Full wwPDB X-ray Structure Validation Report ⓘ

Aug 31, 2023 – 12:34 PM EDT

PDB ID	:	2LDX
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:

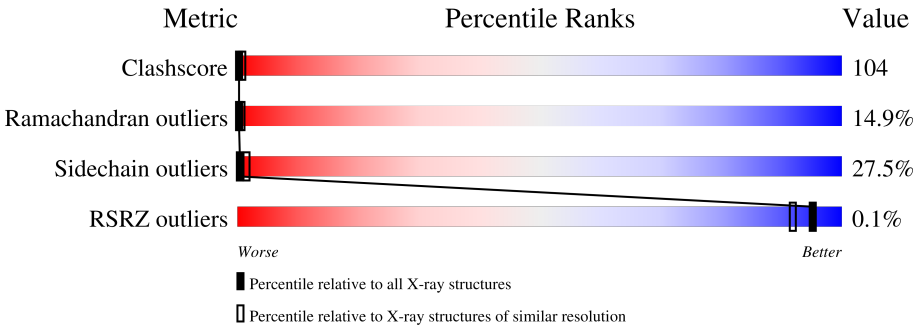
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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 <=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	13% 50% 26% 11%
1	B	331	12% 51% 25% 11%
1	C	331	12% 51% 26% 11%
1	D	331	12% 51% 26% 11%

2 Entry composition (i)

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.

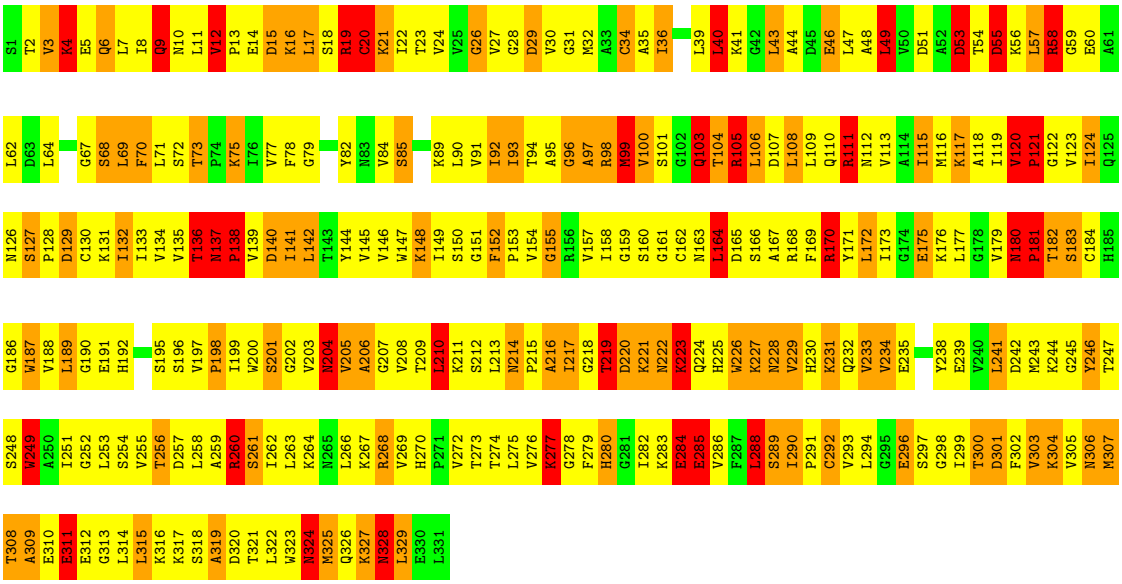
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	29	Total O 29 29	0	0
2	D	2	Total O 2 2	0	0

3 Residue-property plots (i)

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.

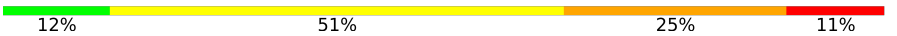
• Molecule 1: APO-LACTATE DEHYDROGENASE

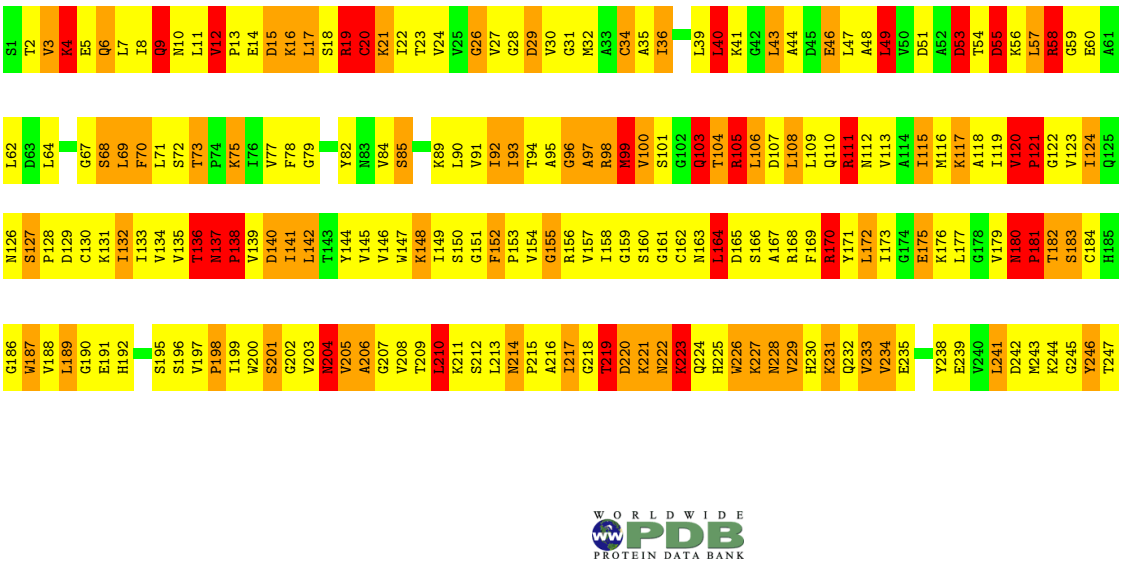
Chain A:



• Molecule 1: APO-LACTATE DEHYDROGENASE

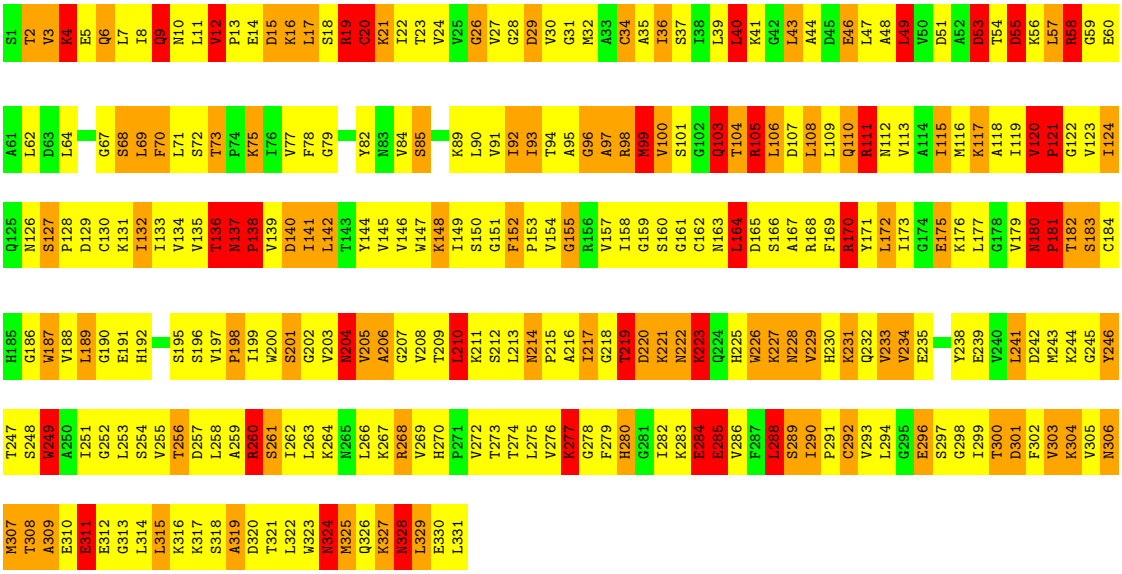
Chain B:





