



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:44 PM UTC

PDB ID : 2LDX / pdb_00002ldx
Title : CHARACTERIZATION OF THE ANTIGENIC SITES ON THE REFINED
3-ANGSTROMS RESOLUTION STRUCTURE OF MOUSE TESTICULAR
LACTATE DEHYDROGENASE C4
Authors : Griffith, J.P.; Rossmann, M.G.
Deposited on : 1987-11-25
Resolution : 2.96 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

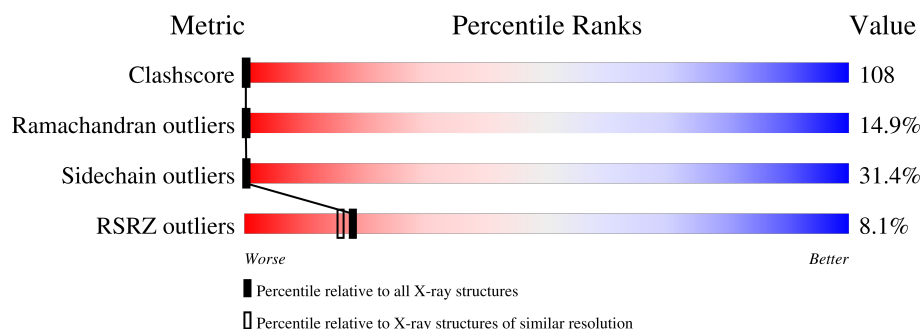
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.96 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	331	8% 11% 39% 33% 17%
1	B	331	8% 11% 40% 32% 17%
1	C	331	8% 9% 40% 33% 18%
1	D	331	9% 10% 40% 32% 18%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10091 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 APO-LACTATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	0	0
			2515	1603	432	468	12			
1	B	331	Total	C	N	O	S	0	0	0
			2515	1603	432	468	12			
1	C	331	Total	C	N	O	S	0	0	0
			2515	1603	432	468	12			
1	D	331	Total	C	N	O	S	0	0	0
			2515	1603	432	468	12			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	29	ASP	ASN	conflict	UNP P00342
A	55	ASP	ASN	conflict	UNP P00342
A	65	GLN	LEU	conflict	UNP P00342
A	103	GLN	GLU	conflict	UNP P00342
A	123	VAL	ILE	conflict	UNP P00342
A	124	ILE	VAL	conflict	UNP P00342
A	134	VAL	ILE	conflict	UNP P00342
A	221	LYS	SER	conflict	UNP P00342
A	222	ASN	ASP	conflict	UNP P00342
A	224	GLN	GLU	conflict	UNP P00342
A	242	ASP	ASN	conflict	UNP P00342
A	296	GLU	GLN	conflict	UNP P00342
A	328	ASN	ASP	conflict	UNP P00342
A	330	GLU	GLN	conflict	UNP P00342
B	29	ASP	ASN	conflict	UNP P00342
B	55	ASP	ASN	conflict	UNP P00342
B	65	GLN	LEU	conflict	UNP P00342
B	103	GLN	GLU	conflict	UNP P00342
B	123	VAL	ILE	conflict	UNP P00342
B	124	ILE	VAL	conflict	UNP P00342
B	134	VAL	ILE	conflict	UNP P00342

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Chain	Residue	Modelled	Actual	Comment	Reference
B	221	LYS	SER	conflict	UNP P00342
B	222	ASN	ASP	conflict	UNP P00342
B	224	GLN	GLU	conflict	UNP P00342
B	242	ASP	ASN	conflict	UNP P00342
B	296	GLU	GLN	conflict	UNP P00342
B	328	ASN	ASP	conflict	UNP P00342
B	330	GLU	GLN	conflict	UNP P00342
C	29	ASP	ASN	conflict	UNP P00342
C	55	ASP	ASN	conflict	UNP P00342
C	65	GLN	LEU	conflict	UNP P00342
C	103	GLN	GLU	conflict	UNP P00342
C	123	VAL	ILE	conflict	UNP P00342
C	124	ILE	VAL	conflict	UNP P00342
C	134	VAL	ILE	conflict	UNP P00342
C	221	LYS	SER	conflict	UNP P00342
C	222	ASN	ASP	conflict	UNP P00342
C	224	GLN	GLU	conflict	UNP P00342
C	242	ASP	ASN	conflict	UNP P00342
C	296	GLU	GLN	conflict	UNP P00342
C	328	ASN	ASP	conflict	UNP P00342
C	330	GLU	GLN	conflict	UNP P00342
D	29	ASP	ASN	conflict	UNP P00342
D	55	ASP	ASN	conflict	UNP P00342
D	65	GLN	LEU	conflict	UNP P00342
D	103	GLN	GLU	conflict	UNP P00342
D	123	VAL	ILE	conflict	UNP P00342
D	124	ILE	VAL	conflict	UNP P00342
D	134	VAL	ILE	conflict	UNP P00342
D	221	LYS	SER	conflict	UNP P00342
D	222	ASN	ASP	conflict	UNP P00342
D	224	GLN	GLU	conflict	UNP P00342
D	242	ASP	ASN	conflict	UNP P00342
D	296	GLU	GLN	conflict	UNP P00342
D	328	ASN	ASP	conflict	UNP P00342
D	330	GLU	GLN	conflict	UNP P00342

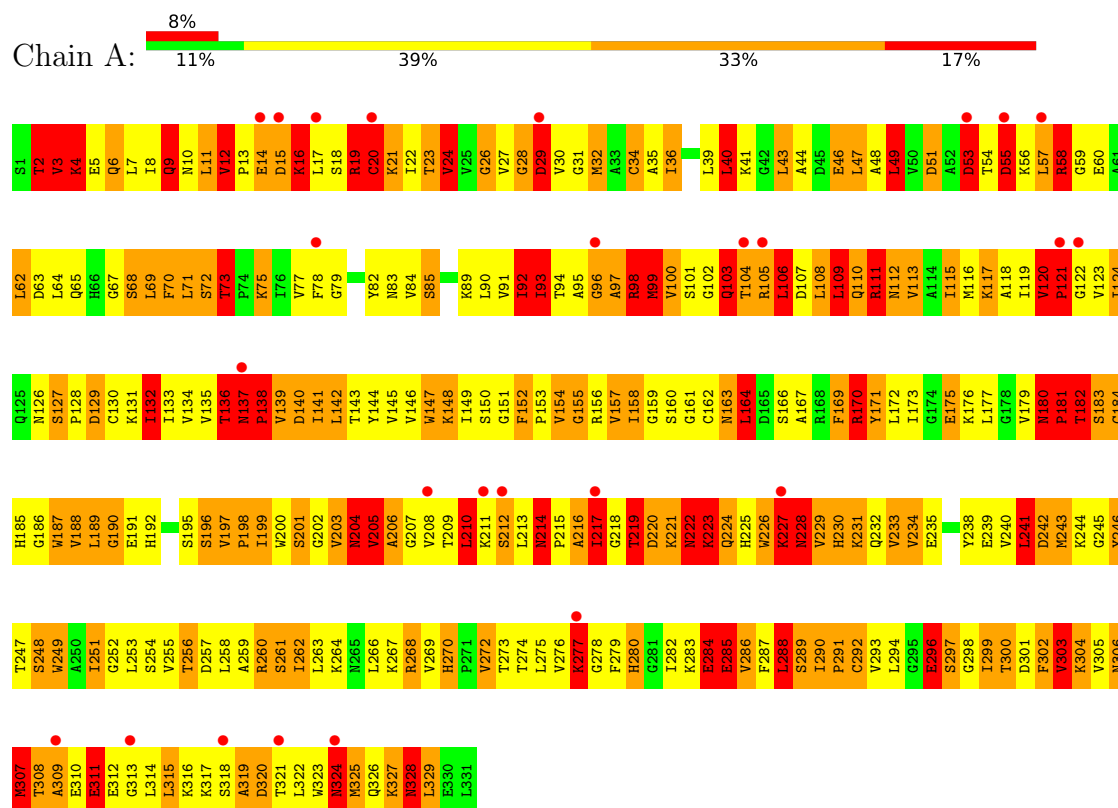
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	29	Total O 29 29	0	0
2	D	2	Total O 2 2	0	0

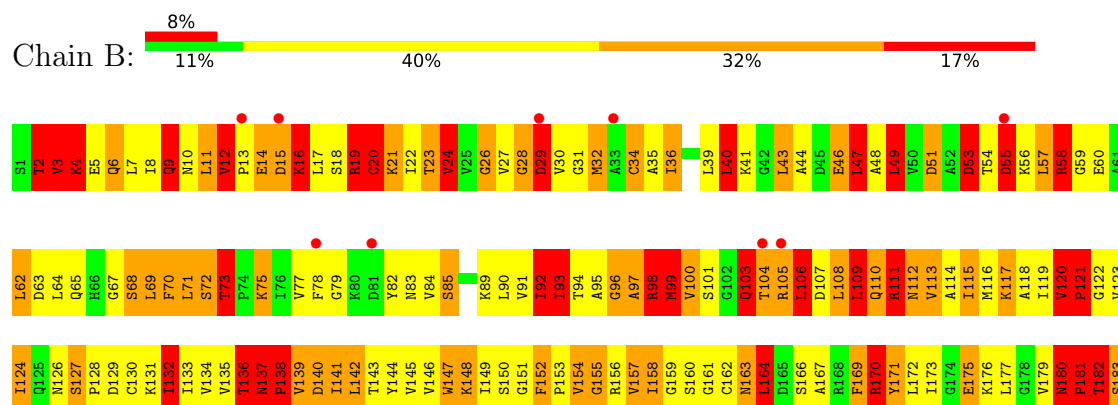
3 Residue-property plots

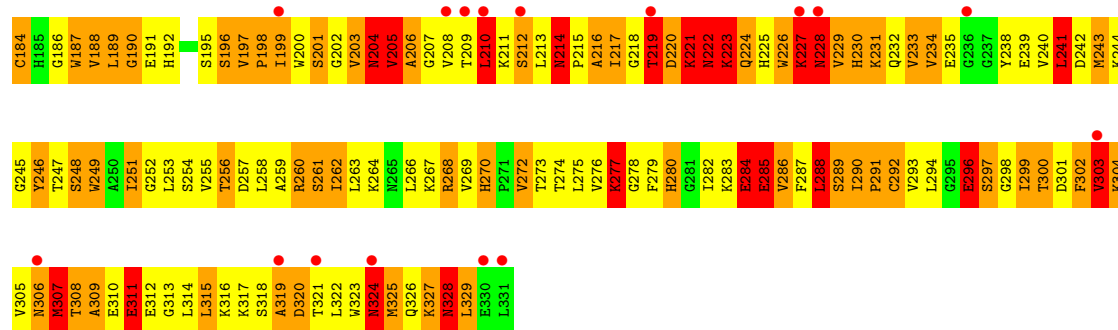
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: APO-LACTATE DEHYDROGENASE

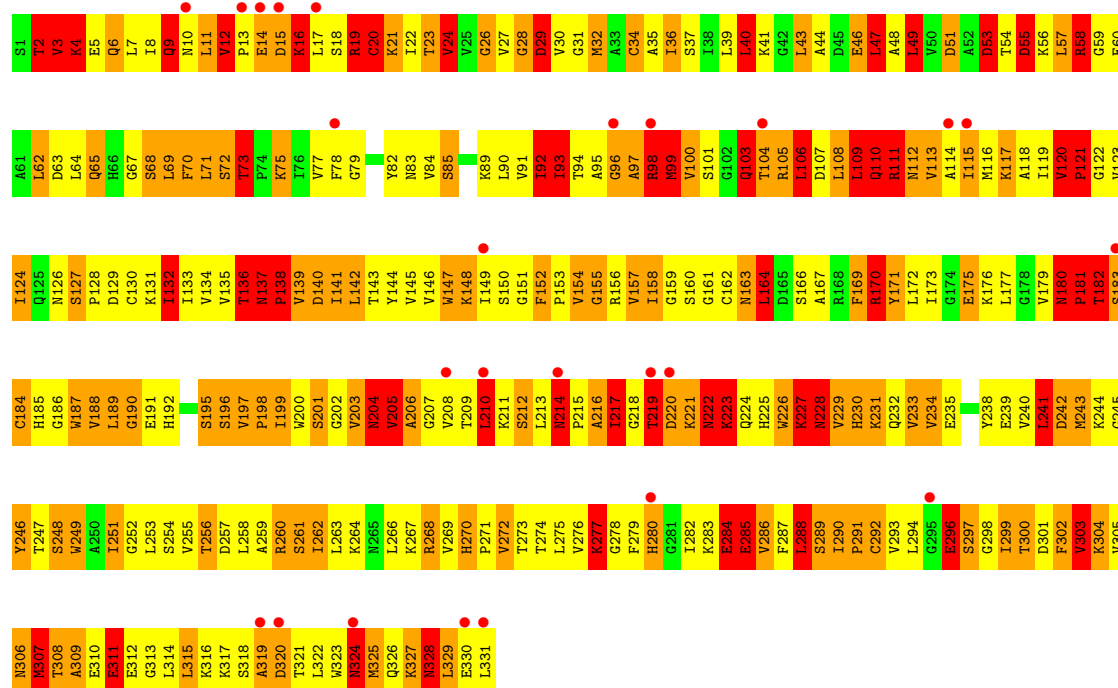


• Molecule 1: APO-LACTATE DEHYDROGENASE

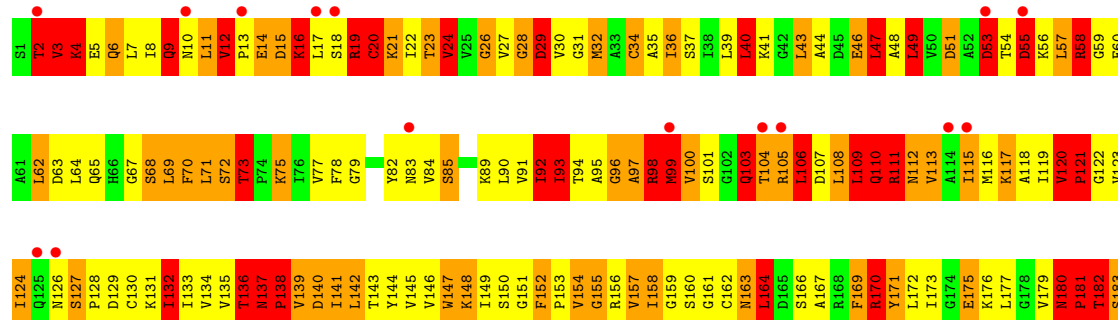


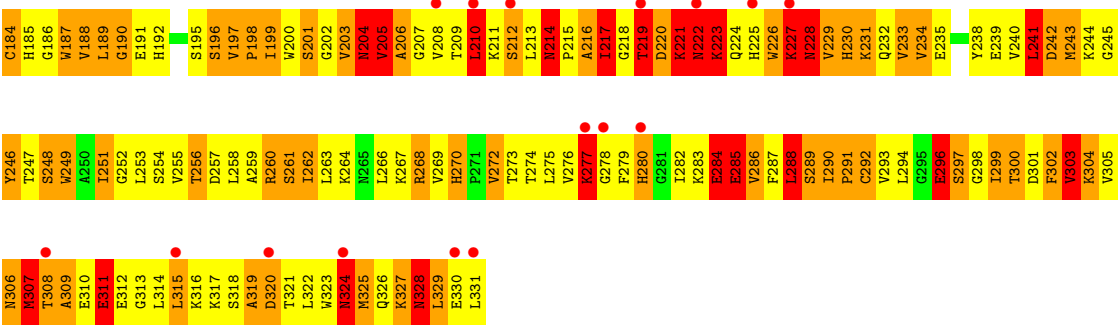


● Molecule 1: APO-LACTATE DEHYDROGENASE



● Molecule 1: APO-LACTATE DEHYDROGENASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	84.80Å 76.60Å 63.90Å 109.70° 89.50° 96.50°	Depositor
Resolution (Å)	10.00 – 2.96 10.00 – 2.96	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.96) 63.7 (10.00-2.96)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	306.79 (at 2.89Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.256 , (Not available) 0.261 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	44.1	Xtriage
Anisotropy	0.259	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.20 , 44.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	10091	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.91% 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	1.37	12/2556 (0.5%)	2.52	174/3465 (5.0%)
1	B	1.37	11/2556 (0.4%)	2.52	173/3465 (5.0%)
1	C	1.37	12/2556 (0.5%)	2.52	176/3465 (5.1%)
1	D	1.37	13/2556 (0.5%)	2.52	174/3465 (5.0%)
All	All	1.37	48/10224 (0.5%)	2.52	697/13860 (5.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	3
1	C	0	3
1	D	0	3
All	All	0	12

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	137	ASN	CA-CB	7.96	1.66	1.53
1	C	137	ASN	CA-CB	7.90	1.66	1.53
1	A	137	ASN	CA-CB	7.88	1.65	1.53
1	D	137	ASN	CA-CB	7.83	1.65	1.53
1	A	28	GLY	N-CA	6.82	1.52	1.45
1	B	28	GLY	N-CA	6.71	1.52	1.45
1	D	28	GLY	N-CA	6.67	1.52	1.45
1	C	28	GLY	N-CA	6.60	1.52	1.45
1	A	136	THR	C-O	6.57	1.32	1.24
1	B	136	THR	C-O	6.51	1.32	1.24
1	C	136	THR	C-O	6.44	1.32	1.24
1	D	136	THR	C-O	6.42	1.32	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	137	ASN	C-O	6.35	1.32	1.24
1	D	137	ASN	C-O	6.30	1.32	1.24
1	B	137	ASN	C-O	6.28	1.32	1.24
1	A	137	ASN	C-O	6.25	1.32	1.24
1	D	58	ARG	CZ-NH1	5.90	1.41	1.32
1	B	58	ARG	CZ-NH1	5.84	1.41	1.32
1	A	58	ARG	CZ-NH1	5.83	1.41	1.32
1	C	58	ARG	CZ-NH1	5.82	1.40	1.32
1	C	170	ARG	CD-NE	-5.56	1.38	1.46
1	C	93	ILE	CA-CB	5.52	1.60	1.53
1	D	93	ILE	CA-CB	5.50	1.60	1.53
1	B	170	ARG	CD-NE	-5.50	1.38	1.46
1	A	93	ILE	CA-CB	5.47	1.59	1.53
1	D	170	ARG	CD-NE	-5.47	1.38	1.46
1	A	170	ARG	CD-NE	-5.43	1.38	1.46
1	B	93	ILE	CA-CB	5.42	1.59	1.53
1	D	2	THR	CA-CB	5.42	1.62	1.53
1	A	218	GLY	N-CA	5.41	1.53	1.45
1	A	2	THR	CA-CB	5.39	1.62	1.53
1	C	58	ARG	CD-NE	-5.38	1.38	1.46
1	C	2	THR	CA-CB	5.36	1.62	1.53
1	D	218	GLY	N-CA	5.33	1.53	1.45
1	B	218	GLY	N-CA	5.33	1.53	1.45
1	B	2	THR	CA-CB	5.30	1.62	1.53
1	D	58	ARG	CD-NE	-5.30	1.38	1.46
1	C	218	GLY	N-CA	5.29	1.53	1.45
1	A	58	ARG	CD-NE	-5.28	1.38	1.46
1	B	58	ARG	CD-NE	-5.28	1.38	1.46
1	A	72	SER	C-N	-5.22	1.29	1.33
1	D	72	SER	C-N	-5.18	1.29	1.33
1	B	72	SER	C-N	-5.10	1.29	1.33
1	D	75	LYS	N-CA	5.02	1.52	1.46
1	D	217	ILE	CA-CB	5.01	1.61	1.54
1	C	72	SER	C-N	-5.01	1.29	1.33
1	C	217	ILE	CA-CB	5.01	1.61	1.54
1	A	217	ILE	CA-CB	5.00	1.61	1.54

