Full wwPDB X-ray Structure Validation Report (i)

Aug 21, 2023 – 11:56 AM EDT

PDB ID	:	2Q49
Title	:	Ensemble refinement of the protein crystal structure of gene product from Arabidopsis thaliana At2g19940
Authors	:	Levin, E.J.; Kondrashov, D.A.; Wesenberg, G.E.; Phillips Jr., G.N.; Center for Eukaryotic Structural Genomics (CESG)
Deposited on	:	2007-05-31
Resolution	:	2.19 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 (i) 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 (1)) were used in the production of this report:

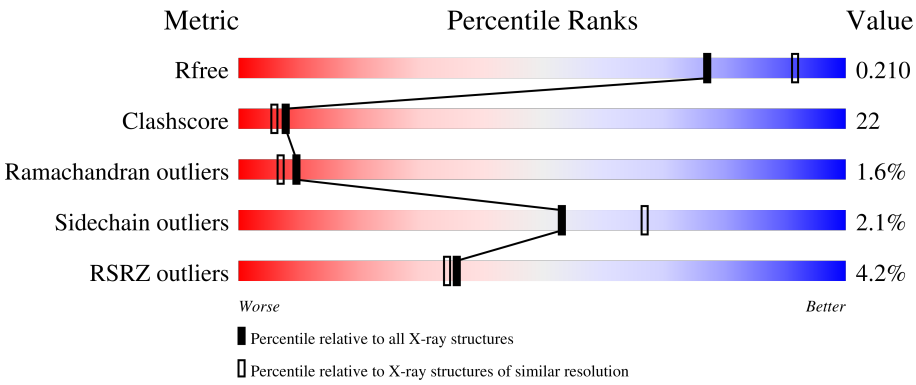
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.19 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	1-A	359	2%, 61%, 34%, • •
1	1-B	359	6%, 57%, 38%, • •
1	1-C	359	7%, 53%, 42%, • •
1	1-D	359	3%, 64%, 30%, • •
1	2-A	359	2%, 65%, 30%, • •

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Mol	Chain	Length	Quality of chain
1	2-B	359	6% 61% 33%
1	2-C	359	7% 52% 41%
1	2-D	359	3% 62% 31%
1	3-A	359	2% 58% 37%
1	3-B	359	6% 56% 36%
1	3-C	359	7% 55% 38%
1	3-D	359	3% 60% 35%
1	4-A	359	2% 58% 37%
1	4-B	359	6% 51% 42%
1	4-C	359	7% 53% 39%
1	4-D	359	3% 63% 32%
1	5-A	359	2% 63% 31%
1	5-B	359	6% 53% 41%
1	5-C	359	7% 59% 35%
1	5-D	359	3% 60% 35%
1	6-A	359	2% 62% 32%
1	6-B	359	6% 56% 37%
1	6-C	359	7% 56% 36%
1	6-D	359	3% 64% 31%
1	7-A	359	2% 60% 35%
1	7-B	359	6% 56% 38%
1	7-C	359	7% 57% 37%
1	7-D	359	3% 60% 35%
1	8-A	359	2% 63% 32%
1	8-B	359	6% 55% 37%

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Mol	Chain	Length	Quality of chain
1	8-C	359	7% 60% 34%
1	8-D	359	3% 61% 33%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 93408 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 Probable N-acetyl-gamma-glutamyl-phosphate reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	1-A	345	2680	1700	467	501	12	0	0	0
1	2-A	345	2680	1700	467	501	12	0	0	0
1	3-A	345	2680	1700	467	501	12	0	0	0
1	4-A	345	2680	1700	467	501	12	0	0	0
1	5-A	345	2680	1700	467	501	12	0	0	0
1	6-A	345	2680	1700	467	501	12	0	0	0
1	7-A	345	2680	1700	467	501	12	0	0	0
1	8-A	345	2680	1700	467	501	12	0	0	0
1	1-B	345	2680	1700	467	501	12	0	0	0
1	2-B	345	2680	1700	467	501	12	0	0	0
1	3-B	345	2680	1700	467	501	12	0	0	0
1	4-B	345	2680	1700	467	501	12	0	0	0
1	5-B	345	2680	1700	467	501	12	0	0	0
1	6-B	345	2680	1700	467	501	12	0	0	0
1	7-B	345	2680	1700	467	501	12	0	0	0
1	8-B	345	2680	1700	467	501	12	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	1-C	345	2680	1700	467	501	12	0	0	0
1	2-C	345	2680	1700	467	501	12	0	0	0
1	3-C	345	2680	1700	467	501	12	0	0	0
1	4-C	345	2680	1700	467	501	12	0	0	0
1	5-C	345	2680	1700	467	501	12	0	0	0
1	6-C	345	2680	1700	467	501	12	0	0	0
1	7-C	345	2680	1700	467	501	12	0	0	0
1	8-C	345	2680	1700	467	501	12	0	0	0
1	1-D	345	2680	1700	467	501	12	0	0	0
1	2-D	345	2680	1700	467	501	12	0	0	0
1	3-D	345	2680	1700	467	501	12	0	0	0
1	4-D	345	2680	1700	467	501	12	0	0	0
1	5-D	345	2680	1700	467	501	12	0	0	0
1	6-D	345	2680	1700	467	501	12	0	0	0
1	7-D	345	2680	1700	467	501	12	0	0	0
1	8-D	345	2680	1700	467	501	12	0	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	1-A	270	270	270	0	0
2	2-A	263	263	263	0	0
2	3-A	268	268	268	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	4-A	267	Total O 267 267	0	0
2	5-A	262	Total O 262 262	0	0
2	6-A	267	Total O 267 267	0	0
2	7-A	269	Total O 269 269	0	0
2	8-A	267	Total O 267 267	0	0
2	1-B	225	Total O 225 225	0	0
2	2-B	227	Total O 227 227	0	0
2	3-B	216	Total O 216 216	0	0
2	4-B	224	Total O 224 224	0	0
2	5-B	223	Total O 223 223	0	0
2	6-B	225	Total O 225 225	0	0
2	7-B	223	Total O 223 223	0	0
2	8-B	222	Total O 222 222	0	0
2	1-C	220	Total O 220 220	0	0
2	2-C	231	Total O 231 231	0	0
2	3-C	228	Total O 228 228	0	0
2	4-C	223	Total O 223 223	0	0
2	5-C	229	Total O 229 229	0	0
2	6-C	224	Total O 224 224	0	0
2	7-C	224	Total O 224 224	0	0
2	8-C	231	Total O 231 231	0	0

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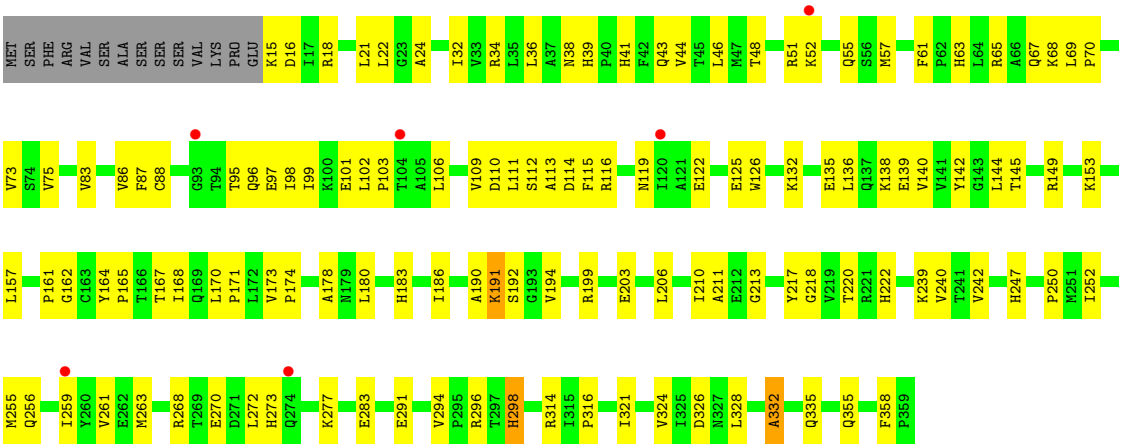
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	1-D	241	241	241	0	0
			Total	O		
2	2-D	235	235	235	0	0
			Total	O		
2	3-D	244	244	244	0	0
			Total	O		
2	4-D	242	242	242	0	0
			Total	O		
2	5-D	242	242	242	0	0
			Total	O		
2	6-D	240	240	240	0	0
			Total	O		
2	7-D	240	240	240	0	0
			Total	O		
2	8-D	236	236	236	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.

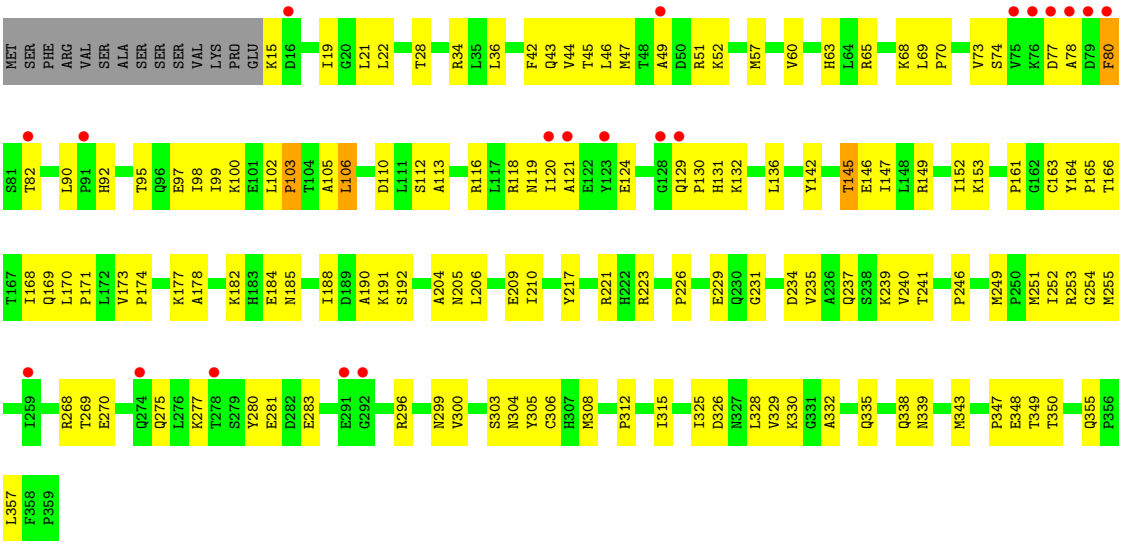
• Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

Chain 1-A:



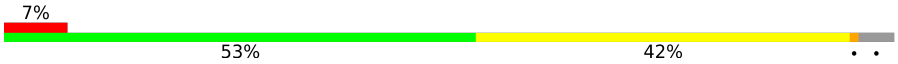
• Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

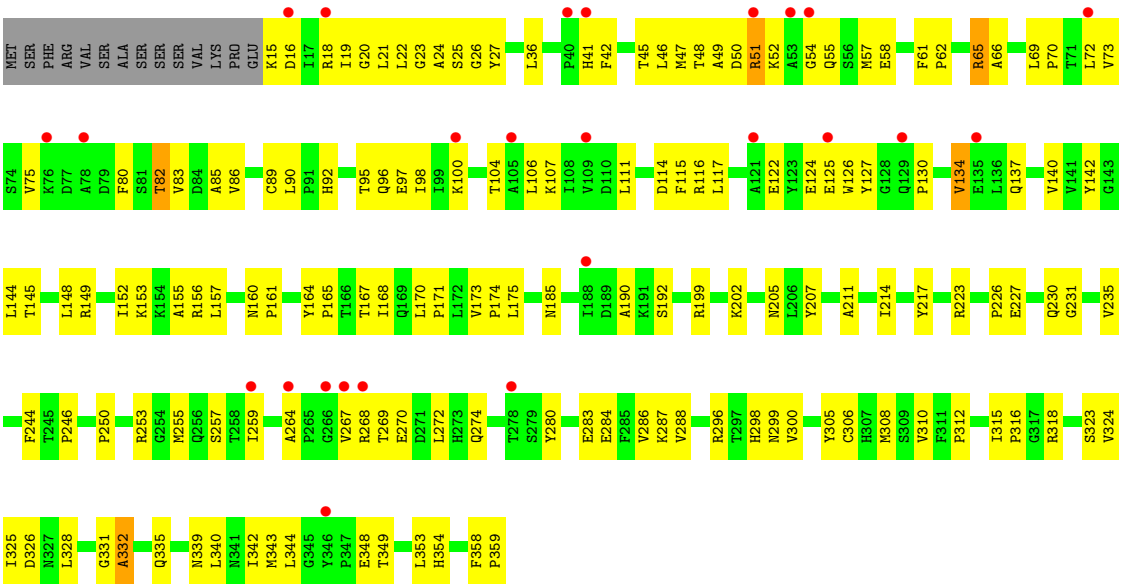
Chain 1-B:



• Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

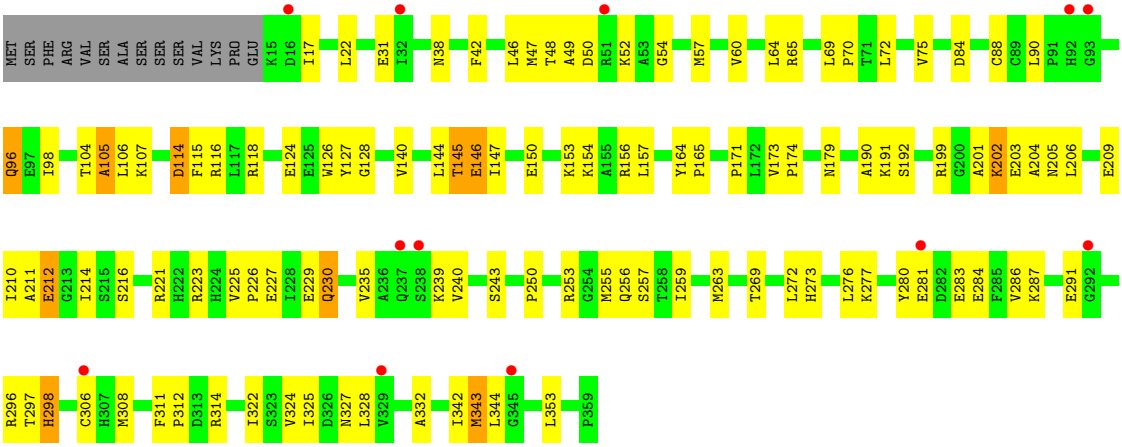
Chain 1-C:





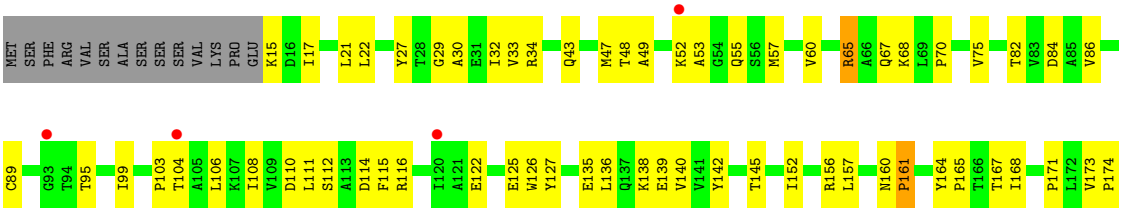
- Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

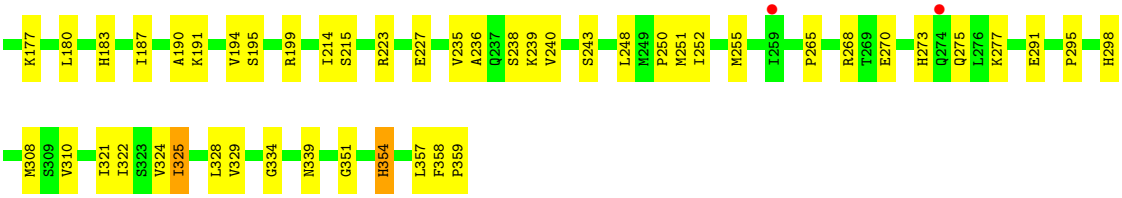
Chain 1-D:



- Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

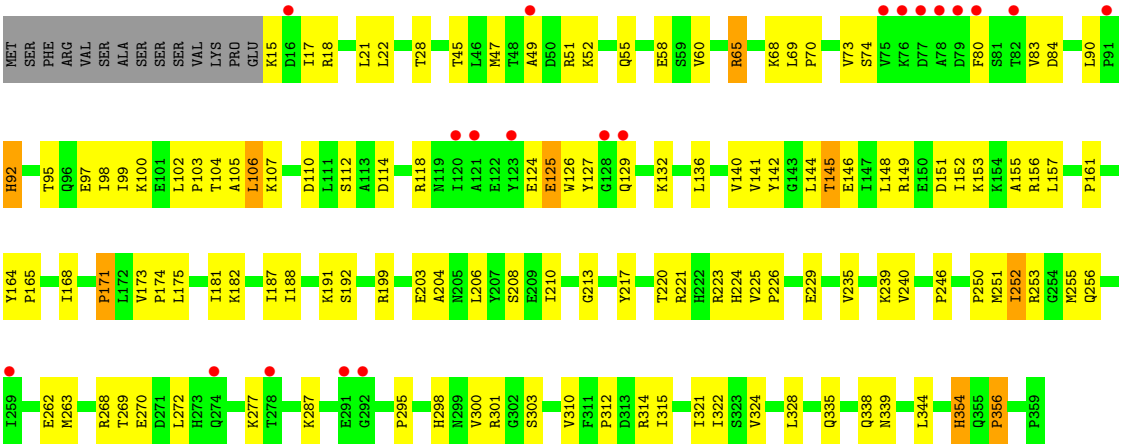
Chain 2-A:





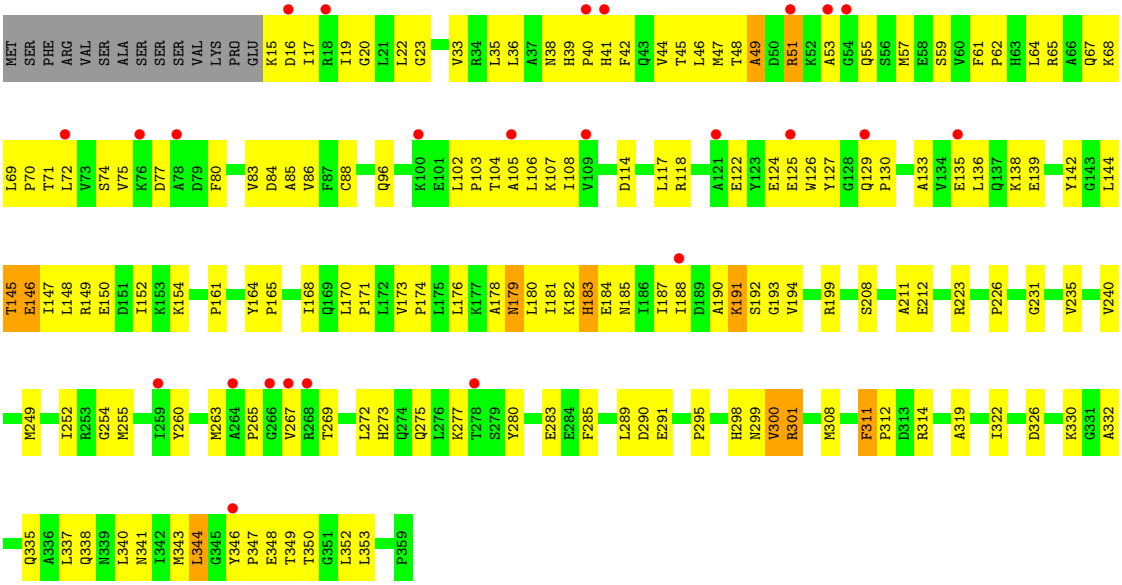
• Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

Chain 2-B:



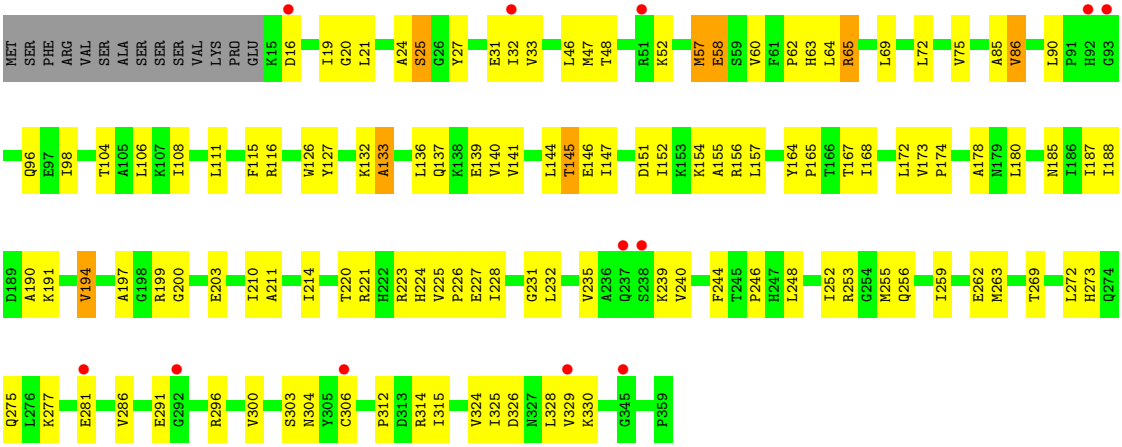
• Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

Chain 2-C:



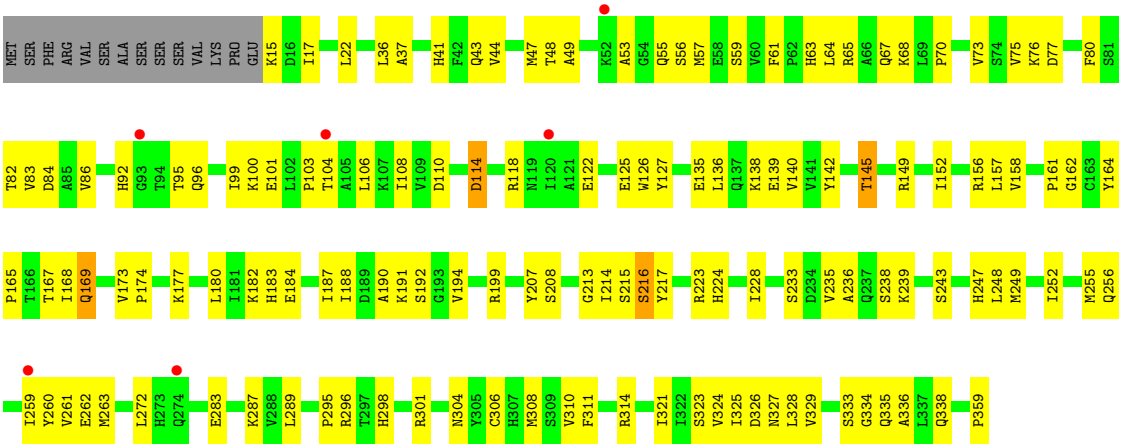
• Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

Chain 2-D:



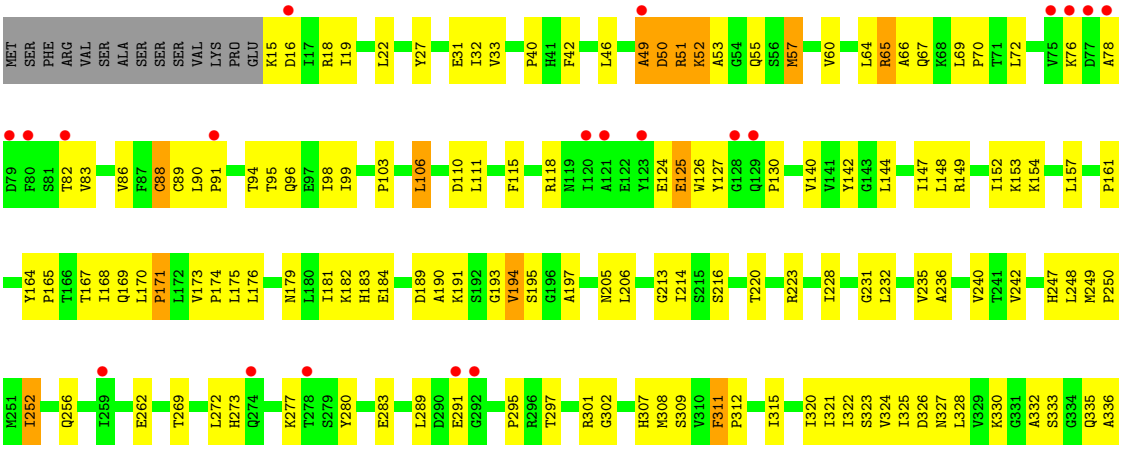
• Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

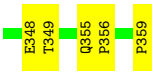
Chain 3-A:



• Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

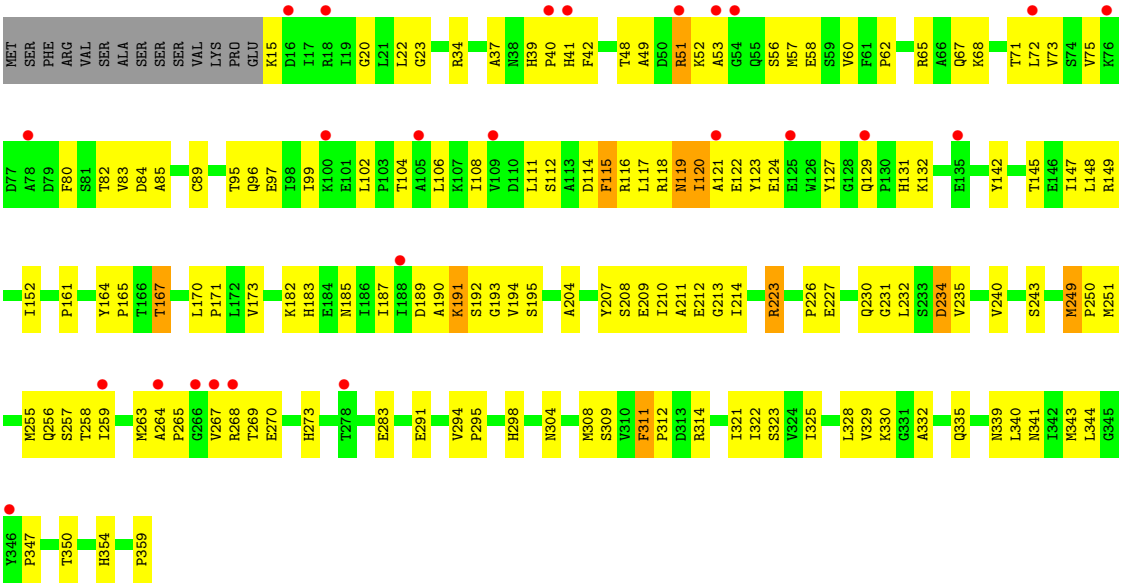
Chain 3-B:





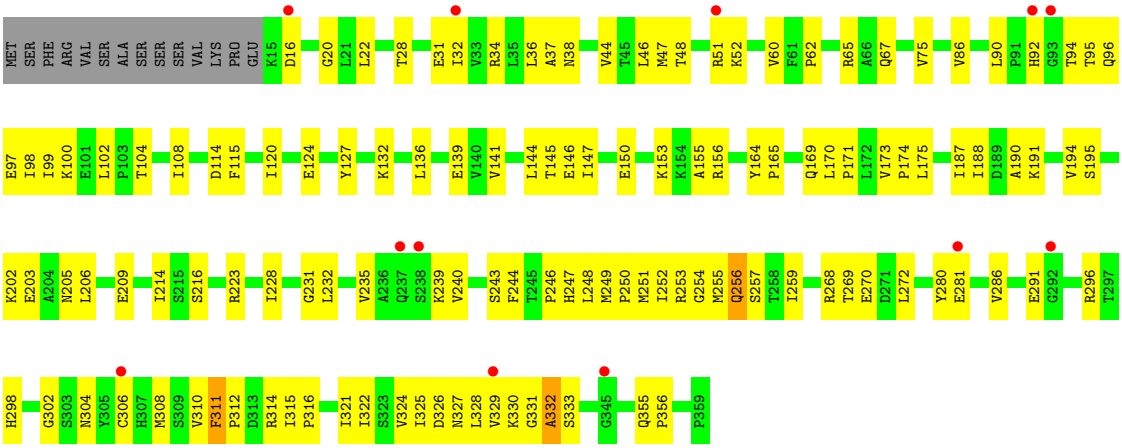
• Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

Chain 3-C:



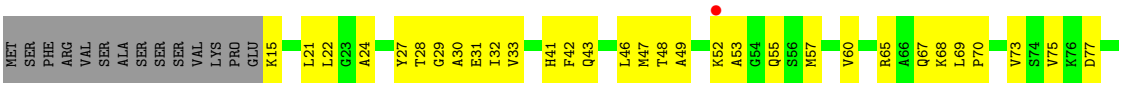
• Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

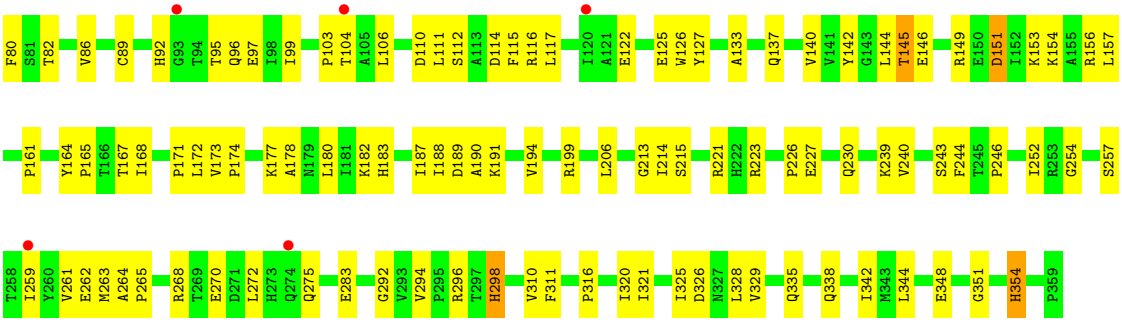
Chain 3-D:



• Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

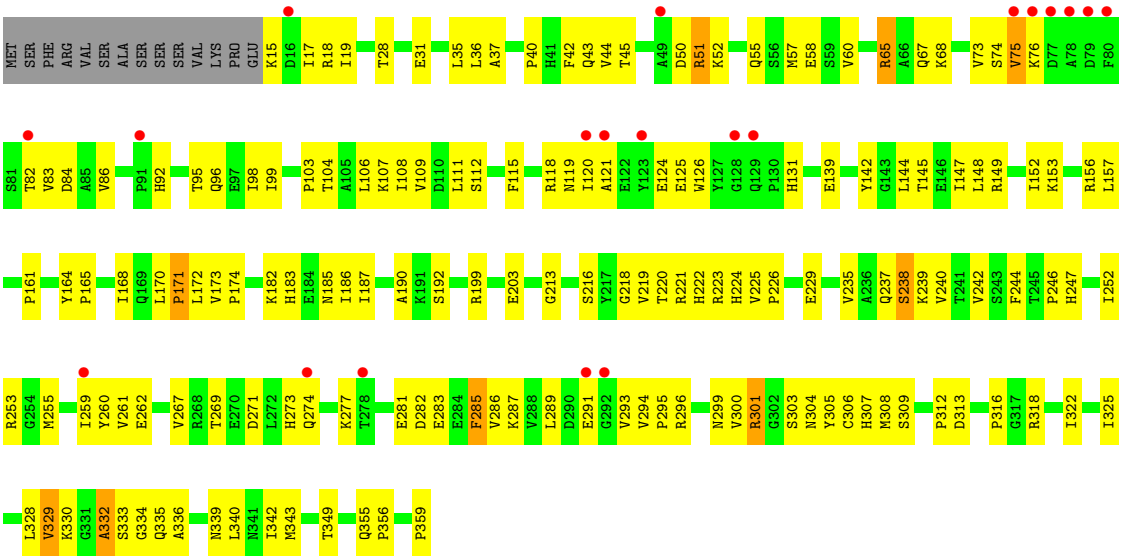
Chain 4-A:





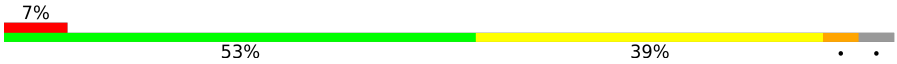
- Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

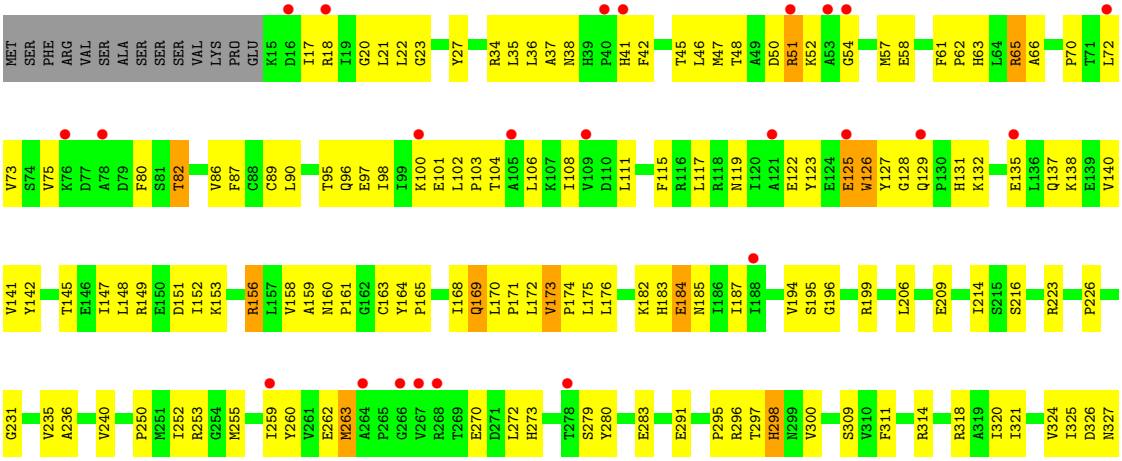
Chain 4-B:

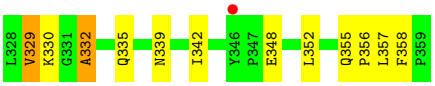


- Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

Chain 4-C:

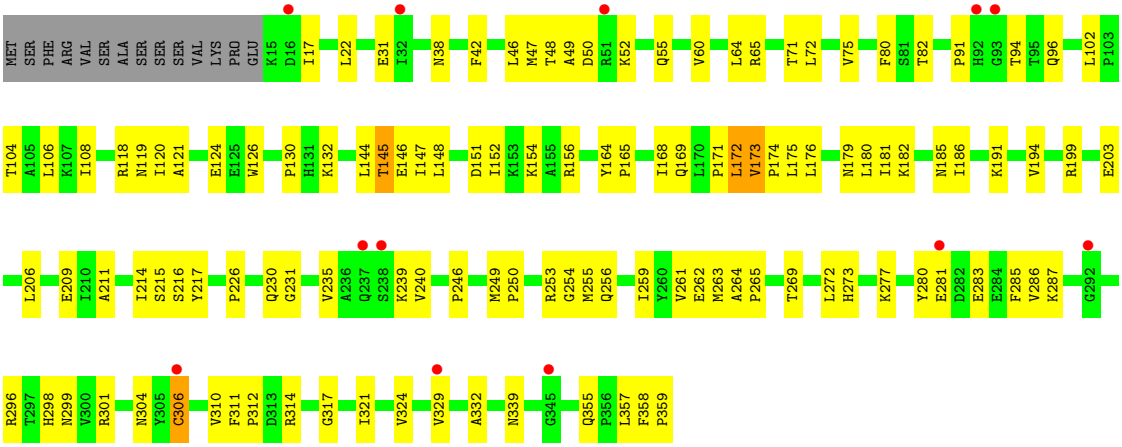






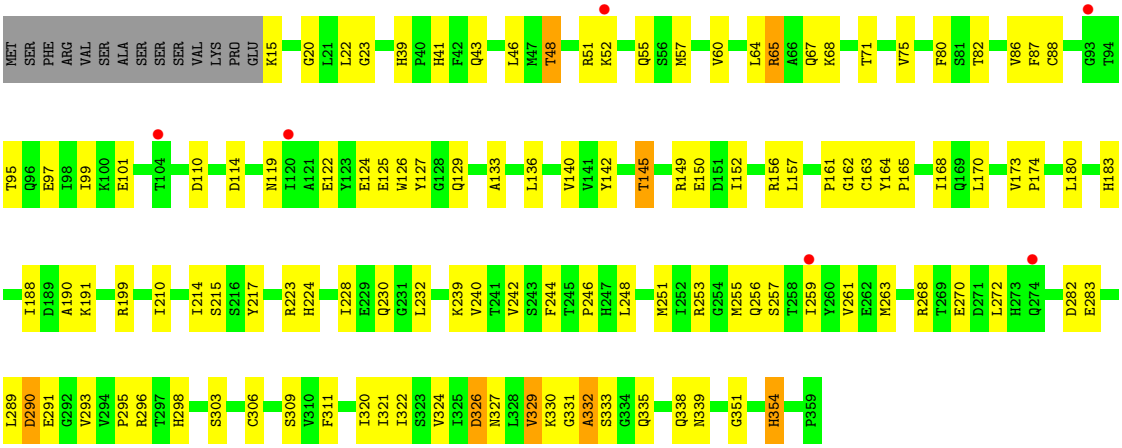
• Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

Chain 4-D:



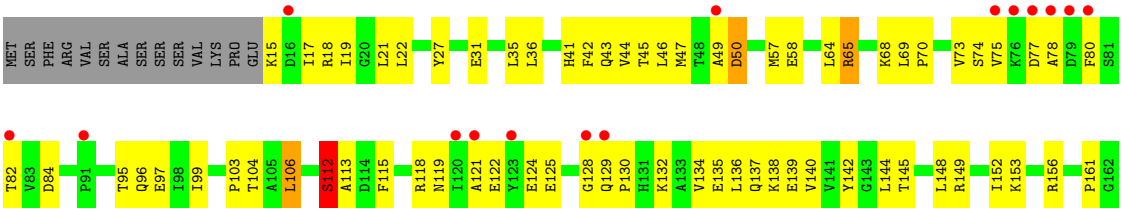
• Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

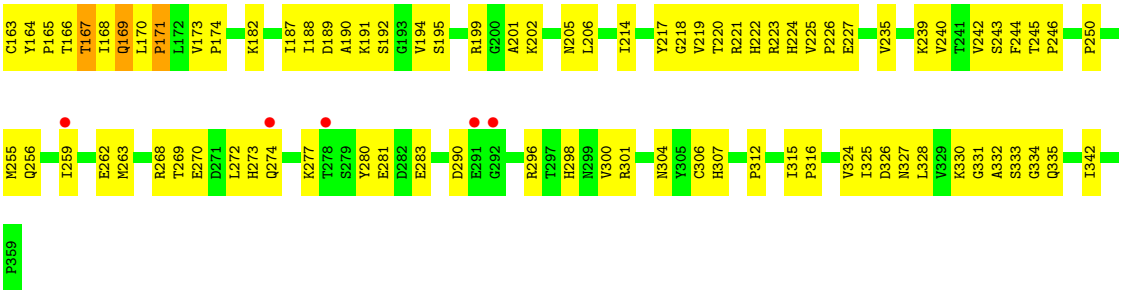
Chain 5-A:



• Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

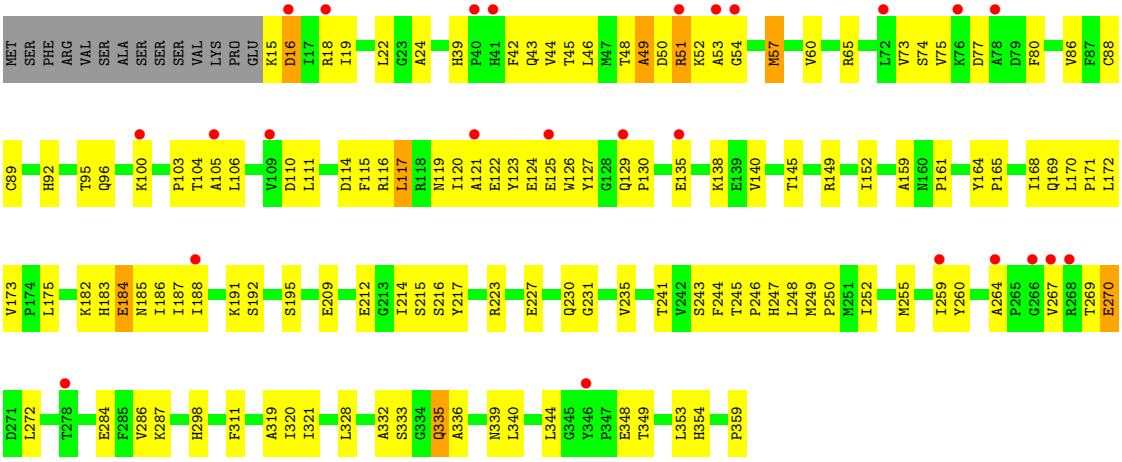
Chain 5-B:





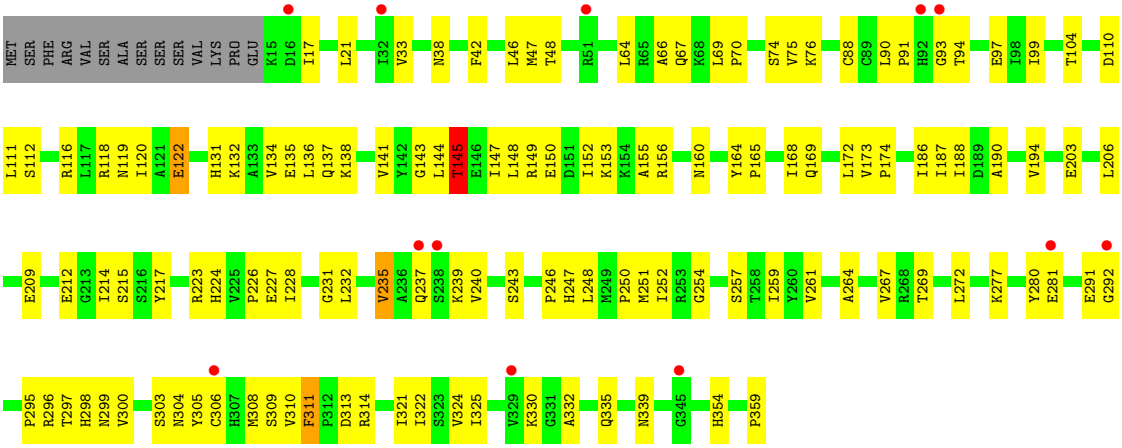
• Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

Chain 5-C:



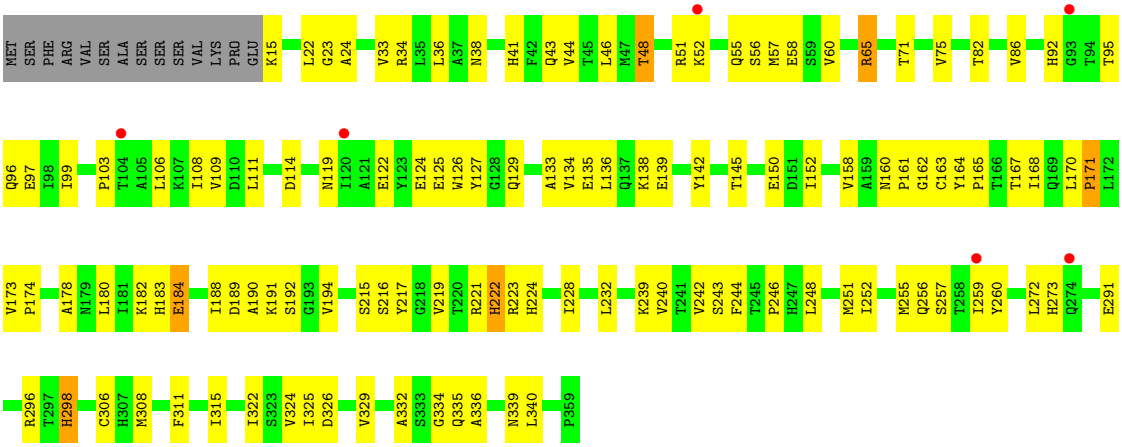
• Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

Chain 5-D:



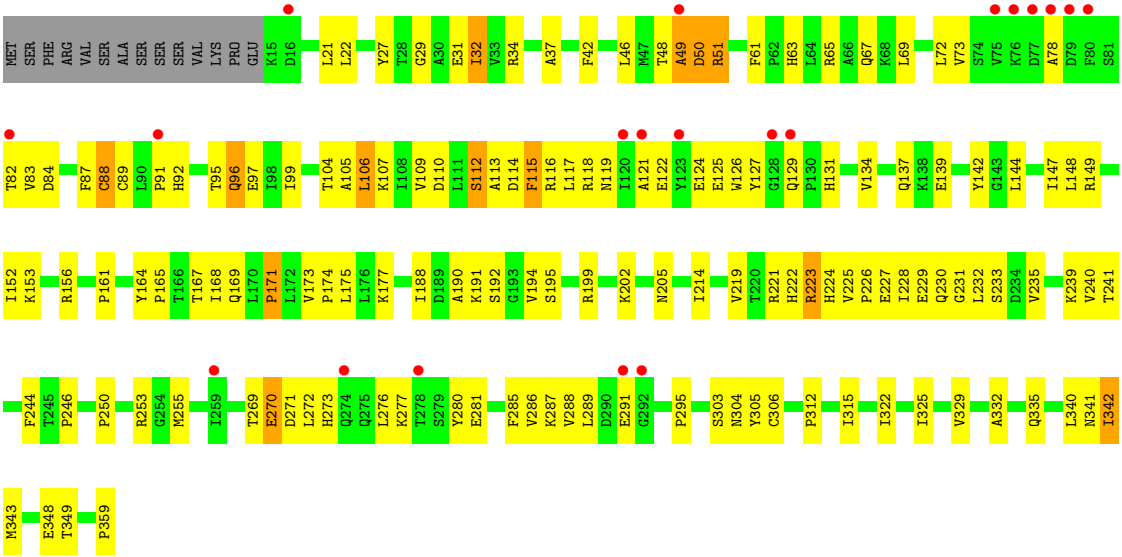
• Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

Chain 6-A:



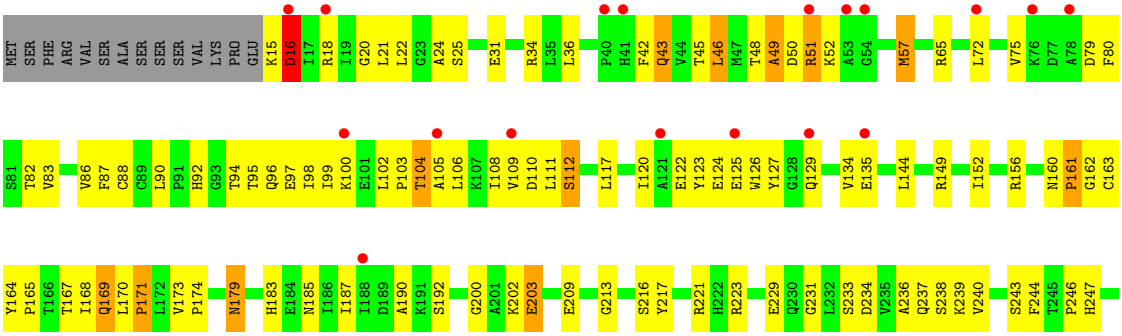
• Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

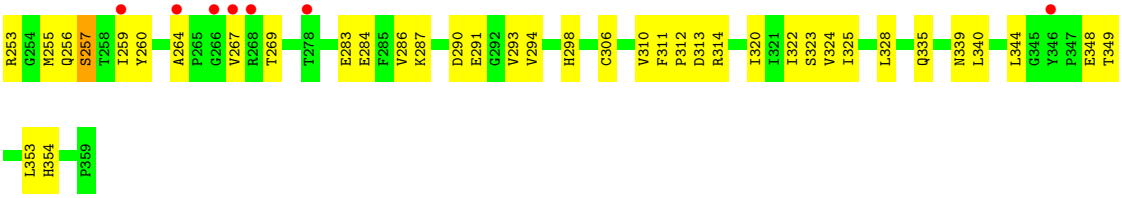
Chain 6-B:



• Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

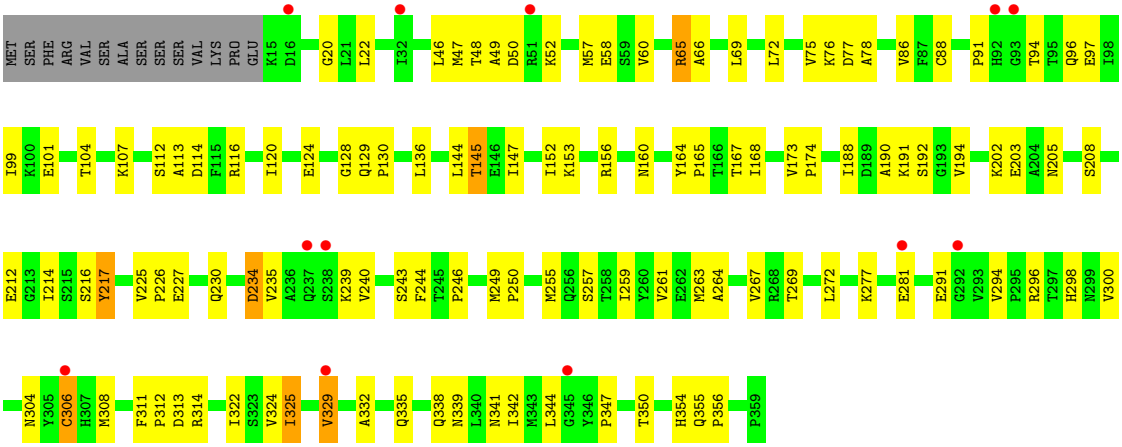
Chain 6-C:





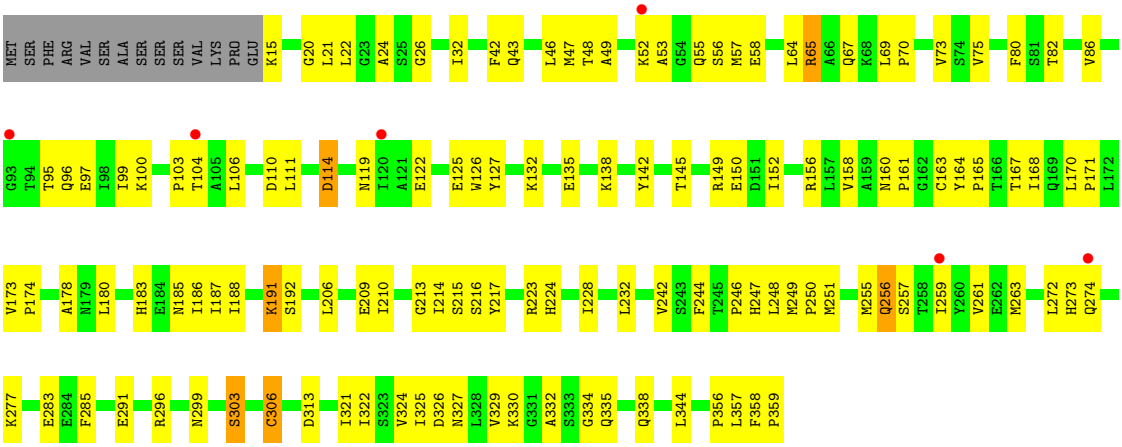
• Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

Chain 6-D:



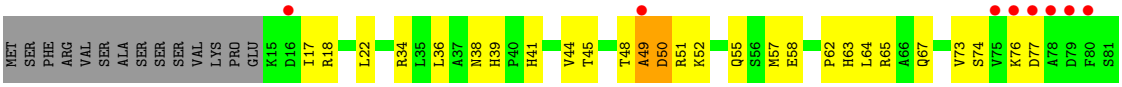
• Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

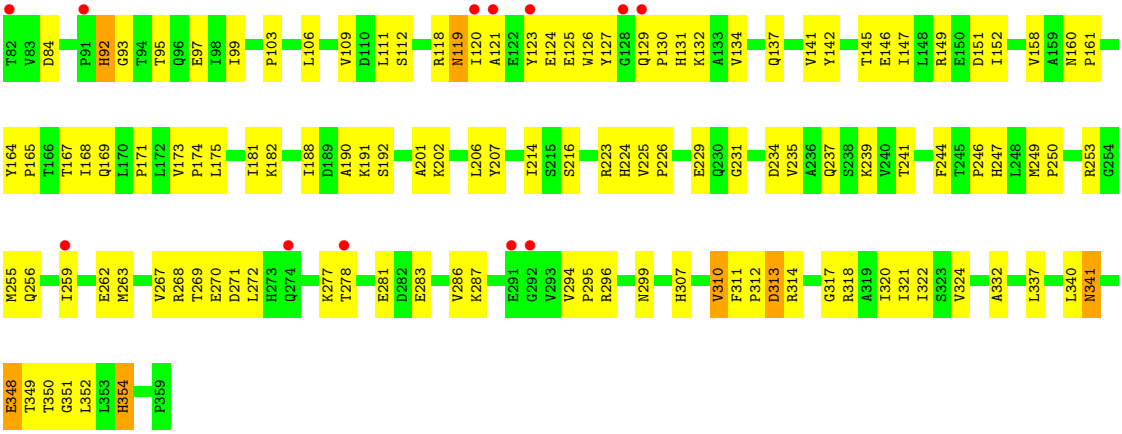
Chain 7-A:



• Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

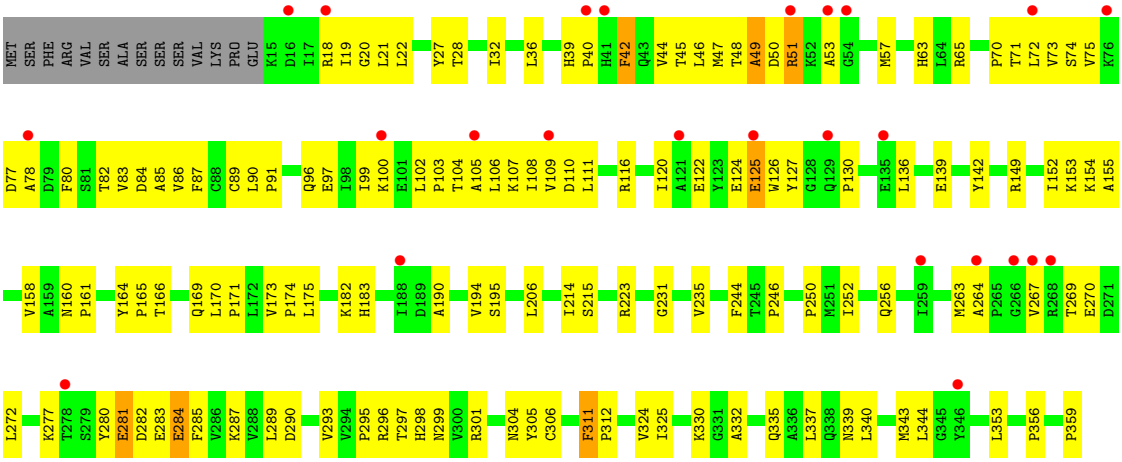
Chain 7-B:





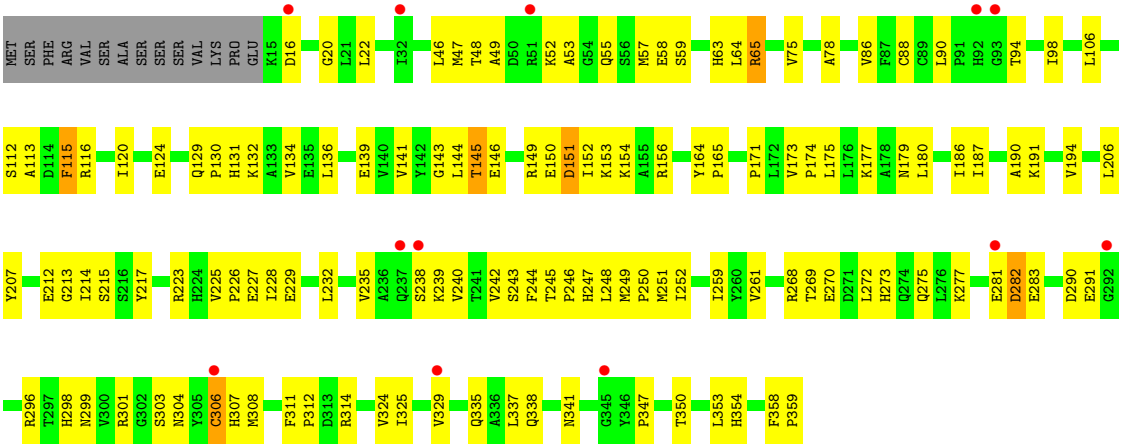
• Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

Chain 7-C:



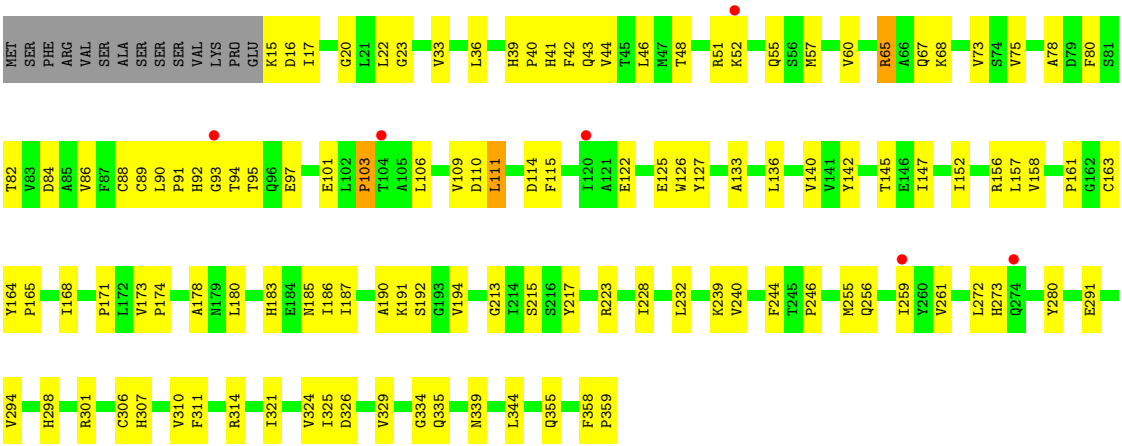
• Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

Chain 7-D:



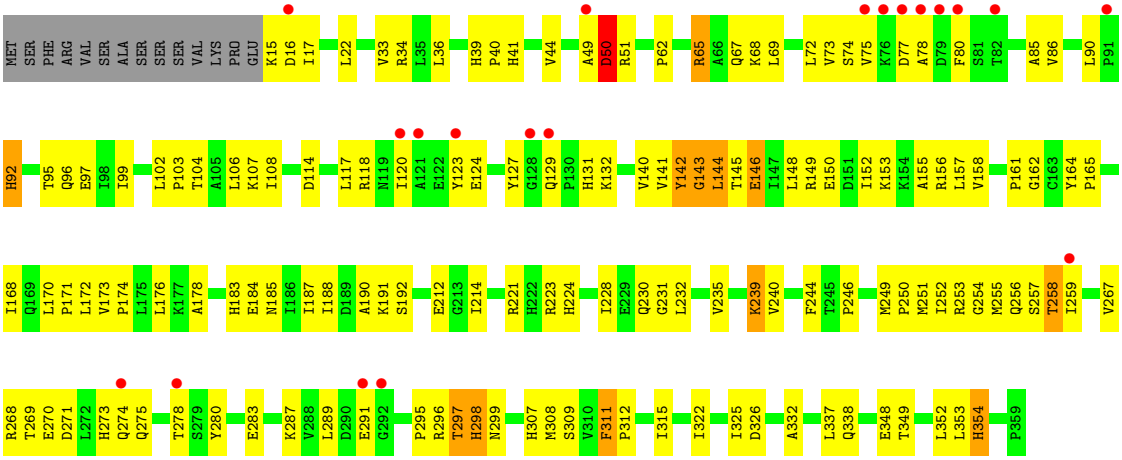
• Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

Chain 8-A:



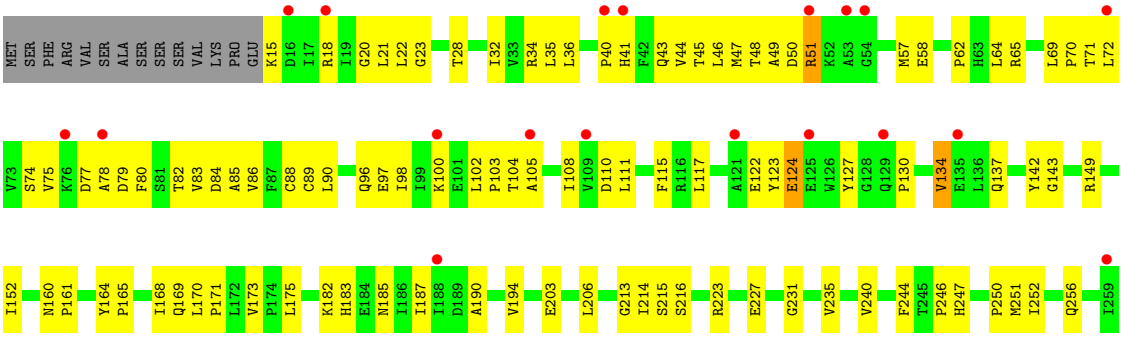
- Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

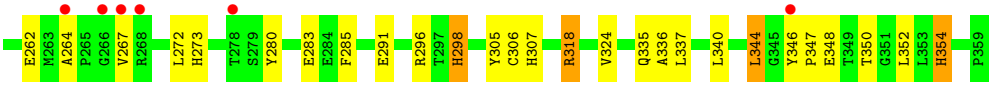
Chain 8-B:



- Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

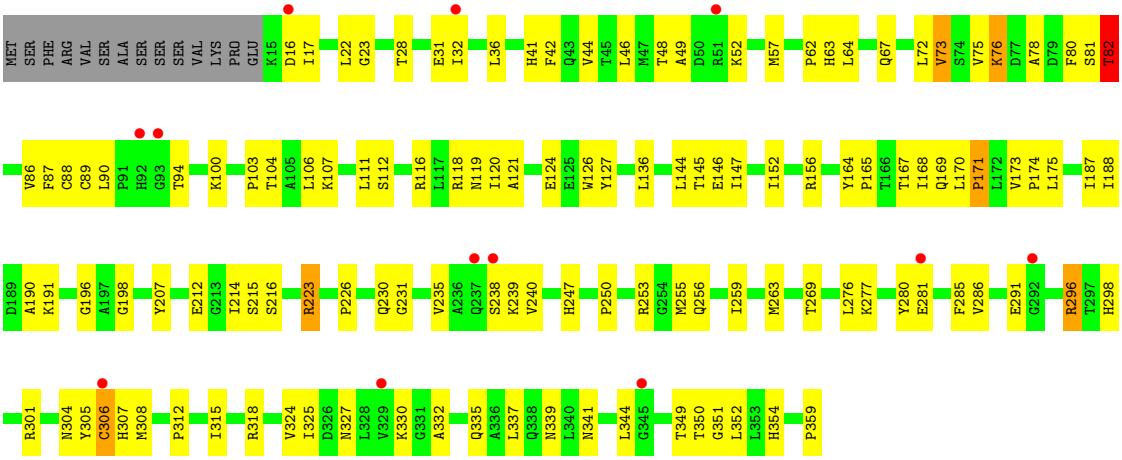
Chain 8-C:





• Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

Chain 8-D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	84.60Å 107.07Å 85.75Å 90.00° 118.88° 90.00°	Depositor
Resolution (Å)	27.31 – 2.19 27.54 – 2.19	Depositor EDS
% Data completeness (in resolution range)	92.9 (27.31-2.19) 92.9 (27.54-2.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.61 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.152 , 0.212 0.154 , 0.210	Depositor DCC
R_{free} test set	3240 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å^2)	26.0	Xtriage
Anisotropy	0.860	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 73.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.002 for -h-l,k,h 0.002 for l,k,-h-l 0.018 for h,-k,-h-l 0.017 for -h-l,-k,l 0.016 for l,-k,h	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	93408	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.08% 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 (i)

5.1 Standard geometry (i)

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	1-A	0.45	0/2734	0.68	1/3709 (0.0%)
1	1-B	0.45	0/2734	0.66	0/3709
1	1-C	0.44	0/2734	0.66	0/3709
1	1-D	0.45	0/2734	0.67	0/3709
1	2-A	0.46	0/2734	0.68	0/3709
1	2-B	0.45	0/2734	0.66	0/3709
1	2-C	0.44	0/2734	0.66	0/3709
1	2-D	0.47	0/2734	0.67	0/3709
1	3-A	0.45	0/2734	0.67	0/3709
1	3-B	0.46	0/2734	0.67	0/3709
1	3-C	0.44	0/2734	0.66	0/3709
1	3-D	0.47	0/2734	0.68	0/3709
1	4-A	0.45	0/2734	0.68	0/3709
1	4-B	0.46	0/2734	0.67	0/3709
1	4-C	0.43	0/2734	0.66	0/3709
1	4-D	0.47	0/2734	0.68	0/3709
1	5-A	0.47	0/2734	0.71	1/3709 (0.0%)
1	5-B	0.47	0/2734	0.70	0/3709
1	5-C	0.46	0/2734	0.70	0/3709
1	5-D	0.49	0/2734	0.69	0/3709
1	6-A	0.48	0/2734	0.70	1/3709 (0.0%)
1	6-B	0.48	1/2734 (0.0%)	0.71	0/3709
1	6-C	0.46	0/2734	0.70	0/3709
1	6-D	0.50	1/2734 (0.0%)	0.70	0/3709
1	7-A	0.47	0/2734	0.72	2/3709 (0.1%)
1	7-B	0.48	0/2734	0.70	0/3709
1	7-C	0.46	0/2734	0.68	0/3709
1	7-D	0.49	0/2734	0.73	0/3709
1	8-A	0.47	0/2734	0.71	1/3709 (0.0%)
1	8-B	0.47	0/2734	0.69	0/3709
1	8-C	0.46	0/2734	0.69	0/3709
1	8-D	0.53	1/2734 (0.0%)	0.72	0/3709
All	All	0.46	3/87488 (0.0%)	0.69	6/118688 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	8-D	306	CYS	CB-SG	-8.15	1.68	1.82
1	6-B	88	CYS	CB-SG	6.15	1.92	1.82
1	6-D	306	CYS	CB-SG	-5.67	1.72	1.81

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	7-A	326	ASP	N-CA-C	-5.49	96.17	111.00
1	1-A	326	ASP	N-CA-C	-5.36	96.52	111.00
1	8-A	326	ASP	N-CA-C	-5.33	96.61	111.00
1	7-A	285	PHE	N-CA-C	5.11	124.78	111.00
1	6-A	326	ASP	N-CA-C	-5.05	97.36	111.00
1	5-A	326	ASP	N-CA-C	-5.01	97.48	111.00

There are no chirality outliers.

There are no planarity outliers.

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	1-A	2680	0	2718	104	0
1	1-B	2680	0	2718	113	0
1	1-C	2680	0	2718	135	0
1	1-D	2680	0	2718	101	0
1	2-A	2680	0	2718	104	0
1	2-B	2680	0	2718	101	0
1	2-C	2680	0	2718	155	0
1	2-D	2680	0	2718	104	0
1	3-A	2680	0	2718	158	0
1	3-B	2680	0	2718	147	0
1	3-C	2680	0	2718	154	0
1	3-D	2680	0	2718	115	0
1	4-A	2680	0	2718	113	0
1	4-B	2680	0	2718	169	0
1	4-C	2680	0	2718	145	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	4-D	2680	0	2718	109	0
1	5-A	2680	0	2718	109	0
1	5-B	2680	0	2718	144	0
1	5-C	2680	0	2718	119	0
1	5-D	2680	0	2718	124	0
1	6-A	2680	0	2718	100	0
1	6-B	2680	0	2718	134	0
1	6-C	2680	0	2718	127	0
1	6-D	2680	0	2718	100	0
1	7-A	2680	0	2718	128	0
1	7-B	2680	0	2718	126	0
1	7-C	2680	0	2718	137	0
1	7-D	2680	0	2718	131	0
1	8-A	2680	0	2718	100	0
1	8-B	2680	0	2718	141	0
1	8-C	2680	0	2718	108	0
1	8-D	2680	0	2718	113	0
2	1-A	270	0	0	10	0
2	1-B	225	0	0	17	0
2	1-C	220	0	0	11	0
2	1-D	241	0	0	11	0
2	2-A	263	0	0	10	0
2	2-B	227	0	0	15	0
2	2-C	231	0	0	16	0
2	2-D	235	0	0	12	0
2	3-A	268	0	0	11	0
2	3-B	216	0	0	8	0
2	3-C	228	0	0	14	0
2	3-D	244	0	0	13	0
2	4-A	267	0	0	12	0
2	4-B	224	0	0	21	0
2	4-C	223	0	0	13	0
2	4-D	242	0	0	16	0
2	5-A	262	0	0	17	0
2	5-B	223	0	0	14	0
2	5-C	229	0	0	15	0
2	5-D	242	0	0	20	0
2	6-A	267	0	0	16	0
2	6-B	225	0	0	13	0
2	6-C	224	0	0	10	0
2	6-D	240	0	0	13	0
2	7-A	269	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	7-B	223	0	0	9	0
2	7-C	224	0	0	11	0
2	7-D	240	0	0	13	0
2	8-A	267	0	0	11	0
2	8-B	222	0	0	12	0
2	8-C	231	0	0	11	0
2	8-D	236	0	0	11	0
All	All	93408	0	86976	3764	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