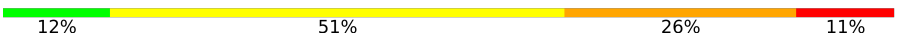
• Molecule 1: APO-LACTATE DEHYDROGENASE

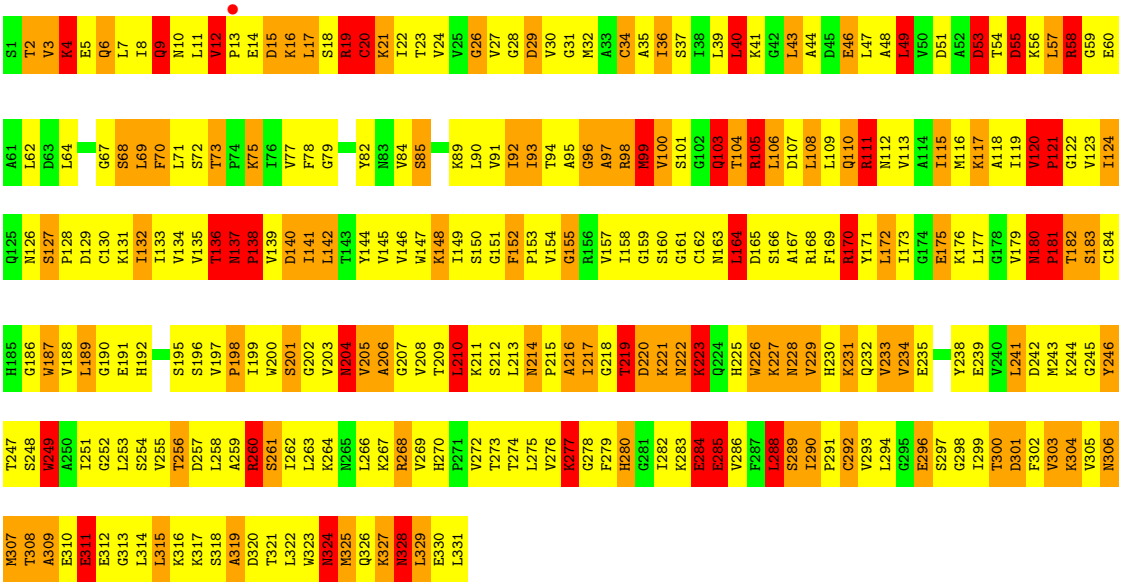
Chain C:



• Molecule 1: APO-LACTATE DEHYDROGENASE

Chain D:





4 Data and refinement statistics (i)

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 – 2.91	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.96) 62.3 (10.00-2.91)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 , 11.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	1.06	3/2556 (0.1%)	1.96	68/3465 (2.0%)
1	B	1.06	3/2556 (0.1%)	1.96	68/3465 (2.0%)
1	C	1.06	3/2556 (0.1%)	1.96	67/3465 (1.9%)
1	D	1.06	3/2556 (0.1%)	1.96	68/3465 (2.0%)
All	All	1.06	12/10224 (0.1%)	1.96	271/13860 (2.0%)

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 (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	58	ARG	CZ-NH1	6.12	1.41	1.33
1	B	58	ARG	CZ-NH1	6.06	1.41	1.33
1	A	58	ARG	CZ-NH1	6.04	1.41	1.33
1	C	58	ARG	CZ-NH1	6.03	1.40	1.33
1	D	34	CYS	CB-SG	-5.67	1.72	1.81
1	B	34	CYS	CB-SG	-5.57	1.72	1.81
1	C	34	CYS	CB-SG	-5.55	1.72	1.81
1	A	34	CYS	CB-SG	-5.55	1.72	1.81
1	B	285	GLU	CB-CG	-5.28	1.42	1.52
1	D	285	GLU	CB-CG	-5.28	1.42	1.52
1	A	285	GLU	CB-CG	-5.27	1.42	1.52
1	C	285	GLU	CB-CG	-5.26	1.42	1.52

