:LYS:HE3	2:H:274:ILE:HD11	1.78	0.64
2:D:333:ARG:HB2	2:D:339:GLY:HA3	1.78	0.64
1:I:300:ASN:HA	1:I:305:ASN:HB3	1.78	0.64
2:J:194:ARG:HH21	2:J:194:ARG:CB	2.11	0.64
2:J:322:VAL:HB	2:J:323:LEU:HD23	1.78	0.64
2:L:318:ILE:C	2:L:322:VAL:HG21	2.23	0.64
1:M:223:ALA:O	1:M:227:PRO:HG3	1.98	0.64
2:N:342:THR:HG22	2:N:345:SER:H	1.61	0.64
2:H:322:VAL:HB	2:H:323:LEU:HD23	1.80	0.64
2:J:36:ILE:HG22	2:J:298:LEU:HD23	1.78	0.64
2:J:349:ALA:O	2:J:353:ARG:HD3	1.97	0.64
2:B:347:THR:O	2:B:351:ILE:HG13	1.98	0.64
2:H:349:ALA:O	2:H:353:ARG:HD3	1.98	0.64
2:L:102:THR:O	2:L:106:THR:HG23	1.98	0.64
1:O:175:ARG:HG3	1:O:175:ARG:NH1	2.08	0.64
2:B:5:GLN:NE2	2:B:6:PRO:HD2	2.12	0.64
2:H:326:ILE:HG21	2:H:350:VAL:HA	1.80	0.64
1:K:175:ARG:HG3	1:K:175:ARG:NH1	2.05	0.64
1:K:175:ARG:CG	1:K:175:ARG:NH1	2.55	0.64
2:B:224:SER:O	2:B:228:VAL:HG23	1.98	0.63
2:D:273:LYS:HE3	2:D:274:ILE:HD11	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:181:VAL:HB	1:E:235:THR:CG2	2.22	0.63
2:H:194:ARG:HH21	2:H:194:ARG:CB	2.10	0.63
1:M:222:GLN:HG3	1:M:229:GLN:OE1	1.98	0.63
2:L:347:THR:O	2:L:351:ILE:HG13	1.98	0.63
2:B:342:THR:HG22	2:B:345:SER:H	1.61	0.63
1:C:113:LEU:HD13	1:C:256:LEU:HD22	1.79	0.63
1:E:222:GLN:HG3	1:E:229:GLN:OE1	1.98	0.63
2:F:159:LEU:HD22	1:G:143:SER:HB3	1.80	0.63
2:J:273:LYS:HE3	2:J:274:ILE:HD11	1.80	0.63
1:C:345:LYS:O	1:C:349:MET:HG3	1.99	0.63
1:I:175:ARG:NH1	1:I:231:ASP:OD1	2.32	0.63
1:M:143:SER:HB3	2:P:159:LEU:HD22	1.81	0.63
1:M:300:ASN:HA	1:M:305:ASN:HB3	1.80	0.63
2:N:322:VAL:C	2:N:326:ILE:HG23	2.23	0.63
2:F:347:THR:O	2:F:351:ILE:HG13	1.98	0.63
2:B:291:ASP:O	2:B:343:THR:HG22	1.98	0.63
1:K:113:LEU:HD13	1:K:256:LEU:HD22	1.79	0.63
1:C:246:ILE:HD11	2:D:253:LEU:HD12	1.81	0.63
1:I:135:GLU:OE2	2:J:189:LYS:HE2	1.99	0.63
1:I:305:ASN:HA	1:I:308:ALA:HB3	1.81	0.63
2:L:322:VAL:HB	2:L:323:LEU:HD23	1.79	0.63
1:O:123:ILE:HD13	1:O:250:LEU:HB3	1.81	0.63
2:P:326:ILE:HD11	2:P:346:PHE:CE1	2.34	0.63
2:F:245:LEU:HD23	2:F:246:TYR:CE1	2.34	0.63
2:H:322:VAL:C	2:H:326:ILE:HG23	2.24	0.63
1:E:325:THR:HG22	1:E:331:GLY:HA3	1.81	0.62
2:J:69:ILE:HD12	2:J:70:PRO:HD2	1.79	0.62
2:P:322:VAL:HB	2:P:323:LEU:HD23	1.81	0.62
2:B:349:ALA:O	2:B:353:ARG:HD3	1.99	0.62
2:D:36:ILE:HG22	2:D:298:LEU:HD23	1.80	0.62
2:J:322:VAL:HG23	2:J:323:LEU:N	2.13	0.62
2:J:333:ARG:HB2	2:J:339:GLY:HA3	1.81	0.62
2:N:194:ARG:HG3	2:N:194:ARG:NH2	2.03	0.62
1:G:113:LEU:HD13	1:G:256:LEU:HD22	1.82	0.62
1:K:300:ASN:HA	1:K:305:ASN:HB3	1.81	0.62
2:L:351:ILE:HA	2:L:354:LEU:HB2	1.80	0.62
1:K:175:ARG:NH1	1:K:231:ASP:OD1	2.32	0.62
2:B:194:ARG:HG3	2:B:194:ARG:NH2	2.08	0.62
1:I:181:VAL:HB	1:I:235:THR:CG2	2.23	0.62
2:L:326:ILE:HG21	2:L:350:VAL:HA	1.82	0.62
1:C:222:GLN:HG3	1:C:229:GLN:OE1	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:175:ARG:NH1	1:G:231:ASP:OD1	2.33	0.62
1:G:305:ASN:HA	1:G:308:ALA:HB3	1.81	0.62
1:E:54:ILE:H	1:E:54:ILE:CD1	1.88	0.62
2:F:326:ILE:HG21	2:F:350:VAL:HA	1.81	0.62
2:D:69:ILE:HD12	2:D:70:PRO:HD2	1.81	0.62
1:M:10:LEU:CD2	1:M:11:PRO:HD2	2.30	0.62
1:M:311:ILE:O	1:M:315:VAL:HG13	1.99	0.62
2:H:97:ARG:HH11	2:H:101:LEU:HD12	1.64	0.62
2:N:36:ILE:HG22	2:N:298:LEU:HD23	1.81	0.62
1:K:222:GLN:HG3	1:K:229:GLN:OE1	1.99	0.61
2:L:194:ARG:HG3	2:L:194:ARG:NH2	2.10	0.61
1:C:175:ARG:HG3	1:C:175:ARG:NH1	2.10	0.61
1:E:79:GLY:HA2	1:E:291:MET:HE1	1.81	0.61
2:J:326:ILE:HG21	2:J:350:VAL:HA	1.80	0.61
2:N:159:LEU:HD21	1:O:144:VAL:CG1	2.28	0.61
2:B:326:ILE:HG21	2:B:350:VAL:HA	1.81	0.61
1:C:90:HIS:CB	2:D:193:GLN:HG3	2.31	0.61
1:E:300:ASN:HA	1:E:305:ASN:HB3	1.81	0.61
1:M:305:ASN:HA	1:M:308:ALA:HB3	1.82	0.61
2:L:97:ARG:CG	2:L:98:SER:H	2.13	0.61
2:J:347:THR:O	2:J:351:ILE:HG13	1.99	0.61
2:N:273:LYS:HE3	2:N:274:ILE:HD11	1.82	0.61
2:P:66:LEU:CD2	2:P:97:ARG:HH21	2.14	0.61
2:P:349:ALA:O	2:P:353:ARG:HD3	2.00	0.61
1:A:18:PHE:CZ	1:E:44:ASN:ND2	2.64	0.61
1:K:151:LEU:HD23	2:L:157:ILE:HG12	1.83	0.61
1:K:245:ASN:OD1	1:K:276:VAL:HG21	2.00	0.61
1:G:222:GLN:HG3	1:G:229:GLN:OE1	2.00	0.61
1:I:275:HIS:ND1	1:I:278:LEU:CD1	2.61	0.61
2:D:189:LYS:HD2	2:D:190:SER:N	2.10	0.61
2:J:291:ASP:O	2:J:343:THR:HG22	2.01	0.61
1:M:146:GLY:O	2:N:161:THR:HA	2.01	0.61
2:N:333:ARG:HB2	2:N:339:GLY:HA3	1.83	0.61
1:A:155:THR:O	1:A:159:THR:CG2	2.48	0.61
2:H:97:ARG:NH1	2:H:101:LEU:CD1	2.63	0.61
2:J:287:ILE:HD11	2:J:292:LYS:CD	2.30	0.61
1:K:55:LYS:HB3	1:K:57:THR:HG22	1.81	0.61
1:O:181:VAL:HB	1:O:235:THR:CG2	2.23	0.61
2:P:333:ARG:HB2	2:P:339:GLY:HA3	1.81	0.61
1:I:113:LEU:HD13	1:I:256:LEU:HD22	1.82	0.60
1:I:222:GLN:HG3	1:I:229:GLN:OE1	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:325:THR:HG22	1:I:331:GLY:HA3	1.82	0.60
2:J:97:ARG:HH21	2:J:102:THR:HG23	1.66	0.60
1:O:175:ARG:NH1	1:O:231:ASP:OD1	2.35	0.60
2:B:97:ARG:NH2	2:B:102:THR:HG23	2.16	0.60
2:J:97:ARG:HH21	2:J:102:THR:CG2	2.14	0.60
2:D:194:ARG:HG3	2:D:194:ARG:NH2	2.07	0.60
2:D:326:ILE:HG21	2:D:350:VAL:HA	1.82	0.60
2:H:6:PRO:O	2:H:10:ARG:HG2	2.01	0.60
1:O:222:GLN:HG3	1:O:229:GLN:OE1	2.01	0.60
1:G:79:GLY:HA2	1:G:291:MET:HE1	1.82	0.60
1:I:300:ASN:OD1	1:I:305:ASN:HB2	2.02	0.60
2:B:69:ILE:HD12	2:B:70:PRO:HD2	1.83	0.60
1:C:163:ALA:HB2	1:C:198:ILE:HD13	1.84	0.60
1:I:79:GLY:HA2	1:I:291:MET:HE1	1.84	0.60
2:L:291:ASP:O	2:L:343:THR:HG22	2.02	0.60
1:M:305:ASN:HA	1:M:308:ALA:CB	2.32	0.60
1:C:305:ASN:HA	1:C:308:ALA:HB3	1.83	0.60
2:F:273:LYS:HE3	2:F:274:ILE:HD11	1.84	0.60
2:L:322:VAL:HG23	2:L:323:LEU:N	2.16	0.60
2:N:118:SER:OG	2:N:129:VAL:HG13	2.02	0.60
1:G:55:LYS:HB3	1:G:56:GLN:NE2	2.15	0.60
1:M:155:THR:O	1:M:159:THR:CG2	2.50	0.60
1:C:175:ARG:NH1	1:C:231:ASP:OD1	2.35	0.59
1:C:300:ASN:OD1	1:C:305:ASN:HB2	2.02	0.59
1:A:144:VAL:HG12	2:D:159:LEU:HD21	1.83	0.59
1:A:305:ASN:HA	1:A:308:ALA:CB	2.31	0.59
2:B:40:VAL:HG22	2:B:299:LEU:HD13	1.84	0.59
2:B:175:TYR:O	2:B:179:ILE:HG12	2.02	0.59
2:P:97:ARG:CZ	2:P:102:THR:HG23	2.32	0.59
1:A:18:PHE:HZ	1:E:44:ASN:HD22	1.51	0.59
2:F:97:ARG:NH1	2:F:101:LEU:CD1	2.66	0.59
1:G:155:THR:O	1:G:159:THR:HG22	2.02	0.59
2:N:291:ASP:O	2:N:343:THR:HG22	2.02	0.59
2:H:39:SER:O	2:H:43:ILE:HG13	2.03	0.59
1:I:163:ALA:HB2	1:I:198:ILE:HD13	1.84	0.59
2:B:194:ARG:HH21	2:B:194:ARG:CB	2.15	0.59
1:O:79:GLY:HA2	1:O:291:MET:HE1	1.84	0.59
2:P:322:VAL:C	2:P:326:ILE:HG23	2.28	0.59
1:E:175:ARG:NH1	1:E:231:ASP:OD1	2.36	0.59
2:F:6:PRO:O	2:F:10:ARG:HG2	2.03	0.59
2:H:36:ILE:HG22	2:H:298:LEU:HD23	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:123:ILE:HD13	1:M:250:LEU:HB3	1.82	0.59
1:O:292:ILE:O	1:O:295:SER:HB3	2.03	0.59
2:H:347:THR:O	2:H:351:ILE:HG13	2.02	0.59
2:F:333:ARG:HB2	2:F:339:GLY:HA3	1.84	0.59
2:P:36:ILE:HG22	2:P:298:LEU:HD23	1.85	0.59
2:P:97:ARG:HG3	2:P:98:SER:N	2.17	0.59
2:D:322:VAL:HG23	2:D:323:LEU:N	2.16	0.58
2:D:326:ILE:HD11	2:D:346:PHE:CE1	2.38	0.58
2:F:102:THR:O	2:F:106:THR:HG23	2.03	0.58
2:F:322:VAL:HG23	2:F:323:LEU:N	2.16	0.58
1:K:181:VAL:HB	1:K:235:THR:CG2	2.25	0.58
1:M:221:MET:SD	2:N:261:SER:HA	2.42	0.58
2:N:347:THR:O	2:N:351:ILE:HG13	2.02	0.58
1:C:181:VAL:HB	1:C:235:THR:CG2	2.24	0.58
1:C:305:ASN:HA	1:C:308:ALA:CB	2.32	0.58
2:D:291:ASP:C	2:D:343:THR:HG22	2.28	0.58
1:E:223:ALA:O	1:E:227:PRO:HG3	2.03	0.58
1:K:223:ALA:O	1:K:227:PRO:HG3	2.03	0.58
1:A:175:ARG:NH1	1:A:231:ASP:OD1	2.37	0.58
1:E:245:ASN:OD1	1:E:276:VAL:HG21	2.03	0.58
1:E:305:ASN:HA	1:E:308:ALA:HB3	1.84	0.58
2:H:326:ILE:HD11	2:H:346:PHE:CE1	2.38	0.58
1:I:140:GLU:HB3	2:J:195:LEU:CD2	2.34	0.58
1:I:155:THR:O	1:I:159:THR:HG23	2.03	0.58
2:L:89:ALA:O	2:L:91:PRO:HD3	2.04	0.58
1:A:323:LYS:O	1:A:324:HIS:HB2	2.03	0.58
1:K:305:ASN:HA	1:K:308:ALA:CB	2.34	0.58
1:M:149:GLU:HG3	2:N:159:LEU:HD12	1.86	0.58
1:M:151:LEU:HA	2:N:156:SER:O	2.02	0.58
2:P:318:ILE:CA	2:P:322:VAL:HG11	2.34	0.58
2:B:273:LYS:HE3	2:B:274:ILE:HD11	1.86	0.58
2:J:97:ARG:NH2	2:J:102:THR:HG23	2.18	0.58
1:K:305:ASN:HA	1:K:308:ALA:HB3	1.85	0.58
2:L:194:ARG:HH21	2:L:194:ARG:CB	2.16	0.58
2:D:287:ILE:HD11	2:D:292:LYS:CD	2.33	0.58
1:G:305:ASN:HA	1:G:308:ALA:CB	2.33	0.58
1:I:155:THR:O	1:I:159:THR:CG2	2.51	0.58
1:K:292:ILE:O	1:K:295:SER:HB3	2.03	0.58
2:B:182:PRO:HD2	2:B:237:ASP:O	2.03	0.58
1:O:305:ASN:HA	1:O:308:ALA:HB3	1.86	0.58
1:K:151:LEU:CD2	2:L:157:ILE:HG12	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:175:ARG:HG3	1:E:175:ARG:NH1	2.09	0.57
1:G:55:LYS:N	1:G:55:LYS:HD2	2.18	0.57
1:G:300:ASN:OD1	1:G:305:ASN:HB2	2.02	0.57
2:H:97:ARG:CG	2:H:98:SER:H	2.15	0.57
2:D:318:ILE:CA	2:D:322:VAL:HG11	2.33	0.57
2:J:326:ILE:HD11	2:J:346:PHE:CE1	2.38	0.57
1:M:175:ARG:NH1	1:M:231:ASP:OD1	2.37	0.57
1:A:275:HIS:CE1	1:A:278:LEU:HD12	2.40	0.57
1:I:90:HIS:CB	2:J:193:GLN:HG3	2.35	0.57
2:L:175:TYR:O	2:L:179:ILE:HG12	2.04	0.57
2:B:273:LYS:HG3	2:B:274:ILE:HD12	1.85	0.57
2:F:287:ILE:HG13	2:F:292:LYS:HB2	1.87	0.57
2:D:88:LEU:HD13	2:D:99:LEU:HD23	1.87	0.57
1:E:113:LEU:HD13	1:E:256:LEU:HD22	1.87	0.57
2:F:39:SER:O	2:F:43:ILE:HG13	2.04	0.57
1:G:155:THR:O	1:G:159:THR:CG2	2.52	0.57
1:A:324:HIS:CG	1:A:341:GLU:HG3	2.40	0.57
2:D:6:PRO:O	2:D:10:ARG:HG2	2.03	0.57
1:I:54:ILE:HG23	1:I:59:HIS:HB3	1.86	0.57
1:M:116:VAL:HG23	1:M:319:ILE:CD1	2.35	0.57
1:M:199:THR:HA	1:M:211:VAL:HG11	1.86	0.57
1:C:151:LEU:HD23	2:D:157:ILE:HG12	1.87	0.57
1:C:79:GLY:HA2	1:C:291:MET:CE	2.35	0.57
1:E:54:ILE:HD12	1:E:54:ILE:N	2.04	0.57
2:F:44:PHE:CD2	2:F:49:VAL:HG21	2.39	0.57
1:I:278:LEU:HD22	1:I:280:ILE:HG12	1.85	0.57
1:I:292:ILE:O	1:I:295:SER:HB3	2.05	0.57
2:L:351:ILE:HG23	2:L:354:LEU:HD23	1.86	0.57
2:N:326:ILE:HD11	2:N:346:PHE:CE1	2.39	0.57
2:B:67:THR:OG1	2:B:97:ARG:HB3	2.04	0.57
1:E:314:ALA:HB2	1:E:346:LEU:HD13	1.86	0.57
2:H:287:ILE:HD11	2:H:292:LYS:CD	2.28	0.57
1:I:54:ILE:HG22	1:I:56:GLN:O	2.04	0.57
1:O:56:GLN:C	1:O:58:ASP:H	2.12	0.57
1:O:113:LEU:HD13	1:O:256:LEU:HD22	1.86	0.57
2:B:333:ARG:HB2	2:B:339:GLY:HA3	1.86	0.57
1:K:163:ALA:HB2	1:K:198:ILE:HD13	1.86	0.57
2:N:12:THR:HB	2:N:81:LEU:CD1	2.35	0.57
1:O:163:ALA:HB2	1:O:198:ILE:HD13	1.87	0.57
1:C:195:ARG:O	1:C:199:THR:HG23	2.05	0.56
1:I:199:THR:HA	1:I:211:VAL:HG11	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:6:PRO:O	2:B:10:ARG:HG2	2.05	0.56
2:B:47:ALA:HB2	2:B:354:LEU:HD21	1.87	0.56
1:E:123:ILE:HD13	1:E:250:LEU:HB3	1.86	0.56
1:E:163:ALA:HB2	1:E:198:ILE:HD13	1.86	0.56
2:J:6:PRO:O	2:J:10:ARG:HG2	2.05	0.56
2:L:69:ILE:HD12	2:L:70:PRO:HD2	1.86	0.56
1:A:311:ILE:O	1:A:315:VAL:HG13	2.05	0.56
2:D:245:LEU:HD23	2:D:246:TYR:CE1	2.39	0.56
2:D:347:THR:O	2:D:351:ILE:HG13	2.05	0.56
1:E:90:HIS:HB3	2:F:193:GLN:HG3	1.86	0.56
1:E:139:LEU:HD23	1:E:151:LEU:HD12	1.87	0.56
1:I:189:LEU:HB3	2:J:154:VAL:HG11	1.87	0.56
2:N:39:SER:O	2:N:43:ILE:HG13	2.05	0.56
1:O:25:GLY:HA2	1:O:81:TRP:CZ2	2.39	0.56
2:F:318:ILE:CA	2:F:322:VAL:HG11	2.34	0.56
1:K:325:THR:HG22	1:K:331:GLY:HA3	1.87	0.56
2:N:322:VAL:HG23	2:N:323:LEU:N	2.20	0.56
2:P:39:SER:O	2:P:43:ILE:HG13	2.06	0.56
1:A:222:GLN:HG3	1:A:229:GLN:OE1	2.06	0.56
1:G:20:VAL:HG13	1:G:47:ILE:HG23	1.88	0.56
1:I:280:ILE:HD12	1:I:280:ILE:O	2.05	0.56
2:B:97:ARG:NH2	2:B:102:THR:CG2	2.69	0.56
1:G:123:ILE:HD13	1:G:250:LEU:HB3	1.86	0.56
1:M:325:THR:CG2	1:M:329:ILE:HG13	2.35	0.56
2:N:97:ARG:HG3	2:N:98:SER:N	2.16	0.56
1:A:223:ALA:O	1:A:227:PRO:HG3	2.05	0.56
2:B:40:VAL:HG22	2:B:299:LEU:CD1	2.36	0.56
2:B:291:ASP:C	2:B:343:THR:HG22	2.31	0.56
1:C:155:THR:O	1:C:159:THR:CG2	2.54	0.56
1:E:199:THR:HA	1:E:211:VAL:HG11	1.86	0.56
2:H:318:ILE:CA	2:H:322:VAL:HG11	2.34	0.56
2:F:291:ASP:O	2:F:343:THR:HG22	2.06	0.56
2:N:274:ILE:HG22	2:N:275:SER:N	2.20	0.56
1:E:292:ILE:O	1:E:295:SER:HB3	2.06	0.56
2:H:12:THR:HB	2:H:81:LEU:CD1	2.36	0.56
2:J:318:ILE:CA	2:J:322:VAL:HG11	2.35	0.56
1:M:10:LEU:HD22	1:M:11:PRO:HD2	1.88	0.56
1:M:300:ASN:OD1	1:M:305:ASN:HB2	2.06	0.56
1:E:79:GLY:HA2	1:E:291:MET:CE	2.36	0.56
2:F:47:ALA:HB2	2:F:354:LEU:HD11	1.87	0.56
2:L:318:ILE:CA	2:L:322:VAL:HG11	2.33	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:47:ALA:HB2	2:B:354:LEU:HD11	1.88	0.55
1:E:175:ARG:CG	1:E:175:ARG:NH1	2.59	0.55
2:J:47:ALA:CA	2:J:354:LEU:HD21	2.35	0.55
1:M:84:PRO:HB3	2:N:220:LEU:HD11	1.87	0.55
1:M:235:THR:HG21	1:M:243:LEU:HD12	1.89	0.55
1:C:276:VAL:O	2:D:226:LEU:HD12	2.06	0.55
1:E:246:ILE:HD11	2:F:253:LEU:HD12	1.88	0.55
1:E:305:ASN:HA	1:E:308:ALA:CB	2.37	0.55
2:L:135:ARG:CD	2:L:247:GLY:HA3	2.32	0.55
2:P:47:ALA:CB	2:P:354:LEU:HD11	2.36	0.55
2:D:166:GLU:O	2:D:167:ARG:HB2	2.05	0.55
2:H:291:ASP:O	2:H:343:THR:HG22	2.07	0.55
1:M:195:ARG:O	1:M:199:THR:HG23	2.07	0.55
2:P:63:VAL:O	2:P:64:ASN:HB2	2.05	0.55
1:K:281:LYS:O	1:K:281:LYS:HD2	2.06	0.55
2:P:322:VAL:HG23	2:P:323:LEU:N	2.21	0.55
1:A:79:GLY:HA2	1:A:291:MET:CE	2.36	0.55
1:A:246:ILE:HD11	2:B:253:LEU:HD12	1.88	0.55
1:C:223:ALA:O	1:C:227:PRO:HG3	2.07	0.55
1:G:58:ASP:HA	1:G:92:SER:HB2	1.88	0.55
1:G:116:VAL:HG23	1:G:319:ILE:CD1	2.37	0.55
1:K:246:ILE:HD11	2:L:253:LEU:HD12	1.89	0.55
2:L:6:PRO:O	2:L:10:ARG:HG2	2.06	0.55
2:N:5:GLN:HG3	2:N:6:PRO:HD2	1.89	0.55
1:K:79:GLY:HA2	1:K:291:MET:CE	2.37	0.55
2:L:332:ASN:HA	2:L:341:ALA:HB2	1.89	0.55
2:N:6:PRO:O	2:N:10:ARG:HG2	2.07	0.55
1:O:54:ILE:CG2	1:O:59:HIS:HB3	2.37	0.55
1:O:199:THR:HA	1:O:211:VAL:HG11	1.88	0.55
1:E:149:GLU:HG3	2:F:159:LEU:HD12	1.89	0.55
1:I:305:ASN:HA	1:I:308:ALA:CB	2.37	0.55
1:M:155:THR:HG22	2:N:153:VAL:HG13	1.88	0.55
1:M:292:ILE:O	1:M:295:SER:HB3	2.07	0.55
1:E:143:SER:HB3	2:H:159:LEU:CD2	2.32	0.55
1:G:199:THR:HA	1:G:211:VAL:HG11	1.88	0.55
1:I:55:LYS:HD3	1:I:55:LYS:N	2.20	0.55
1:M:181:VAL:HB	1:M:235:THR:CG2	2.29	0.55
2:N:287:ILE:HG13	2:N:292:LYS:HB2	1.89	0.55
2:N:318:ILE:CA	2:N:322:VAL:HG11	2.33	0.55
2:B:318:ILE:CA	2:B:322:VAL:HG11	2.37	0.54
2:F:97:ARG:NH2	2:F:102:THR:CG2	2.70	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:175:TYR:O	2:F:179:ILE:HG12	2.06	0.54
1:G:25:GLY:HA2	1:G:81:TRP:CZ2	2.43	0.54
2:J:291:ASP:C	2:J:343:THR:HG22	2.32	0.54
1:K:276:VAL:O	2:L:226:LEU:HD12	2.07	0.54
1:M:113:LEU:CD1	1:M:256:LEU:HD22	2.37	0.54
1:O:235:THR:HG21	1:O:243:LEU:HD12	1.88	0.54
1:A:90:HIS:CB	2:B:193:GLN:HG3	2.37	0.54
2:H:67:THR:OG1	2:H:97:ARG:HB3	2.07	0.54
1:I:277:GLY:O	1:I:279:ASP:N	2.40	0.54
1:M:139:LEU:HD23	1:M:151:LEU:HD12	1.87	0.54
2:N:63:VAL:O	2:N:64:ASN:HB2	2.06	0.54
2:N:332:ASN:HA	2:N:341:ALA:HB2	1.89	0.54
1:O:305:ASN:HA	1:O:308:ALA:CB	2.38	0.54
2:P:126:TYR:HB2	2:P:257:LEU:O	2.08	0.54
2:H:97:ARG:NH1	2:H:101:LEU:HD12	2.22	0.54
2:H:224:SER:O	2:H:228:VAL:HG23	2.07	0.54
2:J:245:LEU:HD23	2:J:246:TYR:CE1	2.43	0.54
2:P:97:ARG:CG	2:P:98:SER:N	2.71	0.54
1:A:288:PRO:O	1:A:292:ILE:HG13	2.08	0.54
1:C:292:ILE:O	1:C:295:SER:HB3	2.08	0.54
2:D:224:SER:O	2:D:228:VAL:HG23	2.07	0.54
1:E:300:ASN:OD1	1:E:305:ASN:HB2	2.07	0.54
1:I:175:ARG:HG3	1:I:175:ARG:NH1	2.11	0.54
2:L:342:THR:HG23	2:L:344:SER:H	1.73	0.54
1:O:116:VAL:HG23	1:O:319:ILE:CD1	2.37	0.54
2:H:322:VAL:HG23	2:H:323:LEU:N	2.20	0.54
1:I:223:ALA:O	1:I:227:PRO:HG3	2.07	0.54
2:N:102:THR:O	2:N:106:THR:HG23	2.07	0.54
1:O:195:ARG:O	1:O:199:THR:HG23	2.08	0.54
2:D:63:VAL:O	2:D:64:ASN:HB2	2.08	0.54
2:F:97:ARG:HH22	2:F:102:THR:HG23	1.73	0.54
2:H:175:TYR:O	2:H:179:ILE:HG12	2.07	0.54
1:K:300:ASN:OD1	1:K:305:ASN:HB2	2.07	0.54
2:N:157:ILE:CD1	1:O:151:LEU:HD11	2.38	0.54
1:E:88:THR:HB	2:F:189:LYS:HE3	1.89	0.54
2:L:5:GLN:HA	2:L:5:GLN:HE21	1.73	0.54
1:M:155:THR:O	1:M:159:THR:HG23	2.08	0.54
1:G:235:THR:HG21	1:G:243:LEU:HD12	1.90	0.54
1:I:25:GLY:HA2	1:I:81:TRP:CZ2	2.42	0.54
2:N:41:LYS:HG2	2:N:53:TRP:NE1	2.23	0.54
1:O:300:ASN:OD1	1:O:305:ASN:HB2	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:PHE:HZ	1:E:44:ASN:HD21	1.53	0.54
2:F:63:VAL:O	2:F:64:ASN:HB2	2.08	0.54
1:G:163:ALA:HB2	1:G:198:ILE:HD13	1.89	0.54
1:I:314:ALA:HB2	1:I:346:LEU:HD13	1.88	0.54
2:L:194:ARG:CG	2:L:194:ARG:NH2	2.61	0.54
2:B:326:ILE:HD11	2:B:346:PHE:CE1	2.44	0.53
2:F:41:LYS:HG2	2:F:53:TRP:NE1	2.22	0.53
2:H:150:CYS:HB2	2:H:151:PRO:CD	2.38	0.53
2:H:291:ASP:C	2:H:343:THR:HG22	2.32	0.53
1:I:325:THR:CG2	1:I:329:ILE:HG13	2.37	0.53
2:N:221:ILE:O	2:N:225:VAL:HG13	2.08	0.53
2:F:274:ILE:HG22	2:F:275:SER:N	2.24	0.53
2:F:348:GLU:O	2:F:352:LYS:HG2	2.09	0.53
1:G:79:GLY:HA2	1:G:291:MET:CE	2.37	0.53
1:G:181:VAL:HB	1:G:235:THR:CG2	2.27	0.53
1:I:140:GLU:HB3	2:J:195:LEU:HD21	1.91	0.53
1:M:148:VAL:HB	2:N:160:ILE:CG2	2.31	0.53
2:N:44:PHE:CD2	2:N:49:VAL:HG21	2.44	0.53
1:E:116:VAL:HG23	1:E:319:ILE:CD1	2.38	0.53
1:E:148:VAL:HB	2:F:160:ILE:HG22	1.90	0.53
1:E:325:THR:CG2	1:E:329:ILE:HG13	2.36	0.53
2:L:291:ASP:C	2:L:343:THR:HG22	2.33	0.53
2:P:291:ASP:O	2:P:343:THR:HG22	2.08	0.53
1:G:56:GLN:C	1:G:58:ASP:N	2.65	0.53
2:F:118:SER:OG	2:F:129:VAL:HG13	2.08	0.53
1:G:325:THR:CG2	1:G:329:ILE:HG13	2.39	0.53
1:K:199:THR:HA	1:K:211:VAL:HG11	1.89	0.53
2:L:66:LEU:HD21	2:L:97:ARG:HH21	1.74	0.53
2:L:326:ILE:O	2:L:326:ILE:HD12	2.08	0.53
2:P:88:LEU:HD13	2:P:99:LEU:HD23	1.89	0.53
1:A:245:ASN:OD1	1:A:276:VAL:HG21	2.09	0.53
2:D:342:THR:HG23	2:D:344:SER:H	1.74	0.53
1:I:116:VAL:HG23	1:I:319:ILE:CD1	2.39	0.53
2:P:44:PHE:CD2	2:P:49:VAL:HG21	2.44	0.53
1:C:314:ALA:HB2	1:C:346:LEU:HD13	1.90	0.53
1:E:195:ARG:O	1:E:199:THR:HG23	2.09	0.53
1:K:25:GLY:HA2	1:K:81:TRP:CZ2	2.43	0.53
1:K:45:ILE:HG23	1:K:46:PRO:HD2	1.90	0.53
1:M:79:GLY:HA2	1:M:291:MET:CE	2.38	0.53
2:H:332:ASN:HA	2:H:341:ALA:HB2	1.90	0.53
1:K:123:ILE:HD13	1:K:250:LEU:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:325:THR:CG2	1:K:329:ILE:HG13	2.39	0.53
1:M:25:GLY:HA2	1:M:81:TRP:CZ2	2.44	0.53
2:P:332:ASN:HA	2:P:341:ALA:HB2	1.91	0.53
2:B:12:THR:HB	2:B:81:LEU:CD1	2.39	0.53
2:F:291:ASP:C	2:F:343:THR:HG22	2.34	0.53
2:P:334:THR:HG22	2:P:335:GLY:H	1.72	0.53
1:C:323:LYS:O	1:C:324:HIS:HB2	2.09	0.52
2:D:39:SER:O	2:D:43:ILE:HG13	2.09	0.52
2:L:326:ILE:HD11	2:L:346:PHE:CE1	2.44	0.52
2:H:88:LEU:HD13	2:H:99:LEU:HD23	1.91	0.52
1:I:175:ARG:CG	1:I:175:ARG:NH1	2.59	0.52
2:N:189:LYS:O	2:N:190:SER:C	2.52	0.52
1:O:79:GLY:HA2	1:O:291:MET:CE	2.39	0.52
1:A:199:THR:HA	1:A:211:VAL:HG11	1.90	0.52
1:C:55:LYS:HB3	1:C:57:THR:HG22	1.90	0.52
2:D:5:GLN:HA	2:D:5:GLN:HE21	1.72	0.52
1:E:25:GLY:HA2	1:E:81:TRP:CZ2	2.44	0.52
1:I:20:VAL:HG13	1:I:47:ILE:HG23	1.90	0.52
1:M:54:ILE:H	1:M:54:ILE:HD12	1.74	0.52
2:F:12:THR:HB	2:F:81:LEU:CD1	2.40	0.52
1:G:54:ILE:CD1	1:G:54:ILE:N	2.72	0.52
2:H:12:THR:HB	2:H:81:LEU:HD12	1.92	0.52
2:H:334:THR:HG22	2:H:335:GLY:H	1.73	0.52
2:J:224:SER:O	2:J:228:VAL:HG23	2.09	0.52
2:L:63:VAL:O	2:L:64:ASN:HB2	2.09	0.52
1:M:314:ALA:HB2	1:M:346:LEU:HD13	1.89	0.52
1:C:245:ASN:OD1	1:C:276:VAL:HG21	2.09	0.52
2:H:126:TYR:HB2	2:H:257:LEU:O	2.10	0.52
2:H:245:LEU:HD23	2:H:246:TYR:CE1	2.44	0.52
2:H:97:ARG:CG	2:H:98:SER:N	2.70	0.52
2:N:270:ILE:HD12	2:N:270:ILE:N	2.25	0.52
2:B:245:LEU:HD23	2:B:246:TYR:CE1	2.44	0.52
2:B:342:THR:HG22	2:B:345:SER:HB3	1.90	0.52
2:D:12:THR:HB	2:D:81:LEU:CD1	2.40	0.52
1:I:195:ARG:O	1:I:199:THR:HG23	2.10	0.52
1:K:15:GLY:O	1:O:301:HIS:CE1	2.56	0.52
2:N:291:ASP:C	2:N:343:THR:HG22	2.35	0.52
1:O:314:ALA:HB2	1:O:346:LEU:HD13	1.92	0.52
1:C:199:THR:HA	1:C:211:VAL:HG11	1.92	0.52
1:C:311:ILE:O	1:C:315:VAL:HG13	2.10	0.52
1:A:155:THR:O	1:A:159:THR:HG22	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:342:THR:HG23	2:B:344:SER:H	1.74	0.52
1:G:314:ALA:HB2	1:G:346:LEU:HD13	1.92	0.52
1:M:148:VAL:N	2:N:160:ILE:O	2.34	0.52
2:N:157:ILE:HD11	1:O:151:LEU:CD1	2.40	0.52
2:N:326:ILE:HG12	2:N:350:VAL:CG2	2.40	0.52
2:P:135:ARG:CD	2:P:247:GLY:HA3	2.29	0.52
1:C:347:SER:HA	1:G:14:TYR:CE1	2.45	0.52
1:E:235:THR:HG21	1:E:243:LEU:HD12	1.90	0.52
1:I:310:ARG:HG2	1:I:349:MET:CE	2.35	0.52
2:J:175:TYR:O	2:J:179:ILE:HG12	2.10	0.52
1:M:163:ALA:HB2	1:M:198:ILE:HD13	1.91	0.52
1:G:38:THR:HG22	1:G:343:ILE:CD1	2.40	0.51
1:M:325:THR:HG22	1:M:331:GLY:HA3	1.92	0.51
1:O:155:THR:O	1:O:159:THR:CG2	2.57	0.51
1:A:275:HIS:ND1	1:A:278:LEU:CD1	2.66	0.51
1:C:235:THR:HG21	1:C:243:LEU:HD12	1.92	0.51
2:F:70:PRO:O	2:F:74:VAL:HG23	2.11	0.51
2:H:97:ARG:CZ	2:H:102:THR:HG23	2.40	0.51
2:J:12:THR:HB	2:J:81:LEU:CD1	2.39	0.51
1:M:88:THR:CB	2:N:189:LYS:HE3	2.34	0.51
1:M:175:ARG:HG3	1:M:175:ARG:NH1	2.09	0.51
1:M:202:GLY:HA3	1:M:211:VAL:HG21	1.91	0.51
1:A:175:ARG:HG3	1:A:175:ARG:NH1	2.15	0.51
2:B:159:LEU:CD2	1:C:143:SER:HB3	2.35	0.51
2:B:195:LEU:HD23	2:B:195:LEU:C	2.36	0.51
2:D:332:ASN:HA	2:D:341:ALA:HB2	1.92	0.51
2:F:12:THR:HB	2:F:81:LEU:HD12	1.91	0.51
2:N:69:ILE:HG22	2:N:106:THR:HG21	1.93	0.51
1:E:149:GLU:HG3	2:F:159:LEU:CD1	2.40	0.51
1:E:311:ILE:O	1:E:315:VAL:HG13	2.10	0.51
2:H:67:THR:HG21	2:H:97:ARG:N	2.25	0.51
1:I:123:ILE:HD13	1:I:250:LEU:HB3	1.92	0.51
2:J:135:ARG:CD	2:J:247:GLY:HA3	2.34	0.51
2:P:166:GLU:O	2:P:167:ARG:HB2	2.10	0.51
2:P:273:LYS:HE3	2:P:274:ILE:CD1	2.40	0.51
1:K:235:THR:HG21	1:K:243:LEU:HD12	1.93	0.51
2:N:145:ILE:HD12	1:O:141:HIS:ND1	2.26	0.51
1:M:20:VAL:HG13	1:M:47:ILE:HG23	1.93	0.51
2:P:224:SER:O	2:P:228:VAL:HG23	2.10	0.51
1:A:314:ALA:HB2	1:A:346:LEU:HD13	1.93	0.51
1:C:135:GLU:OE2	2:D:189:LYS:HE2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:324:HIS:CG	1:C:341:GLU:HG3	2.46	0.51
2:J:342:THR:HG23	2:J:344:SER:H	1.75	0.51
2:L:348:GLU:O	2:L:352:LYS:HG2	2.10	0.51
1:A:143:SER:HB3	2:D:159:LEU:HD22	1.93	0.51