All (3764) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:ASP:HA	1:A:154:LYS:HE2	1.37	1.06
1:C:67:GLN:HE21	1:C:69:LEU:HD21	1.21	1.04
1:B:15:LYS:HD2	1:B:43:GLN:HB2	1.38	1.03
1:B:306:CYS:HA	1:B:325:ILE:HG22	1.42	1.01
1:D:306:CYS:HB3	1:D:325:ILE:HG22	1.42	1.01
1:C:125:GLU:HG3	1:C:126:TRP:H	1.23	1.00
1:D:151:ASP:HA	1:D:154:LYS:HE2	1.43	0.99
1:B:73:VAL:HG12	1:B:74:SER:H	1.28	0.98
1:D:202:LYS:HB2	1:D:205:ASN:ND2	1.80	0.97
1:A:191:LYS:HB3	1:A:247:HIS:HB2	1.44	0.97
1:C:257:SER:HB3	1:C:259:ILE:HD11	1.43	0.96
1:A:15:LYS:HD2	1:A:43:GLN:HB2	1.47	0.96
1:C:51:ARG:H	1:C:51:ARG:HE	0.97	0.95
1:C:51:ARG:H	1:C:51:ARG:HD2	1.31	0.95
1:D:170:LEU:HD12	1:D:306:CYS:SG	2.06	0.95
1:C:51:ARG:H	1:C:51:ARG:HD2	1.29	0.95
1:D:310:VAL:HG22	1:D:321:ILE:HG12	1.46	0.95
1:B:221:ARG:HD3	2:B:474:HOH:O	1.65	0.95
1:C:86:VAL:HB	1:C:108:ILE:HD13	1.45	0.95
1:A:63:HIS:HD2	1:B:356:PRO:HB2	1.27	0.94
1:D:151:ASP:HA	1:D:154:LYS:HE2	1.47	0.94
1:C:51:ARG:H	1:C:51:ARG:HD2	1.32	0.94
1:C:22:LEU:HA	1:C:48:THR:HB	1.46	0.94
1:A:15:LYS:HD2	1:A:43:GLN:HB2	1.50	0.94
1:A:256:GLN:HB2	1:A:324:VAL:HG12	1.46	0.93
1:A:145:THR:HG21	1:A:338:GLN:NE2	1.84	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:GLN:HB2	1:B:324:VAL:HG12	1.49	0.93
1:D:310:VAL:HG22	1:D:321:ILE:HG12	1.51	0.92
1:B:73:VAL:HG12	1:B:74:SER:H	1.31	0.92
1:C:50:ASP:H	1:C:51:ARG:NH2	1.68	0.92
1:D:75:VAL:HG23	1:D:76:LYS:HD2	1.51	0.92
1:A:249:MET:HE3	1:D:214:ILE:HG21	1.50	0.92
1:A:215:SER:HB3	1:D:296:ARG:HG3	1.53	0.91
1:B:73:VAL:HG12	1:B:74:SER:H	1.36	0.91
1:B:73:VAL:HG12	1:B:74:SER:H	1.34	0.91
1:B:46:LEU:HD11	1:B:78:ALA:HB1	1.53	0.91
1:D:173:VAL:HG13	1:D:235:VAL:HG11	1.52	0.91
1:C:51:ARG:H	1:C:51:ARG:HE	1.12	0.90
1:C:51:ARG:H	1:C:51:ARG:HE	1.12	0.90
1:B:220:THR:HG22	1:B:221:ARG:HG3	1.54	0.90
1:B:195:SER:HB2	1:B:252:ILE:O	1.71	0.89
1:A:91:PRO:HD2	1:A:94:THR:HG21	1.54	0.89
1:B:173:VAL:HG13	1:B:235:VAL:HG21	1.55	0.89
1:A:298:HIS:HA	1:A:301:ARG:HD3	1.54	0.89
1:C:103:PRO:HG2	1:C:106:LEU:HG	1.53	0.89
1:C:306:CYS:HB3	1:C:325:ILE:HG22	1.55	0.89
1:B:221:ARG:HD3	2:B:473:HOH:O	1.73	0.89
1:D:151:ASP:HA	1:D:154:LYS:HE2	1.54	0.89
1:B:192:SER:HB3	1:B:255:MET:HE2	1.55	0.88
1:B:18:ARG:HD3	2:B:509:HOH:O	1.74	0.88
1:B:73:VAL:HG12	1:B:74:SER:H	1.38	0.87
1:C:141:VAL:HB	1:C:158:VAL:HG22	1.55	0.87
1:B:221:ARG:HG2	2:C:419:HOH:O	1.74	0.87
1:B:103:PRO:HG2	1:B:106:LEU:HD22	1.54	0.87
1:A:96:GLN:HB2	1:A:132:LYS:HE3	1.58	0.86
1:B:74:SER:HB3	1:B:77:ASP:HB2	1.57	0.86
1:B:149:ARG:HD3	1:B:348:GLU:OE1	1.76	0.86
1:B:206:LEU:HA	1:D:206:LEU:HA	1.58	0.86
1:C:96:GLN:HE21	1:C:114:ASP:HB3	1.41	0.86
1:B:256:GLN:NE2	1:B:322:ILE:HG23	1.90	0.86
1:B:269:THR:HA	1:B:272:LEU:HD12	1.56	0.86
1:B:221:ARG:HD3	2:B:472:HOH:O	1.75	0.86
1:A:259:ILE:HB	1:A:321:ILE:HB	1.58	0.85
1:A:256:GLN:HB3	1:D:214:ILE:HD11	1.58	0.85
1:B:221:ARG:HD3	2:B:472:HOH:O	1.73	0.85
1:B:304:ASN:HA	1:B:329:VAL:HG11	1.57	0.85
1:C:86:VAL:H	1:C:108:ILE:HG12	1.41	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:ARG:H	1:B:51:ARG:HD2	1.42	0.85
1:D:75:VAL:HG23	2:D:400:HOH:O	1.77	0.85
1:A:145:THR:HG21	1:A:338:GLN:NE2	1.92	0.85
1:C:149:ARG:HD3	1:C:348:GLU:OE1	1.77	0.85
1:B:188:ILE:HG12	1:B:259:ILE:HG12	1.58	0.84
1:D:47:MET:HE1	1:D:69:LEU:HB3	1.59	0.84
1:C:182:LYS:HB3	1:C:184:GLU:OE1	1.77	0.84
1:B:273:HIS:ND1	1:B:291:GLU:HG3	1.93	0.83
1:A:23:GLY:H	1:A:48:THR:HG22	1.40	0.82
1:B:103:PRO:HG2	1:B:106:LEU:HD22	1.59	0.82
1:C:22:LEU:HD11	1:C:80:PHE:HE2	1.44	0.82
1:D:168:ILE:HD11	1:D:188:ILE:HG21	1.60	0.82
1:B:173:VAL:HG13	1:B:235:VAL:HG21	1.61	0.82
1:B:49:ALA:HB3	1:B:72:LEU:HD13	1.61	0.82
1:D:173:VAL:HG13	1:D:235:VAL:HG11	1.61	0.82
1:A:15:LYS:HE3	2:A:428:HOH:O	1.79	0.82
1:C:173:VAL:HG13	1:C:235:VAL:HG21	1.62	0.82
1:B:103:PRO:HG2	1:B:106:LEU:HD22	1.61	0.82
1:D:88:CYS:HB2	1:D:110:ASP:HA	1.61	0.82
1:C:22:LEU:HA	1:C:48:THR:HB	1.59	0.82
1:A:310:VAL:HG13	1:A:321:ILE:HG13	1.62	0.82
1:B:142:TYR:CZ	1:B:161:PRO:HB3	2.14	0.82
1:A:191:LYS:CB	1:A:247:HIS:HB2	2.09	0.82
1:C:296:ARG:O	1:C:324:VAL:HG21	1.80	0.81
1:C:51:ARG:H	1:C:51:ARG:HD2	1.45	0.81
1:B:84:ASP:C	1:B:106:LEU:HG	2.00	0.81
1:B:103:PRO:HG2	1:B:106:LEU:HD22	1.62	0.81
1:C:50:ASP:H	1:C:51:ARG:HH21	1.26	0.81
1:D:75:VAL:HG23	2:D:404:HOH:O	1.81	0.81
1:C:115:PHE:HB3	1:C:140:VAL:HG11	1.63	0.80
1:B:117:LEU:HD13	1:B:122:GLU:HB3	1.63	0.80
1:A:15:LYS:HE3	2:A:426:HOH:O	1.81	0.80
1:D:75:VAL:HG23	2:D:398:HOH:O	1.82	0.80
1:C:65:ARG:HD2	2:C:531:HOH:O	1.81	0.80
1:C:315:ILE:HG23	1:C:316:PRO:HD2	1.63	0.80
1:C:67:GLN:NE2	1:C:69:LEU:HD21	1.95	0.80
1:C:50:ASP:N	1:C:51:ARG:HH21	1.80	0.80
1:C:48:THR:HG21	1:C:75:VAL:HG22	1.64	0.80
1:C:124:GLU:HG2	1:C:130:PRO:HA	1.62	0.79
1:C:51:ARG:H	1:C:51:ARG:HE	1.26	0.79
1:D:99:ILE:HG23	1:D:108:ILE:HD13	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51:ARG:H	1:C:51:ARG:NE	1.78	0.79
1:A:49:ALA:O	1:A:53:ALA:HB2	1.83	0.79
1:A:47:MET:HE2	1:A:70:PRO:HD2	1.65	0.79
1:A:23:GLY:H	1:A:48:THR:HG22	1.46	0.79
1:D:165:PRO:HG2	1:D:227:GLU:OE1	1.83	0.78
1:B:296:ARG:HB2	1:B:299:ASN:HD22	1.48	0.78
1:C:259:ILE:HB	1:C:321:ILE:HB	1.63	0.78
1:C:35:LEU:HD22	1:C:352:LEU:HD23	1.64	0.78
1:B:220:THR:HG22	1:B:221:ARG:HG3	1.65	0.78
1:A:111:LEU:HA	1:A:160:ASN:HB3	1.63	0.78
1:B:322:ILE:HG22	1:B:322:ILE:O	1.81	0.78
1:C:80:PHE:HB3	1:C:106:LEU:HD11	1.65	0.78
1:D:281:GLU:HB3	2:D:589:HOH:O	1.84	0.78
1:B:173:VAL:HG13	1:B:235:VAL:HG21	1.64	0.78
1:A:211:ALA:HA	1:A:250:PRO:HB3	1.64	0.78
1:B:231:GLY:O	1:B:235:VAL:HG23	1.84	0.78
1:B:354:HIS:H	1:B:354:HIS:CD2	1.98	0.77
1:B:195:SER:HB3	1:B:327:ASN:HD21	1.48	0.77
1:B:39:HIS:HD1	1:B:41:HIS:H	1.30	0.77
1:D:282:ASP:HB2	2:D:590:HOH:O	1.85	0.77
1:B:280:TYR:HD1	1:B:283:GLU:HG3	1.48	0.77
1:A:191:LYS:HG3	1:A:247:HIS:ND1	2.00	0.77
1:C:282:ASP:HB3	2:C:555:HOH:O	1.83	0.77
1:A:192:SER:HB2	1:A:255:MET:HE2	1.67	0.77
1:B:19:ILE:HD11	1:B:42:PHE:HB3	1.67	0.77
1:B:176:LEU:HD13	1:B:236:ALA:HB2	1.66	0.77
1:B:90:LEU:HD12	1:B:95:THR:HA	1.67	0.77
1:B:269:THR:HG21	1:B:312:PRO:HA	1.65	0.77
1:D:298:HIS:HA	1:D:301:ARG:HH11	1.48	0.77
1:B:73:VAL:HG12	1:B:74:SER:H	1.48	0.77
1:C:173:VAL:HG13	1:C:235:VAL:HG11	1.67	0.76
1:B:304:ASN:HA	1:B:330:LYS:HB2	1.67	0.76
1:C:262:GLU:HA	1:C:318:ARG:HA	1.68	0.76
2:C:422:HOH:O	1:D:62:PRO:HG3	1.85	0.76
1:C:145:THR:HG21	1:C:338:GLN:NE2	1.99	0.76
1:D:341:ASN:HD21	1:D:350:THR:HB	1.50	0.76
1:D:75:VAL:HG23	2:D:400:HOH:O	1.86	0.76
1:A:49:ALA:O	1:A:53:ALA:HB2	1.86	0.76
1:A:97:GLU:O	1:A:101:GLU:HG2	1.85	0.76
1:D:188:ILE:HG12	1:D:259:ILE:HG23	1.67	0.76
1:D:281:GLU:HB3	2:D:591:HOH:O	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:203:GLU:O	1:C:209:GLU:HG3	1.86	0.76
1:B:142:TYR:CZ	1:B:161:PRO:HB3	2.20	0.76
1:D:34:ARG:NH2	1:D:329:VAL:HG22	2.00	0.76
1:C:50:ASP:H	1:C:51:ARG:HH21	1.31	0.75
1:D:75:VAL:HG23	2:D:402:HOH:O	1.87	0.75
1:B:142:TYR:CZ	1:B:161:PRO:HB3	2.21	0.75
1:C:88:CYS:HB2	1:C:110:ASP:HA	1.68	0.75
1:D:281:GLU:HB3	2:D:585:HOH:O	1.86	0.75
1:B:305:TYR:HB3	1:B:307:HIS:CD2	2.21	0.75
1:A:49:ALA:O	1:A:53:ALA:HB2	1.87	0.75
1:C:51:ARG:H	1:C:51:ARG:NE	1.85	0.75
1:A:185:ASN:ND2	2:A:602:HOH:O	2.19	0.74
1:D:188:ILE:HG23	1:D:259:ILE:HG13	1.68	0.74
1:B:52:LYS:HA	1:B:55:GLN:NE2	2.02	0.74
1:C:125:GLU:HG3	1:C:126:TRP:N	2.02	0.74
1:B:173:VAL:HG13	1:B:235:VAL:HG21	1.69	0.74
1:D:104:THR:O	1:D:156:ARG:HD2	1.88	0.74
1:A:52:LYS:HD3	1:A:60:VAL:HG22	1.70	0.74
1:A:260:TYR:HB3	2:A:375:HOH:O	1.86	0.74
1:C:269:THR:HG21	1:C:312:PRO:HA	1.68	0.74
1:C:127:TYR:CE1	1:C:223:ARG:HD3	2.23	0.74
1:C:243:SER:O	2:C:363:HOH:O	2.05	0.74
1:C:39:HIS:HE2	1:C:337:LEU:HD11	1.52	0.74
1:C:106:LEU:HD13	1:C:108:ILE:HD11	1.70	0.74
1:B:149:ARG:O	1:B:153:LYS:HG3	1.87	0.74
1:B:120:ILE:HG23	1:B:131:HIS:HB2	1.68	0.73
1:C:284:GLU:O	1:C:287:LYS:HE2	1.87	0.73
1:C:20:GLY:HA3	1:C:86:VAL:HG22	1.70	0.73
1:C:107:LYS:HE2	1:C:156:ARG:HA	1.70	0.73
1:D:173:VAL:HG13	1:D:235:VAL:HG21	1.68	0.73
1:B:256:GLN:HB2	1:B:324:VAL:HG12	1.69	0.73
1:B:142:TYR:O	1:B:158:VAL:HG13	1.87	0.73
1:C:15:LYS:HG2	1:C:16:ASP:H	1.52	0.73
1:C:48:THR:HG21	1:C:75:VAL:HG22	1.69	0.73
1:A:142:TYR:CZ	1:A:161:PRO:HB3	2.24	0.73
1:A:135:GLU:HG2	2:A:447:HOH:O	1.87	0.73
1:A:97:GLU:HB3	1:A:132:LYS:HD2	1.69	0.73
1:C:22:LEU:HA	1:C:48:THR:HB	1.70	0.73
1:B:18:ARG:NH1	1:B:82:THR:HB	2.03	0.73
1:C:175:LEU:HD22	1:C:272:LEU:HD22	1.71	0.73
1:A:63:HIS:CD2	1:B:356:PRO:HB2	2.19	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:GLN:NE2	1:A:322:ILE:HG23	2.03	0.73
1:B:152:ILE:HG23	1:B:158:VAL:HG21	1.70	0.73
1:B:95:THR:HB	1:B:114:ASP:OD2	1.87	0.73
1:D:46:LEU:HD21	1:D:78:ALA:HB1	1.71	0.73
1:C:340:LEU:O	1:C:344:LEU:HD13	1.89	0.73
1:B:306:CYS:SG	1:B:325:ILE:HG22	2.29	0.72
1:C:245:THR:OG1	2:C:363:HOH:O	2.05	0.72
1:A:52:LYS:HD3	1:A:60:VAL:HG22	1.71	0.72
1:B:273:HIS:CE1	1:B:277:LYS:HD2	2.25	0.72
1:C:124:GLU:OE1	1:C:130:PRO:HA	1.88	0.72
1:D:145:THR:HG21	1:D:338:GLN:HG2	1.71	0.72
1:C:95:THR:HB	1:C:114:ASP:OD2	1.88	0.72
1:B:175:LEU:HD22	1:B:181:ILE:HG23	1.70	0.72
1:D:281:GLU:HB3	2:D:593:HOH:O	1.89	0.72
1:A:214:ILE:H	1:D:297:THR:HB	1.53	0.72
1:C:263:MET:SD	1:C:272:LEU:HD11	2.30	0.72
1:D:144:LEU:HD23	1:D:147:ILE:HG13	1.72	0.72
1:B:304:ASN:HA	1:B:329:VAL:CG1	2.20	0.72
1:A:64:LEU:HD22	1:A:67:GLN:HE21	1.53	0.72
1:C:161:PRO:HG2	1:C:335:GLN:NE2	2.04	0.72
1:C:118:ARG:H	1:C:230:GLN:HE22	1.36	0.72
1:B:103:PRO:HG2	1:B:106:LEU:HD22	1.72	0.72
1:C:299:ASN:ND2	2:C:370:HOH:O	2.10	0.72
1:A:215:SER:HB3	1:D:296:ARG:HG2	1.71	0.72
1:B:354:HIS:H	1:B:354:HIS:CD2	2.08	0.72
1:A:301:ARG:HG3	2:A:376:HOH:O	1.88	0.72
1:A:135:GLU:HG2	2:A:445:HOH:O	1.89	0.72
1:B:291:GLU:HG3	2:B:581:HOH:O	1.90	0.72
1:B:73:VAL:HG12	1:B:74:SER:N	2.04	0.71
1:D:306:CYS:SG	1:D:325:ILE:HG22	2.29	0.71
1:C:48:THR:HG23	1:C:75:VAL:HG22	1.70	0.71
1:B:21:LEU:O	1:B:47:MET:HA	1.90	0.71
1:B:83:VAL:HG23	1:B:106:LEU:HD11	1.72	0.71
1:C:71:THR:HB	2:C:537:HOH:O	1.89	0.71
1:B:147:ILE:HB	1:B:148:LEU:HD12	1.72	0.71
1:A:256:GLN:O	1:A:256:GLN:HG2	1.89	0.71
1:C:22:LEU:HD13	1:C:86:VAL:HG13	1.72	0.71
1:D:62:PRO:HD2	2:D:406:HOH:O	1.90	0.71
1:B:73:VAL:HG12	1:B:74:SER:N	2.04	0.71
1:C:50:ASP:N	1:C:51:ARG:HH21	1.88	0.71
1:D:202:LYS:HD2	1:D:205:ASN:ND2	2.04	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:PRO:HG2	1:C:335:GLN:NE2	2.05	0.71
1:D:167:THR:HG22	1:D:325:ILE:HG12	1.72	0.71
1:D:182:LYS:HE2	2:D:568:HOH:O	1.91	0.71
1:A:97:GLU:HB3	1:A:132:LYS:HD2	1.73	0.71
1:A:239:LYS:HE3	2:A:613:HOH:O	1.90	0.71
1:A:310:VAL:HG22	1:A:321:ILE:HG23	1.71	0.71
1:C:194:VAL:HG21	2:C:382:HOH:O	1.89	0.71
1:C:42:PHE:CE1	1:C:344:LEU:HD23	2.26	0.71
1:D:34:ARG:HH22	1:D:329:VAL:HG22	1.56	0.71
1:B:73:VAL:HG12	1:B:74:SER:N	2.05	0.71
1:D:212:GLU:HA	2:D:390:HOH:O	1.90	0.71
1:A:67:GLN:NE2	1:B:355:GLN:HG3	2.05	0.70
1:A:142:TYR:CZ	1:A:161:PRO:HB3	2.26	0.70
1:C:183:HIS:ND1	2:C:475:HOH:O	2.23	0.70
1:D:75:VAL:HG23	2:D:399:HOH:O	1.89	0.70
1:B:244:PHE:CZ	1:B:246:PRO:HG3	2.26	0.70
1:A:136:LEU:HD12	1:A:139:GLU:HG2	1.72	0.70
1:A:273:HIS:CE1	1:A:277:LYS:HD2	2.26	0.70
1:C:39:HIS:HD1	1:C:41:HIS:H	1.37	0.70
1:B:273:HIS:HE1	1:B:277:LYS:HD2	1.56	0.70
1:D:164:TYR:HB2	1:D:165:PRO:HD3	1.73	0.70
1:D:91:PRO:HG2	1:D:94:THR:HB	1.73	0.70
1:C:170:LEU:HB2	1:C:171:PRO:HD3	1.71	0.70
1:C:71:THR:HB	2:C:537:HOH:O	1.91	0.70
1:D:49:ALA:HB3	1:D:72:LEU:HD13	1.73	0.70
1:C:144:LEU:HD21	1:C:169:GLN:HB3	1.74	0.70
1:B:253:ARG:HG2	1:B:328:LEU:HD12	1.74	0.70
1:A:239:LYS:HE3	2:A:612:HOH:O	1.91	0.70
1:D:215:SER:OG	2:D:382:HOH:O	2.08	0.70
1:D:303:SER:O	2:D:373:HOH:O	2.09	0.70
1:B:73:VAL:HG12	1:B:74:SER:N	2.06	0.70
1:A:142:TYR:CZ	1:A:161:PRO:HB3	2.27	0.70
1:B:15:LYS:HD2	1:B:43:GLN:HB2	1.74	0.70
1:C:51:ARG:H	1:C:51:ARG:NE	1.88	0.70
1:B:175:LEU:HD22	1:B:272:LEU:HD22	1.72	0.70
1:D:231:GLY:O	1:D:235:VAL:HG23	1.92	0.70
1:D:52:LYS:HD3	1:D:60:VAL:HG22	1.74	0.70
1:A:239:LYS:HE3	2:A:608:HOH:O	1.92	0.69
1:B:173:VAL:HG22	1:B:235:VAL:HG21	1.73	0.69
1:A:48:THR:HG22	2:A:560:HOH:O	1.92	0.69
1:A:52:LYS:HD3	1:A:60:VAL:HG22	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:HIS:ND1	2:A:602:HOH:O	2.26	0.69
1:C:265:PRO:HA	2:C:579:HOH:O	1.92	0.69
1:C:167:THR:HG22	1:C:325:ILE:CG1	2.22	0.69
1:C:256:GLN:NE2	1:C:322:ILE:HG23	2.08	0.69
1:D:152:ILE:HD13	1:D:339:ASN:OD1	1.93	0.69
1:C:191:LYS:NZ	1:C:258:THR:H	1.89	0.69
1:B:173:VAL:HB	1:B:174:PRO:HD3	1.75	0.69
1:C:37:ALA:HB3	1:D:355:GLN:HG3	1.74	0.69
1:A:142:TYR:CZ	1:A:161:PRO:HB3	2.26	0.69
1:B:68:LYS:HA	2:B:424:HOH:O	1.93	0.69
1:A:239:LYS:HE3	2:A:613:HOH:O	1.93	0.69
1:A:136:LEU:HD12	1:A:139:GLU:HG2	1.73	0.69
1:A:167:THR:HG22	1:A:325:ILE:HG23	1.74	0.69
1:B:218:GLY:O	1:B:222:HIS:HB2	1.93	0.69
1:C:161:PRO:HG2	1:C:335:GLN:NE2	2.07	0.69
1:D:297:THR:HG22	2:D:360:HOH:O	1.91	0.69
1:D:299:ASN:ND2	2:D:428:HOH:O	2.21	0.69
1:B:139:GLU:OE2	1:B:156:ARG:HD3	1.92	0.69
1:D:152:ILE:HD13	1:D:339:ASN:OD1	1.93	0.69
1:B:168:ILE:O	1:B:171:PRO:HD2	1.92	0.69
1:C:203:GLU:O	1:C:206:LEU:HG	1.93	0.69
1:B:51:ARG:HB2	2:B:415:HOH:O	1.92	0.69
1:B:92:HIS:HB3	2:B:533:HOH:O	1.93	0.69
1:B:307:HIS:O	1:B:323:SER:HA	1.93	0.69
1:B:65:ARG:NE	2:B:510:HOH:O	2.26	0.69
1:C:51:ARG:HD2	1:C:51:ARG:N	2.07	0.68
1:B:175:LEU:HD13	1:B:181:ILE:HD13	1.74	0.68
1:C:83:VAL:HG12	1:C:85:ALA:H	1.58	0.68
1:A:306:CYS:HB2	1:A:325:ILE:HG22	1.73	0.68
1:A:41:HIS:ND1	2:A:420:HOH:O	2.25	0.68
1:D:91:PRO:HG2	1:D:94:THR:OG1	1.93	0.68
1:B:314:ARG:HG3	1:B:314:ARG:HH11	1.58	0.68
1:A:239:LYS:HE3	2:A:616:HOH:O	1.93	0.68
1:C:145:THR:HG22	1:C:146:GLU:N	2.07	0.68
1:D:152:ILE:HD13	1:D:339:ASN:OD1	1.92	0.68
1:B:118:ARG:HB2	1:B:118:ARG:NH1	2.09	0.68
1:C:270:GLU:HG2	2:C:573:HOH:O	1.92	0.68
1:B:149:ARG:NH1	1:B:348:GLU:OE1	2.26	0.68
1:D:202:LYS:HB2	1:D:205:ASN:HD22	1.53	0.68
1:B:68:LYS:HA	2:B:424:HOH:O	1.94	0.68
1:B:173:VAL:HB	1:B:174:PRO:HD3	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:GLU:OE1	1:C:130:PRO:HA	1.93	0.68
1:A:65:ARG:HD2	1:B:287:LYS:HG3	1.75	0.68
1:B:51:ARG:HB2	2:B:417:HOH:O	1.93	0.68
1:B:68:LYS:HA	2:B:422:HOH:O	1.94	0.68
1:B:296:ARG:HD3	2:B:408:HOH:O	1.94	0.68
1:C:103:PRO:HG2	1:C:106:LEU:HG	1.76	0.68
1:A:57:MET:SD	1:A:61:PHE:HB2	2.34	0.68
1:A:142:TYR:CZ	1:A:161:PRO:HB3	2.29	0.68
1:B:325:ILE:HD12	1:B:326:ASP:C	2.14	0.68
1:A:191:LYS:HG3	1:A:247:HIS:HD1	1.58	0.68
1:D:104:THR:O	1:D:156:ARG:HD2	1.93	0.68
1:C:35:LEU:HD22	1:C:352:LEU:HD23	1.75	0.68
1:C:67:GLN:HE21	1:C:69:LEU:CD2	2.04	0.68
1:C:191:LYS:HZ3	1:C:256:GLN:HG2	1.58	0.68
1:B:217:TYR:O	1:B:246:PRO:HD2	1.94	0.68
1:C:51:ARG:HD2	1:C:51:ARG:N	2.09	0.68
1:B:21:LEU:HD13	1:B:32:ILE:HG21	1.75	0.68
1:D:281:GLU:HA	2:D:588:HOH:O	1.93	0.68
1:C:23:GLY:H	1:C:48:THR:HB	1.58	0.68
1:A:149:ARG:NH1	1:A:348:GLU:OE1	2.26	0.68
1:C:22:LEU:HB3	1:C:90:LEU:HD21	1.75	0.68
1:C:122:GLU:HA	1:C:125:GLU:HG2	1.75	0.68
1:B:65:ARG:NH1	1:B:65:ARG:HB2	2.08	0.68
1:B:214:ILE:HD11	1:C:256:GLN:HB3	1.74	0.68
1:A:218:GLY:HA3	1:A:222:HIS:CD2	2.29	0.67
1:A:153:LYS:HE2	1:A:342:ILE:HB	1.75	0.67
1:B:203:GLU:OE2	2:B:561:HOH:O	2.10	0.67
1:D:91:PRO:HG2	1:D:94:THR:OG1	1.94	0.67
1:C:167:THR:HG22	1:C:325:ILE:HG12	1.75	0.67
1:C:149:ARG:HD3	1:C:348:GLU:OE1	1.94	0.67
1:B:269:THR:HG21	1:B:312:PRO:HB3	1.76	0.67
1:B:36:LEU:HD12	1:B:44:VAL:CG2	2.25	0.67
1:B:90:LEU:HD12	1:B:95:THR:HA	1.74	0.67
1:B:231:GLY:O	1:B:235:VAL:HG23	1.95	0.67
1:C:257:SER:O	1:C:259:ILE:HG13	1.95	0.67
1:A:191:LYS:CG	1:A:247:HIS:HB2	2.25	0.67
1:D:306:CYS:HB3	1:D:325:ILE:CG2	2.21	0.67
1:B:49:ALA:HB3	1:B:72:LEU:HD13	1.77	0.67
1:D:81:SER:O	1:D:82:THR:HG23	1.94	0.67
1:B:315:ILE:HD13	1:C:185:ASN:HA	1.76	0.67
1:C:35:LEU:HD22	1:C:352:LEU:HD23	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:ASN:HB2	2:A:430:HOH:O	1.95	0.67
1:C:269:THR:HG21	1:C:312:PRO:HA	1.77	0.67
1:A:359:PRO:OXT	1:B:252:ILE:HG21	1.94	0.67
1:C:173:VAL:HG22	1:C:235:VAL:HG21	1.77	0.67
1:B:43:GLN:O	1:B:45:THR:HG23	1.95	0.67
1:C:49:ALA:HA	1:C:51:ARG:NH1	2.09	0.67
1:C:51:ARG:H	1:C:51:ARG:CD	1.99	0.67
1:A:301:ARG:HH12	1:B:252:ILE:HD12	1.60	0.67
1:B:161:PRO:HG2	1:B:335:GLN:NE2	2.09	0.67
1:A:192:SER:HB2	1:A:255:MET:HE2	1.76	0.67
1:A:144:LEU:HD12	1:A:335:GLN:OE1	1.95	0.67
1:B:183:HIS:O	1:B:240:VAL:HG13	1.95	0.67
1:C:176:LEU:HD22	1:C:236:ALA:HB2	1.76	0.67
1:D:173:VAL:HB	1:D:174:PRO:HD3	1.76	0.67
1:C:51:ARG:HD2	1:C:51:ARG:N	2.08	0.67
1:D:75:VAL:HG23	2:D:399:HOH:O	1.93	0.67
1:D:291:GLU:HG3	2:D:504:HOH:O	1.94	0.67
1:B:354:HIS:H	1:B:354:HIS:CD2	2.13	0.66
1:A:216:SER:H	1:D:256:GLN:NE2	1.92	0.66
1:A:164:TYR:CE1	1:A:190:ALA:HB1	2.30	0.66
1:D:145:THR:O	1:D:149:ARG:HB2	1.95	0.66
1:A:192:SER:HB2	1:A:255:MET:HE2	1.76	0.66
1:A:274:GLN:HE22	1:A:277:LYS:HE2	1.60	0.66
1:D:243:SER:O	2:D:367:HOH:O	2.13	0.66
1:B:17:ILE:HG23	1:B:84:ASP:HB2	1.77	0.66
1:B:125:GLU:HG3	1:B:126:TRP:N	2.10	0.66
1:C:161:PRO:HG2	1:C:335:GLN:HE21	1.60	0.66
1:C:175:LEU:HD22	1:C:272:LEU:HD22	1.78	0.66
1:A:136:LEU:O	1:A:139:GLU:HG2	1.94	0.66
1:C:31:GLU:CD	1:C:253:ARG:HH22	1.97	0.66
1:C:284:GLU:O	1:C:287:LYS:HE2	1.95	0.66
1:B:141:VAL:HG21	1:B:151:ASP:O	1.96	0.66
1:A:91:PRO:O	1:A:94:THR:HB	1.95	0.66
1:D:171:PRO:O	1:D:174:PRO:HD2	1.95	0.66
1:A:48:THR:HG22	2:A:556:HOH:O	1.95	0.66
1:A:142:TYR:CZ	1:A:161:PRO:HB3	2.31	0.66
1:A:301:ARG:HH12	1:B:252:ILE:CD1	2.09	0.66
1:D:270:GLU:H	1:D:270:GLU:CD	1.99	0.66
1:B:28:THR:HG23	2:B:419:HOH:O	1.96	0.66
1:B:73:VAL:HG12	1:B:74:SER:N	2.08	0.66
1:C:127:TYR:CE1	1:C:223:ARG:HD3	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:VAL:HG12	1:B:74:SER:N	2.10	0.66
1:A:187:ILE:HB	1:A:260:TYR:HB2	1.78	0.66
1:B:194:VAL:HA	1:B:248:LEU:HD11	1.77	0.66
1:D:165:PRO:HD3	1:D:224:HIS:ND1	2.11	0.66
1:B:68:LYS:HA	2:B:423:HOH:O	1.96	0.66
1:B:192:SER:HB2	1:B:255:MET:HE2	1.77	0.66
1:A:115:PHE:HB3	1:A:140:VAL:HG11	1.77	0.66
1:C:337:LEU:HD23	1:C:352:LEU:HD21	1.77	0.66
1:A:38:ASN:HB2	2:A:431:HOH:O	1.96	0.66
1:B:295:PRO:HG2	1:B:322:ILE:HG22	1.77	0.66
1:A:187:ILE:HD11	1:D:318:ARG:CZ	2.25	0.66
1:A:215:SER:HB3	1:D:296:ARG:HG3	1.77	0.66
1:C:173:VAL:HG13	1:C:235:VAL:HG11	1.78	0.66
1:B:168:ILE:HD13	1:B:188:ILE:HD13	1.78	0.66
1:D:57:MET:HE2	1:D:72:LEU:HD11	1.77	0.66
1:C:51:ARG:H	1:C:51:ARG:CD	2.05	0.66
1:B:168:ILE:HD13	1:B:188:ILE:HD13	1.78	0.66
1:C:284:GLU:HG3	1:C:285:PHE:N	2.08	0.66
1:A:15:LYS:HD2	1:A:43:GLN:HB2	1.77	0.66
1:D:164:TYR:HB2	1:D:165:PRO:HD3	1.77	0.66
1:B:36:LEU:HD22	1:B:42:PHE:HB2	1.76	0.66
1:C:142:TYR:O	1:C:148:LEU:HD22	1.95	0.66
1:C:50:ASP:H	1:C:51:ARG:HH21	1.41	0.66
1:C:49:ALA:HA	1:C:51:ARG:NH1	2.11	0.66
1:D:281:GLU:HG2	2:D:587:HOH:O	1.94	0.66
1:D:31:GLU:CD	1:D:253:ARG:HH22	1.98	0.66
1:A:136:LEU:HD21	1:A:157:LEU:HD22	1.78	0.66
1:B:297:THR:HA	1:B:324:VAL:HG21	1.78	0.66
1:B:269:THR:HA	1:B:272:LEU:CD1	2.24	0.66
1:C:26:GLY:N	2:C:421:HOH:O	2.25	0.65
1:B:140:VAL:HG22	1:B:157:LEU:HD23	1.77	0.65
1:A:47:MET:HE1	1:A:69:LEU:HB3	1.77	0.65
1:C:51:ARG:HE	1:C:51:ARG:N	1.82	0.65
1:C:80:PHE:HB3	1:C:106:LEU:HD11	1.77	0.65
1:C:122:GLU:HA	1:C:125:GLU:HG2	1.77	0.65
1:C:95:THR:HB	1:C:114:ASP:OD2	1.96	0.65
1:B:174:PRO:HA	1:B:177:LYS:HE2	1.78	0.65
1:A:100:LYS:O	1:A:100:LYS:HD3	1.96	0.65
1:B:192:SER:HB2	1:B:255:MET:HE2	1.79	0.65
1:D:194:VAL:HG23	1:D:248:LEU:HD11	1.78	0.65
1:B:118:ARG:HG2	2:B:539:HOH:O	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:GLN:OE1	1:B:69:LEU:HD11	1.97	0.65
1:D:264:ALA:HB3	1:D:267:VAL:HG21	1.78	0.65
1:A:207:TYR:HD1	1:C:194:VAL:HG11	1.62	0.65
1:A:252:ILE:HD11	1:C:211:ALA:HB3	1.78	0.65
1:C:182:LYS:HE3	1:C:263:MET:O	1.97	0.65
1:A:22:LEU:HB2	1:A:88:CYS:HA	1.78	0.65
1:A:52:LYS:HD3	1:A:60:VAL:HG22	1.78	0.65
1:D:49:ALA:CB	1:D:72:LEU:HD13	2.27	0.65
1:C:118:ARG:NH2	2:C:447:HOH:O	2.29	0.65
1:A:142:TYR:CZ	1:A:161:PRO:HB3	2.30	0.65
1:C:165:PRO:HG2	1:C:227:GLU:OE1	1.95	0.65
1:B:303:SER:HB3	1:B:305:TYR:HD2	1.61	0.65
1:A:142:TYR:CZ	1:A:161:PRO:HB3	2.31	0.65
1:C:22:LEU:HD13	1:C:86:VAL:HG13	1.78	0.65
1:A:325:ILE:O	1:A:325:ILE:HG13	1.95	0.65
1:C:153:LYS:HA	1:C:342:ILE:O	1.97	0.65
1:C:86:VAL:HB	1:C:108:ILE:CD1	2.23	0.65
1:C:104:THR:HA	1:C:156:ARG:CZ	2.27	0.65
1:C:23:GLY:HA2	1:C:51:ARG:HH12	1.62	0.65
1:C:191:LYS:HZ3	1:C:256:GLN:CG	2.10	0.65
2:C:419:HOH:O	1:D:62:PRO:HG3	1.97	0.65
1:B:148:LEU:HD12	1:B:148:LEU:N	2.12	0.65
1:A:210:ILE:HD12	1:A:248:LEU:HD21	1.79	0.65
1:A:277:LYS:HE3	2:A:506:HOH:O	1.95	0.65
1:A:168:ILE:CD1	1:A:188:ILE:HG21	2.27	0.65
1:C:182:LYS:HB3	1:C:184:GLU:OE2	1.97	0.65
1:C:22:LEU:HD12	1:C:86:VAL:HG11	1.78	0.65
1:B:173:VAL:HB	1:B:174:PRO:HD3	1.79	0.65
1:C:122:GLU:HA	1:C:125:GLU:HG2	1.79	0.64
1:D:168:ILE:HD13	1:D:188:ILE:HD13	1.80	0.64
1:A:296:ARG:NE	1:A:298:HIS:HB2	2.12	0.64
1:A:257:SER:O	1:A:259:ILE:HG13	1.98	0.64
1:C:347:PRO:HB2	1:C:350:THR:OG1	1.97	0.64
1:C:16:ASP:HB2	1:C:41:HIS:HB3	1.79	0.64
1:A:152:ILE:HD13	1:A:339:ASN:OD1	1.98	0.64
1:C:125:GLU:HG3	1:C:126:TRP:CD1	2.32	0.64
1:C:86:VAL:O	1:C:108:ILE:HG23	1.96	0.64
1:C:270:GLU:HG2	2:C:569:HOH:O	1.98	0.64
1:A:296:ARG:CD	1:A:298:HIS:HB2	2.28	0.64
1:C:183:HIS:ND1	2:C:477:HOH:O	2.30	0.64
1:A:161:PRO:HG2	1:A:335:GLN:NE2	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:LEU:HD21	1:A:157:LEU:HD22	1.79	0.64
1:B:289:LEU:HD12	1:B:309:SER:HB2	1.80	0.64
1:B:118:ARG:HG2	2:B:536:HOH:O	1.97	0.64
1:B:294:VAL:HG22	1:B:311:PHE:CZ	2.31	0.64
1:C:161:PRO:HG2	1:C:335:GLN:NE2	2.13	0.64
1:C:18:ARG:HE	1:C:45:THR:HG21	1.61	0.64
1:C:145:THR:HB	1:C:330:LYS:NZ	2.13	0.64
1:C:170:LEU:HB2	1:C:171:PRO:HD3	1.80	0.64
1:C:182:LYS:HD3	2:C:474:HOH:O	1.97	0.64
1:B:74:SER:HB3	1:B:77:ASP:OD2	1.96	0.64
1:A:15:LYS:HD2	1:A:43:GLN:HB2	1.80	0.64
1:C:51:ARG:HH22	1:C:90:LEU:HD22	1.63	0.64
1:C:164:TYR:HB2	1:C:165:PRO:HD3	1.80	0.64
1:B:170:LEU:HB2	1:B:171:PRO:HD3	1.79	0.64
1:D:133:ALA:HA	2:D:539:HOH:O	1.98	0.64
1:B:289:LEU:HD13	1:B:293:VAL:HG12	1.79	0.64
1:C:169:GLN:OE1	1:C:231:GLY:HA3	1.98	0.64
1:C:48:THR:HG21	1:C:75:VAL:HG22	1.79	0.64
1:D:168:ILE:CD1	1:D:188:ILE:HG21	2.27	0.64
1:A:145:THR:HG21	1:A:338:GLN:CD	2.17	0.63
1:B:21:LEU:O	1:B:47:MET:HA	1.97	0.63
1:D:269:THR:HG21	1:D:312:PRO:HB3	1.80	0.63
1:B:19:ILE:HB	1:B:44:VAL:HA	1.81	0.63
1:B:107:LYS:HB3	1:B:343:MET:HE2	1.80	0.63
1:C:214:ILE:HG22	1:C:250:PRO:HD3	1.80	0.63
1:C:127:TYR:HB3	1:C:129:GLN:NE2	2.12	0.63
1:B:214:ILE:HD11	1:C:191:LYS:HD3	1.81	0.63
1:D:256:GLN:HA	1:D:324:VAL:HG12	1.80	0.63
1:B:19:ILE:HB	1:B:44:VAL:HA	1.80	0.63
1:B:316:PRO:HB2	2:B:495:HOH:O	1.99	0.63
1:C:22:LEU:HD22	1:C:88:CYS:SG	2.39	0.63
1:A:21:LEU:HD13	1:A:32:ILE:HG21	1.80	0.63