All (271) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	58	ARG	CD-NE-CZ	21.41	153.58	123.60
1	D	58	ARG	CD-NE-CZ	21.38	153.54	123.60
1	C	58	ARG	CD-NE-CZ	21.38	153.53	123.60
1	B	58	ARG	CD-NE-CZ	21.36	153.51	123.60
1	D	170	ARG	NE-CZ-NH1	20.61	130.61	120.30
1	C	170	ARG	NE-CZ-NH1	20.60	130.60	120.30
1	B	170	ARG	NE-CZ-NH1	20.59	130.59	120.30
1	A	170	ARG	NE-CZ-NH1	20.45	130.53	120.30
1	D	285	GLU	CA-CB-CG	14.50	145.31	113.40
1	B	285	GLU	CA-CB-CG	14.49	145.28	113.40
1	C	285	GLU	CA-CB-CG	14.46	145.22	113.40
1	A	285	GLU	CA-CB-CG	14.45	145.19	113.40
1	D	137	ASN	N-CA-C	11.56	142.22	111.00
1	B	137	ASN	N-CA-C	11.55	142.20	111.00
1	C	137	ASN	N-CA-C	11.55	142.20	111.00
1	A	137	ASN	N-CA-C	11.54	142.16	111.00
1	B	58	ARG	CA-CB-CG	10.76	137.08	113.40
1	C	58	ARG	CA-CB-CG	10.76	137.06	113.40
1	D	58	ARG	CA-CB-CG	10.75	137.06	113.40
1	A	58	ARG	CA-CB-CG	10.73	137.01	113.40
1	A	170	ARG	CD-NE-CZ	10.27	137.98	123.60
1	C	170	ARG	CD-NE-CZ	10.24	137.93	123.60
1	D	170	ARG	CD-NE-CZ	10.20	137.88	123.60
1	B	170	ARG	CD-NE-CZ	10.20	137.87	123.60
1	A	218	GLY	C-N-CA	9.24	144.79	121.70
1	C	138	PRO	CA-N-CD	-9.23	98.57	111.50
1	B	218	GLY	C-N-CA	9.23	144.76	121.70
1	C	218	GLY	C-N-CA	9.22	144.75	121.70
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	D	218	GLY	C-N-CA	9.20	144.71	121.70
1	B	120	VAL	CB-CA-C	9.20	128.87	111.40
1	A	120	VAL	CB-CA-C	9.19	128.86	111.40
1	D	120	VAL	CB-CA-C	9.19	128.86	111.40
1	C	120	VAL	CB-CA-C	9.17	128.82	111.40
1	B	138	PRO	CA-N-CD	-9.16	98.68	111.50
1	C	111	ARG	NE-CZ-NH1	8.87	124.73	120.30
1	C	75	LYS	CA-CB-CG	8.80	132.76	113.40
1	C	99	MET	CA-CB-CG	8.79	128.25	113.30
1	A	75	LYS	CA-CB-CG	8.79	132.73	113.40
1	A	99	MET	CA-CB-CG	8.79	128.24	113.30
1	D	99	MET	CA-CB-CG	8.78	128.23	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	75	LYS	CA-CB-CG	8.78	132.72	113.40
1	C	46	GLU	OE1-CD-OE2	-8.78	112.76	123.30
1	B	46	GLU	OE1-CD-OE2	-8.78	112.77	123.30
1	A	111	ARG	NE-CZ-NH1	8.78	124.69	120.30
1	D	75	LYS	CA-CB-CG	8.78	132.71	113.40
1	D	46	GLU	OE1-CD-OE2	-8.77	112.77	123.30
1	B	99	MET	CA-CB-CG	8.76	128.19	113.30
1	B	111	ARG	NE-CZ-NH1	8.76	124.68	120.30
1	A	46	GLU	OE1-CD-OE2	-8.69	112.87	123.30
1	D	111	ARG	NE-CZ-NH1	8.62	124.61	120.30
1	A	324	ASN	N-CA-CB	8.35	125.64	110.60
1	C	324	ASN	N-CA-CB	8.35	125.63	110.60
1	D	324	ASN	N-CA-CB	8.35	125.62	110.60
1	B	324	ASN	N-CA-CB	8.31	125.55	110.60
1	B	170	ARG	NE-CZ-NH2	-8.28	116.16	120.30
1	C	170	ARG	NE-CZ-NH2	-8.26	116.17	120.30
1	D	170	ARG	NE-CZ-NH2	-8.25	116.17	120.30
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	D	138	PRO	CB-CA-C	8.09	132.22	112.00
1	A	170	ARG	NE-CZ-NH2	-8.07	116.26	120.30
1	A	268	ARG	NE-CZ-NH1	7.98	124.29	120.30
1	D	268	ARG	NE-CZ-NH1	7.98	124.29	120.30
1	C	268	ARG	NE-CZ-NH1	7.95	124.27	120.30
1	A	136	THR	CA-C-O	-7.86	103.59	120.10
1	C	136	THR	CA-C-O	-7.85	103.62	120.10
1	D	136	THR	CA-C-O	-7.84	103.64	120.10
1	B	136	THR	CA-C-O	-7.83	103.66	120.10
1	B	268	ARG	NE-CZ-NH1	7.82	124.21	120.30
1	B	175	GLU	CA-CB-CG	7.78	130.52	113.40
1	A	105	ARG	NE-CZ-NH1	7.78	124.19	120.30
1	C	105	ARG	NE-CZ-NH1	7.76	124.18	120.30
1	A	175	GLU	CA-CB-CG	7.75	130.46	113.40
1	D	175	GLU	CA-CB-CG	7.75	130.45	113.40
1	C	175	GLU	CA-CB-CG	7.75	130.44	113.40
1	C	204	ASN	C-N-CA	7.69	140.92	121.70
1	D	204	ASN	C-N-CA	7.68	140.91	121.70
1	A	204	ASN	C-N-CA	7.68	140.90	121.70
1	B	105	ARG	NE-CZ-NH1	7.67	124.13	120.30
1	B	204	ASN	C-N-CA	7.67	140.87	121.70
1	D	105	ARG	NE-CZ-NH1	7.66	124.13	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	34	CYS	CA-CB-SG	7.54	127.56	114.00
1	A	34	CYS	CA-CB-SG	7.50	127.50	114.00
1	B	34	CYS	CA-CB-SG	7.49	127.48	114.00
1	C	223	LYS	C-N-CA	7.49	140.41	121.70
1	D	34	CYS	CA-CB-SG	7.48	127.47	114.00
1	D	223	LYS	C-N-CA	7.48	140.41	121.70
1	B	223	LYS	C-N-CA	7.48	140.39	121.70
1	A	223	LYS	C-N-CA	7.46	140.35	121.70
1	A	137	ASN	CA-C-N	7.41	137.85	117.10
1	B	137	ASN	CA-C-N	7.40	137.82	117.10
1	B	155	GLY	N-CA-C	-7.40	94.61	113.10
1	C	137	ASN	CA-C-N	7.39	137.81	117.10
1	D	137	ASN	CA-C-N	7.39	137.80	117.10
1	C	155	GLY	N-CA-C	-7.37	94.68	113.10
1	D	155	GLY	N-CA-C	-7.35	94.72	113.10
1	A	155	GLY	N-CA-C	-7.34	94.74	113.10
1	B	260	ARG	NE-CZ-NH1	7.31	123.96	120.30
1	A	34	CYS	CB-CA-C	7.30	125.00	110.40
1	D	34	CYS	CB-CA-C	7.30	125.00	110.40
1	B	34	CYS	CB-CA-C	7.29	124.98	110.40
1	A	260	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	C	34	CYS	CB-CA-C	7.28	124.95	110.40
1	C	260	ARG	NE-CZ-NH1	7.18	123.89	120.30
1	D	260	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	C	17	LEU	CA-CB-CG	6.96	131.31	115.30
1	A	175	GLU	OE1-CD-OE2	-6.96	114.95	123.30
1	D	55	ASP	CB-CG-OD1	6.95	124.56	118.30
1	B	43	LEU	CB-CA-C	6.94	123.39	110.20
1	B	137	ASN	O-C-N	-6.94	107.91	121.10
1	A	17	LEU	CA-CB-CG	6.94	131.26	115.30
1	A	43	LEU	CB-CA-C	6.94	123.38	110.20
1	D	17	LEU	CA-CB-CG	6.93	131.25	115.30
1	D	175	GLU	OE1-CD-OE2	-6.93	114.98	123.30
1	B	17	LEU	CA-CB-CG	6.93	131.24	115.30
1	A	55	ASP	CB-CG-OD1	6.93	124.53	118.30
1	B	175	GLU	OE1-CD-OE2	-6.93	114.99	123.30
1	C	55	ASP	CB-CG-OD1	6.93	124.53	118.30
1	D	43	LEU	CB-CA-C	6.92	123.36	110.20
1	C	137	ASN	O-C-N	-6.92	107.96	121.10
1	D	137	ASN	O-C-N	-6.92	107.96	121.10
1	C	175	GLU	OE1-CD-OE2	-6.91	115.00	123.30
1	C	43	LEU	CB-CA-C	6.90	123.31	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	137	ASN	O-C-N	-6.89	108.00	121.10
1	B	55	ASP	CB-CG-OD1	6.85	124.46	118.30
1	B	129	ASP	CB-CG-OD1	6.65	124.29	118.30
1	A	136	THR	CA-C-N	6.62	131.77	117.20
1	B	170	ARG	CG-CD-NE	6.62	125.70	111.80
1	D	49	LEU	CB-CA-C	6.61	122.76	110.20
1	B	136	THR	CA-C-N	6.61	131.74	117.20
1	C	49	LEU	CB-CA-C	6.61	122.76	110.20
1	C	129	ASP	CB-CG-OD1	6.61	124.25	118.30
1	D	288	LEU	CA-CB-CG	6.61	130.50	115.30