1:C:325:THR:CG2	1:C:329:ILE:HG13	2.38	0.51
2:J:47:ALA:HA	2:J:354:LEU:HD21	1.91	0.51
2:B:41:LYS:HG2	2:B:53:TRP:NE1	2.26	0.51
2:D:70:PRO:O	2:D:74:VAL:HG23	2.11	0.51
2:D:334:THR:HG22	2:D:335:GLY:H	1.75	0.51
1:K:311:ILE:O	1:K:315:VAL:HG13	2.10	0.51
1:M:45:ILE:HG12	1:M:307:TYR:CD2	2.45	0.51
2:N:334:THR:HG22	2:N:335:GLY:H	1.76	0.51
2:D:71:ASP:N	2:D:72:PRO:CD	2.74	0.51
1:E:54:ILE:HD13	1:E:81:TRP:CZ2	2.46	0.51
2:F:303:VAL:HG21	2:F:319:GLN:HB2	1.93	0.51
1:G:292:ILE:O	1:G:295:SER:HB3	2.11	0.51
2:H:321:ALA:C	2:H:325:THR:HG22	2.35	0.51
1:I:311:ILE:O	1:I:315:VAL:HG13	2.11	0.51
2:P:41:LYS:HG2	2:P:53:TRP:NE1	2.26	0.51
2:P:44:PHE:O	2:P:49:VAL:HG22	2.11	0.51
2:P:97:ARG:NH2	2:P:102:THR:HG23	2.26	0.51
2:P:342:THR:HG23	2:P:344:SER:H	1.75	0.51
2:B:332:ASN:HA	2:B:341:ALA:HB2	1.92	0.50
1:E:45:ILE:HG12	1:E:307:TYR:CD2	2.47	0.50
2:F:189:LYS:O	2:F:190:SER:C	2.54	0.50
2:H:15:PRO:HG3	2:H:22:TYR:CZ	2.46	0.50
1:K:323:LYS:O	1:K:324:HIS:HB2	2.11	0.50
2:P:274:ILE:HG22	2:P:275:SER:N	2.26	0.50
2:B:183:ARG:HD2	2:B:237:ASP:OD2	2.12	0.50
1:I:79:GLY:HA2	1:I:291:MET:CE	2.41	0.50
2:J:5:GLN:HG3	2:J:6:PRO:CD	2.38	0.50
2:F:166:GLU:HG2	2:F:166:GLU:O	2.11	0.50
2:N:58:VAL:HG12	2:N:69:ILE:HD11	1.92	0.50
2:D:221:ILE:O	2:D:225:VAL:HG13	2.12	0.50
2:F:135:ARG:HD3	2:F:247:GLY:CA	2.34	0.50
2:F:135:ARG:CD	2:F:247:GLY:HA3	2.34	0.50
2:H:5:GLN:CD	2:H:6:PRO:HD2	2.36	0.50
2:L:287:ILE:HD11	2:L:292:LYS:CD	2.34	0.50
1:M:116:VAL:HG23	1:M:319:ILE:HD13	1.93	0.50
1:M:175:ARG:CG	1:M:175:ARG:NH1	2.61	0.50
1:E:155:THR:O	1:E:159:THR:CG2	2.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:152:LYS:O	2:H:155:GLN:HA	2.12	0.50
1:G:223:ALA:O	1:G:227:PRO:HG3	2.11	0.50
2:L:62:PHE:HE1	2:L:96:HIS:HB3	1.76	0.50
2:L:66:LEU:HD21	2:L:97:ARG:NH2	2.26	0.50
2:P:189:LYS:O	2:P:190:SER:C	2.54	0.50
1:A:175:ARG:CG	1:A:175:ARG:NH1	2.65	0.50
1:C:90:HIS:HB3	2:D:193:GLN:HG3	1.93	0.50
1:C:175:ARG:CG	1:C:175:ARG:NH1	2.61	0.50
2:D:135:ARG:CD	2:D:247:GLY:HA3	2.35	0.50
2:D:195:LEU:C	2:D:195:LEU:HD23	2.36	0.50
2:H:44:PHE:CD2	2:H:49:VAL:HG21	2.47	0.50
2:H:348:GLU:O	2:H:352:LYS:HG2	2.10	0.50
2:J:332:ASN:HA	2:J:341:ALA:HB2	1.93	0.50
1:K:90:HIS:CB	2:L:193:GLN:HG3	2.42	0.50
2:P:58:VAL:HG12	2:P:69:ILE:HD11	1.94	0.50
2:P:135:ARG:HD3	2:P:247:GLY:CA	2.31	0.50
2:F:221:ILE:O	2:F:225:VAL:HG13	2.12	0.50
2:P:67:THR:OG1	2:P:97:ARG:HB3	2.11	0.50
2:B:322:VAL:CG2	2:B:323:LEU:N	2.71	0.50
1:C:87:GLN:HB3	1:C:276:VAL:HG12	1.93	0.50
1:C:116:VAL:HG23	1:C:319:ILE:CD1	2.42	0.50
2:P:136:GLU:OE2	2:P:138:THR:HB	2.12	0.50
2:B:44:PHE:CD2	2:B:49:VAL:HG21	2.47	0.50
1:E:155:THR:HG22	2:F:153:VAL:HG13	1.94	0.50
2:J:63:VAL:O	2:J:64:ASN:HB2	2.11	0.50
1:M:54:ILE:HD13	1:M:81:TRP:CZ2	2.38	0.50
1:M:146:GLY:O	2:N:162:ARG:N	2.42	0.50
1:M:304:LEU:O	1:M:305:ASN:CG	2.54	0.50
2:N:182:PRO:HD2	2:N:237:ASP:O	2.12	0.50
1:O:54:ILE:HG22	1:O:59:HIS:HB3	1.94	0.50
2:P:287:ILE:HG13	2:P:292:LYS:HB2	1.94	0.50
2:J:44:PHE:CD2	2:J:49:VAL:HG21	2.47	0.49
2:N:228:VAL:HG12	2:N:257:LEU:CD1	2.42	0.49
2:N:228:VAL:HG22	2:N:235:TYR:CD1	2.46	0.49
1:O:156:ARG:HG2	1:O:157:PRO:HD3	1.94	0.49
2:B:71:ASP:N	2:B:72:PRO:CD	2.75	0.49
1:E:202:GLY:HA3	1:E:211:VAL:HG21	1.94	0.49
2:F:88:LEU:HD13	2:F:99:LEU:HD23	1.94	0.49
2:J:334:THR:HG22	2:J:335:GLY:H	1.77	0.49
2:L:62:PHE:CE1	2:L:96:HIS:HB3	2.47	0.49
2:L:166:GLU:O	2:L:167:ARG:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:334:THR:HG22	2:F:335:GLY:H	1.77	0.49
2:J:89:ALA:O	2:J:91:PRO:HD3	2.12	0.49
1:K:116:VAL:HG23	1:K:319:ILE:CD1	2.42	0.49
2:L:15:PRO:HG3	2:L:22:TYR:CZ	2.47	0.49
2:L:316:ASP:O	2:L:320:ASN:HB3	2.12	0.49
2:N:12:THR:HB	2:N:81:LEU:HD12	1.94	0.49
2:N:195:LEU:HD23	2:N:195:LEU:C	2.37	0.49
1:O:151:LEU:CD2	2:P:157:ILE:HG12	2.42	0.49
1:O:325:THR:CG2	1:O:329:ILE:HG13	2.39	0.49
2:P:316:ASP:O	2:P:320:ASN:HB3	2.11	0.49
1:A:235:THR:HG21	1:A:243:LEU:HD12	1.94	0.49
2:D:100:ASN:O	2:D:104:ARG:HG3	2.12	0.49
2:F:40:VAL:HG22	2:F:299:LEU:CD1	2.42	0.49
1:G:311:ILE:O	1:G:315:VAL:HG13	2.13	0.49
1:K:155:THR:O	1:K:159:THR:CG2	2.60	0.49
1:K:314:ALA:HB2	1:K:346:LEU:HD13	1.95	0.49
2:L:126:TYR:HB2	2:L:257:LEU:O	2.12	0.49
1:E:221:MET:SD	2:F:261:SER:HA	2.53	0.49
1:G:139:LEU:HD23	1:G:151:LEU:HD12	1.94	0.49
2:P:291:ASP:C	2:P:343:THR:HG22	2.37	0.49
2:D:316:ASP:O	2:D:320:ASN:HB3	2.13	0.49
2:J:41:LYS:HG2	2:J:53:TRP:NE1	2.28	0.49
2:L:71:ASP:N	2:L:72:PRO:CD	2.74	0.49
2:N:157:ILE:HD13	1:O:151:LEU:HD11	1.93	0.49
1:O:38:THR:HG22	1:O:343:ILE:CD1	2.40	0.49
2:D:342:THR:HG23	2:D:344:SER:N	2.28	0.49
1:K:155:THR:HG22	2:L:153:VAL:HG13	1.94	0.49
2:F:44:PHE:O	2:F:49:VAL:HG22	2.12	0.49
1:I:235:THR:HG21	1:I:243:LEU:HD12	1.95	0.49
2:J:88:LEU:HD13	2:J:99:LEU:HD23	1.94	0.49
1:K:304:LEU:O	1:K:305:ASN:CG	2.56	0.49
1:O:349:MET:HE2	1:O:349:MET:HB3	1.68	0.49
2:P:100:ASN:O	2:P:104:ARG:HG3	2.12	0.49
2:F:228:VAL:HG12	2:F:257:LEU:CD1	2.43	0.49
2:H:58:VAL:HG12	2:H:69:ILE:HD11	1.94	0.49
2:H:273:LYS:HE3	2:H:274:ILE:CD1	2.43	0.49
2:L:39:SER:O	2:L:43:ILE:HG13	2.12	0.49
1:M:54:ILE:CA	1:M:62:GLY:HA3	2.30	0.49
2:N:70:PRO:O	2:N:74:VAL:HG23	2.13	0.49
2:B:58:VAL:HG12	2:B:69:ILE:HD11	1.95	0.48
2:D:199:LEU:HD23	2:D:199:LEU:C	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:332:ASN:HA	2:F:341:ALA:HB2	1.95	0.48
1:I:324:HIS:CG	1:I:341:GLU:HG3	2.48	0.48
2:J:39:SER:O	2:J:43:ILE:HG13	2.12	0.48
2:L:58:VAL:HG12	2:L:69:ILE:HD11	1.94	0.48
2:L:224:SER:O	2:L:228:VAL:HG23	2.12	0.48
2:L:342:THR:HG22	2:L:345:SER:HB3	1.95	0.48
1:M:90:HIS:HB3	2:N:193:GLN:CG	2.43	0.48
2:N:16:ASN:HB2	2:N:21:LYS:O	2.13	0.48
2:P:221:ILE:O	2:P:225:VAL:HG13	2.14	0.48
2:D:97:ARG:HH21	2:D:102:THR:CG2	2.24	0.48
1:E:323:LYS:O	1:E:324:HIS:HB2	2.13	0.48
2:F:326:ILE:HG21	2:F:350:VAL:HG22	1.95	0.48
2:H:150:CYS:HB2	2:H:151:PRO:HD2	1.94	0.48
1:K:135:GLU:OE2	2:L:189:LYS:HE2	2.13	0.48
2:L:100:ASN:O	2:L:104:ARG:HG3	2.14	0.48
2:N:130:ASP:HB3	2:N:236:THR:HB	1.96	0.48
2:N:342:THR:HG23	2:N:344:SER:H	1.78	0.48
2:P:199:LEU:HD23	2:P:199:LEU:C	2.38	0.48
2:D:351:ILE:HA	2:D:354:LEU:HB2	1.94	0.48
1:M:38:THR:HG22	1:M:343:ILE:CD1	2.39	0.48
2:N:194:ARG:CB	2:N:194:ARG:NH2	2.75	0.48
2:P:326:ILE:HG12	2:P:350:VAL:CG2	2.43	0.48
1:A:135:GLU:OE2	2:B:189:LYS:HE2	2.14	0.48
2:H:190:SER:O	2:H:194:ARG:HG2	2.13	0.48
1:K:195:ARG:O	1:K:199:THR:HG23	2.13	0.48
2:L:70:PRO:O	2:L:74:VAL:HG23	2.13	0.48
2:L:245:LEU:HD23	2:L:246:TYR:CE1	2.48	0.48
1:M:87:GLN:HA	1:M:274:ARG:HB3	1.95	0.48
1:A:113:LEU:CD1	1:A:256:LEU:HD22	2.41	0.48
2:B:136:GLU:OE2	2:B:138:THR:HB	2.13	0.48
2:B:199:LEU:C	2:B:199:LEU:HD23	2.39	0.48
1:E:304:LEU:O	1:E:305:ASN:CG	2.57	0.48
2:J:118:SER:OG	2:J:129:VAL:HG13	2.14	0.48
2:L:162:ARG:HH11	2:L:162:ARG:HB2	1.78	0.48
2:P:270:ILE:HD12	2:P:270:ILE:N	2.28	0.48
1:C:20:VAL:HG13	1:C:47:ILE:HG23	1.95	0.48
1:C:45:ILE:HG23	1:C:46:PRO:HD2	1.96	0.48
2:F:157:ILE:HD11	1:G:151:LEU:CD1	2.44	0.48
1:G:246:ILE:HD11	2:H:253:LEU:HD12	1.96	0.48
1:I:168:ASP:OD2	1:M:12:LYS:HE3	2.13	0.48
1:K:147:VAL:HG22	2:L:161:THR:HG22	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:202:GLY:HA3	1:K:211:VAL:HG21	1.95	0.48
2:P:194:ARG:CB	2:P:194:ARG:NH2	2.75	0.48
1:A:38:THR:HG22	1:A:343:ILE:CD1	2.39	0.48
2:F:159:LEU:HD23	1:G:144:VAL:HG12	1.94	0.48
2:H:41:LYS:HG2	2:H:53:TRP:NE1	2.28	0.48
2:H:162:ARG:NH1	2:H:162:ARG:HB2	2.28	0.48
2:L:66:LEU:CD2	2:L:97:ARG:NH2	2.76	0.48
2:L:221:ILE:O	2:L:225:VAL:HG13	2.13	0.48
1:O:175:ARG:CG	1:O:175:ARG:NH1	2.61	0.48
1:C:45:ILE:HG12	1:C:307:TYR:CD2	2.48	0.48
2:F:58:VAL:HG12	2:F:69:ILE:HD11	1.96	0.48
1:G:153:VAL:HA	2:H:154:VAL:O	2.13	0.48
2:J:321:ALA:C	2:J:325:THR:HG22	2.39	0.48
1:M:150:SER:O	2:N:157:ILE:HA	2.14	0.48
2:N:159:LEU:HD22	1:O:143:SER:HB3	1.94	0.48
1:O:119:ARG:NH2	2:P:230:THR:O	2.47	0.48
1:E:321:GLU:O	1:E:323:LYS:N	2.46	0.48
2:H:44:PHE:O	2:H:49:VAL:HG22	2.14	0.48
1:I:18:PHE:CE1	1:M:44:ASN:ND2	2.81	0.48
2:J:12:THR:HB	2:J:81:LEU:HD12	1.95	0.48
1:K:12:LYS:HB2	1:K:12:LYS:HE3	1.51	0.48
1:K:120:ILE:HA	1:K:121:PRO:HD3	1.70	0.48
2:L:321:ALA:C	2:L:325:THR:HG22	2.39	0.48
2:L:342:THR:HG23	2:L:344:SER:N	2.28	0.48
1:M:54:ILE:HA	1:M:62:GLY:CA	2.31	0.48
1:O:139:LEU:HD23	1:O:151:LEU:HD12	1.94	0.48
2:P:321:ALA:C	2:P:325:THR:HG22	2.39	0.48
2:D:182:PRO:HD2	2:D:237:ASP:O	2.14	0.48
1:E:324:HIS:CG	1:E:341:GLU:HG3	2.49	0.48
2:F:7:SER:HA	2:F:10:ARG:HG2	1.96	0.48
2:F:162:ARG:HB2	2:F:162:ARG:NH1	2.29	0.48
1:G:281:LYS:CG	1:G:282:GLY:N	2.77	0.48
2:H:150:CYS:CB	2:H:151:PRO:CD	2.91	0.48
2:J:71:ASP:N	2:J:72:PRO:CD	2.76	0.48
2:L:88:LEU:HD13	2:L:99:LEU:HD23	1.96	0.48
2:L:113:VAL:HB	2:L:268:ALA:HB3	1.94	0.48
2:L:162:ARG:HB2	2:L:162:ARG:NH1	2.29	0.48
1:M:181:VAL:HG11	1:M:243:LEU:HD11	1.96	0.48
2:B:135:ARG:HD3	2:B:247:GLY:CA	2.36	0.47
1:C:25:GLY:HA2	1:C:81:TRP:CZ2	2.49	0.47
1:C:123:ILE:HD13	1:C:250:LEU:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:LEU:HD23	1:C:151:LEU:HD12	1.96	0.47
2:D:71:ASP:N	2:D:72:PRO:HD2	2.29	0.47
2:F:97:ARG:HH22	2:F:102:THR:CG2	2.27	0.47
2:J:166:GLU:O	2:J:167:ARG:HB2	2.13	0.47
2:L:12:THR:HB	2:L:81:LEU:CD1	2.43	0.47
1:M:146:GLY:O	2:N:161:THR:CA	2.62	0.47
2:N:245:LEU:HD23	2:N:246:TYR:CE1	2.49	0.47
2:N:321:ALA:C	2:N:325:THR:HG22	2.38	0.47
2:N:348:GLU:O	2:N:352:LYS:HG2	2.13	0.47
1:O:120:ILE:HA	1:O:121:PRO:HD3	1.71	0.47
2:P:342:THR:HG23	2:P:344:SER:N	2.29	0.47
1:A:45:ILE:HG12	1:A:307:TYR:CD2	2.48	0.47
2:D:67:THR:O	2:D:102:THR:HG21	2.13	0.47
2:D:190:SER:O	2:D:194:ARG:HG2	2.15	0.47
2:D:318:ILE:C	2:D:322:VAL:HG11	2.39	0.47
2:D:321:ALA:C	2:D:325:THR:HG22	2.40	0.47
2:H:39:SER:OG	2:H:347:THR:HG22	2.15	0.47
1:I:277:GLY:O	1:I:278:LEU:C	2.57	0.47
1:M:54:ILE:HD12	1:M:54:ILE:N	2.29	0.47
2:N:40:VAL:HG22	2:N:299:LEU:CD1	2.44	0.47
2:P:245:LEU:HD23	2:P:246:TYR:CE1	2.49	0.47
1:C:151:LEU:CD2	2:D:157:ILE:HG12	2.44	0.47
2:F:150:CYS:CB	2:F:151:PRO:CD	2.92	0.47
2:H:40:VAL:HG22	2:H:299:LEU:CD1	2.44	0.47
2:J:273:LYS:HE3	2:J:274:ILE:CD1	2.44	0.47
2:N:39:SER:OG	2:N:347:THR:HG22	2.14	0.47
2:N:66:LEU:HD21	2:N:97:ARG:NH2	2.29	0.47
2:P:40:VAL:HG22	2:P:299:LEU:CD1	2.44	0.47
1:A:116:VAL:HG23	1:A:319:ILE:CD1	2.44	0.47
2:F:190:SER:O	2:F:194:ARG:HG2	2.14	0.47
2:F:326:ILE:HG12	2:F:350:VAL:CG2	2.44	0.47
2:L:44:PHE:CD2	2:L:49:VAL:HG21	2.48	0.47
2:N:69:ILE:CG2	2:N:106:THR:HG21	2.45	0.47
2:N:109:LEU:HD13	2:N:269:ASN:HB3	1.97	0.47
2:P:71:ASP:N	2:P:72:PRO:CD	2.77	0.47
1:A:195:ARG:O	1:A:199:THR:HG23	2.13	0.47
2:B:287:ILE:HD11	2:B:292:LYS:CD	2.39	0.47
2:B:322:VAL:HG23	2:B:323:LEU:HG	1.97	0.47
1:E:8:ARG:C	1:E:10:LEU:H	2.22	0.47
2:F:150:CYS:SG	2:H:153:VAL:HG21	2.54	0.47
2:J:195:LEU:HD23	2:J:195:LEU:C	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:69:ILE:HG22	2:L:106:THR:HG21	1.97	0.47
1:O:55:LYS:N	1:O:55:LYS:HD2	2.29	0.47
2:P:39:SER:OG	2:P:347:THR:HG22	2.14	0.47
1:A:155:THR:O	1:A:159:THR:HG23	2.13	0.47
2:B:162:ARG:NH1	2:B:162:ARG:HB2	2.30	0.47
2:D:12:THR:HB	2:D:81:LEU:HD12	1.97	0.47
2:H:70:PRO:O	2:H:74:VAL:HG23	2.14	0.47
2:H:109:LEU:HD13	2:H:269:ASN:HB3	1.97	0.47
2:H:118:SER:OG	2:H:129:VAL:HG13	2.14	0.47
2:H:162:ARG:HB2	2:H:162:ARG:HH11	1.80	0.47
2:H:194:ARG:NH2	2:H:194:ARG:CB	2.77	0.47
2:J:190:SER:O	2:J:194:ARG:HG2	2.15	0.47
2:J:316:ASP:O	2:J:320:ASN:HB3	2.15	0.47
1:O:54:ILE:N	1:O:54:ILE:HD12	2.29	0.47
1:O:189:LEU:HD12	1:O:189:LEU:HA	1.75	0.47
1:A:292:ILE:O	1:A:295:SER:HB3	2.14	0.47
2:B:316:ASP:O	2:B:320:ASN:HB3	2.15	0.47
1:C:88:THR:HB	2:D:189:LYS:HE3	1.96	0.47
1:C:113:LEU:CD1	1:C:256:LEU:HD22	2.44	0.47
1:C:155:THR:O	1:C:159:THR:HG23	2.14	0.47
2:D:274:ILE:HG22	2:D:275:SER:N	2.29	0.47
2:F:66:LEU:HD21	2:F:97:ARG:HH21	1.79	0.47
2:F:130:ASP:HB3	2:F:236:THR:HB	1.95	0.47
2:J:342:THR:HG23	2:J:344:SER:N	2.30	0.47
1:K:139:LEU:HD23	1:K:151:LEU:HD12	1.97	0.47
1:K:149:GLU:HG3	2:L:159:LEU:HD12	1.97	0.47
2:L:67:THR:O	2:L:102:THR:HG21	2.15	0.47
1:M:88:THR:CG2	2:N:189:LYS:HE3	2.45	0.47
2:N:316:ASP:O	2:N:320:ASN:HB3	2.14	0.47
1:O:55:LYS:HD3	1:O:59:HIS:NE2	2.28	0.47
2:P:97:ARG:NH2	2:P:102:THR:CG2	2.78	0.47
2:P:150:CYS:HB2	2:P:151:PRO:CD	2.44	0.47
2:P:265:THR:HA	2:P:266:PRO:HD3	1.67	0.47
2:H:5:GLN:HA	2:H:6:PRO:HD3	1.82	0.47
2:J:70:PRO:O	2:J:74:VAL:HG23	2.14	0.47
1:M:123:ILE:CD1	1:M:250:LEU:HB3	2.45	0.47
2:N:67:THR:O	2:N:102:THR:HG21	2.13	0.47
1:A:54:ILE:HD12	1:A:54:ILE:N	2.30	0.47
2:F:100:ASN:O	2:F:104:ARG:HG3	2.15	0.47
2:H:189:LYS:O	2:H:190:SER:C	2.57	0.47
1:I:304:LEU:O	1:I:305:ASN:CG	2.58	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:58:VAL:HG12	2:J:69:ILE:HD11	1.96	0.47
2:J:209:LYS:HE2	2:J:209:LYS:HB3	1.75	0.47
2:N:224:SER:O	2:N:228:VAL:HG23	2.14	0.47
1:O:87:GLN:HA	1:O:274:ARG:HB3	1.97	0.47
2:D:44:PHE:O	2:D:49:VAL:HG22	2.15	0.47
2:F:67:THR:O	2:F:102:THR:HG21	2.15	0.47
2:F:71:ASP:N	2:F:72:PRO:CD	2.78	0.47
2:F:182:PRO:HD2	2:F:237:ASP:O	2.15	0.47
1:K:20:VAL:HG13	1:K:47:ILE:HG23	1.97	0.47
2:N:126:TYR:HB2	2:N:257:LEU:O	2.15	0.47
1:O:223:ALA:O	1:O:227:PRO:HG3	2.16	0.47
2:B:326:ILE:HD12	2:B:326:ILE:O	2.15	0.46
1:C:38:THR:HG22	1:C:343:ILE:CD1	2.43	0.46
2:H:274:ILE:HG22	2:H:275:SER:N	2.29	0.46
2:H:342:THR:HG23	2:H:344:SER:H	1.80	0.46
1:M:324:HIS:CG	1:M:341:GLU:HG3	2.50	0.46
1:O:324:HIS:CG	1:O:341:GLU:HG3	2.50	0.46
2:B:159:LEU:HD21	1:C:144:VAL:HG12	1.97	0.46
2:D:162:ARG:NH1	2:D:162:ARG:HB2	2.30	0.46
2:F:166:GLU:O	2:F:167:ARG:HB2	2.15	0.46
1:G:154:MET:HE2	1:G:154:MET:HB2	1.81	0.46
2:H:221:ILE:O	2:H:225:VAL:HG13	2.15	0.46
2:J:182:PRO:HD2	2:J:237:ASP:O	2.15	0.46
2:J:189:LYS:O	2:J:190:SER:C	2.58	0.46
2:L:135:ARG:HD3	2:L:247:GLY:CA	2.34	0.46
1:M:323:LYS:O	1:M:324:HIS:HB2	2.14	0.46
2:N:44:PHE:O	2:N:49:VAL:HG22	2.14	0.46
1:O:246:ILE:HD11	2:P:253:LEU:HD12	1.97	0.46
1:O:325:THR:HG22	1:O:331:GLY:CA	2.43	0.46
1:A:154:MET:HE2	1:A:154:MET:HB2	1.79	0.46
2:L:16:ASN:HB2	2:L:21:LYS:O	2.15	0.46
1:O:20:VAL:HG13	1:O:47:ILE:HG23	1.98	0.46
1:O:311:ILE:O	1:O:315:VAL:HG13	2.15	0.46
2:B:321:ALA:C	2:B:325:THR:HG22	2.40	0.46
2:D:194:ARG:CB	2:D:194:ARG:NH2	2.77	0.46
1:K:324:HIS:CG	1:K:341:GLU:HG3	2.50	0.46
1:O:123:ILE:CD1	1:O:250:LEU:HB3	2.44	0.46
2:B:287:ILE:HD12	2:B:287:ILE:HA	1.73	0.46
2:B:342:THR:HG23	2:B:344:SER:N	2.31	0.46
1:E:149:GLU:OE1	1:G:149:GLU:OE1	2.34	0.46
2:D:331:GLU:HA	2:D:340:THR:OG1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:90:HIS:HB3	2:F:193:GLN:OE1	2.16	0.46
2:F:342:THR:HG23	2:F:344:SER:H	1.80	0.46
1:G:181:VAL:HG11	1:G:243:LEU:HD11	1.98	0.46
1:G:195:ARG:O	1:G:199:THR:HG23	2.16	0.46
2:H:67:THR:O	2:H:102:THR:HG21	2.16	0.46
2:H:181:ARG:HA	2:H:182:PRO:HD3	1.84	0.46
1:I:246:ILE:HD11	2:J:253:LEU:HD12	1.98	0.46
2:J:40:VAL:HG22	2:J:299:LEU:CD1	2.46	0.46
2:P:70:PRO:O	2:P:74:VAL:HG23	2.15	0.46
1:C:147:VAL:HG22	2:D:161:THR:HG22	1.97	0.46
2:D:348:GLU:O	2:D:352:LYS:HG2	2.15	0.46
1:G:87:GLN:HA	1:G:274:ARG:HB3	1.98	0.46
1:G:162:ILE:HD12	1:G:162:ILE:HA	1.73	0.46
2:J:323:LEU:H	2:J:323:LEU:CD2	2.21	0.46
1:M:93:LEU:HD23	1:M:93:LEU:HA	1.83	0.46
2:D:58:VAL:HG12	2:D:69:ILE:HD11	1.96	0.46
2:D:183:ARG:HD2	2:D:237:ASP:OD2	2.16	0.46
1:E:120:ILE:HA	1:E:121:PRO:HD3	1.71	0.46
1:I:139:LEU:HD23	1:I:151:LEU:HD12	1.98	0.46
1:I:275:HIS:CG	1:I:278:LEU:HD12	2.49	0.46
2:J:162:ARG:NH1	2:J:162:ARG:HB2	2.30	0.46
2:L:334:THR:HG22	2:L:335:GLY:H	1.80	0.46
2:N:273:LYS:HE3	2:N:274:ILE:CD1	2.45	0.46
2:F:194:ARG:NH2	2:F:194:ARG:CB	2.78	0.46
2:F:228:VAL:HG22	2:F:235:TYR:CD1	2.50	0.46
2:F:326:ILE:HD12	2:F:326:ILE:O	2.16	0.46
2:H:135:ARG:HD3	2:H:247:GLY:CA	2.38	0.46
1:A:324:HIS:CG	1:A:341:GLU:CG	2.99	0.46
2:D:162:ARG:HB2	2:D:162:ARG:HH11	1.80	0.46
2:F:265:THR:HA	2:F:266:PRO:HD3	1.74	0.46
2:J:221:ILE:O	2:J:225:VAL:HG13	2.16	0.46
2:N:190:SER:O	2:N:194:ARG:HG2	2.16	0.46
2:N:326:ILE:HD12	2:N:326:ILE:O	2.16	0.46
2:B:26:PHE:O	2:B:27:ILE:HB	2.15	0.45
2:B:97:ARG:HH21	2:B:102:THR:CG2	2.27	0.45
2:D:41:LYS:HG2	2:D:53:TRP:NE1	2.30	0.45
2:F:153:VAL:HG21	2:H:150:CYS:SG	2.56	0.45
1:I:120:ILE:HA	1:I:121:PRO:HD3	1.72	0.45
2:L:189:LYS:O	2:L:190:SER:C	2.59	0.45
1:M:28:VAL:HG23	1:M:281:LYS:HE2	1.97	0.45
2:P:303:VAL:HG21	2:P:319:GLN:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:LYS:HD3	1:A:281:LYS:HA	1.73	0.45
2:B:71:ASP:N	2:B:72:PRO:HD2	2.32	0.45
2:F:49:VAL:HA	2:F:50:PRO:HD3	1.72	0.45
1:G:155:THR:HG22	2:H:153:VAL:HG13	1.99	0.45
2:H:63:VAL:O	2:H:64:ASN:HB2	2.16	0.45
2:H:135:ARG:CD	2:H:247:GLY:HA3	2.38	0.45
1:I:45:ILE:HG23	1:I:46:PRO:HD2	1.97	0.45
2:J:71:ASP:N	2:J:72:PRO:HD2	2.31	0.45
2:J:274:ILE:HG22	2:J:275:SER:N	2.30	0.45
1:K:126:ILE:HD13	1:K:169:PHE:HE1	1.81	0.45
2:L:60:PRO:HG3	2:L:99:LEU:HD13	1.98	0.45
2:D:5:GLN:OE1	2:D:307:ASN:O	2.35	0.45
2:D:287:ILE:HD12	2:D:287:ILE:HA	1.79	0.45
2:H:59:SER:HA	2:H:60:PRO:HD3	1.78	0.45
2:H:139:GLU:H	2:H:139:GLU:HG2	1.60	0.45
1:I:242:ILE:HD11	2:J:221:ILE:HD13	1.97	0.45
2:J:199:LEU:C	2:J:199:LEU:HD23	2.41	0.45
1:M:154:MET:HE2	1:M:154:MET:HB2	1.77	0.45
1:A:304:LEU:O	1:A:305:ASN:CG	2.60	0.45
2:D:273:LYS:HE3	2:D:274:ILE:CD1	2.45	0.45
1:E:87:GLN:HA	1:E:274:ARG:HB3	1.98	0.45
2:J:47:ALA:CB	2:J:354:LEU:HD11	2.40	0.45
2:J:135:ARG:HD3	2:J:247:GLY:CA	2.35	0.45
2:J:326:ILE:HD12	2:J:326:ILE:O	2.17	0.45
2:L:265:THR:HA	2:L:266:PRO:HD3	1.75	0.45
2:L:273:LYS:HE3	2:L:274:ILE:CD1	2.45	0.45
2:N:5:GLN:HA	2:N:6:PRO:HD3	1.73	0.45
2:N:322:VAL:HG23	2:N:323:LEU:HG	1.98	0.45
2:P:118:SER:OG	2:P:129:VAL:HG13	2.16	0.45
2:B:5:GLN:CD	2:B:6:PRO:HD2	2.42	0.45
2:D:44:PHE:CD2	2:D:49:VAL:HG21	2.51	0.45
1:E:13:LYS:HD2	1:E:18:PHE:CE1	2.52	0.45
2:F:69:ILE:HG22	2:F:106:THR:HG21	1.98	0.45
2:F:318:ILE:O	2:F:318:ILE:HG22	2.16	0.45
1:M:149:GLU:HA	2:N:158:LYS:O	2.17	0.45
2:P:67:THR:O	2:P:102:THR:HG21	2.16	0.45
1:A:25:GLY:HA2	1:A:81:TRP:CZ2	2.52	0.45
2:B:70:PRO:O	2:B:74:VAL:HG23	2.17	0.45
1:C:325:THR:HG22	1:C:331:GLY:CA	2.46	0.45
2:D:60:PRO:HG3	2:D:99:LEU:HD13	1.98	0.45
2:D:97:ARG:NH2	2:D:102:THR:HG23	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:145:ILE:HD12	1:G:141:HIS:ND1	2.32	0.45
2:H:43:ILE:HD13	2:H:350:VAL:HG11	1.97	0.45
2:H:90:THR:HG22	2:H:91:PRO:O	2.17	0.45
2:H:331:GLU:HA	2:H:340:THR:OG1	2.16	0.45
2:L:181:ARG:HA	2:L:182:PRO:HD3	1.79	0.45
1:O:60:LYS:HE3	1:O:60:LYS:HB2	1.82	0.45
1:E:151:LEU:HA	2:F:156:SER:O	2.17	0.45
1:E:279:ASP:N	1:E:279:ASP:OD1	2.50	0.45
2:F:294:ASN:HA	2:F:295:PRO:HD3	1.73	0.45
1:I:154:MET:HE2	1:I:154:MET:HB2	1.87	0.45
1:K:149:GLU:HG3	2:L:159:LEU:CD1	2.47	0.45
2:L:43:ILE:HD13	2:L:350:VAL:HG11	1.99	0.45
2:N:331:GLU:HA	2:N:340:THR:OG1	2.17	0.45
2:P:150:CYS:CB	2:P:151:PRO:CD	2.94	0.45
1:C:155:THR:O	1:C:159:THR:HG22	2.16	0.45
1:C:304:LEU:O	1:C:305:ASN:CG	2.60	0.45
1:E:45:ILE:HG23	1:E:46:PRO:HD2	1.99	0.45
1:E:54:ILE:HD13	1:E:81:TRP:HZ2	1.81	0.45
2:F:181:ARG:HA	2:F:182:PRO:HD3	1.70	0.45
2:H:199:LEU:HD23	2:H:199:LEU:C	2.42	0.45
2:L:189:LYS:HB2	2:L:246:TYR:OH	2.17	0.45
1:M:287:ASN:CB	1:M:326:THR:HG21	2.47	0.45
2:P:195:LEU:HD23	2:P:195:LEU:C	2.41	0.45
1:A:175:ARG:HG3	1:A:231:ASP:OD1	2.16	0.45
1:A:182:HIS:HE2	1:A:213:SER:HB3	1.81	0.45
2:B:166:GLU:O	2:B:166:GLU:HG2	2.16	0.45
2:D:49:VAL:HG12	2:D:314:HIS:ND1	2.32	0.45
2:D:67:THR:HG21	2:D:97:ARG:N	2.32	0.45
2:F:16:ASN:HB2	2:F:21:LYS:O	2.17	0.45
2:H:26:PHE:O	2:H:27:ILE:HB	2.17	0.45
2:H:49:VAL:HA	2:H:50:PRO:HD3	1.72	0.45
2:H:342:THR:HG22	2:H:345:SER:HB3	1.99	0.45
1:K:45:ILE:HG12	1:K:307:TYR:CD2	2.52	0.45
1:K:87:GLN:HA	1:K:274:ARG:HB3	1.98	0.45
1:M:54:ILE:HG23	1:M:62:GLY:C	2.41	0.45
2:P:71:ASP:N	2:P:72:PRO:HD2	2.32	0.45
2:B:135:ARG:CD	2:B:247:GLY:HA3	2.37	0.45
2:B:273:LYS:HE3	2:B:274:ILE:CD1	2.45	0.45
2:D:303:VAL:HG21	2:D:319:GLN:HB2	1.99	0.45
1:I:323:LYS:O	1:I:324:HIS:HB2	2.17	0.45
2:J:109:LEU:HD13	2:J:269:ASN:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:155:THR:O	1:M:159:THR:HG22	2.16	0.45
2:P:190:SER:O	2:P:194:ARG:HG2	2.16	0.45
2:P:326:ILE:HD11	2:P:346:PHE:CD1	2.51	0.45
1:A:55:LYS:HD3	1:A:59:HIS:ND1	2.32	0.44
2:B:326:ILE:HG12	2:B:350:VAL:CG2	2.47	0.44
2:D:69:ILE:HG22	2:D:106:THR:HG21	1.98	0.44
1:E:38:THR:HG22	1:E:343:ILE:CD1	2.43	0.44
2:F:326:ILE:HD11	2:F:346:PHE:CD1	2.52	0.44
1:G:281:LYS:HD3	1:G:282:GLY:N	2.32	0.44
2:H:130:ASP:HB3	2:H:236:THR:HB	1.99	0.44
2:J:15:PRO:HG3	2:J:22:TYR:CZ	2.52	0.44
1:K:88:THR:HB	2:L:189:LYS:HE3	1.98	0.44
1:M:80:LEU:HD21	1:M:271:PRO:HG2	1.98	0.44
2:N:100:ASN:O	2:N:104:ARG:HG3	2.17	0.44
2:N:135:ARG:HD3	2:N:247:GLY:CA	2.32	0.44
2:N:135:ARG:CD	2:N:247:GLY:HA3	2.32	0.44
2:N:150:CYS:CB	2:N:151:PRO:CD	2.95	0.44
2:B:49:VAL:HA	2:B:50:PRO:HD3	1.73	0.44
1:E:194:PHE:O	1:E:198:ILE:HG12	2.17	0.44
1:G:324:HIS:CG	1:G:341:GLU:HG3	2.52	0.44
2:J:326:ILE:HG12	2:J:350:VAL:CG2	2.48	0.44
2:N:15:PRO:HG3	2:N:22:TYR:CZ	2.52	0.44
2:N:150:CYS:SG	2:P:153:VAL:HG21	2.56	0.44
2:N:265:THR:HA	2:N:266:PRO:HD3	1.67	0.44
2:P:228:VAL:HG22	2:P:235:TYR:CD1	2.52	0.44
1:A:140:GLU:OE2	2:B:194:ARG:HA	2.17	0.44
2:B:190:SER:O	2:B:194:ARG:HG2	2.18	0.44
2:D:209:LYS:HE2	2:D:209:LYS:HB3	1.73	0.44
2:D:265:THR:HA	2:D:266:PRO:HD3	1.69	0.44
2:J:194:ARG:NH2	2:J:194:ARG:CB	2.79	0.44
2:L:173:PHE:CD2	2:L:184:VAL:HG11	2.52	0.44
2:L:323:LEU:H	2:L:323:LEU:CD2	2.21	0.44
1:M:324:HIS:HA	1:M:333:SER:OG	2.17	0.44
1:A:275:HIS:CE1	1:A:278:LEU:CD1	3.01	0.44
2:B:12:THR:HB	2:B:81:LEU:HD12	1.99	0.44