1:A:252:ILE:CD1	1:C:208:SER:HA	2.29	0.63
1:A:41:HIS:ND1	2:A:420:HOH:O	2.30	0.63
1:A:217:TYR:O	1:A:246:PRO:HD2	1.98	0.63
1:C:160:ASN:OD1	1:C:335:GLN:HG2	1.97	0.63
1:B:153:LYS:HG2	1:B:342:ILE:HB	1.78	0.63
1:A:161:PRO:HG2	1:A:335:GLN:NE2	2.14	0.63
1:C:315:ILE:CG2	1:C:316:PRO:HD2	2.27	0.63
1:B:186:ILE:HA	1:B:261:VAL:HG12	1.80	0.63
1:C:83:VAL:HG12	1:C:85:ALA:H	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:LYS:HA	2:B:518:HOH:O	1.98	0.63
1:B:161:PRO:HG2	1:B:335:GLN:NE2	2.14	0.63
1:B:229:GLU:OE2	1:B:241:THR:HA	1.98	0.63
1:C:96:GLN:O	1:C:100:LYS:HB2	1.99	0.63
1:C:127:TYR:CE1	1:C:223:ARG:HD3	2.34	0.63
1:B:169:GLN:OE1	1:B:231:GLY:HA3	1.99	0.63
1:D:171:PRO:HD3	1:D:308:MET:HE1	1.80	0.63
1:A:34:ARG:HG3	1:B:355:GLN:HB2	1.81	0.63
1:A:211:ALA:HA	1:A:250:PRO:CB	2.29	0.63
1:A:259:ILE:HD12	1:A:259:ILE:N	2.13	0.63
1:C:284:GLU:O	1:C:287:LYS:HE2	1.99	0.62
1:A:48:THR:HG21	1:A:75:VAL:HG22	1.79	0.62
1:D:253:ARG:HD3	1:D:326:ASP:OD2	1.99	0.62
1:B:167:THR:HG22	1:B:325:ILE:HG12	1.79	0.62
1:B:118:ARG:HB2	1:B:118:ARG:HH11	1.63	0.62
1:C:311:PHE:HB2	1:C:320:ILE:HB	1.81	0.62
1:B:64:LEU:HD22	1:B:67:GLN:HG3	1.79	0.62
1:C:354:HIS:CD2	1:C:354:HIS:H	2.15	0.62
1:A:186:ILE:HB	1:A:242:VAL:HG12	1.81	0.62
1:C:122:GLU:HA	1:C:125:GLU:HG2	1.81	0.62
1:A:68:LYS:HD2	1:A:68:LYS:N	2.14	0.62
1:B:182:LYS:HE2	1:B:262:GLU:OE2	2.00	0.62
1:A:230:GLN:NE2	2:A:477:HOH:O	2.32	0.62
1:C:125:GLU:HG3	1:C:126:TRP:N	2.15	0.62
1:D:253:ARG:HH12	1:D:328:LEU:HB2	1.64	0.62
1:B:103:PRO:HG2	1:B:106:LEU:HD22	1.80	0.62
1:A:168:ILE:HD13	1:A:188:ILE:HD13	1.81	0.62
1:C:161:PRO:HG2	1:C:335:GLN:HE21	1.63	0.62
1:D:164:TYR:HB2	1:D:165:PRO:HD3	1.80	0.62
1:A:15:LYS:HD2	1:A:43:GLN:HB2	1.80	0.62
1:C:173:VAL:HB	1:C:174:PRO:HD3	1.80	0.62
1:B:168:ILE:O	1:B:171:PRO:HD2	1.99	0.62
1:B:214:ILE:HG22	1:B:250:PRO:HD3	1.81	0.62
1:B:244:PHE:CZ	1:B:246:PRO:HG3	2.35	0.62
1:B:97:GLU:HG3	1:B:132:LYS:HE3	1.80	0.62
1:A:252:ILE:HD11	1:C:211:ALA:HB3	1.81	0.62
1:A:86:VAL:HB	1:A:108:ILE:HG12	1.80	0.62
1:B:97:GLU:HG3	1:B:132:LYS:HE3	1.82	0.62
1:C:117:LEU:HD22	1:C:123:TYR:HD1	1.64	0.62
1:A:168:ILE:CD1	1:A:188:ILE:HG21	2.29	0.62
1:B:118:ARG:HH11	1:B:118:ARG:CB	2.13	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:TYR:O	1:B:127:TYR:HB2	1.99	0.62
1:A:57:MET:CE	1:A:60:VAL:HB	2.29	0.62
1:B:190:ALA:HB3	1:B:246:PRO:HA	1.81	0.62
1:A:252:ILE:HG21	1:B:359:PRO:OXT	1.99	0.62
1:B:144:LEU:HD11	1:B:170:LEU:HD21	1.82	0.62
1:C:49:ALA:HB3	1:C:72:LEU:HD13	1.82	0.62
1:A:256:GLN:OE1	1:D:214:ILE:HG13	2.00	0.62
1:D:144:LEU:HD23	1:D:147:ILE:HG13	1.82	0.62
1:C:36:LEU:HD12	1:C:44:VAL:HG22	1.82	0.62
1:A:259:ILE:HB	1:A:321:ILE:HB	1.81	0.62
1:B:152:ILE:HD13	1:B:339:ASN:OD1	2.00	0.62
1:C:173:VAL:HB	1:C:174:PRO:HD3	1.82	0.62
1:A:48:THR:HG21	1:A:75:VAL:CG2	2.30	0.62
1:B:199:ARG:HD3	1:D:203:GLU:OE2	2.00	0.62
1:B:310:VAL:HA	1:B:320:ILE:O	1.98	0.62
1:C:298:HIS:O	1:C:301:ARG:HD3	1.99	0.62
1:C:48:THR:HG21	1:C:75:VAL:HG22	1.81	0.62
1:C:308:MET:HA	1:C:322:ILE:O	2.00	0.62
1:C:264:ALA:HB3	1:C:267:VAL:HG21	1.80	0.62
1:C:269:THR:HA	1:C:272:LEU:HG	1.82	0.62
1:C:18:ARG:O	1:C:83:VAL:HG13	2.00	0.62
1:A:22:LEU:HA	1:A:48:THR:HG22	1.82	0.62
1:D:20:GLY:O	1:D:86:VAL:HG13	2.00	0.61
1:A:192:SER:HB2	1:A:255:MET:HE2	1.81	0.61
1:B:252:ILE:HD11	1:D:211:ALA:HB3	1.81	0.61
1:D:269:THR:HG21	1:D:312:PRO:HB3	1.81	0.61
1:D:173:VAL:HG13	1:D:235:VAL:HG11	1.82	0.61
1:C:47:MET:CE	1:C:70:PRO:HD2	2.30	0.61
1:B:36:LEU:HD22	1:B:42:PHE:HB2	1.82	0.61
1:C:168:ILE:O	1:C:171:PRO:HD2	2.00	0.61
1:C:83:VAL:HG12	1:C:85:ALA:H	1.66	0.61
1:A:242:VAL:O	1:D:314:ARG:HD3	2.00	0.61
1:B:226:PRO:HA	2:B:407:HOH:O	2.00	0.61
1:C:49:ALA:HB3	1:C:72:LEU:HD13	1.83	0.61
1:C:127:TYR:CE1	1:C:223:ARG:HD3	2.35	0.61
1:C:140:VAL:HG22	1:C:157:LEU:HD23	1.81	0.61
1:A:259:ILE:HG22	1:A:261:VAL:HG13	1.81	0.61
1:A:199:ARG:HH21	1:C:209:GLU:CD	2.04	0.61
1:C:115:PHE:HB2	1:C:159:ALA:HB2	1.83	0.61
1:C:239:LYS:HD3	1:C:240:VAL:N	2.13	0.61
1:C:301:ARG:O	1:C:356:PRO:HA	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ARG:O	1:A:83:VAL:HB	1.99	0.61
2:A:366:HOH:O	1:C:194:VAL:HG22	2.00	0.61
1:A:48:THR:HG21	1:A:75:VAL:HG22	1.82	0.61
1:D:47:MET:HE1	1:D:69:LEU:HB3	1.81	0.61
1:A:174:PRO:HG3	2:A:590:HOH:O	2.00	0.61
1:D:272:LEU:HD12	1:D:310:VAL:HG11	1.83	0.61
1:D:257:SER:HB3	1:D:259:ILE:HD11	1.81	0.61
1:A:47:MET:HE1	1:A:69:LEU:HB3	1.81	0.61
1:C:80:PHE:HB3	1:C:106:LEU:HD11	1.83	0.61
1:C:51:ARG:HB2	1:C:52:LYS:HD2	1.83	0.61
1:A:295:PRO:HD3	1:A:309:SER:HB2	1.82	0.61
1:B:214:ILE:HD11	1:C:256:GLN:HB3	1.83	0.61
1:C:83:VAL:HG12	1:C:84:ASP:N	2.16	0.61
1:A:96:GLN:HG3	1:A:114:ASP:HB3	1.83	0.61
1:C:17:ILE:HB	1:C:42:PHE:HD1	1.65	0.61
1:C:49:ALA:HA	1:C:51:ARG:NH1	2.15	0.61
1:C:325:ILE:HD12	1:C:325:ILE:O	2.01	0.61
1:D:95:THR:HB	1:D:114:ASP:OD2	2.01	0.61
1:B:296:ARG:HG3	1:C:215:SER:HB3	1.83	0.61
1:D:143:GLY:HA2	1:D:152:ILE:HD11	1.81	0.61
1:B:32:ILE:HG13	1:B:89:CYS:SG	2.41	0.61
1:C:45:THR:O	1:C:46:LEU:HB2	2.01	0.61
1:B:74:SER:HB3	1:B:77:ASP:OD2	2.00	0.61
1:C:340:LEU:O	1:C:344:LEU:HD13	2.01	0.61
1:B:125:GLU:HG3	1:B:126:TRP:HD1	1.64	0.61
1:A:310:VAL:HG12	1:A:311:PHE:H	1.66	0.61
1:B:173:VAL:HG22	1:B:235:VAL:CG2	2.31	0.61
1:C:253:ARG:HD3	1:C:326:ASP:OD2	2.01	0.60
1:A:187:ILE:HA	1:A:243:SER:HB3	1.83	0.60
1:A:174:PRO:HG3	2:A:591:HOH:O	2.00	0.60
1:B:96:GLN:HA	1:B:115:PHE:CE2	2.36	0.60
1:A:127:TYR:CE1	1:A:223:ARG:HD3	2.35	0.60
1:C:164:TYR:HB2	1:C:165:PRO:HD3	1.83	0.60
1:C:80:PHE:HB3	1:C:106:LEU:HD11	1.82	0.60
1:B:52:LYS:HG2	1:B:60:VAL:HG22	1.81	0.60
1:B:167:THR:HG23	1:B:325:ILE:HD13	1.83	0.60
1:C:22:LEU:HD11	1:C:80:PHE:CE2	2.36	0.60
1:B:286:VAL:O	1:B:287:LYS:HD3	2.01	0.60
1:B:294:VAL:HG11	1:C:216:SER:O	2.00	0.60
1:C:359:PRO:OXT	1:D:252:ILE:HG21	2.01	0.60
1:A:135:GLU:O	1:A:138:LYS:HG2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:PHE:CZ	1:B:322:ILE:HD12	2.36	0.60
1:B:280:TYR:HD1	1:B:283:GLU:HG3	1.66	0.60
1:C:170:LEU:HB2	1:C:171:PRO:HD3	1.82	0.60
1:C:171:PRO:HG3	1:C:308:MET:HE1	1.83	0.60
1:C:127:TYR:CE1	1:C:223:ARG:HD3	2.37	0.60
1:C:264:ALA:HB3	1:C:267:VAL:HG21	1.83	0.60
1:C:286:VAL:O	1:C:287:LYS:HD3	2.02	0.60
1:C:42:PHE:HE1	1:C:344:LEU:HD23	1.65	0.60
1:D:316:PRO:HG2	2:D:510:HOH:O	2.02	0.60
1:A:57:MET:HE3	1:A:57:MET:HA	1.82	0.60
1:B:221:ARG:HD3	2:B:473:HOH:O	2.00	0.60
1:C:164:TYR:HB2	1:C:165:PRO:HD3	1.83	0.60
1:C:183:HIS:HB3	2:C:471:HOH:O	2.02	0.60
1:D:129:GLN:HB2	1:D:132:LYS:NZ	2.15	0.60
1:B:244:PHE:CZ	1:B:246:PRO:HG3	2.36	0.60
1:D:281:GLU:HB3	2:D:584:HOH:O	2.02	0.60
1:A:191:LYS:HD2	1:A:191:LYS:N	2.16	0.60
1:D:269:THR:HG21	1:D:312:PRO:HB3	1.83	0.60
1:D:57:MET:HG2	1:D:72:LEU:HD21	1.82	0.60
1:B:65:ARG:HD3	1:B:65:ARG:C	2.21	0.60
1:C:51:ARG:HE	1:C:51:ARG:N	1.97	0.60
1:D:173:VAL:HG13	1:D:235:VAL:HG21	1.83	0.60
1:B:163:CYS:O	1:B:167:THR:HG23	2.01	0.60
1:B:149:ARG:NH1	1:B:348:GLU:OE1	2.35	0.60
1:C:286:VAL:O	1:C:287:LYS:HD3	2.02	0.60
1:D:259:ILE:HD12	1:D:259:ILE:N	2.16	0.60
1:A:49:ALA:O	1:A:53:ALA:HB2	2.01	0.60
1:B:173:VAL:HB	1:B:174:PRO:HD3	1.82	0.60
1:B:213:GLY:O	1:B:250:PRO:HD3	2.02	0.60
1:D:144:LEU:HD23	1:D:147:ILE:HG13	1.83	0.60
1:B:263:MET:SD	1:B:272:LEU:HD11	2.41	0.60
1:B:107:LYS:HD2	1:B:343:MET:HE2	1.84	0.60
1:C:164:TYR:HB2	1:C:165:PRO:HD3	1.84	0.60
1:B:68:LYS:N	1:B:68:LYS:HD2	2.17	0.60
1:D:172:LEU:O	1:D:174:PRO:N	2.35	0.60
1:D:259:ILE:HD12	1:D:259:ILE:N	2.16	0.60
1:D:130:PRO:HD2	1:D:132:LYS:HZ1	1.67	0.60
1:C:149:ARG:NH1	1:C:348:GLU:OE1	2.35	0.60
1:C:115:PHE:HB3	1:C:140:VAL:HG11	1.84	0.60
1:C:182:LYS:HE2	1:C:265:PRO:HD3	1.84	0.60
1:D:164:TYR:HB2	1:D:165:PRO:HD3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:ARG:HH12	1:A:348:GLU:CD	2.05	0.60
1:C:161:PRO:HG2	1:C:335:GLN:NE2	2.15	0.60
1:D:342:ILE:C	1:D:344:LEU:H	2.04	0.59
1:D:151:ASP:HA	1:D:154:LYS:CE	2.25	0.59
1:D:277:LYS:O	1:D:281:GLU:HG2	2.02	0.59
1:B:33:VAL:HG12	1:B:67:GLN:NE2	2.17	0.59
1:C:23:GLY:O	1:C:89:CYS:HB2	2.01	0.59
1:B:304:ASN:CA	1:B:330:LYS:HB2	2.32	0.59
1:A:243:SER:HB2	1:D:313:ASP:OD1	2.02	0.59
1:A:57:MET:HE3	1:A:57:MET:HA	1.82	0.59
1:B:16:ASP:OD2	1:B:41:HIS:HB3	2.02	0.59
1:B:100:LYS:HA	1:B:136:LEU:HD22	1.83	0.59
1:D:203:GLU:OE2	2:D:516:HOH:O	2.17	0.59
1:C:92:HIS:O	1:C:94:THR:HG23	2.01	0.59
1:A:192:SER:CB	1:A:255:MET:HE2	2.31	0.59
1:C:290:ASP:HB2	1:C:293:VAL:CG2	2.33	0.59
1:B:257:SER:O	1:B:258:THR:C	2.39	0.59
1:B:296:ARG:HB2	1:B:299:ASN:ND2	2.17	0.59
1:B:90:LEU:CD1	1:B:95:THR:HA	2.32	0.59
1:C:269:THR:HG21	1:C:312:PRO:CA	2.32	0.59
1:D:173:VAL:HG22	1:D:235:VAL:HG21	1.84	0.59
1:D:281:GLU:HA	2:D:582:HOH:O	2.02	0.59
1:B:308:MET:HB3	1:B:323:SER:HB3	1.83	0.59
1:C:71:THR:HB	2:C:534:HOH:O	2.02	0.59
1:B:304:ASN:OD1	1:B:330:LYS:HA	2.03	0.59
1:D:119:ASN:HB3	1:D:122:GLU:HB2	1.84	0.59
1:C:36:LEU:HD22	1:C:42:PHE:HB2	1.84	0.59
1:C:50:ASP:H	1:C:51:ARG:HH21	1.50	0.59
1:D:291:GLU:OE2	2:D:592:HOH:O	2.17	0.59
1:A:203:GLU:O	1:A:206:LEU:HG	2.02	0.59
1:A:259:ILE:CG2	1:A:261:VAL:HG13	2.32	0.59
1:C:96:GLN:O	1:C:100:LYS:HB2	2.03	0.59
1:B:168:ILE:HD13	1:B:188:ILE:HD13	1.84	0.59
1:A:243:SER:HB2	1:D:315:ILE:HD12	1.85	0.59
1:A:215:SER:CB	1:D:296:ARG:HG3	2.30	0.59
1:D:90:LEU:HB3	1:D:91:PRO:HD2	1.85	0.59
1:D:168:ILE:HG12	1:D:188:ILE:HG21	1.83	0.59
1:C:314:ARG:HG3	1:C:314:ARG:HH11	1.66	0.59
1:B:63:HIS:NE2	1:B:64:LEU:HG	2.18	0.59
1:A:22:LEU:HA	1:A:48:THR:HB	1.84	0.59
1:A:174:PRO:HG3	2:A:589:HOH:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:GLN:NE2	1:B:258:THR:OG1	2.27	0.59
1:B:349:THR:HB	1:B:353:LEU:HD21	1.84	0.59
1:C:215:SER:O	1:C:247:HIS:HA	2.01	0.59
1:D:354:HIS:H	1:D:354:HIS:CD2	2.19	0.59
1:B:120:ILE:HG23	1:B:131:HIS:HB2	1.84	0.59
1:B:103:PRO:HG2	1:B:106:LEU:HD22	1.83	0.59
1:C:49:ALA:HB3	1:C:72:LEU:HD13	1.85	0.59
1:B:153:LYS:HD2	2:B:550:HOH:O	2.03	0.59
1:B:274:GLN:HE22	1:B:277:LYS:HE2	1.66	0.59
1:D:91:PRO:HG2	1:D:94:THR:CB	2.31	0.59
1:A:259:ILE:HB	1:A:321:ILE:HB	1.85	0.59
1:B:142:TYR:CZ	1:B:161:PRO:HB3	2.38	0.59
1:D:173:VAL:HB	1:D:174:PRO:HD3	1.84	0.59
1:B:304:ASN:CA	1:B:329:VAL:HG11	2.32	0.59
1:B:187:ILE:HG23	1:B:243:SER:HB3	1.84	0.59
1:D:167:THR:HG22	1:D:325:ILE:HG23	1.84	0.59
1:B:330:LYS:HD2	1:B:335:GLN:HB2	1.83	0.59
1:C:167:THR:HB	1:C:323:SER:OG	2.02	0.59
1:B:289:LEU:HD12	1:B:295:PRO:HD3	1.85	0.59
1:B:163:CYS:HA	1:B:331:GLY:HA3	1.84	0.59
1:D:230:GLN:O	1:D:234:ASP:HB2	2.03	0.59
1:B:22:LEU:HD23	1:B:48:THR:OG1	2.03	0.59
1:D:214:ILE:HG22	1:D:250:PRO:HD3	1.84	0.59
1:C:142:TYR:O	1:C:148:LEU:HD12	2.03	0.59
1:A:182:LYS:HB2	1:A:262:GLU:HG3	1.84	0.59
1:A:187:ILE:HG12	1:A:243:SER:HB3	1.84	0.59
1:A:321:ILE:N	1:A:321:ILE:HD12	2.18	0.59
1:B:86:VAL:HB	1:B:108:ILE:HG12	1.83	0.59
1:D:170:LEU:CD1	1:D:306:CYS:SG	2.87	0.59
1:A:328:LEU:O	1:A:332:ALA:HB3	2.03	0.59
1:A:216:SER:HB3	1:A:247:HIS:CD2	2.38	0.59
1:A:314:ARG:HG3	1:A:314:ARG:HH11	1.68	0.59
1:D:203:GLU:O	1:D:209:GLU:HG3	2.02	0.58
1:A:48:THR:HG21	1:A:75:VAL:CG2	2.32	0.58
1:B:164:TYR:HB2	1:B:165:PRO:HD3	1.85	0.58
1:A:150:GLU:HG2	2:A:471:HOH:O	2.02	0.58
1:B:286:VAL:HA	1:B:306:CYS:SG	2.43	0.58
1:C:22:LEU:HD21	1:C:80:PHE:HZ	1.67	0.58
1:A:95:THR:HB	1:A:114:ASP:OD2	2.03	0.58
1:B:269:THR:HG21	1:B:312:PRO:HB3	1.84	0.58
1:A:187:ILE:HD12	1:D:187:ILE:HD12	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:ALA:HA	1:C:51:ARG:HH11	1.67	0.58
1:D:273:HIS:CE1	1:D:277:LYS:HD3	2.38	0.58
1:D:173:VAL:HG13	1:D:235:VAL:HG21	1.85	0.58
1:B:218:GLY:O	1:B:222:HIS:HB2	2.02	0.58
1:C:90:LEU:HD13	1:C:98:ILE:HD12	1.85	0.58
1:A:99:ILE:HG23	1:A:108:ILE:HD13	1.85	0.58
1:C:39:HIS:ND1	1:C:40:PRO:HD2	2.17	0.58
1:C:22:LEU:HD11	1:C:80:PHE:CE2	2.38	0.58
1:D:269:THR:HG21	1:D:312:PRO:HB3	1.84	0.58
1:D:273:HIS:O	1:D:277:LYS:HB2	2.03	0.58
1:D:280:TYR:HD1	1:D:283:GLU:HG3	1.69	0.58
1:B:298:HIS:CD2	2:B:372:HOH:O	2.56	0.58
1:C:269:THR:HG21	1:C:312:PRO:CA	2.33	0.58
1:A:109:VAL:HG11	1:A:336:ALA:HB1	1.85	0.58
1:D:144:LEU:HD12	1:D:335:GLN:OE1	2.02	0.58
1:B:322:ILE:O	1:B:322:ILE:CG2	2.52	0.58
1:C:49:ALA:HB3	1:C:72:LEU:HD13	1.85	0.58
1:C:120:ILE:HG22	1:C:124:GLU:OE2	2.03	0.58
1:D:145:THR:HG21	1:D:338:GLN:CG	2.33	0.58
1:B:28:THR:HG23	2:B:421:HOH:O	2.04	0.58
1:C:17:ILE:HB	1:C:42:PHE:CD1	2.38	0.58
1:C:15:LYS:HG2	1:C:16:ASP:N	2.19	0.58
1:C:20:GLY:N	1:C:83:VAL:HG11	2.18	0.58
1:C:123:TYR:O	1:C:127:TYR:HB2	2.03	0.58
1:B:336:ALA:HA	1:B:339:ASN:HD22	1.68	0.58
1:C:357:LEU:HG	1:D:253:ARG:NE	2.18	0.58
1:D:31:GLU:CD	1:D:253:ARG:HH22	2.06	0.58
1:B:36:LEU:HD12	1:B:44:VAL:HG22	1.85	0.58
1:C:83:VAL:HG12	1:C:84:ASP:H	1.69	0.58
1:D:75:VAL:HG11	1:D:90:LEU:HD21	1.86	0.58
1:A:259:ILE:HB	1:A:321:ILE:HB	1.84	0.58
1:A:194:VAL:O	1:A:194:VAL:HG22	2.03	0.58
1:B:105:ALA:O	1:B:106:LEU:HB2	2.02	0.58
1:A:57:MET:HE3	1:A:57:MET:HA	1.85	0.58
1:A:172:LEU:HD21	1:A:259:ILE:HG21	1.85	0.58
1:A:253:ARG:HD3	1:A:326:ASP:OD2	2.03	0.58
1:D:277:LYS:O	1:D:281:GLU:HG2	2.02	0.58
1:C:104:THR:HA	1:C:156:ARG:NH1	2.18	0.58
1:B:317:GLY:N	2:B:499:HOH:O	2.34	0.58
1:B:22:LEU:HD11	1:B:80:PHE:HE1	1.69	0.58
1:A:57:MET:CE	1:A:60:VAL:HB	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:THR:HG21	1:C:338:GLN:CD	2.23	0.58
1:A:162:GLY:C	1:A:165:PRO:HD2	2.24	0.58
1:B:170:LEU:HB2	1:B:171:PRO:HD3	1.84	0.58
1:D:171:PRO:HG2	1:D:172:LEU:H	1.68	0.58
1:B:202:LYS:HD2	1:B:205:ASN:ND2	2.19	0.58
1:C:354:HIS:CD2	1:C:354:HIS:H	2.19	0.58
1:A:244:PHE:CZ	1:A:246:PRO:HG3	2.38	0.58
1:D:175:LEU:HD23	1:D:275:GLN:HG2	1.86	0.58
1:B:145:THR:HB	1:B:338:GLN:NE2	2.19	0.58
1:D:253:ARG:NH1	1:D:328:LEU:HB2	2.19	0.58
1:D:31:GLU:HG3	1:D:328:LEU:HB3	1.85	0.58
1:A:64:LEU:HD22	1:A:67:GLN:NE2	2.19	0.58
1:D:306:CYS:SG	1:D:330:LYS:HG2	2.44	0.58
1:A:31:GLU:HG3	1:A:328:LEU:HB3	1.86	0.58
1:C:48:THR:HG21	1:C:75:VAL:CG2	2.34	0.58
1:D:292:GLY:HA2	1:D:311:PHE:CD2	2.38	0.58
1:D:167:THR:HG22	1:D:325:ILE:HD12	1.86	0.58
1:C:290:ASP:HB2	1:C:293:VAL:HG21	1.85	0.58
1:C:96:GLN:O	1:C:100:LYS:HB2	2.03	0.58
1:C:125:GLU:HG3	1:C:126:TRP:N	2.19	0.58
1:D:164:TYR:HB2	1:D:165:PRO:HD3	1.86	0.58
1:B:52:LYS:HA	1:B:55:GLN:NE2	2.18	0.58
1:B:149:ARG:HG2	1:B:153:LYS:HE3	1.85	0.58
1:C:192:SER:HB2	1:C:255:MET:HE2	1.86	0.58
1:D:164:TYR:HB2	1:D:165:PRO:HD3	1.86	0.58
1:A:65:ARG:HD2	1:B:307:HIS:CE1	2.38	0.58
1:B:28:THR:HG21	2:B:425:HOH:O	2.03	0.58
1:C:21:LEU:HB3	1:C:47:MET:HG2	1.85	0.58
1:A:243:SER:HB2	1:D:315:ILE:HD12	1.84	0.58
2:A:386:HOH:O	1:D:221:ARG:HG3	2.04	0.58
1:A:168:ILE:HD13	1:A:188:ILE:HG21	1.86	0.58
1:A:213:GLY:HA3	1:D:298:HIS:CD2	2.38	0.58
1:C:269:THR:HG21	1:C:312:PRO:HA	1.85	0.58
1:B:182:LYS:HG3	1:B:262:GLU:HB3	1.86	0.58
1:B:244:PHE:CZ	1:B:246:PRO:HG3	2.39	0.58
1:C:135:GLU:O	1:C:138:LYS:HG2	2.04	0.58
1:D:304:ASN:O	1:D:330:LYS:HB2	2.04	0.58
1:C:354:HIS:CD2	1:C:354:HIS:H	2.20	0.58
1:D:20:GLY:O	1:D:86:VAL:HG13	2.03	0.58
1:B:146:GLU:HA	1:B:149:ARG:NH1	2.19	0.58
1:A:24:ALA:O	1:A:57:MET:HE1	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:VAL:O	1:B:326:ASP:HB2	2.04	0.57
1:C:170:LEU:HB2	1:C:171:PRO:HD3	1.86	0.57
1:D:36:LEU:HD13	1:D:44:VAL:CG2	2.34	0.57
1:D:49:ALA:CB	1:D:72:LEU:HD13	2.34	0.57
1:D:188:ILE:N	1:D:188:ILE:HD12	2.19	0.57
1:B:169:GLN:OE1	1:B:231:GLY:HA3	2.04	0.57
1:C:344:LEU:HB3	1:C:346:TYR:CD1	2.39	0.57
1:C:257:SER:O	1:C:259:ILE:HG13	2.04	0.57
1:D:144:LEU:HD23	1:D:147:ILE:HG13	1.86	0.57
1:A:289:LEU:HD11	1:A:295:PRO:HB3	1.86	0.57
1:C:34:ARG:NH2	1:C:329:VAL:HG22	2.19	0.57
1:B:120:ILE:HG23	1:B:131:HIS:HB2	1.86	0.57
1:C:135:GLU:O	1:C:138:LYS:HG2	2.04	0.57
1:C:337:LEU:HG	1:C:352:LEU:HD11	1.85	0.57
1:A:263:MET:HG2	1:A:272:LEU:HD11	1.86	0.57
1:A:127:TYR:CE1	1:A:223:ARG:HD3	2.39	0.57
1:B:120:ILE:HD12	1:B:134:VAL:HA	1.86	0.57
1:D:107:LYS:HG3	1:D:343:MET:O	2.03	0.57
1:A:174:PRO:HG3	2:A:585:HOH:O	2.02	0.57
1:B:90:LEU:HD13	1:B:98:ILE:HD12	1.85	0.57
1:B:90:LEU:CD1	1:B:95:THR:HA	2.34	0.57
1:C:152:ILE:HD13	1:C:339:ASN:OD1	2.05	0.57
1:C:48:THR:HG21	1:C:75:VAL:CG2	2.34	0.57
1:C:288:VAL:HA	1:C:308:MET:O	2.03	0.57
1:D:165:PRO:HD3	1:D:224:HIS:ND1	2.20	0.57
1:D:132:LYS:HE2	2:D:546:HOH:O	2.04	0.57
1:B:171:PRO:O	1:B:276:LEU:HD21	2.04	0.57
1:C:164:TYR:CZ	1:C:246:PRO:HB3	2.40	0.57
1:C:229:GLU:OE1	1:C:239:LYS:HE2	2.05	0.57
1:B:147:ILE:HG21	1:B:173:VAL:HG11	1.86	0.57
1:C:99:ILE:HA	1:C:102:LEU:HG	1.87	0.57
1:D:214:ILE:C	1:D:214:ILE:HD12	2.25	0.57
1:A:103:PRO:HD2	1:A:106:LEU:HD12	1.85	0.57
1:A:104:THR:O	1:A:156:ARG:HD2	2.05	0.57
1:A:15:LYS:HD2	1:A:43:GLN:HB2	1.86	0.57
1:C:80:PHE:HB3	1:C:106:LEU:HD11	1.87	0.57
1:D:152:ILE:HD13	1:D:339:ASN:OD1	2.03	0.57
1:D:281:GLU:HA	2:D:589:HOH:O	2.03	0.57
1:B:163:CYS:HA	1:B:331:GLY:CA	2.34	0.57
1:B:189:ASP:O	1:B:191:LYS:HD2	2.04	0.57
1:C:188:ILE:HG23	1:C:259:ILE:HG12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:LEU:HB3	1:C:47:MET:HG2	1.85	0.57
1:C:175:LEU:HD22	1:C:272:LEU:HD22	1.86	0.57
1:D:146:GLU:HA	1:D:149:ARG:NH1	2.18	0.57
1:A:161:PRO:HG2	1:A:335:GLN:NE2	2.19	0.57
1:B:33:VAL:HG13	1:B:67:GLN:HE22	1.68	0.57
1:B:296:ARG:O	1:B:299:ASN:HB2	2.04	0.57
1:D:144:LEU:HD12	1:D:335:GLN:HE22	1.69	0.57
1:C:90:LEU:HD13	1:C:98:ILE:HD12	1.86	0.57
1:C:164:TYR:HB2	1:C:165:PRO:HD3	1.87	0.57
1:C:191:LYS:NZ	1:C:256:GLN:HG2	2.18	0.57
1:A:194:VAL:O	1:A:194:VAL:HG22	2.05	0.57
1:C:129:GLN:OE1	1:C:132:LYS:HE3	2.04	0.57
1:D:172:LEU:O	1:D:173:VAL:C	2.43	0.57
1:D:277:LYS:O	1:D:281:GLU:HG2	2.04	0.57
1:C:270:GLU:HG2	2:C:579:HOH:O	2.03	0.57
1:D:296:ARG:H	1:D:299:ASN:HD22	1.53	0.57
1:A:65:ARG:HH11	1:B:287:LYS:HB3	1.68	0.57
1:C:18:ARG:O	1:C:83:VAL:HG13	2.04	0.57
1:C:142:TYR:CZ	1:C:161:PRO:HB3	2.40	0.57
1:D:185:ASN:HB2	1:D:262:GLU:OE2	2.05	0.57
1:C:34:ARG:HD3	1:D:356:PRO:O	2.05	0.57
1:B:139:GLU:OE2	1:B:156:ARG:HD3	2.05	0.57
1:C:153:LYS:HG2	1:C:342:ILE:O	2.05	0.57
1:A:257:SER:HB3	1:A:259:ILE:HD11	1.86	0.57
1:B:164:TYR:HB2	1:B:165:PRO:HD3	1.87	0.57
1:A:215:SER:HB3	1:D:296:ARG:HG2	1.85	0.57
1:C:28:THR:HG22	1:C:89:CYS:SG	2.45	0.57
1:D:22:LEU:HG	1:D:86:VAL:HG11	1.86	0.57
1:D:306:CYS:O	1:D:307:HIS:HD2	1.88	0.57
1:A:294:VAL:HG22	1:A:311:PHE:HZ	1.70	0.57
1:B:252:ILE:N	1:C:212:GLU:OE1	2.36	0.57
1:D:146:GLU:HG2	1:D:286:VAL:HG21	1.86	0.57
1:A:65:ARG:NH1	1:B:287:LYS:HB3	2.20	0.57
1:D:263:MET:HG2	1:D:272:LEU:HD11	1.86	0.57
1:C:46:LEU:HD23	1:C:83:VAL:HG21	1.87	0.57
1:A:214:ILE:HD11	1:D:256:GLN:HB3	1.86	0.57
1:A:217:TYR:O	1:A:246:PRO:HD2	2.05	0.57
1:C:152:ILE:HD13	1:C:339:ASN:OD1	2.05	0.56
1:A:167:THR:HG22	1:A:325:ILE:CG1	2.35	0.56
1:B:173:VAL:HB	1:B:174:PRO:HD3	1.87	0.56
1:D:269:THR:HG21	1:D:312:PRO:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:MET:HE2	1:A:70:PRO:HD2	1.87	0.56
1:B:57:MET:HG2	1:B:64:LEU:HD12	1.87	0.56
1:B:182:LYS:HB3	1:B:184:GLU:OE1	2.04	0.56
1:B:164:TYR:HB2	1:B:165:PRO:HD3	1.87	0.56
1:A:111:LEU:HA	1:A:160:ASN:HB3	1.87	0.56
1:D:214:ILE:C	1:D:214:ILE:HD12	2.25	0.56
1:A:95:THR:HG21	1:A:110:ASP:OD2	2.05	0.56
1:C:125:GLU:HG3	1:C:126:TRP:N	2.20	0.56
1:B:173:VAL:HG13	1:B:235:VAL:HG21	1.87	0.56
1:C:152:ILE:HD13	1:C:339:ASN:OD1	2.05	0.56
1:B:194:VAL:HG22	1:B:194:VAL:O	2.05	0.56
1:B:256:GLN:HB2	1:B:324:VAL:HG12	1.86	0.56
1:A:215:SER:HB3	1:D:296:ARG:HG2	1.87	0.56
1:B:144:LEU:HD23	1:B:147:ILE:HG13	1.86	0.56
1:B:149:ARG:HH12	1:B:348:GLU:CD	2.08	0.56
1:A:310:VAL:HG12	1:A:311:PHE:N	2.20	0.56
1:B:192:SER:HB2	1:B:255:MET:HE2	1.87	0.56
1:A:180:LEU:HD11	1:A:275:GLN:HE21	1.70	0.56
1:D:126:TRP:CH2	1:D:221:ARG:HG2	2.39	0.56
1:A:140:VAL:HG22	1:A:157:LEU:HD23	1.87	0.56
1:B:191:LYS:NZ	1:C:189:ASP:OD2	2.39	0.56
1:C:83:VAL:HG12	1:C:84:ASP:N	2.20	0.56
1:D:268:ARG:HB3	1:D:270:GLU:OE1	2.05	0.56
1:C:253:ARG:HD3	1:C:326:ASP:OD2	2.05	0.56
1:D:169:GLN:OE1	1:D:231:GLY:HA3	2.05	0.56
1:B:189:ASP:OD2	1:C:191:LYS:NZ	2.38	0.56
1:C:173:VAL:HG22	1:C:235:VAL:HG21	1.88	0.56
1:A:82:THR:HG21	2:A:558:HOH:O	2.04	0.56
1:B:73:VAL:HG21	2:B:526:HOH:O	2.05	0.56
1:C:21:LEU:HA	1:C:87:PHE:O	2.06	0.56
1:C:217:TYR:O	1:C:246:PRO:HD2	2.06	0.56
1:A:26:GLY:CA	2:A:423:HOH:O	2.52	0.56
1:B:164:TYR:HB2	1:B:165:PRO:HD3	1.87	0.56
1:C:71:THR:HB	2:C:530:HOH:O	2.04	0.56
1:B:127:TYR:CE1	1:B:223:ARG:HD3	2.40	0.56
1:B:145:THR:HG22	1:B:149:ARG:HG2	1.87	0.56
1:C:124:GLU:OE1	1:C:130:PRO:HA	2.05	0.56
1:D:104:THR:O	1:D:105:ALA:HB2	2.06	0.56
1:B:168:ILE:O	1:B:171:PRO:HD2	2.05	0.56
1:C:83:VAL:HG12	1:C:84:ASP:N	2.21	0.56
1:C:180:LEU:HD22	1:C:267:VAL:HG13	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:273:HIS:CD2	1:C:291:GLU:HG3	2.41	0.56
1:A:82:THR:HG21	2:A:559:HOH:O	2.05	0.56
1:B:86:VAL:HG23	1:B:107:LYS:O	2.06	0.56
1:A:183:HIS:HB2	1:A:240:VAL:HG22	1.87	0.56
1:D:151:ASP:HA	1:D:154:LYS:CE	2.32	0.56
1:B:49:ALA:CB	1:B:72:LEU:HD13	2.35	0.56
1:A:65:ARG:HD2	2:B:492:HOH:O	2.05	0.56
1:D:306:CYS:HB3	1:D:325:ILE:HG22	1.86	0.56
1:B:99:ILE:HA	1:B:102:LEU:HG	1.88	0.56
1:C:96:GLN:NE2	1:C:114:ASP:HB3	2.16	0.56
1:B:173:VAL:O	1:B:235:VAL:HG11	2.06	0.56
1:A:95:THR:HG21	1:A:110:ASP:CG	2.25	0.56
1:B:296:ARG:H	1:B:299:ASN:HD22	1.54	0.56
1:D:358:PHE:HA	1:D:359:PRO:C	2.25	0.56
1:B:139:GLU:CD	2:B:437:HOH:O	2.42	0.56
1:B:268:ARG:HB2	1:B:270:GLU:HG2	1.87	0.56
1:C:252:ILE:HG21	1:D:359:PRO:OXT	2.05	0.56
1:D:111:LEU:HA	1:D:160:ASN:HB3	1.87	0.56
1:C:152:ILE:HD13	1:C:339:ASN:OD1	2.05	0.56
1:D:249:MET:HA	1:D:249:MET:HE2	1.88	0.56
1:D:281:GLU:HG3	2:D:438:HOH:O	2.05	0.56
1:A:48:THR:HG21	1:A:75:VAL:HG22	1.88	0.56
1:B:105:ALA:O	1:B:106:LEU:HB2	2.04	0.56
1:A:304:ASN:OD1	1:A:334:GLY:HA3	2.05	0.56
1:B:31:GLU:HG3	1:B:328:LEU:HB3	1.86	0.56
1:B:329:VAL:HG12	1:B:334:GLY:HA3	1.86	0.56
1:C:169:GLN:O	1:C:173:VAL:HG23	2.06	0.56
1:A:34:ARG:NH1	2:A:395:HOH:O	2.38	0.56
1:B:199:ARG:HD3	1:D:203:GLU:OE2	2.06	0.56
1:D:104:THR:O	1:D:156:ARG:HD2	2.04	0.56
1:B:168:ILE:HD13	1:B:188:ILE:HD13	1.88	0.56
1:C:299:ASN:OD1	1:D:63:HIS:HB3	2.06	0.56
1:A:194:VAL:O	1:A:194:VAL:HG22	2.06	0.56
1:A:289:LEU:CD1	1:A:295:PRO:HB3	2.35	0.56
1:C:118:ARG:H	1:C:230:GLN:NE2	2.04	0.56
1:D:281:GLU:HA	2:D:591:HOH:O	2.05	0.56
1:D:203:GLU:OE2	2:D:521:HOH:O	2.18	0.56
1:D:137:GLN:O	1:D:137:GLN:HG3	2.04	0.56
1:C:111:LEU:HA	1:C:160:ASN:HB3	1.88	0.56
1:B:351:GLY:O	1:B:352:LEU:HG	2.05	0.56
1:D:111:LEU:O	1:D:116:ARG:NH2	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:ARG:HH11	1:B:287:LYS:HD2	1.71	0.56
1:C:23:GLY:N	1:C:48:THR:HB	2.20	0.56
1:A:82:THR:HG22	1:A:82:THR:O	2.06	0.56
1:B:43:GLN:O	1:B:45:THR:HG23	2.06	0.56
1:C:168:ILE:C	1:C:171:PRO:HD2	2.26	0.56
1:C:300:VAL:HG21	1:C:325:ILE:HA	1.87	0.56
1:A:109:VAL:HG21	1:A:340:LEU:HB2	1.87	0.56