1	C	136	THR	CA-C-N	6.60	131.73	117.20
1	D	170	ARG	CG-CD-NE	6.60	125.66	111.80
1	B	288	LEU	CA-CB-CG	6.60	130.47	115.30
1	D	136	THR	CA-C-N	6.60	131.71	117.20
1	A	170	ARG	CG-CD-NE	6.59	125.64	111.80
1	B	49	LEU	CB-CA-C	6.59	122.72	110.20
1	A	49	LEU	CB-CA-C	6.58	122.71	110.20
1	A	129	ASP	CB-CG-OD1	6.58	124.22	118.30
1	A	288	LEU	CA-CB-CG	6.58	130.43	115.30
1	C	170	ARG	CG-CD-NE	6.58	125.61	111.80
1	D	129	ASP	CB-CG-OD1	6.57	124.22	118.30
1	C	288	LEU	CA-CB-CG	6.57	130.42	115.30
1	B	46	GLU	CG-CD-OE1	6.55	131.41	118.30
1	D	46	GLU	CG-CD-OE1	6.53	131.37	118.30
1	A	46	GLU	CG-CD-OE1	6.53	131.35	118.30
1	C	268	ARG	CA-CB-CG	6.53	127.76	113.40
1	A	268	ARG	CA-CB-CG	6.52	127.75	113.40
1	B	268	ARG	CA-CB-CG	6.52	127.74	113.40
1	C	46	GLU	CG-CD-OE1	6.51	131.32	118.30
1	D	268	ARG	CA-CB-CG	6.49	127.67	113.40
1	A	129	ASP	CA-CB-CG	6.36	127.39	113.40
1	B	129	ASP	CA-CB-CG	6.35	127.36	113.40
1	C	129	ASP	CA-CB-CG	6.34	127.36	113.40
1	D	129	ASP	CA-CB-CG	6.33	127.33	113.40
1	A	170	ARG	NH1-CZ-NH2	-6.24	112.54	119.40
1	D	170	ARG	NH1-CZ-NH2	-6.24	112.53	119.40
1	C	219	THR	N-CA-CB	6.24	122.15	110.30
1	C	170	ARG	NH1-CZ-NH2	-6.23	112.54	119.40
1	D	219	THR	N-CA-CB	6.23	122.13	110.30
1	B	170	ARG	NH1-CZ-NH2	-6.21	112.56	119.40
1	A	219	THR	N-CA-CB	6.20	122.08	110.30
1	B	219	THR	N-CA-CB	6.18	122.04	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	328	ASN	C-N-CA	6.08	136.91	121.70
1	B	328	ASN	C-N-CA	6.08	136.91	121.70
1	D	328	ASN	C-N-CA	6.08	136.91	121.70
1	C	328	ASN	C-N-CA	6.07	136.88	121.70
1	A	324	ASN	O-C-N	6.06	132.39	122.70
1	D	324	ASN	O-C-N	6.04	132.37	122.70
1	C	46	GLU	N-CA-CB	6.04	121.47	110.60
1	C	324	ASN	O-C-N	6.04	132.36	122.70
1	B	324	ASN	O-C-N	6.03	132.34	122.70
1	D	260	ARG	CD-NE-CZ	6.02	132.03	123.60
1	B	46	GLU	N-CA-CB	6.01	121.42	110.60
1	D	46	GLU	N-CA-CB	6.00	121.41	110.60
1	C	260	ARG	CD-NE-CZ	6.00	132.00	123.60
1	A	46	GLU	N-CA-CB	6.00	121.39	110.60
1	B	260	ARG	CD-NE-CZ	5.95	131.94	123.60
1	A	260	ARG	CD-NE-CZ	5.95	131.93	123.60
1	C	152	PHE	CA-CB-CG	5.85	127.95	113.90
1	A	152	PHE	CA-CB-CG	5.83	127.89	113.90
1	D	152	PHE	CA-CB-CG	5.82	127.87	113.90
1	B	152	PHE	CA-CB-CG	5.81	127.84	113.90
1	D	168	ARG	NE-CZ-NH1	-5.74	117.43	120.30
1	A	21	LYS	CB-CA-C	-5.74	98.93	110.40
1	C	168	ARG	NE-CZ-NH1	-5.71	117.44	120.30
1	D	21	LYS	CB-CA-C	-5.70	99.00	110.40
1	B	21	LYS	CB-CA-C	-5.69	99.02	110.40
1	B	168	ARG	NE-CZ-NH1	-5.69	117.45	120.30
1	B	285	GLU	CB-CG-CD	5.68	129.55	114.20
1	D	285	GLU	CB-CG-CD	5.68	129.53	114.20
1	C	21	LYS	CB-CA-C	-5.67	99.06	110.40
1	A	285	GLU	CB-CG-CD	5.67	129.50	114.20
1	A	165	ASP	CB-CG-OD2	-5.66	113.20	118.30
1	C	285	GLU	CB-CG-CD	5.66	129.49	114.20
1	A	168	ARG	NE-CZ-NH1	-5.65	117.47	120.30
1	B	165	ASP	CB-CG-OD2	-5.64	113.22	118.30
1	C	165	ASP	CB-CG-OD2	-5.62	113.24	118.30
1	D	165	ASP	CB-CG-OD2	-5.56	113.30	118.30
1	C	142	LEU	CB-CA-C	5.53	120.70	110.20
1	B	142	LEU	CB-CA-C	5.50	120.66	110.20
1	A	142	LEU	CB-CA-C	5.50	120.65	110.20
1	A	9	GLN	C-N-CA	5.49	135.43	121.70
1	D	9	GLN	C-N-CA	5.49	135.42	121.70
1	D	142	LEU	CB-CA-C	5.48	120.62	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	9	GLN	C-N-CA	5.47	135.37	121.70
1	B	9	GLN	C-N-CA	5.46	135.35	121.70
1	D	104	THR	CA-CB-CG2	5.39	119.94	112.40
1	C	53	ASP	CB-CG-OD2	5.36	123.12	118.30
1	A	104	THR	CA-CB-CG2	5.35	119.89	112.40
1	C	301	ASP	CB-CG-OD1	5.35	123.11	118.30
1	B	104	THR	CA-CB-CG2	5.34	119.87	112.40
1	A	301	ASP	CB-CG-OD1	5.32	123.09	118.30
1	C	104	THR	CA-CB-CG2	5.31	119.84	112.40
1	D	46	GLU	CB-CG-CD	5.31	128.53	114.20
1	C	46	GLU	CB-CG-CD	5.31	128.53	114.20
1	B	46	GLU	CB-CG-CD	5.29	128.49	114.20
1	A	53	ASP	CB-CG-OD2	5.29	123.06	118.30
1	B	53	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	46	GLU	CB-CG-CD	5.28	128.45	114.20
1	D	301	ASP	CB-CG-OD1	5.27	123.04	118.30
1	D	53	ASP	CB-CG-OD2	5.24	123.02	118.30
1	B	301	ASP	CB-CG-OD1	5.21	122.99	118.30
1	A	20	CYS	C-N-CA	5.21	134.73	121.70
1	B	20	CYS	C-N-CA	5.20	134.71	121.70
1	C	20	CYS	C-N-CA	5.20	134.71	121.70
1	C	180	ASN	CB-CA-C	5.20	120.80	110.40
1	A	40	LEU	CB-CA-C	5.20	120.07	110.20
1	D	20	CYS	C-N-CA	5.20	134.69	121.70
1	D	180	ASN	CB-CA-C	5.18	120.77	110.40
1	B	111	ARG	NH1-CZ-NH2	-5.17	113.71	119.40
1	B	180	ASN	CB-CA-C	5.16	120.73	110.40
1	A	180	ASN	CB-CA-C	5.16	120.72	110.40
1	B	40	LEU	CB-CA-C	5.15	119.99	110.20
1	C	40	LEU	CB-CA-C	5.15	119.98	110.20
1	A	311	GLU	CG-CD-OE1	5.14	128.58	118.30
1	B	311	GLU	CG-CD-OE1	5.14	128.59	118.30
1	D	40	LEU	CB-CA-C	5.13	119.96	110.20
1	C	111	ARG	NH1-CZ-NH2	-5.13	113.75	119.40
1	D	172	LEU	CA-CB-CG	5.13	127.10	115.30
1	A	172	LEU	CA-CB-CG	5.13	127.09	115.30
1	D	311	GLU	CG-CD-OE1	5.13	128.56	118.30
1	C	311	GLU	CG-CD-OE1	5.12	128.54	118.30
1	A	111	ARG	NH1-CZ-NH2	-5.11	113.78	119.40
1	C	172	LEU	CA-CB-CG	5.11	127.05	115.30
1	B	172	LEU	CA-CB-CG	5.11	127.04	115.30
1	D	12	VAL	CB-CA-C	5.09	121.06	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	284	GLU	CA-CB-CG	5.08	124.57	113.40
1	B	284	GLU	CA-CB-CG	5.07	124.55	113.40
1	A	284	GLU	CA-CB-CG	5.07	124.54	113.40
1	C	284	GLU	CA-CB-CG	5.07	124.55	113.40
1	D	111	ARG	NH1-CZ-NH2	-5.07	113.83	119.40
1	B	156	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	C	121	PRO	CA-N-CD	-5.05	104.43	111.50
1	D	216	ALA	CB-CA-C	5.05	117.68	110.10
1	C	12	VAL	CB-CA-C	5.04	120.98	111.40
1	B	12	VAL	CB-CA-C	5.04	120.97	111.40
1	A	12	VAL	CB-CA-C	5.03	120.96	111.40
1	A	121	PRO	CA-N-CD	-5.03	104.46	111.50
1	B	121	PRO	CA-N-CD	-5.03	104.46	111.50
1	A	4	LYS	N-CA-CB	5.02	119.64	110.60
1	A	216	ALA	CB-CA-C	5.02	117.62	110.10
1	D	4	LYS	N-CA-CB	5.02	119.63	110.60
1	C	4	LYS	N-CA-CB	5.01	119.62	110.60
1	B	4	LYS	N-CA-CB	5.00	119.61	110.60
1	D	121	PRO	CA-N-CD	-5.00	104.50	111.50