1:G:202:GLY:HA3	1:G:211:VAL:HG21	1.99	0.44
2:H:166:GLU:O	2:H:167:ARG:HB2	2.17	0.44
2:H:228:VAL:HG12	2:H:257:LEU:CD1	2.46	0.44
2:L:71:ASP:N	2:L:72:PRO:HD2	2.32	0.44
2:L:287:ILE:HD12	2:L:287:ILE:HA	1.79	0.44
1:M:143:SER:HB3	2:P:159:LEU:CD2	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:88:LEU:HD13	2:N:99:LEU:HD23	1.99	0.44
2:P:162:ARG:NH1	2:P:162:ARG:HB2	2.33	0.44
2:P:182:PRO:HD2	2:P:237:ASP:O	2.17	0.44
2:P:316:ASP:O	2:P:320:ASN:CB	2.66	0.44
2:P:331:GLU:HA	2:P:340:THR:OG1	2.17	0.44
2:B:109:LEU:HD13	2:B:269:ASN:HB3	2.00	0.44
2:D:316:ASP:O	2:D:320:ASN:CB	2.66	0.44
1:E:162:ILE:HD12	1:E:162:ILE:HA	1.76	0.44
2:F:103:LEU:HD12	2:F:103:LEU:HA	1.82	0.44
2:F:331:GLU:HA	2:F:340:THR:OG1	2.17	0.44
1:G:189:LEU:HA	1:G:189:LEU:HD12	1.73	0.44
2:H:270:ILE:HD12	2:H:270:ILE:N	2.33	0.44
2:J:294:ASN:HA	2:J:295:PRO:HD3	1.75	0.44
2:L:49:VAL:HA	2:L:50:PRO:HD3	1.69	0.44
1:M:182:HIS:HE2	1:M:213:SER:HB3	1.81	0.44
1:A:120:ILE:HA	1:A:121:PRO:HD3	1.69	0.44
2:B:351:ILE:HA	2:B:354:LEU:HB2	1.98	0.44
1:C:133:GLU:OE1	1:C:155:THR:HG23	2.17	0.44
1:E:155:THR:O	1:E:159:THR:HG23	2.17	0.44
2:H:71:ASP:N	2:H:72:PRO:HD2	2.32	0.44
2:H:342:THR:HG23	2:H:344:SER:N	2.33	0.44
1:I:156:ARG:N	1:I:157:PRO:CD	2.81	0.44
2:J:69:ILE:HG22	2:J:106:THR:HG21	2.00	0.44
2:L:41:LYS:HG2	2:L:53:TRP:NE1	2.33	0.44
2:L:318:ILE:O	2:L:318:ILE:HG22	2.16	0.44
1:M:45:ILE:HG23	1:M:46:PRO:HD2	2.00	0.44
2:N:71:ASP:N	2:N:72:PRO:CD	2.81	0.44
1:O:323:LYS:O	1:O:324:HIS:HB2	2.18	0.44
1:A:43:GLU:OE2	1:A:346:LEU:HG	2.18	0.44
2:B:294:ASN:HA	2:B:295:PRO:HD3	1.74	0.44
1:C:149:GLU:HG3	2:D:159:LEU:HD12	1.99	0.44
2:D:103:LEU:HD12	2:D:103:LEU:HA	1.83	0.44
2:F:322:VAL:HG23	2:F:323:LEU:HG	2.00	0.44
1:G:90:HIS:HB3	2:H:193:GLN:OE1	2.18	0.44
1:G:104:TYR:CZ	1:G:161:ARG:HD2	2.53	0.44
1:G:304:LEU:O	1:G:305:ASN:CG	2.60	0.44
2:H:299:LEU:HD12	2:H:299:LEU:HA	1.86	0.44
2:N:166:GLU:O	2:N:167:ARG:HB2	2.16	0.44
1:O:45:ILE:HG12	1:O:307:TYR:CD2	2.52	0.44
2:P:264:LEU:HD21	2:P:337:LEU:HD21	1.98	0.44
2:D:294:ASN:HA	2:D:295:PRO:HD3	1.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:316:ASP:O	2:F:320:ASN:HB3	2.17	0.44
2:J:166:GLU:O	2:J:166:GLU:HG2	2.18	0.44
2:J:348:GLU:O	2:J:352:LYS:HG2	2.17	0.44
2:L:166:GLU:O	2:L:166:GLU:HG2	2.17	0.44
2:L:321:ALA:C	2:L:322:VAL:HG22	2.43	0.44
1:C:221:MET:SD	2:D:261:SER:HA	2.58	0.44
2:F:26:PHE:CE2	2:F:37:SER:HB3	2.53	0.44
1:G:323:LYS:O	1:G:324:HIS:HB2	2.17	0.44
1:K:60:LYS:HE3	1:K:60:LYS:HB2	1.83	0.44
2:L:190:SER:O	2:L:194:ARG:HG2	2.17	0.44
1:M:148:VAL:HG11	2:N:196:ALA:HB2	2.00	0.44
2:N:199:LEU:HD23	2:N:199:LEU:C	2.43	0.44
2:N:299:LEU:HD12	2:N:299:LEU:HA	1.80	0.44
1:O:155:THR:O	1:O:159:THR:HG22	2.17	0.44
2:P:209:LYS:HE2	2:P:209:LYS:HB3	1.78	0.44
2:B:342:THR:HG23	2:B:345:SER:H	1.82	0.43
1:C:104:TYR:CZ	1:C:161:ARG:HD2	2.53	0.43
2:F:71:ASP:N	2:F:72:PRO:HD2	2.33	0.43
2:F:326:ILE:HG12	2:F:350:VAL:HG23	2.00	0.43
2:H:69:ILE:HG22	2:H:106:THR:HG21	1.99	0.43
2:L:12:THR:HB	2:L:81:LEU:HD12	1.98	0.43
1:A:54:ILE:HG22	1:A:56:GLN:O	2.19	0.43
1:C:104:TYR:CE1	1:C:161:ARG:HD2	2.54	0.43
2:F:342:THR:HG23	2:F:344:SER:N	2.34	0.43
1:G:120:ILE:HA	1:G:121:PRO:HD3	1.72	0.43
2:H:16:ASN:HB2	2:H:21:LYS:O	2.18	0.43
2:J:100:ASN:O	2:J:104:ARG:HG3	2.18	0.43
2:J:228:VAL:HG12	2:J:257:LEU:CD1	2.48	0.43
2:L:97:ARG:CG	2:L:98:SER:N	2.80	0.43
2:N:130:ASP:O	2:N:181:ARG:NH2	2.51	0.43
2:N:166:GLU:O	2:N:166:GLU:HG2	2.18	0.43
2:N:173:PHE:CD2	2:N:184:VAL:HG11	2.53	0.43
2:N:175:TYR:O	2:N:179:ILE:HG12	2.18	0.43
2:P:318:ILE:O	2:P:318:ILE:HG22	2.18	0.43
1:A:60:LYS:HB2	1:A:60:LYS:HE3	1.84	0.43
2:B:15:PRO:HG3	2:B:22:TYR:CZ	2.52	0.43
2:B:189:LYS:O	2:B:190:SER:C	2.61	0.43
1:C:194:PHE:O	1:C:198:ILE:HG12	2.19	0.43
2:D:321:ALA:C	2:D:322:VAL:HG22	2.43	0.43
1:E:325:THR:HG22	1:E:331:GLY:CA	2.48	0.43
2:H:68:THR:CG2	2:H:69:ILE:N	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:162:ARG:HB2	2:J:162:ARG:HH11	1.83	0.43
1:K:344:ASN:O	1:K:348:THR:HG23	2.18	0.43
2:B:69:ILE:HG22	2:B:106:THR:HG21	2.00	0.43
1:E:90:HIS:HB2	2:F:193:GLN:HG3	1.97	0.43
1:E:279:ASP:O	1:E:280:ILE:C	2.61	0.43
2:F:97:ARG:HH12	2:F:101:LEU:HD13	1.83	0.43
1:G:123:ILE:CD1	1:G:250:LEU:HB3	2.48	0.43
1:I:38:THR:HG22	1:I:343:ILE:CD1	2.44	0.43
2:J:26:PHE:O	2:J:27:ILE:HB	2.18	0.43
2:J:67:THR:O	2:J:102:THR:HG21	2.18	0.43
2:N:162:ARG:HB2	2:N:162:ARG:NH1	2.34	0.43
1:A:194:PHE:O	1:A:198:ILE:HG12	2.18	0.43
2:F:321:ALA:C	2:F:325:THR:HG22	2.44	0.43
2:H:60:PRO:HG3	2:H:99:LEU:HD13	2.01	0.43
1:I:280:ILE:H	1:I:280:ILE:HG13	1.62	0.43
1:I:321:GLU:O	1:I:323:LYS:N	2.52	0.43
2:L:103:LEU:HD12	2:L:103:LEU:HA	1.82	0.43
2:L:316:ASP:O	2:L:320:ASN:CB	2.66	0.43
2:N:326:ILE:HG12	2:N:350:VAL:HG23	2.00	0.43
1:A:17:ARG:NH1	1:A:48:ASP:OD1	2.52	0.43
1:A:156:ARG:N	1:A:157:PRO:CD	2.81	0.43
2:B:162:ARG:HB2	2:B:162:ARG:HH11	1.84	0.43
2:D:326:ILE:O	2:D:326:ILE:HD12	2.19	0.43
1:G:275:HIS:O	1:G:276:VAL:C	2.62	0.43
1:O:155:THR:O	1:O:159:THR:HG23	2.18	0.43
1:A:162:ILE:HD12	1:A:162:ILE:HA	1.74	0.43
2:D:59:SER:HA	2:D:60:PRO:HD3	1.80	0.43
2:D:189:LYS:O	2:D:190:SER:C	2.61	0.43
1:G:113:LEU:CD1	1:G:256:LEU:HD22	2.47	0.43
2:H:13:GLY:O	2:H:14:LYS:HB3	2.19	0.43
2:H:71:ASP:N	2:H:72:PRO:CD	2.81	0.43
2:H:136:GLU:OE2	2:H:138:THR:HB	2.18	0.43
2:H:318:ILE:O	2:H:318:ILE:HG22	2.18	0.43
1:I:93:LEU:HD23	1:I:93:LEU:HA	1.86	0.43
1:M:245:ASN:CB	2:N:225:VAL:HG22	2.49	0.43
1:O:202:GLY:HA3	1:O:211:VAL:HG21	2.01	0.43
1:C:321:GLU:O	1:C:323:LYS:N	2.52	0.43
2:D:136:GLU:OE2	2:D:138:THR:HB	2.18	0.43
2:H:209:LYS:HE2	2:H:209:LYS:HB3	1.72	0.43
2:J:16:ASN:HB2	2:J:21:LYS:O	2.19	0.43
2:J:270:ILE:N	2:J:270:ILE:HD12	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:322:VAL:CG2	2:J:323:LEU:N	2.75	0.43
2:L:209:LYS:HE2	2:L:209:LYS:HB3	1.73	0.43
2:N:58:VAL:O	2:N:59:SER:C	2.62	0.43
2:N:228:VAL:HG22	2:N:235:TYR:CE1	2.53	0.43
2:N:233:SER:HA	2:N:236:THR:HG23	2.00	0.43
2:N:287:ILE:CG1	2:N:292:LYS:HB2	2.48	0.43
2:P:181:ARG:HA	2:P:182:PRO:HD3	1.78	0.43
2:P:287:ILE:HD12	2:P:287:ILE:HA	1.85	0.43
2:D:270:ILE:N	2:D:270:ILE:HD12	2.34	0.43
1:E:279:ASP:C	1:E:280:ILE:HG12	2.44	0.43
1:G:151:LEU:HB3	2:H:155:GLN:NE2	2.34	0.43
1:K:133:GLU:HG2	1:K:153:VAL:O	2.19	0.43
2:L:317:GLN:O	2:L:322:VAL:HG13	2.19	0.43
1:M:241:THR:HG22	1:M:242:ILE:N	2.33	0.43
1:A:325:THR:CG2	1:A:329:ILE:HG13	2.45	0.43
2:B:265:THR:HA	2:B:266:PRO:HD3	1.69	0.43
2:B:321:ALA:C	2:B:322:VAL:HG22	2.44	0.43
2:D:109:LEU:HD13	2:D:269:ASN:HB3	2.00	0.43
2:D:175:TYR:O	2:D:179:ILE:HG12	2.19	0.43
2:D:323:LEU:H	2:D:323:LEU:CD2	2.22	0.43
1:I:90:HIS:CG	2:J:193:GLN:HG3	2.54	0.43
1:K:140:GLU:OE2	2:L:194:ARG:HA	2.19	0.43
1:M:60:LYS:HE3	1:M:60:LYS:HB2	1.84	0.43
2:N:49:VAL:HG12	2:N:314:HIS:ND1	2.33	0.43
2:N:157:ILE:CD1	1:O:151:LEU:CD1	2.97	0.43
2:P:348:GLU:O	2:P:352:LYS:HG2	2.19	0.43
1:A:20:VAL:HG13	1:A:47:ILE:HG23	2.01	0.42
1:A:321:GLU:O	1:A:323:LYS:N	2.52	0.42
2:B:166:GLU:O	2:B:167:ARG:HB2	2.19	0.42
2:B:209:LYS:HE2	2:B:209:LYS:HB3	1.76	0.42
2:B:212:PRO:HG2	1:O:228:HIS:HD2	1.77	0.42
2:D:322:VAL:HG23	2:D:323:LEU:HG	2.01	0.42
1:E:181:VAL:HG11	1:E:243:LEU:HD11	2.00	0.42
2:H:195:LEU:HD23	2:H:195:LEU:C	2.44	0.42
1:K:77:LEU:HD23	1:K:77:LEU:HA	1.84	0.42
2:L:318:ILE:C	2:L:322:VAL:HG11	2.44	0.42
2:N:342:THR:HG23	2:N:344:SER:N	2.33	0.42
2:D:139:GLU:H	2:D:139:GLU:HG2	1.65	0.42
2:F:299:LEU:HD12	2:F:299:LEU:HA	1.81	0.42
2:H:318:ILE:C	2:H:322:VAL:HG11	2.45	0.42
2:J:126:TYR:HB2	2:J:257:LEU:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:55:LYS:HD3	1:K:55:LYS:HA	1.90	0.42
1:K:116:VAL:HG23	1:K:319:ILE:HD13	2.01	0.42
1:K:162:ILE:HD12	1:K:162:ILE:HA	1.81	0.42
2:L:228:VAL:HG12	2:L:257:LEU:CD1	2.48	0.42
2:L:331:GLU:HA	2:L:340:THR:OG1	2.19	0.42
2:N:71:ASP:N	2:N:72:PRO:HD2	2.35	0.42
2:N:326:ILE:HD11	2:N:346:PHE:CD1	2.54	0.42
2:P:40:VAL:HG22	2:P:299:LEU:HD13	2.01	0.42
2:P:49:VAL:HA	2:P:50:PRO:HD3	1.69	0.42
1:A:75:ILE:HD12	1:A:75:ILE:HG23	1.84	0.42
2:B:126:TYR:HB2	2:B:257:LEU:O	2.19	0.42
2:B:342:THR:HG22	2:B:345:SER:CB	2.49	0.42
1:E:288:PRO:O	1:E:292:ILE:HG13	2.19	0.42
2:F:264:LEU:HD21	2:F:337:LEU:HD21	2.00	0.42
1:I:45:ILE:HG12	1:I:307:TYR:CD2	2.54	0.42
1:I:126:ILE:HD13	1:I:169:PHE:HE1	1.84	0.42
2:J:318:ILE:C	2:J:322:VAL:HG11	2.45	0.42
1:M:90:HIS:HB2	2:N:193:GLN:HG3	1.99	0.42
2:P:294:ASN:HA	2:P:295:PRO:HD3	1.75	0.42
2:D:113:VAL:HB	2:D:268:ALA:HB3	2.02	0.42
1:E:116:VAL:HG23	1:E:319:ILE:HD13	2.00	0.42
1:G:344:ASN:O	1:G:348:THR:HG23	2.19	0.42
1:I:181:VAL:HG11	1:I:243:LEU:HD11	2.01	0.42
2:J:342:THR:HG22	2:J:345:SER:HB3	2.00	0.42
1:K:155:THR:O	1:K:159:THR:HG23	2.19	0.42
2:L:182:PRO:HD2	2:L:237:ASP:O	2.19	0.42
1:O:344:ASN:O	1:O:348:THR:HG23	2.20	0.42
2:B:228:VAL:HG12	2:B:257:LEU:CD1	2.50	0.42
1:C:202:GLY:HA3	1:C:211:VAL:HG21	2.02	0.42
2:D:16:ASN:HB2	2:D:21:LYS:O	2.20	0.42
2:D:118:SER:OG	2:D:129:VAL:HG13	2.20	0.42
2:D:318:ILE:O	2:D:318:ILE:HG22	2.19	0.42
2:D:326:ILE:HG21	2:D:350:VAL:HG22	2.01	0.42
2:D:351:ILE:HG23	2:D:354:LEU:HD23	2.00	0.42
2:F:157:ILE:CD1	1:G:151:LEU:HD11	2.49	0.42
2:H:166:GLU:O	2:H:166:GLU:HG2	2.19	0.42
1:K:148:VAL:HB	2:L:160:ILE:HG22	2.00	0.42
1:K:242:ILE:HD11	2:L:221:ILE:HD13	2.01	0.42
1:O:104:TYR:CZ	1:O:161:ARG:HD2	2.55	0.42
1:A:287:ASN:CB	1:A:326:THR:HG21	2.49	0.42
2:B:63:VAL:O	2:B:64:ASN:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:LEU:HD23	1:C:77:LEU:HA	1.91	0.42
1:C:154:MET:HE2	1:C:154:MET:HB2	1.70	0.42
1:C:182:HIS:HE2	1:C:213:SER:HB3	1.84	0.42
2:F:321:ALA:C	2:F:322:VAL:HG22	2.44	0.42
2:H:326:ILE:HD11	2:H:346:PHE:CD1	2.54	0.42
2:H:326:ILE:HG12	2:H:350:VAL:CG2	2.50	0.42
1:I:113:LEU:CD1	1:I:256:LEU:HD22	2.49	0.42
2:J:326:ILE:HD11	2:J:346:PHE:CD1	2.55	0.42
1:O:162:ILE:HD12	1:O:162:ILE:HA	1.73	0.42
1:A:218:ASN:O	1:A:222:GLN:HB2	2.20	0.42
2:B:103:LEU:HD12	2:B:103:LEU:HA	1.81	0.42
2:B:326:ILE:HG12	2:B:350:VAL:HG23	2.02	0.42
1:E:20:VAL:HG13	1:E:47:ILE:HG23	2.00	0.42
2:F:334:THR:HB	2:F:336:ASP:OD1	2.20	0.42
2:H:334:THR:HB	2:H:336:ASP:OD1	2.20	0.42
1:I:90:HIS:HB3	2:J:193:GLN:HG3	2.00	0.42
2:J:44:PHE:O	2:J:49:VAL:HG22	2.20	0.42
1:M:245:ASN:HB3	2:N:225:VAL:HG22	2.01	0.42
2:B:299:LEU:HD12	2:B:299:LEU:HA	1.95	0.42
1:C:175:ARG:HG3	1:C:231:ASP:OD1	2.20	0.42
1:C:288:PRO:O	1:C:292:ILE:HG13	2.20	0.42
2:D:326:ILE:HD11	2:D:346:PHE:CD1	2.55	0.42
1:E:277:GLY:HA3	2:F:226:LEU:HD12	2.01	0.42
2:F:287:ILE:CG1	2:F:292:LYS:HB2	2.48	0.42
2:H:5:GLN:CG	2:H:6:PRO:HD2	2.49	0.42
2:J:321:ALA:C	2:J:322:VAL:HG22	2.45	0.42
1:K:90:HIS:HB3	2:L:193:GLN:HG3	2.01	0.42
2:L:40:VAL:HG22	2:L:299:LEU:CD1	2.50	0.42
2:L:326:ILE:HG12	2:L:350:VAL:CG2	2.50	0.42
1:M:276:VAL:HG11	2:N:222:ASP:HB3	2.02	0.42
2:N:303:VAL:HG21	2:N:319:GLN:HB2	2.01	0.42
2:B:26:PHE:O	2:B:27:ILE:CB	2.66	0.42
2:B:287:ILE:HG13	2:B:292:LYS:HB2	2.02	0.42
2:D:228:VAL:HG12	2:D:257:LEU:CD1	2.49	0.42
1:E:123:ILE:CD1	1:E:250:LEU:HB3	2.50	0.42
2:F:195:LEU:HD23	2:F:195:LEU:C	2.44	0.42
1:G:194:PHE:O	1:G:198:ILE:HG12	2.20	0.42
2:H:172:ALA:HB2	2:H:241:VAL:CG1	2.49	0.42
1:I:202:GLY:HA3	1:I:211:VAL:HG21	2.01	0.42
2:J:303:VAL:HG21	2:J:319:GLN:HB2	2.01	0.42
2:J:331:GLU:HA	2:J:340:THR:OG1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:80:LEU:HD21	1:K:271:PRO:HG2	2.02	0.42
2:L:44:PHE:O	2:L:49:VAL:HG22	2.20	0.42
2:L:136:GLU:OE2	2:L:138:THR:HB	2.20	0.42
2:N:139:GLU:H	2:N:139:GLU:HG2	1.70	0.42
2:P:323:LEU:H	2:P:323:LEU:CD2	2.22	0.42
2:B:316:ASP:O	2:B:320:ASN:CB	2.68	0.42
2:D:135:ARG:HD3	2:D:247:GLY:CA	2.36	0.42
2:F:194:ARG:CG	2:F:194:ARG:NH2	2.58	0.42
2:F:199:LEU:HD23	2:F:199:LEU:C	2.45	0.42
2:F:260:GLY:O	2:F:261:SER:HB3	2.19	0.42
1:G:156:ARG:HG2	1:G:157:PRO:HD3	2.02	0.42
1:I:288:PRO:O	1:I:292:ILE:HG13	2.20	0.42
2:J:47:ALA:HB2	2:J:354:LEU:HD21	2.02	0.42
2:L:136:GLU:HA	2:L:168:VAL:HG11	2.01	0.42
2:N:26:PHE:O	2:N:27:ILE:HB	2.19	0.42
1:O:45:ILE:HG23	1:O:46:PRO:HD2	2.01	0.42
2:P:26:PHE:O	2:P:27:ILE:HB	2.19	0.42
2:P:194:ARG:CG	2:P:194:ARG:NH2	2.56	0.42
1:C:15:GLY:O	1:G:301:HIS:CE1	2.61	0.41
2:F:66:LEU:CD2	2:F:97:ARG:HH21	2.32	0.41
2:H:11:TYR:CD1	2:H:309:MET:HA	2.55	0.41
2:J:59:SER:HA	2:J:60:PRO:HD3	1.79	0.41
1:K:123:ILE:CD1	1:K:250:LEU:HB3	2.49	0.41
1:K:287:ASN:HA	1:K:288:PRO:HD3	1.89	0.41
2:L:139:GLU:H	2:L:139:GLU:HG2	1.67	0.41
1:M:344:ASN:O	1:M:348:THR:HG23	2.19	0.41
2:N:64:ASN:C	2:N:66:LEU:H	2.28	0.41
2:P:69:ILE:HG22	2:P:106:THR:HG21	2.02	0.41
2:P:162:ARG:HB2	2:P:162:ARG:HH11	1.84	0.41
2:P:233:SER:HA	2:P:236:THR:HG23	2.02	0.41
2:B:35:GLU:H	2:B:35:GLU:HG2	1.71	0.41
2:B:47:ALA:CA	2:B:354:LEU:HD21	2.50	0.41
2:D:5:GLN:HA	2:D:6:PRO:HD3	1.95	0.41
2:F:273:LYS:HE3	2:F:274:ILE:CD1	2.48	0.41
2:H:5:GLN:NE2	2:H:308:HIS:HA	2.35	0.41
2:H:40:VAL:HG22	2:H:299:LEU:HD13	2.02	0.41
2:H:100:ASN:O	2:H:104:ARG:HG3	2.20	0.41
2:H:189:LYS:HB2	2:H:246:TYR:OH	2.20	0.41
1:I:182:HIS:HE2	1:I:213:SER:HB3	1.85	0.41
2:L:97:ARG:HH11	2:L:101:LEU:HD12	1.84	0.41
1:M:104:TYR:CE1	1:M:161:ARG:HD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:274:ILE:CG2	2:N:275:SER:N	2.83	0.41
1:O:304:LEU:O	1:O:305:ASN:CG	2.63	0.41
1:A:133:GLU:OE1	1:A:155:THR:HG23	2.20	0.41
1:A:283:GLN:O	1:A:285:VAL:HG13	2.19	0.41
2:B:150:CYS:HB2	2:B:151:PRO:CD	2.51	0.41
2:B:214:LEU:HD12	2:B:214:LEU:HA	1.89	0.41
2:F:130:ASP:O	2:F:181:ARG:NH2	2.53	0.41
2:F:299:LEU:O	2:F:302:SER:HB2	2.20	0.41
2:H:97:ARG:HH11	2:H:101:LEU:CD1	2.27	0.41
1:M:126:ILE:HD13	1:M:169:PHE:HE1	1.85	0.41
2:P:317:GLN:O	2:P:322:VAL:HG13	2.21	0.41
2:B:318:ILE:C	2:B:322:VAL:HG11	2.45	0.41
2:D:40:VAL:HG22	2:D:299:LEU:CD1	2.50	0.41
2:D:85:LYS:HE2	2:D:88:LEU:HD21	2.02	0.41
1:I:162:ILE:HD12	1:I:162:ILE:HA	1.79	0.41
1:I:301:HIS:HE1	1:M:15:GLY:O	2.02	0.41
2:J:265:THR:HA	2:J:266:PRO:HD3	1.70	0.41
2:J:287:ILE:HG13	2:J:292:LYS:HB2	2.01	0.41
1:K:156:ARG:N	1:K:157:PRO:CD	2.83	0.41
2:L:59:SER:HA	2:L:60:PRO:HD3	1.80	0.41
2:L:228:VAL:HG22	2:L:235:TYR:CD1	2.56	0.41
1:M:90:HIS:HB3	2:N:193:GLN:OE1	2.21	0.41
2:N:264:LEU:HD21	2:N:337:LEU:HD21	2.01	0.41
1:A:250:LEU:HD12	1:A:250:LEU:HA	1.92	0.41
2:B:13:GLY:O	2:B:14:LYS:HB3	2.20	0.41
1:C:87:GLN:HA	1:C:274:ARG:HB3	2.03	0.41
2:D:49:VAL:HA	2:D:50:PRO:HD3	1.72	0.41
1:E:321:GLU:C	1:E:323:LYS:H	2.28	0.41
2:F:318:ILE:C	2:F:322:VAL:HG11	2.46	0.41
1:G:325:THR:HG22	1:G:331:GLY:CA	2.47	0.41
2:H:321:ALA:C	2:H:322:VAL:HG22	2.46	0.41
1:I:156:ARG:HG2	1:I:157:PRO:HD3	2.03	0.41
2:J:322:VAL:HG23	2:J:323:LEU:HG	2.01	0.41
1:K:346:LEU:HD12	1:K:346:LEU:HA	1.90	0.41
2:L:109:LEU:HD13	2:L:269:ASN:HB3	2.03	0.41
1:M:149:GLU:HG3	2:N:159:LEU:HD13	2.01	0.41
1:O:116:VAL:HG23	1:O:319:ILE:HD13	2.00	0.41
1:O:181:VAL:HG11	1:O:243:LEU:HD11	2.02	0.41
2:D:172:ALA:HB2	2:D:241:VAL:CG1	2.50	0.41
2:J:150:CYS:HB2	2:J:151:PRO:CD	2.51	0.41
2:J:316:ASP:O	2:J:320:ASN:CB	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:318:ILE:O	2:J:318:ILE:HG22	2.21	0.41
2:L:62:PHE:CZ	2:L:67:THR:HG22	2.56	0.41
1:M:321:GLU:O	1:M:323:LYS:N	2.52	0.41
2:N:40:VAL:HG22	2:N:299:LEU:HD13	2.03	0.41
2:N:136:GLU:OE2	2:N:138:THR:HB	2.21	0.41
2:P:58:VAL:O	2:P:59:SER:C	2.63	0.41
2:B:60:PRO:HG3	2:B:99:LEU:HD13	2.03	0.41
1:C:55:LYS:HD3	1:C:55:LYS:HA	1.82	0.41
2:D:326:ILE:HG12	2:D:350:VAL:CG2	2.50	0.41
2:F:69:ILE:CG2	2:F:106:THR:HG21	2.51	0.41
2:F:109:LEU:HD13	2:F:269:ASN:HB3	2.02	0.41
2:H:194:ARG:CG	2:H:194:ARG:NH2	2.55	0.41
2:H:287:ILE:HG13	2:H:292:LYS:HB2	2.03	0.41
2:J:136:GLU:OE2	2:J:138:THR:HB	2.20	0.41
1:K:189:LEU:HA	1:K:189:LEU:HD12	1.75	0.41
2:L:26:PHE:O	2:L:27:ILE:HB	2.20	0.41
1:M:254:PRO:HD2	1:M:278:LEU:HD23	2.02	0.41
2:N:181:ARG:HA	2:N:182:PRO:HD3	1.74	0.41
2:N:318:ILE:O	2:N:318:ILE:HG22	2.21	0.41
2:P:175:TYR:O	2:P:179:ILE:HG12	2.21	0.41
1:A:77:LEU:HD23	1:A:77:LEU:HA	1.92	0.41
2:B:118:SER:OG	2:B:129:VAL:HG13	2.20	0.41
1:G:45:ILE:HG23	1:G:46:PRO:HD2	2.03	0.41
2:J:40:VAL:HG22	2:J:299:LEU:HD13	2.02	0.41
1:K:140:GLU:HB3	2:L:195:LEU:HD21	2.02	0.41
1:K:182:HIS:HE2	1:K:213:SER:HB3	1.86	0.41
2:N:189:LYS:HB2	2:N:246:TYR:OH	2.21	0.41
1:O:45:ILE:HA	1:O:46:PRO:HD3	1.88	0.41
1:O:126:ILE:HD13	1:O:169:PHE:HE1	1.85	0.41
2:B:334:THR:HG22	2:B:335:GLY:H	1.84	0.41
1:C:37:ARG:HH11	1:C:37:ARG:HD3	1.76	0.41
1:C:140:GLU:OE2	2:D:194:ARG:HA	2.20	0.41
1:C:140:GLU:HB3	2:D:195:LEU:CD2	2.50	0.41
1:C:156:ARG:N	1:C:157:PRO:CD	2.84	0.41
2:D:136:GLU:HA	2:D:168:VAL:HG11	2.03	0.41
2:F:162:ARG:HB2	2:F:162:ARG:HH11	1.86	0.41
2:F:287:ILE:HA	2:F:287:ILE:HD12	1.81	0.41
2:F:323:LEU:H	2:F:323:LEU:CD2	2.12	0.41
1:G:45:ILE:HG12	1:G:307:TYR:CD2	2.56	0.41
1:G:54:ILE:H	1:G:54:ILE:CD1	2.02	0.41
1:G:175:ARG:CG	1:G:175:ARG:NH1	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:39:SER:HB2	2:H:347:THR:CG2	2.51	0.41
2:H:250:LEU:HD23	2:H:250:LEU:HA	1.81	0.41
2:H:287:ILE:HA	2:H:287:ILE:HD12	1.80	0.41
1:I:80:LEU:HD21	1:I:271:PRO:HG2	2.02	0.41
1:I:155:THR:O	1:I:159:THR:HG22	2.21	0.41
1:I:319:ILE:O	1:I:319:ILE:HD12	2.21	0.41
2:J:60:PRO:HG3	2:J:99:LEU:HD13	2.03	0.41
2:J:183:ARG:HD2	2:J:237:ASP:OD2	2.20	0.41
1:M:12:LYS:HB3	1:M:19:THR:HB	2.03	0.41
1:M:43:GLU:OE2	1:M:346:LEU:HG	2.21	0.41
1:M:149:GLU:CG	2:N:159:LEU:CD1	2.98	0.41
1:M:162:ILE:HD12	1:M:162:ILE:HA	1.73	0.41
2:N:7:SER:HA	2:N:10:ARG:HG2	2.03	0.41
1:O:194:PHE:O	1:O:198:ILE:HG12	2.21	0.41
1:O:221:MET:SD	2:P:262:LEU:HD22	2.61	0.41
2:B:59:SER:HA	2:B:60:PRO:HD3	1.80	0.41
2:B:322:VAL:CG2	2:B:323:LEU:H	2.34	0.41
1:C:17:ARG:NH1	1:C:48:ASP:CG	2.79	0.41
2:D:133:LEU:HD23	2:D:251:SER:HB3	2.03	0.41
1:E:279:ASP:HB2	1:E:280:ILE:H	1.67	0.41
2:F:317:GLN:O	2:F:322:VAL:HG13	2.21	0.41
2:H:182:PRO:HD2	2:H:237:ASP:O	2.21	0.41
2:H:228:VAL:HG22	2:H:235:TYR:CD1	2.56	0.41
2:H:319:GLN:C	2:H:322:VAL:HG22	2.46	0.41
1:M:133:GLU:HG2	1:M:153:VAL:O	2.21	0.41
2:N:172:ALA:HB2	2:N:241:VAL:CG1	2.50	0.41
2:P:319:GLN:C	2:P:322:VAL:HG22	2.46	0.41
2:B:39:SER:HB2	2:B:347:THR:HG21	2.03	0.40
1:C:226:LYS:N	1:C:227:PRO:HD3	2.36	0.40
2:D:126:TYR:HB2	2:D:257:LEU:O	2.20	0.40
1:E:278:LEU:HD22	1:E:278:LEU:HA	1.74	0.40
1:E:280:ILE:HG22	1:E:327:ARG:CZ	2.51	0.40
1:E:346:LEU:HD12	1:E:346:LEU:HA	1.94	0.40
2:F:39:SER:OG	2:F:347:THR:HG22	2.20	0.40
2:H:69:ILE:CD1	2:H:70:PRO:HD2	2.50	0.40
1:I:344:ASN:O	1:I:348:THR:HG23	2.20	0.40
2:L:5:GLN:HE21	2:L:5:GLN:CA	2.33	0.40
2:N:13:GLY:O	2:N:14:LYS:HB3	2.21	0.40
2:N:49:VAL:HA	2:N:50:PRO:HD3	1.70	0.40
2:P:62:PHE:CZ	2:P:67:THR:HG22	2.56	0.40
1:A:104:TYR:CE1	1:A:161:ARG:HD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:VAL:HG11	1:A:243:LEU:HD11	2.04	0.40
2:B:39:SER:O	2:B:43:ILE:HG13	2.22	0.40
2:B:189:LYS:HB2	2:B:246:TYR:OH	2.21	0.40
2:H:316:ASP:O	2:H:320:ASN:HB3	2.22	0.40
1:I:133:GLU:HG2	1:I:153:VAL:O	2.22	0.40
2:L:195:LEU:C	2:L:195:LEU:HD23	2.46	0.40
2:L:274:ILE:HG22	2:L:275:SER:N	2.36	0.40
2:N:26:PHE:CD2	2:N:28:GLU:HG2	2.57	0.40
1:O:275:HIS:O	1:O:276:VAL:C	2.64	0.40
2:P:342:THR:HG22	2:P:345:SER:HB3	2.02	0.40
1:A:45:ILE:HG23	1:A:46:PRO:HD2	2.04	0.40
1:A:202:GLY:HA3	1:A:211:VAL:HG21	2.03	0.40
2:B:43:ILE:HD13	2:B:350:VAL:HG11	2.03	0.40
2:D:181:ARG:HA	2:D:182:PRO:HD3	1.80	0.40
2:D:228:VAL:HG22	2:D:235:TYR:CD1	2.57	0.40
2:D:319:GLN:C	2:D:322:VAL:HG22	2.47	0.40
2:F:59:SER:HA	2:F:60:PRO:HD3	1.77	0.40
1:G:60:LYS:HE3	1:G:60:LYS:HB2	1.83	0.40
1:G:241:THR:HG21	2:H:189:LYS:NZ	2.36	0.40
1:G:293:LEU:HD23	1:G:293:LEU:HA	1.89	0.40
2:J:159:LEU:CD2	1:K:143:SER:HB3	2.44	0.40
2:J:172:ALA:HB2	2:J:241:VAL:CG1	2.51	0.40
1:K:56:GLN:H	1:K:56:GLN:CD	2.29	0.40
2:L:287:ILE:HG13	2:L:292:LYS:HB2	2.02	0.40
2:L:299:LEU:HD12	2:L:299:LEU:HA	1.84	0.40
2:D:317:GLN:O	2:D:322:VAL:HG13	2.21	0.40
2:D:326:ILE:C	2:D:328:SER:H	2.29	0.40
2:F:15:PRO:HG3	2:F:22:TYR:CZ	2.57	0.40
2:J:7:SER:HA	2:J:10:ARG:HG2	2.04	0.40
1:M:104:TYR:CZ	1:M:161:ARG:HD2	2.57	0.40
2:N:316:ASP:O	2:N:320:ASN:CB	2.70	0.40
2:P:172:ALA:HB2	2:P:241:VAL:CG1	2.52	0.40
2:P:318:ILE:C	2:P:322:VAL:HG11	2.46	0.40
2:P:334:THR:HB	2:P:336:ASP:OD1	2.20	0.40
1:E:344:ASN:O	1:E:348:THR:HG23	2.21	0.40
2:F:7:SER:HA	2:F:10:ARG:CG	2.50	0.40
2:F:26:PHE:O	2:F:27:ILE:HB	2.22	0.40
2:F:224:SER:O	2:F:228:VAL:HG23	2.21	0.40
2:H:35:GLU:H	2:H:35:GLU:HG2	1.71	0.40
2:J:319:GLN:C	2:J:322:VAL:HG22	2.47	0.40
1:M:8:ARG:C	1:M:10:LEU:H	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:26:ASP:OD2	1:M:26:ASP:C	2.65	0.40
2:N:270:ILE:N	2:N:270:ILE:CD1	2.83	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	331/349 (95%)	311 (94%)	16 (5%)	4 (1%)	10	27
1	C	334/349 (96%)	315 (94%)	16 (5%)	3 (1%)	14	35
1	E	337/349 (97%)	320 (95%)	12 (4%)	5 (2%)	8	22
1	G	330/349 (95%)	309 (94%)	14 (4%)	7 (2%)	5	15
1	I	331/349 (95%)	310 (94%)	16 (5%)	5 (2%)	8	22
1	K	334/349 (96%)	315 (94%)	15 (4%)	4 (1%)	10	27
1	M	333/349 (95%)	315 (95%)	15 (4%)	3 (1%)	14	35
1	O	328/349 (94%)	309 (94%)	16 (5%)	3 (1%)	14	35
2	B	342/354 (97%)	310 (91%)	23 (7%)	9 (3%)	4	11
2	D	341/354 (96%)	307 (90%)	25 (7%)	9 (3%)	4	11
2	F	341/354 (96%)	307 (90%)	26 (8%)	8 (2%)	5	13
2	H	341/354 (96%)	304 (89%)	29 (8%)	8 (2%)	5	13
2	J	341/354 (96%)	309 (91%)	24 (7%)	8 (2%)	5	13
2	L	342/354 (97%)	306 (90%)	27 (8%)	9 (3%)	4	11
2	N	341/354 (96%)	301 (88%)	30 (9%)	10 (3%)	3	9
2	P	322/354 (91%)	289 (90%)	27 (8%)	6 (2%)	6	17
All	All	5369/5624 (96%)	4937 (92%)	331 (6%)	101 (2%)	6	17