All (697) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	58	ARG	CD-NE-CZ	20.84	153.58	124.40
1	D	58	ARG	CD-NE-CZ	20.81	153.54	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	58	ARG	CD-NE-CZ	20.80	153.53	124.40
1	B	58	ARG	CD-NE-CZ	20.79	153.51	124.40
1	D	285	GLU	CA-CB-CG	15.60	145.31	114.10
1	B	285	GLU	CA-CB-CG	15.59	145.28	114.10
1	C	285	GLU	CA-CB-CG	15.56	145.22	114.10
1	A	285	GLU	CA-CB-CG	15.55	145.19	114.10
1	A	129	ASP	CA-CB-CG	14.79	127.39	112.60
1	B	129	ASP	CA-CB-CG	14.77	127.36	112.60
1	C	129	ASP	CA-CB-CG	14.76	127.36	112.60
1	D	129	ASP	CA-CB-CG	14.73	127.33	112.60
1	D	137	ASN	N-CA-C	14.66	142.22	109.81
1	B	137	ASN	N-CA-C	14.65	142.20	109.81
1	C	137	ASN	N-CA-C	14.65	142.20	109.81
1	A	137	ASN	N-CA-C	14.64	142.16	109.81
1	C	152	PHE	CA-CB-CG	14.15	127.95	113.80
1	A	152	PHE	CA-CB-CG	14.09	127.89	113.80
1	D	152	PHE	CA-CB-CG	14.07	127.87	113.80
1	B	152	PHE	CA-CB-CG	14.04	127.84	113.80
1	A	218	GLY	CA-C-N	12.17	144.79	121.54
1	A	218	GLY	C-N-CA	12.17	144.79	121.54
1	B	218	GLY	CA-C-N	12.16	144.76	121.54
1	B	218	GLY	C-N-CA	12.16	144.76	121.54
1	C	218	GLY	CA-C-N	12.15	144.75	121.54
1	C	218	GLY	C-N-CA	12.15	144.75	121.54
1	D	218	GLY	CA-C-N	12.13	144.71	121.54
1	D	218	GLY	C-N-CA	12.13	144.71	121.54
1	A	136	THR	CA-C-O	-11.83	103.59	120.51
1	C	136	THR	CA-C-O	-11.81	103.62	120.51
1	D	136	THR	CA-C-O	-11.80	103.64	120.51
1	B	136	THR	CA-C-O	-11.78	103.66	120.51
1	B	137	ASN	O-C-N	-11.66	107.91	121.32
1	C	137	ASN	O-C-N	-11.62	107.96	121.32
1	D	137	ASN	O-C-N	-11.62	107.96	121.32
1	A	137	ASN	O-C-N	-11.58	108.00	121.32
1	B	58	ARG	CA-CB-CG	11.49	137.08	114.10
1	C	58	ARG	CA-CB-CG	11.48	137.06	114.10
1	D	58	ARG	CA-CB-CG	11.48	137.06	114.10
1	A	58	ARG	CA-CB-CG	11.45	137.01	114.10
1	B	169	PHE	CA-CB-CG	10.82	124.62	113.80
1	D	169	PHE	CA-CB-CG	10.81	124.61	113.80
1	A	169	PHE	CA-CB-CG	10.78	124.58	113.80
1	C	169	PHE	CA-CB-CG	10.77	124.57	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	324	ASN	N-CA-CB	10.54	125.64	109.94
1	C	204	ASN	CA-C-N	10.53	140.92	121.97
1	C	204	ASN	C-N-CA	10.53	140.92	121.97
1	C	324	ASN	N-CA-CB	10.53	125.63	109.94
1	D	324	ASN	N-CA-CB	10.52	125.62	109.94
1	D	204	ASN	CA-C-N	10.52	140.91	121.97
1	D	204	ASN	C-N-CA	10.52	140.91	121.97
1	A	204	ASN	CA-C-N	10.52	140.90	121.97
1	A	204	ASN	C-N-CA	10.52	140.90	121.97
1	C	55	ASP	CA-CB-CG	10.51	123.11	112.60
1	B	204	ASN	CA-C-N	10.50	140.87	121.97
1	B	204	ASN	C-N-CA	10.50	140.87	121.97
1	B	324	ASN	N-CA-CB	10.48	125.55	109.94
1	A	55	ASP	CA-CB-CG	10.45	123.05	112.60
1	B	55	ASP	CA-CB-CG	10.45	123.05	112.60
1	D	55	ASP	CA-CB-CG	10.42	123.02	112.60
1	B	285	GLU	CB-CG-CD	9.97	129.55	112.60
1	D	285	GLU	CB-CG-CD	9.96	129.53	112.60
1	A	285	GLU	CB-CG-CD	9.94	129.50	112.60
1	C	285	GLU	CB-CG-CD	9.94	129.49	112.60
1	A	324	ASN	O-C-N	9.91	132.39	122.09
1	C	223	LYS	CA-C-N	9.88	140.41	121.54
1	C	223	LYS	C-N-CA	9.88	140.41	121.54
1	D	324	ASN	O-C-N	9.88	132.37	122.09
1	D	223	LYS	CA-C-N	9.88	140.41	121.54
1	D	223	LYS	C-N-CA	9.88	140.41	121.54
1	C	324	ASN	O-C-N	9.87	132.36	122.09
1	B	223	LYS	CA-C-N	9.87	140.39	121.54
1	B	223	LYS	C-N-CA	9.87	140.39	121.54
1	B	324	ASN	O-C-N	9.86	132.34	122.09
1	A	223	LYS	CA-C-N	9.85	140.35	121.54
1	A	223	LYS	C-N-CA	9.85	140.35	121.54
1	A	170	ARG	CD-NE-CZ	9.70	137.98	124.40
1	C	170	ARG	CD-NE-CZ	9.66	137.93	124.40
1	D	170	ARG	CD-NE-CZ	9.63	137.88	124.40
1	B	170	ARG	CD-NE-CZ	9.62	137.87	124.40
1	B	120	VAL	CB-CA-C	9.62	128.87	111.36
1	A	120	VAL	CB-CA-C	9.61	128.86	111.36
1	D	120	VAL	CB-CA-C	9.61	128.86	111.36
1	C	120	VAL	CB-CA-C	9.60	128.82	111.36
1	D	53	ASP	CA-CB-CG	9.43	122.03	112.60
1	D	46	GLU	CB-CG-CD	9.37	128.53	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	46	GLU	CB-CG-CD	9.37	128.53	112.60
1	B	53	ASP	CA-CB-CG	9.36	121.96	112.60
1	C	53	ASP	CA-CB-CG	9.36	121.96	112.60
1	A	53	ASP	CA-CB-CG	9.36	121.96	112.60
1	B	46	GLU	CB-CG-CD	9.35	128.49	112.60
1	C	75	LYS	CA-CB-CG	9.33	132.76	114.10
1	A	46	GLU	CB-CG-CD	9.32	128.45	112.60
1	A	75	LYS	CA-CB-CG	9.31	132.73	114.10
1	B	75	LYS	CA-CB-CG	9.31	132.72	114.10
1	D	75	LYS	CA-CB-CG	9.30	132.71	114.10
1	C	138	PRO	CA-N-CD	-9.23	98.57	111.50
1	D	138	PRO	CA-N-CD	-9.22	98.59	111.50
1	A	138	PRO	CA-N-CD	-9.21	98.61	111.50
1	B	138	PRO	CA-N-CD	-9.16	98.68	111.50
1	D	170	ARG	NE-CZ-NH1	9.11	130.61	121.50
1	C	170	ARG	NE-CZ-NH1	9.10	130.60	121.50
1	B	170	ARG	NE-CZ-NH1	9.09	130.59	121.50
1	A	170	ARG	NE-CZ-NH1	9.03	130.53	121.50
1	A	28	GLY	CA-C-O	-8.93	113.55	121.41
1	A	196	SER	CA-C-N	-8.93	116.53	122.60
1	A	196	SER	C-N-CA	-8.93	116.53	122.60
1	D	28	GLY	CA-C-O	-8.91	113.57	121.41
1	C	196	SER	CA-C-N	-8.89	116.56	122.60
1	C	196	SER	C-N-CA	-8.89	116.56	122.60
1	B	28	GLY	CA-C-O	-8.88	113.59	121.41
1	C	28	GLY	CA-C-O	-8.88	113.60	121.41
1	D	196	SER	CA-C-N	-8.88	116.56	122.60
1	D	196	SER	C-N-CA	-8.88	116.56	122.60
1	B	196	SER	CA-C-N	-8.85	116.58	122.60
1	B	196	SER	C-N-CA	-8.85	116.58	122.60
1	A	28	GLY	N-CA-C	-8.83	101.03	111.36
1	D	28	GLY	N-CA-C	-8.82	101.04	111.36
1	B	28	GLY	N-CA-C	-8.82	101.04	111.36
1	C	28	GLY	N-CA-C	-8.80	101.06	111.36
1	A	104	THR	CB-CA-C	8.77	120.58	109.80
1	D	104	THR	CB-CA-C	8.74	120.55	109.80
1	C	104	THR	CB-CA-C	8.74	120.55	109.80
1	B	104	THR	CB-CA-C	8.70	120.50	109.80
1	A	180	ASN	CA-CB-CG	8.43	121.03	112.60
1	B	180	ASN	CA-CB-CG	8.39	120.99	112.60
1	C	180	ASN	CA-CB-CG	8.38	120.98	112.60
1	D	180	ASN	CA-CB-CG	8.37	120.97	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	92	ILE	CB-CA-C	8.36	120.67	110.73
1	C	92	ILE	CB-CA-C	8.35	120.66	110.73
1	D	137	ASN	CA-CB-CG	-8.34	104.26	112.60
1	C	137	ASN	CA-CB-CG	-8.32	104.28	112.60
1	A	92	ILE	CB-CA-C	8.32	120.63	110.73
1	B	92	ILE	CB-CA-C	8.30	120.61	110.73
1	B	137	ASN	CA-CB-CG	-8.24	104.36	112.60
1	A	137	ASN	CA-CB-CG	-8.24	104.36	112.60
1	B	175	GLU	CA-CB-CG	8.21	130.52	114.10
1	A	175	GLU	CA-CB-CG	8.18	130.46	114.10
1	C	175	GLU	CA-CB-CG	8.17	130.44	114.10
1	D	175	GLU	CA-CB-CG	8.17	130.45	114.10
1	B	138	PRO	CB-CA-C	8.12	132.31	112.00
1	C	138	PRO	CB-CA-C	8.12	132.31	112.00
1	A	138	PRO	CB-CA-C	8.10	132.26	112.00
1	B	175	GLU	CB-CG-CD	8.09	126.36	112.60
1	D	138	PRO	CB-CA-C	8.09	132.22	112.00
1	C	175	GLU	CB-CG-CD	8.05	126.29	112.60
1	A	328	ASN	CA-C-N	8.05	136.91	121.54
1	A	328	ASN	C-N-CA	8.05	136.91	121.54
1	B	328	ASN	CA-C-N	8.05	136.91	121.54
1	B	328	ASN	C-N-CA	8.05	136.91	121.54
1	D	328	ASN	CA-C-N	8.05	136.91	121.54
1	D	328	ASN	C-N-CA	8.05	136.91	121.54
1	A	138	PRO	CA-C-N	8.04	130.98	120.60
1	A	138	PRO	C-N-CA	8.04	130.98	120.60
1	D	175	GLU	CB-CG-CD	8.04	126.27	112.60
1	C	328	ASN	CA-C-N	8.03	136.88	121.54
1	C	328	ASN	C-N-CA	8.03	136.88	121.54
1	A	175	GLU	CB-CG-CD	8.03	126.25	112.60
1	D	138	PRO	CA-C-N	8.03	130.96	120.60
1	D	138	PRO	C-N-CA	8.03	130.96	120.60
1	A	20	CYS	N-CA-C	8.03	123.62	107.41
1	B	20	CYS	N-CA-C	8.03	123.62	107.41
1	B	138	PRO	CA-C-N	8.02	130.94	120.60
1	B	138	PRO	C-N-CA	8.02	130.94	120.60
1	C	138	PRO	CA-C-N	8.00	130.92	120.60
1	C	138	PRO	C-N-CA	8.00	130.92	120.60
1	D	20	CYS	N-CA-C	8.00	123.57	107.41
1	C	20	CYS	N-CA-C	7.99	123.55	107.41
1	B	92	ILE	CA-C-O	7.90	128.05	120.31
1	C	92	ILE	CA-C-O	7.90	128.05	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	92	ILE	CA-C-O	7.84	127.99	120.31
1	B	155	GLY	N-CA-C	-7.84	94.61	113.18
1	C	155	GLY	N-CA-C	-7.80	94.68	113.18
1	D	92	ILE	CA-C-O	7.80	127.95	120.31
1	D	155	GLY	N-CA-C	-7.79	94.72	113.18
1	D	34	CYS	N-CA-C	-7.78	103.76	113.18
1	A	155	GLY	N-CA-C	-7.78	94.74	113.18
1	C	34	CYS	N-CA-C	-7.78	103.77	113.18
1	A	34	CYS	N-CA-C	-7.74	103.81	113.18
1	B	34	CYS	N-CA-C	-7.74	103.81	113.18
1	A	324	ASN	CA-C-O	-7.74	112.62	120.90
1	C	324	ASN	CA-C-O	-7.68	112.68	120.90
1	B	324	ASN	CA-C-O	-7.68	112.69	120.90
1	D	324	ASN	CA-C-O	-7.67	112.70	120.90
1	A	34	CYS	CB-CA-C	7.57	125.00	109.95
1	D	34	CYS	CB-CA-C	7.56	125.00	109.95
1	B	34	CYS	CB-CA-C	7.55	124.98	109.95
1	C	34	CYS	CB-CA-C	7.54	124.95	109.95
1	C	311	GLU	CB-CG-CD	7.49	125.33	112.60
1	D	49	LEU	CB-CA-C	7.47	122.76	110.74
1	C	49	LEU	CB-CA-C	7.47	122.76	110.74
1	D	311	GLU	CB-CG-CD	7.46	125.28	112.60
1	B	49	LEU	CB-CA-C	7.44	122.72	110.74
1	A	49	LEU	CB-CA-C	7.43	122.71	110.74
1	A	311	GLU	CB-CG-CD	7.43	125.24	112.60
1	B	311	GLU	CB-CG-CD	7.41	125.20	112.60
1	A	83	ASN	CA-CB-CG	-7.29	105.31	112.60
1	C	83	ASN	CA-CB-CG	-7.29	105.31	112.60
1	A	9	GLN	CA-C-N	7.27	135.43	121.54
1	A	9	GLN	C-N-CA	7.27	135.43	121.54
1	D	9	GLN	CA-C-N	7.27	135.42	121.54
1	D	9	GLN	C-N-CA	7.27	135.42	121.54
1	C	180	ASN	CB-CA-C	7.25	120.80	109.42
1	B	83	ASN	CA-CB-CG	-7.24	105.36	112.60
1	D	83	ASN	CA-CB-CG	-7.24	105.36	112.60
1	C	9	GLN	CA-C-N	7.24	135.37	121.54
1	C	9	GLN	C-N-CA	7.24	135.37	121.54
1	B	9	GLN	CA-C-N	7.23	135.35	121.54
1	B	9	GLN	C-N-CA	7.23	135.35	121.54
1	D	180	ASN	CB-CA-C	7.23	120.77	109.42
1	B	180	ASN	CB-CA-C	7.20	120.73	109.42
1	A	180	ASN	CB-CA-C	7.20	120.72	109.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	24	VAL	CB-CA-C	7.20	120.14	110.42
1	C	24	VAL	CB-CA-C	7.17	120.10	110.42
1	A	248	SER	N-CA-C	7.16	120.29	108.48
1	B	270	HIS	O-C-N	7.16	126.86	121.85
1	B	24	VAL	CB-CA-C	7.16	120.08	110.42
1	B	248	SER	N-CA-C	7.15	120.28	108.48
1	A	40	LEU	CB-CA-C	7.14	120.07	111.22
1	C	270	HIS	O-C-N	7.14	126.85	121.85
1	D	248	SER	N-CA-C	7.13	120.24	108.48
1	A	270	HIS	O-C-N	7.12	126.83	121.85
1	A	24	VAL	CB-CA-C	7.12	120.03	110.42
1	C	248	SER	N-CA-C	7.11	120.21	108.48
1	C	99	MET	CA-CB-CG	7.08	128.25	114.10
1	B	40	LEU	CB-CA-C	7.07	119.99	111.22
1	A	99	MET	CA-CB-CG	7.07	128.24	114.10
1	D	99	MET	CA-CB-CG	7.07	128.23	114.10
1	C	40	LEU	CB-CA-C	7.06	119.98	111.22
1	D	270	HIS	O-C-N	7.06	126.79	121.85
1	B	99	MET	CA-CB-CG	7.05	128.19	114.10
1	D	40	LEU	CB-CA-C	7.04	119.96	111.22
1	A	120	VAL	N-CA-CB	-7.03	101.37	111.21
1	B	328	ASN	N-CA-C	7.01	120.45	110.14
1	D	328	ASN	N-CA-C	7.01	120.45	110.14
1	A	223	LYS	CA-C-O	7.01	130.54	120.51
1	D	284	GLU	CB-CG-CD	7.00	124.50	112.60
1	D	120	VAL	N-CA-CB	-7.00	101.41	111.21
1	B	120	VAL	N-CA-CB	-7.00	101.42	111.21
1	D	223	LYS	CA-C-O	6.99	130.50	120.51
1	C	223	LYS	CA-C-O	6.99	130.50	120.51
1	A	284	GLU	CB-CG-CD	6.98	124.47	112.60
1	B	223	LYS	CA-C-O	6.98	130.50	120.51
1	C	328	ASN	N-CA-C	6.97	120.39	110.14
1	A	328	ASN	N-CA-C	6.97	120.38	110.14
1	C	284	GLU	CB-CG-CD	6.97	124.44	112.60
1	B	204	ASN	CA-CB-CG	6.96	119.56	112.60
1	C	120	VAL	N-CA-CB	-6.96	101.46	111.21
1	B	284	GLU	CB-CG-CD	6.96	124.43	112.60
1	A	204	ASN	CA-CB-CG	6.92	119.52	112.60
1	C	219	THR	N-CA-CB	6.90	122.15	110.49
1	D	204	ASN	CA-CB-CG	6.90	119.50	112.60
1	D	219	THR	N-CA-CB	6.89	122.13	110.49
1	C	204	ASN	CA-CB-CG	6.88	119.48	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	29	ASP	CA-CB-CG	6.88	119.48	112.60
1	A	219	THR	N-CA-CB	6.86	122.08	110.49
1	D	214	ASN	CA-CB-CG	6.86	119.46	112.60
1	D	29	ASP	CA-CB-CG	6.85	119.45	112.60
1	C	214	ASN	CA-CB-CG	6.84	119.44	112.60
1	B	219	THR	N-CA-CB	6.83	122.04	110.49
1	C	268	ARG	CA-CB-CG	6.83	127.76	114.10
1	B	43	LEU	CB-CA-C	6.83	123.39	109.67
1	A	268	ARG	CA-CB-CG	6.82	127.75	114.10
1	B	29	ASP	CA-CB-CG	6.82	119.42	112.60
1	A	43	LEU	CB-CA-C	6.82	123.38	109.67
1	B	214	ASN	CA-CB-CG	6.82	119.42	112.60
1	C	29	ASP	CA-CB-CG	6.82	119.42	112.60
1	B	268	ARG	CA-CB-CG	6.82	127.74	114.10
1	A	110	GLN	CA-C-N	6.81	129.41	120.28
1	A	110	GLN	C-N-CA	6.81	129.41	120.28
1	D	43	LEU	CB-CA-C	6.81	123.36	109.67
1	A	214	ASN	CA-CB-CG	6.81	119.41	112.60
1	B	110	GLN	CA-C-N	6.81	129.40	120.28
1	B	110	GLN	C-N-CA	6.81	129.40	120.28
1	D	110	GLN	CA-C-N	6.80	129.40	120.28
1	D	110	GLN	C-N-CA	6.80	129.40	120.28
1	C	110	GLN	CA-C-N	6.79	129.38	120.28
1	C	110	GLN	C-N-CA	6.79	129.38	120.28
1	C	43	LEU	CB-CA-C	6.79	123.31	109.67
1	D	268	ARG	CA-CB-CG	6.79	127.67	114.10
1	A	299	ILE	N-CA-CB	6.69	118.01	110.72
1	D	299	ILE	N-CA-CB	6.66	117.98	110.72
1	B	230	HIS	CA-CB-CG	-6.64	107.16	113.80
1	C	299	ILE	N-CA-CB	6.60	117.92	110.72
1	B	299	ILE	N-CA-CB	6.60	117.91	110.72
1	D	230	HIS	CA-CB-CG	-6.58	107.22	113.80
1	C	98	ARG	N-CA-C	6.57	119.61	107.99
1	C	46	GLU	N-CA-CB	6.57	121.47	110.77
1	A	230	HIS	CA-CB-CG	-6.56	107.24	113.80
1	C	230	HIS	CA-CB-CG	-6.56	107.24	113.80
1	B	98	ARG	N-CA-C	6.55	119.59	107.99
1	A	53	ASP	CB-CA-C	6.55	119.85	111.40
1	D	53	ASP	CB-CA-C	6.54	119.84	111.40
1	B	53	ASP	CB-CA-C	6.54	119.84	111.40
1	D	21	LYS	N-CA-C	6.54	120.07	110.59
1	D	98	ARG	N-CA-C	6.54	119.56	107.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	46	GLU	N-CA-CB	6.53	121.42	110.77
1	A	98	ARG	N-CA-C	6.53	119.54	107.99
1	D	46	GLU	N-CA-CB	6.53	121.41	110.77
1	B	21	LYS	N-CA-C	6.52	120.04	110.59
1	A	46	GLU	N-CA-CB	6.52	121.39	110.77
1	A	21	LYS	N-CA-C	6.51	120.02	110.59
1	C	53	ASP	CB-CA-C	6.51	119.79	111.40
1	B	11	LEU	CA-C-N	6.50	134.15	122.13
1	B	11	LEU	C-N-CA	6.50	134.15	122.13
1	C	21	LYS	N-CA-C	6.49	120.00	110.59
1	A	11	LEU	CA-C-N	6.46	134.07	122.13
1	A	11	LEU	C-N-CA	6.46	134.07	122.13
1	C	11	LEU	CA-C-N	6.43	134.03	122.13
1	C	11	LEU	C-N-CA	6.43	134.03	122.13
1	D	11	LEU	CA-C-N	6.43	134.02	122.13
1	D	11	LEU	C-N-CA	6.43	134.02	122.13
1	D	32	MET	N-CA-C	6.40	119.57	111.69
1	C	32	MET	N-CA-C	6.40	119.56	111.69
1	D	299	ILE	N-CA-C	-6.39	99.37	108.58
1	B	299	ILE	N-CA-C	-6.38	99.39	108.58
1	A	299	ILE	N-CA-C	-6.38	99.40	108.58
1	A	228	ASN	CA-C-O	-6.37	113.80	120.55
1	A	32	MET	N-CA-C	6.36	119.52	111.69
1	C	299	ILE	N-CA-C	-6.36	99.42	108.58
1	C	228	ASN	CA-C-O	-6.35	113.82	120.55
1	A	147	TRP	CA-C-N	6.33	129.01	120.65
1	A	147	TRP	C-N-CA	6.33	129.01	120.65
1	D	147	TRP	CA-C-N	6.33	129.00	120.65
1	D	147	TRP	C-N-CA	6.33	129.00	120.65
1	C	147	TRP	CA-C-N	6.33	129.00	120.65
1	C	147	TRP	C-N-CA	6.33	129.00	120.65
1	A	20	CYS	CA-C-N	6.32	134.73	122.03
1	A	20	CYS	C-N-CA	6.32	134.73	122.03
1	B	32	MET	N-CA-C	6.31	119.45	111.69
1	B	147	TRP	CA-C-N	6.31	128.98	120.65
1	B	147	TRP	C-N-CA	6.31	128.98	120.65
1	B	20	CYS	CA-C-N	6.31	134.71	122.03
1	B	20	CYS	C-N-CA	6.31	134.71	122.03
1	C	20	CYS	CA-C-N	6.31	134.71	122.03
1	C	20	CYS	C-N-CA	6.31	134.71	122.03
1	A	197	VAL	N-CA-C	-6.30	101.83	107.56
1	D	20	CYS	CA-C-N	6.30	134.69	122.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	20	CYS	C-N-CA	6.30	134.69	122.03
1	B	228	ASN	CA-C-O	-6.28	113.90	120.55
1	D	228	ASN	CA-C-O	-6.27	113.90	120.55
1	B	170	ARG	CG-CD-NE	6.23	125.70	112.00
1	D	197	VAL	N-CA-C	-6.22	101.89	107.56
1	B	288	LEU	N-CA-C	-6.22	100.35	109.18
1	B	197	VAL	N-CA-C	-6.21	101.91	107.56
1	C	197	VAL	N-CA-C	-6.21	101.91	107.56
1	D	170	ARG	CG-CD-NE	6.21	125.66	112.00
1	A	170	ARG	CG-CD-NE	6.20	125.64	112.00
1	A	288	LEU	N-CA-C	-6.20	100.38	109.18
1	C	170	ARG	CG-CD-NE	6.19	125.61	112.00
1	B	240	VAL	CB-CA-C	-6.16	104.11	111.81
1	D	288	LEU	N-CA-C	-6.16	100.44	109.18
1	A	154	VAL	N-CA-C	-6.15	100.77	109.63
1	B	154	VAL	N-CA-C	-6.15	100.78	109.63
1	D	240	VAL	CB-CA-C	-6.14	104.13	111.81
1	C	240	VAL	CB-CA-C	-6.14	104.14	111.81
1	A	240	VAL	CB-CA-C	-6.13	104.15	111.81
1	A	21	LYS	CB-CA-C	-6.13	98.93	110.51
1	C	154	VAL	N-CA-C	-6.12	100.81	109.63
1	D	154	VAL	N-CA-C	-6.12	100.82	109.63
1	C	288	LEU	N-CA-C	-6.12	100.49	109.18
1	D	21	LYS	CB-CA-C	-6.09	99.00	110.51
1	B	21	LYS	CB-CA-C	-6.08	99.02	110.51
1	A	311	GLU	N-CA-C	-6.07	103.99	111.33
1	C	21	LYS	CB-CA-C	-6.06	99.06	110.51
1	C	311	GLU	N-CA-C	-6.03	104.03	111.33
1	D	212	SER	CA-C-O	-6.00	114.02	120.92
1	B	311	GLU	N-CA-C	-5.98	104.09	111.33
1	A	190	GLY	N-CA-C	-5.98	104.17	111.35
1	D	311	GLU	N-CA-C	-5.98	104.09	111.33
1	A	73	THR	O-C-N	5.98	126.40	121.44
1	D	190	GLY	N-CA-C	-5.97	104.18	111.35
1	D	324	ASN	N-CA-C	-5.97	103.94	111.11
1	C	324	ASN	N-CA-C	-5.97	103.94	111.11
1	A	212	SER	CA-C-O	-5.96	114.06	120.92
1	A	324	ASN	N-CA-C	-5.96	103.96	111.11
1	C	212	SER	CA-C-O	-5.96	114.07	120.92
1	B	190	GLY	N-CA-C	-5.93	104.24	111.35
1	B	212	SER	CA-C-O	-5.92	114.11	120.92
1	C	190	GLY	N-CA-C	-5.92	104.25	111.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	142	LEU	CB-CA-C	5.90	120.70	110.79
1	B	324	ASN	N-CA-C	-5.89	104.04	111.11
1	D	243	MET	N-CA-C	5.88	120.56	111.56
1	A	243	MET	N-CA-C	5.88	120.55	111.56
1	C	243	MET	N-CA-C	5.87	120.55	111.56
1	B	142	LEU	CB-CA-C	5.87	120.66	110.79
1	D	73	THR	O-C-N	5.87	126.31	121.44
1	A	142	LEU	CB-CA-C	5.87	120.65	110.79
1	B	106	LEU	N-CA-C	-5.86	104.28	112.25
1	C	73	THR	O-C-N	5.86	126.30	121.44
1	D	142	LEU	CB-CA-C	5.85	120.62	110.79
1	A	106	LEU	N-CA-C	-5.84	104.30	112.25
1	B	73	THR	O-C-N	5.84	126.29	121.44
1	B	243	MET	N-CA-C	5.84	120.50	111.56
1	D	287	PHE	CA-CB-CG	5.83	119.64	113.80
1	B	222	ASN	CA-C-N	5.83	132.67	121.54
1	B	222	ASN	C-N-CA	5.83	132.67	121.54
1	A	222	ASN	CA-C-N	5.82	132.65	121.54
1	A	222	ASN	C-N-CA	5.82	132.65	121.54
1	C	287	PHE	CA-CB-CG	5.82	119.62	113.80
1	C	222	ASN	CA-C-N	5.81	132.64	121.54
1	C	222	ASN	C-N-CA	5.81	132.64	121.54
1	C	106	LEU	N-CA-C	-5.80	104.36	112.25
1	D	222	ASN	CA-C-N	5.80	132.63	121.54
1	D	222	ASN	C-N-CA	5.80	132.63	121.54
1	D	106	LEU	N-CA-C	-5.80	104.36	112.25
1	A	287	PHE	CA-CB-CG	5.80	119.60	113.80
1	B	51	ASP	CA-CB-CG	5.79	118.39	112.60
1	B	287	PHE	CA-CB-CG	5.77	119.57	113.80
1	D	291	PRO	CB-CA-C	5.76	117.84	111.56
1	B	224	GLN	CA-C-N	5.76	132.54	121.54
1	B	224	GLN	C-N-CA	5.76	132.54	121.54
1	B	291	PRO	CB-CA-C	5.76	117.84	111.56
1	C	224	GLN	CA-C-N	5.76	132.54	121.54
1	C	224	GLN	C-N-CA	5.76	132.54	121.54
1	A	291	PRO	CB-CA-C	5.76	117.83	111.56
1	C	228	ASN	O-C-N	5.75	128.22	122.12
1	D	182	THR	N-CA-C	-5.75	105.93	113.12
1	D	51	ASP	CA-CB-CG	5.74	118.34	112.60
1	D	285	GLU	CA-C-N	5.74	129.78	122.37
1	D	285	GLU	C-N-CA	5.74	129.78	122.37
1	C	291	PRO	CB-CA-C	5.74	117.82	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	182	THR	N-CA-C	-5.74	105.95	113.12
1	C	51	ASP	CA-CB-CG	5.74	118.34	112.60
1	A	51	ASP	CA-CB-CG	5.73	118.33	112.60
1	A	224	GLN	CA-C-N	5.73	132.48	121.54
1	A	224	GLN	C-N-CA	5.73	132.48	121.54
1	B	182	THR	N-CA-C	-5.73	105.96	113.12
1	D	224	GLN	CA-C-N	5.73	132.48	121.54
1	D	224	GLN	C-N-CA	5.73	132.48	121.54
1	B	285	GLU	CA-C-N	5.72	129.75	122.37
1	B	285	GLU	C-N-CA	5.72	129.75	122.37
1	C	34	CYS	CA-CB-SG	5.72	127.56	114.40
1	A	3	VAL	N-CA-C	-5.72	104.93	110.42
1	A	228	ASN	O-C-N	5.71	128.17	122.12
1	C	182	THR	N-CA-C	-5.71	105.98	113.12
1	A	285	GLU	CA-C-N	5.71	129.73	122.37
1	A	285	GLU	C-N-CA	5.71	129.73	122.37
1	C	285	GLU	CA-C-N	5.70	129.73	122.37
1	C	285	GLU	C-N-CA	5.70	129.73	122.37
1	A	34	CYS	CA-CB-SG	5.70	127.50	114.40
1	B	228	ASN	O-C-N	5.69	128.15	122.12
1	D	3	VAL	N-CA-C	-5.69	104.96	110.42
1	B	34	CYS	CA-CB-SG	5.69	127.48	114.40
1	D	34	CYS	CA-CB-SG	5.68	127.47	114.40
1	C	222	ASN	CA-CB-CG	5.67	118.27	112.60
1	C	3	VAL	N-CA-C	-5.67	104.98	110.42
1	D	14	GLU	CA-C-O	5.66	128.61	120.51
1	D	197	VAL	CB-CA-C	5.66	117.51	110.95
1	B	46	GLU	CG-CD-OE1	5.66	131.41	118.40
1	D	228	ASN	O-C-N	5.65	128.11	122.12
1	A	14	GLU	CA-C-O	5.64	128.58	120.51
1	B	3	VAL	N-CA-C	-5.64	105.00	110.42
1	D	46	GLU	CG-CD-OE1	5.64	131.37	118.40
1	A	46	GLU	CG-CD-OE1	5.63	131.35	118.40
1	B	222	ASN	CA-CB-CG	5.62	118.22	112.60
1	C	14	GLU	CA-C-O	5.62	128.54	120.51
1	C	46	GLU	CG-CD-OE1	5.62	131.32	118.40
1	A	240	VAL	O-C-N	5.61	127.72	121.94
1	B	14	GLU	CA-C-O	5.60	128.52	120.51
1	C	216	ALA	N-CA-C	-5.60	106.80	113.97
1	D	216	ALA	N-CA-C	-5.60	106.81	113.97
1	A	222	ASN	CA-CB-CG	5.59	118.19	112.60
1	A	197	VAL	CB-CA-C	5.59	117.43	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	320	ASP	CA-C-O	-5.58	115.16	120.90
1	D	222	ASN	CA-CB-CG	5.58	118.18	112.60
1	C	197	VAL	CB-CA-C	5.57	117.41	110.95
1	C	199	ILE	CB-CA-C	5.57	120.42	111.29
1	D	199	ILE	CB-CA-C	5.56	120.41	111.29
1	B	111	ARG	O-C-N	5.56	128.02	122.12
1	D	104	THR	CA-CB-CG2	5.55	119.94	110.50
1	B	197	VAL	CB-CA-C	5.55	117.39	110.95
1	B	199	ILE	CB-CA-C	5.55	120.39	111.29
1	A	216	ALA	N-CA-C	-5.55	106.87	113.97
1	C	240	VAL	O-C-N	5.55	127.65	121.94
1	A	199	ILE	CB-CA-C	5.54	120.38	111.29
1	B	216	ALA	N-CA-C	-5.54	106.88	113.97
1	C	23	THR	CA-C-N	-5.54	115.11	122.98
1	C	23	THR	C-N-CA	-5.54	115.11	122.98
1	B	241	LEU	CB-CA-C	5.53	119.57	110.88
1	A	104	THR	CA-CB-CG2	5.53	119.89	110.50
1	D	296	GLU	CB-CG-CD	5.52	121.98	112.60
1	B	63	ASP	N-CA-C	-5.52	105.18	111.14
1	B	104	THR	CA-CB-CG2	5.51	119.87	110.50
1	B	320	ASP	CA-C-O	-5.51	115.22	120.90
1	C	83	ASN	OD1-CG-ND2	5.51	128.12	122.60
1	D	320	ASP	CA-C-O	-5.51	115.22	120.90
1	C	212	SER	N-CA-C	-5.51	100.70	109.96
1	B	240	VAL	O-C-N	5.51	127.61	121.94
1	D	240	VAL	O-C-N	5.51	127.61	121.94
1	A	241	LEU	CB-CA-C	5.51	119.53	110.88
1	C	111	ARG	O-C-N	5.50	127.95	122.12
1	A	63	ASP	N-CA-C	-5.50	105.20	111.14
1	A	23	THR	CA-C-N	-5.50	115.17	122.98
1	A	23	THR	C-N-CA	-5.50	115.17	122.98
1	C	320	ASP	CA-C-O	-5.50	115.24	120.90
1	C	104	THR	CA-CB-CG2	5.49	119.84	110.50
1	A	83	ASN	OD1-CG-ND2	5.49	128.09	122.60
1	B	23	THR	CA-C-N	-5.49	115.19	122.98
1	B	23	THR	C-N-CA	-5.49	115.19	122.98
1	B	296	GLU	CB-CG-CD	5.49	121.93	112.60
1	D	83	ASN	OD1-CG-ND2	5.49	128.09	122.60
1	B	212	SER	N-CA-C	-5.49	100.74	109.96
1	A	212	SER	N-CA-C	-5.48	100.75	109.96
1	C	241	LEU	CB-CA-C	5.48	119.49	110.88
1	B	112	ASN	CA-CB-CG	-5.48	107.12	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	23	THR	CA-C-N	-5.48	115.20	122.98
1	D	23	THR	C-N-CA	-5.48	115.20	122.98
1	D	241	LEU	CB-CA-C	5.47	119.47	110.88
1	D	63	ASP	N-CA-C	-5.47	105.23	111.14
1	C	296	GLU	CB-CG-CD	5.47	121.89	112.60
1	A	296	GLU	CB-CG-CD	5.46	121.89	112.60
1	D	111	ARG	O-C-N	5.46	127.91	122.12
1	C	63	ASP	N-CA-C	-5.46	105.24	111.14
1	D	212	SER	N-CA-C	-5.46	100.79	109.96
1	D	260	ARG	CD-NE-CZ	5.45	132.03	124.40
1	D	139	VAL	N-CA-C	-5.44	104.65	110.36
1	A	111	ARG	O-C-N	5.44	127.89	122.12
1	A	227	LYS	N-CA-C	-5.44	104.75	111.33
1	C	139	VAL	N-CA-C	-5.43	104.66	110.36
1	C	260	ARG	CD-NE-CZ	5.43	132.00	124.40
1	B	83	ASN	OD1-CG-ND2	5.43	128.03	122.60
1	A	139	VAL	N-CA-C	-5.43	104.66	110.36
1	C	112	ASN	CA-CB-CG	-5.43	107.17	112.60
1	B	53	ASP	CA-C-N	5.42	131.89	121.54
1	B	53	ASP	C-N-CA	5.42	131.89	121.54
1	A	4	LYS	N-CA-CB	5.42	119.64	110.49
1	C	121	PRO	CA-N-CD	-5.41	104.43	112.00
1	D	4	LYS	N-CA-CB	5.41	119.63	110.49
1	D	53	ASP	CA-C-N	5.41	131.87	121.54
1	D	53	ASP	C-N-CA	5.41	131.87	121.54
1	D	112	ASN	CA-CB-CG	-5.41	107.19	112.60
1	C	4	LYS	N-CA-CB	5.40	119.62	110.49
1	A	154	VAL	O-C-N	5.40	128.35	122.63
1	C	303	VAL	CB-CA-C	5.40	118.43	110.77
1	B	4	LYS	N-CA-CB	5.39	119.61	110.49
1	D	132	ILE	N-CA-C	5.39	115.66	108.11
1	A	132	ILE	N-CA-C	5.39	115.66	108.11
1	A	112	ASN	CA-CB-CG	-5.39	107.21	112.60
1	A	121	PRO	CA-N-CD	-5.39	104.46	112.00
1	B	121	PRO	CA-N-CD	-5.39	104.46	112.00
1	C	53	ASP	CA-C-N	5.39	131.83	121.54
1	C	53	ASP	C-N-CA	5.39	131.83	121.54
1	D	203	VAL	N-CA-CB	-5.39	105.94	112.35
1	D	303	VAL	CB-CA-C	5.38	118.41	110.77
1	A	53	ASP	CA-C-N	5.38	131.82	121.54
1	A	53	ASP	C-N-CA	5.38	131.82	121.54
1	B	260	ARG	CD-NE-CZ	5.38	131.94	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	203	VAL	N-CA-CB	-5.38	105.95	112.35
1	A	260	ARG	CD-NE-CZ	5.38	131.93	124.40
1	B	139	VAL	N-CA-C	-5.38	104.71	110.36
1	A	303	VAL	CB-CA-C	5.37	118.40	110.77
1	D	227	LYS	N-CA-C	-5.37	104.84	111.33
1	D	121	PRO	CA-N-CD	-5.36	104.50	112.00
1	B	132	ILE	N-CA-C	5.36	115.61	108.11
1	B	227	LYS	N-CA-C	-5.36	104.85	111.33
1	C	154	VAL	O-C-N	5.36	128.31	122.63
1	C	307	MET	N-CA-C	-5.36	101.73	110.20
1	B	303	VAL	CB-CA-C	5.35	118.36	110.77
1	C	227	LYS	N-CA-C	-5.34	104.87	111.33
1	B	154	VAL	O-C-N	5.34	128.29	122.63
1	D	12	VAL	CB-CA-C	5.33	121.06	111.36
1	B	307	MET	N-CA-C	-5.33	101.78	110.20
1	A	203	VAL	N-CA-CB	-5.33	106.01	112.35
1	A	307	MET	N-CA-C	-5.32	101.79	110.20
1	B	205	VAL	CA-C-N	5.32	131.69	121.54
1	B	205	VAL	C-N-CA	5.32	131.69	121.54
1	C	132	ILE	N-CA-C	5.32	115.55	108.11
1	A	205	VAL	CA-C-N	5.31	131.69	121.54
1	A	205	VAL	C-N-CA	5.31	131.69	121.54
1	C	164	LEU	N-CA-CB	-5.31	101.51	110.49
1	B	286	VAL	O-C-N	5.31	129.00	122.95
1	B	164	LEU	N-CA-CB	-5.30	101.53	110.49
1	D	307	MET	N-CA-C	-5.30	101.82	110.20
1	A	164	LEU	N-CA-CB	-5.30	101.53	110.49
1	A	297	SER	N-CA-C	5.30	119.38	113.02
1	B	203	VAL	N-CA-CB	-5.30	106.05	112.35
1	D	164	LEU	N-CA-CB	-5.30	101.54	110.49
1	D	154	VAL	O-C-N	5.29	128.24	122.63
1	C	286	VAL	O-C-N	5.29	128.98	122.95
1	D	297	SER	N-CA-C	5.29	119.36	113.02
1	C	12	VAL	CB-CA-C	5.29	120.98	111.36
1	C	205	VAL	CA-C-N	5.29	131.64	121.54
1	C	205	VAL	C-N-CA	5.29	131.64	121.54
1	D	205	VAL	CA-C-N	5.29	131.63	121.54
1	D	205	VAL	C-N-CA	5.29	131.63	121.54
1	D	272	VAL	N-CA-CB	-5.28	104.48	112.35
1	C	297	SER	N-CA-C	5.28	119.36	113.02
1	B	12	VAL	CB-CA-C	5.28	120.97	111.36
1	B	268	ARG	N-CA-CB	5.28	118.47	109.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	272	VAL	N-CA-CB	-5.28	104.48	112.35
1	A	12	VAL	CB-CA-C	5.28	120.96	111.36
1	A	268	ARG	N-CA-CB	5.28	118.47	109.87
1	C	302	PHE	CA-CB-CG	5.27	119.07	113.80
1	A	272	VAL	N-CA-CB	-5.27	104.50	112.35
1	C	268	ARG	N-CA-CB	5.26	118.44	109.87
1	B	272	VAL	N-CA-CB	-5.26	104.52	112.35
1	D	112	ASN	CB-CA-C	5.26	120.05	110.11
1	D	302	PHE	CA-CB-CG	5.25	119.05	113.80
1	D	286	VAL	O-C-N	5.25	128.93	122.95
1	C	188	VAL	CA-C-O	-5.25	114.93	120.39
1	A	112	ASN	CB-CA-C	5.24	120.01	110.11
1	B	297	SER	N-CA-C	5.24	119.30	113.02
1	D	284	GLU	CA-CB-CG	5.24	124.57	114.10
1	A	302	PHE	CA-CB-CG	5.23	119.03	113.80
1	C	163	ASN	CA-CB-CG	-5.23	107.37	112.60
1	D	268	ARG	N-CA-CB	5.23	118.39	109.87
1	A	188	VAL	CA-C-O	-5.22	114.96	120.39
1	B	284	GLU	CA-CB-CG	5.22	124.55	114.10
1	A	284	GLU	CA-CB-CG	5.22	124.54	114.10
1	C	284	GLU	CA-CB-CG	5.22	124.55	114.10
1	C	112	ASN	CB-CA-C	5.22	119.97	110.11
1	B	112	ASN	CB-CA-C	5.22	119.97	110.11
1	A	286	VAL	O-C-N	5.21	128.89	122.95
1	B	2	THR	CB-CA-C	-5.21	100.71	109.83
1	B	184	CYS	N-CA-C	-5.21	101.39	109.72
1	A	163	ASN	CA-CB-CG	-5.20	107.40	112.60
1	A	170	ARG	NH1-CZ-NH2	-5.20	112.54	119.30
1	D	170	ARG	NH1-CZ-NH2	-5.20	112.53	119.30
1	B	302	PHE	CA-CB-CG	5.20	119.00	113.80
1	C	170	ARG	NH1-CZ-NH2	-5.20	112.54	119.30
1	B	163	ASN	CA-CB-CG	-5.18	107.42	112.60
1	D	163	ASN	CA-CB-CG	-5.18	107.42	112.60
1	C	272	VAL	CA-C-O	-5.18	116.56	121.64
1	B	170	ARG	NH1-CZ-NH2	-5.18	112.56	119.30
1	C	184	CYS	N-CA-C	-5.18	101.43	109.72
1	A	184	CYS	N-CA-C	-5.18	101.43	109.72
1	D	2	THR	CB-CA-C	-5.17	100.78	109.83
1	D	184	CYS	N-CA-C	-5.17	101.45	109.72
1	B	272	VAL	CA-C-O	-5.17	116.58	121.64
1	A	2	THR	CB-CA-C	-5.16	100.80	109.83
1	B	188	VAL	CA-C-O	-5.16	115.03	120.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	218	GLY	CA-C-O	5.16	129.54	120.57
1	C	2	THR	CB-CA-C	-5.15	100.82	109.83
1	B	157	VAL	N-CA-CB	-5.15	105.79	111.66
1	D	188	VAL	CA-C-O	-5.15	115.04	120.39
1	A	104	THR	CA-C-N	5.14	131.35	121.54
1	A	104	THR	C-N-CA	5.14	131.35	121.54
1	C	104	THR	CA-C-N	5.14	131.35	121.54
1	C	104	THR	C-N-CA	5.14	131.35	121.54
1	C	157	VAL	N-CA-CB	-5.13	105.81	111.66
1	B	104	THR	CA-C-N	5.13	131.33	121.54
1	B	104	THR	C-N-CA	5.13	131.33	121.54
1	B	218	GLY	CA-C-O	5.13	129.49	120.57
1	B	212	SER	CB-CA-C	5.12	117.99	109.53
1	D	216	ALA	CB-CA-C	5.12	117.68	109.07
1	A	157	VAL	N-CA-CB	-5.12	105.82	111.66
1	A	184	CYS	CA-C-O	-5.12	115.33	121.11
1	B	307	MET	CB-CA-C	5.12	118.17	109.53
1	A	272	VAL	CA-C-O	-5.11	116.63	121.64
1	D	218	GLY	CA-C-O	5.11	129.47	120.57
1	D	272	VAL	CA-C-O	-5.11	116.63	121.64
1	D	104	THR	CA-C-N	5.11	131.30	121.54
1	D	104	THR	C-N-CA	5.11	131.30	121.54
1	B	277	LYS	CA-C-O	-5.11	113.21	120.51
1	C	212	SER	CB-CA-C	5.11	117.96	109.53
1	D	184	CYS	CA-C-O	-5.11	115.34	121.11
1	C	307	MET	CB-CA-C	5.10	118.15	109.53
1	A	212	SER	CB-CA-C	5.10	117.95	109.53
1	A	218	GLY	CA-C-O	5.10	129.44	120.57
1	C	184	CYS	CA-C-O	-5.09	115.35	121.11
1	A	216	ALA	CB-CA-C	5.09	117.62	109.07
1	A	109	LEU	N-CA-C	5.09	119.13	111.96
1	D	109	LEU	N-CA-C	5.08	119.12	111.96
1	C	277	LYS	CA-C-O	-5.08	113.25	120.51
1	D	212	SER	CB-CA-C	5.08	117.91	109.53
1	D	157	VAL	N-CA-CB	-5.07	105.88	111.66
1	C	16	LYS	CA-CB-CG	5.07	124.24	114.10
1	D	307	MET	CB-CA-C	5.07	118.09	109.53
1	B	284	GLU	CA-C-N	5.07	131.22	121.54
1	B	284	GLU	C-N-CA	5.07	131.22	121.54
1	B	16	LYS	CA-CB-CG	5.06	124.23	114.10
1	B	109	LEU	N-CA-C	5.06	119.10	111.96
1	D	16	LYS	CA-CB-CG	5.06	124.23	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	216	ALA	CB-CA-C	5.06	117.57	109.07
1	C	216	ALA	CB-CA-C	5.06	117.57	109.07
1	B	184	CYS	CA-C-O	-5.06	115.39	121.11
1	C	47	LEU	CB-CA-C	5.06	118.26	110.62
1	A	284	GLU	CA-C-N	5.06	131.20	121.54
1	A	284	GLU	C-N-CA	5.06	131.20	121.54
1	D	284	GLU	CA-C-N	5.06	131.20	121.54
1	D	284	GLU	C-N-CA	5.06	131.20	121.54
1	A	16	LYS	CA-CB-CG	5.05	124.21	114.10
1	C	109	LEU	N-CA-C	5.05	119.08	111.96
1	C	284	GLU	CA-C-N	5.05	131.19	121.54
1	C	284	GLU	C-N-CA	5.05	131.19	121.54
1	D	47	LEU	CB-CA-C	5.05	118.25	110.62
1	A	307	MET	CB-CA-C	5.04	118.05	109.53
1	A	242	ASP	CA-CB-CG	5.04	117.64	112.60
1	B	47	LEU	CB-CA-C	5.04	118.23	110.62
1	D	277	LYS	CA-C-O	-5.04	113.31	120.51
1	C	195	SER	N-CA-C	-5.02	105.64	112.26
1	C	242	ASP	CA-CB-CG	5.02	117.62	112.60
1	A	277	LYS	CA-C-O	-5.02	113.33	120.51
1	C	110	GLN	N-CA-C	-5.01	105.94	111.71
1	A	110	GLN	N-CA-C	-5.01	105.95	111.71
1	D	242	ASP	CA-CB-CG	5.00	117.60	112.60

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	136	THR	Mainchain
1	A	181	PRO	Mainchain
1	A	311	GLU	Mainchain
1	B	136	THR	Mainchain
1	B	181	PRO	Mainchain
1	B	311	GLU	Mainchain
1	C	136	THR	Mainchain
1	C	181	PRO	Mainchain
1	C	311	GLU	Mainchain
1	D	136	THR	Mainchain
1	D	181	PRO	Mainchain
1	D	311	GLU	Mainchain

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	2515	0	2613	697	0
1	B	2515	0	2613	691	0
1	C	2515	0	2613	695	39
1	D	2515	0	2613	699	35
2	A	29	0	0	1	4
2	D	2	0	0	3	0
All	All	10091	0	10452	2218	39

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 108.