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 (i)

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	2611	672	0
1	B	2515	0	2611	668	0
1	C	2515	0	2611	671	39
1	D	2515	0	2611	679	35
2	A	29	0	0	1	4
2	D	2	0	0	3	0
All	All	10091	0	10444	2129	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 104.

All (2129) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:177:LEU:HD23	1:D:4:LYS:HZ3	1.25	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:B:177:LEU:CD2	1:D:4:LYS:NZ	2.28	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: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:C:209:THR:CB	1:D:201:SER:O	2.13	0.96
1:A:177:LEU:HD23	1:C:4:LYS:HZ3	1.28	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:208:VAL:HA	1:D:208:VAL:CB	1.96	0.96
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:104:THR:HG22	1:D:238:TYR:HE1	1.32	0.92
1:A:204:ASN:CG	1:B:208:VAL:HG23	1.90	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:C:208:VAL:HG23	1:D:204:ASN:CG	1.90	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
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:C:204:ASN:CG	1:D:208:VAL:HG23	1.90	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: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:A:208:VAL:HG23	1:B:204:ASN:CG	1.90	0.89
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:CYS:HA	1:A:89:LYS:HD3	1.52	0.89
1:C:204:ASN:OD1	1:D:204:ASN:OD1	1.91	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: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: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
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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:A:7:LEU:HG	1:C:211:LYS:CD	2.07	0.84
1:A:208:VAL:C	1:B:208:VAL:HG13	1.98	0.84
1:C:260:ARG:NH1	1:C:268:ARG:HH12	1.75	0.84
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:C:208:VAL:HG13	1:D:208:VAL:C	1.98	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:HG13	1:B:208:VAL:C	1.98	0.83
1:A:208:VAL:HG12	1:B:212:SER:HB2	0.85	0.83
1:C:208:VAL:C	1:D:208:VAL:HG13	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:B:227:LYS:HE2	1:B:231:LYS:NZ	1.95	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: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:A:204:ASN:CG	1:B:208:VAL:CG2	2.50	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:D:227:LYS:HE2	1:D:231:LYS:HZ1	1.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:208:VAL:CG2	1:D:204:ASN:CG	2.50	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: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:208:VAL:CG2	1:B:204:ASN:CG	2.50	0.80
1:A:216:ALA:HB1	1:C:6:GLN:NE2	1.95	0.80
1:B:177:LEU:CD2	1:D:4:LYS:HZ3	1.89	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:C:204:ASN:CG	1:D:208:VAL:CG2	2.50	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:137:ASN:C	1:B:139:VAL:H	1.87	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:137:ASN:C	1:A:139:VAL:H	1.87	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:228:ASN:HA	1:B:231:LYS:HZ3	1.49	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
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:D:137:ASN:C	1:D:139:VAL:H	1.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:228:ASN:HA	1:C:231:LYS:HZ3	1.50	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: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: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
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:D:228:ASN:HA	1:D:231:LYS:HZ3	1.51	0.74
1:B:260:ARG:HH11	1:B:268:ARG:HH22	1.35	0.74
1:C:137:ASN:C	1:C:139:VAL:H	1.87	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:A:227:LYS:HZ3	1:A:228:ASN:HB2	1.53	0.73
1:C:227:LYS:HE2	1:C:231:LYS:HZ1	1.53	0.73
1:D:227:LYS:HD3	1:D:228:ASN:H	1.52	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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
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:B:227:LYS:HE2	1:B:231:LYS:HZ1	1.54	0.71
1:A:177:LEU:CD2	1:C:4:LYS:HZ3	1.93	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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:177:LEU:HD23	1:C:4:LYS:HE2	1.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:32:MET:HE1	1:D:60:GLU:HB3	1.76	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
1:C:227:LYS:HZ3	1:C:228:ASN:HB2	1.57	0.67
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:D:275:LEU:HD11	1:D:285:GLU:HA	1.78	0.66
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:32:MET:HE1	1:B:60:GLU:HB3	1.78	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
1:D:220:ASP:O	1:D:221:LYS:HB3	1.95	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:C:32:MET:HE1	1:C:60:GLU:HB3	1.77	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: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:A:210:LEU:HD23	1:B:306:ASN:ND2	2.12	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:300:THR:HG22	1:B:301:ASP:OD1	1.97	0.64
1:C:4:LYS:HA	1:C:4:LYS:HZ2	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:32:MET:HE1	1:A:60:GLU:HB3	1.80	0.64
1:A:177:LEU:HD22	1:C:4:LYS:NZ	2.12	0.64
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
1:A:314:LEU:O	1:A:317:LYS:HB3	1.97	0.63
1:C:291:PRO:HB2	1:C:303:VAL:HG12	1.79	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: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: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:98:ARG:HG2	1:B:99:MET:HE1	1.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:ASN:HA	1:A:211:LYS:O	1.99	0.62
1:C:98:ARG:HG2	1:C:99:MET:HE1	1.81	0.62
1:C:204:ASN:OD1	1:D:204:ASN:CG	2.38	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
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: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:98:ARG:HG2	1:A:99:MET:HE1	1.81	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:98:ARG:HG2	1:D:99:MET:HE1	1.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:204:ASN:OD1	1:B:204:ASN:CG	2.38	0.61
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:C:219:THR:HG21	1:C:222:ASN:C	2.21	0.61
1:D:219:THR:HG21	1:D:222:ASN:C	2.21	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:204:ASN:CG	1:D:204:ASN:OD1	2.38	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:204:ASN:CG	1:B:204:ASN:OD1	2.38	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:ASN:ND2	1:A:10:ASN:H	1.97	0.61
1:A:219:THR:HG21	1:A:222:ASN:C	2.21	0.61
1:B:98:ARG:HB3	1:B:99:MET:SD	2.40	0.61
1:B:219:THR:HG21	1:B:222:ASN:C	2.21	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:D:221:LYS:C	1:D:223:LYS:H	2.03	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:A:34:CYS:HB2	1:A:252:GLY:HA2	1.83	0.60
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: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:A:221:LYS:C	1:A:223:LYS:H	2.03	0.60
1:C:207:GLY:HA2	1:D:204:ASN:HD21	1.66	0.60
1:D:4:LYS:HA	1:D:4:LYS:HZ2	1.65	0.60
1:D:98:ARG:HB3	1:D:99:MET:SD	2.41	0.60
1:A:208:VAL:HG22	1:B:207:GLY:C	2.22	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:208:VAL:HG22	1:D:207:GLY:C	2.22	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: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:A:207:GLY:C	1:B:208:VAL:HG22	2.22	0.60
1:C:34:CYS:HB2	1:C:252:GLY:HA2	1.84	0.60
1:C:207:GLY:C	1:D:208:VAL:HG22	2.22	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:94:THR:C	1:A:98:ARG:HH12	2.06	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:187:TRP:NE1	1:B:291:PRO:HB3	2.18	0.59
1:D:94:THR:C	1:D:98:ARG:HH12	2.06	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: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:94:THR:C	1:B:98:ARG:HH12	2.06	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: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:C:187:TRP:NE1	1:C:291:PRO:HB3	2.18	0.58
1:C:221:LYS:C	1:C:223:LYS:H	2.03	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: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:221:LYS:C	1:B:223:LYS:H	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:94:THR:C	1:C:98:ARG:HH12	2.06	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:D:137:ASN:C	1:D:139:VAL:N	2.56	0.58
1:A:137:ASN:C	1:A:139:VAL:N	2.56	0.58
1:A:187:TRP:NE1	1:A:291:PRO:HB3	2.18	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:ASN:C	1:B:139:VAL:N	2.56	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
1:C:131:LYS:HE2	1:C:298:GLY:HA2	1.85	0.57
1:C:137:ASN:C	1:C:139:VAL:N	2.56	0.57
1:C:208:VAL:HB	1:D:212:SER:CA	2.33	0.57
1:C:4:LYS:HZ2	1:C:4:LYS:CA	2.17	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: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: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: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:231:LYS:HZ3	1:D:231:LYS:HB2	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: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: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: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
1:D:41:LYS:HB3	1:D:43:LEU:CD1	2.32	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:131:LYS:HZ2	1:D:262:ILE:HG21	1.71	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:C:131:LYS:HZ3	1:C:158:ILE:HD12	1.69	0.56
1:D:119:ILE:O	1:D:123:VAL:HG13	2.06	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:D:4:LYS:HZ2	1:D:4:LYS:CA	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:A:41:LYS:HB3	1:A:43:LEU:CD1	2.32	0.56
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:276:VAL:HG11	1:C:288:LEU:HD13	1.87	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: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:B:217:ILE:C	1:B:219:THR:N	2.60	0.56
1:C:137:ASN:HB3	1:C:138:PRO:HG2	1.88	0.56
1:D:32:MET:CE	1:D:60:GLU:HB3	2.34	0.56
1:D:78:PHE:CD1	1:D:79:GLY:N	2.74	0.56
1:D:227:LYS:CE	1:D:231:LYS:HZ1	2.17	0.56
1:A:9:GLN:O	1:D:302:PHE:N	2.29	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:C:217:ILE:C	1:C:219:THR:N	2.60	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: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:C:202:GLY:HA2	1:D:208:VAL:C	2.27	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:A:107:ASP:C	1:A:109:LEU:H	2.10	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
1:C:208:VAL:C	1:D:202:GLY:HA2	2.27	0.55
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:107:ASP:C	1:D:109:LEU:H	2.10	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:217:ILE:C	1:A:219:THR:N	2.60	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: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:D:217:ILE:C	1:D:219:THR:N	2.60	0.55
1:B:4:LYS:HE2	1:D:177:LEU:CA	2.36	0.55
1:B:208:VAL:C	1:B:210:LEU:H	2.10	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:177:LEU:CD2	1:C:4:LYS:HZ1	2.16	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:107:ASP:C	1:B:109:LEU:H	2.10	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:C:106:LEU:H	1:C:106:LEU:HD12	1.72	0.54