All (101) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	304	LEU
1	C	58	ASP
1	C	304	LEU
1	E	276	VAL
1	E	304	LEU
2	F	54	GLU
1	G	14	TYR
1	G	15	GLY
1	G	304	LEU
1	I	278	LEU
1	I	304	LEU
1	K	304	LEU
1	M	304	LEU
2	N	54	GLU
1	O	304	LEU
2	P	54	GLU
2	P	321	ALA
1	A	14	TYR
1	A	322	GLY
2	B	13	GLY
2	B	54	GLU
2	B	167	ARG
2	B	321	ALA
2	B	322	VAL
2	D	13	GLY
2	D	54	GLU
2	D	167	ARG
2	D	321	ALA
2	D	322	VAL
1	E	279	ASP
1	E	322	GLY
2	F	13	GLY
2	F	167	ARG
2	F	321	ALA
2	F	322	VAL
1	G	57	THR
2	H	13	GLY
2	H	54	GLU
2	H	167	ARG
2	H	321	ALA
2	H	322	VAL
1	I	322	GLY

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Mol	Chain	Res	Type
2	J	13	GLY
2	J	54	GLU
2	J	167	ARG
2	J	321	ALA
2	J	322	VAL
1	K	58	ASP
2	L	13	GLY
2	L	54	GLU
2	L	167	ARG
2	L	321	ALA
2	L	322	VAL
1	M	322	GLY
2	N	13	GLY
2	N	98	SER
2	N	167	ARG
2	N	321	ALA
2	N	322	VAL
2	P	167	ARG
2	P	322	VAL
2	B	190	SER
2	H	190	SER
1	I	59	HIS
2	J	190	SER
1	K	57	THR
1	K	322	GLY
2	L	190	SER
2	N	190	SER
2	P	190	SER
1	C	322	GLY
2	D	190	SER
2	F	190	SER
1	G	55	LYS
1	G	322	GLY
2	L	48	ASN
2	B	27	ILE
2	D	27	ILE
2	D	48	ASN
2	F	27	ILE
1	I	276	VAL
2	J	27	ILE
1	A	55	LYS
2	B	14	LYS