All (2218) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:SER:HB2	1:D:208:VAL:CG1	1.20	1.63
1:A:208:VAL:CG1	1:B:212:SER:HB2	1.20	1.61
1:C:208:VAL:CG1	1:D:212:SER:HB2	1.20	1.60
1:A:212:SER:HB2	1:B:208:VAL:CG1	1.20	1.60
1:A:210:LEU:CB	1:B:202:GLY:HA3	1.59	1.32
1:A:202:GLY:HA3	1:B:210:LEU:CB	1.59	1.30
1:A:201:SER:O	1:B:209:THR:HB	1.21	1.30
1:A:208:VAL:HG13	1:B:208:VAL:CA	1.61	1.30
1:C:208:VAL:HG13	1:D:208:VAL:CA	1.61	1.29
1:C:210:LEU:CB	1:D:202:GLY:HA3	1.59	1.29
1:C:202:GLY:HA3	1:D:210:LEU:CB	1.59	1.29
1:A:210:LEU:HB2	1:B:202:GLY:CA	1.62	1.28
1:C:208:VAL:CA	1:D:208:VAL:HG13	1.61	1.28
1:C:208:VAL:HA	1:D:208:VAL:CG1	1.63	1.28
1:A:202:GLY:CA	1:B:210:LEU:HB2	1.62	1.28
1:A:209:THR:HB	1:B:201:SER:O	1.21	1.28
1:C:208:VAL:CG1	1:D:208:VAL:HA	1.63	1.28
1:A:208:VAL:CG1	1:B:208:VAL:HA	1.63	1.27
1:A:208:VAL:CA	1:B:208:VAL:HG13	1.62	1.27
1:A:208:VAL:CG1	1:B:212:SER:CB	2.13	1.26
1:C:201:SER:O	1:D:209:THR:HB	1.21	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:202:GLY:CA	1:D:210:LEU:HB2	1.62	1.26
1:C:210:LEU:HB2	1:D:202:GLY:CA	1.62	1.26
1:A:208:VAL:HA	1:B:208:VAL:CG1	1.64	1.26
1:A:212:SER:CB	1:B:208:VAL:CG1	2.14	1.25
1:B:17:LEU:HD21	1:C:297:SER:CB	1.65	1.25
1:B:297:SER:CB	1:C:17:LEU:HD21	1.65	1.25
1:A:17:LEU:HD21	1:D:297:SER:CB	1.65	1.25
1:C:208:VAL:CG1	1:D:212:SER:CB	2.14	1.25
1:C:212:SER:CB	1:D:208:VAL:CG1	2.13	1.25
1:A:297:SER:CB	1:D:17:LEU:HD21	1.65	1.25
1:C:209:THR:HB	1:D:201:SER:O	1.21	1.24
1:A:12:VAL:HB	1:A:13:PRO:HD3	1.25	1.18
1:C:212:SER:CB	1:D:208:VAL:HG12	1.74	1.18
1:A:212:SER:CB	1:B:208:VAL:HG12	1.74	1.17
1:C:210:LEU:HA	1:D:306:ASN:HD21	1.08	1.17
1:D:12:VAL:HB	1:D:13:PRO:HD3	1.25	1.16
1:B:17:LEU:HD21	1:C:297:SER:HB3	1.20	1.15
1:C:306:ASN:HD21	1:D:210:LEU:HA	1.08	1.15
1:C:208:VAL:HG12	1:D:212:SER:CB	1.74	1.14
1:B:12:VAL:HB	1:B:13:PRO:HD3	1.25	1.13
1:A:177:LEU:CD2	1:C:4:LYS:HZ3	1.61	1.13
1:A:208:VAL:HG12	1:B:212:SER:CB	1.74	1.13
1:B:297:SER:HB3	1:C:17:LEU:HD21	1.20	1.13
1:C:212:SER:HB2	1:D:208:VAL:HG11	1.29	1.12
1:A:297:SER:HB3	1:D:17:LEU:CD2	1.80	1.12
1:B:297:SER:HB3	1:C:17:LEU:CD2	1.80	1.11
1:A:17:LEU:HD21	1:D:297:SER:HB3	1.19	1.11
1:A:17:LEU:CD2	1:D:297:SER:HB3	1.80	1.10
1:B:17:LEU:CD2	1:C:297:SER:HB3	1.80	1.10
1:C:12:VAL:HB	1:C:13:PRO:HD3	1.25	1.10
1:A:306:ASN:HD21	1:B:210:LEU:HA	1.08	1.10
1:B:177:LEU:CD2	1:D:4:LYS:HZ3	1.63	1.10
1:A:297:SER:HB3	1:D:17:LEU:HD21	1.19	1.10
1:C:208:VAL:HG11	1:D:212:SER:HB2	1.29	1.08
1:A:4:LYS:HZ3	1:C:177:LEU:HD23	1.16	1.07
1:A:210:LEU:HA	1:B:306:ASN:HD21	1.08	1.07
1:A:212:SER:HB2	1:B:208:VAL:HG11	1.29	1.07
1:B:4:LYS:HZ3	1:D:177:LEU:HD23	1.14	1.07
1:B:4:LYS:HZ3	1:D:177:LEU:CD2	1.67	1.07
1:A:208:VAL:HG11	1:B:212:SER:HB2	1.29	1.06
1:B:177:LEU:HD23	1:D:4:LYS:HZ3	1.13	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:LEU:HD23	1:C:4:LYS:HZ3	1.13	1.06
1:B:279:PHE:CZ	1:C:9:GLN:NE2	2.28	1.02
1:A:4:LYS:HZ3	1:C:177:LEU:CD2	1.73	1.01
1:A:9:GLN:NE2	1:D:279:PHE:CZ	2.28	1.01
1:A:279:PHE:CZ	1:D:9:GLN:NE2	2.28	1.01
1:B:9:GLN:NE2	1:C:279:PHE:CZ	2.28	1.01
1:C:137:ASN:HA	1:C:139:VAL:HG13	1.43	1.00
1:D:137:ASN:HA	1:D:139:VAL:HG13	1.43	1.00
1:C:208:VAL:CG1	1:D:209:THR:H	1.75	1.00
1:C:208:VAL:HG13	1:D:209:THR:N	1.76	1.00
1:C:209:THR:H	1:D:208:VAL:CG1	1.76	0.99
1:C:209:THR:N	1:D:208:VAL:HG13	1.77	0.99
1:A:208:VAL:CG1	1:B:209:THR:H	1.75	0.99
1:A:209:THR:N	1:B:208:VAL:HG13	1.77	0.98
1:C:36:ILE:HA	1:C:39:LEU:HD12	1.45	0.98
1:A:11:LEU:HG	1:D:302:PHE:CZ	1.99	0.98
1:A:302:PHE:CZ	1:D:11:LEU:HG	1.99	0.98
1:B:137:ASN:HA	1:B:139:VAL:HG13	1.43	0.98
1:A:209:THR:H	1:B:208:VAL:CG1	1.75	0.97
1:A:208:VAL:HG13	1:B:209:THR:N	1.77	0.97
1:A:279:PHE:HZ	1:D:9:GLN:HE21	1.11	0.97
1:B:302:PHE:CZ	1:C:11:LEU:HG	1.99	0.97
1:D:172:LEU:HD22	1:D:232:GLN:HE21	1.29	0.97
1:B:11:LEU:HG	1:C:302:PHE:CZ	1.99	0.97
1:C:208:VAL:HG13	1:D:208:VAL:HA	0.99	0.97
1:A:208:VAL:HG13	1:B:208:VAL:HA	0.99	0.97
1:A:208:VAL:HA	1:B:208:VAL:HG13	0.99	0.97
1:A:177:LEU:CD2	1:C:4:LYS:NZ	2.28	0.96
1:C:172:LEU:HD22	1:C:232:GLN:HE21	1.28	0.96
1:C:208:VAL:HA	1:D:208:VAL:HG13	0.99	0.96
1:C:208:VAL:HG23	1:D:204:ASN:CG	1.90	0.96
1:A:4:LYS:NZ	1:C:177:LEU:CD2	2.28	0.96
1:A:172:LEU:HD22	1:A:232:GLN:HE21	1.29	0.96
1:A:204:ASN:CG	1:B:208:VAL:HG23	1.90	0.96
1:C:209:THR:CB	1:D:201:SER:O	2.13	0.96
1:A:209:THR:CB	1:B:201:SER:O	2.13	0.96
1:A:36:ILE:HA	1:A:39:LEU:HD12	1.46	0.96
1:A:120:VAL:HG21	1:A:146:VAL:HG12	1.46	0.96
1:A:137:ASN:HA	1:A:139:VAL:HG13	1.43	0.96
1:C:208:VAL:CB	1:D:208:VAL:HA	1.96	0.96
1:C:227:LYS:HE2	1:C:231:LYS:HZ1	1.28	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:208:VAL:HA	1:D:208:VAL:CB	1.96	0.96
1:C:204:ASN:CG	1:D:208:VAL:HG23	1.90	0.95
1:A:177:LEU:HD23	1:C:4:LYS:NZ	1.80	0.95
1:B:4:LYS:NZ	1:D:177:LEU:HD23	1.80	0.95
1:A:208:VAL:CB	1:B:208:VAL:HA	1.96	0.95
1:A:4:LYS:NZ	1:C:177:LEU:HD23	1.80	0.95
1:A:208:VAL:HA	1:B:208:VAL:CB	1.96	0.95
1:C:201:SER:O	1:D:209:THR:CB	2.13	0.95
1:B:177:LEU:HD23	1:D:4:LYS:NZ	1.80	0.95
1:A:208:VAL:HG23	1:B:204:ASN:CG	1.90	0.95
1:A:301:ASP:OD2	1:D:8:ILE:HG23	1.66	0.95
1:B:4:LYS:NZ	1:D:177:LEU:CD2	2.28	0.95
1:A:201:SER:O	1:B:209:THR:CB	2.13	0.95
1:C:120:VAL:HG21	1:C:146:VAL:HG12	1.46	0.95
1:D:19:ARG:CG	2:D:409:HOH:O	2.13	0.95
1:A:104:THR:HG22	1:A:238:TYR:HE1	1.32	0.94
1:C:189:LEU:HD21	1:C:199:ILE:HD13	1.49	0.94
1:D:189:LEU:HD21	1:D:199:ILE:HD13	1.49	0.94
1:A:189:LEU:HD21	1:A:199:ILE:HD13	1.49	0.94
1:B:8:ILE:HG23	1:C:301:ASP:OD2	1.67	0.94
1:B:120:VAL:HG21	1:B:146:VAL:HG12	1.46	0.94
1:B:177:LEU:CD2	1:D:4:LYS:NZ	2.28	0.94
1:D:36:ILE:HA	1:D:39:LEU:HD12	1.46	0.94
1:B:189:LEU:HD21	1:B:199:ILE:HD13	1.49	0.94
1:B:301:ASP:OD2	1:C:8:ILE:HG23	1.66	0.94
1:A:8:ILE:HG23	1:D:301:ASP:OD2	1.66	0.94
1:D:120:VAL:HG21	1:D:146:VAL:HG12	1.46	0.94
1:B:36:ILE:HA	1:B:39:LEU:HD12	1.46	0.94
1:B:104:THR:HG22	1:B:238:TYR:HE1	1.33	0.93
1:B:172:LEU:HD22	1:B:232:GLN:HE21	1.29	0.93
1:B:302:PHE:HD1	1:C:9:GLN:HG2	1.33	0.93
1:C:104:THR:HG22	1:C:238:TYR:HE1	1.32	0.92
1:B:99:MET:HE3	1:B:246:TYR:HB2	1.52	0.92
1:D:104:THR:HG22	1:D:238:TYR:HE1	1.32	0.92
1:B:9:GLN:HE21	1:C:279:PHE:HZ	1.11	0.92
1:A:9:GLN:HG2	1:D:302:PHE:HD1	1.33	0.92
1:B:279:PHE:HZ	1:C:9:GLN:HE21	1.11	0.92
1:A:302:PHE:HD1	1:D:9:GLN:HG2	1.33	0.91
1:A:9:GLN:HE21	1:D:279:PHE:HZ	1.11	0.91
1:B:9:GLN:HG2	1:C:302:PHE:HD1	1.33	0.91
1:D:20:CYS:HA	1:D:89:LYS:HD3	1.52	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:CYS:HA	1:C:89:LYS:HD3	1.52	0.91
1:A:17:LEU:CG	1:D:297:SER:HB3	2.01	0.91
1:B:17:LEU:CG	1:C:297:SER:HB3	2.01	0.91
1:B:22:ILE:HD13	1:B:44:ALA:HB2	1.53	0.90
1:C:99:MET:HE3	1:C:246:TYR:HB2	1.52	0.90
1:B:227:LYS:HE2	1:B:231:LYS:HZ1	1.36	0.90
1:B:297:SER:HB3	1:C:17:LEU:CG	2.01	0.90
1:A:297:SER:HB3	1:D:17:LEU:CG	2.01	0.90
1:D:288:LEU:HD21	1:D:315:LEU:HD21	1.54	0.89
1:C:22:ILE:HD13	1:C:44:ALA:HB2	1.53	0.89
1:D:99:MET:HE3	1:D:246:TYR:HB2	1.52	0.89
1:A:20:CYS:HA	1:A:89:LYS:HD3	1.52	0.89
1:A:99:MET:HE3	1:A:246:TYR:HB2	1.52	0.89
1:C:204:ASN:OD1	1:D:204:ASN:OD1	1.91	0.89
1:A:208:VAL:C	1:B:208:VAL:HG13	1.98	0.89
1:A:302:PHE:CD1	1:D:9:GLN:HG2	2.09	0.88
1:B:288:LEU:HD21	1:B:315:LEU:HD21	1.54	0.88
1:C:208:VAL:HG13	1:D:208:VAL:C	1.98	0.88
1:A:208:VAL:HG13	1:B:208:VAL:C	1.98	0.88
1:C:208:VAL:C	1:D:208:VAL:HG13	1.98	0.88
1:A:269:VAL:HG12	1:B:183:SER:OG	1.74	0.88
1:C:264:LYS:HB2	1:C:266:LEU:HD13	1.56	0.88
1:D:22:ILE:HD13	1:D:44:ALA:HB2	1.53	0.88
1:A:22:ILE:HD13	1:A:44:ALA:HB2	1.53	0.88
1:A:211:LYS:CE	1:C:7:LEU:HG	2.04	0.88
1:B:20:CYS:HA	1:B:89:LYS:HD3	1.52	0.88
1:B:302:PHE:CD1	1:C:9:GLN:HG2	2.09	0.88
1:A:183:SER:OG	1:B:269:VAL:HG12	1.74	0.88
1:B:211:LYS:CE	1:D:7:LEU:HG	2.04	0.87
1:C:269:VAL:HG12	1:D:183:SER:OG	1.74	0.87
1:A:212:SER:HA	1:B:208:VAL:HB	1.56	0.87
1:B:264:LYS:HB2	1:B:266:LEU:HD13	1.56	0.87
1:C:288:LEU:HD21	1:C:315:LEU:HD21	1.54	0.87
1:A:9:GLN:HG2	1:D:302:PHE:CD1	2.09	0.87
1:A:204:ASN:OD1	1:B:204:ASN:OD1	1.91	0.87
1:A:7:LEU:HG	1:C:211:LYS:CE	2.04	0.87
1:A:217:ILE:C	1:A:219:THR:H	1.78	0.87
1:A:288:LEU:HD21	1:A:315:LEU:HD21	1.54	0.87
1:A:208:VAL:HB	1:B:212:SER:HA	1.56	0.87
1:C:208:VAL:HB	1:D:212:SER:HA	1.56	0.87
1:A:210:LEU:CA	1:B:306:ASN:HD21	1.88	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:LEU:HG	1:D:211:LYS:CE	2.04	0.87
1:C:183:SER:OG	1:D:269:VAL:HG12	1.74	0.87
1:C:146:VAL:HA	1:C:149:ILE:HG22	1.57	0.86
1:C:217:ILE:C	1:C:219:THR:H	1.78	0.86
1:B:9:GLN:HG2	1:C:302:PHE:CD1	2.09	0.86
1:B:94:THR:HG22	1:B:135:VAL:HB	1.58	0.86
1:B:217:ILE:C	1:B:219:THR:H	1.78	0.86
1:D:264:LYS:HB2	1:D:266:LEU:HD13	1.56	0.86
1:A:306:ASN:HD21	1:B:210:LEU:CA	1.88	0.86
1:C:212:SER:HA	1:D:208:VAL:HB	1.56	0.86
1:D:206:ALA:HB3	1:D:211:LYS:HB2	1.58	0.86
1:C:206:ALA:HB3	1:C:211:LYS:HB2	1.58	0.86
1:A:12:VAL:HB	1:A:13:PRO:CD	2.07	0.85
1:A:264:LYS:HB2	1:A:266:LEU:HD13	1.56	0.85
1:C:306:ASN:ND2	1:D:210:LEU:HA	1.90	0.85
1:C:210:LEU:CA	1:D:306:ASN:HD21	1.88	0.85
1:A:208:VAL:CG2	1:B:204:ASN:CG	2.50	0.85
1:A:94:THR:HG22	1:A:135:VAL:HB	1.57	0.85
1:A:146:VAL:HA	1:A:149:ILE:HG22	1.57	0.85
1:A:211:LYS:CD	1:C:7:LEU:HG	2.07	0.85
1:B:12:VAL:HB	1:B:13:PRO:CD	2.06	0.85
1:B:206:ALA:HB3	1:B:211:LYS:HB2	1.58	0.85
1:B:146:VAL:HA	1:B:149:ILE:HG22	1.57	0.85
1:C:210:LEU:HA	1:D:306:ASN:ND2	1.90	0.85
1:B:211:LYS:CD	1:D:7:LEU:HG	2.07	0.85
1:D:146:VAL:HA	1:D:149:ILE:HG22	1.57	0.85
1:A:212:SER:HB2	1:B:208:VAL:HG12	0.85	0.85
1:D:217:ILE:C	1:D:219:THR:H	1.78	0.85
1:C:208:VAL:CG2	1:D:204:ASN:CG	2.50	0.85
1:A:210:LEU:HA	1:B:306:ASN:ND2	1.90	0.84
1:D:260:ARG:NH1	1:D:268:ARG:HH12	1.75	0.84
1:C:306:ASN:HD21	1:D:210:LEU:CA	1.88	0.84
1:D:94:THR:HG22	1:D:135:VAL:HB	1.58	0.84
1:C:204:ASN:CG	1:D:208:VAL:CG2	2.50	0.84
1:A:208:VAL:HG13	1:B:209:THR:H	1.37	0.84
1:C:188:VAL:HA	1:C:198:PRO:HA	1.59	0.84
1:A:260:ARG:NH1	1:A:268:ARG:HH12	1.75	0.84
1:D:227:LYS:HE2	1:D:231:LYS:HZ1	1.42	0.84
1:A:7:LEU:HG	1:C:211:LYS:CD	2.07	0.84
1:C:260:ARG:NH1	1:C:268:ARG:HH12	1.75	0.84
1:A:204:ASN:CG	1:B:208:VAL:CG2	2.50	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:LEU:HD21	1:C:297:SER:OG	1.77	0.84
1:C:208:VAL:HG12	1:D:212:SER:HB2	0.85	0.84
1:A:206:ALA:HB3	1:A:211:LYS:HB2	1.58	0.83
1:C:94:THR:HG22	1:C:135:VAL:HB	1.58	0.83
1:A:208:VAL:HG11	1:B:212:SER:CB	1.94	0.83
1:A:208:VAL:HG12	1:B:212:SER:HB2	0.85	0.83
1:C:212:SER:HB2	1:D:208:VAL:HG12	0.84	0.83
1:D:41:LYS:HB3	1:D:43:LEU:HD13	1.60	0.83
1:A:17:LEU:HD21	1:D:297:SER:OG	1.77	0.83
1:A:209:THR:H	1:B:208:VAL:HG13	1.37	0.83
1:C:120:VAL:HG22	1:C:121:PRO:HD2	1.61	0.83
1:A:211:LYS:HD3	1:C:7:LEU:HG	1.61	0.83
1:A:306:ASN:ND2	1:B:210:LEU:HA	1.90	0.83
1:B:7:LEU:HG	1:D:211:LYS:CD	2.07	0.83
1:A:7:LEU:HG	1:C:211:LYS:HD3	1.60	0.83
1:C:202:GLY:HA2	1:D:208:VAL:O	1.79	0.83
1:A:297:SER:OG	1:D:17:LEU:HD21	1.77	0.83
1:B:7:LEU:HG	1:D:211:LYS:HD3	1.60	0.83
1:C:121:PRO:HA	1:C:124:ILE:HG23	1.60	0.83
1:B:188:VAL:HA	1:B:198:PRO:HA	1.59	0.83
1:C:208:VAL:O	1:D:202:GLY:HA2	1.79	0.83
1:A:120:VAL:HG22	1:A:121:PRO:HD2	1.60	0.82
1:B:211:LYS:HD3	1:D:7:LEU:HG	1.61	0.82
1:B:260:ARG:NH1	1:B:268:ARG:HH12	1.75	0.82
1:B:297:SER:OG	1:C:17:LEU:HD21	1.77	0.82
1:D:188:VAL:HA	1:D:198:PRO:HA	1.59	0.82
1:D:121:PRO:HA	1:D:124:ILE:HG23	1.60	0.82
1:A:188:VAL:HA	1:A:198:PRO:HA	1.59	0.82
1:C:12:VAL:HB	1:C:13:PRO:CD	2.07	0.82
1:D:12:VAL:HB	1:D:13:PRO:CD	2.07	0.82
1:D:120:VAL:HG22	1:D:121:PRO:HD2	1.61	0.82
1:D:137:ASN:C	1:D:139:VAL:H	1.87	0.82
1:D:227:LYS:HE2	1:D:231:LYS:NZ	1.95	0.82
1:C:208:VAL:HG11	1:D:212:SER:CB	1.94	0.82
1:A:41:LYS:HB3	1:A:43:LEU:HD13	1.60	0.81
1:B:177:LEU:HD23	1:D:4:LYS:CE	2.10	0.81
1:A:121:PRO:HA	1:A:124:ILE:HG23	1.60	0.81
1:B:41:LYS:HB3	1:B:43:LEU:HD13	1.60	0.81
1:A:202:GLY:HA2	1:B:208:VAL:O	1.79	0.81
1:A:227:LYS:HE2	1:A:231:LYS:NZ	1.95	0.81
1:A:6:GLN:NE2	1:C:216:ALA:HB1	1.96	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:PRO:HA	1:B:124:ILE:HG23	1.60	0.81
1:B:6:GLN:NE2	1:D:216:ALA:HB1	1.96	0.81
1:C:227:LYS:HE2	1:C:231:LYS:NZ	1.95	0.81
1:A:208:VAL:O	1:B:202:GLY:HA2	1.79	0.81
1:B:4:LYS:CE	1:D:177:LEU:HD23	2.11	0.81
1:A:137:ASN:C	1:A:139:VAL:H	1.87	0.81
1:B:137:ASN:C	1:B:139:VAL:H	1.87	0.81
1:C:204:ASN:HD22	1:C:204:ASN:H	1.27	0.81
1:D:204:ASN:H	1:D:204:ASN:HD22	1.28	0.81
1:A:191:GLU:HB3	1:A:195:SER:HB2	1.63	0.81
1:A:204:ASN:H	1:A:204:ASN:HD22	1.28	0.81
1:B:216:ALA:HB1	1:D:6:GLN:NE2	1.96	0.81
1:D:191:GLU:HB3	1:D:195:SER:HB2	1.63	0.81
1:A:4:LYS:CE	1:C:177:LEU:HD23	2.11	0.80
1:A:177:LEU:HD23	1:C:4:LYS:CE	2.11	0.80
1:C:210:LEU:HB2	1:D:202:GLY:HA3	0.83	0.80
1:C:208:VAL:HG21	1:D:211:LYS:O	1.81	0.80
1:D:19:ARG:HG3	2:D:409:HOH:O	1.74	0.80
1:C:260:ARG:HD2	1:C:268:ARG:NH2	1.96	0.80
1:A:49:LEU:HD12	1:A:78:PHE:HB2	1.62	0.80
1:C:41:LYS:HB3	1:C:43:LEU:HD13	1.60	0.80
1:C:191:GLU:HB3	1:C:195:SER:HB2	1.63	0.80
1:B:49:LEU:HD12	1:B:78:PHE:HB2	1.62	0.80
1:C:49:LEU:HD12	1:C:78:PHE:HB2	1.62	0.80
1:C:209:THR:H	1:D:208:VAL:HG13	1.37	0.80
1:C:211:LYS:O	1:D:208:VAL:HG21	1.81	0.80
1:A:177:LEU:CD2	1:C:4:LYS:HE2	2.12	0.80
1:B:120:VAL:HG22	1:B:121:PRO:HD2	1.60	0.80
1:B:191:GLU:HB3	1:B:195:SER:HB2	1.63	0.80
1:C:137:ASN:C	1:C:139:VAL:H	1.87	0.80
1:A:260:ARG:HD2	1:A:268:ARG:NH2	1.97	0.80
1:C:208:VAL:CB	1:D:212:SER:HB2	2.12	0.80
1:C:212:SER:HB2	1:D:208:VAL:CB	2.12	0.80
1:A:4:LYS:HE2	1:C:177:LEU:CD2	2.12	0.80
1:A:216:ALA:HB1	1:C:6:GLN:NE2	1.95	0.80
1:B:227:LYS:HE2	1:B:231:LYS:NZ	1.95	0.80
1:B:177:LEU:CD2	1:D:4:LYS:HE2	2.12	0.80
1:B:181:PRO:O	1:D:69:LEU:HD13	1.82	0.80
1:A:69:LEU:CD1	1:C:181:PRO:O	2.31	0.79
1:A:181:PRO:O	1:C:69:LEU:CD1	2.30	0.79
1:B:260:ARG:HD2	1:B:268:ARG:NH2	1.97	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:PRO:O	1:C:69:LEU:HD13	1.82	0.79
1:C:212:SER:CB	1:D:208:VAL:HG11	1.94	0.79
1:A:69:LEU:HD13	1:C:181:PRO:O	1.83	0.79
1:A:208:VAL:HG21	1:B:211:LYS:O	1.81	0.79
1:B:4:LYS:HE2	1:D:177:LEU:CD2	2.12	0.79
1:C:46:GLU:HB2	1:C:75:LYS:HE3	1.65	0.79
1:D:49:LEU:HD12	1:D:78:PHE:HB2	1.62	0.79
1:D:260:ARG:HD2	1:D:268:ARG:NH2	1.97	0.79
1:A:208:VAL:CB	1:B:212:SER:HB2	2.12	0.79
1:B:69:LEU:CD1	1:D:181:PRO:O	2.31	0.79
1:D:246:TYR:HE1	1:D:248:SER:HB3	1.48	0.79
1:B:46:GLU:HB2	1:B:75:LYS:HE3	1.65	0.79
1:B:181:PRO:O	1:D:69:LEU:CD1	2.31	0.79
1:C:202:GLY:HA3	1:D:210:LEU:HB2	0.83	0.79
1:A:46:GLU:HB2	1:A:75:LYS:HE3	1.65	0.79
1:A:246:TYR:HE1	1:A:248:SER:HB3	1.48	0.78
1:A:211:LYS:O	1:B:208:VAL:HG21	1.81	0.78
1:B:134:VAL:HG21	1:B:146:VAL:HG21	1.65	0.78
1:B:69:LEU:HD13	1:D:181:PRO:O	1.82	0.78
1:C:246:TYR:HE1	1:C:248:SER:HB3	1.48	0.78
1:C:214:ASN:O	1:C:217:ILE:HB	1.82	0.78
1:B:214:ASN:O	1:B:217:ILE:HB	1.83	0.78
1:D:46:GLU:HB2	1:D:75:LYS:HE3	1.65	0.78
1:B:246:TYR:HE1	1:B:248:SER:HB3	1.48	0.78
1:D:44:ALA:O	1:D:73:THR:HB	1.84	0.78
1:A:212:SER:HB2	1:B:208:VAL:CB	2.12	0.78
1:B:158:ILE:HG12	1:B:299:ILE:HD11	1.66	0.78
1:A:44:ALA:O	1:A:73:THR:HB	1.84	0.77
1:A:134:VAL:HG21	1:A:146:VAL:HG21	1.66	0.77
1:C:44:ALA:O	1:C:73:THR:HB	1.84	0.77
1:A:210:LEU:HB2	1:B:202:GLY:HA3	0.83	0.77
1:C:134:VAL:HG21	1:C:146:VAL:HG21	1.66	0.77
1:A:214:ASN:O	1:A:217:ILE:HB	1.83	0.77
1:D:158:ILE:HG12	1:D:299:ILE:HD11	1.66	0.77
1:D:214:ASN:O	1:D:217:ILE:HB	1.83	0.77
1:B:204:ASN:HD22	1:B:204:ASN:H	1.28	0.77
1:B:44:ALA:O	1:B:73:THR:HB	1.84	0.77
1:A:172:LEU:HD22	1:A:232:GLN:NE2	2.00	0.77
1:A:212:SER:CB	1:B:208:VAL:HG11	1.94	0.77
1:A:246:TYR:CE1	1:A:248:SER:HB3	2.20	0.77
1:B:4:LYS:CE	1:D:177:LEU:CD2	2.63	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:VAL:CG1	1:B:209:THR:N	2.43	0.77
1:B:177:LEU:CD2	1:D:4:LYS:CE	2.63	0.77
1:C:172:LEU:HD22	1:C:232:GLN:NE2	2.00	0.77
1:B:246:TYR:CE1	1:B:248:SER:HB3	2.20	0.76
1:C:246:TYR:CE1	1:C:248:SER:HB3	2.20	0.76
1:A:4:LYS:CE	1:C:177:LEU:CD2	2.63	0.76
1:D:246:TYR:CE1	1:D:248:SER:HB3	2.20	0.76
1:A:227:LYS:HE2	1:A:231:LYS:HZ1	1.50	0.76
1:A:158:ILE:HG12	1:A:299:ILE:HD11	1.65	0.76
1:C:208:VAL:HG13	1:D:209:THR:H	1.36	0.76
1:D:134:VAL:HG21	1:D:146:VAL:HG21	1.66	0.76
1:A:177:LEU:CD2	1:C:4:LYS:CE	2.63	0.76
1:B:172:LEU:HD22	1:B:232:GLN:NE2	2.00	0.76
1:C:208:VAL:CG1	1:D:209:THR:N	2.42	0.76
1:A:202:GLY:HA3	1:B:210:LEU:HB2	0.83	0.76
1:C:158:ILE:HG12	1:C:299:ILE:HD11	1.66	0.76
1:A:57:LEU:HB3	1:A:78:PHE:CZ	2.22	0.75
1:D:131:LYS:CE	1:D:298:GLY:HA2	2.16	0.75
1:D:19:ARG:HG2	2:D:409:HOH:O	1.80	0.75
1:C:131:LYS:CE	1:C:298:GLY:HA2	2.17	0.75
1:B:131:LYS:CE	1:B:298:GLY:HA2	2.17	0.75
1:B:177:LEU:HA	1:D:4:LYS:HE2	1.69	0.75
1:C:57:LEU:HB3	1:C:78:PHE:CZ	2.21	0.75
1:A:4:LYS:HE2	1:C:177:LEU:HA	1.69	0.75
1:A:177:LEU:HA	1:C:4:LYS:HE2	1.69	0.75
1:D:131:LYS:HE3	1:D:298:GLY:HA2	1.69	0.75
1:B:131:LYS:HE3	1:B:298:GLY:HA2	1.69	0.75
1:D:172:LEU:HD22	1:D:232:GLN:NE2	2.00	0.75
1:A:106:LEU:HD22	1:A:325:MET:HE3	1.69	0.75
1:A:228:ASN:HA	1:A:231:LYS:HZ3	1.50	0.75
1:B:227:LYS:HD3	1:B:228:ASN:H	1.52	0.75
1:D:306:ASN:H	1:D:306:ASN:HD22	1.35	0.75
1:B:57:LEU:HB3	1:B:78:PHE:CZ	2.22	0.74
1:B:211:LYS:HE3	1:D:7:LEU:HG	1.68	0.74
1:C:106:LEU:HD22	1:C:325:MET:HE3	1.69	0.74
1:C:204:ASN:ND2	1:D:208:VAL:HG23	2.02	0.74
1:B:4:LYS:HE2	1:D:177:LEU:HA	1.69	0.74
1:C:306:ASN:HD22	1:C:306:ASN:H	1.35	0.74
1:A:204:ASN:ND2	1:B:208:VAL:HG23	2.01	0.74
1:A:208:VAL:HG23	1:B:204:ASN:ND2	2.02	0.74
1:A:131:LYS:CE	1:A:298:GLY:HA2	2.16	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:LEU:HG	1:C:211:LYS:HE3	1.68	0.74
1:B:306:ASN:H	1:B:306:ASN:HD22	1.35	0.74
1:C:208:VAL:HG23	1:D:204:ASN:ND2	2.01	0.74
1:D:57:LEU:HB3	1:D:78:PHE:CZ	2.22	0.74
1:B:260:ARG:HH11	1:B:268:ARG:HH22	1.35	0.74
1:B:106:LEU:HD22	1:B:325:MET:HE3	1.69	0.74
1:A:306:ASN:H	1:A:306:ASN:HD22	1.35	0.73
1:C:227:LYS:HD3	1:C:228:ASN:H	1.52	0.73
1:B:7:LEU:HG	1:D:211:LYS:HE3	1.68	0.73
1:A:131:LYS:HE3	1:A:298:GLY:HA2	1.69	0.73
1:A:211:LYS:HE3	1:C:7:LEU:HG	1.68	0.73
1:A:227:LYS:HD3	1:A:228:ASN:H	1.52	0.73
1:D:227:LYS:HD3	1:D:228:ASN:H	1.52	0.73
1:A:21:LYS:HG3	1:A:46:GLU:HB3	1.70	0.73
1:A:120:VAL:HG21	1:A:146:VAL:CG1	2.19	0.73
1:C:131:LYS:HE3	1:C:298:GLY:HA2	1.69	0.73
1:C:260:ARG:HH11	1:C:268:ARG:HH22	1.36	0.73
1:A:260:ARG:HH11	1:A:268:ARG:HH22	1.36	0.72
1:D:106:LEU:HD22	1:D:325:MET:HE3	1.69	0.72
1:C:21:LYS:HG3	1:C:46:GLU:HB3	1.70	0.72
1:A:27:VAL:HB	1:A:32:MET:SD	2.29	0.72
1:B:82:TYR:CD2	1:B:123:VAL:HG12	2.25	0.72
1:C:27:VAL:HB	1:C:32:MET:SD	2.29	0.72
1:A:209:THR:N	1:B:208:VAL:CG1	2.43	0.72
1:B:27:VAL:HB	1:B:32:MET:SD	2.29	0.72
1:C:120:VAL:HG21	1:C:146:VAL:CG1	2.19	0.72
1:D:228:ASN:HA	1:D:231:LYS:HZ3	1.53	0.72
1:D:120:VAL:HG21	1:D:146:VAL:CG1	2.19	0.72
1:D:154:VAL:CG2	1:D:274:THR:HG22	2.20	0.72
1:B:21:LYS:HG3	1:B:46:GLU:HB3	1.70	0.72
1:B:120:VAL:HG13	1:B:121:PRO:HD2	1.72	0.72
1:D:21:LYS:HG3	1:D:46:GLU:HB3	1.70	0.72
1:D:27:VAL:HB	1:D:32:MET:SD	2.29	0.72
1:C:231:LYS:HZ3	1:C:231:LYS:HB2	1.55	0.71
1:A:120:VAL:HG13	1:A:121:PRO:HD2	1.72	0.71
1:A:82:TYR:CD2	1:A:123:VAL:HG12	2.25	0.71
1:A:154:VAL:CG2	1:A:274:THR:HG22	2.19	0.71
1:B:217:ILE:HG12	1:B:219:THR:HA	1.73	0.71
1:D:82:TYR:CD2	1:D:123:VAL:HG12	2.25	0.71
1:D:260:ARG:HH11	1:D:268:ARG:HH22	1.36	0.71
1:C:154:VAL:CG2	1:C:274:THR:HG22	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:307:MET:HB3	1:C:311:GLU:HB3	1.72	0.71
1:D:217:ILE:HG12	1:D:219:THR:HA	1.72	0.71
1:A:217:ILE:HG12	1:A:219:THR:HA	1.73	0.71
1:C:217:ILE:HG12	1:C:219:THR:HA	1.73	0.71
1:B:154:VAL:CG2	1:B:274:THR:HG22	2.19	0.71
1:C:227:LYS:CE	1:C:231:LYS:HZ1	2.04	0.71
1:C:120:VAL:HG13	1:C:121:PRO:HD2	1.71	0.70
1:D:227:LYS:HZ3	1:D:228:ASN:HB2	1.54	0.70
1:B:4:LYS:HD2	1:D:177:LEU:HA	1.73	0.70
1:C:120:VAL:CG2	1:C:121:PRO:HD2	2.21	0.70
1:B:177:LEU:HA	1:D:4:LYS:HD2	1.73	0.70
1:C:82:TYR:CD2	1:C:123:VAL:HG12	2.25	0.70
1:D:307:MET:HB3	1:D:311:GLU:HB3	1.72	0.70
1:B:252:GLY:O	1:B:256:THR:HG22	1.92	0.70
1:C:210:LEU:H	1:D:202:GLY:HA2	1.57	0.70
1:C:252:GLY:O	1:C:256:THR:HG22	1.92	0.70
1:B:131:LYS:HD3	1:B:262:ILE:HG21	1.73	0.70
1:D:120:VAL:HG13	1:D:121:PRO:HD2	1.71	0.70
1:B:99:MET:O	1:B:100:VAL:HG23	1.92	0.70
1:B:228:ASN:HA	1:B:231:LYS:HZ3	1.55	0.70
1:D:32:MET:HE2	1:D:60:GLU:HB3	1.74	0.70
1:B:120:VAL:HG21	1:B:146:VAL:CG1	2.19	0.70
1:B:307:MET:HB3	1:B:311:GLU:HB3	1.72	0.70
1:A:99:MET:O	1:A:100:VAL:HG23	1.92	0.69
1:B:120:VAL:CG2	1:B:121:PRO:HD2	2.21	0.69
1:B:227:LYS:HZ3	1:B:228:ASN:HB2	1.56	0.69
1:D:120:VAL:CG2	1:D:121:PRO:HD2	2.21	0.69
1:A:202:GLY:HA2	1:B:210:LEU:H	1.57	0.69
1:A:252:GLY:O	1:A:256:THR:HG22	1.92	0.69
1:B:32:MET:HE2	1:B:60:GLU:HB3	1.74	0.69
1:A:307:MET:HB3	1:A:311:GLU:HB3	1.72	0.69
1:B:249:TRP:CD1	1:D:64:LEU:CD2	2.76	0.69
1:C:131:LYS:HD3	1:C:262:ILE:HG21	1.73	0.69
1:D:252:GLY:O	1:D:256:THR:HG22	1.92	0.69
1:C:104:THR:HG22	1:C:238:TYR:CE1	2.23	0.69
1:D:99:MET:O	1:D:100:VAL:HG23	1.92	0.69
1:A:120:VAL:CG2	1:A:121:PRO:HD2	2.21	0.69
1:A:131:LYS:HD3	1:A:262:ILE:HG21	1.73	0.69
1:A:210:LEU:H	1:B:202:GLY:HA2	1.57	0.69
1:C:99:MET:O	1:C:100:VAL:HG23	1.92	0.69
1:C:170:ARG:O	1:C:173:ILE:HG22	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:202:GLY:HA2	1:D:210:LEU:H	1.57	0.69
1:A:249:TRP:CD1	1:C:64:LEU:CD2	2.76	0.69
1:B:177:LEU:HD23	1:D:4:LYS:HE2	1.75	0.69
1:C:307:MET:HB3	1:C:311:GLU:CB	2.23	0.69
1:A:177:LEU:HA	1:C:4:LYS:HD2	1.73	0.69
1:B:64:LEU:CD2	1:D:249:TRP:CD1	2.76	0.69
1:A:4:LYS:CE	1:A:4:LYS:HA	2.23	0.68
1:A:64:LEU:CD2	1:C:249:TRP:CD1	2.76	0.68
1:C:4:LYS:CE	1:C:4:LYS:HA	2.23	0.68
1:A:104:THR:HG22	1:A:238:TYR:CE1	2.23	0.68
1:A:202:GLY:N	1:B:210:LEU:HB2	2.09	0.68
1:C:209:THR:N	1:D:208:VAL:CG1	2.43	0.68
1:A:307:MET:HB3	1:A:311:GLU:CB	2.23	0.68
1:C:212:SER:CA	1:D:208:VAL:HG11	2.23	0.68
1:A:32:MET:HE2	1:A:60:GLU:HB3	1.73	0.68
1:A:177:LEU:HD23	1:C:4:LYS:HE2	1.75	0.68
1:C:32:MET:HE2	1:C:60:GLU:HB3	1.74	0.68
1:D:170:ARG:O	1:D:173:ILE:HG22	1.93	0.68
1:D:259:ALA:HA	1:D:262:ILE:HD12	1.76	0.68
1:A:4:LYS:HD2	1:C:177:LEU:HA	1.73	0.68
1:A:170:ARG:O	1:A:173:ILE:HG22	1.93	0.68
1:A:212:SER:CA	1:B:208:VAL:HG11	2.23	0.68
1:B:259:ALA:HA	1:B:262:ILE:HD12	1.76	0.68
1:A:208:VAL:HG11	1:B:212:SER:CA	2.23	0.68
1:B:307:MET:HB3	1:B:311:GLU:CB	2.23	0.68
1:D:4:LYS:CE	1:D:4:LYS:HA	2.23	0.68
1:D:307:MET:HB3	1:D:311:GLU:CB	2.23	0.68
1:A:211:LYS:HD3	1:C:7:LEU:CG	2.24	0.68
1:A:227:LYS:HZ3	1:A:228:ASN:HB2	1.58	0.68
1:A:259:ALA:HA	1:A:262:ILE:HD12	1.76	0.68
1:A:7:LEU:CG	1:C:211:LYS:HD3	2.24	0.68
1:B:4:LYS:CE	1:B:4:LYS:HA	2.23	0.68
1:C:208:VAL:HG11	1:D:212:SER:CA	2.23	0.68
1:A:210:LEU:HB2	1:B:202:GLY:N	2.09	0.67
1:D:131:LYS:HD3	1:D:262:ILE:HG21	1.73	0.67
1:A:4:LYS:HE2	1:C:177:LEU:HD23	1.75	0.67
1:C:202:GLY:N	1:D:210:LEU:HB2	2.08	0.67
1:C:204:ASN:OD1	1:D:204:ASN:CG	2.38	0.67
1:B:170:ARG:O	1:B:173:ILE:HG22	1.93	0.67
1:C:56:LYS:HE3	1:C:60:GLU:HG3	1.76	0.67
1:B:7:LEU:CG	1:D:211:LYS:HD3	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:VAL:HG22	1:A:121:PRO:CD	2.25	0.67
1:A:210:LEU:HB3	1:B:202:GLY:HA3	1.74	0.67
1:B:112:ASN:O	1:B:115:ILE:HG22	1.95	0.67
1:C:121:PRO:CG	1:C:149:ILE:HG23	2.25	0.67
1:D:112:ASN:O	1:D:115:ILE:HG22	1.95	0.67
1:B:56:LYS:HE3	1:B:60:GLU:HG3	1.76	0.67
1:B:121:PRO:CG	1:B:149:ILE:HG23	2.25	0.67
1:B:220:ASP:O	1:B:221:LYS:HB3	1.95	0.67
1:C:259:ALA:HA	1:C:262:ILE:HD12	1.76	0.67
1:D:56:LYS:HE3	1:D:60:GLU:HG3	1.76	0.67
1:C:112:ASN:O	1:C:115:ILE:HG22	1.95	0.66
1:A:104:THR:O	1:A:105:ARG:HG3	1.95	0.66
1:B:211:LYS:HD3	1:D:7:LEU:CG	2.24	0.66
1:D:121:PRO:CG	1:D:149:ILE:HG23	2.25	0.66
1:A:56:LYS:HE3	1:A:60:GLU:HG3	1.76	0.66
1:A:220:ASP:O	1:A:221:LYS:HB3	1.95	0.66
1:B:104:THR:HG22	1:B:238:TYR:CE1	2.23	0.66
1:C:210:LEU:HB2	1:D:202:GLY:N	2.09	0.66
1:A:204:ASN:OD1	1:B:204:ASN:CG	2.38	0.66
1:C:120:VAL:HG22	1:C:121:PRO:CD	2.25	0.66
1:B:120:VAL:HG22	1:B:121:PRO:CD	2.25	0.66
1:C:104:THR:O	1:C:105:ARG:HG3	1.95	0.66
1:D:120:VAL:HG22	1:D:121:PRO:CD	2.25	0.66
1:A:302:PHE:HZ	1:D:11:LEU:HG	1.59	0.66
1:C:275:LEU:HD11	1:C:285:GLU:HA	1.78	0.66
1:B:201:SER:HB3	1:B:311:GLU:OE1	1.96	0.66
1:C:219:THR:HG21	1:C:222:ASN:C	2.21	0.66
1:D:219:THR:HG21	1:D:222:ASN:C	2.21	0.66
1:A:201:SER:HB3	1:A:311:GLU:OE1	1.96	0.66
1:C:201:SER:HB3	1:C:311:GLU:OE1	1.96	0.66
1:C:204:ASN:CG	1:D:204:ASN:OD1	2.38	0.66
1:C:227:LYS:HZ3	1:C:228:ASN:HB2	1.59	0.66
1:C:228:ASN:HA	1:C:231:LYS:HZ3	1.60	0.66
1:A:204:ASN:CG	1:B:204:ASN:OD1	2.38	0.66
1:D:201:SER:HB3	1:D:311:GLU:OE1	1.96	0.66
1:A:57:LEU:HD12	1:A:78:PHE:CG	2.31	0.66
1:A:249:TRP:CD1	1:C:64:LEU:HD21	2.31	0.66
1:A:275:LEU:HD11	1:A:285:GLU:HA	1.78	0.66
1:B:219:THR:HG21	1:B:222:ASN:C	2.21	0.66
1:D:275:LEU:HD11	1:D:285:GLU:HA	1.78	0.66
1:A:219:THR:HG21	1:A:222:ASN:C	2.21	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:208:VAL:CG1	1:D:212:SER:CA	2.74	0.65
1:A:208:VAL:CG1	1:B:212:SER:CA	2.74	0.65
1:B:275:LEU:HD11	1:B:285:GLU:HA	1.78	0.65
1:C:202:GLY:O	1:D:207:GLY:HA3	1.96	0.65
1:D:57:LEU:HD12	1:D:78:PHE:CD2	2.32	0.65
1:D:57:LEU:HD12	1:D:78:PHE:CG	2.31	0.65
1:D:221:LYS:C	1:D:223:LYS:H	2.03	0.65
1:A:121:PRO:CG	1:A:149:ILE:HG23	2.25	0.65
1:A:212:SER:CA	1:B:208:VAL:CG1	2.74	0.65
1:C:57:LEU:HD12	1:C:78:PHE:CD2	2.31	0.65
1:C:212:SER:CA	1:D:208:VAL:CG1	2.74	0.65
1:D:104:THR:O	1:D:105:ARG:HG3	1.95	0.65
1:A:64:LEU:HD21	1:C:249:TRP:CD1	2.32	0.65
1:A:112:ASN:O	1:A:115:ILE:HG22	1.95	0.65
1:A:141:ILE:O	1:A:145:VAL:HG23	1.97	0.65
1:A:209:THR:H	1:B:208:VAL:HG12	1.59	0.65
1:B:7:LEU:O	1:B:7:LEU:HD23	1.97	0.65
1:C:220:ASP:O	1:C:221:LYS:HB3	1.95	0.65
1:D:104:THR:HG22	1:D:238:TYR:CE1	2.23	0.65
1:A:202:GLY:O	1:B:207:GLY:HA3	1.97	0.65
1:A:208:VAL:HG12	1:B:209:THR:H	1.59	0.65
1:B:104:THR:O	1:B:105:ARG:HG3	1.95	0.65
1:C:141:ILE:O	1:C:145:VAL:HG23	1.97	0.65
1:D:300:THR:HG22	1:D:301:ASP:OD1	1.97	0.65
1:A:57:LEU:HG	1:A:78:PHE:CE1	2.32	0.65
1:B:64:LEU:HD21	1:D:249:TRP:CD1	2.32	0.65
1:C:7:LEU:O	1:C:7:LEU:HD23	1.97	0.65
1:C:57:LEU:HD12	1:C:78:PHE:CG	2.31	0.65
1:A:221:LYS:C	1:A:223:LYS:H	2.03	0.65
1:C:207:GLY:HA3	1:D:202:GLY:O	1.96	0.65
1:C:210:LEU:HD23	1:D:306:ASN:ND2	2.12	0.65
1:C:214:ASN:N	1:C:215:PRO:HD2	2.12	0.65
1:D:57:LEU:HG	1:D:78:PHE:CE1	2.32	0.65
1:B:141:ILE:O	1:B:145:VAL:HG23	1.97	0.65
1:B:227:LYS:CE	1:B:231:LYS:HZ1	2.09	0.65
1:C:207:GLY:C	1:D:208:VAL:HG22	2.22	0.65
1:C:219:THR:HG22	1:C:220:ASP:N	2.12	0.65
1:A:300:THR:HG22	1:A:301:ASP:OD1	1.97	0.65
1:B:214:ASN:N	1:B:215:PRO:HD2	2.12	0.65
1:B:314:LEU:O	1:B:317:LYS:HB3	1.97	0.65
1:C:300:THR:HG22	1:C:301:ASP:OD1	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:220:ASP:O	1:D:221:LYS:HB3	1.95	0.65
1:A:207:GLY:C	1:B:208:VAL:HG22	2.22	0.65
1:B:57:LEU:HG	1:B:78:PHE:CE1	2.32	0.65
1:B:249:TRP:CD1	1:D:64:LEU:HD21	2.31	0.65
1:D:7:LEU:HD23	1:D:7:LEU:O	1.97	0.65
1:B:57:LEU:HD12	1:B:78:PHE:CD2	2.31	0.64
1:A:207:GLY:HA3	1:B:202:GLY:O	1.97	0.64
1:A:208:VAL:HG22	1:B:207:GLY:C	2.22	0.64
1:B:57:LEU:HD12	1:B:78:PHE:CG	2.31	0.64
1:D:219:THR:HG22	1:D:220:ASP:N	2.12	0.64
1:A:72:SER:OG	1:D:260:ARG:NH2	2.26	0.64
1:A:291:PRO:HB2	1:A:303:VAL:HG12	1.79	0.64
1:A:306:ASN:ND2	1:B:210:LEU:HD23	2.12	0.64
1:B:219:THR:HG22	1:B:220:ASP:N	2.12	0.64
1:C:4:LYS:NZ	1:C:4:LYS:HA	2.13	0.64
1:D:141:ILE:O	1:D:145:VAL:HG23	1.97	0.64
1:B:11:LEU:HG	1:C:302:PHE:HZ	1.59	0.64
1:B:302:PHE:HZ	1:C:11:LEU:HG	1.59	0.64
1:C:57:LEU:HG	1:C:78:PHE:CE1	2.32	0.64
1:C:208:VAL:HG22	1:D:207:GLY:C	2.22	0.64
1:A:210:LEU:HD23	1:B:306:ASN:ND2	2.12	0.64
1:A:94:THR:C	1:A:98:ARG:HH12	2.06	0.64
1:A:217:ILE:CG1	1:A:219:THR:HA	2.28	0.64
1:A:260:ARG:NH2	1:D:72:SER:OG	2.26	0.64
1:B:260:ARG:NH2	1:C:72:SER:OG	2.26	0.64
1:C:142:LEU:O	1:C:146:VAL:HG22	1.98	0.64
1:C:212:SER:HA	1:D:208:VAL:CB	2.27	0.64
1:C:306:ASN:ND2	1:D:210:LEU:HD23	2.12	0.64
1:A:4:LYS:NZ	1:A:4:LYS:HA	2.13	0.64
1:A:57:LEU:HD12	1:A:78:PHE:CD2	2.31	0.64
1:A:219:THR:HG22	1:A:220:ASP:N	2.12	0.64
1:B:4:LYS:HE2	1:D:177:LEU:HD23	1.75	0.64
1:B:217:ILE:CG1	1:B:219:THR:HA	2.28	0.64
1:B:231:LYS:HZ3	1:B:231:LYS:HB2	1.61	0.64
1:B:300:THR:HG22	1:B:301:ASP:OD1	1.97	0.64
1:D:4:LYS:NZ	1:D:4:LYS:HA	2.13	0.64
1:D:314:LEU:O	1:D:317:LYS:HB3	1.97	0.64
1:A:177:LEU:HD22	1:C:4:LYS:NZ	2.12	0.64
1:D:94:THR:C	1:D:98:ARG:HH12	2.06	0.63
1:D:291:PRO:HB2	1:D:303:VAL:HG12	1.79	0.63
1:A:214:ASN:N	1:A:215:PRO:HD2	2.12	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:LEU:O	1:A:317:LYS:HB3	1.97	0.63
1:B:94:THR:C	1:B:98:ARG:HH12	2.06	0.63
1:C:291:PRO:HB2	1:C:303:VAL:HG12	1.79	0.63
1:C:221:LYS:C	1:C:223:LYS:H	2.03	0.63
1:C:314:LEU:O	1:C:317:LYS:HB3	1.97	0.63
1:A:142:LEU:O	1:A:146:VAL:HG22	1.98	0.63
1:B:278:GLY:HA2	1:B:282:ILE:O	1.99	0.63
1:C:306:ASN:OD1	1:D:209:THR:O	2.17	0.63
1:C:204:ASN:OD1	1:D:204:ASN:ND2	2.31	0.63
1:D:214:ASN:N	1:D:215:PRO:HD2	2.12	0.63
1:A:7:LEU:HD23	1:A:7:LEU:O	1.97	0.63
1:B:291:PRO:HB2	1:B:303:VAL:HG12	1.79	0.63
1:C:204:ASN:ND2	1:D:204:ASN:OD1	2.31	0.63
1:C:278:GLY:HA2	1:C:282:ILE:O	1.99	0.63
1:D:36:ILE:O	1:D:40:LEU:HD23	1.99	0.63
1:D:142:LEU:O	1:D:146:VAL:HG22	1.98	0.63
1:A:208:VAL:HA	1:B:208:VAL:HA	1.81	0.63
1:A:306:ASN:OD1	1:B:209:THR:O	2.17	0.63
1:B:221:LYS:C	1:B:223:LYS:H	2.03	0.63
1:C:187:TRP:HE1	1:C:291:PRO:HB3	1.64	0.63
1:B:4:LYS:NZ	1:B:4:LYS:HA	2.13	0.63
1:C:36:ILE:O	1:C:40:LEU:HD23	1.99	0.63
1:C:94:THR:C	1:C:98:ARG:HH12	2.06	0.63
1:A:278:GLY:HA2	1:A:282:ILE:O	1.99	0.62
1:B:4:LYS:NZ	1:D:177:LEU:HD22	2.13	0.62
1:C:204:ASN:HA	1:C:211:LYS:O	1.99	0.62
1:C:208:VAL:CB	1:D:212:SER:HA	2.27	0.62
1:D:204:ASN:HA	1:D:211:LYS:O	1.99	0.62
1:A:204:ASN:OD1	1:B:204:ASN:ND2	2.31	0.62
1:B:72:SER:OG	1:C:260:ARG:NH2	2.26	0.62
1:B:120:VAL:CG1	1:B:121:PRO:HD2	2.29	0.62
1:C:209:THR:H	1:D:208:VAL:HG12	1.59	0.62
1:D:278:GLY:HA2	1:D:282:ILE:O	1.99	0.62
1:A:204:ASN:ND2	1:B:204:ASN:OD1	2.31	0.62
1:B:36:ILE:O	1:B:40:LEU:HD23	1.99	0.62
1:B:142:LEU:O	1:B:146:VAL:HG22	1.98	0.62
1:D:120:VAL:CB	1:D:121:PRO:HD2	2.29	0.62
1:D:187:TRP:HE1	1:D:291:PRO:HB3	1.64	0.62
1:A:204:ASN:HA	1:A:211:LYS:O	1.99	0.62
1:C:209:THR:O	1:D:306:ASN:OD1	2.17	0.62
1:D:154:VAL:HG21	1:D:274:THR:HG22	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:217:ILE:CG1	1:D:219:THR:HA	2.28	0.62
1:B:51:ASP:HB2	1:B:57:LEU:HD23	1.82	0.62
1:C:120:VAL:CG1	1:C:121:PRO:HD2	2.29	0.62
1:C:217:ILE:CG1	1:C:219:THR:HA	2.28	0.62
1:A:120:VAL:CB	1:A:121:PRO:HD2	2.29	0.62
1:A:120:VAL:CG1	1:A:121:PRO:HD2	2.29	0.62
1:A:154:VAL:HG21	1:A:274:THR:HG22	1.81	0.62
1:A:212:SER:HA	1:B:208:VAL:CB	2.27	0.62
1:A:221:LYS:HG3	1:A:222:ASN:N	2.15	0.62
1:C:10:ASN:H	1:C:10:ASN:ND2	1.98	0.62
1:C:137:ASN:C	1:C:139:VAL:N	2.56	0.62
1:C:208:VAL:HG12	1:D:209:THR:H	1.59	0.62
1:A:187:TRP:HE1	1:A:291:PRO:HB3	1.64	0.62
1:C:51:ASP:HB2	1:C:57:LEU:HD23	1.82	0.62
1:C:93:ILE:HD11	1:C:132:ILE:HG21	1.82	0.62
1:C:120:VAL:CB	1:C:121:PRO:HD2	2.30	0.62
1:D:93:ILE:HD11	1:D:132:ILE:HG21	1.82	0.62
1:A:36:ILE:O	1:A:40:LEU:HD23	1.99	0.62
1:A:209:THR:O	1:B:306:ASN:OD1	2.17	0.62
1:B:93:ILE:HD11	1:B:132:ILE:HG21	1.82	0.62
1:C:36:ILE:O	1:C:39:LEU:HB2	2.00	0.62
1:B:4:LYS:CD	1:D:177:LEU:HA	2.30	0.62
1:B:204:ASN:HA	1:B:211:LYS:O	1.99	0.62
1:B:221:LYS:HG3	1:B:222:ASN:N	2.15	0.62
1:D:51:ASP:HB2	1:D:57:LEU:HD23	1.82	0.62
1:D:120:VAL:CG1	1:D:121:PRO:HD2	2.29	0.62
1:B:120:VAL:CB	1:B:121:PRO:HD2	2.29	0.62
1:B:154:VAL:HG21	1:B:274:THR:HG22	1.81	0.62
1:B:277:LYS:O	1:B:283:LYS:HA	2.00	0.62
1:A:4:LYS:CD	1:C:177:LEU:HA	2.30	0.61
1:A:36:ILE:O	1:A:39:LEU:HB2	2.00	0.61
1:A:93:ILE:HD11	1:A:132:ILE:HG21	1.82	0.61
1:A:98:ARG:HB3	1:A:99:MET:SD	2.40	0.61
1:C:208:VAL:HA	1:D:208:VAL:HA	1.81	0.61
1:C:277:LYS:O	1:C:283:LYS:HA	2.00	0.61
1:A:208:VAL:CB	1:B:212:SER:HA	2.27	0.61
1:B:36:ILE:O	1:B:39:LEU:HB2	2.00	0.61
1:B:187:TRP:HE1	1:B:291:PRO:HB3	1.64	0.61
1:C:204:ASN:HD22	1:C:204:ASN:N	1.98	0.61
1:D:36:ILE:O	1:D:39:LEU:HB2	2.00	0.61
1:A:20:CYS:CA	1:A:89:LYS:HD3	2.28	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:ILE:O	1:A:255:VAL:HG23	2.01	0.61
1:C:221:LYS:HG3	1:C:222:ASN:N	2.15	0.61
1:A:4:LYS:NZ	1:C:177:LEU:HD22	2.12	0.61
1:A:11:LEU:HG	1:D:302:PHE:HZ	1.59	0.61
1:A:51:ASP:HB2	1:A:57:LEU:HD23	1.82	0.61
1:A:277:LYS:O	1:A:283:LYS:HA	2.00	0.61
1:C:204:ASN:HD21	1:D:207:GLY:HA2	1.66	0.61
1:C:208:VAL:HA	1:D:208:VAL:CA	2.30	0.61
1:D:251:ILE:O	1:D:255:VAL:HG23	2.00	0.61
1:A:204:ASN:HD21	1:B:207:GLY:HA2	1.66	0.61
1:A:208:VAL:HG11	1:B:212:SER:N	2.15	0.61