1:B:161:PRO:HG2	1:B:335:GLN:NE2	2.21	0.56
1:A:306:CYS:HA	1:A:324:VAL:O	2.06	0.56
1:D:164:TYR:HB2	1:D:165:PRO:HD3	1.88	0.56
1:D:62:PRO:HD2	2:D:404:HOH:O	2.05	0.56
1:C:231:GLY:O	1:C:235:VAL:HG23	2.06	0.56
1:B:223:ARG:O	1:B:224:HIS:CD2	2.59	0.56
1:A:111:LEU:HA	1:A:160:ASN:CB	2.34	0.56
1:B:182:LYS:HD2	1:B:262:GLU:HG2	1.87	0.56
1:B:140:VAL:HG22	1:B:157:LEU:HD23	1.87	0.56
1:C:97:GLU:HG3	2:C:415:HOH:O	2.06	0.56
1:A:98:ILE:O	1:A:102:LEU:HD13	2.06	0.56
1:A:182:LYS:HD2	1:A:262:GLU:CD	2.26	0.56
1:B:149:ARG:O	1:B:153:LYS:HG3	2.06	0.56
1:B:306:CYS:SG	1:B:330:LYS:HG2	2.45	0.56
1:B:124:GLU:HG2	1:B:129:GLN:O	2.05	0.56
1:B:190:ALA:HB3	1:B:245:THR:O	2.06	0.56
1:C:149:ARG:NH2	1:C:283:GLU:OE2	2.37	0.56
1:A:65:ARG:HD2	1:B:307:HIS:NE2	2.21	0.56
1:B:187:ILE:HD12	1:C:187:ILE:HD12	1.88	0.56
1:D:16:ASP:OD2	1:D:41:HIS:HB3	2.06	0.56
1:B:185:ASN:HA	1:C:315:ILE:HD13	1.87	0.55
1:A:103:PRO:HD2	1:A:106:LEU:HD12	1.88	0.55
1:B:105:ALA:HB3	2:B:538:HOH:O	2.05	0.55
1:B:127:TYR:CE1	1:B:223:ARG:HD3	2.41	0.55
1:C:39:HIS:CE1	1:C:42:PHE:H	2.24	0.55
1:C:232:LEU:HD13	1:C:240:VAL:HG11	1.87	0.55
1:A:164:TYR:HB2	1:A:165:PRO:HD3	1.87	0.55
1:A:189:ASP:OD1	1:A:191:LYS:HE3	2.06	0.55
1:B:156:ARG:HB3	2:B:378:HOH:O	2.05	0.55
1:A:145:THR:HG21	1:A:338:GLN:HG2	1.88	0.55
1:C:264:ALA:HB3	1:C:267:VAL:HG21	1.88	0.55
1:C:257:SER:HB3	1:C:259:ILE:CD1	2.28	0.55
1:C:290:ASP:HB2	1:C:293:VAL:HG21	1.88	0.55
1:B:310:VAL:HG12	1:B:321:ILE:HG12	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:VAL:O	1:A:194:VAL:HG22	2.06	0.55
1:B:52:LYS:HG3	1:B:55:GLN:NE2	2.21	0.55
1:D:145:THR:HA	1:D:152:ILE:HD12	1.88	0.55
1:A:68:LYS:HD2	1:A:68:LYS:N	2.21	0.55
1:B:141:VAL:CG2	1:B:155:ALA:HB2	2.36	0.55
1:B:142:TYR:CZ	1:B:161:PRO:HB3	2.41	0.55
1:B:145:THR:O	1:B:149:ARG:HG3	2.06	0.55
1:B:164:TYR:HB2	1:B:165:PRO:HD3	1.88	0.55
1:D:171:PRO:C	1:D:174:PRO:HD2	2.25	0.55
1:D:285:PHE:HA	1:D:305:TYR:CD1	2.41	0.55
1:B:291:GLU:HA	2:B:569:HOH:O	2.06	0.55
1:D:314:ARG:HH11	1:D:314:ARG:HG3	1.71	0.55
1:C:92:HIS:HB2	2:C:541:HOH:O	2.06	0.55
1:C:110:ASP:HB3	1:C:158:VAL:O	2.06	0.55
1:C:142:TYR:CZ	1:C:161:PRO:HB3	2.41	0.55
1:D:213:GLY:O	1:D:214:ILE:HG23	2.05	0.55
1:B:176:LEU:HB2	1:B:235:VAL:HG11	1.87	0.55
1:B:184:GLU:HG3	1:B:185:ASN:ND2	2.22	0.55
1:D:285:PHE:CE2	1:D:349:THR:HG22	2.42	0.55
1:D:48:THR:OG1	1:D:75:VAL:HG22	2.07	0.55
1:B:315:ILE:HD13	1:C:185:ASN:HA	1.89	0.55
1:A:118:ARG:NH1	1:A:118:ARG:HB2	2.21	0.55
1:B:149:ARG:HG2	1:B:153:LYS:HE3	1.87	0.55
1:C:289:LEU:HD11	1:C:295:PRO:HB3	1.88	0.55
1:D:214:ILE:HG22	1:D:248:LEU:O	2.06	0.55
1:D:286:VAL:HG22	1:D:306:CYS:SG	2.46	0.55
1:B:164:TYR:HB2	1:B:165:PRO:HD3	1.88	0.55
1:C:142:TYR:HE2	1:C:144:LEU:HD22	1.72	0.55
1:C:273:HIS:HE2	1:C:290:ASP:HA	1.70	0.55
1:C:308:MET:HA	1:C:322:ILE:O	2.07	0.55
1:A:145:THR:HG21	1:A:338:GLN:HE21	1.70	0.55
1:A:182:LYS:HE3	1:A:263:MET:O	2.07	0.55
1:C:34:ARG:HG3	1:D:355:GLN:HB2	1.88	0.55
1:A:52:LYS:HG2	2:A:361:HOH:O	2.06	0.55
1:B:142:TYR:OH	1:B:227:GLU:HG2	2.06	0.55
1:B:223:ARG:HG3	2:B:470:HOH:O	2.07	0.55
1:B:303:SER:HB3	1:B:305:TYR:CD2	2.42	0.55
1:D:216:SER:O	1:D:217:TYR:HB3	2.06	0.55
1:C:100:LYS:HE3	2:C:549:HOH:O	2.07	0.55
1:D:350:THR:O	1:D:352:LEU:HG	2.06	0.55
1:C:27:TYR:N	2:C:516:HOH:O	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:214:ILE:C	1:D:214:ILE:HD12	2.27	0.55
2:B:465:HOH:O	1:C:297:THR:HG22	2.07	0.55
1:A:56:SER:C	1:A:58:GLU:H	2.08	0.55
1:A:242:VAL:O	1:D:314:ARG:HD3	2.06	0.55
1:B:229:GLU:OE2	1:B:241:THR:HA	2.06	0.55
1:B:73:VAL:CG1	1:B:74:SER:H	2.13	0.55
1:C:16:ASP:O	1:C:17:ILE:HD13	2.06	0.55
1:C:48:THR:HG23	1:C:75:VAL:HG22	1.89	0.55
1:B:32:ILE:HD13	1:B:333:SER:HB2	1.89	0.55
1:B:115:PHE:O	1:B:140:VAL:HG11	2.07	0.55
1:C:22:LEU:HA	1:C:48:THR:HB	1.87	0.55
1:B:299:ASN:ND2	2:B:386:HOH:O	2.39	0.55
1:C:23:GLY:O	1:C:89:CYS:HB2	2.06	0.55
1:C:38:ASN:HD21	1:D:355:GLN:HE21	1.54	0.55
1:C:116:ARG:HD3	1:C:227:GLU:OE2	2.07	0.55
1:B:144:LEU:HD12	1:B:335:GLN:OE1	2.07	0.55
1:A:164:TYR:CE1	1:A:190:ALA:HB1	2.41	0.55
1:D:214:ILE:HD12	1:D:214:ILE:O	2.07	0.55
1:D:120:ILE:O	1:D:124:GLU:HG3	2.07	0.55
1:A:57:MET:CE	1:A:60:VAL:HB	2.36	0.55
1:A:228:ILE:O	1:A:232:LEU:HG	2.06	0.55
1:D:160:ASN:ND2	1:D:332:ALA:O	2.40	0.55
1:B:296:ARG:HD3	2:B:409:HOH:O	2.06	0.55
1:A:48:THR:CG2	2:A:560:HOH:O	2.54	0.55
1:B:249:MET:HG3	1:B:251:MET:CE	2.36	0.55
1:B:295:PRO:HG2	1:B:322:ILE:CG2	2.37	0.55
1:A:191:LYS:HD2	1:A:191:LYS:N	2.22	0.55
1:B:21:LEU:O	1:B:47:MET:HA	2.07	0.55
1:C:22:LEU:HD13	1:C:86:VAL:CG1	2.36	0.55
1:C:273:HIS:HE1	1:C:277:LYS:HD3	1.72	0.55
1:A:56:SER:O	1:A:59:SER:HB3	2.07	0.55
1:A:63:HIS:NE2	1:A:64:LEU:HG	2.22	0.55
1:A:173:VAL:HB	1:A:174:PRO:HD3	1.88	0.55
1:B:96:GLN:HA	1:B:115:PHE:CZ	2.42	0.55
1:D:194:VAL:HG23	1:D:248:LEU:HD11	1.89	0.55
1:B:269:THR:HG21	1:B:312:PRO:HA	1.89	0.55
1:A:296:ARG:NH1	2:A:518:HOH:O	2.37	0.55
1:D:164:TYR:HB2	1:D:165:PRO:HD3	1.89	0.55
1:B:46:LEU:HD21	1:B:78:ALA:HB1	1.88	0.55
1:C:231:GLY:O	1:C:234:ASP:HB2	2.07	0.55
1:B:58:GLU:O	1:B:62:PRO:HA	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:VAL:HG11	1:D:216:SER:O	2.07	0.54
1:A:116:ARG:HD3	1:A:227:GLU:OE2	2.08	0.54
1:A:308:MET:HA	1:A:322:ILE:O	2.07	0.54
1:D:93:GLY:HA2	2:D:544:HOH:O	2.06	0.54
1:B:99:ILE:HD12	1:B:115:PHE:HE2	1.72	0.54
1:C:111:LEU:HA	1:C:160:ASN:HB3	1.90	0.54
1:A:296:ARG:HB3	1:A:298:HIS:ND1	2.23	0.54
1:C:18:ARG:HE	1:C:45:THR:HG21	1.72	0.54
1:C:15:LYS:HD3	1:C:40:PRO:O	2.06	0.54
1:C:22:LEU:HD13	1:C:86:VAL:CG1	2.37	0.54
1:C:67:GLN:HG2	1:C:69:LEU:HG	1.88	0.54
1:D:173:VAL:HB	1:D:174:PRO:HD3	1.88	0.54
1:A:187:ILE:HA	1:A:243:SER:HB3	1.88	0.54
1:B:127:TYR:CE1	1:B:223:ARG:HD3	2.42	0.54
1:A:82:THR:HG22	1:A:82:THR:O	2.05	0.54
1:B:306:CYS:SG	1:B:330:LYS:CG	2.95	0.54
1:C:161:PRO:HG2	1:C:335:GLN:NE2	2.23	0.54
1:C:356:PRO:C	1:C:358:PHE:H	2.09	0.54
1:D:96:GLN:HG3	2:D:548:HOH:O	2.07	0.54
1:A:251:MET:HB2	1:D:212:GLU:HA	1.88	0.54
1:A:263:MET:HG2	1:A:272:LEU:HD11	1.89	0.54
1:B:300:VAL:HG21	1:B:325:ILE:HA	1.89	0.54
1:C:237:GLN:NE2	2:C:563:HOH:O	2.40	0.54
1:C:311:PHE:HD1	1:C:320:ILE:O	1.91	0.54
1:D:96:GLN:HG3	2:D:545:HOH:O	2.07	0.54
1:A:48:THR:HG21	1:A:75:VAL:HG22	1.89	0.54
1:C:252:ILE:HG21	1:D:359:PRO:OXT	2.07	0.54
1:B:43:GLN:O	1:B:45:THR:HG23	2.06	0.54
1:C:149:ARG:NH1	1:C:348:GLU:OE1	2.40	0.54
1:B:269:THR:HG21	1:B:312:PRO:HA	1.89	0.54
1:B:121:ALA:O	1:B:125:GLU:HG2	2.08	0.54
1:C:115:PHE:CD1	1:C:140:VAL:HG21	2.43	0.54
1:B:83:VAL:O	1:B:106:LEU:HD21	2.08	0.54
1:B:342:ILE:HG13	1:B:342:ILE:O	2.07	0.54
1:B:314:ARG:HG3	1:B:314:ARG:NH1	2.21	0.54
1:A:33:VAL:HG12	1:A:67:GLN:HE22	1.72	0.54
1:D:144:LEU:CD2	1:D:147:ILE:HG13	2.37	0.54
1:D:25:SER:HB2	2:D:443:HOH:O	2.07	0.54
1:A:330:LYS:NZ	1:A:338:GLN:OE1	2.40	0.54
1:B:142:TYR:CZ	1:B:161:PRO:HB3	2.42	0.54
1:D:306:CYS:HA	1:D:324:VAL:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:269:THR:HG21	1:D:312:PRO:HB3	1.88	0.54
1:D:269:THR:HG23	2:D:576:HOH:O	2.06	0.54
1:C:176:LEU:HG	1:C:181:ILE:HD11	1.89	0.54
1:C:263:MET:SD	1:C:319:ALA:HB2	2.48	0.54
1:A:215:SER:HB3	2:D:429:HOH:O	2.07	0.54
1:A:235:VAL:HG13	1:A:236:ALA:N	2.23	0.54
1:B:256:GLN:HB2	1:B:324:VAL:HG12	1.88	0.54
1:C:119:ASN:O	1:C:122:GLU:HB3	2.07	0.54
1:C:147:ILE:HB	1:C:148:LEU:HD12	1.89	0.54
1:C:340:LEU:O	1:C:344:LEU:HD13	2.08	0.54
1:D:175:LEU:HD13	1:D:272:LEU:HD22	1.90	0.54
1:A:256:GLN:HA	1:A:324:VAL:HG12	1.88	0.54
1:B:50:ASP:OD1	1:B:75:VAL:HG23	2.08	0.54
1:B:199:ARG:O	1:B:199:ARG:HG2	2.08	0.54
1:D:67:GLN:O	1:D:69:LEU:HG	2.07	0.54
1:C:253:ARG:CZ	1:C:328:LEU:HD12	2.38	0.54
1:C:51:ARG:HH22	1:C:90:LEU:CD2	2.20	0.54
1:C:325:ILE:C	1:C:325:ILE:HD12	2.28	0.54
1:A:164:TYR:HB2	1:A:165:PRO:HD3	1.88	0.54
1:A:306:CYS:HA	1:A:324:VAL:O	2.08	0.54
1:A:307:HIS:NE2	1:B:65:ARG:HD2	2.22	0.54
1:B:183:HIS:HB2	1:B:240:VAL:HG22	1.89	0.54
1:A:22:LEU:HA	1:A:48:THR:HB	1.89	0.54
1:B:142:TYR:CZ	1:B:161:PRO:HB3	2.42	0.54
1:C:47:MET:HE3	1:C:69:LEU:HB3	1.90	0.54
1:D:254:GLY:HA2	2:D:517:HOH:O	2.07	0.54
1:D:256:GLN:HA	1:D:324:VAL:HG12	1.88	0.54
1:D:135:GLU:O	1:D:138:LYS:HG3	2.08	0.54
1:A:242:VAL:O	1:D:314:ARG:HD3	2.08	0.54
1:B:84:ASP:O	1:B:106:LEU:HG	2.07	0.54
1:B:149:ARG:HG3	1:B:348:GLU:OE1	2.08	0.54
1:B:156:ARG:HB3	2:B:379:HOH:O	2.07	0.54
1:C:108:ILE:HG22	1:C:109:VAL:N	2.23	0.54
1:A:182:LYS:HD2	1:A:262:GLU:CG	2.38	0.54
1:A:151:ASP:HA	1:A:154:LYS:CE	2.24	0.54
1:D:311:PHE:HE2	2:D:411:HOH:O	1.89	0.54
1:B:218:GLY:HA3	1:B:222:HIS:HD2	1.73	0.54
1:C:20:GLY:N	1:C:83:VAL:HG11	2.23	0.54
1:D:239:LYS:HD2	1:D:240:VAL:N	2.23	0.54
1:B:216:SER:HA	1:B:247:HIS:HA	1.90	0.54
1:D:201:ALA:C	1:D:202:LYS:HD2	2.28	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:TYR:CE1	1:A:223:ARG:HD3	2.42	0.54
1:D:104:THR:O	1:D:156:ARG:HD2	2.06	0.54
1:A:239:LYS:HE2	2:A:496:HOH:O	2.07	0.54
1:A:89:CYS:SG	1:A:111:LEU:HD13	2.48	0.54
1:B:52:LYS:HA	1:B:55:GLN:HE21	1.72	0.54
1:D:217:TYR:O	1:D:246:PRO:HD2	2.08	0.54
1:B:256:GLN:HB2	1:B:324:VAL:CG1	2.32	0.54
1:C:22:LEU:HD21	1:C:80:PHE:CZ	2.42	0.54
1:A:187:ILE:HD12	1:D:187:ILE:HD12	1.88	0.54
1:C:48:THR:CG2	1:C:75:VAL:HG22	2.38	0.54
1:C:161:PRO:HG2	1:C:335:GLN:NE2	2.23	0.54
1:B:321:ILE:HD12	1:B:321:ILE:N	2.22	0.54
1:C:22:LEU:HD11	1:C:80:PHE:CE2	2.43	0.54
1:A:82:THR:HG22	1:A:82:THR:O	2.07	0.54
1:A:91:PRO:HD2	1:A:94:THR:CG2	2.34	0.54
1:B:92:HIS:HB2	2:B:532:HOH:O	2.08	0.54
1:B:250:PRO:O	1:D:207:TYR:CZ	2.61	0.54
1:B:280:TYR:CD1	1:B:283:GLU:HG3	2.37	0.54
1:C:337:LEU:HD23	1:C:352:LEU:HD21	1.89	0.54
1:A:174:PRO:HG3	2:A:592:HOH:O	2.06	0.54
1:C:20:GLY:H	1:C:83:VAL:HG11	1.72	0.54
1:D:239:LYS:HD2	1:D:240:VAL:N	2.23	0.54
1:A:57:MET:HE3	1:A:60:VAL:HB	1.89	0.54
1:C:61:PHE:CE1	1:C:199:ARG:NH1	2.76	0.54
1:B:22:LEU:HD13	1:B:86:VAL:CG1	2.38	0.54
1:B:164:TYR:HB2	1:B:165:PRO:HD3	1.89	0.54
1:D:231:GLY:O	1:D:235:VAL:HG23	2.07	0.54
1:A:21:LEU:HD13	1:A:32:ILE:HG21	1.90	0.54
1:A:270:GLU:H	1:A:270:GLU:CD	2.10	0.54
1:B:17:ILE:HG23	1:B:84:ASP:HB2	1.88	0.54
1:D:209:GLU:OE1	2:D:492:HOH:O	2.19	0.54
1:D:215:SER:OG	2:D:383:HOH:O	2.18	0.54
1:C:285:PHE:HA	1:C:305:TYR:CD1	2.43	0.54
1:A:67:GLN:C	1:A:68:LYS:HD2	2.29	0.53
1:B:173:VAL:HB	1:B:174:PRO:HD3	1.90	0.53
1:C:103:PRO:C	1:C:105:ALA:H	2.11	0.53
1:D:194:VAL:HA	1:D:248:LEU:HD11	1.89	0.53
1:A:92:HIS:HD1	1:A:92:HIS:H	1.56	0.53
1:A:287:LYS:HG3	1:B:65:ARG:HD2	1.90	0.53
1:C:68:LYS:HD2	1:C:68:LYS:N	2.23	0.53
1:C:171:PRO:HG3	1:C:308:MET:CE	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:195:SER:HB2	1:C:328:LEU:HD11	1.90	0.53
1:A:48:THR:HG21	1:A:75:VAL:HG22	1.90	0.53
1:B:328:LEU:O	1:B:332:ALA:HB3	2.08	0.53
1:D:286:VAL:O	1:D:287:LYS:HD3	2.08	0.53
1:D:97:GLU:O	1:D:101:GLU:HG2	2.08	0.53
1:C:107:LYS:NZ	1:C:153:LYS:O	2.38	0.53
1:D:46:LEU:HD12	1:D:47:MET:N	2.23	0.53
1:B:173:VAL:HA	1:B:235:VAL:HG11	1.90	0.53
1:C:164:TYR:HB2	1:C:165:PRO:HD3	1.90	0.53
1:C:300:VAL:HG23	2:C:505:HOH:O	2.06	0.53
1:B:111:LEU:HD11	1:B:336:ALA:HB1	1.90	0.53
1:B:147:ILE:HD12	1:B:173:VAL:HG11	1.89	0.53
1:C:15:LYS:HG2	1:C:16:ASP:H	1.73	0.53
1:C:167:THR:HG21	1:C:255:MET:HG2	1.90	0.53
1:C:170:LEU:N	1:C:171:PRO:CD	2.70	0.53
1:A:20:GLY:HA3	1:A:86:VAL:HG22	1.90	0.53
1:B:34:ARG:O	1:B:38:ASN:ND2	2.41	0.53
1:C:46:LEU:HD12	2:C:428:HOH:O	2.07	0.53
1:D:229:GLU:HG2	1:D:242:VAL:HG22	1.89	0.53
1:A:192:SER:HB2	1:A:255:MET:HE2	1.89	0.53
1:B:230:GLN:OE1	2:B:433:HOH:O	2.18	0.53
1:A:122:GLU:HA	1:A:125:GLU:HG2	1.90	0.53
1:B:83:VAL:HG23	1:B:106:LEU:HD11	1.90	0.53
1:C:173:VAL:HB	1:C:174:PRO:HD3	1.90	0.53
1:A:118:ARG:NH1	1:A:118:ARG:CB	2.72	0.53
1:A:236:ALA:C	1:A:238:SER:H	2.11	0.53
1:C:96:GLN:HA	1:C:115:PHE:CZ	2.44	0.53
1:C:141:VAL:O	1:C:158:VAL:HG13	2.09	0.53
1:C:183:HIS:CE1	1:C:184:GLU:HG3	2.43	0.53
1:D:182:LYS:HB2	1:D:262:GLU:CG	2.39	0.53
1:A:251:MET:HB2	1:D:212:GLU:HA	1.90	0.53
1:A:311:PHE:CE1	1:A:322:ILE:HD12	2.44	0.53
1:D:48:THR:OG1	1:D:75:VAL:HG22	2.08	0.53
1:B:104:THR:O	1:B:156:ARG:HD2	2.08	0.53
1:C:79:ASP:OD1	1:C:82:THR:HG23	2.08	0.53
1:B:120:ILE:HG23	1:B:131:HIS:CB	2.39	0.53
1:B:164:TYR:HB2	1:B:165:PRO:HD3	1.91	0.53
1:A:169:GLN:OE1	1:A:228:ILE:HA	2.08	0.53
1:A:252:ILE:HD12	1:C:208:SER:HA	1.91	0.53
1:C:194:VAL:HG12	1:C:251:MET:O	2.08	0.53
1:D:302:GLY:N	1:D:326:ASP:OD2	2.35	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:269:THR:HG23	2:D:578:HOH:O	2.08	0.53
1:D:119:ASN:O	1:D:122:GLU:HB3	2.09	0.53
1:D:173:VAL:HB	1:D:174:PRO:HD3	1.89	0.53
1:B:27:TYR:HD2	1:B:195:SER:O	1.91	0.53
1:A:274:GLN:NE2	1:A:277:LYS:HE2	2.22	0.53
1:C:61:PHE:CE1	1:C:199:ARG:NH1	2.77	0.53
1:A:182:LYS:HD2	1:A:262:GLU:HG3	1.89	0.53
1:C:191:LYS:HD2	1:C:256:GLN:O	2.08	0.53
1:B:51:ARG:HD2	1:B:51:ARG:N	2.19	0.53
1:C:18:ARG:HB3	1:C:45:THR:OG1	2.08	0.53
1:A:95:THR:HG21	1:A:110:ASP:OD2	2.09	0.53
1:B:119:ASN:HB3	1:B:122:GLU:HB3	1.89	0.53
1:A:48:THR:HG21	1:A:75:VAL:HG22	1.91	0.53
1:A:152:ILE:HG23	1:A:158:VAL:HG21	1.90	0.53
1:B:107:LYS:HB3	1:B:343:MET:CE	2.38	0.53
1:B:17:ILE:HG23	1:B:84:ASP:HB2	1.90	0.53
1:C:296:ARG:HD2	1:C:298:HIS:ND1	2.23	0.53
1:D:263:MET:HG2	1:D:272:LEU:HD11	1.90	0.53
1:A:17:ILE:HG23	1:A:84:ASP:HB2	1.91	0.53
1:A:136:LEU:HD12	1:A:136:LEU:O	2.08	0.53
1:A:217:TYR:CE1	1:A:248:LEU:HB2	2.43	0.53
1:A:243:SER:HB2	1:D:315:ILE:CD1	2.38	0.53
1:B:52:LYS:HD3	1:B:60:VAL:HG22	1.91	0.53
1:C:259:ILE:N	1:C:259:ILE:HD12	2.23	0.53
1:D:281:GLU:HA	2:D:583:HOH:O	2.07	0.53
1:A:48:THR:CG2	2:A:562:HOH:O	2.56	0.53
1:A:247:HIS:NE2	1:D:256:GLN:NE2	2.56	0.53
1:B:191:LYS:O	1:B:255:MET:HA	2.09	0.53
1:A:37:ALA:HB2	1:A:67:GLN:NE2	2.24	0.53
1:B:161:PRO:HG2	1:B:335:GLN:NE2	2.24	0.53
1:C:52:LYS:HE2	1:C:60:VAL:HG13	1.91	0.53
1:D:104:THR:O	1:D:156:ARG:HD2	2.08	0.53
1:B:149:ARG:O	1:B:153:LYS:HG3	2.09	0.53
1:D:49:ALA:CB	1:D:72:LEU:HD13	2.38	0.53
1:A:152:ILE:HG23	1:A:158:VAL:HG21	1.91	0.53
1:A:191:LYS:HE2	1:D:191:LYS:HE3	1.91	0.53
1:D:242:VAL:HG23	1:D:242:VAL:O	2.09	0.53
1:A:91:PRO:HB2	1:A:94:THR:OG1	2.08	0.53
1:A:136:LEU:HD21	1:A:157:LEU:HD22	1.91	0.53
1:C:20:GLY:N	1:C:83:VAL:HG11	2.24	0.53
1:C:255:MET:O	1:C:324:VAL:HA	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:90:LEU:HD13	1:D:98:ILE:HD12	1.91	0.53
1:D:211:ALA:O	1:D:212:GLU:O	2.27	0.53
1:B:149:ARG:O	1:B:153:LYS:HG3	2.09	0.53
1:D:32:ILE:HA	1:D:333:SER:OG	2.09	0.53
1:A:178:ALA:HB3	1:A:180:LEU:HG	1.91	0.53
1:D:298:HIS:HA	1:D:301:ARG:NH1	2.19	0.53
1:C:20:GLY:O	1:C:86:VAL:HA	2.09	0.53
1:D:52:LYS:HD2	1:D:52:LYS:N	2.24	0.53
1:A:97:GLU:O	1:A:101:GLU:HG2	2.08	0.53
1:B:301:ARG:NH1	1:C:212:GLU:O	2.42	0.53
1:A:235:VAL:HG13	1:A:236:ALA:H	1.74	0.53
1:B:126:TRP:CD1	1:B:226:PRO:HG3	2.44	0.53
1:C:97:GLU:O	1:C:100:LYS:HB3	2.09	0.53
1:C:270:GLU:N	1:C:270:GLU:OE1	2.41	0.53
1:B:222:HIS:O	1:B:224:HIS:N	2.42	0.53
1:C:168:ILE:C	1:C:171:PRO:HD2	2.29	0.53
1:C:103:PRO:O	1:C:105:ALA:N	2.41	0.53
1:A:52:LYS:HD3	1:A:60:VAL:CG2	2.38	0.53
1:A:233:SER:OG	1:A:239:LYS:HD2	2.09	0.53
1:D:90:LEU:HD13	1:D:98:ILE:HD12	1.91	0.53
1:C:117:LEU:HA	1:C:230:GLN:OE1	2.08	0.53
1:A:173:VAL:HB	1:A:174:PRO:HD3	1.91	0.53
1:C:340:LEU:O	1:C:344:LEU:HD13	2.09	0.53
1:D:325:ILE:HD13	1:D:325:ILE:H	1.73	0.53
1:A:22:LEU:HD11	1:A:80:PHE:CE1	2.43	0.53
1:A:270:GLU:H	1:A:270:GLU:CD	2.11	0.52
1:C:124:GLU:HG2	1:C:130:PRO:HA	1.89	0.52
1:D:132:LYS:HE2	2:D:538:HOH:O	2.09	0.52
1:A:95:THR:HG21	1:A:110:ASP:OD2	2.09	0.52
1:B:289:LEU:HB2	1:B:309:SER:OG	2.09	0.52
1:D:20:GLY:O	1:D:86:VAL:HG13	2.09	0.52
1:B:35:LEU:CD1	1:B:334:GLY:HA2	2.39	0.52
1:B:235:VAL:HG12	1:B:235:VAL:O	2.10	0.52
1:D:281:GLU:HG2	2:D:589:HOH:O	2.09	0.52
1:A:82:THR:HG22	1:A:82:THR:O	2.09	0.52
1:A:217:TYR:O	1:A:246:PRO:HB2	2.08	0.52
1:D:22:LEU:HG	1:D:86:VAL:HG11	1.90	0.52
1:A:103:PRO:HD2	1:A:106:LEU:HD12	1.91	0.52
1:A:82:THR:HG22	1:A:82:THR:O	2.09	0.52
1:C:301:ARG:NH2	2:C:518:HOH:O	2.42	0.52
1:D:296:ARG:NE	2:D:502:HOH:O	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:PRO:HG2	1:B:322:ILE:HG22	1.92	0.52
1:C:191:LYS:NZ	1:C:258:THR:N	2.57	0.52
1:A:199:ARG:O	1:A:199:ARG:HG2	2.10	0.52
1:B:17:ILE:HG23	1:B:84:ASP:OD2	2.09	0.52
1:B:96:GLN:HA	1:B:115:PHE:CZ	2.44	0.52
1:C:18:ARG:HH11	1:C:45:THR:HB	1.75	0.52
1:D:120:ILE:O	1:D:124:GLU:HG3	2.10	0.52
1:C:108:ILE:CG2	1:C:109:VAL:N	2.72	0.52
1:D:136:LEU:HD12	1:D:139:GLU:HG2	1.91	0.52
1:C:65:ARG:HD2	2:C:534:HOH:O	2.08	0.52
1:C:117:LEU:HA	1:C:230:GLN:HE22	1.73	0.52
1:C:58:GLU:OE1	1:C:58:GLU:HA	2.09	0.52
1:C:191:LYS:HB3	1:C:249:MET:SD	2.49	0.52
1:D:48:THR:OG1	1:D:75:VAL:HG22	2.09	0.52
1:B:289:LEU:HD11	1:B:295:PRO:HB3	1.92	0.52
1:D:304:ASN:HA	1:D:329:VAL:HG12	1.90	0.52
1:B:31:GLU:HB3	1:B:333:SER:HB2	1.90	0.52
1:C:349:THR:HB	1:C:353:LEU:HD21	1.91	0.52
1:C:256:GLN:HE21	1:C:322:ILE:HG23	1.73	0.52
1:C:291:GLU:HG3	2:C:574:HOH:O	2.09	0.52
1:A:24:ALA:O	1:A:57:MET:HE1	2.09	0.52
1:D:171:PRO:HD3	1:D:308:MET:CE	2.39	0.52
1:D:275:GLN:HA	1:D:275:GLN:HE21	1.75	0.52
1:B:65:ARG:HB2	1:B:65:ARG:HH11	1.75	0.52
1:B:251:MET:HB2	1:C:212:GLU:HA	1.91	0.52
1:C:47:MET:SD	1:C:57:MET:HE2	2.50	0.52
1:C:264:ALA:HB3	1:C:267:VAL:HG21	1.92	0.52
1:B:170:LEU:HB2	1:B:171:PRO:HD3	1.91	0.52
1:D:151:ASP:HA	1:D:154:LYS:CE	2.30	0.52
1:D:176:LEU:HD21	1:D:181:ILE:HD11	1.91	0.52
1:A:48:THR:HG21	1:A:75:VAL:HG22	1.91	0.52
1:D:132:LYS:HB2	1:D:132:LYS:HZ2	1.74	0.52
1:A:150:GLU:HG2	2:A:469:HOH:O	2.08	0.52
1:A:67:GLN:C	1:A:68:LYS:HD2	2.30	0.52
1:A:135:GLU:O	1:A:138:LYS:HG2	2.09	0.52
1:A:126:TRP:HZ3	1:A:221:ARG:O	1.93	0.52
1:A:213:GLY:HA3	1:D:298:HIS:CE1	2.44	0.52
1:B:287:LYS:HE2	1:B:305:TYR:CE1	2.45	0.52
1:B:22:LEU:HD11	1:B:80:PHE:HE1	1.74	0.52
1:D:48:THR:OG1	1:D:75:VAL:HG22	2.10	0.52
1:A:162:GLY:C	1:A:165:PRO:HD2	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:ASP:OD1	1:B:112:SER:HB3	2.09	0.52
1:C:216:SER:HB3	1:C:247:HIS:NE2	2.24	0.52
1:B:73:VAL:CG1	1:B:74:SER:H	2.15	0.52
1:B:311:PHE:CE1	1:B:322:ILE:HD12	2.45	0.52
1:C:22:LEU:HD11	1:C:80:PHE:CE2	2.34	0.52
1:C:107:LYS:HG2	1:C:343:MET:HB3	1.91	0.52
1:A:57:MET:HE3	1:A:57:MET:HA	1.91	0.52
1:C:347:PRO:HB2	1:C:350:THR:OG1	2.08	0.52
1:A:326:ASP:O	1:A:328:LEU:N	2.43	0.52
1:C:191:LYS:HZ1	1:C:258:THR:H	1.56	0.52
1:B:203:GLU:CD	2:B:561:HOH:O	2.47	0.52
1:B:295:PRO:HG2	1:B:322:ILE:CG2	2.39	0.52
1:C:96:GLN:HG3	1:C:114:ASP:OD2	2.09	0.52
1:C:165:PRO:HG2	1:C:227:GLU:CD	2.30	0.52
1:C:253:ARG:NE	1:C:328:LEU:HD12	2.24	0.52
1:A:163:CYS:HB2	1:A:255:MET:SD	2.49	0.52
1:B:249:MET:SD	1:C:214:ILE:HG21	2.49	0.52
1:D:31:GLU:CD	1:D:253:ARG:HH22	2.13	0.52
1:A:15:LYS:HD2	1:A:43:GLN:HB2	1.92	0.52
1:A:135:GLU:HA	1:A:138:LYS:HE2	1.91	0.52
1:B:92:HIS:HB2	2:B:537:HOH:O	2.10	0.52
1:B:214:ILE:HB	1:B:249:MET:HE2	1.90	0.52
1:A:161:PRO:HG2	1:A:335:GLN:NE2	2.25	0.52
1:A:270:GLU:H	1:A:270:GLU:CD	2.12	0.52
1:B:144:LEU:HB3	1:B:148:LEU:HD13	1.92	0.52
1:A:22:LEU:HD23	1:A:48:THR:HG21	1.91	0.52
1:A:152:ILE:HG21	1:A:339:ASN:OD1	2.10	0.52
1:C:145:THR:O	1:C:149:ARG:HG3	2.10	0.52
1:A:306:CYS:HA	1:A:324:VAL:O	2.10	0.52
1:C:349:THR:HB	1:C:353:LEU:HD21	1.92	0.52
1:D:304:ASN:OD1	1:D:330:LYS:HA	2.08	0.52
1:B:249:MET:SD	1:C:214:ILE:HG21	2.49	0.52
1:C:18:ARG:HH11	1:C:45:THR:HB	1.75	0.52
1:A:270:GLU:H	1:A:270:GLU:CD	2.13	0.52
1:B:216:SER:O	1:C:294:VAL:HG11	2.09	0.52
1:A:167:THR:HG22	1:A:325:ILE:CG2	2.40	0.52
1:B:239:LYS:HD3	1:B:240:VAL:N	2.25	0.52
1:C:357:LEU:HG	1:D:253:ARG:CZ	2.40	0.52
1:B:15:LYS:HB3	1:B:41:HIS:O	2.09	0.52
1:C:18:ARG:HB3	1:C:45:THR:OG1	2.09	0.52
1:C:48:THR:HG22	1:C:49:ALA:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:GLU:HG3	1:C:126:TRP:CD1	2.45	0.52
1:B:18:ARG:HE	1:B:45:THR:HG21	1.75	0.52
1:B:120:ILE:HG13	1:B:134:VAL:HG13	1.92	0.52
1:C:183:HIS:ND1	2:C:472:HOH:O	2.34	0.52
1:B:80:PHE:HB3	1:B:106:LEU:HD21	1.92	0.52
1:B:315:ILE:HD13	1:C:185:ASN:HA	1.92	0.52
1:D:144:LEU:HD21	1:D:169:GLN:HB3	1.91	0.52
1:A:48:THR:HG21	1:A:75:VAL:CG2	2.39	0.52
1:C:19:ILE:HG22	1:C:20:GLY:O	2.10	0.52
1:C:244:PHE:CE2	1:C:246:PRO:HG3	2.44	0.52
1:D:192:SER:HB2	1:D:255:MET:HE2	1.92	0.52
1:C:144:LEU:CD2	1:C:147:ILE:HG13	2.39	0.52
1:C:102:LEU:HD12	1:C:108:ILE:HD13	1.90	0.52
1:A:122:GLU:HA	1:A:125:GLU:HG2	1.92	0.52
1:A:259:ILE:O	1:A:320:ILE:HA	2.10	0.52
1:B:18:ARG:HB2	1:B:83:VAL:HA	1.91	0.52
1:B:187:ILE:HD12	1:B:187:ILE:N	2.24	0.52
1:A:46:LEU:HD12	2:A:428:HOH:O	2.10	0.52
1:B:95:THR:C	1:B:97:GLU:H	2.13	0.52
1:C:102:LEU:HD12	1:C:108:ILE:HD13	1.91	0.52
1:C:28:THR:O	1:C:32:ILE:HG12	2.09	0.52
1:D:190:ALA:C	1:D:191:LYS:HD2	2.31	0.52
1:D:52:LYS:HD3	2:D:409:HOH:O	2.10	0.52
1:C:125:GLU:HG3	1:C:126:TRP:CD1	2.45	0.52
1:D:126:TRP:CZ3	1:D:221:ARG:HG3	2.45	0.52
1:A:67:GLN:C	1:A:68:LYS:HD2	2.31	0.52
1:B:17:ILE:HG13	1:B:344:LEU:HD13	1.90	0.52
1:C:51:ARG:H	1:C:51:ARG:CD	2.00	0.52
1:C:142:TYR:CE2	1:C:144:LEU:HB2	2.45	0.52
1:D:24:ALA:O	1:D:25:SER:OG	2.23	0.52
1:B:46:LEU:HD11	1:B:78:ALA:CB	2.35	0.52
1:C:341:ASN:OD1	1:C:350:THR:HB	2.10	0.52
1:C:273:HIS:CD2	1:C:291:GLU:HG3	2.45	0.52
1:B:170:LEU:HB2	1:B:171:PRO:HD3	1.91	0.52
1:B:311:PHE:HB3	1:B:312:PRO:HD2	1.92	0.52
1:C:136:LEU:O	1:C:139:GLU:HG2	2.10	0.52
1:C:256:GLN:HG3	1:C:324:VAL:HG12	1.92	0.52
1:D:240:VAL:HG12	1:D:242:VAL:HG13	1.91	0.52
1:A:93:GLY:H	1:A:114:ASP:CG	2.13	0.52
1:D:146:GLU:HG2	1:D:286:VAL:HG21	1.91	0.51
1:D:269:THR:HG23	2:D:571:HOH:O	2.08	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:GLU:HA	1:A:125:GLU:HG2	1.92	0.51
1:B:173:VAL:HG13	1:B:235:VAL:CG2	2.39	0.51
1:B:183:HIS:HB2	1:B:240:VAL:HG22	1.92	0.51
1:D:94:THR:HA	2:D:545:HOH:O	2.09	0.51
1:C:65:ARG:HG3	1:C:66:ALA:N	2.25	0.51
1:D:217:TYR:O	1:D:246:PRO:HD2	2.10	0.51
1:C:296:ARG:HB3	1:C:298:HIS:ND1	2.25	0.51
1:D:22:LEU:HD12	1:D:88:CYS:SG	2.50	0.51
1:D:107:LYS:HG3	1:D:344:LEU:HD21	1.93	0.51
1:C:274:GLN:OE1	2:C:486:HOH:O	2.18	0.51
1:D:115:PHE:CD1	1:D:140:VAL:HG21	2.45	0.51
1:D:239:LYS:HD2	1:D:240:VAL:H	1.75	0.51
1:A:135:GLU:O	1:A:138:LYS:HG2	2.09	0.51
1:C:68:LYS:HD2	1:C:68:LYS:N	2.25	0.51
1:C:118:ARG:N	1:C:230:GLN:HE22	2.05	0.51
1:C:270:GLU:HG2	2:C:577:HOH:O	2.09	0.51
1:A:48:THR:CG2	2:A:560:HOH:O	2.56	0.51
1:D:48:THR:OG1	1:D:75:VAL:HG22	2.10	0.51
1:B:19:ILE:CG1	1:B:42:PHE:HB3	2.39	0.51
1:B:27:TYR:O	1:B:31:GLU:HG2	2.09	0.51
1:C:216:SER:HA	1:C:247:HIS:HA	1.93	0.51
1:C:256:GLN:HG3	1:C:324:VAL:CG1	2.40	0.51
1:D:269:THR:HG21	1:D:312:PRO:CA	2.40	0.51
1:B:145:THR:HG21	1:B:338:GLN:HE21	1.75	0.51
1:B:124:GLU:HG3	1:B:129:GLN:C	2.31	0.51
1:B:268:ARG:HB2	1:B:270:GLU:HG2	1.91	0.51
1:C:38:ASN:ND2	2:C:371:HOH:O	2.42	0.51
1:C:144:LEU:HA	1:C:161:PRO:HG3	1.93	0.51