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Mol	Chain	Res	Type
2	B	48	ASN
2	D	14	LYS
1	G	276	VAL
2	H	14	LYS
2	H	27	ILE
2	L	27	ILE
1	M	280	ILE
2	N	27	ILE
2	N	48	ASN
1	O	322	GLY
2	P	27	ILE
2	J	14	LYS
2	L	14	LYS
2	N	14	LYS
2	F	14	LYS
1	E	280	ILE
1	O	276	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	279/289 (96%)	246 (88%)	33 (12%)	5	13
1	C	283/289 (98%)	244 (86%)	39 (14%)	3	9
1	E	285/289 (99%)	240 (84%)	45 (16%)	2	7
1	G	278/289 (96%)	241 (87%)	37 (13%)	4	10
1	I	279/289 (96%)	240 (86%)	39 (14%)	3	9
1	K	283/289 (98%)	243 (86%)	40 (14%)	3	9
1	M	281/289 (97%)	247 (88%)	34 (12%)	5	12
1	O	276/289 (96%)	243 (88%)	33 (12%)	5	12
2	B	292/297 (98%)	260 (89%)	32 (11%)	6	15
2	D	291/297 (98%)	259 (89%)	32 (11%)	6	15
2	F	291/297 (98%)	262 (90%)	29 (10%)	7	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	291/297 (98%)	260 (89%)	31 (11%)	6	16
2	J	291/297 (98%)	261 (90%)	30 (10%)	7	18
2	L	292/297 (98%)	260 (89%)	32 (11%)	6	15
2	N	291/297 (98%)	263 (90%)	28 (10%)	8	20
2	P	275/297 (93%)	245 (89%)	30 (11%)	6	16
All	All	4558/4688 (97%)	4014 (88%)	544 (12%)	5	13