1:B:251:ILE:O	1:B:255:VAL:HG23	2.01	0.61
1:B:177:LEU:HD22	1:D:4:LYS:NZ	2.13	0.61
1:B:227:LYS:NZ	1:B:228:ASN:HB2	2.15	0.61
1:C:208:VAL:CA	1:D:208:VAL:HA	2.30	0.61
1:C:251:ILE:O	1:C:255:VAL:HG23	2.00	0.61
1:D:277:LYS:O	1:D:283:LYS:HA	2.00	0.61
1:A:207:GLY:HA2	1:B:204:ASN:HD21	1.65	0.61
1:A:208:VAL:CA	1:B:208:VAL:HA	2.30	0.61
1:A:208:VAL:HA	1:B:208:VAL:CA	2.30	0.61
1:B:196:SER:O	1:B:230:HIS:NE2	2.34	0.61
1:D:12:VAL:CB	1:D:13:PRO:HD3	2.17	0.61
1:A:243:MET:HE3	1:C:59:GLY:HA2	1.83	0.61
1:B:177:LEU:HA	1:D:4:LYS:CD	2.30	0.61
1:B:260:ARG:HD2	1:B:268:ARG:HH22	1.65	0.61
1:C:20:CYS:CA	1:C:89:LYS:HD3	2.28	0.61
1:C:154:VAL:HG21	1:C:274:THR:HG22	1.82	0.61
1:C:212:SER:N	1:D:208:VAL:HG11	2.15	0.61
1:C:227:LYS:NZ	1:C:228:ASN:HB2	2.15	0.61
1:C:260:ARG:HD2	1:C:268:ARG:HH22	1.64	0.61
1:D:221:LYS:HG3	1:D:222:ASN:N	2.15	0.61
1:B:98:ARG:HB3	1:B:99:MET:SD	2.40	0.61
1:D:10:ASN:ND2	1:D:10:ASN:H	1.98	0.61
1:B:51:ASP:CB	1:B:57:LEU:HD23	2.31	0.61
1:C:51:ASP:CB	1:C:57:LEU:HD23	2.31	0.61
1:A:227:LYS:NZ	1:A:228:ASN:HB2	2.15	0.60
1:A:260:ARG:HD2	1:A:268:ARG:HH22	1.64	0.60
1:C:208:VAL:HG11	1:D:212:SER:N	2.15	0.60
1:D:137:ASN:C	1:D:139:VAL:N	2.56	0.60
1:A:34:CYS:HB2	1:A:252:GLY:HA2	1.83	0.60
1:B:243:MET:HE3	1:D:59:GLY:HA2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:260:ARG:HD2	1:D:268:ARG:HH22	1.65	0.60
1:C:98:ARG:HB3	1:C:99:MET:SD	2.41	0.60
1:C:107:ASP:C	1:C:109:LEU:H	2.10	0.60
1:A:59:GLY:HA2	1:C:243:MET:HE3	1.83	0.60
1:A:137:ASN:C	1:A:139:VAL:N	2.56	0.60
1:B:204:ASN:HD22	1:B:204:ASN:N	1.98	0.60
1:D:196:SER:O	1:D:230:HIS:NE2	2.34	0.60
1:A:51:ASP:CB	1:A:57:LEU:HD23	2.31	0.60
1:A:177:LEU:HA	1:C:4:LYS:CD	2.30	0.60
1:A:212:SER:N	1:B:208:VAL:HG11	2.15	0.60
1:C:207:GLY:HA2	1:D:204:ASN:HD21	1.66	0.60
1:D:98:ARG:HB3	1:D:99:MET:SD	2.41	0.60
1:D:231:LYS:HZ3	1:D:231:LYS:HB2	1.66	0.60
1:B:34:CYS:HB2	1:B:252:GLY:HA2	1.83	0.60
1:B:219:THR:HG21	1:B:222:ASN:CA	2.32	0.60
1:B:9:GLN:NE2	1:C:279:PHE:HZ	1.86	0.60
1:C:202:GLY:HA2	1:D:208:VAL:C	2.27	0.60
1:A:107:ASP:C	1:A:109:LEU:H	2.10	0.60
1:B:98:ARG:O	1:B:99:MET:HG2	2.02	0.60
1:C:98:ARG:O	1:C:99:MET:HG2	2.02	0.60
1:C:208:VAL:C	1:D:202:GLY:HA2	2.27	0.60
1:A:219:THR:HG21	1:A:222:ASN:CA	2.32	0.60
1:D:20:CYS:CA	1:D:89:LYS:HD3	2.28	0.60
1:D:98:ARG:O	1:D:99:MET:HG2	2.02	0.60
1:A:196:SER:O	1:A:230:HIS:NE2	2.34	0.60
1:C:34:CYS:HB2	1:C:252:GLY:HA2	1.84	0.60
1:C:41:LYS:HB3	1:C:43:LEU:CD1	2.32	0.59
1:A:98:ARG:O	1:A:99:MET:HG2	2.02	0.59
1:B:208:VAL:C	1:B:210:LEU:H	2.10	0.59
1:D:51:ASP:CB	1:D:57:LEU:HD23	2.31	0.59
1:D:227:LYS:NZ	1:D:228:ASN:HB2	2.16	0.59
1:C:196:SER:O	1:C:230:HIS:NE2	2.34	0.59
1:D:204:ASN:HD22	1:D:204:ASN:N	1.98	0.59
1:B:10:ASN:ND2	1:B:10:ASN:H	1.98	0.59
1:C:12:VAL:CB	1:C:13:PRO:HD3	2.17	0.59
1:B:41:LYS:HB3	1:B:43:LEU:CD1	2.32	0.59
1:B:20:CYS:CA	1:B:89:LYS:HD3	2.28	0.59
1:B:107:ASP:C	1:B:109:LEU:H	2.10	0.59
1:A:10:ASN:ND2	1:A:10:ASN:H	1.97	0.59
1:A:202:GLY:HA2	1:B:208:VAL:C	2.27	0.59
1:B:187:TRP:NE1	1:B:291:PRO:HB3	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:SER:HG	1:D:269:VAL:HG12	1.66	0.59
1:C:208:VAL:C	1:C:210:LEU:H	2.10	0.59
1:D:227:LYS:CE	1:D:231:LYS:HZ1	2.14	0.59
1:A:30:VAL:HG13	1:A:251:ILE:CG2	2.33	0.59
1:A:60:GLU:OE2	1:C:244:LYS:NZ	2.33	0.59
1:A:131:LYS:HE2	1:A:298:GLY:HA2	1.85	0.59
1:A:208:VAL:C	1:B:202:GLY:HA2	2.27	0.59
1:A:248:SER:O	1:A:251:ILE:HG22	2.03	0.59
1:D:22:ILE:O	1:D:47:LEU:HA	2.03	0.59
1:A:302:PHE:CE2	1:D:11:LEU:HG	2.38	0.59
1:B:30:VAL:HG13	1:B:251:ILE:CG2	2.33	0.59
1:B:187:TRP:HD1	1:B:189:LEU:CD1	2.16	0.59
1:B:279:PHE:HZ	1:C:9:GLN:NE2	1.86	0.59
1:D:107:ASP:C	1:D:109:LEU:H	2.10	0.59
1:D:208:VAL:C	1:D:210:LEU:H	2.10	0.59
1:A:120:VAL:O	1:A:123:VAL:HG13	2.04	0.58
1:A:204:ASN:HD22	1:A:204:ASN:N	1.98	0.58
1:B:59:GLY:HA2	1:D:243:MET:HE3	1.83	0.58
1:C:187:TRP:NE1	1:C:291:PRO:HB3	2.18	0.58
1:D:30:VAL:HG13	1:D:251:ILE:CG2	2.33	0.58
1:D:34:CYS:HB2	1:D:252:GLY:HA2	1.84	0.58
1:B:22:ILE:O	1:B:47:LEU:HA	2.03	0.58
1:B:131:LYS:HE2	1:B:298:GLY:HA2	1.85	0.58
1:B:177:LEU:HA	1:D:4:LYS:CE	2.33	0.58
1:B:248:SER:O	1:B:251:ILE:HG22	2.03	0.58
1:C:219:THR:HG21	1:C:222:ASN:CA	2.32	0.58
1:D:219:THR:HG21	1:D:222:ASN:CA	2.32	0.58
1:D:289:SER:O	1:D:290:ILE:HD12	2.03	0.58
1:A:187:TRP:HD1	1:A:189:LEU:CD1	2.17	0.58
1:B:11:LEU:HG	1:C:302:PHE:CE2	2.38	0.58
1:D:187:TRP:NE1	1:D:291:PRO:HB3	2.18	0.58
1:B:120:VAL:O	1:B:123:VAL:HG13	2.03	0.58
1:B:164:LEU:HD13	1:B:192:HIS:CE1	2.38	0.58
1:C:22:ILE:O	1:C:47:LEU:HA	2.03	0.58
1:A:208:VAL:C	1:A:210:LEU:H	2.10	0.58
1:A:212:SER:CB	1:B:208:VAL:CB	2.78	0.58
1:B:4:LYS:CE	1:D:177:LEU:HA	2.33	0.58
1:B:289:SER:O	1:B:290:ILE:HD12	2.03	0.58
1:C:15:ASP:O	1:C:16:LYS:HG2	2.03	0.58
1:C:210:LEU:HB3	1:D:202:GLY:HA3	1.74	0.58
1:C:248:SER:O	1:C:251:ILE:HG22	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:310:GLU:C	1:C:313:GLY:H	2.12	0.58
1:D:120:VAL:O	1:D:123:VAL:HG13	2.03	0.58
1:A:4:LYS:CE	1:C:177:LEU:HA	2.33	0.58
1:A:11:LEU:HG	1:D:302:PHE:CE2	2.38	0.58
1:B:241:LEU:C	1:B:241:LEU:HD12	2.29	0.58
1:D:310:GLU:C	1:D:313:GLY:H	2.12	0.58
1:A:187:TRP:NE1	1:A:291:PRO:HB3	2.18	0.58
1:A:241:LEU:C	1:A:241:LEU:HD12	2.29	0.58
1:A:275:LEU:HG	1:A:277:LYS:HB3	1.86	0.58
1:B:15:ASP:O	1:B:16:LYS:HG2	2.03	0.58
1:B:254:SER:O	1:B:257:ASP:HB3	2.04	0.58
1:C:138:PRO:O	1:C:142:LEU:HG	2.04	0.58
1:C:164:LEU:HD13	1:C:192:HIS:CE1	2.38	0.58
1:C:275:LEU:HG	1:C:277:LYS:HB3	1.86	0.58
1:D:138:PRO:O	1:D:142:LEU:HG	2.04	0.58
1:C:30:VAL:HG13	1:C:251:ILE:CG2	2.33	0.58
1:D:197:VAL:HG22	1:D:198:PRO:O	2.04	0.58
1:D:275:LEU:HG	1:D:277:LYS:HB3	1.86	0.58
1:A:22:ILE:O	1:A:47:LEU:HA	2.03	0.58
1:A:32:MET:CE	1:A:60:GLU:HB3	2.34	0.58
1:A:177:LEU:HA	1:C:4:LYS:CE	2.33	0.58
1:B:227:LYS:HD3	1:B:228:ASN:N	2.19	0.58
1:B:275:LEU:HG	1:B:277:LYS:HB3	1.86	0.58
1:C:39:LEU:HD22	1:C:71:LEU:HD13	1.86	0.58
1:C:189:LEU:HD21	1:C:199:ILE:CD1	2.30	0.58
1:C:241:LEU:C	1:C:241:LEU:HD12	2.29	0.58
1:D:15:ASP:O	1:D:16:LYS:HG2	2.03	0.58
1:D:131:LYS:HE2	1:D:298:GLY:HA2	1.85	0.58
1:A:9:GLN:NE2	1:D:279:PHE:HZ	1.86	0.57
1:A:24:VAL:HG12	1:A:92:ILE:HG23	1.86	0.57
1:A:138:PRO:O	1:A:142:LEU:HG	2.04	0.57
1:A:254:SER:O	1:A:257:ASP:HB3	2.04	0.57
1:B:187:TRP:HD1	1:B:189:LEU:HD12	1.69	0.57
1:C:187:TRP:HD1	1:C:189:LEU:CD1	2.17	0.57
1:C:187:TRP:HD1	1:C:189:LEU:HD12	1.69	0.57
1:C:197:VAL:HG22	1:C:198:PRO:O	2.04	0.57
1:A:15:ASP:O	1:A:16:LYS:HG2	2.03	0.57
1:A:187:TRP:HD1	1:A:189:LEU:HD12	1.69	0.57
1:B:32:MET:CE	1:B:60:GLU:HB3	2.35	0.57
1:B:302:PHE:CE2	1:C:11:LEU:HG	2.38	0.57
1:C:24:VAL:HG12	1:C:92:ILE:HG23	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:LYS:HE2	1:C:298:GLY:HA2	1.85	0.57
1:C:208:VAL:HB	1:D:212:SER:CA	2.33	0.57
1:D:248:SER:O	1:D:251:ILE:HG22	2.03	0.57
1:A:164:LEU:HD13	1:A:192:HIS:CE1	2.39	0.57
1:A:197:VAL:C	1:A:198:PRO:O	2.46	0.57
1:A:289:SER:O	1:A:290:ILE:HD12	2.03	0.57
1:B:177:LEU:HD22	1:D:4:LYS:CE	2.34	0.57
1:C:152:PHE:HB2	1:C:153:PRO:HD2	1.86	0.57
1:D:227:LYS:HD3	1:D:228:ASN:N	2.19	0.57
1:A:197:VAL:HG22	1:A:198:PRO:O	2.04	0.57
1:A:219:THR:HG22	1:A:220:ASP:H	1.69	0.57
1:B:115:ILE:O	1:B:119:ILE:HD13	2.05	0.57
1:C:115:ILE:O	1:C:119:ILE:HD13	2.04	0.57
1:C:116:MET:O	1:C:118:ALA:N	2.37	0.57
1:D:152:PHE:HB2	1:D:153:PRO:HD2	1.86	0.57
1:D:189:LEU:HD21	1:D:199:ILE:CD1	2.30	0.57
1:A:310:GLU:C	1:A:313:GLY:H	2.12	0.57
1:B:219:THR:HG22	1:B:220:ASP:H	1.69	0.57
1:B:249:TRP:HD1	1:D:64:LEU:CD2	2.18	0.57
1:B:310:GLU:C	1:B:313:GLY:H	2.12	0.57
1:C:219:THR:HG22	1:C:220:ASP:H	1.69	0.57
1:D:116:MET:O	1:D:118:ALA:N	2.37	0.57
1:D:131:LYS:HZ2	1:D:262:ILE:HG21	1.70	0.57
1:A:302:PHE:N	1:D:9:GLN:O	2.29	0.57
1:B:116:MET:O	1:B:118:ALA:N	2.37	0.57
1:B:16:LYS:C	1:B:17:LEU:HD22	2.30	0.57
1:C:289:SER:O	1:C:290:ILE:HD12	2.03	0.57
1:D:39:LEU:HD22	1:D:71:LEU:HD13	1.86	0.57
1:D:115:ILE:O	1:D:119:ILE:HD13	2.04	0.57
1:D:241:LEU:C	1:D:241:LEU:HD12	2.29	0.57
1:A:116:MET:O	1:A:118:ALA:N	2.37	0.57
1:A:212:SER:CA	1:B:208:VAL:HB	2.33	0.57
1:B:138:PRO:O	1:B:142:LEU:HG	2.04	0.57
1:B:197:VAL:HG22	1:B:198:PRO:O	2.04	0.57
1:B:229:VAL:O	1:B:233:VAL:HG23	2.05	0.57
1:C:120:VAL:O	1:C:123:VAL:HG13	2.04	0.57
1:D:16:LYS:C	1:D:17:LEU:HD22	2.30	0.57
1:A:227:LYS:HD3	1:A:228:ASN:N	2.19	0.57
1:B:39:LEU:HD22	1:B:71:LEU:HD13	1.86	0.57
1:B:131:LYS:HZ2	1:B:262:ILE:HG21	1.70	0.57
1:B:152:PHE:HB2	1:B:153:PRO:HD2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:LYS:C	1:C:17:LEU:HD22	2.30	0.57
1:D:41:LYS:HB3	1:D:43:LEU:CD1	2.32	0.57
1:D:187:TRP:HD1	1:D:189:LEU:HD12	1.69	0.57
1:A:208:VAL:HB	1:B:212:SER:CA	2.33	0.56
1:A:221:LYS:O	1:A:223:LYS:N	2.37	0.56
1:A:276:VAL:HG11	1:A:288:LEU:HD13	1.87	0.56
1:C:120:VAL:HG13	1:C:121:PRO:CD	2.35	0.56
1:D:187:TRP:HD1	1:D:189:LEU:CD1	2.17	0.56
1:D:254:SER:O	1:D:257:ASP:HB3	2.04	0.56
1:A:177:LEU:HD22	1:C:4:LYS:CE	2.34	0.56
1:B:4:LYS:CE	1:D:177:LEU:HD22	2.34	0.56
1:B:24:VAL:HG12	1:B:92:ILE:HG23	1.86	0.56
1:B:249:TRP:HZ2	1:D:32:MET:HG3	1.71	0.56
1:B:276:VAL:HG11	1:B:288:LEU:HD13	1.87	0.56
1:B:302:PHE:N	1:C:9:GLN:O	2.29	0.56
1:D:24:VAL:HG12	1:D:92:ILE:HG23	1.86	0.56
1:A:16:LYS:C	1:A:17:LEU:HD22	2.30	0.56
1:A:115:ILE:O	1:A:119:ILE:HD13	2.04	0.56
1:A:229:VAL:O	1:A:233:VAL:HG23	2.05	0.56
1:C:119:ILE:O	1:C:123:VAL:HG13	2.06	0.56
1:C:254:SER:O	1:C:257:ASP:HB3	2.04	0.56
1:D:164:LEU:HD13	1:D:192:HIS:CE1	2.39	0.56
1:A:39:LEU:HD22	1:A:71:LEU:HD13	1.86	0.56
1:B:9:GLN:O	1:C:302:PHE:N	2.29	0.56
1:C:202:GLY:HA3	1:D:210:LEU:HB3	1.74	0.56
1:C:229:VAL:O	1:C:233:VAL:HG23	2.05	0.56
1:D:120:VAL:HG13	1:D:121:PRO:CD	2.35	0.56
1:A:131:LYS:HZ2	1:A:262:ILE:HG21	1.70	0.56
1:D:119:ILE:O	1:D:123:VAL:HG13	2.06	0.56
1:D:308:THR:O	1:D:309:ALA:C	2.48	0.56
1:B:119:ILE:O	1:B:123:VAL:HG13	2.06	0.56
1:A:16:LYS:O	1:A:17:LEU:HD13	2.06	0.56
1:A:152:PHE:HB2	1:A:153:PRO:HD2	1.86	0.56
1:A:302:PHE:CE2	1:D:11:LEU:HD12	2.41	0.56
1:B:17:LEU:CD1	1:C:297:SER:HB3	2.36	0.56
1:C:227:LYS:HD3	1:C:228:ASN:N	2.19	0.56
1:A:11:LEU:HD12	1:D:302:PHE:CE2	2.41	0.56
1:B:212:SER:O	1:B:215:PRO:HD2	2.06	0.56
1:B:302:PHE:CE2	1:C:11:LEU:HD12	2.41	0.56
1:B:308:THR:O	1:B:309:ALA:C	2.48	0.56
1:A:41:LYS:HB3	1:A:43:LEU:CD1	2.32	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:LEU:CD2	1:C:249:TRP:HD1	2.18	0.56
1:A:119:ILE:O	1:A:123:VAL:HG13	2.06	0.56
1:B:11:LEU:HD12	1:C:302:PHE:CE2	2.41	0.56
1:B:297:SER:HB3	1:C:17:LEU:CD1	2.36	0.56
1:C:32:MET:CE	1:C:60:GLU:HB3	2.34	0.56
1:C:39:LEU:C	1:C:41:LYS:H	2.14	0.56
1:C:131:LYS:HZ2	1:C:262:ILE:HG21	1.71	0.56
1:C:276:VAL:HG11	1:C:288:LEU:HD13	1.87	0.56
1:C:308:THR:O	1:C:309:ALA:C	2.48	0.56
1:D:39:LEU:C	1:D:41:LYS:H	2.14	0.56
1:D:158:ILE:HG12	1:D:299:ILE:CD1	2.35	0.56
1:A:17:LEU:CD1	1:D:297:SER:HB3	2.36	0.56
1:A:32:MET:HG3	1:C:249:TRP:HZ2	1.71	0.56
1:A:39:LEU:C	1:A:41:LYS:H	2.14	0.56
1:A:324:ASN:O	1:A:327:LYS:N	2.38	0.56
1:B:78:PHE:CD1	1:B:79:GLY:N	2.74	0.56
1:C:137:ASN:HB3	1:C:138:PRO:HG2	1.88	0.56
1:C:272:VAL:C	1:C:289:SER:HB2	2.31	0.56
1:D:78:PHE:CD1	1:D:79:GLY:N	2.74	0.56
1:A:9:GLN:O	1:D:302:PHE:N	2.29	0.55
1:A:308:THR:O	1:A:309:ALA:C	2.48	0.55
1:B:16:LYS:O	1:B:17:LEU:HD13	2.06	0.55
1:B:158:ILE:HG12	1:B:299:ILE:CD1	2.36	0.55
1:C:2:THR:O	1:C:6:GLN:HB2	2.06	0.55
1:C:46:GLU:CB	1:C:75:LYS:HE3	2.36	0.55
1:D:229:VAL:O	1:D:233:VAL:HG23	2.05	0.55
1:A:78:PHE:CD1	1:A:79:GLY:N	2.74	0.55
1:A:169:PHE:CD2	1:A:188:VAL:HG23	2.42	0.55
1:C:208:VAL:O	1:D:201:SER:O	2.24	0.55
1:C:258:LEU:O	1:C:262:ILE:HG13	2.06	0.55
1:D:272:VAL:C	1:D:289:SER:HB2	2.32	0.55
1:D:276:VAL:HG11	1:D:288:LEU:HD13	1.87	0.55
1:A:249:TRP:HZ2	1:C:32:MET:HG3	1.71	0.55
1:A:303:VAL:CG2	1:D:7:LEU:HD23	2.36	0.55
1:B:137:ASN:HB3	1:B:138:PRO:HG2	1.88	0.55
1:B:221:LYS:O	1:B:223:LYS:N	2.37	0.55
1:A:7:LEU:HD23	1:D:303:VAL:CG2	2.37	0.55
1:A:30:VAL:HG13	1:A:251:ILE:HG23	1.89	0.55
1:B:272:VAL:C	1:B:289:SER:HB2	2.32	0.55
1:B:277:LYS:HG3	1:B:278:GLY:N	2.22	0.55
1:C:78:PHE:CD1	1:C:79:GLY:N	2.74	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:GLU:CB	1:D:75:LYS:HE3	2.36	0.55
1:D:282:ILE:CD1	1:D:319:ALA:HB2	2.37	0.55
1:A:208:VAL:O	1:B:201:SER:O	2.24	0.55
1:A:212:SER:O	1:A:215:PRO:HD2	2.06	0.55
1:C:212:SER:O	1:C:215:PRO:HD2	2.06	0.55
1:D:32:MET:CE	1:D:60:GLU:HB3	2.34	0.55
1:A:4:LYS:CE	1:C:177:LEU:HD22	2.34	0.55
1:A:46:GLU:CB	1:A:75:LYS:HE3	2.36	0.55
1:A:258:LEU:O	1:A:262:ILE:HG13	2.07	0.55
1:B:244:LYS:NZ	1:D:60:GLU:OE2	2.33	0.55
1:B:282:ILE:CD1	1:B:319:ALA:HB2	2.37	0.55
1:D:112:ASN:O	1:D:115:ILE:N	2.40	0.55
1:D:212:SER:O	1:D:215:PRO:HD2	2.06	0.55
1:D:258:LEU:O	1:D:262:ILE:HG13	2.06	0.55
1:A:116:MET:O	1:A:120:VAL:HG12	2.07	0.55
1:A:137:ASN:H	1:A:142:LEU:HD12	1.72	0.55
1:A:272:VAL:C	1:A:289:SER:HB2	2.32	0.55
1:B:39:LEU:C	1:B:41:LYS:H	2.14	0.55
1:C:30:VAL:HG13	1:C:251:ILE:HG23	1.89	0.55
1:C:137:ASN:H	1:C:142:LEU:HD12	1.72	0.55
1:C:208:VAL:CB	1:D:212:SER:CB	2.78	0.55
1:C:212:SER:CA	1:D:208:VAL:HB	2.33	0.55
1:C:282:ILE:CD1	1:C:319:ALA:HB2	2.37	0.55
1:D:16:LYS:O	1:D:17:LEU:HD13	2.06	0.55
1:D:275:LEU:CD1	1:D:277:LYS:HB3	2.37	0.55
1:A:124:ILE:HD12	1:A:152:PHE:CE2	2.42	0.55
1:A:282:ILE:CD1	1:A:319:ALA:HB2	2.37	0.55
1:A:297:SER:HB3	1:D:17:LEU:CD1	2.36	0.55
1:B:2:THR:O	1:B:6:GLN:HB2	2.05	0.55
1:B:7:LEU:HD23	1:C:303:VAL:CG2	2.37	0.55
1:B:30:VAL:HG13	1:B:251:ILE:HG23	1.89	0.55
1:B:116:MET:O	1:B:120:VAL:HG12	2.07	0.55
1:B:124:ILE:HD12	1:B:152:PHE:CE2	2.42	0.55
1:C:112:ASN:O	1:C:115:ILE:N	2.40	0.55
1:D:2:THR:O	1:D:6:GLN:HB2	2.06	0.55
1:D:124:ILE:HD12	1:D:152:PHE:CE2	2.42	0.55
1:B:4:LYS:HE2	1:D:177:LEU:CA	2.36	0.55
1:C:124:ILE:HD12	1:C:152:PHE:CE2	2.42	0.55
1:C:158:ILE:HG12	1:C:299:ILE:CD1	2.35	0.55
1:C:169:PHE:CD2	1:C:188:VAL:HG23	2.42	0.55
1:C:308:THR:HG22	1:C:311:GLU:CD	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:LYS:HE2	1:C:177:LEU:CB	2.37	0.55
1:B:4:LYS:HE2	1:D:177:LEU:CB	2.37	0.55
1:B:32:MET:HG3	1:D:249:TRP:HZ2	1.70	0.55
1:B:177:LEU:CB	1:D:4:LYS:HE2	2.37	0.55
1:B:258:LEU:O	1:B:262:ILE:HG13	2.06	0.55
1:B:303:VAL:CG2	1:C:7:LEU:HD23	2.37	0.55
1:C:16:LYS:O	1:C:17:LEU:HD13	2.06	0.55
1:D:197:VAL:C	1:D:198:PRO:O	2.46	0.55
1:A:36:ILE:CA	1:A:39:LEU:HD12	2.30	0.54
1:B:112:ASN:O	1:B:115:ILE:N	2.40	0.54
1:B:275:LEU:CD1	1:B:277:LYS:HB3	2.37	0.54
1:C:201:SER:O	1:D:208:VAL:O	2.24	0.54
1:D:200:TRP:O	1:D:201:SER:C	2.50	0.54
1:D:308:THR:HG22	1:D:311:GLU:CD	2.32	0.54
1:C:97:ALA:O	1:C:108:LEU:HD13	2.08	0.54
1:D:169:PHE:CD2	1:D:188:VAL:HG23	2.42	0.54
1:A:208:VAL:CB	1:B:212:SER:CB	2.78	0.54
1:A:208:VAL:N	1:B:208:VAL:HG22	2.22	0.54
1:A:249:TRP:HD1	1:C:64:LEU:CD2	2.18	0.54
1:B:137:ASN:H	1:B:142:LEU:HD12	1.72	0.54
1:B:169:PHE:CD2	1:B:188:VAL:HG23	2.41	0.54
1:B:200:TRP:O	1:B:201:SER:C	2.51	0.54
1:C:106:LEU:H	1:C:106:LEU:HD12	1.72	0.54
1:D:97:ALA:O	1:D:108:LEU:HD13	2.08	0.54
1:A:177:LEU:CB	1:C:4:LYS:HE2	2.37	0.54
1:D:30:VAL:HG13	1:D:251:ILE:HG23	1.89	0.54
1:D:116:MET:O	1:D:120:VAL:HG12	2.07	0.54
1:A:2:THR:O	1:A:6:GLN:HB2	2.06	0.54
1:A:158:ILE:HG12	1:A:299:ILE:CD1	2.35	0.54
1:A:308:THR:HG22	1:A:311:GLU:CD	2.32	0.54
1:C:200:TRP:O	1:C:201:SER:C	2.50	0.54
1:A:137:ASN:HB3	1:A:138:PRO:HG2	1.88	0.54
1:A:208:VAL:HG22	1:B:208:VAL:N	2.23	0.54
1:B:308:THR:HG22	1:B:311:GLU:CD	2.32	0.54
1:D:137:ASN:O	1:D:139:VAL:HG22	2.08	0.54
1:D:137:ASN:HB3	1:D:138:PRO:HG2	1.88	0.54
1:D:275:LEU:HD11	1:D:277:LYS:HB3	1.90	0.54
1:A:121:PRO:HA	1:A:124:ILE:CG2	2.37	0.54
1:A:202:GLY:HA3	1:B:210:LEU:HB3	1.74	0.54
1:B:64:LEU:CD2	1:D:249:TRP:HD1	2.18	0.54
1:B:97:ALA:O	1:B:108:LEU:HD13	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:282:ILE:HD13	1:C:319:ALA:HB2	1.90	0.54
1:D:109:LEU:O	1:D:113:VAL:HG12	2.08	0.54
1:D:219:THR:HG22	1:D:220:ASP:H	1.69	0.54
1:A:277:LYS:HG3	1:A:278:GLY:N	2.21	0.54
1:B:12:VAL:CB	1:B:13:PRO:HD3	2.17	0.54
1:B:106:LEU:HD12	1:B:106:LEU:H	1.73	0.54
1:C:100:VAL:O	1:C:103:GLN:HB3	2.08	0.54
1:C:109:LEU:O	1:C:113:VAL:HG12	2.08	0.54
1:C:116:MET:O	1:C:120:VAL:HG12	2.07	0.54
1:D:282:ILE:HD13	1:D:319:ALA:HB2	1.90	0.54
1:A:112:ASN:O	1:A:115:ILE:N	2.40	0.54
1:A:137:ASN:O	1:A:139:VAL:HG22	2.08	0.54
1:B:60:GLU:OE2	1:D:244:LYS:NZ	2.33	0.54
1:B:100:VAL:O	1:B:103:GLN:HB3	2.07	0.54
1:B:137:ASN:O	1:B:139:VAL:HG22	2.08	0.54
1:B:177:LEU:CA	1:D:4:LYS:HE2	2.36	0.54
1:C:137:ASN:O	1:C:139:VAL:HG22	2.08	0.54
1:A:129:ASP:HB3	2:A:347:HOH:O	2.08	0.54
1:A:201:SER:O	1:B:208:VAL:O	2.25	0.54
1:B:120:VAL:HG13	1:B:121:PRO:CD	2.35	0.54
1:B:324:ASN:O	1:B:327:LYS:N	2.38	0.54
1:D:21:LYS:HD2	1:D:46:GLU:CD	2.33	0.54
1:D:100:VAL:O	1:D:103:GLN:HB3	2.07	0.54
1:A:200:TRP:O	1:A:201:SER:C	2.51	0.53
1:A:275:LEU:CD1	1:A:277:LYS:HB3	2.37	0.53
1:C:189:LEU:HD23	1:C:315:LEU:HD11	1.91	0.53
1:C:275:LEU:HD11	1:C:277:LYS:HB3	1.90	0.53
1:C:277:LYS:HG3	1:C:278:GLY:N	2.21	0.53
1:C:318:SER:O	1:C:319:ALA:C	2.51	0.53
1:D:277:LYS:HG3	1:D:278:GLY:N	2.22	0.53
1:D:318:SER:O	1:D:319:ALA:C	2.51	0.53
1:A:120:VAL:HG13	1:A:121:PRO:CD	2.35	0.53
1:D:106:LEU:H	1:D:106:LEU:HD12	1.72	0.53
1:A:189:LEU:HD23	1:A:315:LEU:HD11	1.90	0.53
1:B:211:LYS:CD	1:D:7:LEU:CG	2.85	0.53
1:C:275:LEU:CD1	1:C:277:LYS:HB3	2.37	0.53
1:D:137:ASN:H	1:D:142:LEU:HD12	1.72	0.53
1:A:4:LYS:HE2	1:C:177:LEU:CA	2.36	0.53
1:B:109:LEU:O	1:B:113:VAL:HG12	2.08	0.53
1:D:126:ASN:O	1:D:128:PRO:HD3	2.09	0.53
1:A:21:LYS:HD2	1:A:46:GLU:CD	2.33	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:LEU:CG	1:A:277:LYS:HB3	2.39	0.53
1:A:279:PHE:HZ	1:D:9:GLN:NE2	1.86	0.53
1:B:275:LEU:HD11	1:B:277:LYS:HB3	1.90	0.53
1:B:275:LEU:CG	1:B:277:LYS:HB3	2.38	0.53
1:C:208:VAL:HG22	1:D:208:VAL:N	2.22	0.53
1:A:137:ASN:C	1:A:137:ASN:HD22	2.16	0.53
1:A:275:LEU:HD11	1:A:277:LYS:HB3	1.90	0.53
1:D:93:ILE:CD1	1:D:120:VAL:HG23	2.39	0.53
1:A:17:LEU:HD11	1:D:297:SER:CB	2.39	0.53
1:A:19:ARG:HB3	1:A:20:CYS:SG	2.49	0.53
1:A:90:LEU:HD21	1:A:133:ILE:HD12	1.91	0.53
1:A:100:VAL:O	1:A:103:GLN:HB3	2.07	0.53
1:A:204:ASN:H	1:A:204:ASN:ND2	2.03	0.53
1:B:21:LYS:HD2	1:B:46:GLU:CD	2.33	0.53
1:C:221:LYS:O	1:C:223:LYS:N	2.37	0.53
1:A:97:ALA:O	1:A:108:LEU:HD13	2.07	0.53
1:A:109:LEU:O	1:A:113:VAL:HG12	2.08	0.53
1:C:19:ARG:HB3	1:C:20:CYS:SG	2.49	0.53
1:C:90:LEU:HD21	1:C:133:ILE:HD12	1.90	0.53
1:C:275:LEU:CG	1:C:277:LYS:HB3	2.38	0.53
1:D:137:ASN:C	1:D:137:ASN:HD22	2.16	0.53
1:D:284:GLU:O	1:D:286:VAL:N	2.35	0.53
1:A:27:VAL:HG21	1:A:57:LEU:HD22	1.91	0.53
1:A:177:LEU:CA	1:C:4:LYS:HE2	2.36	0.53
1:A:318:SER:O	1:A:319:ALA:C	2.51	0.53
1:B:189:LEU:HD21	1:B:199:ILE:CD1	2.30	0.53
1:C:21:LYS:HD2	1:C:46:GLU:CD	2.33	0.53
1:C:93:ILE:CD1	1:C:120:VAL:HG23	2.39	0.53
1:A:6:GLN:HE22	1:C:216:ALA:HB1	1.73	0.53
1:B:4:LYS:HE2	1:D:177:LEU:HD22	1.91	0.53
1:B:19:ARG:HB3	1:B:20:CYS:SG	2.49	0.53
1:B:93:ILE:CD1	1:B:120:VAL:HG23	2.39	0.53
1:B:297:SER:CB	1:C:17:LEU:HD11	2.39	0.53
1:C:212:SER:CB	1:D:208:VAL:CB	2.78	0.53
1:A:12:VAL:CB	1:A:13:PRO:HD3	2.17	0.52
1:A:93:ILE:CD1	1:A:120:VAL:HG23	2.39	0.52
1:A:177:LEU:HD22	1:C:4:LYS:HE2	1.91	0.52
1:B:46:GLU:CB	1:B:75:LYS:HE3	2.36	0.52
1:B:269:VAL:HG23	1:B:292:CYS:C	2.35	0.52
1:D:275:LEU:CG	1:D:277:LYS:HB3	2.39	0.52
1:A:106:LEU:H	1:A:106:LEU:HD12	1.72	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:PHE:CB	1:A:153:PRO:HD2	2.40	0.52
1:A:227:LYS:CE	1:A:231:LYS:HZ1	2.20	0.52
1:A:231:LYS:HZ3	1:A:231:LYS:HB2	1.73	0.52
1:A:282:ILE:HD13	1:A:319:ALA:HB2	1.91	0.52
1:B:8:ILE:CG2	1:C:301:ASP:OD2	2.51	0.52
1:B:216:ALA:HB1	1:D:6:GLN:HE22	1.73	0.52
1:D:324:ASN:O	1:D:327:LYS:N	2.38	0.52
1:B:17:LEU:HD11	1:C:297:SER:CB	2.39	0.52
1:B:318:SER:O	1:B:319:ALA:C	2.51	0.52
1:C:126:ASN:O	1:C:128:PRO:HD3	2.09	0.52
1:A:28:GLY:O	1:A:30:VAL:N	2.42	0.52
1:A:230:HIS:O	1:A:234:VAL:HG12	2.09	0.52
1:B:276:VAL:HG21	1:B:288:LEU:CD1	2.39	0.52
1:B:282:ILE:HD13	1:B:319:ALA:HB2	1.90	0.52
1:D:158:ILE:HG22	1:D:159:GLY:H	1.75	0.52
1:D:276:VAL:HG21	1:D:288:LEU:CD1	2.39	0.52
1:A:126:ASN:O	1:A:128:PRO:HD3	2.09	0.52
1:A:245:GLY:O	1:A:246:TYR:HB3	2.10	0.52
1:A:269:VAL:HG23	1:A:292:CYS:C	2.34	0.52
1:A:276:VAL:HG21	1:A:288:LEU:CD1	2.39	0.52
1:A:297:SER:CB	1:D:17:LEU:HD11	2.39	0.52
1:C:28:GLY:O	1:C:30:VAL:N	2.42	0.52
1:C:96:GLY:HA2	1:C:115:ILE:CG1	2.40	0.52
1:C:276:VAL:HG21	1:C:288:LEU:CD1	2.39	0.52
1:D:221:LYS:O	1:D:223:LYS:N	2.37	0.52
1:C:158:ILE:HG22	1:C:159:GLY:H	1.75	0.52
1:B:27:VAL:HG21	1:B:57:LEU:HD22	1.91	0.52
1:B:90:LEU:HD21	1:B:133:ILE:HD12	1.90	0.52
1:B:106:LEU:HD22	1:B:325:MET:CE	2.39	0.52
1:B:137:ASN:C	1:B:139:VAL:N	2.56	0.52
1:B:189:LEU:HD23	1:B:315:LEU:HD11	1.90	0.52
1:C:324:ASN:O	1:C:326:GLN:N	2.43	0.52
1:A:23:THR:HA	1:A:48:ALA:O	2.09	0.52
1:A:306:ASN:ND2	1:A:306:ASN:H	2.06	0.52
1:B:96:GLY:HA2	1:B:115:ILE:CG1	2.40	0.52
1:B:152:PHE:CB	1:B:153:PRO:HD2	2.40	0.52
1:B:204:ASN:H	1:B:204:ASN:ND2	2.03	0.52
1:B:245:GLY:O	1:B:246:TYR:HB3	2.10	0.52
1:C:208:VAL:CB	1:D:212:SER:CA	2.88	0.52
1:C:208:VAL:N	1:D:208:VAL:HG22	2.23	0.52
1:D:204:ASN:H	1:D:204:ASN:ND2	2.03	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:245:GLY:O	1:D:246:TYR:HB3	2.10	0.52
1:B:126:ASN:O	1:B:128:PRO:HD3	2.09	0.52
1:B:230:HIS:O	1:B:234:VAL:HG12	2.10	0.52
1:A:211:LYS:CD	1:C:7:LEU:CG	2.85	0.52
1:B:23:THR:HA	1:B:48:ALA:O	2.09	0.52
1:B:28:GLY:O	1:B:30:VAL:N	2.42	0.52
1:B:32:MET:O	1:B:35:ALA:HB3	2.10	0.52
1:C:208:VAL:CG2	1:D:208:VAL:HA	2.40	0.52
1:D:269:VAL:HG23	1:D:292:CYS:C	2.35	0.52
1:A:186:GLY:HA2	1:A:203:VAL:HG22	1.92	0.51
1:C:197:VAL:C	1:C:198:PRO:O	2.46	0.51
1:D:19:ARG:HB3	1:D:20:CYS:SG	2.49	0.51
1:D:28:GLY:O	1:D:30:VAL:N	2.42	0.51
1:A:297:SER:HB3	1:D:17:LEU:HD11	1.92	0.51
1:A:303:VAL:CG2	1:D:7:LEU:CD2	2.89	0.51
1:C:27:VAL:HG21	1:C:57:LEU:HD22	1.91	0.51
1:C:177:LEU:CD1	1:C:205:VAL:HG21	2.40	0.51
1:D:23:THR:HA	1:D:48:ALA:O	2.09	0.51
1:D:324:ASN:O	1:D:326:GLN:N	2.43	0.51
1:B:308:THR:HG23	1:B:310:GLU:OE2	2.11	0.51
1:C:202:GLY:CA	1:D:210:LEU:H	2.23	0.51
1:C:208:VAL:HA	1:D:208:VAL:CG2	2.41	0.51
1:C:230:HIS:O	1:C:234:VAL:HG12	2.10	0.51
1:D:27:VAL:HG21	1:D:57:LEU:HD22	1.91	0.51
1:A:7:LEU:CD2	1:D:303:VAL:CG2	2.89	0.51
1:A:9:GLN:CG	1:D:302:PHE:HD1	2.16	0.51
1:A:17:LEU:HD11	1:D:297:SER:HB3	1.92	0.51
1:B:158:ILE:HG22	1:B:159:GLY:H	1.75	0.51
1:B:231:LYS:NZ	1:B:231:LYS:HB2	2.25	0.51
1:B:306:ASN:ND2	1:B:306:ASN:H	2.06	0.51
1:C:188:VAL:C	1:C:189:LEU:HD13	2.36	0.51
1:D:32:MET:O	1:D:35:ALA:HB3	2.10	0.51
1:D:177:LEU:CD1	1:D:205:VAL:HG21	2.40	0.51
1:A:4:LYS:HE2	1:C:177:LEU:HD22	1.91	0.51
1:A:96:GLY:HA2	1:A:115:ILE:HG12	1.92	0.51
1:A:188:VAL:C	1:A:189:LEU:HD13	2.36	0.51
1:A:189:LEU:HD21	1:A:199:ILE:CD1	2.30	0.51
1:A:208:VAL:CB	1:B:212:SER:CA	2.88	0.51
1:A:210:LEU:CB	1:B:202:GLY:CA	2.49	0.51
1:B:7:LEU:CD2	1:C:303:VAL:CG2	2.89	0.51
1:B:36:ILE:CA	1:B:39:LEU:HD12	2.30	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:MET:HB3	1:B:120:VAL:HG11	1.92	0.51
1:C:58:ARG:O	1:C:62:LEU:HD12	2.11	0.51
1:C:210:LEU:H	1:D:202:GLY:CA	2.23	0.51
1:C:269:VAL:HG23	1:C:292:CYS:C	2.35	0.51
1:D:90:LEU:HD21	1:D:133:ILE:HD12	1.91	0.51
1:D:96:GLY:HA2	1:D:115:ILE:HG12	1.92	0.51
1:D:106:LEU:HD22	1:D:325:MET:CE	2.39	0.51
1:D:152:PHE:CB	1:D:153:PRO:HD2	2.39	0.51
1:D:189:LEU:HD23	1:D:315:LEU:HD11	1.90	0.51
1:D:230:HIS:O	1:D:234:VAL:HG12	2.10	0.51
1:A:131:LYS:HZ2	1:A:262:ILE:CG2	2.23	0.51
1:A:158:ILE:HG22	1:A:159:GLY:H	1.75	0.51
1:A:177:LEU:CD1	1:A:205:VAL:HG21	2.40	0.51
1:A:244:LYS:NZ	1:C:60:GLU:OE2	2.33	0.51
1:B:186:GLY:HA2	1:B:203:VAL:HG22	1.92	0.51
1:D:17:LEU:O	1:D:18:SER:HB3	2.11	0.51
1:D:116:MET:HB3	1:D:120:VAL:HG11	1.92	0.51
1:A:146:VAL:CA	1:A:149:ILE:HG22	2.37	0.51
1:A:308:THR:HG23	1:A:310:GLU:OE2	2.11	0.51
1:C:32:MET:O	1:C:35:ALA:HB3	2.10	0.51
1:C:208:VAL:HG23	1:D:204:ASN:CB	2.41	0.51
1:C:212:SER:CA	1:D:208:VAL:CB	2.88	0.51
1:A:7:LEU:HA	1:C:211:LYS:HE3	1.93	0.51
1:A:58:ARG:O	1:A:62:LEU:HD12	2.11	0.51
1:B:197:VAL:C	1:B:198:PRO:O	2.46	0.51
1:B:284:GLU:O	1:B:286:VAL:N	2.35	0.51
1:B:303:VAL:CG2	1:C:7:LEU:CD2	2.89	0.51
1:D:96:GLY:HA2	1:D:115:ILE:CG1	2.40	0.51
1:A:32:MET:O	1:A:35:ALA:HB3	2.10	0.51
1:A:90:LEU:HD11	1:A:133:ILE:HD11	1.93	0.51
1:A:96:GLY:HA2	1:A:115:ILE:CG1	2.40	0.51
1:A:324:ASN:O	1:A:326:GLN:N	2.43	0.51
1:B:17:LEU:O	1:B:18:SER:HB3	2.11	0.51
1:B:177:LEU:CD1	1:B:205:VAL:HG21	2.40	0.51
1:B:188:VAL:C	1:B:189:LEU:HD13	2.36	0.51
1:B:324:ASN:O	1:B:326:GLN:N	2.43	0.51
1:C:116:MET:HB3	1:C:120:VAL:HG11	1.92	0.51
1:D:306:ASN:ND2	1:D:306:ASN:H	2.06	0.51
1:A:301:ASP:OD2	1:D:8:ILE:CG2	2.51	0.51
1:B:297:SER:HB3	1:C:17:LEU:HD11	1.92	0.51
1:C:23:THR:HA	1:C:48:ALA:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:245:GLY:O	1:C:246:TYR:HB3	2.10	0.51
1:D:186:GLY:HA2	1:D:203:VAL:HG22	1.93	0.51
1:D:308:THR:HG23	1:D:310:GLU:OE2	2.11	0.51
1:A:198:PRO:O	1:A:199:ILE:HG23	2.11	0.50
1:C:308:THR:HG23	1:C:310:GLU:OE2	2.11	0.50
1:D:188:VAL:C	1:D:189:LEU:HD13	2.36	0.50
1:A:231:LYS:NZ	1:A:231:LYS:HB2	2.25	0.50
1:B:17:LEU:HD11	1:C:297:SER:HB3	1.92	0.50
1:C:96:GLY:HA2	1:C:115:ILE:HG12	1.92	0.50
1:D:139:VAL:HG11	1:D:160:SER:OG	2.12	0.50
1:A:177:LEU:HD13	1:A:205:VAL:HG21	1.93	0.50
1:A:216:ALA:HB1	1:C:6:GLN:HE22	1.73	0.50
1:B:177:LEU:HD13	1:B:205:VAL:HG21	1.93	0.50
1:C:90:LEU:HD11	1:C:133:ILE:CD1	2.41	0.50
1:C:146:VAL:CA	1:C:149:ILE:HG22	2.37	0.50
1:D:90:LEU:HD11	1:D:133:ILE:HD11	1.93	0.50
1:D:212:SER:C	1:D:215:PRO:HD2	2.36	0.50
1:A:90:LEU:HD11	1:A:133:ILE:CD1	2.42	0.50
1:A:208:VAL:CG2	1:B:208:VAL:HA	2.41	0.50
1:B:68:SER:O	1:B:70:PHE:N	2.45	0.50
1:B:96:GLY:HA2	1:B:115:ILE:HG12	1.93	0.50
1:B:212:SER:C	1:B:215:PRO:HD2	2.36	0.50
1:C:139:VAL:HG11	1:C:160:SER:OG	2.12	0.50
1:C:177:LEU:HD13	1:C:205:VAL:HG21	1.92	0.50
1:C:186:GLY:HA2	1:C:203:VAL:HG22	1.92	0.50
1:C:198:PRO:O	1:C:199:ILE:HG23	2.11	0.50
1:D:231:LYS:NZ	1:D:231:LYS:HB2	2.25	0.50
1:A:106:LEU:HD22	1:A:325:MET:CE	2.39	0.50
1:B:58:ARG:O	1:B:62:LEU:HD12	2.11	0.50
1:C:68:SER:O	1:C:70:PHE:N	2.45	0.50
1:C:190:GLY:CA	1:C:288:LEU:HD23	2.42	0.50
1:D:198:PRO:O	1:D:199:ILE:HG23	2.11	0.50
1:A:137:ASN:HB3	1:A:138:PRO:CG	2.42	0.50
1:B:127:SER:O	1:B:130:CYS:HB3	2.12	0.50
1:B:162:CYS:O	1:B:163:ASN:C	2.55	0.50
1:B:177:LEU:HD22	1:D:4:LYS:HE2	1.91	0.50
1:B:249:TRP:CD1	1:D:64:LEU:HD23	2.47	0.50
1:C:204:ASN:H	1:C:204:ASN:ND2	2.03	0.50
1:C:324:ASN:O	1:C:327:LYS:N	2.38	0.50
1:A:7:LEU:HD23	1:D:303:VAL:HG22	1.94	0.50
1:A:116:MET:HB3	1:A:120:VAL:HG11	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:LYS:HE3	1:C:7:LEU:HA	1.94	0.50
1:B:6:GLN:HE22	1:D:216:ALA:HB1	1.73	0.50
1:B:137:ASN:HB3	1:B:138:PRO:CG	2.42	0.50
1:C:17:LEU:O	1:C:18:SER:HB3	2.11	0.50
1:C:212:SER:C	1:C:215:PRO:HD2	2.36	0.50
1:C:306:ASN:ND2	1:C:306:ASN:H	2.06	0.50
1:D:137:ASN:HB3	1:D:138:PRO:CG	2.42	0.50
1:D:146:VAL:CA	1:D:149:ILE:HG22	2.37	0.50
1:A:68:SER:O	1:A:70:PHE:N	2.44	0.50
1:A:147:TRP:HZ3	1:A:148:LYS:HZ1	1.58	0.50
1:A:211:LYS:HE2	1:B:304:LYS:O	2.12	0.50
1:A:212:SER:CA	1:B:208:VAL:CB	2.88	0.50
1:A:96:GLY:HA2	1:A:115:ILE:HD13	1.94	0.50
1:B:7:LEU:CG	1:D:211:LYS:CD	2.84	0.50
1:B:18:SER:O	1:B:19:ARG:HG2	2.12	0.50
1:B:57:LEU:C	1:B:59:GLY:H	2.20	0.50
1:C:127:SER:O	1:C:130:CYS:HB3	2.12	0.50
1:D:36:ILE:CA	1:D:39:LEU:HD12	2.30	0.50
1:A:190:GLY:CA	1:A:288:LEU:HD23	2.42	0.49
1:B:198:PRO:O	1:B:199:ILE:HG23	2.11	0.49
1:D:58:ARG:O	1:D:62:LEU:HD12	2.11	0.49
1:D:177:LEU:HD13	1:D:205:VAL:HG21	1.92	0.49
1:A:17:LEU:O	1:A:18:SER:HB3	2.11	0.49
1:A:127:SER:O	1:A:130:CYS:HB3	2.12	0.49
1:A:204:ASN:CB	1:B:208:VAL:HG23	2.41	0.49
1:A:208:VAL:HA	1:B:208:VAL:CG2	2.41	0.49
1:A:297:SER:HB3	1:D:17:LEU:HG	1.91	0.49
1:A:304:LYS:O	1:B:211:LYS:HE2	2.12	0.49
1:A:322:LEU:O	1:A:326:GLN:HG3	2.12	0.49
1:B:64:LEU:HD23	1:D:249:TRP:CD1	2.46	0.49
1:B:90:LEU:HD11	1:B:133:ILE:HD11	1.94	0.49
1:B:190:GLY:CA	1:B:288:LEU:HD23	2.42	0.49
1:C:36:ILE:CA	1:C:39:LEU:HD12	2.30	0.49
1:C:121:PRO:HA	1:C:124:ILE:CG2	2.37	0.49
1:C:137:ASN:C	1:C:137:ASN:HD22	2.16	0.49
1:D:112:ASN:O	1:D:113:VAL:C	2.54	0.49
1:D:127:SER:O	1:D:130:CYS:HB3	2.12	0.49
1:D:190:GLY:CA	1:D:288:LEU:HD23	2.42	0.49
1:A:212:SER:C	1:A:215:PRO:HD2	2.36	0.49
1:C:106:LEU:HD22	1:C:325:MET:CE	2.39	0.49
1:C:155:GLY:O	1:C:299:ILE:HD12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:SER:O	1:A:19:ARG:HG2	2.12	0.49
1:A:284:GLU:O	1:A:286:VAL:N	2.35	0.49
1:B:7:LEU:HD23	1:C:303:VAL:HG22	1.94	0.49
1:B:7:LEU:HA	1:D:211:LYS:HE3	1.93	0.49
1:D:68:SER:O	1:D:70:PHE:N	2.45	0.49
1:D:131:LYS:HZ2	1:D:262:ILE:CG2	2.26	0.49
1:A:96:GLY:O	1:A:115:ILE:HD13	2.12	0.49
1:B:155:GLY:O	1:B:299:ILE:HD12	2.13	0.49
1:C:57:LEU:C	1:C:59:GLY:H	2.20	0.49
1:C:152:PHE:CB	1:C:153:PRO:HD2	2.40	0.49
1:C:211:LYS:HE2	1:D:304:LYS:O	2.12	0.49
1:D:121:PRO:HA	1:D:124:ILE:CG2	2.37	0.49
1:D:270:HIS:N	1:D:292:CYS:O	2.41	0.49
1:A:64:LEU:HD23	1:C:249:TRP:CD1	2.47	0.49
1:A:208:VAL:HG23	1:B:204:ASN:CB	2.41	0.49
1:A:291:PRO:HB2	1:A:303:VAL:CG1	2.42	0.49
1:B:96:GLY:HA2	1:B:115:ILE:HD13	1.94	0.49
1:C:137:ASN:HB3	1:C:138:PRO:CG	2.42	0.49
1:C:162:CYS:O	1:C:163:ASN:C	2.55	0.49
1:C:322:LEU:O	1:C:326:GLN:HG3	2.12	0.49
1:D:162:CYS:O	1:D:163:ASN:C	2.55	0.49
1:D:320:ASP:O	1:D:321:THR:C	2.56	0.49
1:A:162:CYS:O	1:A:163:ASN:C	2.55	0.49
1:A:210:LEU:H	1:B:202:GLY:CA	2.23	0.49
1:B:19:ARG:HB2	1:C:296:GLU:OE2	2.13	0.49
1:B:90:LEU:HD11	1:B:133:ILE:CD1	2.42	0.49
1:B:96:GLY:O	1:B:115:ILE:HD13	2.12	0.49
1:B:303:VAL:HG22	1:C:7:LEU:HD23	1.94	0.49
1:B:322:LEU:O	1:B:326:GLN:HG3	2.12	0.49
1:C:291:PRO:HB2	1:C:303:VAL:CG1	2.42	0.49
1:D:90:LEU:HD11	1:D:133:ILE:CD1	2.42	0.49
1:D:96:GLY:O	1:D:115:ILE:HD13	2.12	0.49
1:D:137:ASN:HB3	1:D:138:PRO:HB2	1.95	0.49
1:A:15:ASP:C	1:A:16:LYS:HG2	2.38	0.49
1:A:107:ASP:C	1:A:109:LEU:N	2.71	0.49
1:A:112:ASN:O	1:A:113:VAL:C	2.55	0.49
1:A:139:VAL:HG11	1:A:160:SER:OG	2.12	0.49
1:A:303:VAL:HG22	1:D:7:LEU:HD23	1.94	0.49
1:B:9:GLN:CG	1:C:302:PHE:HD1	2.16	0.49
1:B:296:GLU:OE2	1:C:19:ARG:HB2	2.13	0.49
1:C:15:ASP:C	1:C:16:LYS:HG2	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:284:GLU:O	1:C:286:VAL:N	2.35	0.49
1:A:202:GLY:CA	1:B:210:LEU:CB	2.49	0.49
1:C:131:LYS:HZ3	1:C:158:ILE:HD12	1.77	0.49
1:D:15:ASP:C	1:D:16:LYS:HG2	2.38	0.49
1:D:122:GLY:O	1:D:126:ASN:ND2	2.46	0.49
1:A:27:VAL:HG23	1:A:56:LYS:HE2	1.95	0.49
1:A:147:TRP:CE3	1:A:148:LYS:HE3	2.48	0.49
1:A:155:GLY:O	1:A:299:ILE:HD12	2.12	0.49
1:A:249:TRP:CD1	1:C:64:LEU:HD23	2.46	0.49
1:B:139:VAL:HG11	1:B:160:SER:OG	2.12	0.49
1:B:211:LYS:HE3	1:D:7:LEU:HA	1.94	0.49
1:B:234:VAL:HG13	1:B:235:GLU:H	1.78	0.49
1:C:96:GLY:HA2	1:C:115:ILE:HD13	1.94	0.49
1:C:112:ASN:O	1:C:113:VAL:C	2.55	0.49
1:D:18:SER:O	1:D:19:ARG:HG2	2.12	0.49
1:B:15:ASP:C	1:B:16:LYS:HG2	2.38	0.48
1:B:297:SER:HB3	1:C:17:LEU:HG	1.91	0.48
1:C:96:GLY:O	1:C:115:ILE:HD13	2.12	0.48
1:C:304:LYS:O	1:D:211:LYS:HE2	2.12	0.48
1:D:291:PRO:CB	1:D:303:VAL:HG12	2.43	0.48
1:A:296:GLU:OE2	1:D:19:ARG:HB2	2.13	0.48
1:B:11:LEU:CG	1:C:302:PHE:CZ	2.87	0.48
1:B:32:MET:CG	1:D:249:TRP:HZ2	2.26	0.48
1:B:147:TRP:CE3	1:B:148:LYS:HE3	2.48	0.48
1:B:320:ASP:O	1:B:321:THR:C	2.56	0.48
1:C:18:SER:O	1:C:19:ARG:HG2	2.12	0.48
1:A:122:GLY:O	1:A:126:ASN:ND2	2.46	0.48
1:A:131:LYS:HZ2	1:A:262:ILE:HG12	1.77	0.48
1:A:302:PHE:CZ	1:D:11:LEU:CG	2.87	0.48
1:B:116:MET:O	1:B:117:LYS:C	2.57	0.48
1:B:328:ASN:O	1:B:329:LEU:HB2	2.13	0.48
1:C:23:THR:HG21	1:C:85:SER:OG	2.13	0.48
1:C:328:ASN:O	1:C:329:LEU:HB2	2.13	0.48
1:D:23:THR:HG21	1:D:85:SER:OG	2.13	0.48
1:A:4:LYS:C	1:A:6:GLN:H	2.22	0.48
1:A:8:ILE:HD13	1:D:303:VAL:HG23	1.96	0.48
1:A:234:VAL:HG13	1:A:235:GLU:H	1.78	0.48
1:A:320:ASP:O	1:A:321:THR:C	2.56	0.48
1:A:328:ASN:O	1:A:329:LEU:HB2	2.12	0.48
1:B:30:VAL:C	1:B:32:MET:N	2.70	0.48
1:B:121:PRO:HG3	1:B:149:ILE:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:GLY:O	1:B:126:ASN:ND2	2.46	0.48
1:B:131:LYS:HZ2	1:B:262:ILE:CG2	2.25	0.48
1:B:146:VAL:CA	1:B:149:ILE:HG22	2.37	0.48
1:B:249:TRP:HZ2	1:D:32:MET:CG	2.26	0.48
1:C:122:GLY:O	1:C:126:ASN:ND2	2.46	0.48
1:C:320:ASP:O	1:C:321:THR:C	2.56	0.48
1:D:121:PRO:HG3	1:D:149:ILE:HG23	1.95	0.48
1:D:322:LEU:O	1:D:326:GLN:HG3	2.12	0.48
1:D:328:ASN:O	1:D:329:LEU:HB2	2.13	0.48
1:A:11:LEU:CD1	1:D:302:PHE:CE2	2.97	0.48
1:A:239:GLU:O	1:A:243:MET:HG3	2.14	0.48
1:A:249:TRP:HZ2	1:C:32:MET:CG	2.26	0.48
1:A:302:PHE:CE2	1:D:11:LEU:CD1	2.97	0.48