1:C:208:VAL:C	1:C:210:LEU:H	2.10	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:A:202:GLY:HA2	1:B:208:VAL:C	2.27	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:D:208:VAL:C	1:D:210:LEU:H	2.10	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:208:VAL:C	1:B:202:GLY:HA2	2.27	0.54
1:A:131:LYS:HZ3	1:A:158:ILE:HD12	1.71	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:C:204:ASN:H	1:C:204:ASN:ND2	2.03	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:131:LYS:HZ2	1:A:262:ILE:HG21	1.73	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:VAL:C	1:A:210:LEU:H	2.10	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:100:VAL:O	1:D:103:GLN:HB3	2.07	0.54
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:310:GLU:C	1:C:313:GLY:H	2.12	0.53
1:D:277:LYS:HG3	1:D:278:GLY:N	2.22	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:107:ASP:C	1:C:109:LEU:H	2.10	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:D:310:GLU:C	1:D:313:GLY:H	2.12	0.53
1:A:4:LYS:HE2	1:C:177:LEU:CA	2.36	0.53
1:A:241:LEU:C	1:A:241:LEU:HD12	2.29	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:106:LEU:HD22	1:D:325:MET:CE	2.39	0.53
1:A:275:LEU:HD11	1:A:277:LYS:HB3	1.90	0.53
1:B:106:LEU:HD22	1:B:325:MET:CE	2.39	0.53
1:B:241:LEU:C	1:B:241:LEU:HD12	2.29	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:C:106:LEU:HD22	1:C:325:MET:CE	2.39	0.53
1:C:131:LYS:HZ2	1:C:262:ILE:HG21	1.73	0.53
1:C:221:LYS:O	1:C:223:LYS:N	2.37	0.53
1:C:241:LEU:C	1:C:241:LEU:HD12	2.29	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:204:ASN:H	1:D:204:ASN:ND2	2.03	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:106:LEU:HD22	1:A:325:MET:CE	2.39	0.53
1:A:177:LEU:CA	1:C:4:LYS:HE2	2.36	0.53
1:B:189:LEU:HD21	1:B:199:ILE:CD1	2.30	0.53
1:B:204:ASN:H	1:B:204:ASN:ND2	2.03	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:A:197:VAL:C	1:A:198:PRO:O	2.46	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:B:310:GLU:C	1:B:313:GLY:H	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:310:GLU:C	1:A:313:GLY:H	2.12	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:C:197:VAL:C	1:C:198:PRO:O	2.46	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: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: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:16:LYS:C	1:D:17:LEU:HD22	2.30	0.52
1:D:221:LYS:O	1:D:223:LYS:N	2.37	0.52
1:C:16:LYS:C	1:C:17:LEU:HD22	2.30	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: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:D:241:LEU:C	1:D:241:LEU:HD12	2.29	0.52
1:A:23:THR:HA	1:A:48:ALA:O	2.09	0.52
1:A:177:LEU:HD22	1:C:4:LYS:HZ1	1.74	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:245:GLY:O	1:B:246:TYR:HB3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:245:GLY:O	1:D:246:TYR:HB3	2.10	0.52
1:A:147:TRP:HZ3	1:A:148:LYS:HZ1	1.55	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:A:186:GLY:HA2	1:A:203:VAL:HG22	1.92	0.51
1:C:231:LYS:NZ	1:C:231:LYS:HB2	2.25	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:308:THR:O	1:D:309:ALA:C	2.48	0.51
1:D:324:ASN:O	1:D:326:GLN:N	2.43	0.51
1:B:197:VAL:C	1:B:198:PRO:O	2.46	0.51
1:B:231:LYS:NZ	1:B:231:LYS:HB2	2.25	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:16:LYS:C	1:B:17:LEU:HD22	2.30	0.51
1:B:158:ILE:HG22	1:B:159:GLY:H	1.75	0.51
1:B:306:ASN:ND2	1:B:306:ASN:H	2.06	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:116:MET:HB3	1:B:120:VAL:HG11	1.92	0.51
1:B:308:THR:O	1:B:309:ALA:C	2.48	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: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: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: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:C:272:VAL:C	1:C:289:SER:HB2	2.31	0.51
1:C:308:THR:O	1:C:309:ALA:C	2.48	0.51
1:D:17:LEU:O	1:D:18:SER:HB3	2.11	0.51
1:D:39:LEU:C	1:D:41:LYS:H	2.14	0.51
1:D:116:MET:HB3	1:D:120:VAL:HG11	1.92	0.51
1:A:39:LEU:C	1:A:41:LYS:H	2.14	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:39:LEU:C	1:C:41:LYS:H	2.14	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: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:16:LYS:C	1:A:17:LEU:HD22	2.30	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:308:THR:O	1:A:309:ALA:C	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:245:GLY:O	1:C:246:TYR:HB3	2.10	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
1:C:204:ASN:CB	1:D:208:VAL:HG23	2.41	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:B:272:VAL:C	1:B:289:SER:HB2	2.32	0.50
1:C:308:THR:HG23	1:C:310:GLU:OE2	2.11	0.50
1:D:272:VAL:C	1:D:289:SER:HB2	2.32	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:C:231:LYS:HZ3	1:C:231:LYS:HB2	1.76	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: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:A:272:VAL:C	1:A:289:SER:HB2	2.32	0.50
1:B:39:LEU:C	1:B:41:LYS:H	2.14	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: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:C:227:LYS:CE	1:C:231:LYS:HZ1	2.22	0.50
1:D:197:VAL:C	1:D:198:PRO:O	2.46	0.50
1:D:231:LYS:NZ	1:D:231:LYS:HB2	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:308:THR:HG22	1:C:311:GLU:CD	2.32	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
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:B:231:LYS:HZ3	1:B:231:LYS:HB2	1.77	0.50
1:C:17:LEU:O	1:C:18:SER:HB3	2.11	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: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:D:200:TRP:O	1:D:201:SER:C	2.50	0.50
1:D:308:THR:HG22	1:D:311:GLU:CD	2.32	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:TRP:O	1:B:201:SER:C	2.51	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:D:127:SER:O	1:D:130:CYS:HB3	2.12	0.49
1:D:131:LYS:HZ3	1:D:158:ILE:HD12	1.77	0.49
1:D:190:GLY:CA	1:D:288:LEU:HD23	2.42	0.49
1:A:308:THR:HG22	1:A:311:GLU:CD	2.32	0.49
1:C:155:GLY:O	1:C:299:ILE:HD12	2.12	0.49
1:C:200:TRP:O	1:C:201:SER:C	2.50	0.49
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: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: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:322:LEU:O	1:C:326:GLN:HG3	2.12	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:227:LYS:CE	1:B:231:LYS:HZ1	2.23	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:21:LYS:HD2	1:D:46:GLU:CD	2.33	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:GLU:OE2	1:C:19:ARG:HB2	2.13	0.49
1:B:308:THR:HG22	1:B:311:GLU:CD	2.32	0.49
1:C:284:GLU:O	1:C:286:VAL:N	2.35	0.49
1:A:21:LYS:HD2	1:A:46:GLU:CD	2.33	0.49
1:A:202:GLY:CA	1:B:210:LEU:CB	2.49	0.49
1:D:122:GLY:O	1:D:126:ASN:ND2	2.46	0.49
1:D:318:SER:O	1:D:319:ALA:C	2.51	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:200:TRP:O	1:A:201:SER:C	2.51	0.49
1:A:249:TRP:CD1	1:C:64:LEU:HD23	2.46	0.49
1:B:21:LYS:HD2	1:B:46:GLU:CD	2.33	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:318:SER:O	1:C:319:ALA:C	2.51	0.49
1:D:18:SER:O	1:D:19:ARG:HG2	2.12	0.49
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: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:302:PHE:CZ	1:D:11:LEU:CG	2.87	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:8:ILE:HD13	1:D:303:VAL:HG23	1.96	0.48
1:A:137:ASN:C	1:A:137:ASN:HD22	2.16	0.48
1:A:234:VAL:HG13	1:A:235:GLU:H	1.78	0.48
1:A:328:ASN:O	1:A:329:LEU:HB2	2.12	0.48
1:B:121:PRO:HG3	1:B:149:ILE:HG23	1.95	0.48
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:99:MET:CE	1:C:246:TYR:HB2	2.43	0.48
1:C:122:GLY:O	1:C:126:ASN:ND2	2.46	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:99:MET:CE	1:B:246:TYR:HB2	2.43	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: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:137:ASN:HB3	1:B:138:PRO:HB2	1.95	0.48
1:C:21:LYS:HD2	1:C:46:GLU:CD	2.33	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:318:SER:O	1:A:319:ALA:C	2.51	0.48
1:B:177:LEU:HD22	1:D:4:LYS:HZ1	1.78	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: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: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
1:B:17:LEU:HG	1:C:297:SER:HB3	1.91	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:D:99:MET:CE	1:D:246:TYR:HB2	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:99:MET:CE	1:A:246:TYR:HB2	2.43	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:B:318:SER:O	1:B:319:ALA:C	2.51	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:177:LEU:CD2	1:D:4:LYS:HZ1	2.20	0.47
1:B:302:PHE:CE2	1:C:11:LEU:CD1	2.97	0.47
1:C:49:LEU:HD13	1:C:57:LEU:HD11	1.96	0.47
1:C:150:SER:OG	1:C:151:GLY:N	2.48	0.47
1:D:49:LEU:HD13	1:D:57:LEU:HD11	1.96	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
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:291:PRO:HB2	1:D:303:VAL:CG1	2.42	0.47
1:A:150:SER:OG	1:A:151:GLY:N	2.48	0.47
1:B:161:GLY:CA	1:B:273:THR:HG23	2.44	0.47
1:C:208:VAL:HB	1:D:212:SER:CB	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:VAL:HG23	1:B:292:CYS:C	2.35	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:D:269:VAL:HG23	1:D:292:CYS:C	2.35	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:A:269:VAL:HG23	1:A:292:CYS:C	2.34	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:320:ASP:HA	1:C:323:TRP:HB3	1.97	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: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: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:249:TRP:HD1	1:D:64:LEU:HD23	1.78	0.47
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: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:188:VAL:C	1:D:189:LEU:HD13	2.36	0.47
1:A:58:ARG:O	1:C:243:MET:HE3	2.15	0.46
1:A:212:SER:CB	1:B:208:VAL:HB	2.44	0.46
1:B:58:ARG:O	1:D:243:MET:HE3	2.15	0.46
1:B:135:VAL:HG13	1:B:251:ILE:HD11	1.96	0.46
1:D:135:VAL:HG13	1:D:251:ILE:HD11	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:208:VAL:CG2	1:D:204:ASN:CB	2.93	0.46
1:C:269:VAL:HG23	1:C:292:CYS:C	2.35	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:188:VAL:C	1:B:189:LEU:HD13	2.36	0.46
1:B:253:LEU:O	1:B:256:THR:HG23	2.15	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
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: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: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:188:VAL:C	1:C:189:LEU:HD13	2.36	0.46
1:C:310:GLU:O	1:C:313:GLY:N	2.48	0.46
1:D:320:ASP:HA	1:D:323:TRP:HB3	1.97	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: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:30:VAL:O	1:C:34:CYS:HB3	2.16	0.46
1:C:121:PRO:HG3	1:C:149:ILE:HG23	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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: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: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:188:VAL:C	1:A:189:LEU:HD13	2.36	0.46
1:B:172:LEU:O	1:B:175:GLU:HB3	2.16	0.46
1:B:243:MET:HE3	1:D:58:ARG:O	2.14	0.46
1:C:170:ARG:HA	1:C:173:ILE:CG2	2.46	0.46