1:B:31:GLU:HB3	1:B:333:SER:OG	2.11	0.51
1:B:111:LEU:HD11	1:B:336:ALA:HB1	1.92	0.51
1:B:118:ARG:CB	1:B:118:ARG:HH11	2.24	0.51
1:C:15:LYS:HB3	1:C:41:HIS:HA	1.93	0.51
1:C:124:GLU:HG2	1:C:129:GLN:O	2.10	0.51
1:C:95:THR:HG22	1:C:115:PHE:HE2	1.75	0.51
1:C:135:GLU:HG2	2:C:457:HOH:O	2.09	0.51
1:A:249:MET:CE	1:D:214:ILE:HG21	2.31	0.51
1:A:251:MET:HB2	1:D:212:GLU:HA	1.91	0.51
1:A:256:GLN:HE21	1:A:322:ILE:HG23	1.70	0.51
1:B:277:LYS:O	1:B:281:GLU:HB3	2.11	0.51
1:C:155:ALA:O	1:C:343:MET:HE2	2.11	0.51
1:C:173:VAL:HB	1:C:174:PRO:HD3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:100:LYS:HA	1:D:136:LEU:HD22	1.92	0.51
1:B:315:ILE:HD13	1:C:185:ASN:HA	1.93	0.51
1:C:264:ALA:HB3	1:C:267:VAL:HG21	1.92	0.51
1:A:48:THR:CG2	2:A:556:HOH:O	2.57	0.51
1:C:190:ALA:C	1:C:191:LYS:HD2	2.31	0.51
1:C:301:ARG:HA	1:C:326:ASP:OD2	2.11	0.51
1:A:47:MET:HE2	1:A:70:PRO:HD2	1.92	0.51
1:A:252:ILE:HG21	1:B:359:PRO:OXT	2.10	0.51
1:A:80:PHE:C	1:A:82:THR:H	2.13	0.51
1:C:46:LEU:HD12	2:C:433:HOH:O	2.09	0.51
1:D:251:MET:HE3	1:D:254:GLY:HA3	1.93	0.51
1:C:260:TYR:HB3	2:C:372:HOH:O	2.09	0.51
1:D:306:CYS:HA	1:D:324:VAL:O	2.10	0.51
1:A:294:VAL:HG22	1:A:311:PHE:CZ	2.46	0.51
1:C:280:TYR:HD1	1:C:283:GLU:HG3	1.75	0.51
1:C:92:HIS:HB2	2:C:531:HOH:O	2.09	0.51
1:C:349:THR:HB	1:C:353:LEU:HD21	1.93	0.51
1:A:95:THR:HG21	1:A:110:ASP:CG	2.31	0.51
1:A:135:GLU:HA	1:A:138:LYS:HE2	1.92	0.51
1:A:117:LEU:HA	1:A:230:GLN:OE1	2.10	0.51
1:C:111:LEU:HA	1:C:160:ASN:HB3	1.92	0.51
1:C:185:ASN:HB3	1:C:318:ARG:NH2	2.25	0.51
1:A:174:PRO:HG3	2:A:584:HOH:O	2.09	0.51
1:D:131:HIS:O	1:D:134:VAL:HG23	2.10	0.51
1:A:163:CYS:HB2	1:A:255:MET:SD	2.49	0.51
1:A:168:ILE:HD11	1:A:188:ILE:HG21	1.92	0.51
1:B:63:HIS:CG	1:B:64:LEU:N	2.79	0.51
1:C:63:HIS:HB3	1:D:299:ASN:OD1	2.11	0.51
1:B:141:VAL:HG21	1:B:155:ALA:HB2	1.93	0.51
1:D:62:PRO:C	1:D:64:LEU:H	2.13	0.51
1:C:125:GLU:HG3	1:C:126:TRP:CD1	2.45	0.51
1:C:144:LEU:HG	1:C:147:ILE:HG13	1.92	0.51
1:B:308:MET:HA	1:B:322:ILE:O	2.11	0.51
1:C:49:ALA:HA	1:C:51:ARG:NH1	2.25	0.51
1:B:267:VAL:HG13	1:B:271:ASP:OD2	2.10	0.51
1:C:119:ASN:HB3	1:C:122:GLU:HB3	1.92	0.51
1:A:149:ARG:NH2	1:A:283:GLU:OE2	2.37	0.51
1:B:274:GLN:NE2	1:B:277:LYS:HE2	2.26	0.51
1:D:187:ILE:HG12	1:D:243:SER:HB3	1.91	0.51
1:B:83:VAL:HG23	1:B:106:LEU:HD21	1.93	0.51
1:D:46:LEU:HD12	1:D:47:MET:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:TYR:CE1	1:A:223:ARG:HD3	2.46	0.51
1:B:289:LEU:HB2	1:B:309:SER:OG	2.11	0.51
1:D:239:LYS:HD2	1:D:240:VAL:N	2.26	0.51
1:B:182:LYS:HB3	1:B:184:GLU:OE1	2.10	0.51
1:C:48:THR:HG21	1:C:75:VAL:HG22	1.91	0.51
1:C:170:LEU:CB	1:C:171:PRO:HD3	2.40	0.51
1:B:19:ILE:HD11	1:B:42:PHE:HB3	1.92	0.51
1:B:168:ILE:O	1:B:171:PRO:HD2	2.11	0.51
1:B:144:LEU:CD2	1:B:169:GLN:HB3	2.41	0.51
1:D:116:ARG:HD3	1:D:227:GLU:CD	2.31	0.51
1:C:200:GLY:HA3	2:C:399:HOH:O	2.11	0.51
1:D:186:ILE:HB	1:D:242:VAL:HG12	1.92	0.51
1:D:358:PHE:CD2	1:D:359:PRO:HA	2.45	0.51
1:A:103:PRO:HD2	1:A:106:LEU:HD12	1.93	0.51
1:C:161:PRO:HG2	1:C:335:GLN:HE21	1.73	0.51
1:C:116:ARG:HD3	1:C:227:GLU:CD	2.31	0.51
1:C:173:VAL:HG13	1:C:235:VAL:HG21	1.91	0.51
1:C:48:THR:CG2	1:C:75:VAL:HG22	2.41	0.51
1:A:47:MET:CE	1:A:70:PRO:HD2	2.40	0.51
1:D:306:CYS:SG	1:D:325:ILE:CG2	2.98	0.51
1:D:308:MET:HA	1:D:322:ILE:O	2.11	0.51
1:B:277:LYS:HD2	2:B:579:HOH:O	2.10	0.51
1:D:21:LEU:HB3	1:D:47:MET:HG2	1.93	0.51
1:D:164:TYR:CE1	1:D:190:ALA:HB1	2.44	0.51
1:D:291:GLU:CD	2:D:598:HOH:O	2.48	0.51
1:B:142:TYR:CZ	1:B:161:PRO:HB3	2.46	0.51
1:C:65:ARG:NE	2:C:527:HOH:O	2.43	0.51
1:D:173:VAL:N	1:D:174:PRO:CD	2.74	0.51
1:D:174:PRO:HB2	1:D:276:LEU:HD23	1.92	0.51
1:B:73:VAL:CG1	1:B:74:SER:H	2.17	0.51
1:D:306:CYS:HA	1:D:324:VAL:O	2.11	0.51
1:A:136:LEU:HD12	1:A:136:LEU:O	2.11	0.51
1:A:164:TYR:HB2	1:A:165:PRO:HD3	1.92	0.51
1:B:213:GLY:O	1:B:250:PRO:HD3	2.10	0.51
1:C:50:ASP:CB	1:C:51:ARG:HH21	2.24	0.51
1:C:153:LYS:HG2	1:C:342:ILE:HB	1.92	0.51
1:B:124:GLU:HA	1:B:129:GLN:O	2.10	0.51
1:C:18:ARG:HH11	1:C:45:THR:HB	1.76	0.51
1:C:34:ARG:HG3	1:D:355:GLN:HB2	1.92	0.51
1:D:202:LYS:HE3	1:D:205:ASN:HD22	1.76	0.51
1:D:300:VAL:HG21	1:D:325:ILE:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:HIS:C	1:A:94:THR:H	2.15	0.51
1:B:291:GLU:HA	2:B:575:HOH:O	2.09	0.51
1:C:100:LYS:HE3	2:C:556:HOH:O	2.11	0.51
1:A:135:GLU:HB2	2:A:579:HOH:O	2.10	0.51
1:C:173:VAL:HG13	1:C:235:VAL:CG2	2.40	0.51
1:C:344:LEU:N	1:C:344:LEU:HD12	2.26	0.51
1:B:100:LYS:HA	1:B:136:LEU:HD22	1.93	0.51
1:A:259:ILE:HD12	1:A:259:ILE:N	2.26	0.51
1:B:175:LEU:HB3	1:B:181:ILE:HG12	1.93	0.51
1:A:116:ARG:HD3	1:A:227:GLU:OE2	2.11	0.51
1:D:185:ASN:ND2	1:D:262:GLU:OE2	2.44	0.51
1:B:19:ILE:HD11	1:B:42:PHE:HB3	1.93	0.51
1:C:212:GLU:OE2	1:C:212:GLU:HA	2.11	0.51
1:B:121:ALA:O	1:B:125:GLU:HG2	2.10	0.51
1:A:67:GLN:HE21	1:B:355:GLN:HG3	1.72	0.50
1:A:95:THR:HB	1:A:114:ASP:OD2	2.10	0.50
1:B:109:VAL:HG11	1:B:336:ALA:HB1	1.93	0.50
1:B:202:LYS:HE3	2:B:393:HOH:O	2.11	0.50
1:D:147:ILE:O	1:D:148:LEU:HD23	2.12	0.50
1:D:299:ASN:HB2	2:D:428:HOH:O	2.11	0.50
1:A:24:ALA:O	1:A:57:MET:HE1	2.10	0.50
1:A:168:ILE:HD13	1:A:188:ILE:HG21	1.92	0.50
1:C:344:LEU:N	1:C:344:LEU:HD12	2.26	0.50
1:D:113:ALA:HA	1:D:116:ARG:CZ	2.41	0.50
1:D:130:PRO:HD2	1:D:132:LYS:NZ	2.26	0.50
1:B:95:THR:CG2	1:B:99:ILE:HD12	2.41	0.50
1:C:45:THR:HA	1:C:70:PRO:HG2	1.93	0.50
1:D:48:THR:HG22	1:D:73:VAL:CG2	2.41	0.50
1:C:48:THR:HG21	1:C:75:VAL:CG2	2.41	0.50
1:B:187:ILE:HD12	1:C:187:ILE:HD12	1.94	0.50
1:C:341:ASN:CG	1:C:350:THR:HB	2.31	0.50
1:A:182:LYS:HD2	1:A:262:GLU:OE1	2.11	0.50
1:A:152:ILE:HD13	1:A:339:ASN:OD1	2.11	0.50
1:D:306:CYS:HB2	1:D:325:ILE:HG22	1.91	0.50
1:A:313:ASP:OD1	1:D:243:SER:HB2	2.12	0.50
1:B:310:VAL:CG1	1:B:321:ILE:HG12	2.41	0.50
1:C:125:GLU:HG3	1:C:126:TRP:N	2.25	0.50
1:B:15:LYS:NZ	2:B:511:HOH:O	2.42	0.50
1:D:167:THR:CG2	1:D:325:ILE:HG12	2.42	0.50
1:A:149:ARG:NH2	1:A:283:GLU:OE2	2.37	0.50
1:B:254:GLY:HA2	2:B:382:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:MET:HE1	1:C:69:LEU:HD22	1.93	0.50
1:A:21:LEU:HD13	1:A:32:ILE:HG21	1.93	0.50
1:A:161:PRO:HG2	1:A:335:GLN:NE2	2.26	0.50
1:A:254:GLY:HA2	1:A:326:ASP:HA	1.94	0.50
1:C:63:HIS:HA	1:D:299:ASN:HB3	1.93	0.50
1:C:330:LYS:HB3	2:C:366:HOH:O	2.12	0.50
1:B:73:VAL:CG1	1:B:74:SER:H	2.11	0.50
1:B:87:PHE:CE1	1:B:109:VAL:HB	2.46	0.50
1:B:92:HIS:HB2	2:B:533:HOH:O	2.11	0.50
1:D:48:THR:OG1	1:D:75:VAL:HG22	2.11	0.50
1:D:132:LYS:HD2	1:D:132:LYS:N	2.26	0.50
1:A:122:GLU:HA	1:A:125:GLU:HG2	1.93	0.50
1:B:162:GLY:C	1:B:165:PRO:HD2	2.32	0.50
1:B:296:ARG:CB	1:B:299:ASN:HD22	2.18	0.50
1:C:344:LEU:HB3	1:C:346:TYR:HD1	1.73	0.50
1:D:291:GLU:HG3	2:D:504:HOH:O	2.11	0.50
1:A:239:LYS:NZ	2:A:609:HOH:O	2.44	0.50
1:C:118:ARG:NH2	2:C:547:HOH:O	2.44	0.50
1:C:145:THR:HB	1:C:330:LYS:HZ2	1.76	0.50
1:C:280:TYR:HD1	1:C:283:GLU:HG3	1.76	0.50
1:D:60:VAL:HG12	1:D:199:ARG:HH12	1.76	0.50
1:B:140:VAL:HG22	1:B:157:LEU:CD2	2.41	0.50
1:B:168:ILE:C	1:B:171:PRO:HD2	2.31	0.50
1:A:96:GLN:HG3	1:A:114:ASP:HB3	1.93	0.50
1:A:206:LEU:HA	1:C:206:LEU:HA	1.93	0.50
1:B:168:ILE:C	1:B:171:PRO:HD2	2.32	0.50
1:D:144:LEU:HD12	1:D:335:GLN:OE1	2.12	0.50
1:D:165:PRO:HG3	1:D:228:ILE:HG13	1.92	0.50
1:B:124:GLU:HA	1:B:129:GLN:O	2.10	0.50
1:A:242:VAL:O	1:D:314:ARG:HD3	2.11	0.50
1:D:269:THR:HG21	1:D:312:PRO:CA	2.41	0.50
1:C:183:HIS:CG	2:C:475:HOH:O	2.65	0.50
1:C:192:SER:HB2	1:C:255:MET:HE2	1.94	0.50
1:A:327:ASN:O	1:A:331:GLY:HA3	2.10	0.50
1:A:191:LYS:HD2	1:A:191:LYS:N	2.27	0.50
1:D:173:VAL:HB	1:D:174:PRO:HD3	1.93	0.50
1:B:274:GLN:NE2	1:B:278:THR:OG1	2.45	0.50
1:C:46:LEU:HA	2:C:435:HOH:O	2.11	0.50
1:C:15:LYS:HB2	1:C:40:PRO:O	2.11	0.50
1:C:273:HIS:CD2	1:C:291:GLU:HG3	2.47	0.50
1:D:304:ASN:HA	1:D:330:LYS:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:GLU:OE2	1:B:329:VAL:HG22	2.12	0.50
1:B:229:GLU:HB3	1:B:239:LYS:HE2	1.92	0.50
1:C:104:THR:C	1:C:106:LEU:H	2.14	0.50
1:A:268:ARG:HB3	1:A:270:GLU:OE1	2.11	0.50
1:A:306:CYS:HA	1:A:324:VAL:O	2.11	0.50
1:B:140:VAL:HB	2:B:536:HOH:O	2.10	0.50
1:D:303:SER:HB3	1:D:305:TYR:HD2	1.77	0.50
1:B:190:ALA:C	1:B:191:LYS:HD2	2.31	0.50
1:D:97:GLU:HB2	2:D:541:HOH:O	2.10	0.50
1:D:168:ILE:HD13	1:D:188:ILE:HD13	1.92	0.50
1:B:294:VAL:HG22	1:B:311:PHE:HZ	1.76	0.50
1:D:217:TYR:O	1:D:246:PRO:HD2	2.12	0.50
1:A:163:CYS:HB2	1:A:255:MET:SD	2.51	0.50
1:A:177:LYS:HG3	1:A:235:VAL:HG23	1.94	0.50
1:B:189:ASP:OD1	1:B:191:LYS:HE3	2.12	0.50
1:D:36:LEU:HD13	1:D:44:VAL:HG22	1.92	0.50
1:D:253:ARG:HD3	1:D:326:ASP:OD2	2.12	0.50
1:C:54:GLY:C	2:C:530:HOH:O	2.50	0.50
1:A:161:PRO:HG2	1:A:335:GLN:HE21	1.76	0.50
1:A:164:TYR:HB2	1:A:165:PRO:HD3	1.93	0.50
1:B:46:LEU:HD21	1:B:78:ALA:HB1	1.94	0.50
1:B:104:THR:HA	1:B:156:ARG:NH1	2.27	0.50
1:A:22:LEU:HD11	1:A:80:PHE:CE1	2.47	0.50
1:C:195:SER:HB3	1:C:252:ILE:O	2.12	0.50
1:D:214:ILE:HD12	1:D:214:ILE:O	2.11	0.50
1:A:164:TYR:HB2	1:A:165:PRO:HD3	1.93	0.50
1:B:268:ARG:HB3	1:B:270:GLU:OE2	2.12	0.50
1:D:173:VAL:HB	1:D:174:PRO:HD3	1.93	0.50
1:D:47:MET:HE1	1:D:69:LEU:HB3	1.94	0.50
1:D:60:VAL:HG12	1:D:199:ARG:NH1	2.26	0.50
1:A:199:ARG:HH21	1:C:209:GLU:CD	2.15	0.50
1:B:256:GLN:HB3	1:C:214:ILE:HD11	1.94	0.50
1:C:51:ARG:HD2	1:C:51:ARG:N	2.13	0.50
1:D:188:ILE:HG23	1:D:259:ILE:HG12	1.94	0.50
1:B:126:TRP:CZ2	1:B:226:PRO:HD3	2.47	0.50
1:C:22:LEU:HD13	1:C:86:VAL:HG13	1.94	0.50
1:C:135:GLU:O	1:C:138:LYS:HG2	2.11	0.50
1:C:340:LEU:HG	1:C:344:LEU:HD13	1.93	0.50
1:A:149:ARG:NH2	1:A:283:GLU:OE2	2.36	0.50
1:A:136:LEU:HD11	1:A:156:ARG:NH2	2.27	0.50
1:A:152:ILE:HD13	1:A:339:ASN:OD1	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:THR:HG22	1:C:89:CYS:SG	2.51	0.50
1:D:167:THR:HG22	1:D:325:ILE:CG2	2.41	0.50
1:A:46:LEU:HD12	2:A:429:HOH:O	2.12	0.50
1:A:173:VAL:HB	1:A:174:PRO:HD3	1.93	0.50
1:C:54:GLY:C	2:C:536:HOH:O	2.50	0.50
1:D:135:GLU:HB2	2:D:545:HOH:O	2.11	0.50
1:D:235:VAL:O	1:D:237:GLN:HG3	2.12	0.50
1:B:277:LYS:HD2	2:B:581:HOH:O	2.11	0.50
1:A:46:LEU:HD12	2:A:430:HOH:O	2.12	0.50
1:B:214:ILE:HG13	1:C:256:GLN:OE1	2.12	0.50
1:D:22:LEU:HG	1:D:86:VAL:CG1	2.42	0.50
1:A:244:PHE:CE2	1:A:246:PRO:HG3	2.47	0.50
1:C:268:ARG:HB3	1:C:270:GLU:OE1	2.12	0.49
1:B:18:ARG:HE	1:B:45:THR:HG21	1.76	0.49
1:B:310:VAL:HG13	1:B:321:ILE:HG12	1.94	0.49
1:D:285:PHE:C	1:D:306:CYS:SG	2.90	0.49
1:B:31:GLU:HA	1:B:31:GLU:OE1	2.12	0.49
1:D:354:HIS:H	1:D:354:HIS:CD2	2.30	0.49
1:B:278:THR:HG23	1:B:281:GLU:OE2	2.12	0.49
1:A:173:VAL:HB	1:A:174:PRO:HD3	1.93	0.49
1:B:191:LYS:O	1:B:255:MET:HA	2.11	0.49
1:B:36:LEU:HD22	1:B:42:PHE:HB2	1.94	0.49
1:D:314:ARG:HH11	1:D:314:ARG:HG3	1.77	0.49
1:A:48:THR:OG1	1:A:75:VAL:HG22	2.12	0.49
1:C:148:LEU:HD12	1:C:148:LEU:N	2.27	0.49
1:D:97:GLU:CD	1:D:132:LYS:HD2	2.32	0.49
1:A:73:VAL:HB	1:A:77:ASP:HB2	1.93	0.49
1:A:149:ARG:HD2	2:A:594:HOH:O	2.12	0.49
1:A:183:HIS:HB2	1:A:240:VAL:HG22	1.93	0.49
1:C:131:HIS:NE2	1:C:137:GLN:HG2	2.27	0.49
1:B:206:LEU:HA	1:D:206:LEU:HA	1.93	0.49
1:C:65:ARG:NE	2:C:533:HOH:O	2.46	0.49
1:D:214:ILE:HG22	1:D:250:PRO:HD3	1.94	0.49
1:A:170:LEU:HB3	1:A:308:MET:HE1	1.94	0.49
1:D:144:LEU:CD2	1:D:147:ILE:HG13	2.41	0.49
1:A:168:ILE:HD13	1:A:188:ILE:HD13	1.93	0.49
1:A:314:ARG:HG3	1:A:314:ARG:NH1	2.26	0.49
1:A:104:THR:O	1:A:156:ARG:HD2	2.12	0.49
1:B:95:THR:HB	1:B:114:ASP:OD2	2.12	0.49
1:B:203:GLU:OE2	2:B:565:HOH:O	2.20	0.49
1:B:277:LYS:HD2	2:B:582:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:ILE:CD1	1:C:185:ASN:HA	2.40	0.49
1:D:173:VAL:HB	1:D:174:PRO:HD3	1.93	0.49
1:A:244:PHE:CE2	1:A:246:PRO:HG3	2.48	0.49
1:B:156:ARG:HG2	1:B:157:LEU:N	2.27	0.49
1:C:104:THR:HA	1:C:156:ARG:NH1	2.27	0.49
1:A:168:ILE:HD11	1:A:188:ILE:HG21	1.94	0.49
1:D:47:MET:HE1	1:D:69:LEU:HB3	1.94	0.49
1:C:97:GLU:O	1:C:100:LYS:HB3	2.12	0.49
1:A:210:ILE:HD12	1:A:248:LEU:CD2	2.42	0.49
1:C:269:THR:HG21	1:C:312:PRO:HA	1.95	0.49
1:D:273:HIS:O	1:D:277:LYS:HB2	2.12	0.49
1:A:57:MET:HE3	1:A:60:VAL:HB	1.93	0.49
1:A:88:CYS:O	1:A:111:LEU:HB2	2.13	0.49
1:A:228:ILE:O	1:A:232:LEU:HG	2.12	0.49
1:D:285:PHE:HA	1:D:305:TYR:HD1	1.76	0.49
1:C:280:TYR:HD1	1:C:283:GLU:HG3	1.78	0.49
1:D:296:ARG:HB3	1:D:298:HIS:ND1	2.27	0.49
1:A:140:VAL:HG22	1:A:157:LEU:HD23	1.94	0.49
1:C:341:ASN:HD21	1:C:350:THR:HB	1.77	0.49
1:D:48:THR:OG1	1:D:75:VAL:HG22	2.11	0.49
1:A:64:LEU:HD21	1:B:355:GLN:HB3	1.94	0.49
1:A:304:ASN:OD1	1:A:329:VAL:HG12	2.13	0.49
1:A:296:ARG:HB3	1:A:298:HIS:ND1	2.28	0.49
1:D:214:ILE:HG22	1:D:250:PRO:HD3	1.94	0.49
1:A:95:THR:HG21	1:A:110:ASP:CG	2.33	0.49
1:A:191:LYS:HD2	1:A:191:LYS:N	2.28	0.49
1:B:229:GLU:OE2	1:B:241:THR:HA	2.12	0.49
1:B:229:GLU:OE2	1:B:241:THR:HG23	2.12	0.49
1:D:269:THR:HG21	1:D:312:PRO:CB	2.42	0.49
1:C:21:LEU:HD22	1:C:32:ILE:HG21	1.93	0.49
1:C:17:ILE:HG23	1:C:84:ASP:HB2	1.92	0.49
1:A:149:ARG:NH2	1:A:283:GLU:OE2	2.38	0.49
1:B:164:TYR:CE1	1:B:190:ALA:HB1	2.47	0.49
1:C:145:THR:O	1:C:149:ARG:HB2	2.12	0.49
1:C:191:LYS:HZ2	1:C:258:THR:H	1.58	0.49
1:A:57:MET:CE	1:A:60:VAL:HB	2.42	0.49
1:C:52:LYS:HD2	1:C:52:LYS:N	2.28	0.49
1:C:115:PHE:HD1	1:C:137:GLN:OE1	1.95	0.49
1:C:183:HIS:HB2	1:C:240:VAL:HG22	1.94	0.49
1:A:124:GLU:HG3	1:A:129:GLN:C	2.33	0.49
1:A:183:HIS:HE1	2:A:603:HOH:O	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:ARG:NE	2:C:527:HOH:O	2.46	0.49
1:D:144:LEU:HA	1:D:335:GLN:OE1	2.12	0.49
1:A:263:MET:HG2	1:A:272:LEU:HD11	1.94	0.49
1:D:80:PHE:CD2	1:D:106:LEU:HD11	2.48	0.49
1:C:67:GLN:HG3	2:C:401:HOH:O	2.12	0.49
1:A:333:SER:O	1:A:336:ALA:HB3	2.13	0.49
1:B:103:PRO:O	1:B:106:LEU:HB2	2.12	0.49
1:D:269:THR:HG21	1:D:312:PRO:HB3	1.93	0.49
1:B:18:ARG:O	1:B:83:VAL:HB	2.13	0.49
1:C:27:TYR:CD1	1:D:359:PRO:HD3	2.47	0.49
1:C:297:THR:HA	1:C:324:VAL:HB	1.93	0.49
1:D:48:THR:CB	1:D:75:VAL:HG22	2.42	0.49
1:A:48:THR:CG2	1:A:75:VAL:HG22	2.43	0.49
1:D:120:ILE:HG13	1:D:134:VAL:HG13	1.94	0.49
1:C:110:ASP:OD1	1:C:112:SER:HB3	2.13	0.49
1:B:202:LYS:H	1:D:206:LEU:HD21	1.78	0.49
1:C:166:THR:O	1:C:170:LEU:HG	2.12	0.49
1:A:51:ARG:HG3	2:A:561:HOH:O	2.12	0.49
1:C:185:ASN:HB3	1:C:318:ARG:NH2	2.27	0.49
1:D:190:ALA:C	1:D:191:LYS:HD2	2.33	0.49
1:D:164:TYR:CE1	1:D:190:ALA:HB1	2.47	0.49
1:D:164:TYR:HA	1:D:255:MET:SD	2.52	0.49
1:C:273:HIS:NE2	1:C:289:LEU:O	2.44	0.49
1:A:96:GLN:HG3	1:A:114:ASP:HB3	1.95	0.49
1:C:354:HIS:CD2	1:C:354:HIS:H	2.29	0.49
1:D:52:LYS:NZ	2:D:525:HOH:O	2.45	0.49
1:B:126:TRP:CE2	1:B:226:PRO:HD3	2.48	0.49
1:B:220:THR:HG21	2:B:563:HOH:O	2.10	0.49
1:A:303:SER:O	1:A:329:VAL:HB	2.13	0.49
1:A:296:ARG:HB3	1:A:298:HIS:ND1	2.27	0.49
1:D:301:ARG:HG3	2:D:517:HOH:O	2.11	0.49
1:B:165:PRO:HD3	1:B:224:HIS:ND1	2.28	0.49
1:C:340:LEU:O	1:C:344:LEU:HD13	2.13	0.49
1:A:215:SER:CB	1:D:296:ARG:HG2	2.43	0.49
1:B:253:ARG:NE	1:B:328:LEU:HD12	2.28	0.49
1:C:22:LEU:HA	1:C:48:THR:CB	2.41	0.49
1:B:175:LEU:CD2	1:B:272:LEU:HD22	2.42	0.49
1:D:164:TYR:HA	1:D:255:MET:SD	2.53	0.49
1:C:117:LEU:HD22	1:C:123:TYR:CD1	2.46	0.49
1:A:183:HIS:HE1	2:A:599:HOH:O	1.94	0.49
1:B:164:TYR:HB2	1:B:224:HIS:ND1	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:LYS:C	1:B:239:LYS:HD3	2.33	0.49
1:B:325:ILE:CD1	1:B:327:ASN:HA	2.43	0.49
1:C:88:CYS:HB2	1:C:110:ASP:HA	1.93	0.49
1:C:217:TYR:O	1:C:246:PRO:HB2	2.13	0.49
1:B:199:ARG:O	1:B:199:ARG:HG2	2.13	0.49
1:A:168:ILE:CD1	1:A:188:ILE:HG21	2.43	0.49
1:B:132:LYS:HE2	2:B:429:HOH:O	2.12	0.49
1:A:268:ARG:HB3	1:A:270:GLU:OE1	2.13	0.49
1:C:39:HIS:HE1	1:C:41:HIS:HB2	1.77	0.49
1:B:91:PRO:HD2	1:B:94:THR:OG1	2.13	0.49
1:C:149:ARG:NH2	1:C:283:GLU:OE2	2.39	0.49
1:B:153:LYS:CD	2:B:550:HOH:O	2.60	0.49
1:C:101:GLU:HB2	2:C:533:HOH:O	2.12	0.49
1:C:340:LEU:HG	1:C:344:LEU:HD13	1.95	0.49
1:D:269:THR:HG23	2:D:578:HOH:O	2.11	0.49
1:B:285:PHE:CE2	1:B:349:THR:HG22	2.47	0.49
1:B:22:LEU:HD23	1:B:90:LEU:HD11	1.95	0.49
1:A:324:VAL:O	1:A:325:ILE:HG23	2.12	0.49
1:B:15:LYS:NZ	2:B:517:HOH:O	2.46	0.49
1:C:116:ARG:HD3	1:C:227:GLU:CD	2.33	0.49
1:D:22:LEU:HG	1:D:86:VAL:HG11	1.94	0.49
1:D:120:ILE:O	1:D:124:GLU:HG3	2.13	0.49
1:B:152:ILE:CG2	1:B:342:ILE:HD11	2.43	0.49
1:A:259:ILE:HB	1:A:321:ILE:HB	1.95	0.49
1:B:126:TRP:CH2	1:B:225:VAL:HB	2.48	0.49
1:D:291:GLU:OE2	2:D:596:HOH:O	2.18	0.49
1:A:329:VAL:HG12	1:A:334:GLY:HA3	1.95	0.49
1:B:140:VAL:CG2	1:B:157:LEU:HD23	2.43	0.49
1:C:46:LEU:HD21	1:C:80:PHE:CE2	2.48	0.49
1:A:136:LEU:HD12	1:A:139:GLU:HG2	1.95	0.48
1:C:47:MET:CE	1:C:70:PRO:HD2	2.43	0.48
1:A:152:ILE:HD13	1:A:339:ASN:OD1	2.13	0.48
1:A:160:ASN:O	1:A:161:PRO:O	2.31	0.48
1:B:239:LYS:C	1:B:239:LYS:HD3	2.34	0.48
1:D:22:LEU:HG	1:D:86:VAL:CG1	2.43	0.48
1:B:152:ILE:HG22	1:B:342:ILE:HD11	1.95	0.48
1:B:187:ILE:HB	1:B:260:TYR:HB2	1.95	0.48
1:C:270:GLU:HG2	2:C:573:HOH:O	2.12	0.48
1:D:104:THR:O	1:D:156:ARG:HD2	2.13	0.48
1:D:141:VAL:HG21	1:D:155:ALA:HB2	1.95	0.48
1:A:95:THR:HB	1:A:114:ASP:OD2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:PHE:CE2	1:B:340:LEU:HG	2.48	0.48
1:B:107:LYS:HB3	1:B:343:MET:HE1	1.94	0.48
1:B:192:SER:HB2	1:B:255:MET:HE2	1.94	0.48
1:C:96:GLN:O	1:C:100:LYS:HB2	2.13	0.48
1:C:214:ILE:HG22	1:C:250:PRO:HD3	1.93	0.48
1:C:149:ARG:HH12	1:C:348:GLU:CD	2.16	0.48
1:A:162:GLY:C	1:A:165:PRO:HD2	2.34	0.48
1:C:175:LEU:HD22	1:C:272:LEU:HD22	1.95	0.48
1:D:257:SER:O	1:D:259:ILE:HG13	2.12	0.48
1:B:118:ARG:CB	1:B:118:ARG:HH11	2.26	0.48
1:B:145:THR:HG21	1:B:338:GLN:HE21	1.79	0.48
1:C:171:PRO:HG2	1:C:323:SER:HB2	1.95	0.48
1:A:56:SER:C	1:A:58:GLU:N	2.66	0.48
1:A:95:THR:CG2	1:A:99:ILE:HD12	2.43	0.48
1:B:165:PRO:HD3	1:B:224:HIS:ND1	2.27	0.48
1:B:233:SER:HA	1:B:240:VAL:HG23	1.96	0.48
1:D:48:THR:CB	1:D:75:VAL:HG22	2.43	0.48
1:C:264:ALA:HB3	1:C:267:VAL:HG21	1.94	0.48
2:A:392:HOH:O	1:D:298:HIS:HD2	1.94	0.48
1:A:213:GLY:HA2	1:D:297:THR:OG1	2.13	0.48
1:A:263:MET:HG2	1:A:272:LEU:HD11	1.95	0.48
1:B:19:ILE:CD1	1:B:42:PHE:HB3	2.41	0.48
1:D:229:GLU:O	1:D:230:GLN:C	2.52	0.48
1:B:22:LEU:O	1:B:89:CYS:HB2	2.13	0.48
1:B:295:PRO:HG2	1:B:322:ILE:CG2	2.43	0.48
1:D:314:ARG:HH11	1:D:314:ARG:HG3	1.79	0.48
1:B:111:LEU:HD11	1:B:336:ALA:CB	2.44	0.48
1:B:148:LEU:O	1:B:152:ILE:HG13	2.14	0.48
1:D:285:PHE:HB3	1:D:306:CYS:SG	2.53	0.48
1:C:135:GLU:HB2	2:C:555:HOH:O	2.13	0.48
1:B:295:PRO:HG2	1:B:322:ILE:CG2	2.44	0.48
1:C:286:VAL:O	1:C:287:LYS:HD3	2.13	0.48
1:A:303:SER:HB3	1:A:356:PRO:CA	2.43	0.48
1:C:214:ILE:HG22	1:C:250:PRO:HD3	1.95	0.48
1:A:164:TYR:CE1	1:A:190:ALA:HB1	2.48	0.48
1:A:243:SER:HB2	1:D:315:ILE:CD1	2.43	0.48
1:D:86:VAL:HG12	1:D:108:ILE:HG23	1.95	0.48
1:D:127:TYR:CE1	1:D:223:ARG:HD3	2.48	0.48
1:A:256:GLN:HB2	1:A:324:VAL:HG12	1.96	0.48
1:B:336:ALA:HA	1:B:339:ASN:ND2	2.29	0.48
1:D:203:GLU:O	1:D:209:GLU:HG3	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:GLN:O	1:A:71:THR:HG23	2.14	0.48
1:A:21:LEU:HD13	1:A:32:ILE:HG21	1.94	0.48
1:A:215:SER:CB	1:D:296:ARG:HG2	2.43	0.48
1:B:123:TYR:CE2	1:B:129:GLN:HG3	2.48	0.48
1:D:341:ASN:ND2	1:D:347:PRO:O	2.46	0.48
1:B:153:LYS:HD2	2:B:549:HOH:O	2.14	0.48
1:B:231:GLY:O	1:B:235:VAL:HG23	2.14	0.48
1:C:57:MET:CE	1:C:72:LEU:HD21	2.42	0.48
1:C:169:GLN:OE1	1:C:231:GLY:HA3	2.12	0.48
1:D:196:GLY:C	1:D:198:GLY:H	2.17	0.48
1:C:106:LEU:O	1:C:156:ARG:NH1	2.45	0.48
1:A:173:VAL:HB	1:A:174:PRO:HD3	1.95	0.48
1:B:239:LYS:HD3	1:B:240:VAL:N	2.28	0.48
1:A:55:GLN:N	1:A:55:GLN:OE1	2.46	0.48
1:A:167:THR:HG22	1:A:325:ILE:HG12	1.95	0.48
1:A:173:VAL:HB	1:A:174:PRO:HD3	1.96	0.48
1:C:115:PHE:CB	1:C:159:ALA:HB2	2.42	0.48
1:B:286:VAL:HG22	1:B:306:CYS:SG	2.53	0.48
1:D:354:HIS:H	1:D:354:HIS:CD2	2.32	0.48
1:B:120:ILE:HG23	1:B:131:HIS:CB	2.44	0.48
1:B:311:PHE:CD1	1:B:311:PHE:N	2.82	0.48
1:C:307:HIS:O	1:C:324:VAL:HG22	2.13	0.48
1:A:34:ARG:HG3	1:B:355:GLN:CB	2.44	0.48
1:B:166:THR:HG21	1:B:330:LYS:HG3	1.94	0.48
1:C:22:LEU:HB2	1:C:88:CYS:HA	1.96	0.48
1:C:170:LEU:CB	1:C:171:PRO:HD3	2.42	0.48
1:A:36:LEU:HD12	1:A:44:VAL:HG23	1.96	0.48
1:B:191:LYS:HZ1	1:C:189:ASP:CG	2.15	0.48
1:D:301:ARG:HB2	2:D:517:HOH:O	2.14	0.48
1:C:50:ASP:OD1	1:C:75:VAL:HG23	2.14	0.48
1:C:170:LEU:HB2	1:C:171:PRO:HD3	1.95	0.48
1:C:187:ILE:HB	1:C:260:TYR:HB2	1.95	0.48
1:D:308:MET:HA	1:D:322:ILE:O	2.14	0.48
1:B:239:LYS:C	1:B:239:LYS:HD3	2.34	0.48
1:C:244:PHE:CE2	1:C:246:PRO:HG3	2.49	0.48
1:D:66:ALA:HB3	2:D:367:HOH:O	2.12	0.48
1:C:285:PHE:HB2	2:C:403:HOH:O	2.13	0.48
1:C:287:LYS:HB3	1:D:65:ARG:HD2	1.94	0.48
1:D:94:THR:HA	2:D:541:HOH:O	2.13	0.48
1:D:194:VAL:HA	1:D:248:LEU:HD11	1.96	0.48
1:A:52:LYS:HG2	1:A:55:GLN:HE22	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:PRO:OXT	1:B:252:ILE:HG21	2.13	0.48
1:C:51:ARG:H	1:C:51:ARG:NE	1.95	0.48
1:D:269:THR:HG21	1:D:312:PRO:CA	2.43	0.48
1:B:239:LYS:C	1:B:239:LYS:HD3	2.34	0.48
1:C:272:LEU:HD12	1:C:310:VAL:HG11	1.95	0.48
1:D:116:ARG:HD3	1:D:227:GLU:CD	2.34	0.48
1:A:177:LYS:CG	1:A:235:VAL:HG23	2.43	0.48
1:A:255:MET:HB3	1:A:325:ILE:CD1	2.43	0.48
1:D:314:ARG:HH11	1:D:314:ARG:HG3	1.79	0.48
1:A:104:THR:O	1:A:156:ARG:HD2	2.14	0.48
1:B:168:ILE:C	1:B:171:PRO:HD2	2.34	0.48
1:B:316:PRO:HB2	2:B:497:HOH:O	2.13	0.48
1:A:22:LEU:HD13	1:A:86:VAL:HG13	1.96	0.48
1:A:103:PRO:HD2	1:A:106:LEU:HD12	1.96	0.48
1:A:194:VAL:O	1:A:194:VAL:HG22	2.13	0.48
1:D:239:LYS:HD2	1:D:240:VAL:H	1.76	0.48
1:B:253:ARG:NH1	1:B:326:ASP:OD2	2.39	0.48
1:D:353:LEU:HB2	2:D:459:HOH:O	2.13	0.48
1:D:300:VAL:HG21	1:D:325:ILE:HA	1.95	0.48
1:A:100:LYS:HE3	1:A:101:GLU:OE2	2.14	0.48
1:A:118:ARG:HH11	1:A:118:ARG:HB3	1.79	0.48
1:B:273:HIS:O	1:B:277:LYS:HG3	2.14	0.48
1:C:193:GLY:HA2	1:C:251:MET:HG3	1.94	0.48
1:C:294:VAL:HG13	1:C:322:ILE:HD12	1.95	0.48
1:D:244:PHE:CZ	1:D:246:PRO:HG3	2.49	0.48
1:B:182:LYS:HG2	1:B:262:GLU:O	2.13	0.48
1:B:295:PRO:HG2	1:B:322:ILE:HG21	1.95	0.48
1:C:20:GLY:HA3	1:C:86:VAL:HG22	1.96	0.48
1:C:48:THR:HG21	1:C:75:VAL:HG23	1.94	0.48
1:A:174:PRO:HG3	2:A:590:HOH:O	2.13	0.48
1:B:97:GLU:OE1	1:B:132:LYS:HD2	2.14	0.48
1:C:42:PHE:N	1:C:42:PHE:CD1	2.80	0.48
1:D:239:LYS:HD2	1:D:240:VAL:N	2.29	0.48
1:A:183:HIS:HB2	1:A:240:VAL:HG22	1.96	0.48
1:D:285:PHE:HB3	1:D:304:ASN:O	2.12	0.48
1:A:135:GLU:O	1:A:138:LYS:HG2	2.14	0.48
1:A:167:THR:HG22	1:A:325:ILE:HG12	1.96	0.48
1:B:295:PRO:HG2	1:B:322:ILE:CG2	2.44	0.48
1:D:164:TYR:CE1	1:D:190:ALA:HB1	2.47	0.48
1:D:194:VAL:CA	1:D:248:LEU:HD11	2.43	0.48
1:A:118:ARG:CB	1:A:118:ARG:HH11	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:PHE:CZ	1:B:322:ILE:HD12	2.49	0.48
1:A:48:THR:HA	1:A:73:VAL:O	2.14	0.48
1:B:187:ILE:HG12	1:B:243:SER:HB3	1.96	0.48
1:C:192:SER:HB2	1:C:255:MET:HE2	1.96	0.48
1:B:146:GLU:HG2	1:B:286:VAL:HG21	1.95	0.48
1:B:249:MET:SD	1:C:214:ILE:HG21	2.53	0.48