1:B:112:ASN:O	1:B:113:VAL:C	2.54	0.48
1:C:284:GLU:HG2	1:C:323:TRP:CE2	2.49	0.48
1:D:155:GLY:O	1:D:299:ILE:HD12	2.13	0.48
1:D:234:VAL:HG13	1:D:235:GLU:H	1.78	0.48
1:A:170:ARG:C	1:A:173:ILE:HG22	2.38	0.48
1:A:284:GLU:HG2	1:A:323:TRP:CE2	2.49	0.48
1:B:64:LEU:HD23	1:D:249:TRP:HD1	1.78	0.48
1:B:107:ASP:C	1:B:109:LEU:N	2.71	0.48
1:B:137:ASN:C	1:B:137:ASN:HD22	2.16	0.48
1:B:137:ASN:HB3	1:B:138:PRO:HB2	1.95	0.48
1:D:57:LEU:C	1:D:59:GLY:H	2.20	0.48
1:D:96:GLY:HA2	1:D:115:ILE:HD13	1.94	0.48
1:A:131:LYS:HE2	1:A:158:ILE:HD11	1.96	0.48
1:A:208:VAL:CG2	1:B:207:GLY:C	2.87	0.48
1:B:4:LYS:C	1:B:6:GLN:H	2.21	0.48
1:B:239:GLU:O	1:B:243:MET:HG3	2.14	0.48
1:B:291:PRO:HB2	1:B:303:VAL:CG1	2.42	0.48
1:C:90:LEU:HD11	1:C:133:ILE:HD11	1.93	0.48
1:C:147:TRP:CE3	1:C:148:LYS:HE3	2.49	0.48
1:D:147:TRP:CE3	1:D:148:LYS:HE3	2.49	0.48
1:A:4:LYS:HA	1:A:4:LYS:HZ2	1.79	0.48
1:A:23:THR:HG21	1:A:85:SER:OG	2.14	0.48
1:A:57:LEU:C	1:A:59:GLY:H	2.20	0.48
1:B:11:LEU:CD1	1:C:302:PHE:CE2	2.97	0.48
1:C:234:VAL:HG13	1:C:235:GLU:H	1.78	0.48
1:D:170:ARG:C	1:D:173:ILE:HG22	2.39	0.48
1:A:249:TRP:HD1	1:C:64:LEU:HD23	1.78	0.48
1:B:8:ILE:HD13	1:C:303:VAL:HG23	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:LEU:HG	1:C:297:SER:HB3	1.91	0.48
1:B:21:LYS:HZ3	1:B:85:SER:C	2.21	0.48
1:B:170:ARG:C	1:B:173:ILE:HG22	2.39	0.48
1:C:147:TRP:HZ3	1:C:148:LYS:HZ1	1.59	0.48
1:C:260:ARG:NH1	1:C:268:ARG:NH1	2.56	0.48
1:C:270:HIS:O	1:C:291:PRO:HA	2.14	0.48
1:A:32:MET:CG	1:C:249:TRP:HZ2	2.26	0.48
1:A:64:LEU:HD23	1:C:249:TRP:HD1	1.78	0.48
1:A:291:PRO:CB	1:A:303:VAL:HG12	2.43	0.48
1:B:131:LYS:HE2	1:B:158:ILE:HD11	1.96	0.48
1:C:27:VAL:HG23	1:C:56:LYS:HE2	1.95	0.48
1:C:131:LYS:HE2	1:C:158:ILE:HD11	1.96	0.48
1:C:208:VAL:CG2	1:D:207:GLY:C	2.87	0.48
1:C:291:PRO:CB	1:C:303:VAL:HG12	2.43	0.48
1:D:27:VAL:HG23	1:D:56:LYS:HE2	1.95	0.48
1:A:19:ARG:HB2	1:D:296:GLU:OE2	2.13	0.47
1:A:94:THR:HG22	1:A:135:VAL:CB	2.38	0.47
1:A:207:GLY:C	1:B:208:VAL:CG2	2.87	0.47
1:A:241:LEU:O	1:A:242:ASP:C	2.57	0.47
1:A:253:LEU:O	1:A:256:THR:HG23	2.14	0.47
1:B:23:THR:HG21	1:B:85:SER:OG	2.14	0.47
1:B:203:VAL:O	1:B:213:LEU:HD23	2.14	0.47
1:C:137:ASN:HB3	1:C:138:PRO:HB2	1.95	0.47
1:C:203:VAL:O	1:C:213:LEU:HD23	2.14	0.47
1:C:239:GLU:O	1:C:243:MET:HG3	2.14	0.47
1:D:239:GLU:O	1:D:243:MET:HG3	2.13	0.47
1:D:284:GLU:HG2	1:D:323:TRP:CE2	2.49	0.47
1:A:7:LEU:CG	1:C:211:LYS:CD	2.85	0.47
1:A:49:LEU:HD13	1:A:57:LEU:HD11	1.96	0.47
1:A:131:LYS:NZ	1:A:262:ILE:HG12	2.30	0.47
1:A:202:GLY:CA	1:B:210:LEU:H	2.23	0.47
1:B:27:VAL:HG23	1:B:56:LYS:HE2	1.95	0.47
1:B:49:LEU:HD13	1:B:57:LEU:HD11	1.96	0.47
1:B:302:PHE:CE2	1:C:11:LEU:CD1	2.97	0.47
1:C:4:LYS:C	1:C:6:GLN:H	2.21	0.47
1:C:49:LEU:HD13	1:C:57:LEU:HD11	1.96	0.47
1:C:207:GLY:C	1:D:208:VAL:CG2	2.87	0.47
1:D:49:LEU:HD13	1:D:57:LEU:HD11	1.96	0.47
1:D:241:LEU:O	1:D:242:ASP:C	2.57	0.47
1:A:4:LYS:HA	1:A:4:LYS:HE3	1.97	0.47
1:A:207:GLY:CA	1:A:210:LEU:HB3	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:ARG:NH1	1:A:268:ARG:NH1	2.55	0.47
1:A:270:HIS:O	1:A:291:PRO:HA	2.14	0.47
1:B:284:GLU:HG2	1:B:323:TRP:CE2	2.49	0.47
1:C:253:LEU:O	1:C:256:THR:HG23	2.14	0.47
1:D:4:LYS:C	1:D:6:GLN:H	2.22	0.47
1:D:116:MET:O	1:D:117:LYS:C	2.57	0.47
1:D:291:PRO:HB2	1:D:303:VAL:CG1	2.42	0.47
1:B:161:GLY:CA	1:B:273:THR:HG23	2.44	0.47
1:C:150:SER:OG	1:C:151:GLY:N	2.48	0.47
1:C:208:VAL:HB	1:D:212:SER:CB	2.44	0.47
1:A:116:MET:O	1:A:117:LYS:C	2.57	0.47
1:A:137:ASN:HB3	1:A:138:PRO:HB2	1.95	0.47
1:A:203:VAL:O	1:A:213:LEU:HD23	2.14	0.47
1:C:21:LYS:HZ3	1:C:85:SER:C	2.22	0.47
1:C:107:ASP:C	1:C:109:LEU:N	2.70	0.47
1:C:131:LYS:NZ	1:C:262:ILE:HG12	2.30	0.47
1:C:270:HIS:N	1:C:292:CYS:O	2.41	0.47
1:D:161:GLY:CA	1:D:273:THR:HG23	2.45	0.47
1:A:9:GLN:O	1:D:301:ASP:HA	2.15	0.47
1:A:121:PRO:HG3	1:A:149:ILE:HG23	1.95	0.47
1:A:135:VAL:HG13	1:A:251:ILE:HD11	1.96	0.47
1:B:4:LYS:HA	1:B:4:LYS:HE3	1.97	0.47
1:B:9:GLN:O	1:C:301:ASP:HA	2.15	0.47
1:B:121:PRO:HA	1:B:124:ILE:CG2	2.37	0.47
1:B:131:LYS:NZ	1:B:262:ILE:HG12	2.30	0.47
1:B:164:LEU:O	1:B:167:ALA:HB3	2.15	0.47
1:B:291:PRO:CB	1:B:303:VAL:HG12	2.43	0.47
1:C:170:ARG:C	1:C:173:ILE:HG22	2.39	0.47
1:C:320:ASP:HA	1:C:323:TRP:HB3	1.97	0.47
1:A:7:LEU:HD23	1:A:7:LEU:C	2.40	0.47
1:A:208:VAL:HB	1:B:212:SER:CB	2.44	0.47
1:A:219:THR:CG2	1:A:220:ASP:N	2.78	0.47
1:C:241:LEU:O	1:C:242:ASP:C	2.57	0.47
1:D:131:LYS:HE2	1:D:158:ILE:HD11	1.96	0.47
1:D:270:HIS:O	1:D:291:PRO:HA	2.14	0.47
1:D:310:GLU:O	1:D:313:GLY:N	2.48	0.47
1:A:131:LYS:HZ2	1:A:262:ILE:CG1	2.27	0.47
1:A:303:VAL:HG23	1:D:8:ILE:HD13	1.96	0.47
1:B:207:GLY:CA	1:B:210:LEU:HB3	2.45	0.47
1:B:241:LEU:O	1:B:242:ASP:C	2.57	0.47
1:B:249:TRP:HD1	1:D:64:LEU:HD23	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:HIS:O	1:B:291:PRO:HA	2.14	0.47
1:B:279:PHE:CE1	1:C:9:GLN:NE2	2.81	0.47
1:B:301:ASP:HA	1:C:9:GLN:O	2.15	0.47
1:C:116:MET:O	1:C:117:LYS:C	2.57	0.47
1:C:204:ASN:CB	1:D:208:VAL:HG23	2.41	0.47
1:D:4:LYS:HA	1:D:4:LYS:HE3	1.97	0.47
1:D:105:ARG:HB2	1:D:107:ASP:OD2	2.15	0.47
1:D:203:VAL:O	1:D:213:LEU:HD23	2.14	0.47
1:A:204:ASN:CB	1:B:208:VAL:CG2	2.93	0.47
1:A:208:VAL:CG2	1:B:204:ASN:CB	2.93	0.47
1:B:301:ASP:OD2	1:C:8:ILE:CG2	2.51	0.47
1:C:105:ARG:HB2	1:C:107:ASP:OD2	2.15	0.47
1:C:260:ARG:NH1	1:C:268:ARG:HH22	2.09	0.47
1:D:107:ASP:C	1:D:109:LEU:N	2.71	0.47
1:A:212:SER:CB	1:B:208:VAL:HB	2.44	0.46
1:B:135:VAL:HG13	1:B:251:ILE:HD11	1.96	0.46
1:C:19:ARG:O	1:C:89:LYS:NZ	2.46	0.46
1:C:57:LEU:C	1:C:59:GLY:N	2.73	0.46
1:D:7:LEU:HD23	1:D:7:LEU:C	2.40	0.46
1:D:135:VAL:HG13	1:D:251:ILE:HD11	1.96	0.46
1:A:17:LEU:HB3	1:D:296:GLU:OE1	2.15	0.46
1:A:144:TYR:O	1:A:148:LYS:HB2	2.16	0.46
1:A:164:LEU:O	1:A:167:ALA:HB3	2.15	0.46
1:A:270:HIS:N	1:A:292:CYS:O	2.41	0.46
1:B:9:GLN:O	1:C:301:ASP:HB2	2.16	0.46
1:B:94:THR:HG22	1:B:135:VAL:CB	2.38	0.46
1:B:150:SER:OG	1:B:151:GLY:N	2.48	0.46
1:B:280:HIS:ND1	1:B:280:HIS:O	2.49	0.46
1:B:310:GLU:O	1:B:313:GLY:N	2.48	0.46
1:C:131:LYS:NZ	1:C:158:ILE:HD12	2.30	0.46
1:C:135:VAL:HG13	1:C:251:ILE:HD11	1.96	0.46
1:C:161:GLY:CA	1:C:273:THR:HG23	2.45	0.46
1:D:219:THR:CG2	1:D:220:ASP:N	2.78	0.46
1:A:9:GLN:O	1:D:301:ASP:HB2	2.16	0.46
1:A:105:ARG:HB2	1:A:107:ASP:OD2	2.15	0.46
1:B:253:LEU:O	1:B:256:THR:HG23	2.15	0.46
1:C:30:VAL:C	1:C:32:MET:N	2.70	0.46
1:C:180:ASN:C	1:C:182:THR:H	2.23	0.46
1:C:208:VAL:CG2	1:D:204:ASN:CB	2.93	0.46
1:C:280:HIS:ND1	1:C:280:HIS:O	2.49	0.46
1:D:30:VAL:O	1:D:34:CYS:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:131:LYS:NZ	1:D:262:ILE:HG12	2.30	0.46
1:D:172:LEU:O	1:D:175:GLU:HB3	2.16	0.46
1:D:253:LEU:O	1:D:256:THR:HG23	2.15	0.46
1:A:161:GLY:CA	1:A:273:THR:HG23	2.45	0.46
1:A:208:VAL:C	1:A:210:LEU:N	2.73	0.46
1:B:105:ARG:HB2	1:B:107:ASP:OD2	2.15	0.46
1:B:147:TRP:HZ3	1:B:148:LYS:HZ1	1.60	0.46
1:B:180:ASN:C	1:B:182:THR:H	2.23	0.46
1:B:303:VAL:HG23	1:C:8:ILE:HD13	1.96	0.46
1:C:164:LEU:O	1:C:167:ALA:HB3	2.15	0.46
1:C:208:VAL:C	1:C:210:LEU:N	2.73	0.46
1:C:260:ARG:HD3	1:C:260:ARG:C	2.41	0.46
1:C:310:GLU:O	1:C:313:GLY:N	2.48	0.46
1:D:260:ARG:C	1:D:260:ARG:HD3	2.41	0.46
1:D:320:ASP:HA	1:D:323:TRP:HB3	1.97	0.46
1:A:30:VAL:C	1:A:32:MET:N	2.70	0.46
1:A:30:VAL:O	1:A:34:CYS:HB3	2.16	0.46
1:A:94:THR:O	1:A:98:ARG:NH1	2.46	0.46
1:A:296:GLU:OE1	1:D:17:LEU:HB3	2.15	0.46
1:B:273:THR:HA	1:B:289:SER:HA	1.98	0.46
1:C:103:GLN:O	1:C:104:THR:C	2.59	0.46
1:D:204:ASN:ND2	1:D:204:ASN:N	2.63	0.46
1:B:11:LEU:CG	1:C:302:PHE:CE2	2.99	0.46
1:B:296:GLU:OE1	1:C:17:LEU:HB3	2.15	0.46
1:B:301:ASP:HB2	1:C:9:GLN:O	2.16	0.46
1:C:7:LEU:HD23	1:C:7:LEU:C	2.40	0.46
1:C:30:VAL:O	1:C:34:CYS:HB3	2.16	0.46
1:C:67:GLY:O	1:C:68:SER:C	2.58	0.46
1:C:121:PRO:HG3	1:C:149:ILE:HG23	1.95	0.46
1:C:144:TYR:O	1:C:148:LYS:HB2	2.16	0.46
1:C:172:LEU:O	1:C:175:GLU:HB3	2.16	0.46
1:C:190:GLY:HA2	1:C:288:LEU:HD23	1.98	0.46
1:C:204:ASN:CB	1:D:208:VAL:CG2	2.93	0.46
1:D:67:GLY:O	1:D:68:SER:C	2.59	0.46
1:D:94:THR:O	1:D:98:ARG:NH1	2.46	0.46
1:A:11:LEU:CG	1:D:302:PHE:CE2	2.99	0.46
1:A:17:LEU:HG	1:D:297:SER:HB3	1.91	0.46
1:A:150:SER:OG	1:A:151:GLY:N	2.48	0.46
1:C:207:GLY:CA	1:C:210:LEU:HB3	2.45	0.46
1:C:210:LEU:CB	1:D:202:GLY:CA	2.49	0.46
1:D:180:ASN:C	1:D:182:THR:H	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:207:GLY:CA	1:D:210:LEU:HB3	2.45	0.46
1:D:272:VAL:HG22	1:D:292:CYS:SG	2.56	0.46
1:A:96:GLY:HA2	1:A:115:ILE:CD1	2.46	0.46
1:A:158:ILE:CG1	1:A:299:ILE:HD11	2.42	0.46
1:A:272:VAL:HG22	1:A:292:CYS:SG	2.56	0.46
1:A:310:GLU:O	1:A:313:GLY:N	2.48	0.46
1:B:94:THR:O	1:B:98:ARG:NH1	2.46	0.46
1:B:131:LYS:NZ	1:B:158:ILE:HD12	2.30	0.46
1:B:208:VAL:C	1:B:210:LEU:N	2.73	0.46
1:B:302:PHE:CE2	1:C:11:LEU:CG	2.99	0.46
1:C:96:GLY:HA2	1:C:115:ILE:CD1	2.46	0.46
1:D:208:VAL:C	1:D:210:LEU:N	2.73	0.46
1:B:320:ASP:HA	1:B:323:TRP:HB3	1.97	0.46
1:C:219:THR:CG2	1:C:220:ASP:N	2.78	0.46
1:D:164:LEU:O	1:D:167:ALA:HB3	2.15	0.46
1:D:170:ARG:HA	1:D:173:ILE:CG2	2.46	0.46
1:A:260:ARG:C	1:A:260:ARG:HD3	2.40	0.46
1:B:7:LEU:HD23	1:B:7:LEU:C	2.40	0.46
1:B:103:GLN:O	1:B:104:THR:C	2.59	0.46
1:B:172:LEU:O	1:B:175:GLU:HB3	2.16	0.46
1:C:170:ARG:HA	1:C:173:ILE:CG2	2.46	0.46
1:A:4:LYS:HZ2	1:A:4:LYS:CA	2.30	0.45
1:A:8:ILE:CG2	1:D:301:ASP:OD2	2.51	0.45
1:A:53:ASP:O	1:A:55:ASP:N	2.50	0.45
1:A:67:GLY:O	1:A:68:SER:C	2.59	0.45
1:A:301:ASP:HB2	1:D:9:GLN:O	2.16	0.45
1:B:30:VAL:O	1:B:34:CYS:HB3	2.16	0.45
1:B:67:GLY:O	1:B:68:SER:C	2.59	0.45
1:B:96:GLY:HA2	1:B:115:ILE:CD1	2.46	0.45
1:B:260:ARG:C	1:B:260:ARG:HD3	2.40	0.45
1:C:94:THR:HG22	1:C:135:VAL:CB	2.38	0.45
1:D:57:LEU:C	1:D:59:GLY:N	2.73	0.45
1:A:103:GLN:O	1:A:104:THR:C	2.59	0.45
1:A:131:LYS:NZ	1:A:158:ILE:HD12	2.31	0.45
1:C:273:THR:HA	1:C:289:SER:HA	1.98	0.45
1:D:4:LYS:C	1:D:6:GLN:N	2.75	0.45
1:D:53:ASP:O	1:D:55:ASP:N	2.50	0.45
1:D:94:THR:HG22	1:D:135:VAL:CB	2.38	0.45
1:D:103:GLN:O	1:D:104:THR:C	2.59	0.45
1:D:144:TYR:O	1:D:148:LYS:HB2	2.16	0.45
1:D:260:ARG:NH1	1:D:268:ARG:HH22	2.09	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:280:HIS:ND1	1:D:280:HIS:O	2.49	0.45
1:A:51:ASP:HB2	1:A:57:LEU:CD2	2.46	0.45
1:A:280:HIS:ND1	1:A:280:HIS:O	2.49	0.45
1:B:116:MET:C	1:B:118:ALA:N	2.74	0.45
1:B:144:TYR:O	1:B:148:LYS:HB2	2.16	0.45
1:B:219:THR:CG2	1:B:220:ASP:N	2.78	0.45
1:C:272:VAL:HG22	1:C:292:CYS:SG	2.56	0.45
1:D:155:GLY:HA2	1:D:299:ILE:H	1.81	0.45
1:A:190:GLY:HA2	1:A:288:LEU:HD23	1.98	0.45
1:A:301:ASP:HA	1:D:9:GLN:O	2.15	0.45
1:B:17:LEU:HB3	1:C:296:GLU:OE1	2.15	0.45
1:B:222:ASN:O	1:B:223:LYS:HB2	2.17	0.45
1:B:302:PHE:CZ	1:C:11:LEU:CG	2.87	0.45
1:C:222:ASN:O	1:C:223:LYS:HB2	2.17	0.45
1:D:273:THR:HA	1:D:289:SER:HA	1.97	0.45
1:A:2:THR:HG22	1:A:3:VAL:N	2.32	0.45
1:A:180:ASN:C	1:A:182:THR:H	2.23	0.45
1:A:302:PHE:CE2	1:D:11:LEU:CG	2.99	0.45
1:C:276:VAL:CG1	1:C:288:LEU:HD13	2.47	0.45
1:D:150:SER:OG	1:D:151:GLY:N	2.48	0.45
1:D:190:GLY:HA2	1:D:288:LEU:HD23	1.98	0.45
1:A:57:LEU:C	1:A:59:GLY:N	2.73	0.45
1:A:170:ARG:HA	1:A:173:ILE:CG2	2.46	0.45
1:A:172:LEU:O	1:A:175:GLU:HB3	2.16	0.45
1:A:273:THR:HA	1:A:289:SER:HA	1.97	0.45
1:A:320:ASP:HA	1:A:323:TRP:HB3	1.97	0.45
1:B:309:ALA:O	1:B:312:GLU:HB3	2.17	0.45
1:C:94:THR:O	1:C:98:ARG:NH1	2.46	0.45
1:D:96:GLY:HA2	1:D:115:ILE:CD1	2.46	0.45
1:D:131:LYS:NZ	1:D:158:ILE:HD12	2.31	0.45
1:D:172:LEU:CD2	1:D:232:GLN:HE21	2.16	0.45
1:D:313:GLY:O	1:D:316:LYS:HB2	2.17	0.45
1:A:219:THR:HG21	1:A:222:ASN:N	2.32	0.45
1:A:222:ASN:O	1:A:223:LYS:HB2	2.17	0.45
1:B:103:GLN:OE1	1:B:111:ARG:NH2	2.46	0.45
1:B:323:TRP:O	1:B:324:ASN:C	2.60	0.45
1:D:190:GLY:O	1:D:288:LEU:HD23	2.17	0.45
1:D:217:ILE:HG23	1:D:217:ILE:O	2.17	0.45
1:A:116:MET:C	1:A:118:ALA:N	2.74	0.45
1:A:136:THR:O	1:A:137:ASN:CB	2.65	0.45
1:B:30:VAL:HG13	1:B:251:ILE:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:VAL:O	1:B:132:ILE:HG23	2.17	0.45
1:B:158:ILE:CG1	1:B:299:ILE:HD11	2.42	0.45
1:C:309:ALA:O	1:C:312:GLU:HB3	2.17	0.45
1:D:136:THR:O	1:D:137:ASN:CB	2.65	0.45
1:D:161:GLY:HA2	1:D:273:THR:HG23	1.99	0.45
1:A:120:VAL:O	1:A:121:PRO:C	2.60	0.45
1:A:309:ALA:O	1:A:312:GLU:HB3	2.17	0.45
1:B:2:THR:HG22	1:B:3:VAL:N	2.32	0.45
1:B:53:ASP:O	1:B:55:ASP:N	2.50	0.45
1:B:155:GLY:HA2	1:B:299:ILE:H	1.81	0.45
1:B:272:VAL:HG22	1:B:292:CYS:SG	2.56	0.45
1:C:203:VAL:HG12	1:C:213:LEU:HB2	1.99	0.45
1:C:204:ASN:ND2	1:C:204:ASN:N	2.63	0.45
1:C:212:SER:CB	1:D:208:VAL:HB	2.44	0.45
1:D:116:MET:C	1:D:118:ALA:N	2.74	0.45
1:D:270:HIS:HB3	1:D:272:VAL:HG13	1.99	0.45
1:A:91:VAL:O	1:A:132:ILE:HG23	2.17	0.44
1:C:53:ASP:O	1:C:55:ASP:N	2.50	0.44
1:C:172:LEU:HD13	1:C:232:GLN:HB3	1.99	0.44
1:D:172:LEU:HD13	1:D:232:GLN:HB3	1.99	0.44
1:D:276:VAL:CG1	1:D:288:LEU:HD13	2.47	0.44
1:B:136:THR:O	1:B:137:ASN:CB	2.65	0.44
1:B:170:ARG:HA	1:B:173:ILE:CG2	2.46	0.44
1:B:219:THR:HG21	1:B:222:ASN:N	2.32	0.44
1:B:270:HIS:HB3	1:B:272:VAL:HG13	1.98	0.44
1:B:313:GLY:O	1:B:316:LYS:HB2	2.17	0.44
1:D:275:LEU:CD1	1:D:285:GLU:HA	2.47	0.44
1:A:267:LYS:HA	1:A:294:LEU:O	2.17	0.44
1:B:172:LEU:HD13	1:B:232:GLN:HB3	1.99	0.44
1:B:223:LYS:HB3	1:B:224:GLN:H	1.45	0.44
1:B:310:GLU:O	1:B:311:GLU:C	2.61	0.44
1:C:91:VAL:O	1:C:132:ILE:HG23	2.17	0.44
1:C:313:GLY:O	1:C:316:LYS:HB2	2.17	0.44
1:A:28:GLY:O	1:A:29:ASP:C	2.61	0.44
1:A:146:VAL:HA	1:A:149:ILE:CG2	2.39	0.44
1:A:270:HIS:HB3	1:A:272:VAL:HG13	1.98	0.44
1:B:10:ASN:H	1:B:10:ASN:HD22	1.66	0.44
1:B:190:GLY:O	1:B:288:LEU:HD23	2.17	0.44
1:C:116:MET:C	1:C:118:ALA:N	2.74	0.44
1:C:120:VAL:O	1:C:121:PRO:C	2.60	0.44
1:C:270:HIS:HB3	1:C:272:VAL:HG13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:323:TRP:O	1:C:324:ASN:C	2.60	0.44
1:D:49:LEU:O	1:D:78:PHE:HD1	2.01	0.44
1:D:91:VAL:O	1:D:132:ILE:HG23	2.17	0.44
1:D:98:ARG:CB	1:D:99:MET:SD	3.05	0.44
1:D:203:VAL:HG12	1:D:213:LEU:HB2	2.00	0.44
1:D:222:ASN:O	1:D:223:LYS:HB2	2.17	0.44
1:A:98:ARG:CB	1:A:99:MET:SD	3.05	0.44
1:A:161:GLY:HA2	1:A:273:THR:HG23	1.99	0.44
1:A:234:VAL:O	1:A:235:GLU:C	2.61	0.44
1:A:323:TRP:O	1:A:324:ASN:C	2.60	0.44
1:C:155:GLY:HA2	1:C:299:ILE:H	1.82	0.44
1:C:161:GLY:HA2	1:C:273:THR:HG23	1.99	0.44
1:C:306:ASN:HD22	1:C:306:ASN:N	2.07	0.44
1:D:228:ASN:O	1:D:232:GLN:N	2.43	0.44
1:D:309:ALA:O	1:D:312:GLU:HB3	2.17	0.44
1:C:158:ILE:CG1	1:C:299:ILE:HD11	2.42	0.44
1:C:217:ILE:HG23	1:C:217:ILE:O	2.17	0.44
1:D:2:THR:HG22	1:D:3:VAL:N	2.32	0.44
1:A:155:GLY:HA2	1:A:299:ILE:H	1.81	0.44
1:A:203:VAL:HG12	1:A:213:LEU:HB2	1.99	0.44
1:A:269:VAL:HA	1:A:293:VAL:HA	2.00	0.44
1:B:98:ARG:CB	1:B:99:MET:SD	3.05	0.44
1:B:131:LYS:HZ2	1:B:262:ILE:CG1	2.31	0.44
1:B:267:LYS:HA	1:B:294:LEU:O	2.18	0.44
1:C:98:ARG:CB	1:C:99:MET:SD	3.05	0.44
1:C:136:THR:O	1:C:137:ASN:CB	2.65	0.44
1:C:208:VAL:HG23	1:D:204:ASN:CA	2.48	0.44
1:C:231:LYS:NZ	1:C:231:LYS:HB2	2.25	0.44
1:D:323:TRP:O	1:D:324:ASN:C	2.60	0.44
1:A:155:GLY:HA2	1:A:299:ILE:CD1	2.48	0.44
1:A:204:ASN:ND2	1:A:204:ASN:N	2.63	0.44
1:B:116:MET:C	1:B:120:VAL:HG12	2.43	0.44
1:B:120:VAL:O	1:B:121:PRO:C	2.60	0.44
1:B:270:HIS:N	1:B:292:CYS:O	2.40	0.44
1:C:2:THR:HG22	1:C:3:VAL:N	2.32	0.44
1:C:28:GLY:O	1:C:29:ASP:C	2.61	0.44
1:C:92:ILE:HD11	1:C:94:THR:HG21	1.99	0.44
1:C:190:GLY:O	1:C:288:LEU:HD23	2.17	0.44
1:C:227:LYS:HZ1	1:C:228:ASN:CG	2.26	0.44
1:C:228:ASN:O	1:C:232:GLN:N	2.43	0.44
1:D:131:LYS:HZ2	1:D:262:ILE:CG1	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:GLN:NE2	1:C:279:PHE:CE1	2.80	0.44
1:B:51:ASP:HB2	1:B:57:LEU:CD2	2.46	0.44
1:B:161:GLY:HA2	1:B:273:THR:HG23	1.99	0.44
1:B:189:LEU:HD23	1:B:315:LEU:CD1	2.48	0.44
1:B:190:GLY:HA2	1:B:288:LEU:HD23	1.99	0.44
1:C:314:LEU:H	1:C:314:LEU:HD12	1.83	0.44
1:D:51:ASP:HB2	1:D:57:LEU:CD2	2.47	0.44
1:D:269:VAL:HA	1:D:293:VAL:HA	2.00	0.44
1:A:4:LYS:C	1:A:6:GLN:N	2.75	0.43
1:A:49:LEU:O	1:A:78:PHE:HD1	2.01	0.43
1:A:116:MET:C	1:A:120:VAL:HG12	2.43	0.43
1:A:190:GLY:O	1:A:288:LEU:HD23	2.17	0.43
1:A:208:VAL:HG23	1:B:204:ASN:CA	2.48	0.43
1:B:95:ALA:HA	1:B:98:ARG:HH12	1.83	0.43
1:B:324:ASN:O	1:B:325:MET:C	2.61	0.43
1:C:116:MET:C	1:C:120:VAL:HG12	2.43	0.43
1:C:219:THR:HG21	1:C:222:ASN:N	2.33	0.43
1:D:324:ASN:O	1:D:325:MET:C	2.61	0.43
1:A:30:VAL:HG13	1:A:251:ILE:HG21	1.99	0.43
1:A:204:ASN:CG	1:B:208:VAL:HG22	2.41	0.43
1:A:217:ILE:HG23	1:A:217:ILE:O	2.17	0.43
1:A:310:GLU:O	1:A:311:GLU:C	2.61	0.43
1:A:313:GLY:O	1:A:316:LYS:HB2	2.17	0.43
1:B:28:GLY:O	1:B:29:ASP:C	2.61	0.43
1:B:203:VAL:HG12	1:B:213:LEU:HB2	1.99	0.43
1:C:2:THR:O	1:C:6:GLN:N	2.51	0.43
1:C:49:LEU:O	1:C:78:PHE:HD1	2.01	0.43
1:C:202:GLY:CA	1:D:210:LEU:CB	2.49	0.43
1:D:92:ILE:HD11	1:D:94:THR:HG21	2.00	0.43
1:D:120:VAL:O	1:D:121:PRO:C	2.60	0.43
1:A:172:LEU:HD13	1:A:232:GLN:HB3	1.99	0.43
1:A:304:LYS:H	1:A:304:LYS:HG2	1.68	0.43
1:B:46:GLU:CG	1:B:75:LYS:HE3	2.48	0.43
1:B:269:VAL:HA	1:B:293:VAL:HA	2.00	0.43
1:C:46:GLU:CG	1:C:75:LYS:HE3	2.48	0.43
1:C:155:GLY:HA2	1:C:299:ILE:CD1	2.48	0.43
1:C:267:LYS:HA	1:C:294:LEU:O	2.18	0.43
1:C:310:GLU:O	1:C:311:GLU:C	2.61	0.43
1:D:12:VAL:CB	1:D:13:PRO:CD	2.87	0.43
1:D:155:GLY:HA2	1:D:299:ILE:CD1	2.48	0.43
1:A:103:GLN:OE1	1:A:111:ARG:NH2	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:VAL:CG1	1:A:288:LEU:HD13	2.47	0.43
1:B:137:ASN:CA	1:B:139:VAL:HG13	2.32	0.43
1:B:217:ILE:O	1:B:217:ILE:HG23	2.17	0.43
1:C:4:LYS:C	1:C:6:GLN:N	2.75	0.43
1:C:241:LEU:HD12	1:C:242:ASP:N	2.33	0.43
1:D:46:GLU:CG	1:D:75:LYS:HE3	2.48	0.43
1:D:82:TYR:CE2	1:D:123:VAL:HG12	2.53	0.43
1:D:272:VAL:O	1:D:289:SER:HB2	2.19	0.43
1:A:11:LEU:CG	1:D:302:PHE:CZ	2.87	0.43
1:A:46:GLU:CG	1:A:75:LYS:HE3	2.48	0.43
1:A:171:TYR:O	1:A:172:LEU:C	2.62	0.43
1:A:302:PHE:HD1	1:D:9:GLN:CG	2.16	0.43
1:D:147:TRP:HA	1:D:157:VAL:HG11	2.00	0.43
1:D:264:LYS:HB2	1:D:266:LEU:CD1	2.40	0.43
1:A:204:ASN:CA	1:B:208:VAL:HG23	2.49	0.43
1:B:2:THR:O	1:B:6:GLN:N	2.51	0.43
1:B:28:GLY:O	1:B:31:GLY:N	2.52	0.43
1:B:121:PRO:HG2	1:B:149:ILE:HG23	2.00	0.43
1:B:176:LYS:HE2	1:B:226:TRP:CZ3	2.54	0.43
1:D:171:TYR:O	1:D:172:LEU:C	2.62	0.43
1:D:260:ARG:NH1	1:D:268:ARG:NH1	2.55	0.43
1:D:320:ASP:O	1:D:323:TRP:HB3	2.19	0.43
1:A:2:THR:O	1:A:6:GLN:N	2.51	0.43
1:B:272:VAL:O	1:B:289:SER:HB2	2.19	0.43
1:C:137:ASN:CA	1:C:139:VAL:HG13	2.32	0.43
1:C:204:ASN:CA	1:D:208:VAL:HG23	2.48	0.43
1:D:28:GLY:O	1:D:29:ASP:C	2.61	0.43
1:D:28:GLY:O	1:D:31:GLY:N	2.51	0.43
1:D:30:VAL:HG13	1:D:251:ILE:HG21	1.99	0.43
1:D:176:LYS:HE2	1:D:226:TRP:CZ3	2.54	0.43
1:D:275:LEU:C	1:D:277:LYS:H	2.27	0.43
1:A:28:GLY:O	1:A:31:GLY:N	2.52	0.43
1:A:176:LYS:HE2	1:A:226:TRP:CZ3	2.54	0.43
1:A:314:LEU:HD12	1:A:314:LEU:H	1.83	0.43
1:B:58:ARG:CG	1:B:78:PHE:HE2	2.32	0.43
1:B:276:VAL:CG1	1:B:288:LEU:HD13	2.47	0.43
1:C:28:GLY:O	1:C:31:GLY:N	2.52	0.43
1:C:95:ALA:HA	1:C:98:ARG:HH12	1.83	0.43
1:C:269:VAL:HA	1:C:293:VAL:HA	2.00	0.43
1:D:2:THR:O	1:D:6:GLN:N	2.51	0.43
1:D:219:THR:HG21	1:D:222:ASN:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:310:GLU:O	1:D:311:GLU:C	2.61	0.43
1:D:314:LEU:HD12	1:D:314:LEU:H	1.83	0.43
1:A:92:ILE:HD11	1:A:94:THR:HG21	1.99	0.43
1:A:241:LEU:HD12	1:A:242:ASP:N	2.33	0.43
1:A:272:VAL:O	1:A:289:SER:HB2	2.19	0.43
1:B:92:ILE:HD11	1:B:94:THR:HG21	2.00	0.43
1:B:155:GLY:HA2	1:B:299:ILE:CD1	2.48	0.43
1:C:234:VAL:O	1:C:235:GLU:C	2.61	0.43
1:C:260:ARG:HH11	1:C:268:ARG:NH2	2.12	0.43
1:C:286:VAL:HG11	1:C:319:ALA:HA	2.01	0.43
1:D:26:GLY:HA2	1:D:51:ASP:OD1	2.19	0.43
1:D:30:VAL:C	1:D:32:MET:N	2.70	0.43
1:D:116:MET:C	1:D:120:VAL:HG12	2.43	0.43
1:D:234:VAL:O	1:D:235:GLU:C	2.61	0.43
1:D:267:LYS:HA	1:D:294:LEU:O	2.18	0.43
1:A:9:GLN:NE2	1:D:279:PHE:CE1	2.80	0.43
1:A:56:LYS:HE3	1:A:60:GLU:CG	2.47	0.43
1:A:58:ARG:CG	1:A:78:PHE:HE2	2.32	0.43
1:A:189:LEU:HD23	1:A:315:LEU:CD1	2.49	0.43
1:A:207:GLY:N	1:A:210:LEU:HD13	2.33	0.43
1:B:49:LEU:O	1:B:78:PHE:HD1	2.01	0.43
1:B:57:LEU:C	1:B:59:GLY:N	2.73	0.43
1:B:207:GLY:N	1:B:210:LEU:HD13	2.33	0.43
1:B:302:PHE:HD1	1:C:9:GLN:CG	2.16	0.43
1:C:276:VAL:O	1:C:278:GLY:N	2.52	0.43
1:D:10:ASN:H	1:D:10:ASN:HD22	1.66	0.43
1:D:241:LEU:HD12	1:D:242:ASP:N	2.33	0.43
1:A:2:THR:HB	1:A:5:GLU:H	1.84	0.42
1:A:95:ALA:HA	1:A:98:ARG:HH12	1.83	0.42
1:A:207:GLY:C	1:A:210:LEU:HB3	2.44	0.42
1:B:4:LYS:C	1:B:6:GLN:N	2.74	0.42
1:B:27:VAL:HG22	1:B:51:ASP:OD2	2.19	0.42
1:B:82:TYR:CE2	1:B:123:VAL:HG12	2.53	0.42
1:B:131:LYS:HZ2	1:B:262:ILE:HG12	1.84	0.42
1:B:171:TYR:O	1:B:172:LEU:C	2.62	0.42
1:B:241:LEU:HD12	1:B:242:ASP:N	2.33	0.42
1:B:314:LEU:H	1:B:314:LEU:HD12	1.83	0.42
1:B:320:ASP:O	1:B:323:TRP:HB3	2.19	0.42
1:C:176:LYS:HE2	1:C:226:TRP:CZ3	2.54	0.42
1:C:208:VAL:O	1:C:209:THR:HB	2.19	0.42
1:D:2:THR:HB	1:D:5:GLU:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:131:LYS:HZ2	1:D:262:ILE:HG12	1.84	0.42
1:D:155:GLY:HA2	1:D:299:ILE:HD12	2.02	0.42
1:D:308:THR:N	1:D:311:GLU:HB2	2.34	0.42
1:A:198:PRO:O	1:A:199:ILE:CG2	2.68	0.42
1:A:324:ASN:O	1:A:325:MET:C	2.61	0.42
1:B:312:GLU:O	1:B:316:LYS:HG3	2.19	0.42
1:C:30:VAL:HG13	1:C:251:ILE:HG21	1.99	0.42
1:C:272:VAL:O	1:C:289:SER:HB2	2.18	0.42
1:C:320:ASP:O	1:C:323:TRP:HB3	2.19	0.42
1:D:58:ARG:CG	1:D:78:PHE:HE2	2.32	0.42
1:D:95:ALA:HA	1:D:98:ARG:HH12	1.83	0.42
1:D:137:ASN:CA	1:D:139:VAL:HG13	2.32	0.42
1:D:207:GLY:C	1:D:210:LEU:HB3	2.44	0.42
1:D:306:ASN:HD22	1:D:306:ASN:N	2.07	0.42
1:A:26:GLY:HA2	1:A:51:ASP:OD1	2.19	0.42
1:A:208:VAL:O	1:A:209:THR:HB	2.19	0.42
1:B:191:GLU:HG3	1:B:192:HIS:N	2.35	0.42
1:B:198:PRO:O	1:B:199:ILE:CG2	2.68	0.42
1:B:207:GLY:C	1:B:210:LEU:HB3	2.44	0.42
1:B:275:LEU:CD1	1:B:285:GLU:HA	2.47	0.42
1:C:79:GLY:HA3	1:C:84:VAL:HG21	2.01	0.42
1:C:155:GLY:HA2	1:C:299:ILE:HD12	2.02	0.42
1:C:171:TYR:O	1:C:172:LEU:C	2.62	0.42
1:C:207:GLY:N	1:C:210:LEU:HD13	2.33	0.42
1:C:305:VAL:HB	1:D:210:LEU:HD21	2.01	0.42
1:C:312:GLU:O	1:C:316:LYS:HG3	2.19	0.42
1:D:207:GLY:N	1:D:210:LEU:HD13	2.33	0.42
1:A:82:TYR:CE2	1:A:123:VAL:HG12	2.53	0.42
1:A:275:LEU:C	1:A:277:LYS:H	2.27	0.42
1:A:286:VAL:HG11	1:A:319:ALA:HA	2.02	0.42
1:B:286:VAL:HG11	1:B:319:ALA:HA	2.02	0.42
1:C:30:VAL:HG22	1:C:247:THR:O	2.20	0.42
1:C:82:TYR:CE2	1:C:123:VAL:HG12	2.53	0.42
1:C:191:GLU:HG3	1:C:192:HIS:N	2.35	0.42
1:C:275:LEU:C	1:C:277:LYS:H	2.27	0.42
1:C:324:ASN:O	1:C:325:MET:C	2.61	0.42
1:D:27:VAL:HG22	1:D:51:ASP:OD2	2.19	0.42
1:D:146:VAL:HA	1:D:149:ILE:CG2	2.39	0.42
1:D:189:LEU:HD23	1:D:315:LEU:CD1	2.49	0.42
1:A:16:LYS:O	1:A:17:LEU:HD22	2.19	0.42
1:A:121:PRO:HG2	1:A:149:ILE:HG23	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:GLU:HG3	1:A:192:HIS:N	2.35	0.42
1:A:243:MET:HE3	1:C:59:GLY:CA	2.48	0.42
1:A:306:ASN:HD22	1:A:306:ASN:N	2.07	0.42
1:B:21:LYS:NZ	1:B:85:SER:C	2.77	0.42
1:B:147:TRP:HA	1:B:157:VAL:HG11	2.00	0.42
1:C:16:LYS:O	1:C:17:LEU:HD22	2.19	0.42
1:C:27:VAL:HG22	1:C:51:ASP:OD2	2.19	0.42
1:C:308:THR:N	1:C:311:GLU:HB2	2.35	0.42
1:D:189:LEU:HB2	1:D:190:GLY:H	1.77	0.42
1:D:208:VAL:O	1:D:209:THR:HB	2.19	0.42
1:A:147:TRP:HA	1:A:157:VAL:HG11	2.00	0.42
1:A:241:LEU:O	1:A:245:GLY:HA2	2.20	0.42
1:C:2:THR:HB	1:C:5:GLU:H	1.85	0.42
1:C:189:LEU:HB2	1:C:190:GLY:H	1.77	0.42
1:D:16:LYS:O	1:D:17:LEU:HD22	2.19	0.42
1:D:276:VAL:O	1:D:278:GLY:N	2.52	0.42
1:D:286:VAL:HG11	1:D:319:ALA:HA	2.02	0.42
1:A:140:ASP:OD2	1:A:273:THR:HG21	2.20	0.42
1:A:207:GLY:O	1:B:208:VAL:CG2	2.68	0.42
1:A:308:THR:N	1:A:311:GLU:HB2	2.34	0.42
1:A:324:ASN:HD22	1:A:324:ASN:HA	1.60	0.42
1:B:140:ASP:OD2	1:B:273:THR:HG21	2.20	0.42
1:B:276:VAL:O	1:B:278:GLY:N	2.52	0.42
1:C:21:LYS:NZ	1:C:85:SER:C	2.77	0.42
1:C:131:LYS:CD	1:C:262:ILE:HG21	2.47	0.42
1:C:138:PRO:O	1:C:142:LEU:N	2.42	0.42
1:D:147:TRP:HZ3	1:D:148:LYS:HZ1	1.62	0.42
1:D:312:GLU:O	1:D:316:LYS:HG3	2.19	0.42
1:A:276:VAL:O	1:A:278:GLY:N	2.52	0.42
1:A:288:LEU:HD22	1:A:289:SER:N	2.35	0.42
1:A:312:GLU:O	1:A:316:LYS:HG3	2.19	0.42
1:B:2:THR:HB	1:B:5:GLU:H	1.85	0.42
1:B:16:LYS:O	1:B:17:LEU:HD22	2.19	0.42
1:B:56:LYS:HE3	1:B:60:GLU:CG	2.47	0.42
1:B:310:GLU:O	1:B:314:LEU:N	2.48	0.42
1:C:26:GLY:HA2	1:C:51:ASP:OD1	2.19	0.42
1:C:51:ASP:HB2	1:C:57:LEU:CD2	2.47	0.42
1:C:103:GLN:OE1	1:C:111:ARG:NH2	2.46	0.42
1:D:3:VAL:O	1:D:4:LYS:C	2.62	0.42
1:D:191:GLU:HG3	1:D:192:HIS:N	2.35	0.42
1:A:227:LYS:HZ1	1:A:228:ASN:CG	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:ASP:O	1:A:323:TRP:HB3	2.19	0.42
1:B:234:VAL:O	1:B:235:GLU:C	2.61	0.42
1:B:288:LEU:HD22	1:B:289:SER:N	2.35	0.42
1:C:207:GLY:C	1:C:210:LEU:HB3	2.45	0.42
1:C:207:GLY:O	1:D:208:VAL:CG2	2.68	0.42
1:C:282:ILE:HD13	1:C:319:ALA:CB	2.49	0.42
1:D:70:PHE:CD2	1:D:70:PHE:C	2.98	0.42
1:A:27:VAL:HG22	1:A:51:ASP:OD2	2.19	0.42
1:A:228:ASN:O	1:A:232:GLN:N	2.43	0.42
1:C:121:PRO:HG2	1:C:149:ILE:HG23	2.00	0.42
1:C:160:SER:O	1:C:161:GLY:C	2.63	0.42
1:C:208:VAL:CG2	1:D:207:GLY:O	2.68	0.42
1:C:210:LEU:HD21	1:D:305:VAL:HB	2.01	0.42
1:C:227:LYS:O	1:C:230:HIS:HB3	2.20	0.42
1:C:241:LEU:O	1:C:245:GLY:HA2	2.20	0.42
1:D:30:VAL:HG22	1:D:247:THR:O	2.20	0.42
1:A:21:LYS:NZ	1:A:85:SER:C	2.78	0.41
1:A:142:LEU:O	1:A:143:THR:C	2.63	0.41
1:A:261:SER:OG	1:A:262:ILE:N	2.53	0.41
1:C:208:VAL:HG22	1:D:204:ASN:CG	2.41	0.41
1:C:324:ASN:HD22	1:C:324:ASN:HA	1.60	0.41
1:A:21:LYS:HZ3	1:A:85:SER:C	2.27	0.41
1:A:70:PHE:C	1:A:70:PHE:CD2	2.98	0.41
1:A:223:LYS:HB3	1:A:224:GLN:H	1.45	0.41
1:B:26:GLY:HA2	1:B:51:ASP:OD1	2.19	0.41
1:B:204:ASN:ND2	1:B:204:ASN:N	2.63	0.41
1:B:208:VAL:O	1:B:209:THR:HB	2.20	0.41
1:B:275:LEU:C	1:B:277:LYS:H	2.27	0.41
1:B:314:LEU:O	1:B:315:LEU:C	2.64	0.41
1:C:58:ARG:CG	1:C:78:PHE:HE2	2.32	0.41
1:C:112:ASN:C	1:C:114:ALA:N	2.76	0.41
1:C:137:ASN:CB	1:C:138:PRO:HB2	2.50	0.41
1:C:288:LEU:HD22	1:C:289:SER:N	2.35	0.41
1:D:282:ILE:HD13	1:D:319:ALA:CB	2.49	0.41
1:A:3:VAL:O	1:A:4:LYS:C	2.62	0.41
1:A:9:GLN:O	1:D:301:ASP:CA	2.69	0.41
1:A:59:GLY:CA	1:C:243:MET:HE3	2.48	0.41
1:A:137:ASN:CB	1:A:138:PRO:HB2	2.50	0.41
1:A:208:VAL:CG2	1:B:207:GLY:O	2.68	0.41
1:A:227:LYS:O	1:A:230:HIS:HB3	2.21	0.41
1:A:307:MET:HB3	1:A:311:GLU:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:LYS:HD2	1:B:46:GLU:OE2	2.20	0.41
1:B:112:ASN:C	1:B:114:ALA:N	2.76	0.41
1:B:137:ASN:CB	1:B:138:PRO:HB2	2.50	0.41
1:B:155:GLY:HA2	1:B:299:ILE:HD12	2.02	0.41
1:B:260:ARG:NH1	1:B:268:ARG:NH1	2.55	0.41
1:B:308:THR:N	1:B:311:GLU:HB2	2.34	0.41
1:C:3:VAL:O	1:C:4:LYS:C	2.63	0.41
1:C:58:ARG:N	1:C:78:PHE:CE2	2.89	0.41
1:C:70:PHE:CD2	1:C:70:PHE:C	2.98	0.41
1:D:158:ILE:CG1	1:D:299:ILE:HD11	2.42	0.41
1:A:30:VAL:HG22	1:A:247:THR:O	2.20	0.41
1:A:127:SER:HA	1:A:128:PRO:HD2	1.94	0.41
1:A:301:ASP:CA	1:D:9:GLN:O	2.69	0.41
1:A:305:VAL:HB	1:B:210:LEU:HD21	2.01	0.41
1:B:9:GLN:O	1:C:301:ASP:CA	2.69	0.41
1:C:147:TRP:HA	1:C:157:VAL:HG11	2.00	0.41
1:D:95:ALA:O	1:D:136:THR:HG21	2.21	0.41
1:D:198:PRO:O	1:D:199:ILE:CG2	2.67	0.41
1:D:241:LEU:O	1:D:245:GLY:HA2	2.20	0.41
1:D:307:MET:HB3	1:D:311:GLU:HB2	2.01	0.41
1:A:21:LYS:HD2	1:A:46:GLU:OE2	2.20	0.41
1:B:95:ALA:O	1:B:136:THR:HG21	2.21	0.41
1:B:142:LEU:O	1:B:143:THR:C	2.64	0.41
1:C:222:ASN:O	1:C:223:LYS:CB	2.69	0.41
1:D:21:LYS:NZ	1:D:85:SER:C	2.78	0.41
1:D:138:PRO:O	1:D:142:LEU:N	2.42	0.41
1:D:209:THR:C	1:D:210:LEU:O	2.63	0.41
1:D:310:GLU:OE2	1:D:310:GLU:N	2.53	0.41
1:A:79:GLY:HA3	1:A:84:VAL:HG21	2.01	0.41
1:A:155:GLY:HA2	1:A:299:ILE:HD12	2.02	0.41
1:A:310:GLU:O	1:A:314:LEU:N	2.48	0.41
1:A:314:LEU:O	1:A:315:LEU:C	2.64	0.41
1:A:320:ASP:O	1:A:323:TRP:N	2.54	0.41
1:B:3:VAL:O	1:B:4:LYS:C	2.62	0.41
1:B:30:VAL:HG22	1:B:247:THR:O	2.20	0.41
1:B:260:ARG:NH1	1:B:268:ARG:HH22	2.09	0.41
1:B:297:SER:HB2	1:C:17:LEU:HD11	2.03	0.41
1:C:140:ASP:OD2	1:C:273:THR:HG21	2.20	0.41
1:C:179:VAL:HG12	1:C:184:CYS:SG	2.61	0.41
1:C:189:LEU:HD23	1:C:315:LEU:CD1	2.49	0.41
1:D:179:VAL:HG12	1:D:184:CYS:SG	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:SER:O	1:A:161:GLY:C	2.63	0.41
1:A:222:ASN:O	1:A:223:LYS:CB	2.69	0.41
1:B:200:TRP:CH2	1:B:226:TRP:HB3	2.56	0.41
1:B:222:ASN:O	1:B:223:LYS:CB	2.69	0.41
1:B:241:LEU:O	1:B:245:GLY:HA2	2.20	0.41
1:A:58:ARG:N	1:A:78:PHE:CE2	2.89	0.41
1:A:102:GLY:O	1:A:103:GLN:C	2.64	0.41
1:A:179:VAL:HG12	1:A:184:CYS:SG	2.61	0.41
1:A:297:SER:HB2	1:D:17:LEU:HD11	2.03	0.41
1:B:2:THR:HB	1:B:5:GLU:HG3	2.03	0.41
1:B:17:LEU:CD2	1:C:297:SER:CB	2.52	0.41
1:B:301:ASP:CA	1:C:9:GLN:O	2.69	0.41
1:C:10:ASN:H	1:C:10:ASN:HD22	1.66	0.41
1:C:131:LYS:HZ2	1:C:262:ILE:CG2	2.30	0.41
1:D:94:THR:C	1:D:98:ARG:NH1	2.77	0.41
1:D:142:LEU:O	1:D:143:THR:C	2.63	0.41
1:D:200:TRP:CH2	1:D:226:TRP:HB3	2.56	0.41
1:A:94:THR:C	1:A:98:ARG:NH1	2.77	0.41
1:A:123:VAL:HG22	1:A:124:ILE:HG22	2.03	0.41
1:A:131:LYS:CD	1:A:262:ILE:HG21	2.47	0.41
1:A:318:SER:O	1:A:321:THR:N	2.54	0.41
1:B:70:PHE:C	1:B:70:PHE:CD2	2.98	0.41
1:B:79:GLY:HA3	1:B:84:VAL:HG21	2.02	0.41
1:B:131:LYS:HE3	1:B:298:GLY:CA	2.47	0.41
1:B:137:ASN:C	1:B:137:ASN:ND2	2.79	0.41
1:B:179:VAL:HG12	1:B:184:CYS:SG	2.60	0.41
1:B:209:THR:C	1:B:210:LEU:O	2.64	0.41
1:B:227:LYS:HZ1	1:B:228:ASN:CG	2.28	0.41
1:B:247:THR:O	1:B:247:THR:HG23	2.21	0.41
1:B:318:SER:O	1:B:321:THR:N	2.54	0.41
1:B:324:ASN:HD22	1:B:324:ASN:HA	1.60	0.41
1:C:21:LYS:HD2	1:C:46:GLU:OE2	2.20	0.41
1:C:95:ALA:O	1:C:136:THR:HG21	2.21	0.41
1:C:200:TRP:CH2	1:C:226:TRP:HB3	2.56	0.41
1:C:209:THR:C	1:C:210:LEU:O	2.64	0.41
1:D:36:ILE:HG23	1:D:37:SER:N	2.36	0.41
1:D:53:ASP:OD2	1:D:53:ASP:N	2.54	0.41
1:D:58:ARG:N	1:D:78:PHE:CE2	2.89	0.41
1:D:137:ASN:CB	1:D:138:PRO:HB2	2.50	0.41
1:D:160:SER:O	1:D:161:GLY:C	2.63	0.41
1:D:261:SER:OG	1:D:262:ILE:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:324:ASN:HD22	1:D:324:ASN:HA	1.60	0.41
1:A:53:ASP:OD2	1:A:53:ASP:N	2.54	0.41
1:A:137:ASN:HB3	1:A:138:PRO:CB	2.51	0.41
1:A:275:LEU:CD1	1:A:285:GLU:HA	2.47	0.41
1:B:260:ARG:HH11	1:B:268:ARG:NH2	2.12	0.41
1:D:2:THR:OG1	1:D:5:GLU:HG3	2.21	0.41
1:D:21:LYS:HD2	1:D:46:GLU:OE2	2.20	0.41
1:A:184:CYS:C	1:A:185:HIS:CD2	3.00	0.40
1:A:253:LEU:HD22	1:C:70:PHE:CG	2.56	0.40
1:A:260:ARG:NH1	1:A:268:ARG:HH22	2.09	0.40
1:A:282:ILE:HD13	1:A:319:ALA:CB	2.50	0.40
1:B:2:THR:OG1	1:B:5:GLU:HG3	2.22	0.40
1:B:261:SER:OG	1:B:262:ILE:N	2.54	0.40
1:C:65:GLN:C	1:C:67:GLY:N	2.78	0.40
1:C:123:VAL:HG22	1:C:124:ILE:HG22	2.03	0.40
1:C:198:PRO:O	1:C:199:ILE:CG2	2.67	0.40
1:D:79:GLY:HA3	1:D:84:VAL:HG21	2.01	0.40
1:D:137:ASN:HB3	1:D:138:PRO:CB	2.51	0.40
1:D:318:SER:O	1:D:321:THR:N	2.54	0.40
1:A:2:THR:OG1	1:A:5:GLU:HG3	2.21	0.40
1:A:17:LEU:CD2	1:D:297:SER:CB	2.52	0.40
1:A:47:LEU:HD23	1:A:47:LEU:O	2.22	0.40
1:A:209:THR:C	1:A:210:LEU:O	2.64	0.40
1:A:247:THR:O	1:A:247:THR:HG23	2.22	0.40
1:B:160:SER:O	1:B:161:GLY:C	2.63	0.40
1:B:243:MET:HE3	1:D:59:GLY:CA	2.48	0.40
1:B:282:ILE:HD13	1:B:319:ALA:CB	2.49	0.40
1:C:114:ALA:O	1:C:115:ILE:C	2.64	0.40
1:C:142:LEU:O	1:C:143:THR:C	2.64	0.40
1:C:184:CYS:C	1:C:185:HIS:CD2	2.99	0.40
1:C:207:GLY:O	1:C:211:LYS:N	2.55	0.40
1:C:271:PRO:C	1:C:272:VAL:HG13	2.46	0.40
1:C:310:GLU:C	1:C:312:GLU:N	2.78	0.40
1:D:247:THR:O	1:D:247:THR:HG23	2.22	0.40
1:D:320:ASP:O	1:D:323:TRP:N	2.54	0.40
1:A:95:ALA:O	1:A:136:THR:HG21	2.21	0.40
1:A:210:LEU:HD21	1:B:305:VAL:HB	2.01	0.40
1:B:58:ARG:N	1:B:78:PHE:CE2	2.89	0.40
1:B:59:GLY:CA	1:D:243:MET:HE3	2.48	0.40
1:B:78:PHE:C	1:B:84:VAL:HG11	2.47	0.40
1:B:146:VAL:HA	1:B:149:ILE:CG2	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:GLY:O	1:B:211:LYS:N	2.54	0.40
1:B:320:ASP:O	1:B:323:TRP:N	2.54	0.40
1:C:318:SER:O	1:C:321:THR:N	2.54	0.40
1:D:222:ASN:O	1:D:223:LYS:CB	2.69	0.40
1:D:227:LYS:O	1:D:230:HIS:HB3	2.20	0.40
1:D:261:SER:HA	1:D:266:LEU:HB2	2.04	0.40
1:D:310:GLU:O	1:D:314:LEU:N	2.48	0.40
1:B:94:THR:C	1:B:98:ARG:NH1	2.77	0.40
1:B:228:ASN:O	1:B:229:VAL:C	2.65	0.40
1:C:78:PHE:C	1:C:84:VAL:HG11	2.46	0.40
1:C:228:ASN:O	1:C:229:VAL:C	2.65	0.40
1:C:261:SER:HA	1:C:266:LEU:HB2	2.04	0.40
1:D:46:GLU:HA	1:D:75:LYS:O	2.22	0.40
1:D:47:LEU:O	1:D:47:LEU:HD23	2.22	0.40
1:D:140:ASP:OD2	1:D:273:THR:HG21	2.20	0.40
1:D:184:CYS:C	1:D:185:HIS:CD2	2.99	0.40
1:D:203:VAL:O	1:D:213:LEU:N	2.54	0.40
1:D:288:LEU:HD22	1:D:289:SER:N	2.35	0.40
1:A:70:PHE:CG	1:C:253:LEU:HD22	2.57	0.40
1:C:36:ILE:HG23	1:C:37:SER:N	2.36	0.40
1:C:53:ASP:OD2	1:C:53:ASP:N	2.54	0.40
1:C:247:THR:O	1:C:247:THR:HG23	2.21	0.40
1:D:2:THR:CB	1:D:5:GLU:HG3	2.52	0.40
1:D:207:GLY:O	1:D:211:LYS:N	2.55	0.40