1:D:212:SER:C	1:D:215:PRO:HD2	2.36	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: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:96:GLY:HA2	1:B:115:ILE:CD1	2.46	0.45
1:C:94:THR:HG22	1:C:135:VAL:CB	2.38	0.45
1:C:99:MET:HE3	1:C:246:TYR:HB2	1.98	0.45
1:A:131:LYS:NZ	1:A:158:ILE:HD12	2.31	0.45
1:B:212:SER:C	1:B:215:PRO:HD2	2.36	0.45
1:C:273:THR:HA	1:C:289:SER:HA	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:144:TYR:O	1:B:148:LYS:HB2	2.16	0.45
1:B:162:CYS:O	1:B:163:ASN:C	2.55	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:212:SER:C	1:C:215:PRO:HD2	2.36	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: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: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:57:LEU:C	1:B:59:GLY:H	2.20	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: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:C:137:ASN:C	1:C:137:ASN:HD22	2.16	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:136:THR:O	1:A:137:ASN:CB	2.65	0.45
1:A:212:SER:C	1:A:215:PRO:HD2	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:VAL:HG13	1:B:251:ILE:HG21	1.99	0.45
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:112:ASN:O	1:D:113:VAL:C	2.54	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: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:57:LEU:C	1:C:59:GLY:H	2.20	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: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:131:LYS:NZ	1:C:158:ILE:HD12	2.30	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:C:162:CYS:O	1:C:163:ASN:C	2.55	0.44
1:D:275:LEU:CD1	1:D:285:GLU:HA	2.47	0.44
1:A:107:ASP:C	1:A:109:LEU:N	2.71	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: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:D:162:CYS:O	1:D:163:ASN:C	2.55	0.44
1:D:320:ASP:O	1:D:321:THR:C	2.56	0.44
1:A:112:ASN:O	1:A:113:VAL:C	2.55	0.44
1:A:146:VAL:HA	1:A:149:ILE:CG2	2.39	0.44
1:A:162:CYS:O	1:A:163:ASN:C	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:15:ASP:C	1:C:16:LYS:HG2	2.38	0.44
1:C:270:HIS:HB3	1:C:272:VAL:HG13	1.99	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:131:LYS:NZ	1:D:158:ILE:HD12	2.31	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: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:15:ASP:C	1:D:16:LYS:HG2	2.38	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:A:15:ASP:C	1:A:16:LYS:HG2	2.38	0.44
1:C:112:ASN:O	1:C:113:VAL:C	2.55	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: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:30:VAL:C	1:B:32:MET:N	2.70	0.44
1:B:270:HIS:N	1:B:292:CYS:O	2.40	0.44
1:B:320:ASP:O	1:B:321:THR:C	2.56	0.44
1:C:2:THR:HG22	1:C:3:VAL:N	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:228:ASN:O	1:C:232:GLN:N	2.43	0.44
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:116:MET:O	1:B:117:LYS:C	2.57	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:137:ASN:C	1:D:137:ASN:HD22	2.16	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:H	2.22	0.43
1:A:49:LEU:O	1:A:78:PHE:HD1	2.01	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:A:320:ASP:O	1:A:321:THR:C	2.56	0.43
1:B:15:ASP:C	1:B:16:LYS:HG2	2.38	0.43
1:B:95:ALA:HA	1:B:98:ARG:HH12	1.83	0.43
1:C:219:THR:HG21	1:C:222:ASN:N	2.33	0.43
1:C:320:ASP:O	1:C:321:THR:C	2.56	0.43
1:D:57:LEU:C	1:D:59:GLY:H	2.20	0.43
1:A:30:VAL:HG13	1:A:251:ILE:HG21	1.99	0.43
1:A:217:ILE:HG23	1:A:217:ILE:O	2.17	0.43
1:A:313:GLY:O	1:A:316:LYS:HB2	2.17	0.43
1:B:107:ASP:C	1:B:109:LEU:N	2.71	0.43
1:B:112:ASN:O	1:B:113:VAL:C	2.54	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:107:ASP:C	1:C:109:LEU:N	2.70	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:99:MET:HE3	1:D:246:TYR:HB2	1.99	0.43
1:A:57:LEU:C	1:A:59:GLY:H	2.20	0.43
1:A:170:ARG:C	1:A:173:ILE:HG22	2.38	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:137:ASN:C	1:B:137:ASN:HD22	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:208:VAL:CG2	1:B:207:GLY:C	2.87	0.43
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: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:302:PHE:HD1	1:D:9:GLN:CG	2.16	0.43
1:B:106:LEU:HD22	1:B:325:MET:HE3	2.00	0.43
1:D:106:LEU:HD22	1:D:325:MET:HE3	1.99	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:4:LYS:C	1:B:6:GLN:H	2.21	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:170:ARG:C	1:B:173:ILE:HG22	2.39	0.43
1:B:176:LYS:HE2	1:B:226:TRP:CZ3	2.54	0.43
1:D:170:ARG:C	1:D:173:ILE:HG22	2.39	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:C:208:VAL:CG2	1:D:207:GLY:C	2.87	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:106:LEU:HD22	1:A:325:MET:HE3	2.01	0.43
1:A:241:LEU:HD12	1:A:242:ASP:N	2.33	0.43
1:A:241:LEU:O	1:A:242:ASP:C	2.57	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:4:LYS:C	1:C:6:GLN:H	2.21	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: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: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:207:GLY:C	1:D:208:VAL:CG2	2.87	0.43
1:C:276:VAL:O	1:C:278:GLY:N	2.52	0.43
1:D:4:LYS:C	1:D:6:GLN:H	2.22	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:D:241:LEU:O	1:D:242:ASP:C	2.57	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:B:208:VAL:CG2	2.87	0.42
1:A:243:MET:HE3	1:C:58:ARG:O	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:116:MET:O	1:D:117:LYS:C	2.57	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:30:VAL:C	1:A:32:MET:N	2.70	0.42
1:A:198:PRO:O	1:A:199:ILE:CG2	2.68	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: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:116:MET:O	1:A:117:LYS:C	2.57	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:275:LEU:CD1	1:B:285:GLU:HA	2.47	0.42
1:C:21:LYS:HZ3	1:C:85:SER:C	2.22	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: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: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:170:ARG:C	1:C:173:ILE:HG22	2.39	0.42
1:C:191:GLU:HG3	1:C:192:HIS:N	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:191:GLU:HG3	1:A:192:HIS:N	2.35	0.42
1:A:306:ASN:HD22	1:A:306:ASN:N	2.07	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:7:LEU:HD23	1:A:7:LEU:C	2.40	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:C:241:LEU:O	1:C:242:ASP:C	2.57	0.42
1:D:16:LYS:O	1:D:17:LEU:HD22	2.19	0.42
1:D:107:ASP:C	1:D:109:LEU:N	2.71	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:99:MET:HE2	1:B:246:TYR:HB2	2.02	0.42
1:B:140:ASP:OD2	1:B:273:THR:HG21	2.20	0.42
1:B:241:LEU:O	1:B:242:ASP:C	2.57	0.42
1:B:276:VAL:O	1:B:278:GLY:N	2.52	0.42
1:C:116:MET:O	1:C:117:LYS:C	2.57	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:30:VAL:C	1:D:32:MET:N	2.70	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:180:ASN:C	1:C:182:THR:H	2.23	0.42
1:D:131:LYS:HZ2	1:D:262:ILE:CG2	2.30	0.42
1:D:191:GLU:HG3	1:D:192:HIS:N	2.35	0.42
1:A:320:ASP:O	1:A:323:TRP:HB3	2.19	0.42
1:B:208:VAL:C	1:B:210:LEU:N	2.73	0.42
1:B:288:LEU:HD22	1:B:289:SER:N	2.35	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:7:LEU:HD23	1:D:7:LEU:C	2.40	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:B:260:ARG:C	1:B:260:ARG:HD3	2.40	0.42
1:C:106:LEU:HD22	1:C:325:MET:HE2	2.01	0.42
1:C:121:PRO:HG2	1:C:149:ILE:HG23	2.00	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:99:MET:HE2	1:A:246:TYR:HB2	2.02	0.41
1:A:261:SER:OG	1:A:262:ILE:N	2.53	0.41
1:C:30:VAL:C	1:C:32:MET:N	2.70	0.41
1:C:324:ASN:HD22	1:C:324:ASN:HA	1.60	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:180:ASN:C	1:B:182:THR:H	2.23	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:C:58:ARG:CG	1:C:78:PHE:HE2	2.32	0.41
1:C:137:ASN:CB	1:C:138:PRO:HB2	2.50	0.41
1:C:208:VAL:C	1:C:210:LEU:N	2.73	0.41
1:C:288:LEU:HD22	1:C:289:SER:N	2.35	0.41
1:D:260:ARG:C	1:D:260:ARG:HD3	2.41	0.41
1:D:282:ILE:HD13	1:D:319:ALA:CB	2.49	0.41
1:A:9:GLN:O	1:D:301:ASP:CA	2.69	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:MET:HB3	1:A:311:GLU:HB2	2.01	0.41
1:B:21:LYS:HD2	1:B:46:GLU:OE2	2.20	0.41
1:B:57:LEU:C	1:B:59:GLY:N	2.73	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:58:ARG:N	1:C:78:PHE:CE2	2.89	0.41
1:C:103:GLN:O	1:C:104:THR:C	2.59	0.41
1:C:260:ARG:HD3	1:C:260:ARG:C	2.41	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:67:GLY:O	1:A:68:SER:C	2.59	0.41
1:A:127:SER:HA	1:A:128:PRO:HD2	1.94	0.41
1:A:260:ARG:C	1:A:260:ARG:HD3	2.40	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:67:GLY:O	1:C:68:SER:C	2.58	0.41
1:C:147:TRP:HA	1:C:157:VAL:HG11	2.00	0.41
1:D:67:GLY:O	1:D:68:SER:C	2.59	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:C:222:ASN:O	1:C:223:LYS:CB	2.69	0.41
1:D:138:PRO:O	1:D:142:LEU:N	2.42	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:320:ASP:O	1:A:323:TRP:N	2.54	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:D:208:VAL:C	1:D:210:LEU:N	2.73	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: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:7:LEU:HD23	1:B:7:LEU:C	2.40	0.41
1:B:17:LEU:CD2	1:C:297:SER:CB	2.52	0.41
1:B:103:GLN:O	1:B:104:THR:C	2.59	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:D:200:TRP:CH2	1:D:226:TRP:HB3	2.56	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:67:GLY:O	1:B:68:SER:C	2.59	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:179:VAL:HG12	1:B:184:CYS:SG	2.60	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: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:103:GLN:O	1:D:104:THR:C	2.59	0.41
1:D:137:ASN:CB	1:D:138:PRO:HB2	2.50	0.41
1:D:261:SER:OG	1:D:262:ILE:N	2.54	0.41
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:103:GLN:O	1:A:104:THR:C	2.59	0.41
1:A:137:ASN:HB3	1:A:138:PRO:CB	2.51	0.41
1:A:180:ASN:C	1:A:182:THR:H	2.23	0.41
1:A:275:LEU:CD1	1:A:285:GLU:HA	2.47	0.41
1:B:106:LEU:HD22	1:B:325:MET:HE1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:MET:C	1:B:118:ALA:N	2.74	0.41
1:B:260:ARG:HH11	1:B:268:ARG:NH2	2.12	0.41
1:C:4:LYS:C	1:C:6:GLN:N	2.75	0.41
1:C:57:LEU:C	1:C:59:GLY:N	2.73	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: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: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:C:261:SER:OG	1:C:262:ILE:N	2.53	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:57:LEU:C	1:A:59:GLY:N	2.73	0.40
1:A:247:THR:O	1:A:247:THR:HG23	2.22	0.40
1:B:282:ILE:HD13	1:B:319:ALA:CB	2.49	0.40
1:C:207:GLY:O	1:C:211:LYS:N	2.55	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:146:VAL:HA	1:B:149:ILE:CG2	2.39	0.40
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:7:LEU:HD23	1:C:7:LEU:C	2.40	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:A:208:VAL:C	1:A:210:LEU:N	2.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:180:ASN:C	1:D:182:THR:H	2.23	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:4:LYS:HZ2	1:C:4:LYS:N	2.19	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:116:MET:C	1:D:118:ALA:N	2.74	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 (i)