1:C:42:PHE:N	1:C:42:PHE:HD1	2.12	0.48
1:C:110:ASP:OD2	2:C:389:HOH:O	2.19	0.48
1:C:304:ASN:O	1:C:330:LYS:HB2	2.14	0.48
1:C:23:GLY:O	1:C:89:CYS:HB2	2.14	0.48
1:C:175:LEU:HD22	1:C:272:LEU:HD22	1.94	0.48
1:A:298:HIS:CD2	1:D:212:GLU:O	2.67	0.48
1:D:96:GLN:HA	1:D:96:GLN:HE21	1.79	0.48
1:B:52:LYS:HG2	1:B:60:VAL:HG22	1.96	0.48
1:C:179:ASN:OD1	1:C:179:ASN:N	2.47	0.48
1:A:306:CYS:HA	1:A:324:VAL:O	2.14	0.48
1:B:203:GLU:HG3	1:D:199:ARG:HG2	1.96	0.48
1:A:210:ILE:HD12	1:A:248:LEU:HD21	1.95	0.48
1:C:122:GLU:CA	1:C:125:GLU:HG2	2.43	0.48
1:C:344:LEU:N	1:C:344:LEU:HD12	2.29	0.48
1:B:21:LEU:HD11	1:B:89:CYS:SG	2.53	0.48
1:C:244:PHE:CZ	1:C:246:PRO:HG3	2.49	0.48
1:A:215:SER:O	1:A:247:HIS:HA	2.14	0.48
1:C:311:PHE:CD1	1:C:311:PHE:N	2.82	0.48
1:B:82:THR:O	1:B:82:THR:HG22	2.14	0.47
1:C:65:ARG:HG3	1:C:66:ALA:N	2.29	0.47
1:D:306:CYS:HB3	1:D:325:ILE:CG2	2.44	0.47
1:C:231:GLY:O	1:C:235:VAL:HG23	2.14	0.47
1:D:291:GLU:OE2	2:D:591:HOH:O	2.20	0.47
1:B:18:ARG:HD3	1:B:82:THR:O	2.13	0.47
1:A:253:ARG:HD3	1:A:326:ASP:CG	2.34	0.47
1:B:112:SER:OG	1:B:113:ALA:N	2.46	0.47
1:C:48:THR:HG23	1:C:73:VAL:O	2.13	0.47
1:A:15:LYS:HB3	1:A:41:HIS:O	2.14	0.47
1:C:216:SER:HB3	1:C:247:HIS:CD2	2.49	0.47
1:D:124:GLU:OE2	1:D:130:PRO:HA	2.14	0.47
1:A:48:THR:HA	1:A:73:VAL:O	2.13	0.47
1:A:187:ILE:HD12	1:D:187:ILE:HD12	1.96	0.47
1:B:95:THR:HG22	1:B:99:ILE:HD12	1.95	0.47
1:B:124:GLU:HG3	2:B:435:HOH:O	2.13	0.47
1:A:259:ILE:HG22	1:A:261:VAL:HG13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:TYR:O	1:B:246:PRO:HD2	2.14	0.47
1:C:104:THR:C	1:C:106:LEU:H	2.17	0.47
1:D:263:MET:HG2	1:D:272:LEU:HD11	1.96	0.47
1:B:22:LEU:HD11	1:B:80:PHE:HE1	1.79	0.47
1:C:60:VAL:O	1:C:62:PRO:HD3	2.14	0.47
1:B:183:HIS:HB3	1:B:240:VAL:HG22	1.96	0.47
1:D:172:LEU:HD21	1:D:259:ILE:HG21	1.95	0.47
1:A:167:THR:HG22	1:A:325:ILE:HG12	1.96	0.47
1:A:174:PRO:HG3	2:A:588:HOH:O	2.12	0.47
1:C:202:LYS:HB2	2:C:478:HOH:O	2.13	0.47
1:D:153:LYS:HA	1:D:342:ILE:O	2.14	0.47
1:A:82:THR:HG22	1:A:82:THR:O	2.15	0.47
1:A:103:PRO:HD2	1:A:106:LEU:HD12	1.95	0.47
1:A:244:PHE:CE2	1:A:246:PRO:HG3	2.50	0.47
1:B:354:HIS:H	1:B:354:HIS:HD2	1.57	0.47
1:B:118:ARG:CB	1:B:118:ARG:HH11	2.27	0.47
1:B:168:ILE:HD13	1:B:188:ILE:HD13	1.97	0.47
1:A:115:PHE:CD1	1:A:140:VAL:HG21	2.49	0.47
1:A:194:VAL:O	1:A:194:VAL:HG22	2.14	0.47
1:C:97:GLU:O	1:C:100:LYS:HB3	2.14	0.47
1:A:95:THR:HB	1:A:114:ASP:OD2	2.14	0.47
1:C:183:HIS:HB2	1:C:240:VAL:HG22	1.95	0.47
1:C:269:THR:HA	1:C:272:LEU:CD1	2.44	0.47
1:A:216:SER:HA	1:A:247:HIS:HA	1.96	0.47
1:B:206:LEU:HA	1:D:206:LEU:HA	1.95	0.47
1:C:163:CYS:HB2	1:C:255:MET:CE	2.44	0.47
1:C:295:PRO:HD3	1:C:309:SER:HB3	1.96	0.47
1:D:172:LEU:O	1:D:175:LEU:N	2.47	0.47
1:B:269:THR:HG21	1:B:312:PRO:HA	1.96	0.47
1:D:88:CYS:SG	1:D:99:ILE:HD11	2.53	0.47
1:D:143:GLY:HA2	1:D:152:ILE:CD1	2.44	0.47
1:D:259:ILE:HD12	1:D:259:ILE:H	1.78	0.47
1:C:43:GLN:O	1:C:45:THR:HG23	2.14	0.47
1:C:65:ARG:HB2	1:C:65:ARG:NH1	2.28	0.47
1:C:124:GLU:HG2	1:C:129:GLN:O	2.14	0.47
1:A:82:THR:HG22	1:A:82:THR:O	2.14	0.47
1:A:256:GLN:HB2	1:A:324:VAL:HG12	1.96	0.47
1:B:99:ILE:HA	1:B:102:LEU:HG	1.96	0.47
1:C:102:LEU:HD12	1:C:108:ILE:HD13	1.96	0.47
1:C:244:PHE:CZ	1:C:246:PRO:HG3	2.49	0.47
1:C:134:VAL:O	1:C:137:GLN:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:ILE:CD1	1:D:256:GLN:HB2	2.44	0.47
1:B:118:ARG:HB2	1:B:118:ARG:NH1	2.29	0.47
1:C:187:ILE:HG12	1:C:243:SER:HB3	1.97	0.47
1:B:219:VAL:HG12	1:B:220:THR:N	2.30	0.47
1:C:17:ILE:HB	1:C:42:PHE:HA	1.96	0.47
1:C:170:LEU:N	1:C:171:PRO:CD	2.77	0.47
1:C:174:PRO:HB3	1:C:279:SER:OG	2.15	0.47
1:C:231:GLY:O	1:C:235:VAL:HG23	2.14	0.47
1:B:225:VAL:N	1:B:226:PRO:HD2	2.30	0.47
1:C:168:ILE:HG12	1:C:188:ILE:HG21	1.94	0.47
1:D:257:SER:HB3	1:D:259:ILE:HD11	1.96	0.47
1:A:221:ARG:O	1:A:222:HIS:HB2	2.14	0.47
1:B:194:VAL:HG22	1:B:194:VAL:O	2.14	0.47
1:B:228:ILE:O	1:B:232:LEU:HG	2.15	0.47
1:C:15:LYS:HG2	1:C:16:ASP:N	2.29	0.47
1:A:214:ILE:HG22	1:A:250:PRO:HD3	1.96	0.47
1:B:167:THR:HG21	1:B:255:MET:HG2	1.95	0.47
1:D:337:LEU:O	1:D:341:ASN:HB2	2.14	0.47
1:B:244:PHE:O	1:B:246:PRO:HD3	2.15	0.47
1:B:270:GLU:CD	1:B:270:GLU:H	2.18	0.47
1:C:340:LEU:O	1:C:344:LEU:HB2	2.14	0.47
1:B:22:LEU:HD11	1:B:80:PHE:CE1	2.49	0.47
1:B:113:ALA:HA	1:B:116:ARG:NE	2.29	0.47
1:B:174:PRO:O	1:B:177:LYS:HB3	2.14	0.47
1:D:202:LYS:CB	1:D:205:ASN:ND2	2.67	0.47
1:D:205:ASN:CG	2:D:390:HOH:O	2.53	0.47
1:A:235:VAL:HG13	1:A:236:ALA:N	2.29	0.47
1:B:142:TYR:CE2	1:B:144:LEU:HB2	2.50	0.47
1:C:349:THR:HB	1:C:353:LEU:HD21	1.97	0.47
1:A:259:ILE:N	1:A:259:ILE:CD1	2.77	0.47
1:A:296:ARG:O	1:A:324:VAL:HG21	2.14	0.47
1:C:295:PRO:HG2	1:C:322:ILE:HG22	1.96	0.47
1:D:291:GLU:OE2	2:D:600:HOH:O	2.20	0.47
1:B:126:TRP:CG	1:B:226:PRO:HG3	2.50	0.47
1:B:299:ASN:HB2	2:B:386:HOH:O	2.14	0.47
1:A:228:ILE:O	1:A:232:LEU:HG	2.14	0.47
1:B:31:GLU:CD	1:B:253:ARG:HH22	2.17	0.47
1:C:126:TRP:CZ3	1:C:221:ARG:HG3	2.49	0.47
1:B:268:ARG:HB2	1:B:270:GLU:HG2	1.95	0.47
1:D:167:THR:HG22	1:D:325:ILE:HG12	1.95	0.47
1:A:167:THR:O	1:A:171:PRO:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:HIS:CE1	1:A:277:LYS:HD3	2.50	0.47
1:B:235:VAL:O	1:B:237:GLN:HG3	2.15	0.47
1:D:47:MET:HE2	1:D:70:PRO:HD2	1.96	0.47
1:C:33:VAL:HG11	1:C:64:LEU:HD13	1.97	0.47
1:A:264:ALA:HB1	1:A:265:PRO:HD2	1.95	0.47
1:D:203:GLU:HA	1:D:206:LEU:HG	1.96	0.47
1:C:119:ASN:HB3	1:C:122:GLU:CD	2.34	0.47
1:C:90:LEU:HD12	1:C:95:THR:HA	1.96	0.47
1:D:120:ILE:O	1:D:124:GLU:HG3	2.15	0.47
1:A:99:ILE:HD11	1:A:110:ASP:HB2	1.96	0.47
1:C:62:PRO:HD2	2:C:399:HOH:O	2.14	0.47
1:C:107:LYS:NZ	1:C:155:ALA:O	2.46	0.47
1:C:164:TYR:CE1	1:C:190:ALA:HB1	2.50	0.47
1:C:171:PRO:HG3	1:C:308:MET:SD	2.55	0.47
1:A:17:ILE:HG23	1:A:84:ASP:HB2	1.97	0.47
1:A:86:VAL:CG2	1:A:106:LEU:HD13	2.44	0.47
1:B:220:THR:HG21	1:C:312:PRO:HG2	1.95	0.47
1:C:223:ARG:NH1	2:C:452:HOH:O	2.48	0.47
1:B:73:VAL:CG1	1:B:74:SER:H	2.17	0.47
1:B:223:ARG:O	1:B:224:HIS:HD2	1.98	0.47
1:B:261:VAL:HB	2:B:367:HOH:O	2.13	0.47
1:C:140:VAL:HG11	1:C:159:ALA:HB2	1.97	0.47
1:B:49:ALA:O	1:B:50:ASP:C	2.53	0.47
1:A:38:ASN:ND2	2:A:428:HOH:O	2.48	0.47
1:B:227:GLU:O	1:B:230:GLN:N	2.48	0.47
1:D:116:ARG:HD3	1:D:227:GLU:CD	2.35	0.47
1:A:26:GLY:HA3	2:A:423:HOH:O	2.14	0.47
1:B:312:PRO:O	1:B:313:ASP:C	2.53	0.47
1:C:39:HIS:NE2	1:C:337:LEU:HD11	2.26	0.47
1:C:306:CYS:HA	1:C:324:VAL:O	2.15	0.47
1:D:120:ILE:O	1:D:124:GLU:HG3	2.15	0.47
1:A:199:ARG:O	1:A:199:ARG:HG2	2.15	0.47
1:B:225:VAL:O	1:B:229:GLU:HG3	2.14	0.47
1:B:179:ASN:OD1	1:B:179:ASN:O	2.33	0.47
1:C:190:ALA:HA	1:C:191:LYS:HE3	1.97	0.47
1:C:343:MET:C	1:C:344:LEU:HD12	2.35	0.47
1:C:36:LEU:HD22	1:C:42:PHE:HB2	1.97	0.47
1:C:209:GLU:OE1	2:C:374:HOH:O	2.20	0.47
1:D:186:ILE:HB	2:D:416:HOH:O	2.14	0.47
1:C:100:LYS:HE3	2:C:555:HOH:O	2.14	0.47
1:C:244:PHE:CE2	1:C:246:PRO:HG3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:52:LYS:HD3	1:D:60:VAL:HG22	1.97	0.47
1:A:20:GLY:O	1:A:86:VAL:HA	2.14	0.47
1:A:22:LEU:HD13	1:A:86:VAL:CG1	2.45	0.47
1:C:19:ILE:CD1	1:C:85:ALA:HB3	2.45	0.47
1:C:48:THR:HG23	1:C:73:VAL:O	2.15	0.47
1:C:49:ALA:HA	1:C:51:ARG:HH11	1.80	0.47
2:C:378:HOH:O	1:D:64:LEU:HD23	2.15	0.47
1:C:103:PRO:C	1:C:105:ALA:H	2.16	0.47
1:D:298:HIS:CD2	1:D:301:ARG:HH12	2.33	0.47
1:A:38:ASN:ND2	2:A:427:HOH:O	2.48	0.47
1:A:183:HIS:HB2	1:A:240:VAL:HG22	1.97	0.47
1:B:349:THR:HG23	2:B:504:HOH:O	2.15	0.47
2:C:377:HOH:O	1:D:64:LEU:HD23	2.15	0.47
1:D:286:VAL:HA	1:D:306:CYS:SG	2.55	0.47
1:B:148:LEU:O	1:B:152:ILE:HG13	2.15	0.47
1:A:80:PHE:HD1	1:A:83:VAL:HG21	1.80	0.47
1:A:194:VAL:HG11	1:C:207:TYR:HB3	1.97	0.47
1:B:197:ALA:HB1	1:B:205:ASN:ND2	2.29	0.47
1:C:96:GLN:NE2	1:C:114:ASP:O	2.48	0.47
1:B:281:GLU:HG3	1:B:282:ASP:H	1.79	0.47
1:C:50:ASP:N	1:C:51:ARG:HH21	2.02	0.47
1:D:259:ILE:HG22	1:D:261:VAL:HG13	1.95	0.47
1:A:164:TYR:CE1	1:A:190:ALA:HB1	2.49	0.47
1:B:153:LYS:HA	1:B:342:ILE:O	2.14	0.47
1:B:191:LYS:O	1:B:255:MET:HA	2.14	0.47
2:B:482:HOH:O	1:C:213:GLY:HA2	2.14	0.47
1:B:296:ARG:HG3	1:C:215:SER:HB3	1.97	0.47
1:D:244:PHE:O	1:D:245:THR:OG1	2.29	0.47
1:D:281:GLU:CG	2:D:587:HOH:O	2.59	0.47
1:C:153:LYS:HG2	1:C:342:ILE:HB	1.97	0.47
1:C:358:PHE:CD1	1:C:358:PHE:C	2.88	0.47
1:A:310:VAL:HG22	1:A:321:ILE:HG12	1.97	0.47
1:B:145:THR:HA	1:B:152:ILE:CD1	2.45	0.47
1:C:191:LYS:HB3	1:C:249:MET:CG	2.45	0.47
1:B:242:VAL:O	1:C:314:ARG:HD3	2.15	0.47
1:C:118:ARG:O	1:C:119:ASN:HB2	2.15	0.47
1:D:239:LYS:HD2	1:D:240:VAL:N	2.30	0.47
1:C:62:PRO:HD2	2:C:399:HOH:O	2.14	0.47
1:C:115:PHE:HA	1:C:137:GLN:OE1	2.15	0.47
1:A:20:GLY:O	1:A:86:VAL:HA	2.15	0.47
1:B:167:THR:HG21	1:B:255:MET:HG2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:259:ILE:HG22	1:D:261:VAL:HG13	1.96	0.47
1:D:325:ILE:HD13	1:D:325:ILE:N	2.30	0.47
1:A:183:HIS:HB3	2:A:597:HOH:O	2.14	0.46
1:A:255:MET:HB3	1:A:325:ILE:HD12	1.97	0.46
1:A:357:LEU:HD11	1:B:253:ARG:NH1	2.30	0.46
1:C:38:ASN:ND2	2:C:432:HOH:O	2.47	0.46
1:D:116:ARG:HD3	1:D:227:GLU:CD	2.36	0.46
1:C:51:ARG:H	1:C:51:ARG:CD	2.02	0.46
1:D:96:GLN:HB2	1:D:132:LYS:HE3	1.97	0.46
1:A:183:HIS:HE1	2:A:605:HOH:O	1.97	0.46
1:B:148:LEU:HD12	1:B:148:LEU:H	1.78	0.46
1:B:213:GLY:HA3	1:C:298:HIS:CD2	2.49	0.46
1:B:313:ASP:HB3	1:B:318:ARG:HB2	1.97	0.46
1:C:21:LEU:HA	1:C:87:PHE:O	2.16	0.46
1:C:47:MET:HE3	1:C:70:PRO:HD2	1.97	0.46
1:C:295:PRO:HD3	1:C:309:SER:CB	2.46	0.46
1:C:311:PHE:HD1	1:C:320:ILE:O	1.98	0.46
1:D:172:LEU:O	1:D:174:PRO:HD2	2.15	0.46
1:D:264:ALA:HB1	1:D:265:PRO:CD	2.45	0.46
1:A:80:PHE:C	1:A:82:THR:N	2.68	0.46
1:B:164:TYR:OH	1:B:192:SER:HB3	2.15	0.46
1:C:31:GLU:CD	1:C:253:ARG:NH2	2.67	0.46
1:B:127:TYR:CE1	1:B:223:ARG:HD3	2.51	0.46
1:B:165:PRO:HD3	1:B:224:HIS:ND1	2.30	0.46
1:C:111:LEU:HA	1:C:160:ASN:HB3	1.97	0.46
1:D:22:LEU:HD12	1:D:88:CYS:SG	2.55	0.46
1:D:129:GLN:HB2	1:D:132:LYS:HZ1	1.80	0.46
1:D:269:THR:HG21	1:D:312:PRO:HA	1.98	0.46
1:C:57:MET:HE2	1:C:72:LEU:HD21	1.96	0.46
1:D:31:GLU:CD	1:D:253:ARG:HH22	2.19	0.46
1:D:127:TYR:CE1	1:D:223:ARG:HG2	2.50	0.46
1:B:239:LYS:HD3	1:B:240:VAL:N	2.30	0.46
1:A:177:LYS:NZ	2:A:587:HOH:O	2.48	0.46
1:B:95:THR:CG2	1:B:99:ILE:HD12	2.44	0.46
1:D:46:LEU:HD12	1:D:47:MET:N	2.30	0.46
1:D:48:THR:CB	1:D:75:VAL:HG22	2.45	0.46
1:D:96:GLN:HG3	2:D:541:HOH:O	2.15	0.46
1:B:144:LEU:HD23	1:B:147:ILE:HG13	1.95	0.46
1:D:255:MET:O	1:D:324:VAL:HA	2.15	0.46
1:C:41:HIS:C	1:C:42:PHE:HD1	2.19	0.46
1:C:149:ARG:NE	1:C:348:GLU:OE1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:124:GLU:OE2	1:D:130:PRO:HA	2.14	0.46
1:A:329:VAL:HA	1:A:333:SER:OG	2.15	0.46
1:C:65:ARG:HB2	1:C:65:ARG:NH1	2.29	0.46
1:C:18:ARG:NH2	1:C:82:THR:HB	2.31	0.46
1:C:233:SER:OG	1:C:239:LYS:HA	2.14	0.46
1:C:65:ARG:HB2	1:C:65:ARG:NH1	2.30	0.46
1:B:95:THR:CG2	1:B:99:ILE:HD12	2.45	0.46
1:B:326:ASP:CG	1:B:329:VAL:HG23	2.36	0.46
1:B:125:GLU:HG3	1:B:126:TRP:N	2.30	0.46
1:A:310:VAL:HG12	1:A:311:PHE:N	2.30	0.46
1:B:175:LEU:HD22	1:B:181:ILE:CG2	2.42	0.46
1:C:118:ARG:HG2	2:C:443:HOH:O	2.14	0.46
1:C:344:LEU:HD12	1:C:344:LEU:N	2.30	0.46
1:D:127:TYR:CE1	1:D:223:ARG:HD3	2.51	0.46
1:B:199:ARG:O	1:B:199:ARG:HG2	2.15	0.46
1:C:175:LEU:HD22	1:C:272:LEU:CD2	2.44	0.46
1:D:292:GLY:HA2	1:D:311:PHE:HD2	1.80	0.46
1:D:291:GLU:CD	2:D:596:HOH:O	2.53	0.46
1:B:337:LEU:O	1:B:341:ASN:HB2	2.15	0.46
1:B:67:GLN:HE21	1:B:69:LEU:HD21	1.80	0.46
1:B:163:CYS:HB2	1:B:255:MET:SD	2.56	0.46
1:B:269:THR:HG21	1:B:312:PRO:HB3	1.97	0.46
1:D:96:GLN:HB2	2:D:546:HOH:O	2.14	0.46
1:C:22:LEU:HD11	1:C:80:PHE:CE2	2.51	0.46
1:A:177:LYS:NZ	2:A:593:HOH:O	2.48	0.46
1:A:177:LYS:CG	1:A:235:VAL:HG23	2.45	0.46
1:A:191:LYS:HD2	1:A:191:LYS:N	2.31	0.46
1:C:49:ALA:HA	1:C:51:ARG:HH11	1.80	0.46
1:D:171:PRO:O	1:D:175:LEU:HG	2.16	0.46
1:B:225:VAL:N	1:B:226:PRO:HD2	2.30	0.46
1:B:242:VAL:O	1:C:314:ARG:HD3	2.15	0.46
1:D:118:ARG:NH1	1:D:230:GLN:HG3	2.30	0.46
1:A:171:PRO:O	1:A:174:PRO:HD2	2.16	0.46
1:B:153:LYS:HD2	2:B:554:HOH:O	2.14	0.46
1:C:22:LEU:HD13	1:C:88:CYS:SG	2.55	0.46
1:D:214:ILE:HG22	1:D:250:PRO:HD3	1.98	0.46
1:A:209:GLU:OE2	1:C:27:TYR:HE1	1.99	0.46
1:B:36:LEU:HD12	1:B:44:VAL:HG23	1.98	0.46
1:C:149:ARG:HH22	1:C:283:GLU:CD	2.19	0.46
1:D:281:GLU:N	2:D:587:HOH:O	2.48	0.46
1:C:182:LYS:HD3	1:C:262:GLU:OE1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:TYR:HE2	1:A:222:HIS:HE2	1.56	0.46
1:A:256:GLN:HB2	1:A:324:VAL:HG12	1.98	0.46
1:B:46:LEU:HD21	1:B:78:ALA:HB1	1.98	0.46
1:A:199:ARG:O	1:A:199:ARG:HG2	2.16	0.46
1:C:86:VAL:HG21	1:C:106:LEU:HD13	1.97	0.46
1:C:103:PRO:O	1:C:105:ALA:N	2.48	0.46
1:D:180:LEU:HB3	1:D:272:LEU:HD23	1.96	0.46
1:A:168:ILE:HD11	1:A:188:ILE:HG21	1.96	0.46
1:A:191:LYS:HB3	1:A:249:MET:CG	2.45	0.46
1:A:92:HIS:ND1	1:A:112:SER:HB2	2.31	0.46
1:A:268:ARG:HB3	1:A:270:GLU:OE1	2.16	0.46
1:B:144:LEU:HB3	1:B:148:LEU:CD1	2.46	0.46
1:C:187:ILE:HB	1:C:260:TYR:HB2	1.97	0.46
1:A:183:HIS:HB3	2:A:600:HOH:O	2.16	0.46
1:B:105:ALA:HB2	2:B:537:HOH:O	2.15	0.46
1:B:126:TRP:CZ2	1:B:226:PRO:HD3	2.51	0.46
1:B:291:GLU:HA	2:B:578:HOH:O	2.14	0.46
1:C:120:ILE:HG13	1:C:134:VAL:HG13	1.96	0.46
1:A:249:MET:HE2	1:D:214:ILE:HG12	1.98	0.46
1:B:118:ARG:HB2	1:B:118:ARG:NH1	2.30	0.46
1:C:22:LEU:CA	1:C:48:THR:HB	2.33	0.46
1:D:216:SER:HA	1:D:247:HIS:HA	1.98	0.46
1:C:15:LYS:HG2	1:C:16:ASP:OD1	2.16	0.46
1:A:191:LYS:HD2	1:A:191:LYS:N	2.31	0.46
1:C:135:GLU:HB2	2:C:556:HOH:O	2.15	0.46
1:C:183:HIS:CE1	2:C:475:HOH:O	2.67	0.46
1:B:161:PRO:HG2	1:B:335:GLN:HE22	1.78	0.46
1:B:296:ARG:HD3	2:B:410:HOH:O	2.14	0.46
1:D:132:LYS:HB2	1:D:132:LYS:NZ	2.30	0.46
1:D:150:GLU:HA	1:D:153:LYS:HD3	1.98	0.46
1:A:51:ARG:HG3	2:A:560:HOH:O	2.15	0.46
1:A:127:TYR:CE1	1:A:223:ARG:HD3	2.51	0.46
1:A:170:LEU:N	1:A:171:PRO:HD2	2.31	0.46
1:D:167:THR:CG2	1:D:325:ILE:HD12	2.45	0.46
1:A:95:THR:HG21	1:A:110:ASP:OD2	2.15	0.46
1:B:354:HIS:CD2	1:B:354:HIS:N	2.82	0.46
1:A:23:GLY:HA3	1:A:89:CYS:O	2.15	0.46
1:B:295:PRO:HG2	1:B:322:ILE:HG22	1.98	0.46
1:B:297:THR:HG1	1:C:214:ILE:H	1.60	0.46
1:C:217:TYR:O	1:C:246:PRO:HD2	2.16	0.46
1:A:359:PRO:OXT	1:B:252:ILE:HD13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:249:MET:HG3	1:D:251:MET:HE1	1.98	0.46
1:A:24:ALA:HA	1:A:29:GLY:HA3	1.98	0.46
1:B:125:GLU:HG3	1:B:126:TRP:N	2.30	0.46
1:C:95:THR:HG22	1:C:115:PHE:CE2	2.50	0.46
1:D:17:ILE:HB	1:D:42:PHE:CD1	2.50	0.46
1:D:50:ASP:HB3	2:D:536:HOH:O	2.15	0.46
1:D:304:ASN:HA	1:D:329:VAL:CG1	2.45	0.46
1:B:19:ILE:HB	1:B:44:VAL:HA	1.98	0.46
1:B:166:THR:HG21	1:B:330:LYS:HG3	1.97	0.46
1:C:121:ALA:O	1:C:125:GLU:N	2.48	0.46
2:C:516:HOH:O	1:D:67:GLN:HG3	2.15	0.46
1:A:183:HIS:HB2	1:A:240:VAL:HG22	1.97	0.46
1:A:164:TYR:HB2	1:A:165:PRO:HD3	1.97	0.46
1:A:256:GLN:HG3	1:A:257:SER:N	2.29	0.46
1:B:119:ASN:OD1	1:B:121:ALA:HB3	2.15	0.46
1:D:245:THR:HA	1:D:246:PRO:HD3	1.78	0.46
1:A:183:HIS:HB3	2:A:601:HOH:O	2.16	0.46
1:A:191:LYS:HD2	1:A:191:LYS:N	2.31	0.46
1:B:176:LEU:HB2	1:B:235:VAL:CG1	2.46	0.46
1:B:239:LYS:C	1:B:239:LYS:HD3	2.36	0.46
1:A:136:LEU:O	1:A:139:GLU:HG2	2.16	0.46
1:A:173:VAL:HB	1:A:174:PRO:HD3	1.97	0.46
1:A:355:GLN:HB2	1:B:34:ARG:HG3	1.98	0.46
1:B:191:LYS:HA	1:B:247:HIS:HB2	1.96	0.46
1:B:273:HIS:CE1	1:B:291:GLU:HG3	2.50	0.46
1:C:223:ARG:NH1	2:C:552:HOH:O	2.46	0.46
1:C:294:VAL:HG13	1:C:322:ILE:CD1	2.46	0.46
1:B:118:ARG:HB2	1:B:118:ARG:NH1	2.31	0.46
1:B:289:LEU:HB3	1:B:293:VAL:HB	1.98	0.46
1:D:277:LYS:HE3	1:D:281:GLU:OE2	2.16	0.46
1:B:29:GLY:HA3	2:B:400:HOH:O	2.15	0.46
1:B:175:LEU:HD13	1:B:272:LEU:HD13	1.97	0.46
1:B:269:THR:HG21	1:B:312:PRO:CB	2.45	0.46
1:C:162:GLY:O	1:C:165:PRO:HD2	2.15	0.46
1:A:95:THR:CG2	1:A:99:ILE:HD12	2.45	0.46
1:C:47:MET:HE3	1:C:57:MET:HB2	1.98	0.46
1:C:47:MET:CE	1:C:57:MET:HB2	2.46	0.46
1:C:48:THR:HG22	1:C:49:ALA:N	2.31	0.46
1:C:35:LEU:HD22	1:C:352:LEU:CD2	2.40	0.46
1:C:58:GLU:OE1	1:C:64:LEU:HB2	2.15	0.46
1:A:95:THR:HB	1:A:114:ASP:OD2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:202:LYS:HE3	1:C:205:ASN:HD22	1.81	0.46
1:C:315:ILE:CG2	1:C:318:ARG:HD2	2.45	0.46
1:D:21:LEU:HD13	1:D:32:ILE:HG21	1.98	0.46
1:A:76:LYS:HG2	2:A:547:HOH:O	2.16	0.46
1:A:42:PHE:CZ	1:A:344:LEU:HD12	2.51	0.46
1:B:120:ILE:HD12	1:B:131:HIS:CD2	2.50	0.46
1:C:148:LEU:O	1:C:152:ILE:HG13	2.16	0.46
1:C:195:SER:HB3	1:C:327:ASN:HD21	1.81	0.46
1:D:191:LYS:HB3	1:D:249:MET:CG	2.46	0.46
1:A:65:ARG:HB2	1:A:65:ARG:NH1	2.31	0.46
1:C:172:LEU:HD13	1:C:186:ILE:HD13	1.98	0.46
1:D:295:PRO:HG2	1:D:322:ILE:HG22	1.97	0.46
1:D:306:CYS:HA	1:D:324:VAL:O	2.16	0.46
1:B:73:VAL:HG11	1:B:78:ALA:HB2	1.98	0.46
1:D:46:LEU:HD12	1:D:47:MET:N	2.31	0.46
1:D:104:THR:HG23	1:D:156:ARG:CZ	2.46	0.46
1:B:149:ARG:O	1:B:153:LYS:HG3	2.15	0.46
1:D:269:THR:HG21	1:D:312:PRO:HA	1.98	0.46
1:A:63:HIS:CE1	1:A:64:LEU:HG	2.51	0.46
1:B:113:ALA:HA	1:B:116:ARG:NE	2.31	0.46
1:C:90:LEU:HD13	1:C:98:ILE:HD12	1.96	0.46
1:A:214:ILE:N	1:D:298:HIS:CE1	2.84	0.46
1:B:229:GLU:CD	1:B:241:THR:HA	2.36	0.46
1:B:287:LYS:HB2	1:B:307:HIS:CD2	2.50	0.46
1:C:103:PRO:C	1:C:105:ALA:H	2.19	0.46
1:A:213:GLY:HA3	1:D:298:HIS:CE1	2.51	0.46
1:B:39:HIS:ND1	1:B:40:PRO:HD2	2.31	0.46
1:B:50:ASP:OD2	1:B:75:VAL:HB	2.16	0.46
1:B:308:MET:HA	1:B:322:ILE:O	2.16	0.46
1:B:178:ALA:CB	1:B:275:GLN:HE21	2.29	0.45
1:D:115:PHE:HB3	1:D:140:VAL:HG11	1.98	0.45
1:D:118:ARG:HG3	1:D:230:GLN:OE1	2.16	0.45
1:D:127:TYR:CE1	1:D:223:ARG:HD3	2.51	0.45
1:B:106:LEU:O	1:B:156:ARG:HG3	2.16	0.45
1:C:103:PRO:C	1:C:105:ALA:N	2.68	0.45
1:C:192:SER:HB2	1:C:255:MET:HE2	1.97	0.45
1:D:291:GLU:CD	2:D:591:HOH:O	2.54	0.45
1:A:207:TYR:CD1	1:C:194:VAL:HG11	2.48	0.45
1:B:111:LEU:HD11	1:B:336:ALA:CB	2.46	0.45
1:C:182:LYS:HE3	1:C:264:ALA:HA	1.98	0.45
1:D:270:GLU:H	1:D:270:GLU:CD	2.19	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:ASP:HB2	1:B:51:ARG:HD2	1.96	0.45
1:B:285:PHE:CE2	1:B:349:THR:HG22	2.50	0.45
1:A:68:LYS:HD2	1:A:68:LYS:N	2.31	0.45
1:D:299:ASN:CB	2:D:428:HOH:O	2.62	0.45
1:C:117:LEU:HD22	1:C:123:TYR:HA	1.98	0.45
1:C:233:SER:HA	1:C:236:ALA:HB3	1.97	0.45
1:C:236:ALA:O	1:C:237:GLN:HB2	2.16	0.45
1:D:58:GLU:CD	1:D:65:ARG:HA	2.35	0.45
1:C:164:TYR:CE1	1:C:190:ALA:HB1	2.51	0.45
1:D:171:PRO:O	1:D:175:LEU:HG	2.16	0.45
1:D:351:GLY:O	1:D:352:LEU:HD23	2.16	0.45
1:A:164:TYR:CE1	1:A:190:ALA:HB1	2.52	0.45
1:D:146:GLU:HG2	1:D:286:VAL:CG2	2.46	0.45
1:C:20:GLY:N	1:C:83:VAL:HG11	2.31	0.45
1:C:57:MET:O	1:C:57:MET:HG3	2.16	0.45
1:C:96:GLN:NE2	1:C:131:HIS:CE1	2.84	0.45
1:C:231:GLY:O	1:C:234:ASP:HB2	2.16	0.45
1:D:291:GLU:CD	2:D:600:HOH:O	2.54	0.45
1:B:28:THR:HB	1:B:333:SER:OG	2.15	0.45
1:C:131:HIS:CE1	1:C:137:GLN:HB2	2.50	0.45
1:D:126:TRP:CG	1:D:226:PRO:HG3	2.51	0.45
1:D:228:ILE:O	1:D:232:LEU:HG	2.16	0.45
1:A:92:HIS:H	1:A:92:HIS:HD1	1.62	0.45
1:C:164:TYR:CE1	1:C:190:ALA:HB1	2.52	0.45
1:C:314:ARG:HG3	1:C:314:ARG:NH1	2.31	0.45
1:B:103:PRO:O	1:B:106:LEU:HB2	2.17	0.45
1:A:185:ASN:HA	1:D:315:ILE:HD13	1.99	0.45
1:B:85:ALA:HA	1:B:107:LYS:O	2.16	0.45
1:B:145:THR:CG2	1:B:149:ARG:HG2	2.45	0.45
1:B:249:MET:HG3	1:B:251:MET:HE1	1.97	0.45
1:C:164:TYR:CE1	1:C:190:ALA:HB1	2.51	0.45
1:D:28:THR:CG2	1:D:111:LEU:HD22	2.47	0.45
1:D:126:TRP:CG	1:D:226:PRO:HG3	2.50	0.45
1:D:173:VAL:HG13	1:D:235:VAL:HG21	1.97	0.45
1:C:48:THR:HA	1:C:73:VAL:O	2.15	0.45
1:D:171:PRO:O	1:D:276:LEU:HD21	2.16	0.45
1:C:45:THR:HA	1:C:70:PRO:HG2	1.99	0.45
1:D:172:LEU:HD21	1:D:259:ILE:HG21	1.98	0.45
1:D:178:ALA:HB2	1:D:275:GLN:HE21	1.82	0.45
1:A:334:GLY:O	1:A:338:GLN:HB2	2.16	0.45
1:B:90:LEU:HD13	1:B:98:ILE:HD12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:164:TYR:CE1	1:D:190:ALA:HB1	2.51	0.45
1:C:164:TYR:HB2	1:C:165:PRO:HD3	1.98	0.45
1:D:168:ILE:O	1:D:172:LEU:HG	2.15	0.45
1:A:97:GLU:O	1:A:101:GLU:HG2	2.17	0.45
1:B:161:PRO:HG2	1:B:335:GLN:NE2	2.32	0.45
1:B:164:TYR:HA	1:B:255:MET:SD	2.57	0.45
1:A:48:THR:HG23	2:A:559:HOH:O	2.15	0.45
1:C:171:PRO:HG3	1:C:323:SER:HB2	1.99	0.45
1:D:22:LEU:HG	1:D:86:VAL:CG1	2.46	0.45
1:D:46:LEU:HD21	1:D:78:ALA:HB1	1.99	0.45
1:D:128:GLY:O	1:D:129:GLN:HB3	2.16	0.45
1:D:145:THR:HB	1:D:338:GLN:NE2	2.32	0.45
1:A:161:PRO:HG2	1:A:335:GLN:NE2	2.31	0.45
1:B:259:ILE:HB	1:B:321:ILE:HB	1.98	0.45
1:C:50:ASP:OD1	1:C:75:VAL:HG23	2.16	0.45
1:A:48:THR:HG21	1:A:75:VAL:CG2	2.47	0.45
1:D:48:THR:HG22	1:D:73:VAL:HG23	1.98	0.45
1:D:118:ARG:HG3	1:D:230:GLN:OE1	2.16	0.45
1:B:206:LEU:HB2	1:B:209:GLU:HG2	1.99	0.45
1:A:273:HIS:CG	1:A:291:GLU:HG3	2.52	0.45
1:B:51:ARG:HB2	2:B:417:HOH:O	2.16	0.45
1:C:39:HIS:HD1	1:C:42:PHE:H	1.64	0.45
1:D:20:GLY:HA2	1:D:46:LEU:O	2.17	0.45
1:A:190:ALA:C	1:A:191:LYS:HD2	2.37	0.45
1:A:296:ARG:HD2	1:A:298:HIS:HB2	1.98	0.45
1:B:144:LEU:HD22	1:B:169:GLN:OE1	2.16	0.45
1:B:273:HIS:CG	1:B:291:GLU:HG3	2.50	0.45
1:B:349:THR:HG23	2:B:501:HOH:O	2.17	0.45
1:C:97:GLU:HB2	1:C:132:LYS:HD2	1.98	0.45
1:D:269:THR:HG23	2:D:580:HOH:O	2.16	0.45
1:C:137:GLN:HG3	1:C:137:GLN:O	2.15	0.45
1:B:315:ILE:HD13	1:C:185:ASN:HA	1.98	0.45
1:C:103:PRO:O	1:C:105:ALA:N	2.49	0.45
1:C:120:ILE:HG22	1:C:124:GLU:OE2	2.17	0.45
1:D:94:THR:N	2:D:547:HOH:O	2.50	0.45
1:A:96:GLN:HG3	1:A:114:ASP:HB3	1.99	0.45
1:A:306:CYS:HB2	1:A:325:ILE:HG22	1.97	0.45
1:A:173:VAL:HB	1:A:174:PRO:HD3	1.99	0.45
1:A:22:LEU:HD13	1:A:86:VAL:CG1	2.46	0.45
1:D:311:PHE:N	1:D:311:PHE:CD1	2.84	0.45
1:C:178:ALA:HB1	1:C:275:GLN:NE2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:LYS:HE3	1:B:65:ARG:NH1	2.32	0.45
1:C:304:ASN:OD1	1:C:330:LYS:HA	2.17	0.45
1:C:359:PRO:OXT	1:D:252:ILE:HG21	2.16	0.45
1:D:99:ILE:HA	1:D:102:LEU:HG	1.97	0.45
1:C:48:THR:HG21	1:C:75:VAL:HG22	1.97	0.45
1:D:172:LEU:O	1:D:174:PRO:CD	2.64	0.45
1:A:170:LEU:HD12	1:A:306:CYS:SG	2.57	0.45
1:A:256:GLN:HB3	1:D:214:ILE:HD11	1.99	0.45
1:B:219:VAL:HG11	1:C:311:PHE:CD2	2.52	0.45
1:D:113:ALA:HB2	1:D:116:ARG:NH1	2.31	0.45
1:D:308:MET:HA	1:D:322:ILE:O	2.17	0.45
1:B:296:ARG:HB2	1:B:299:ASN:ND2	2.32	0.45
1:C:49:ALA:O	1:C:53:ALA:N	2.49	0.45
1:C:86:VAL:HG12	1:C:87:PHE:N	2.32	0.45
1:A:140:VAL:HG22	1:A:157:LEU:HD23	1.99	0.45
1:B:106:LEU:HD13	2:B:529:HOH:O	2.16	0.45
1:C:73:VAL:HG13	2:C:426:HOH:O	2.16	0.45
1:C:296:ARG:H	1:C:299:ASN:HD22	1.65	0.45
1:C:306:CYS:CB	1:C:325:ILE:HG22	2.36	0.45
1:D:342:ILE:C	1:D:344:LEU:N	2.69	0.45
1:A:168:ILE:O	1:A:171:PRO:HG2	2.16	0.45
1:C:135:GLU:HG2	2:C:459:HOH:O	2.17	0.45
1:C:149:ARG:HH12	1:C:348:GLU:CD	2.19	0.45
1:A:191:LYS:HA	1:A:247:HIS:O	2.16	0.45
1:D:331:GLY:O	1:D:332:ALA:HB2	2.17	0.45
1:A:22:LEU:HD13	1:A:86:VAL:HG13	1.99	0.45
1:C:58:GLU:OE1	1:C:65:ARG:HB2	2.17	0.45
1:A:20:GLY:HA3	1:A:86:VAL:HG22	1.99	0.45