All (39) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:ARG:CA	1:D:330:GLU:CD[1_566]	0.93	1.27
1:C:330:GLU:CD	1:D:111:ARG:CA[1_566]	0.93	1.27
1:C:111:ARG:CB	1:D:330:GLU:OE2[1_566]	0.97	1.23
1:C:330:GLU:OE2	1:D:111:ARG:CB[1_566]	0.97	1.23
1:C:126:ASN:CA	2:A:345:HOH:O[1_556]	1.06	1.14
1:C:111:ARG:CB	1:D:330:GLU:CD[1_566]	1.06	1.14
1:C:330:GLU:CD	1:D:111:ARG:CB[1_566]	1.06	1.14
1:C:126:ASN:N	2:A:345:HOH:O[1_556]	1.15	1.05
1:C:111:ARG:CA	1:D:330:GLU:OE2[1_566]	1.19	1.01
1:C:330:GLU:OE2	1:D:111:ARG:CA[1_566]	1.19	1.01
1:C:110:GLN:NE2	1:D:110:GLN:NE2[1_566]	1.37	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:GLN:N	1:D:330:GLU:O[1_566]	1.57	0.63
1:C:111:ARG:CG	1:D:330:GLU:OE1[1_566]	1.57	0.63
1:C:330:GLU:OE1	1:D:111:ARG:CG[1_566]	1.57	0.63
1:C:330:GLU:O	1:D:110:GLN:N[1_566]	1.57	0.63
1:C:126:ASN:CB	2:A:345:HOH:O[1_556]	1.59	0.61
1:C:111:ARG:CB	1:D:330:GLU:OE1[1_566]	1.62	0.58
1:C:330:GLU:OE1	1:D:111:ARG:CB[1_566]	1.62	0.58
1:C:111:ARG:CA	1:D:330:GLU:OE1[1_566]	1.66	0.54
1:C:330:GLU:OE1	1:D:111:ARG:CA[1_566]	1.66	0.54
1:C:330:GLU:OE2	1:D:111:ARG:N[1_566]	1.72	0.48
1:C:111:ARG:N	1:D:330:GLU:OE2[1_566]	1.73	0.47
1:C:111:ARG:N	1:D:330:GLU:CG[1_566]	1.77	0.43
1:C:330:GLU:CG	1:D:111:ARG:N[1_566]	1.77	0.43
1:C:126:ASN:CG	2:A:345:HOH:O[1_556]	1.85	0.35
1:C:111:ARG:N	1:D:330:GLU:CD[1_566]	1.88	0.32
1:C:330:GLU:CD	1:D:111:ARG:N[1_566]	1.88	0.32
1:C:111:ARG:CA	1:D:330:GLU:CG[1_566]	1.91	0.29
1:C:330:GLU:CG	1:D:111:ARG:CA[1_566]	1.91	0.29
1:C:110:GLN:NE2	1:D:110:GLN:CD[1_566]	1.93	0.27
1:C:110:GLN:CD	1:D:110:GLN:NE2[1_566]	1.93	0.27
1:C:111:ARG:C	1:D:330:GLU:OE2[1_566]	1.99	0.21
1:C:330:GLU:OE2	1:D:111:ARG:C[1_566]	1.99	0.21
1:C:110:GLN:OE1	1:D:331:LEU:O[1_566]	2.07	0.13
1:C:331:LEU:O	1:D:110:GLN:OE1[1_566]	2.07	0.13
1:C:110:GLN:CA	1:D:330:GLU:O[1_566]	2.13	0.07
1:C:330:GLU:O	1:D:110:GLN:CA[1_566]	2.13	0.07
1:C:111:ARG:CG	1:D:330:GLU:CD[1_566]	2.14	0.06
1:C:330:GLU:CD	1:D:111:ARG:CG[1_566]	2.14	0.06