All (544) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	VAL
1	A	33	THR
1	A	51	THR
1	A	77	LEU
1	A	80	LEU
1	A	93	LEU
1	A	95	VAL
1	A	97	LEU
1	A	98	ARG
1	A	114	LYS
1	A	144	VAL
1	A	154	MET
1	A	156	ARG
1	A	159	THR
1	A	161	ARG
1	A	175	ARG
1	A	211	VAL
1	A	212	SER
1	A	222	GLN
1	A	238	MET
1	A	241	THR
1	A	250	LEU
1	A	276	VAL
1	A	281	LYS
1	A	315	VAL
1	A	319	ILE
1	A	325	THR
1	A	328	ASP
1	A	335	THR
1	A	336	THR

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Mol	Chain	Res	Type
1	A	341	GLU
1	A	346	LEU
1	A	348	THR
2	B	23	THR
2	B	30	ASP
2	B	61	ILE
2	B	66	LEU
2	B	88	LEU
2	B	101	LEU
2	B	102	THR
2	B	103	LEU
2	B	106	THR
2	B	114	ARG
2	B	125	THR
2	B	129	VAL
2	B	135	ARG
2	B	150	CYS
2	B	168	VAL
2	B	181	ARG
2	B	184	VAL
2	B	189	LYS
2	B	194	ARG
2	B	195	LEU
2	B	214	LEU
2	B	225	VAL
2	B	226	LEU
2	B	241	VAL
2	B	283	SER
2	B	286	ASP
2	B	299	LEU
2	B	306	LEU
2	B	323	LEU
2	B	326	ILE
2	B	334	THR
2	B	353	ARG
1	C	20	VAL
1	C	33	THR
1	C	37	ARG
1	C	51	THR
1	C	56	GLN
1	C	58	ASP
1	C	77	LEU