5.3.1 Protein backbone (i)

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

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

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

All (196) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	VAL

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 (i)

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%)	205 (73%)	77 (27%)	0 1
1	B	282/282 (100%)	205 (73%)	77 (27%)	0 1
1	C	282/282 (100%)	204 (72%)	78 (28%)	0 1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	282/282 (100%)	204 (72%)	78 (28%)	0 1
All	All	1128/1128 (100%)	818 (72%)	310 (28%)	0 1

All (310) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
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	29	ASP
1	A	40	LEU
1	A	49	LEU
1	A	53	ASP
1	A	57	LEU
1	A	58	ARG
1	A	73	THR
1	A	77	VAL
1	A	85	SER
1	A	92	ILE
1	A	93	ILE
1	A	98	ARG
1	A	99	MET
1	A	103	GLN
1	A	106	LEU
1	A	108	LEU
1	A	110	GLN
1	A	111	ARG
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

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Mol	Chain	Res	Type
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	249	TRP
1	A	256	THR
1	A	260	ARG
1	A	261	SER
1	A	263	LEU
1	A	277	LYS
1	A	284	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	3	VAL

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Mol	Chain	Res	Type
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	29	ASP
1	B	40	LEU
1	B	49	LEU
1	B	53	ASP
1	B	57	LEU
1	B	58	ARG
1	B	73	THR
1	B	77	VAL
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	110	GLN
1	B	111	ARG
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	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

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Mol	Chain	Res	Type
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	223	LYS
1	B	227	LYS
1	B	228	ASN
1	B	229	VAL
1	B	231	LYS
1	B	241	LEU
1	B	249	TRP
1	B	256	THR
1	B	260	ARG
1	B	261	SER
1	B	263	LEU
1	B	277	LYS
1	B	284	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

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Mol	Chain	Res	Type
1	C	16	LYS
1	C	19	ARG
1	C	20	CYS
1	C	29	ASP
1	C	40	LEU
1	C	49	LEU
1	C	53	ASP
1	C	57	LEU
1	C	58	ARG
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	110	GLN
1	C	111	ARG
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	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

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Mol	Chain	Res	Type
1	C	223	LYS
1	C	227	LYS
1	C	228	ASN
1	C	229	VAL
1	C	231	LYS
1	C	241	LEU
1	C	249	TRP
1	C	256	THR
1	C	260	ARG
1	C	261	SER
1	C	263	LEU
1	C	277	LYS
1	C	284	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	29	ASP
1	D	40	LEU
1	D	49	LEU

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Mol	Chain	Res	Type
1	D	53	ASP
1	D	57	LEU
1	D	58	ARG
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	110	GLN
1	D	111	ARG
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	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
1	D	210	LEU
1	D	214	ASN
1	D	223	LYS
1	D	227	LYS
1	D	228	ASN
1	D	229	VAL
1	D	231	LYS
1	D	241	LEU

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Mol	Chain	Res	Type
1	D	249	TRP
1	D	256	THR
1	D	260	ARG
1	D	261	SER
1	D	263	LEU
1	D	277	LYS
1	D	284	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 (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	10	ASN
1	A	65	GLN
1	A	125	GLN
1	A	185	HIS
1	A	232	GLN
1	A	270	HIS
1	A	306	ASN
1	A	324	ASN
1	A	328	ASN
1	B	6	GLN
1	B	10	ASN
1	B	65	GLN
1	B	125	GLN
1	B	185	HIS
1	B	232	GLN

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Mol	Chain	Res	Type
1	B	270	HIS
1	B	306	ASN
1	B	324	ASN
1	B	328	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	C	328	ASN
1	D	6	GLN
1	D	9	GLN
1	D	10	ASN
1	D	65	GLN
1	D	125	GLN
1	D	185	HIS
1	D	232	GLN
1	D	270	HIS
1	D	306	ASN
1	D	324	ASN
1	D	328	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	0	100	100	2, 15, 33, 45	0
1	B	331/331 (100%)	-0.58	0	100	100	2, 15, 33, 45	0
1	C	331/331 (100%)	-0.56	0	100	100	2, 15, 33, 45	0
1	D	331/331 (100%)	-0.52	1 (0%)	94	87	2, 15, 33, 45	0
All	All	1324/1324 (100%)	-0.56	1 (0%)	95	92	2, 15, 33, 45	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	13	PRO	4.6

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.