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	329/331 (99%)	206 (63%)	74 (22%)	49 (15%)	0	0
1	B	329/331 (99%)	206 (63%)	74 (22%)	49 (15%)	0	0
1	C	329/331 (99%)	205 (62%)	75 (23%)	49 (15%)	0	0
1	D	329/331 (99%)	205 (62%)	75 (23%)	49 (15%)	0	0
All	All	1316/1324 (99%)	822 (62%)	298 (23%)	196 (15%)	0	0

All (196) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	VAL
1	A	29	ASP
1	A	54	THR
1	A	69	LEU
1	A	70	PHE
1	A	117	LYS
1	A	120	VAL
1	A	137	ASN
1	A	138	PRO
1	A	205	VAL
1	A	206	ALA
1	A	210	LEU
1	A	217	ILE
1	A	220	ASP
1	A	221	LYS
1	A	222	ASN
1	A	223	LYS
1	A	225	HIS
1	A	226	TRP
1	A	277	LYS
1	A	280	HIS
1	A	285	GLU
1	A	329	LEU
1	B	12	VAL
1	B	29	ASP
1	B	54	THR
1	B	69	LEU
1	B	70	PHE
1	B	117	LYS
1	B	120	VAL
1	B	137	ASN
1	B	138	PRO
1	B	205	VAL