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Mol	Chain	Res	Type
1	C	80	LEU
1	C	93	LEU
1	C	95	VAL
1	C	97	LEU
1	C	98	ARG
1	C	114	LYS
1	C	144	VAL
1	C	154	MET
1	C	155	THR
1	C	156	ARG
1	C	159	THR
1	C	161	ARG
1	C	175	ARG
1	C	201	ILE
1	C	211	VAL
1	C	212	SER
1	C	222	GLN
1	C	234	VAL
1	C	238	MET
1	C	241	THR
1	C	250	LEU
1	C	305	ASN
1	C	315	VAL
1	C	319	ILE
1	C	325	THR
1	C	328	ASP
1	C	333	SER
1	C	335	THR
1	C	336	THR
1	C	341	GLU
1	C	346	LEU
1	C	348	THR
2	D	5	GLN
2	D	23	THR
2	D	61	ILE
2	D	66	LEU
2	D	88	LEU
2	D	97	ARG
2	D	101	LEU
2	D	102	THR
2	D	103	LEU
2	D	114	ARG

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Mol	Chain	Res	Type
2	D	125	THR
2	D	129	VAL
2	D	150	CYS
2	D	160	ILE
2	D	168	VAL
2	D	181	ARG
2	D	184	VAL
2	D	189	LYS
2	D	194	ARG
2	D	195	LEU
2	D	214	LEU
2	D	225	VAL
2	D	226	LEU
2	D	241	VAL
2	D	283	SER
2	D	286	ASP
2	D	299	LEU
2	D	306	LEU
2	D	323	LEU
2	D	326	ILE
2	D	334	THR
2	D	353	ARG
1	E	8	ARG
1	E	9	THR
1	E	20	VAL
1	E	33	THR
1	E	51	THR
1	E	54	ILE
1	E	59	HIS
1	E	77	LEU
1	E	80	LEU
1	E	93	LEU
1	E	95	VAL
1	E	97	LEU
1	E	98	ARG
1	E	114	LYS
1	E	144	VAL
1	E	154	MET
1	E	156	ARG
1	E	159	THR
1	E	161	ARG
1	E	175	ARG

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Mol	Chain	Res	Type
1	E	201	ILE
1	E	211	VAL
1	E	212	SER
1	E	222	GLN
1	E	234	VAL
1	E	238	MET
1	E	241	THR
1	E	250	LEU
1	E	273	SER
1	E	276	VAL
1	E	278	LEU
1	E	279	ASP
1	E	280	ILE
1	E	305	ASN
1	E	315	VAL
1	E	319	ILE
1	E	325	THR
1	E	328	ASP
1	E	333	SER
1	E	335	THR
1	E	336	THR
1	E	341	GLU
1	E	346	LEU
1	E	348	THR
1	E	349	MET
2	F	23	THR
2	F	61	ILE
2	F	66	LEU
2	F	88	LEU
2	F	101	LEU
2	F	102	THR
2	F	103	LEU
2	F	114	ARG
2	F	125	THR
2	F	129	VAL
2	F	150	CYS
2	F	160	ILE
2	F	168	VAL
2	F	184	VAL
2	F	189	LYS
2	F	194	ARG
2	F	195	LEU

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Mol	Chain	Res	Type
2	F	214	LEU
2	F	225	VAL
2	F	226	LEU
2	F	241	VAL
2	F	283	SER
2	F	286	ASP
2	F	299	LEU
2	F	306	LEU
2	F	323	LEU
2	F	326	ILE
2	F	334	THR
2	F	353	ARG
1	G	13	LYS
1	G	20	VAL
1	G	33	THR
1	G	37	ARG
1	G	51	THR
1	G	53	ASN
1	G	54	ILE
1	G	77	LEU
1	G	80	LEU
1	G	93	LEU
1	G	95	VAL
1	G	97	LEU
1	G	98	ARG
1	G	114	LYS
1	G	144	VAL
1	G	154	MET
1	G	156	ARG
1	G	158	LYS
1	G	159	THR
1	G	161	ARG
1	G	175	ARG
1	G	211	VAL
1	G	212	SER
1	G	222	GLN
1	G	238	MET
1	G	241	THR
1	G	250	LEU
1	G	273	SER
1	G	315	VAL
1	G	319	ILE