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Mol	Chain	Res	Type
1	B	206	ALA
1	B	210	LEU
1	B	217	ILE
1	B	220	ASP
1	B	221	LYS
1	B	222	ASN
1	B	223	LYS
1	B	225	HIS
1	B	226	TRP
1	B	277	LYS
1	B	280	HIS
1	B	285	GLU
1	B	329	LEU
1	C	12	VAL
1	C	29	ASP
1	C	54	THR
1	C	69	LEU
1	C	70	PHE
1	C	117	LYS
1	C	120	VAL
1	C	137	ASN
1	C	138	PRO
1	C	205	VAL
1	C	206	ALA
1	C	210	LEU
1	C	217	ILE
1	C	220	ASP
1	C	221	LYS
1	C	222	ASN
1	C	223	LYS
1	C	225	HIS
1	C	226	TRP
1	C	277	LYS
1	C	280	HIS
1	C	285	GLU
1	C	329	LEU
1	D	12	VAL
1	D	29	ASP
1	D	54	THR
1	D	69	LEU
1	D	70	PHE
1	D	117	LYS

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Mol	Chain	Res	Type
1	D	120	VAL
1	D	137	ASN
1	D	138	PRO
1	D	205	VAL
1	D	206	ALA
1	D	210	LEU
1	D	217	ILE
1	D	220	ASP
1	D	221	LYS
1	D	222	ASN
1	D	223	LYS
1	D	225	HIS
1	D	226	TRP
1	D	277	LYS
1	D	280	HIS
1	D	285	GLU
1	D	329	LEU
1	A	19	ARG
1	A	55	ASP
1	A	100	VAL
1	A	136	THR
1	A	171	TYR
1	A	219	THR
1	B	19	ARG
1	B	55	ASP
1	B	100	VAL
1	B	136	THR
1	B	171	TYR
1	B	219	THR
1	C	19	ARG
1	C	55	ASP
1	C	100	VAL
1	C	136	THR
1	C	171	TYR
1	C	219	THR
1	D	19	ARG
1	D	55	ASP
1	D	100	VAL
1	D	136	THR
1	D	171	TYR
1	D	219	THR
1	A	68	SER

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Mol	Chain	Res	Type
1	A	97	ALA
1	A	101	SER
1	A	105	ARG
1	A	121	PRO
1	A	164	LEU
1	A	246	TYR
1	A	284	GLU
1	A	319	ALA
1	A	325	MET
1	B	68	SER
1	B	97	ALA
1	B	101	SER
1	B	105	ARG
1	B	121	PRO
1	B	164	LEU
1	B	246	TYR
1	B	284	GLU
1	B	319	ALA
1	B	325	MET
1	C	68	SER
1	C	97	ALA
1	C	101	SER
1	C	105	ARG
1	C	121	PRO
1	C	164	LEU
1	C	246	TYR
1	C	284	GLU
1	C	319	ALA
1	C	325	MET
1	D	68	SER
1	D	97	ALA
1	D	101	SER
1	D	105	ARG
1	D	121	PRO
1	D	164	LEU
1	D	246	TYR
1	D	284	GLU
1	D	319	ALA
1	D	325	MET
1	A	103	GLN
1	A	140	ASP
1	A	309	ALA

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Mol	Chain	Res	Type
1	B	103	GLN
1	B	140	ASP
1	B	309	ALA
1	C	103	GLN
1	C	140	ASP
1	C	309	ALA
1	D	103	GLN
1	D	140	ASP
1	D	309	ALA
1	B	249	TRP
1	C	249	TRP
1	A	249	TRP
1	D	249	TRP
1	A	36	ILE
1	B	36	ILE
1	C	36	ILE
1	D	36	ILE
1	A	198	PRO
1	A	233	VAL
1	A	234	VAL
1	B	26	GLY
1	B	198	PRO
1	B	233	VAL
1	B	234	VAL
1	C	26	GLY
1	C	198	PRO
1	C	233	VAL
1	C	234	VAL
1	D	198	PRO
1	D	233	VAL
1	D	234	VAL
1	A	26	GLY
1	A	96	GLY
1	B	96	GLY
1	C	96	GLY
1	D	26	GLY
1	D	96	GLY

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	282/282 (100%)	194 (69%)	88 (31%)	0	0
1	B	282/282 (100%)	193 (68%)	89 (32%)	0	0
1	C	282/282 (100%)	194 (69%)	88 (31%)	0	0
1	D	282/282 (100%)	193 (68%)	89 (32%)	0	0
All	All	1128/1128 (100%)	774 (69%)	354 (31%)	0	0

All (354) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	3	VAL
1	A	4	LYS
1	A	6	GLN
1	A	9	GLN
1	A	12	VAL
1	A	14	GLU
1	A	15	ASP
1	A	16	LYS
1	A	19	ARG
1	A	20	CYS
1	A	24	VAL
1	A	29	ASP
1	A	40	LEU
1	A	47	LEU
1	A	49	LEU
1	A	53	ASP
1	A	57	LEU
1	A	58	ARG
1	A	62	LEU
1	A	65	GLN
1	A	71	LEU
1	A	73	THR
1	A	77	VAL
1	A	85	SER
1	A	92	ILE
1	A	93	ILE
1	A	98	ARG

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Mol	Chain	Res	Type
1	A	99	MET
1	A	103	GLN
1	A	106	LEU
1	A	108	LEU
1	A	109	LEU
1	A	110	GLN
1	A	111	ARG
1	A	113	VAL
1	A	115	ILE
1	A	124	ILE
1	A	127	SER
1	A	132	ILE
1	A	137	ASN
1	A	138	PRO
1	A	141	ILE
1	A	148	LYS
1	A	156	ARG
1	A	158	ILE
1	A	164	LEU
1	A	166	SER
1	A	170	ARG
1	A	180	ASN
1	A	181	PRO
1	A	182	THR
1	A	183	SER
1	A	187	TRP
1	A	189	LEU
1	A	201	SER
1	A	204	ASN
1	A	210	LEU
1	A	214	ASN
1	A	223	LYS
1	A	227	LYS
1	A	228	ASN
1	A	229	VAL
1	A	231	LYS
1	A	241	LEU
1	A	251	ILE
1	A	256	THR
1	A	261	SER
1	A	262	ILE
1	A	263	LEU

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Mol	Chain	Res	Type
1	A	277	LYS
1	A	284	GLU
1	A	285	GLU
1	A	288	LEU
1	A	289	SER
1	A	290	ILE
1	A	292	CYS
1	A	296	GLU
1	A	300	THR
1	A	303	VAL
1	A	304	LYS
1	A	306	ASN
1	A	307	MET
1	A	308	THR
1	A	315	LEU
1	A	324	ASN
1	A	327	LYS
1	A	328	ASN
1	B	2	THR
1	B	3	VAL
1	B	4	LYS
1	B	6	GLN
1	B	9	GLN
1	B	12	VAL
1	B	14	GLU
1	B	15	ASP
1	B	16	LYS
1	B	19	ARG
1	B	20	CYS
1	B	24	VAL
1	B	29	ASP
1	B	40	LEU
1	B	47	LEU
1	B	49	LEU
1	B	53	ASP
1	B	57	LEU
1	B	58	ARG
1	B	62	LEU
1	B	65	GLN
1	B	71	LEU
1	B	73	THR
1	B	77	VAL

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Mol	Chain	Res	Type
1	B	85	SER
1	B	92	ILE
1	B	93	ILE
1	B	98	ARG
1	B	99	MET
1	B	103	GLN
1	B	106	LEU
1	B	108	LEU
1	B	109	LEU
1	B	110	GLN
1	B	111	ARG
1	B	113	VAL
1	B	115	ILE
1	B	124	ILE
1	B	127	SER
1	B	132	ILE
1	B	137	ASN
1	B	138	PRO
1	B	141	ILE
1	B	148	LYS
1	B	156	ARG
1	B	158	ILE
1	B	164	LEU
1	B	166	SER
1	B	170	ARG
1	B	180	ASN
1	B	181	PRO
1	B	182	THR
1	B	183	SER
1	B	187	TRP
1	B	189	LEU
1	B	201	SER
1	B	204	ASN
1	B	210	LEU
1	B	214	ASN
1	B	221	LYS
1	B	223	LYS
1	B	227	LYS
1	B	228	ASN
1	B	229	VAL
1	B	231	LYS
1	B	241	LEU

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Mol	Chain	Res	Type
1	B	251	ILE
1	B	256	THR
1	B	261	SER
1	B	262	ILE
1	B	263	LEU
1	B	277	LYS
1	B	284	GLU
1	B	285	GLU
1	B	288	LEU
1	B	289	SER
1	B	290	ILE
1	B	292	CYS
1	B	296	GLU
1	B	300	THR
1	B	303	VAL
1	B	304	LYS
1	B	306	ASN
1	B	307	MET
1	B	308	THR
1	B	315	LEU
1	B	324	ASN
1	B	327	LYS
1	B	328	ASN
1	C	2	THR
1	C	3	VAL
1	C	4	LYS
1	C	6	GLN
1	C	9	GLN
1	C	12	VAL
1	C	14	GLU
1	C	15	ASP
1	C	16	LYS
1	C	19	ARG
1	C	20	CYS
1	C	24	VAL
1	C	29	ASP
1	C	40	LEU
1	C	47	LEU
1	C	49	LEU
1	C	53	ASP
1	C	57	LEU
1	C	58	ARG

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Mol	Chain	Res	Type
1	C	62	LEU
1	C	65	GLN
1	C	71	LEU
1	C	73	THR
1	C	77	VAL
1	C	85	SER
1	C	92	ILE
1	C	93	ILE
1	C	98	ARG
1	C	99	MET
1	C	103	GLN
1	C	106	LEU
1	C	108	LEU
1	C	109	LEU
1	C	110	GLN
1	C	111	ARG
1	C	113	VAL
1	C	115	ILE
1	C	124	ILE
1	C	127	SER
1	C	132	ILE
1	C	137	ASN
1	C	138	PRO
1	C	141	ILE
1	C	148	LYS
1	C	156	ARG
1	C	158	ILE
1	C	164	LEU
1	C	166	SER
1	C	170	ARG
1	C	180	ASN
1	C	181	PRO
1	C	182	THR
1	C	183	SER
1	C	187	TRP
1	C	189	LEU
1	C	201	SER
1	C	204	ASN
1	C	210	LEU
1	C	214	ASN
1	C	223	LYS
1	C	227	LYS

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Mol	Chain	Res	Type
1	C	228	ASN
1	C	229	VAL
1	C	231	LYS
1	C	241	LEU
1	C	251	ILE
1	C	256	THR
1	C	261	SER
1	C	262	ILE
1	C	263	LEU
1	C	277	LYS
1	C	284	GLU
1	C	285	GLU
1	C	288	LEU
1	C	289	SER
1	C	290	ILE
1	C	292	CYS
1	C	296	GLU
1	C	300	THR
1	C	303	VAL
1	C	304	LYS
1	C	306	ASN
1	C	307	MET
1	C	308	THR
1	C	315	LEU
1	C	324	ASN
1	C	327	LYS
1	C	328	ASN
1	D	2	THR
1	D	3	VAL
1	D	4	LYS
1	D	6	GLN
1	D	9	GLN
1	D	12	VAL
1	D	14	GLU
1	D	15	ASP
1	D	16	LYS
1	D	19	ARG
1	D	20	CYS
1	D	24	VAL
1	D	29	ASP
1	D	40	LEU
1	D	47	LEU

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Mol	Chain	Res	Type
1	D	49	LEU
1	D	53	ASP
1	D	57	LEU
1	D	58	ARG
1	D	62	LEU
1	D	65	GLN
1	D	71	LEU
1	D	73	THR
1	D	77	VAL
1	D	85	SER
1	D	92	ILE
1	D	93	ILE
1	D	98	ARG
1	D	99	MET
1	D	103	GLN
1	D	106	LEU
1	D	108	LEU
1	D	109	LEU
1	D	110	GLN
1	D	111	ARG
1	D	113	VAL
1	D	115	ILE
1	D	124	ILE
1	D	127	SER
1	D	132	ILE
1	D	137	ASN
1	D	138	PRO
1	D	141	ILE
1	D	148	LYS
1	D	156	ARG
1	D	158	ILE
1	D	164	LEU
1	D	166	SER
1	D	170	ARG
1	D	180	ASN
1	D	181	PRO
1	D	182	THR
1	D	183	SER
1	D	187	TRP
1	D	189	LEU
1	D	201	SER
1	D	204	ASN

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Mol	Chain	Res	Type
1	D	210	LEU
1	D	214	ASN
1	D	221	LYS
1	D	223	LYS
1	D	227	LYS
1	D	228	ASN
1	D	229	VAL
1	D	231	LYS
1	D	241	LEU
1	D	251	ILE
1	D	256	THR
1	D	261	SER
1	D	262	ILE
1	D	263	LEU
1	D	277	LYS
1	D	284	GLU
1	D	285	GLU
1	D	288	LEU
1	D	289	SER
1	D	290	ILE
1	D	292	CYS
1	D	296	GLU
1	D	300	THR
1	D	303	VAL
1	D	304	LYS
1	D	306	ASN
1	D	307	MET
1	D	308	THR
1	D	315	LEU
1	D	324	ASN
1	D	327	LYS
1	D	328	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	9	GLN
1	A	10	ASN
1	A	65	GLN
1	A	125	GLN
1	A	163	ASN

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Mol	Chain	Res	Type
1	A	185	HIS
1	A	232	GLN
1	A	270	HIS
1	A	306	ASN
1	A	324	ASN
1	B	6	GLN
1	B	9	GLN
1	B	10	ASN
1	B	65	GLN
1	B	125	GLN
1	B	163	ASN
1	B	185	HIS
1	B	232	GLN
1	B	270	HIS
1	B	306	ASN
1	B	324	ASN
1	C	6	GLN
1	C	9	GLN
1	C	10	ASN
1	C	65	GLN
1	C	125	GLN
1	C	163	ASN
1	C	185	HIS
1	C	232	GLN
1	C	270	HIS
1	C	306	ASN
1	C	324	ASN
1	D	6	GLN
1	D	9	GLN
1	D	10	ASN
1	D	65	GLN
1	D	125	GLN
1	D	163	ASN
1	D	185	HIS
1	D	232	GLN
1	D	270	HIS
1	D	306	ASN
1	D	324	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	331/331 (100%)	0.59	26 (7%)	18 16	2, 15, 33, 45	0
1	B	331/331 (100%)	0.60	25 (7%)	20 18	2, 15, 33, 45	0
1	C	331/331 (100%)	0.60	25 (7%)	20 18	2, 15, 33, 45	0
1	D	331/331 (100%)	0.72	31 (9%)	14 12	2, 15, 33, 45	0
All	All	1324/1324 (100%)	0.63	107 (8%)	18 16	2, 15, 33, 45	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	208	VAL	9.7
1	B	208	VAL	9.0
1	A	208	VAL	8.5
1	C	208	VAL	8.2
1	D	13	PRO	8.0
1	A	212	SER	5.9
1	A	55	ASP	5.3
1	B	55	ASP	5.2
1	D	324	ASN	5.0
1	A	324	ASN	5.0
1	C	104	THR	4.8
1	C	324	ASN	4.3
1	A	29	ASP	4.3
1	C	219	THR	4.1
1	B	227	LYS	4.1
1	A	121	PRO	4.0
1	D	104	THR	4.0
1	C	214	ASN	3.9
1	B	212	SER	3.8
1	C	210	LEU	3.7
1	D	219	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	15	ASP	3.6
1	D	277	LYS	3.6
1	D	212	SER	3.5
1	A	53	ASP	3.5
1	B	210	LEU	3.3
1	D	17	LEU	3.3
1	C	183	SER	3.3
1	C	320	ASP	3.2
1	B	29	ASP	3.2
1	D	210	LEU	3.2
1	C	331	LEU	3.2
1	A	277	LYS	3.1
1	A	57	LEU	3.1
1	D	330	GLU	3.1
1	C	13	PRO	3.1
1	D	114	ALA	3.0
1	A	78	PHE	3.0
1	D	278	GLY	2.9
1	A	105	ARG	2.8
1	D	115	ILE	2.7
1	C	10	ASN	2.7
1	A	313	GLY	2.7
1	A	14	GLU	2.7
1	B	33	ALA	2.7
1	B	15	ASP	2.7
1	B	319	ALA	2.7
1	D	10	ASN	2.7
1	C	14	GLU	2.7
1	D	308	THR	2.6
1	D	222	ASN	2.6
1	D	331	LEU	2.6
1	B	104	THR	2.6
1	C	78	PHE	2.6
1	B	105	ARG	2.5
1	D	105	ARG	2.5
1	D	53	ASP	2.5
1	D	227	LYS	2.5
1	C	17	LEU	2.5
1	B	236	GLY	2.5
1	B	78	PHE	2.5
1	B	324	ASN	2.5
1	D	126	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	330	GLU	2.4
1	D	225	HIS	2.4
1	C	220	ASP	2.4
1	C	149	ILE	2.4
1	B	81	ASP	2.4
1	A	211	LYS	2.4
1	B	13	PRO	2.4
1	B	306	ASN	2.3
1	C	98	ARG	2.3
1	C	15	ASP	2.3
1	D	280	HIS	2.3
1	C	280	HIS	2.3
1	B	209	THR	2.3
1	C	115	ILE	2.3
1	A	321	THR	2.3
1	D	315	LEU	2.2
1	B	219	THR	2.2
1	A	137	ASN	2.2
1	B	331	LEU	2.2
1	D	99	MET	2.2
1	A	309	ALA	2.2
1	A	104	THR	2.2
1	A	227	LYS	2.2
1	D	2	THR	2.2
1	D	18	SER	2.2
1	C	319	ALA	2.2
1	D	125	GLN	2.1
1	B	228	ASN	2.1
1	D	320	ASP	2.1
1	C	114	ALA	2.1
1	B	330	GLU	2.1
1	D	83	ASN	2.1
1	A	96	GLY	2.1
1	C	96	GLY	2.1
1	B	199	ILE	2.1
1	A	122	GLY	2.1
1	A	17	LEU	2.1
1	D	55	ASP	2.1
1	A	217	ILE	2.1
1	C	295	GLY	2.0
1	A	318	SER	2.0
1	B	303	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	20	CYS	2.0
1	B	321	THR	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.