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Mol	Chain	Res	Type
1	G	325	THR
1	G	328	ASP
1	G	335	THR
1	G	336	THR
1	G	341	GLU
1	G	346	LEU
1	G	348	THR
2	H	23	THR
2	H	30	ASP
2	H	61	ILE
2	H	66	LEU
2	H	88	LEU
2	H	101	LEU
2	H	102	THR
2	H	103	LEU
2	H	106	THR
2	H	114	ARG
2	H	125	THR
2	H	129	VAL
2	H	150	CYS
2	H	160	ILE
2	H	168	VAL
2	H	184	VAL
2	H	189	LYS
2	H	194	ARG
2	H	195	LEU
2	H	214	LEU
2	H	225	VAL
2	H	226	LEU
2	H	241	VAL
2	H	283	SER
2	H	286	ASP
2	H	299	LEU
2	H	306	LEU
2	H	323	LEU
2	H	326	ILE
2	H	334	THR
2	H	353	ARG
1	I	20	VAL
1	I	33	THR
1	I	51	THR
1	I	77	LEU

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Mol	Chain	Res	Type
1	I	80	LEU
1	I	93	LEU
1	I	95	VAL
1	I	97	LEU
1	I	98	ARG
1	I	114	LYS
1	I	144	VAL
1	I	156	ARG
1	I	158	LYS
1	I	159	THR
1	I	161	ARG
1	I	175	ARG
1	I	201	ILE
1	I	211	VAL
1	I	212	SER
1	I	222	GLN
1	I	234	VAL
1	I	238	MET
1	I	241	THR
1	I	250	LEU
1	I	273	SER
1	I	276	VAL
1	I	280	ILE
1	I	281	LYS
1	I	305	ASN
1	I	315	VAL
1	I	319	ILE
1	I	325	THR
1	I	328	ASP
1	I	333	SER
1	I	335	THR
1	I	336	THR
1	I	341	GLU
1	I	346	LEU
1	I	348	THR
2	J	23	THR
2	J	30	ASP
2	J	61	ILE
2	J	66	LEU
2	J	88	LEU
2	J	101	LEU
2	J	102	THR

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Mol	Chain	Res	Type
2	J	103	LEU
2	J	114	ARG
2	J	125	THR
2	J	129	VAL
2	J	150	CYS
2	J	160	ILE
2	J	168	VAL
2	J	184	VAL
2	J	189	LYS
2	J	194	ARG
2	J	195	LEU
2	J	214	LEU
2	J	225	VAL
2	J	226	LEU
2	J	241	VAL
2	J	283	SER
2	J	286	ASP
2	J	299	LEU
2	J	306	LEU
2	J	323	LEU
2	J	326	ILE
2	J	334	THR
2	J	353	ARG
1	K	8	ARG
1	K	20	VAL
1	K	33	THR
1	K	37	ARG
1	K	51	THR
1	K	56	GLN
1	K	77	LEU
1	K	80	LEU
1	K	93	LEU
1	K	95	VAL
1	K	97	LEU
1	K	98	ARG
1	K	114	LYS
1	K	144	VAL
1	K	154	MET
1	K	156	ARG
1	K	159	THR
1	K	161	ARG
1	K	175	ARG

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Mol	Chain	Res	Type
1	K	201	ILE
1	K	211	VAL
1	K	212	SER
1	K	222	GLN
1	K	234	VAL
1	K	238	MET
1	K	241	THR
1	K	250	LEU
1	K	273	SER
1	K	276	VAL
1	K	305	ASN
1	K	315	VAL
1	K	319	ILE
1	K	325	THR
1	K	328	ASP
1	K	333	SER
1	K	335	THR
1	K	336	THR
1	K	341	GLU
1	K	346	LEU
1	K	348	THR
2	L	5	GLN
2	L	23	THR
2	L	61	ILE
2	L	66	LEU
2	L	88	LEU
2	L	96	HIS
2	L	101	LEU
2	L	102	THR
2	L	103	LEU
2	L	114	ARG
2	L	125	THR
2	L	129	VAL
2	L	150	CYS
2	L	160	ILE
2	L	168	VAL
2	L	184	VAL
2	L	189	LYS
2	L	194	ARG
2	L	195	LEU
2	L	214	LEU
2	L	225	VAL

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Mol	Chain	Res	Type
2	L	226	LEU
2	L	241	VAL
2	L	283	SER
2	L	286	ASP
2	L	299	LEU
2	L	306	LEU
2	L	323	LEU
2	L	326	ILE
2	L	334	THR
2	L	342	THR
2	L	353	ARG
1	M	20	VAL
1	M	33	THR
1	M	51	THR
1	M	54	ILE
1	M	77	LEU
1	M	80	LEU
1	M	93	LEU
1	M	95	VAL
1	M	97	LEU
1	M	98	ARG
1	M	114	LYS
1	M	144	VAL
1	M	154	MET
1	M	156	ARG
1	M	159	THR
1	M	175	ARG
1	M	211	VAL
1	M	222	GLN
1	M	234	VAL
1	M	238	MET
1	M	241	THR
1	M	250	LEU
1	M	276	VAL
1	M	279	ASP
1	M	315	VAL
1	M	319	ILE
1	M	325	THR
1	M	328	ASP
1	M	335	THR
1	M	336	THR
1	M	341	GLU

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Mol	Chain	Res	Type
1	M	346	LEU
1	M	348	THR
1	M	349	MET
2	N	61	ILE
2	N	66	LEU
2	N	88	LEU
2	N	97	ARG
2	N	101	LEU
2	N	102	THR
2	N	103	LEU
2	N	125	THR
2	N	129	VAL
2	N	150	CYS
2	N	160	ILE
2	N	168	VAL
2	N	184	VAL
2	N	189	LYS
2	N	194	ARG
2	N	195	LEU
2	N	214	LEU
2	N	225	VAL
2	N	226	LEU
2	N	241	VAL
2	N	286	ASP
2	N	299	LEU
2	N	306	LEU
2	N	323	LEU
2	N	326	ILE
2	N	334	THR
2	N	342	THR
2	N	353	ARG
1	O	20	VAL
1	O	33	THR
1	O	51	THR
1	O	77	LEU
1	O	80	LEU
1	O	93	LEU
1	O	95	VAL
1	O	97	LEU
1	O	98	ARG
1	O	114	LYS
1	O	144	VAL

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Mol	Chain	Res	Type
1	O	154	MET
1	O	158	LYS
1	O	159	THR
1	O	161	ARG
1	O	175	ARG
1	O	201	ILE
1	O	211	VAL
1	O	212	SER
1	O	222	GLN
1	O	238	MET
1	O	241	THR
1	O	250	LEU
1	O	305	ASN
1	O	315	VAL
1	O	319	ILE
1	O	325	THR
1	O	328	ASP
1	O	335	THR
1	O	336	THR
1	O	341	GLU
1	O	346	LEU
1	O	348	THR
2	P	61	ILE
2	P	66	LEU
2	P	88	LEU
2	P	97	ARG
2	P	101	LEU
2	P	102	THR
2	P	103	LEU
2	P	114	ARG
2	P	125	THR
2	P	129	VAL
2	P	150	CYS
2	P	160	ILE
2	P	168	VAL
2	P	184	VAL
2	P	189	LYS
2	P	194	ARG
2	P	195	LEU
2	P	214	LEU
2	P	225	VAL
2	P	226	LEU

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Mol	Chain	Res	Type
2	P	241	VAL
2	P	283	SER
2	P	286	ASP
2	P	299	LEU
2	P	306	LEU
2	P	323	LEU
2	P	326	ILE
2	P	334	THR
2	P	342	THR
2	P	353	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	301	HIS
2	B	112	ASN
2	B	155	GLN
2	B	269	ASN
2	D	5	GLN
2	D	112	ASN
2	D	128	ASN
2	D	155	GLN
2	D	244	ASN
2	D	269	ASN
2	F	112	ASN
2	F	155	GLN
2	F	269	ASN
1	G	56	GLN
1	G	283	GLN
1	G	301	HIS
2	H	112	ASN
2	H	137	ASN
2	H	155	GLN
1	I	301	HIS
2	J	112	ASN
2	J	269	ASN
1	K	56	GLN
1	K	90	HIS
1	K	283	GLN
2	L	5	GLN
2	L	96	HIS
2	L	193	GLN

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Mol	Chain	Res	Type
1	O	90	HIS
1	O	283	GLN
1	O	301	HIS
2	P	112	ASN
2	P	269	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	335/349 (95%)	-0.19	2 (0%) 85 85	13, 38, 80, 100	0
1	C	338/349 (96%)	-0.07	4 (1%) 76 75	11, 38, 75, 93	0
1	E	341/349 (97%)	-0.19	3 (0%) 81 80	18, 42, 78, 117	0
1	G	334/349 (95%)	-0.19	2 (0%) 85 85	16, 41, 79, 96	0
1	I	333/349 (95%)	-0.01	4 (1%) 76 75	17, 40, 78, 113	0
1	K	338/349 (96%)	-0.21	5 (1%) 72 70	13, 41, 78, 98	0
1	M	337/349 (96%)	0.89	47 (13%) 6 5	21, 48, 91, 121	0
1	O	332/349 (95%)	-0.19	4 (1%) 76 75	17, 43, 79, 97	0
2	B	346/354 (97%)	0.42	22 (6%) 25 22	21, 60, 102, 119	0
2	D	345/354 (97%)	0.39	24 (6%) 22 19	21, 66, 105, 123	0
2	F	345/354 (97%)	0.51	17 (4%) 35 31	24, 69, 107, 121	0
2	H	345/354 (97%)	0.30	10 (2%) 53 50	24, 69, 108, 127	0
2	J	345/354 (97%)	1.02	57 (16%) 4 4	24, 67, 105, 120	0
2	L	346/354 (97%)	0.42	15 (4%) 40 36	24, 69, 106, 121	0
2	N	345/354 (97%)	1.02	39 (11%) 10 8	28, 77, 111, 122	0
2	P	326/354 (92%)	0.48	14 (4%) 40 36	30, 74, 109, 119	0
All	All	5431/5624 (96%)	0.28	269 (4%) 34 30	11, 53, 103, 127	0

All (269) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	323	LEU	6.2
2	J	30	ASP	5.0
2	L	346	PHE	5.0
1	M	290	ALA	4.9
2	H	350	VAL	4.8

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Mol	Chain	Res	Type	RSRZ
2	F	327	ALA	4.7
2	J	36	ILE	4.6
1	M	275	HIS	4.6
1	M	81	TRP	4.4
2	J	66	LEU	4.4
1	M	62	GLY	4.3
2	D	323	LEU	4.1
1	M	54	ILE	4.0
2	L	44	PHE	4.0
2	J	51	ILE	3.9
2	J	287	ILE	3.9
2	J	327	ALA	3.9
2	N	126	TYR	3.8
1	M	25	GLY	3.7
2	B	63	VAL	3.7
1	C	276	VAL	3.6
1	C	56	GLN	3.6
2	N	192	ILE	3.6
1	M	338	PHE	3.6
1	C	275	HIS	3.5
2	J	318	ILE	3.5
2	N	63	VAL	3.5
1	M	84	PRO	3.4
1	M	80	LEU	3.4
1	M	83	THR	3.4
2	N	69	ILE	3.4
2	J	335	GLY	3.4
2	J	67	THR	3.4
2	J	63	VAL	3.4
1	M	280	ILE	3.3
2	B	348	GLU	3.3
2	J	328	SER	3.3
2	J	315	ALA	3.2
1	K	56	GLN	3.2
2	J	347	THR	3.2
1	M	79	GLY	3.2
2	N	341	ALA	3.2
2	J	62	PHE	3.2
2	J	325	THR	3.2
1	M	24	PRO	3.1
2	J	9	GLY	3.1
2	B	69	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	M	93	LEU	3.1
2	N	327	ALA	3.1
1	M	63	VAL	3.1
2	B	323	LEU	3.1
2	J	286	ASP	3.1
2	N	333	ARG	3.1
2	F	63	VAL	3.1
1	M	324	HIS	3.0
2	J	64	ASN	3.0
2	D	17	PRO	3.0
2	J	24	VAL	3.0
2	L	53	TRP	3.0
2	N	326	ILE	3.0
2	B	347	THR	3.0
1	M	334	SER	3.0
2	J	32	ILE	3.0
1	M	316	HIS	2.9
2	D	330	PRO	2.9
1	M	23	ILE	2.9
2	F	69	ILE	2.9
2	J	326	ILE	2.9
2	D	23	THR	2.9
2	D	58	VAL	2.9
2	F	8	ILE	2.9
2	N	191	THR	2.9
2	L	193	GLN	2.9
1	I	282	GLY	2.9
2	J	65	GLY	2.9
1	M	335	THR	2.9
1	M	22	LEU	2.9
2	F	91	PRO	2.8
2	J	320	ASN	2.8
2	J	101	LEU	2.8
1	M	282	GLY	2.8
2	J	121	GLY	2.8
1	M	276	VAL	2.8
1	M	343	ILE	2.8
2	B	36	ILE	2.8
2	D	287	ILE	2.8
2	J	31	GLY	2.8
2	P	130	ASP	2.8
2	B	321	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	I	275	HIS	2.8
2	D	44	PHE	2.8
2	N	91	PRO	2.7
1	M	32	ILE	2.7
2	J	26	PHE	2.7
2	N	44	PHE	2.7
2	P	121	GLY	2.7
2	B	51	ILE	2.7
1	M	278	LEU	2.7
1	I	274	ARG	2.7
2	B	202	ASN	2.7
2	F	321	ALA	2.7
2	J	39	SER	2.7
2	J	40	VAL	2.7
1	M	328	ASP	2.7
1	M	64	TYR	2.6
2	D	329	GLY	2.6
1	M	285	VAL	2.6
2	P	349	ALA	2.6
1	C	57	THR	2.6
2	D	347	THR	2.6
2	P	351	ILE	2.6
2	J	49	VAL	2.6
2	N	282	GLY	2.6
1	M	40	PHE	2.6
1	I	87	GLN	2.6
2	J	53	TRP	2.6
2	B	286	ASP	2.6
2	D	286	ASP	2.6
2	J	252	ASP	2.6
1	M	272	GLY	2.6
1	E	276	VAL	2.6
1	O	184	ALA	2.6
2	N	321	ALA	2.6
1	G	323	LYS	2.5
2	F	285	PRO	2.5
2	B	327	ALA	2.5
2	J	346	PHE	2.5
2	L	287	ILE	2.5
2	J	348	GLU	2.5
1	M	342	ILE	2.5
2	D	41	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
2	N	43	ILE	2.5
2	N	61	ILE	2.5
1	A	275	HIS	2.5
2	L	23	THR	2.5
2	J	52	GLU	2.5
1	O	18	PHE	2.5
2	N	68	THR	2.4
2	F	36	ILE	2.4
2	J	290	GLN	2.4
2	D	321	ALA	2.4
2	F	326	ILE	2.4
2	J	332	ASN	2.4
2	N	323	LEU	2.4
1	M	337	ASP	2.4
2	D	53	TRP	2.4
2	P	330	PRO	2.4
2	P	350	VAL	2.4
2	D	346	PHE	2.4
2	H	349	ALA	2.4
1	K	275	HIS	2.4
2	J	285	PRO	2.4
2	N	284	ALA	2.4
2	N	293	ALA	2.4
1	E	83	THR	2.4
2	F	68	THR	2.4
2	J	351	ILE	2.4
2	N	67	THR	2.4
2	N	263	GLY	2.4
2	F	193	GLN	2.4
2	P	74	VAL	2.4
2	D	46	ALA	2.4
2	N	297	ALA	2.4
1	M	293	LEU	2.3
2	B	287	ILE	2.3
2	J	69	ILE	2.3
2	F	289	GLY	2.3
2	F	310	GLY	2.3
1	O	274	ARG	2.3
2	J	58	VAL	2.3
2	F	62	PHE	2.3
2	D	69	ILE	2.3
2	J	43	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
2	L	41	LYS	2.3
2	N	285	PRO	2.3
2	D	13	GLY	2.3
2	F	247	GLY	2.3
2	N	226	LEU	2.3
2	J	61	ILE	2.3
2	B	64	ASN	2.3
1	M	327	ARG	2.3
2	B	151	PRO	2.3
2	P	40	VAL	2.3
2	N	122	PHE	2.3
2	B	62	PHE	2.3
2	H	26	PHE	2.3
2	N	346	PHE	2.3
2	J	284	ALA	2.2
2	L	36	ILE	2.2
2	N	349	ALA	2.2
2	P	51	ILE	2.2
1	G	335	THR	2.2
2	J	23	THR	2.2
1	M	274	ARG	2.2
1	O	277	GLY	2.2
2	J	339	GLY	2.2
2	P	31	GLY	2.2
2	H	322	VAL	2.2
2	F	346	PHE	2.2
2	N	272	HIS	2.2
2	D	56	CYS	2.2
2	J	56	CYS	2.2
2	J	60	PRO	2.2
2	N	193	GLN	2.2
1	M	86	ASP	2.2
2	L	9	GLY	2.2
2	N	335	GLY	2.2
2	H	321	ALA	2.2
2	J	46	ALA	2.2
2	J	288	ALA	2.2
2	B	230	THR	2.2
2	H	52	GLU	2.2
1	M	271	PRO	2.2
1	M	113	LEU	2.2
1	M	332	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	M	45	ILE	2.2
2	D	192	ILE	2.2
2	D	326	ILE	2.2
2	H	327	ALA	2.2
1	M	288	PRO	2.2
1	M	125	LEU	2.2
2	B	26	PHE	2.2
2	N	62	PHE	2.2
2	J	73	ALA	2.1
2	H	91	PRO	2.1
2	L	60	PRO	2.1
1	K	87	GLN	2.1
2	L	65	GLY	2.1
1	E	280	ILE	2.1
2	L	37	SER	2.1
2	L	192	ILE	2.1
1	K	42	ALA	2.1
1	M	51	THR	2.1
2	J	337	LEU	2.1
2	N	64	ASN	2.1
2	N	289	GLY	2.1
2	P	329	GLY	2.1
2	H	351	ILE	2.1
2	P	341	ALA	2.1
1	M	339	THR	2.1
2	N	215	THR	2.1
2	N	325	THR	2.1
2	N	115	PRO	2.1
2	D	193	GLN	2.1
2	N	235	TYR	2.1
1	M	52	ILE	2.1
2	N	239	VAL	2.1
2	B	252	ASP	2.1
1	M	65	GLU	2.1
1	A	57	THR	2.1
2	F	124	THR	2.1
2	J	90	THR	2.1
2	J	334	THR	2.1
2	L	91	PRO	2.1
2	J	142	TYR	2.1
2	P	43	ILE	2.1
2	J	322	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	327	ALA	2.0
2	B	325	THR	2.0
2	P	64	ASN	2.0
2	B	339	GLY	2.0
2	D	322	VAL	2.0
2	D	62	PHE	2.0
1	K	323	LYS	2.0
2	L	321	ALA	2.0
2	N	304	MET	2.0
2	B	193	GLN	2.0
2	H	193	GLN	2.0
2	B	61	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.