1:A:290:ASP:HB2	1:A:293:VAL:HG21	1.98	0.45
1:B:182:LYS:HD2	1:B:262:GLU:CD	2.37	0.45
1:C:103:PRO:C	1:C:105:ALA:H	2.19	0.45
1:C:195:SER:HB3	1:C:252:ILE:O	2.17	0.45
1:A:168:ILE:HD11	1:A:188:ILE:HG21	1.96	0.45
1:C:34:ARG:HD3	1:D:356:PRO:O	2.16	0.45
1:D:52:LYS:NZ	2:D:521:HOH:O	2.49	0.45
1:A:191:LYS:HG3	1:A:247:HIS:CG	2.52	0.45
1:B:120:ILE:HD11	1:B:137:GLN:HB3	1.99	0.45
1:B:124:GLU:HG2	1:B:129:GLN:O	2.17	0.45
1:B:313:ASP:HB3	1:B:318:ARG:O	2.17	0.45
1:B:223:ARG:HG3	2:B:468:HOH:O	2.17	0.45
1:B:223:ARG:O	1:B:226:PRO:HD2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:214:ILE:HG22	1:D:250:PRO:HD3	1.99	0.45
1:A:177:LYS:HG3	1:A:235:VAL:HG23	1.98	0.45
1:A:68:LYS:HD2	1:A:68:LYS:N	2.32	0.45
1:A:177:LYS:HG3	1:A:235:VAL:CG2	2.47	0.45
1:A:208:SER:OG	1:C:194:VAL:HG13	2.17	0.45
1:B:88:CYS:SG	1:B:95:THR:HG23	2.57	0.45
1:B:124:GLU:HG3	1:B:130:PRO:HA	1.98	0.45
1:C:117:LEU:HD11	1:C:226:PRO:C	2.37	0.45
1:A:146:GLU:HG3	1:A:283:GLU:OE1	2.16	0.45
1:B:121:ALA:O	1:B:124:GLU:HB3	2.17	0.45
1:C:126:TRP:CG	1:C:226:PRO:HG3	2.52	0.45
1:D:191:LYS:HB3	1:D:249:MET:HG3	1.98	0.45
1:C:191:LYS:HB3	1:C:249:MET:CG	2.46	0.45
1:B:134:VAL:O	1:B:137:GLN:HB3	2.17	0.45
1:A:357:LEU:HD11	1:B:253:ARG:NH1	2.32	0.45
1:D:49:ALA:O	1:D:53:ALA:HB2	2.16	0.45
1:D:115:PHE:HB2	2:D:430:HOH:O	2.16	0.45
1:B:17:ILE:HB	1:B:41:HIS:O	2.16	0.45
1:B:140:VAL:HG13	1:B:157:LEU:O	2.17	0.45
1:B:228:ILE:O	1:B:232:LEU:HG	2.16	0.45
1:D:36:LEU:HD13	1:D:44:VAL:CG2	2.47	0.45
1:D:269:THR:HG21	1:D:312:PRO:CB	2.46	0.45
1:A:86:VAL:HG21	1:A:106:LEU:HD13	1.99	0.45
1:D:269:THR:HG21	1:D:312:PRO:CB	2.47	0.45
1:D:304:ASN:OD1	1:D:330:LYS:HA	2.17	0.45
1:B:57:MET:HA	1:B:72:LEU:HD11	1.98	0.45
1:C:82:THR:HG22	1:C:82:THR:O	2.16	0.45
1:D:31:GLU:OE2	1:D:328:LEU:HB3	2.17	0.45
1:D:244:PHE:CE2	1:D:246:PRO:HG3	2.51	0.45
1:B:252:ILE:HD11	1:D:211:ALA:HB3	1.98	0.45
1:D:102:LEU:HD13	1:D:108:ILE:HD13	1.98	0.45
1:B:217:TYR:O	1:B:218:GLY:C	2.54	0.45
1:B:164:TYR:CZ	1:B:246:PRO:HB3	2.52	0.45
1:A:96:GLN:HG3	1:A:114:ASP:OD2	2.17	0.45
1:D:90:LEU:HD13	1:D:98:ILE:HD12	1.98	0.45
1:A:48:THR:HA	1:A:73:VAL:O	2.17	0.45
1:A:273:HIS:CD2	1:A:291:GLU:HG3	2.52	0.45
1:A:273:HIS:CG	1:A:291:GLU:HG3	2.51	0.45
1:A:39:HIS:HE1	1:A:41:HIS:HB2	1.82	0.45
1:D:145:THR:HA	1:D:152:ILE:HD12	1.98	0.45
1:B:65:ARG:HD3	1:B:66:ALA:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:LYS:HE2	1:B:277:LYS:HB3	1.80	0.45
1:B:311:PHE:CD1	1:B:311:PHE:N	2.85	0.45
1:C:213:GLY:O	1:C:250:PRO:HD3	2.17	0.45
1:D:100:LYS:HA	1:D:136:LEU:HD22	1.98	0.45
1:D:280:TYR:HD1	1:D:283:GLU:HG3	1.81	0.45
1:A:48:THR:HG23	2:A:554:HOH:O	2.15	0.45
1:A:170:LEU:HD23	1:A:170:LEU:HA	1.86	0.45
1:B:118:ARG:HG2	2:B:536:HOH:O	2.16	0.45
1:B:239:LYS:HD3	1:B:240:VAL:N	2.32	0.45
1:C:152:ILE:HD13	1:C:339:ASN:OD1	2.17	0.45
1:D:304:ASN:OD1	1:D:329:VAL:HG12	2.17	0.45
1:A:303:SER:HB3	1:A:356:PRO:HA	1.99	0.45
1:B:39:HIS:NE2	1:B:341:ASN:ND2	2.64	0.45
1:D:106:LEU:O	1:D:156:ARG:HD3	2.17	0.45
1:B:145:THR:HG22	1:B:149:ARG:CG	2.46	0.45
1:A:111:LEU:N	1:A:111:LEU:HD12	2.32	0.45
1:C:41:HIS:C	1:C:42:PHE:HD1	2.21	0.45
1:B:239:LYS:HE3	2:B:475:HOH:O	2.17	0.45
1:C:19:ILE:CD1	1:C:85:ALA:HB3	2.47	0.45
1:C:74:SER:HB3	1:C:77:ASP:OD2	2.17	0.45
1:C:187:ILE:HB	1:C:260:TYR:HB2	1.98	0.45
1:D:32:ILE:HD11	1:D:111:LEU:HD21	1.99	0.45
1:A:80:PHE:HB3	1:A:106:LEU:HD11	1.99	0.45
1:A:335:GLN:NE2	2:A:385:HOH:O	2.40	0.45
1:B:89:CYS:O	1:B:90:LEU:O	2.35	0.45
1:B:90:LEU:HB2	1:B:95:THR:OG1	2.17	0.45
1:C:191:LYS:HZ3	1:C:256:GLN:CB	2.30	0.45
1:B:106:LEU:HD13	2:B:530:HOH:O	2.16	0.45
1:B:300:VAL:O	1:B:301:ARG:C	2.55	0.45
1:D:262:GLU:O	1:D:262:GLU:HG3	2.15	0.45
1:C:18:ARG:HD3	1:C:82:THR:O	2.17	0.45
1:A:296:ARG:HA	1:D:215:SER:HB3	2.00	0.45
1:A:329:VAL:HG12	1:A:334:GLY:HA3	1.98	0.45
1:B:97:GLU:HG3	1:B:132:LYS:HE3	1.98	0.45
1:C:149:ARG:NH2	1:C:283:GLU:OE2	2.50	0.45
1:C:269:THR:HG21	1:C:312:PRO:CA	2.47	0.45
1:D:150:GLU:HA	1:D:153:LYS:HD3	1.98	0.45
1:B:123:TYR:O	1:B:127:TYR:HB2	2.17	0.45
1:B:144:LEU:HD12	1:B:144:LEU:HA	1.79	0.45
1:C:22:LEU:HG	1:C:48:THR:OG1	2.17	0.45
1:B:124:GLU:HG2	1:B:129:GLN:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:ASN:O	1:B:343:MET:HG3	2.17	0.44
1:D:47:MET:HE2	1:D:70:PRO:HG2	2.00	0.44
1:D:65:ARG:HH11	1:D:65:ARG:HG3	1.81	0.44
1:C:150:GLU:O	1:C:154:LYS:HE2	2.17	0.44
1:D:255:MET:HB3	1:D:325:ILE:HD12	1.98	0.44
1:D:118:ARG:HG3	1:D:230:GLN:OE1	2.18	0.44
1:D:144:LEU:CD2	1:D:147:ILE:HG13	2.47	0.44
1:B:106:LEU:HD13	2:B:530:HOH:O	2.16	0.44
1:C:19:ILE:HB	1:C:44:VAL:HA	1.99	0.44
1:C:164:TYR:HB2	1:C:165:PRO:HD3	1.99	0.44
1:A:56:SER:C	1:A:58:GLU:N	2.70	0.44
1:B:124:GLU:OE2	1:B:130:PRO:HG3	2.16	0.44
1:B:143:GLY:O	1:B:145:THR:N	2.49	0.44
1:B:153:LYS:CD	2:B:549:HOH:O	2.65	0.44
1:B:164:TYR:HA	1:B:255:MET:SD	2.57	0.44
1:B:254:GLY:HA2	1:B:325:ILE:O	2.17	0.44
1:A:314:ARG:HG3	1:A:314:ARG:HH11	1.80	0.44
1:B:303:SER:O	1:B:329:VAL:HG21	2.16	0.44
1:C:46:LEU:O	1:C:47:MET:HG3	2.18	0.44
1:C:142:TYR:CZ	1:C:161:PRO:HB3	2.52	0.44
1:C:144:LEU:HD11	1:C:170:LEU:HD21	1.98	0.44
1:D:284:GLU:O	1:D:287:LYS:HE2	2.17	0.44
1:C:49:ALA:O	1:C:53:ALA:N	2.50	0.44
1:B:191:LYS:NZ	1:C:189:ASP:CG	2.70	0.44
1:D:48:THR:CB	1:D:75:VAL:HG22	2.48	0.44
1:A:57:MET:HE3	1:A:60:VAL:HB	2.00	0.44
1:A:167:THR:O	1:A:171:PRO:HG3	2.16	0.44
1:C:34:ARG:HG3	1:D:355:GLN:HB2	1.98	0.44
1:C:356:PRO:C	1:C:358:PHE:N	2.71	0.44
1:D:181:ILE:HA	1:D:263:MET:HA	1.99	0.44
1:D:358:PHE:CD2	1:D:359:PRO:HA	2.52	0.44
1:A:95:THR:CG2	1:A:99:ILE:HD12	2.47	0.44
1:A:163:CYS:HB2	1:A:255:MET:HE3	1.99	0.44
1:B:103:PRO:CG	1:B:106:LEU:HD22	2.41	0.44
1:D:147:ILE:HD11	1:D:280:TYR:OH	2.17	0.44
1:D:223:ARG:O	1:D:226:PRO:HD2	2.17	0.44
1:A:164:TYR:HB2	1:A:165:PRO:HD3	1.99	0.44
1:A:216:SER:O	1:D:294:VAL:HG11	2.17	0.44
1:B:285:PHE:CE1	1:B:304:ASN:HB3	2.52	0.44
1:B:285:PHE:C	1:B:306:CYS:HG	2.19	0.44
1:C:25:SER:HB3	1:C:52:LYS:HD2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:116:ARG:HD3	1:D:227:GLU:OE2	2.17	0.44
1:D:180:LEU:HD12	1:D:275:GLN:HG2	1.98	0.44
1:A:109:VAL:HG22	1:A:158:VAL:HB	1.99	0.44
1:B:190:ALA:HA	1:B:256:GLN:O	2.17	0.44
1:C:143:GLY:HA2	1:C:152:ILE:HD11	2.00	0.44
1:C:262:GLU:OE2	2:C:476:HOH:O	2.21	0.44
1:A:218:GLY:HA3	1:A:222:HIS:HD2	1.76	0.44
1:B:149:ARG:HA	1:B:152:ILE:HD12	2.00	0.44
1:D:64:LEU:HD21	2:D:453:HOH:O	2.17	0.44
1:C:55:GLN:HG2	1:C:59:SER:OG	2.17	0.44
1:A:83:VAL:HG23	1:A:106:LEU:HD21	2.00	0.44
1:A:207:TYR:CE2	1:C:211:ALA:HB2	2.53	0.44
1:B:103:PRO:CG	1:B:106:LEU:HD22	2.40	0.44
1:C:39:HIS:CE1	1:C:41:HIS:H	2.36	0.44
1:C:48:THR:HA	1:C:73:VAL:O	2.17	0.44
1:C:111:LEU:HD12	1:C:111:LEU:N	2.33	0.44
1:B:186:ILE:HG13	2:B:366:HOH:O	2.17	0.44
1:B:340:LEU:HA	1:B:343:MET:SD	2.58	0.44
1:C:61:PHE:CE1	1:C:199:ARG:NH1	2.85	0.44
1:C:169:GLN:HE21	1:C:169:GLN:HB2	1.48	0.44
1:A:190:ALA:C	1:A:191:LYS:HD2	2.38	0.44
1:D:33:VAL:HG11	1:D:69:LEU:HD11	1.99	0.44
1:A:190:ALA:C	1:A:191:LYS:HD2	2.37	0.44
1:B:51:ARG:HB2	2:B:415:HOH:O	2.17	0.44
1:B:92:HIS:HE1	1:B:127:TYR:O	2.00	0.44
1:B:340:LEU:O	1:B:341:ASN:C	2.55	0.44
1:D:281:GLU:HA	2:D:587:HOH:O	2.18	0.44
1:C:74:SER:HB3	1:C:77:ASP:OD2	2.17	0.44
1:C:103:PRO:C	1:C:105:ALA:N	2.70	0.44
1:D:174:PRO:HG2	1:D:280:TYR:HE2	1.83	0.44
1:A:96:GLN:HB2	1:A:132:LYS:HE3	2.00	0.44
1:A:65:ARG:NH1	1:B:287:LYS:HB3	2.32	0.44
1:C:171:PRO:HG3	1:C:308:MET:CE	2.47	0.44
1:D:140:VAL:HG13	1:D:157:LEU:O	2.18	0.44
1:A:48:THR:HG21	1:A:75:VAL:HG23	1.97	0.44
1:A:162:GLY:C	1:A:165:PRO:HD2	2.38	0.44
1:D:164:TYR:CE1	1:D:190:ALA:HB1	2.53	0.44
1:A:24:ALA:HB1	1:A:57:MET:HE3	1.97	0.44
1:A:249:MET:CE	1:D:214:ILE:HG12	2.47	0.44
1:B:49:ALA:O	1:B:50:ASP:C	2.55	0.44
1:A:298:HIS:CA	1:A:301:ARG:HD3	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:PRO:HD2	2:C:404:HOH:O	2.15	0.44
1:C:134:VAL:O	1:C:137:GLN:HB3	2.16	0.44
1:A:69:LEU:HB3	1:A:70:PRO:CD	2.47	0.44
1:D:141:VAL:CG2	1:D:155:ALA:HB2	2.48	0.44
1:C:37:ALA:HB2	1:C:67:GLN:OE1	2.17	0.44
1:D:259:ILE:HG22	1:D:261:VAL:HG13	2.00	0.44
1:D:314:ARG:HG3	1:D:314:ARG:NH1	2.33	0.44
1:A:311:PHE:HD1	1:A:320:ILE:O	2.00	0.44
1:B:118:ARG:CB	1:B:118:ARG:HH11	2.31	0.44
1:C:24:ALA:HB1	1:C:57:MET:HE1	1.99	0.44
1:A:104:THR:O	1:A:156:ARG:HD2	2.17	0.44
1:A:255:MET:HB2	1:A:327:ASN:HB3	1.99	0.44
1:A:299:ASN:O	1:B:63:HIS:HB2	2.18	0.44
1:B:253:ARG:HH11	1:B:326:ASP:CG	2.20	0.44
1:A:52:LYS:HD3	1:A:55:GLN:HE22	1.82	0.44
1:A:88:CYS:HB3	1:A:110:ASP:HA	1.98	0.44
1:C:117:LEU:HA	1:C:230:GLN:NE2	2.32	0.44
1:D:49:ALA:HB1	1:D:52:LYS:HB2	2.00	0.44
1:A:194:VAL:HA	1:A:248:LEU:HD11	1.98	0.44
1:B:107:LYS:HG3	1:B:344:LEU:HD21	1.99	0.44
1:B:141:VAL:HG21	1:B:155:ALA:HB2	1.99	0.44
1:C:180:LEU:HD22	1:C:267:VAL:CG1	2.47	0.44
1:B:280:TYR:HD1	1:B:283:GLU:HG3	1.81	0.44
1:D:92:HIS:CE1	1:D:127:TYR:HD1	2.34	0.44
1:C:57:MET:CE	1:C:72:LEU:HD21	2.47	0.44
2:C:377:HOH:O	1:D:64:LEU:HD23	2.18	0.44
1:D:49:ALA:HB3	1:D:72:LEU:HD13	1.99	0.44
1:D:52:LYS:HD2	1:D:60:VAL:HG22	1.99	0.44
1:B:135:GLU:OE1	1:B:138:LYS:HD2	2.18	0.44
1:C:49:ALA:HA	1:C:51:ARG:HH11	1.79	0.44
1:D:354:HIS:H	1:D:354:HIS:CD2	2.35	0.44
1:A:124:GLU:HG3	1:A:129:GLN:C	2.38	0.44
1:B:239:LYS:HD3	1:B:240:VAL:N	2.33	0.44
1:B:235:VAL:O	1:B:237:GLN:HG3	2.18	0.44
1:B:256:GLN:CB	1:B:324:VAL:HG12	2.33	0.44
1:D:232:LEU:HD12	1:D:242:VAL:HG11	1.99	0.44
1:A:168:ILE:O	1:A:171:PRO:HG2	2.18	0.44
1:B:268:ARG:HB3	1:B:270:GLU:OE2	2.17	0.44
1:C:75:VAL:O	1:C:78:ALA:HB3	2.18	0.44
1:D:263:MET:HE2	1:D:318:ARG:O	2.18	0.44
1:A:39:HIS:CE1	1:A:41:HIS:HB2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:HIS:CD2	1:A:291:GLU:HG3	2.52	0.44
1:A:265:PRO:HG3	2:A:514:HOH:O	2.17	0.44
1:B:124:GLU:HA	1:B:129:GLN:O	2.17	0.44
1:B:225:VAL:HG11	1:C:314:ARG:NE	2.33	0.44
1:C:83:VAL:HG12	1:C:84:ASP:H	1.83	0.44
1:D:90:LEU:HD13	1:D:98:ILE:HD12	2.00	0.44
1:D:150:GLU:O	1:D:153:LYS:HG2	2.18	0.44
1:B:295:PRO:HD3	1:B:309:SER:CB	2.48	0.44
1:A:136:LEU:HD11	1:A:156:ARG:NH2	2.32	0.44
1:B:80:PHE:O	1:B:103:PRO:HG3	2.17	0.44
1:B:170:LEU:N	1:B:171:PRO:CD	2.81	0.44
1:B:96:GLN:OE1	1:B:131:HIS:HA	2.18	0.44
1:D:190:ALA:C	1:D:191:LYS:HD2	2.38	0.44
1:A:191:LYS:HA	1:A:247:HIS:H	1.83	0.44
1:C:169:GLN:OE1	1:C:231:GLY:HA3	2.17	0.44
1:C:74:SER:HB3	1:C:77:ASP:OD2	2.18	0.44
1:C:98:ILE:O	1:C:102:LEU:HG	2.18	0.44
1:C:123:TYR:O	1:C:127:TYR:N	2.50	0.44
1:A:168:ILE:O	1:A:171:PRO:HG2	2.18	0.44
1:B:206:LEU:HA	1:D:205:ASN:O	2.18	0.44
1:B:300:VAL:HB	1:B:305:TYR:O	2.18	0.44
1:C:24:ALA:HB1	1:C:57:MET:HE1	2.00	0.44
1:C:315:ILE:O	1:C:318:ARG:HB2	2.18	0.44
1:D:225:VAL:N	1:D:226:PRO:HD2	2.33	0.44
1:D:175:LEU:HD22	1:D:272:LEU:HD22	1.99	0.44
1:D:195:SER:HB3	1:D:252:ILE:HG23	1.99	0.44
1:A:351:GLY:O	1:A:354:HIS:HE1	2.01	0.44
1:B:296:ARG:HB2	1:B:299:ASN:ND2	2.33	0.44
1:C:269:THR:HG22	1:C:319:ALA:HB2	2.00	0.44
1:D:169:GLN:OE1	1:D:231:GLY:HA3	2.18	0.44
1:C:135:GLU:HB2	2:C:549:HOH:O	2.17	0.44
1:D:164:TYR:OH	1:D:192:SER:HB3	2.17	0.44
1:A:47:MET:CE	1:A:70:PRO:HD2	2.47	0.44
1:B:109:VAL:HG21	1:B:340:LEU:HB2	2.00	0.44
1:C:103:PRO:C	1:C:105:ALA:N	2.71	0.44
1:B:354:HIS:H	1:B:354:HIS:HD2	1.62	0.44
1:C:264:ALA:HB3	1:C:267:VAL:CG2	2.47	0.44
1:D:22:LEU:HA	1:D:48:THR:OG1	2.18	0.44
1:D:308:MET:HA	1:D:322:ILE:O	2.18	0.44
1:A:89:CYS:SG	1:A:111:LEU:HD13	2.57	0.44
1:A:238:SER:O	1:A:240:VAL:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:LEU:HD22	1:B:272:LEU:HD22	2.00	0.44
1:D:136:LEU:HD12	1:D:139:GLU:CG	2.48	0.44
1:A:165:PRO:HD3	1:A:224:HIS:ND1	2.33	0.44
1:D:46:LEU:HD12	1:D:47:MET:N	2.33	0.44
1:A:187:ILE:HG12	1:A:243:SER:CB	2.47	0.44
1:C:142:TYR:HB3	1:C:148:LEU:HD22	2.00	0.44
1:A:253:ARG:HA	1:A:327:ASN:OD1	2.18	0.44
1:B:18:ARG:HD3	1:B:82:THR:O	2.18	0.44
1:B:47:MET:HE1	1:B:69:LEU:HD13	2.00	0.44
1:B:124:GLU:HG3	2:B:435:HOH:O	2.17	0.44
1:D:17:ILE:HB	1:D:42:PHE:CD1	2.52	0.44
1:B:83:VAL:HG23	1:B:106:LEU:CD2	2.47	0.44
1:B:270:GLU:OE1	1:B:271:ASP:N	2.51	0.44
1:B:147:ILE:CG2	1:B:173:VAL:HG11	2.48	0.44
1:B:149:ARG:NH1	1:B:348:GLU:OE1	2.48	0.44
1:C:306:CYS:HA	1:C:324:VAL:O	2.18	0.44
1:A:217:TYR:O	1:A:246:PRO:HD2	2.18	0.44
1:B:15:LYS:HA	2:B:512:HOH:O	2.17	0.44
1:B:287:LYS:HB2	1:B:307:HIS:HD2	1.83	0.44
1:C:123:TYR:O	1:C:127:TYR:HB2	2.18	0.44
1:D:118:ARG:NH1	2:D:548:HOH:O	2.51	0.44
1:A:96:GLN:HB3	1:A:132:LYS:HB2	1.99	0.43
1:A:194:VAL:HG11	1:C:207:TYR:HB3	1.99	0.43
1:A:316:PRO:HG2	2:A:408:HOH:O	2.16	0.43
1:B:92:HIS:HB2	2:B:536:HOH:O	2.18	0.43
1:C:111:LEU:HA	1:C:160:ASN:HB3	1.99	0.43
1:A:22:LEU:N	1:A:22:LEU:HD12	2.32	0.43
1:A:268:ARG:HB3	1:A:270:GLU:OE1	2.18	0.43
1:C:107:LYS:HE2	1:C:343:MET:O	2.18	0.43
1:C:136:LEU:O	1:C:139:GLU:HG2	2.17	0.43
1:C:223:ARG:HG3	2:C:396:HOH:O	2.17	0.43
1:C:311:PHE:CD1	1:C:311:PHE:N	2.86	0.43
1:A:263:MET:HG2	1:A:272:LEU:HD11	2.00	0.43
1:D:190:ALA:O	1:D:247:HIS:N	2.51	0.43
1:A:215:SER:HB3	1:D:296:ARG:HG2	2.00	0.43
1:C:270:GLU:CD	1:C:270:GLU:H	2.20	0.43
1:D:55:GLN:C	1:D:71:THR:HG23	2.39	0.43
1:D:146:GLU:HB3	1:D:280:TYR:HE1	1.83	0.43
1:A:64:LEU:HD23	1:A:67:GLN:HE22	1.83	0.43
1:C:169:GLN:OE1	1:C:231:GLY:HA3	2.17	0.43
1:D:295:PRO:HD3	1:D:309:SER:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:ALA:O	1:B:50:ASP:C	2.56	0.43
1:B:202:LYS:HD2	1:B:205:ASN:ND2	2.32	0.43
1:A:358:PHE:CD2	1:A:359:PRO:HA	2.53	0.43
1:B:244:PHE:CE2	1:B:246:PRO:HG3	2.53	0.43
1:C:21:LEU:O	1:C:47:MET:HA	2.17	0.43
1:D:168:ILE:HG12	1:D:259:ILE:HD11	1.99	0.43
1:A:34:ARG:HD2	2:B:392:HOH:O	2.18	0.43
1:B:314:ARG:HG3	2:B:393:HOH:O	2.18	0.43
1:C:16:ASP:HB3	1:C:346:TYR:OH	2.18	0.43
1:C:223:ARG:O	1:C:226:PRO:HD2	2.17	0.43
1:C:340:LEU:O	1:C:340:LEU:HG	2.18	0.43
1:B:228:ILE:O	1:B:232:LEU:HG	2.18	0.43
1:A:125:GLU:HG3	1:A:126:TRP:CD1	2.53	0.43
1:B:75:VAL:HG11	1:B:98:ILE:HD13	1.98	0.43
1:B:339:ASN:O	1:B:343:MET:HG3	2.17	0.43
1:C:355:GLN:HB3	2:C:375:HOH:O	2.17	0.43
1:D:191:LYS:O	1:D:255:MET:HA	2.17	0.43
1:A:51:ARG:HG3	2:A:555:HOH:O	2.18	0.43
1:A:55:GLN:O	1:A:71:THR:HG23	2.18	0.43
1:A:289:LEU:HD11	1:A:295:PRO:HB3	1.98	0.43
1:B:167:THR:HG21	1:B:255:MET:SD	2.58	0.43
1:D:136:LEU:C	1:D:138:LYS:H	2.20	0.43
1:A:36:LEU:HD12	1:A:44:VAL:HG23	2.00	0.43
1:B:191:LYS:HD2	1:B:191:LYS:N	2.33	0.43
1:B:287:LYS:O	1:B:289:LEU:HD23	2.19	0.43
1:B:124:GLU:OE2	1:B:130:PRO:HG3	2.18	0.43
1:C:21:LEU:HG	1:C:24:ALA:HB2	2.01	0.43
1:C:145:THR:O	1:C:149:ARG:HB2	2.17	0.43
1:A:29:GLY:O	1:A:33:VAL:HG23	2.18	0.43
1:B:118:ARG:HB2	1:B:118:ARG:NH1	2.32	0.43
1:B:303:SER:OG	1:B:356:PRO:HG3	2.18	0.43
1:A:118:ARG:HB2	1:A:118:ARG:CZ	2.48	0.43
1:C:311:PHE:CD1	1:C:311:PHE:N	2.87	0.43
1:D:169:GLN:OE1	1:D:231:GLY:HA3	2.18	0.43
1:A:127:TYR:CE1	1:A:223:ARG:HD3	2.53	0.43
1:A:310:VAL:HG22	1:A:321:ILE:CG2	2.46	0.43
1:C:125:GLU:O	1:C:127:TYR:N	2.51	0.43
1:A:244:PHE:CE2	1:A:246:PRO:HG3	2.53	0.43
1:C:333:SER:O	1:C:336:ALA:N	2.51	0.43
1:D:47:MET:HE2	1:D:70:PRO:HG2	2.00	0.43
1:D:173:VAL:HG13	1:D:235:VAL:CG1	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:GLN:HG3	1:B:114:ASP:HB3	2.01	0.43
1:B:304:ASN:HA	1:B:329:VAL:HG12	2.00	0.43
1:D:264:ALA:HB3	1:D:267:VAL:CG2	2.46	0.43
1:B:256:GLN:HE22	1:B:322:ILE:HG23	1.76	0.43
1:C:244:PHE:CE2	1:C:246:PRO:HG3	2.53	0.43
1:D:217:TYR:CZ	1:D:246:PRO:HB2	2.54	0.43
1:C:273:HIS:CD2	1:C:291:GLU:HG3	2.53	0.43
1:D:36:LEU:HD13	1:D:44:VAL:HG22	2.00	0.43
1:D:87:PHE:HZ	1:D:337:LEU:HA	1.83	0.43
1:D:269:THR:HG21	1:D:312:PRO:HA	2.01	0.43
1:A:15:LYS:HD2	1:A:43:GLN:HB2	2.00	0.43
1:A:96:GLN:CB	1:A:132:LYS:HE3	2.48	0.43
1:A:113:ALA:HB2	1:A:116:ARG:NH1	2.34	0.43
1:B:205:ASN:HB2	1:D:206:LEU:CD2	2.48	0.43
1:A:358:PHE:CD2	1:A:359:PRO:HA	2.53	0.43
1:B:165:PRO:HD3	1:B:224:HIS:ND1	2.34	0.43
1:B:181:ILE:HA	1:B:263:MET:HA	2.01	0.43
1:C:49:ALA:CB	1:C:72:LEU:HD13	2.48	0.43
1:C:192:SER:HA	1:C:254:GLY:O	2.18	0.43
1:C:18:ARG:HD3	1:C:82:THR:O	2.19	0.43
1:C:175:LEU:HD11	1:C:321:ILE:HD11	2.01	0.43
1:D:239:LYS:NZ	1:D:240:VAL:O	2.50	0.43
1:B:136:LEU:HD12	1:B:139:GLU:OE1	2.19	0.43
1:B:149:ARG:O	1:B:153:LYS:HG3	2.18	0.43
1:C:328:LEU:O	1:C:332:ALA:HB3	2.18	0.43
1:D:291:GLU:OE2	2:D:598:HOH:O	2.21	0.43
1:D:296:ARG:HG2	1:D:298:HIS:ND1	2.34	0.43
1:A:46:LEU:HD12	2:A:432:HOH:O	2.19	0.43
1:B:119:ASN:OD1	1:B:121:ALA:N	2.51	0.43
1:B:273:HIS:CD2	1:B:291:GLU:HG3	2.53	0.43
1:C:20:GLY:C	1:C:86:VAL:HG23	2.38	0.43
1:C:124:GLU:HG2	1:C:130:PRO:HA	2.00	0.43
1:C:340:LEU:HA	1:C:340:LEU:HD12	1.84	0.43
1:C:359:PRO:OXT	1:D:252:ILE:HG21	2.19	0.43
1:A:65:ARG:HD2	1:B:287:LYS:HG3	2.00	0.43
1:A:67:GLN:C	1:A:68:LYS:HD2	2.38	0.43
1:D:118:ARG:NH1	1:D:230:GLN:HG3	2.33	0.43
1:D:164:TYR:CE1	1:D:190:ALA:HB1	2.52	0.43
1:B:90:LEU:HD13	1:B:98:ILE:HD12	2.00	0.43
1:C:300:VAL:HB	1:C:305:TYR:O	2.18	0.43
1:D:202:LYS:CB	1:D:205:ASN:HD22	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:LEU:N	1:A:22:LEU:HD12	2.33	0.43
1:C:20:GLY:N	1:C:83:VAL:HG11	2.33	0.43
1:A:97:GLU:OE1	2:A:444:HOH:O	2.21	0.43
1:B:308:MET:HB3	1:B:308:MET:HE2	1.90	0.43
1:C:47:MET:HE2	1:C:70:PRO:HD2	1.99	0.43
1:C:145:THR:O	1:C:149:ARG:HB2	2.18	0.43
1:D:22:LEU:HA	1:D:48:THR:OG1	2.18	0.43
1:D:146:GLU:HG2	1:D:286:VAL:HG21	2.01	0.43
1:B:124:GLU:CD	2:B:435:HOH:O	2.56	0.43
1:B:124:GLU:OE2	1:B:130:PRO:HG3	2.19	0.43
1:B:224:HIS:HB2	1:B:244:PHE:CE2	2.54	0.43
1:C:173:VAL:HG13	1:C:235:VAL:HG21	2.00	0.43
1:A:213:GLY:C	1:D:298:HIS:CE1	2.92	0.43
1:A:259:ILE:HG22	1:A:261:VAL:HG13	2.01	0.43
1:A:273:HIS:CG	1:A:291:GLU:HG3	2.54	0.43
1:B:190:ALA:C	1:B:191:LYS:HD2	2.39	0.43
1:C:344:LEU:N	1:C:344:LEU:HD12	2.34	0.43
1:B:172:LEU:HD21	1:B:259:ILE:HG21	2.01	0.43
1:C:142:TYR:OH	1:C:227:GLU:HG2	2.19	0.43
1:D:231:GLY:O	1:D:235:VAL:HG23	2.18	0.43
1:D:306:CYS:O	1:D:307:HIS:HD2	2.01	0.43
1:B:69:LEU:HB3	1:B:70:PRO:HD2	2.00	0.43
1:B:145:THR:O	1:B:147:ILE:N	2.52	0.43
1:C:202:LYS:HE3	1:C:205:ASN:ND2	2.32	0.43
1:C:182:LYS:C	1:C:184:GLU:H	2.22	0.43
1:C:194:VAL:O	1:C:194:VAL:HG22	2.19	0.43
1:B:27:TYR:N	2:B:416:HOH:O	2.47	0.43
1:A:29:GLY:O	1:A:33:VAL:HG23	2.18	0.43
1:A:140:VAL:HG22	1:A:157:LEU:HD23	2.01	0.43
1:C:37:ALA:CB	1:D:355:GLN:HG3	2.45	0.43
1:B:195:SER:HB2	1:B:328:LEU:HD11	2.00	0.43
1:D:46:LEU:HD23	1:D:47:MET:N	2.33	0.43
1:B:99:ILE:HD12	1:B:115:PHE:CE2	2.52	0.43
1:C:97:GLU:HG3	2:C:536:HOH:O	2.18	0.43
1:A:52:LYS:HG2	1:A:55:GLN:NE2	2.33	0.43
1:B:92:HIS:CG	1:B:93:GLY:N	2.87	0.43
1:C:285:PHE:HA	1:C:305:TYR:HD1	1.84	0.43
1:B:22:LEU:HD11	1:B:80:PHE:CZ	2.54	0.43
1:B:124:GLU:HG3	2:B:433:HOH:O	2.19	0.43
1:D:54:GLY:N	1:D:72:LEU:O	2.36	0.43
1:D:190:ALA:C	1:D:191:LYS:HD2	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:148:LEU:O	1:C:152:ILE:HG13	2.18	0.43
1:A:308:MET:HA	1:A:323:SER:HA	2.00	0.43
1:B:15:LYS:HD3	1:B:40:PRO:O	2.18	0.43
1:B:95:THR:CG2	1:B:99:ILE:HD12	2.48	0.43
1:C:191:LYS:HZ1	1:C:258:THR:N	2.17	0.43
1:B:118:ARG:NH1	1:B:118:ARG:CB	2.81	0.43
1:B:308:MET:HA	1:B:322:ILE:O	2.18	0.43
1:A:150:GLU:HG2	2:A:467:HOH:O	2.19	0.43
1:A:295:PRO:HD3	1:A:309:SER:CB	2.46	0.43
1:C:115:PHE:CG	1:C:140:VAL:HG21	2.53	0.43
1:C:209:GLU:OE1	2:C:375:HOH:O	2.21	0.43
1:A:33:VAL:HG22	1:A:44:VAL:HG21	2.00	0.43
1:A:56:SER:C	1:A:58:GLU:H	2.20	0.43
1:C:90:LEU:HA	1:C:91:PRO:HD3	1.90	0.43
1:C:124:GLU:CD	1:C:130:PRO:HA	2.39	0.43
1:C:183:HIS:HB2	1:C:240:VAL:HG22	2.01	0.43
1:A:22:LEU:HD13	1:A:86:VAL:HG13	2.01	0.43
1:A:273:HIS:CG	1:A:291:GLU:HG3	2.54	0.43
1:B:204:ALA:O	1:B:210:ILE:HD11	2.18	0.43
1:A:214:ILE:HG22	1:A:250:PRO:HD3	2.00	0.43
1:A:298:HIS:NE2	1:D:210:ILE:O	2.47	0.43
1:C:341:ASN:OD1	1:C:347:PRO:O	2.37	0.43
1:D:167:THR:HG22	1:D:325:ILE:CG1	2.44	0.43
1:D:273:HIS:HE1	1:D:277:LYS:HD3	1.83	0.43
1:A:15:LYS:HB3	1:A:41:HIS:O	2.19	0.43
1:A:187:ILE:HD12	1:D:187:ILE:HD12	2.01	0.43
1:A:325:ILE:O	1:A:325:ILE:CG1	2.65	0.43
1:B:172:LEU:HD21	1:B:259:ILE:HG21	2.00	0.43
1:C:129:GLN:NE2	2:C:452:HOH:O	2.52	0.43
1:C:280:TYR:HD1	1:C:283:GLU:HG3	1.83	0.43
1:C:127:TYR:O	1:C:129:GLN:HG2	2.18	0.43
1:C:236:ALA:HB3	1:C:238:SER:O	2.18	0.43
1:A:65:ARG:NH1	1:B:287:LYS:HB3	2.33	0.43
1:B:73:VAL:CG1	1:B:74:SER:H	2.25	0.43
1:B:273:HIS:CD2	1:B:291:GLU:HG3	2.54	0.43
1:C:117:LEU:HD23	1:C:122:GLU:HB3	2.00	0.43
1:C:216:SER:HA	1:C:246:PRO:O	2.19	0.43
1:D:171:PRO:HD3	1:D:308:MET:HE1	2.01	0.43
1:D:296:ARG:HG2	1:D:298:HIS:ND1	2.34	0.43
1:A:110:ASP:OD2	1:A:112:SER:HB3	2.17	0.43
1:A:125:GLU:HG3	1:A:126:TRP:CD1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:HIS:HE1	2:A:607:HOH:O	2.01	0.43
1:A:86:VAL:HB	1:A:108:ILE:HG12	1.99	0.43
1:C:191:LYS:HB3	1:C:249:MET:CE	2.49	0.43
1:C:223:ARG:NH2	2:C:552:HOH:O	2.52	0.43
1:D:38:ASN:ND2	2:D:411:HOH:O	2.49	0.43
1:B:19:ILE:CG1	1:B:42:PHE:HB3	2.49	0.43
1:B:145:THR:HA	1:B:152:ILE:CD1	2.49	0.43
1:D:118:ARG:NH1	2:D:555:HOH:O	2.52	0.43
1:A:125:GLU:HG3	1:A:126:TRP:CD1	2.54	0.43
1:B:128:GLY:O	1:B:129:GLN:HB3	2.18	0.43
1:B:301:ARG:NH1	1:C:212:GLU:HB2	2.34	0.43
1:D:264:ALA:HB3	1:D:267:VAL:HG21	2.01	0.43
1:C:144:LEU:CD2	1:C:169:GLN:HB3	2.46	0.43
1:C:269:THR:HG21	1:C:312:PRO:CA	2.41	0.43
1:A:42:PHE:CZ	1:A:344:LEU:HD12	2.53	0.43
1:A:214:ILE:HG23	1:D:251:MET:SD	2.59	0.43
1:C:51:ARG:NH2	1:C:90:LEU:HD22	2.31	0.43
1:A:178:ALA:HB3	1:A:180:LEU:HG	2.01	0.43
1:A:186:ILE:HG23	1:A:261:VAL:HG12	2.01	0.43
1:B:212:GLU:HA	1:C:251:MET:HB2	2.00	0.43
1:C:15:LYS:N	1:C:43:GLN:HB2	2.34	0.43
1:D:46:LEU:HD12	2:D:431:HOH:O	2.18	0.43
1:A:358:PHE:HB3	1:B:63:HIS:CG	2.54	0.43
1:C:83:VAL:HG12	1:C:85:ALA:H	1.84	0.43
1:D:52:LYS:HD2	1:D:60:VAL:HG22	2.01	0.43
1:D:225:VAL:N	1:D:226:PRO:HD2	2.34	0.43
1:A:214:ILE:HD11	1:D:256:GLN:HB3	2.01	0.43
1:B:98:ILE:O	1:B:102:LEU:HG	2.18	0.43
1:A:95:THR:CG2	1:A:99:ILE:HD12	2.49	0.43
1:A:135:GLU:HB2	2:A:577:HOH:O	2.18	0.43
1:D:28:THR:O	1:D:32:ILE:HG12	2.19	0.43
1:A:188:ILE:HD13	1:A:259:ILE:HG12	2.01	0.43
1:B:58:GLU:HG2	1:B:65:ARG:HA	2.00	0.43
1:C:170:LEU:HB2	1:C:171:PRO:HD3	2.01	0.43
1:A:164:TYR:HA	1:A:255:MET:SD	2.59	0.43
1:A:180:LEU:HB3	1:A:272:LEU:HD23	2.01	0.43
1:B:69:LEU:HB3	1:B:70:PRO:HD2	2.01	0.43
1:B:136:LEU:O	1:B:139:GLU:HG2	2.19	0.43
1:D:144:LEU:HD12	1:D:335:GLN:OE1	2.19	0.43
1:B:177:LYS:HE2	1:B:177:LYS:HB3	1.82	0.43
1:C:18:ARG:HB3	1:C:45:THR:OG1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:VAL:CG1	1:B:77:ASP:HB2	2.49	0.43
1:C:116:ARG:NH2	1:C:160:ASN:O	2.47	0.43
1:C:120:ILE:O	1:C:124:GLU:HG3	2.19	0.43
1:C:122:GLU:O	1:C:126:TRP:HB2	2.19	0.43
1:D:177:LYS:C	1:D:179:ASN:H	2.22	0.43
1:C:111:LEU:HD21	1:C:336:ALA:HB2	2.01	0.43
1:C:337:LEU:HD12	1:C:337:LEU:O	2.18	0.43
1:C:306:CYS:HA	1:C:324:VAL:O	2.19	0.42
1:C:331:GLY:O	1:C:332:ALA:HB2	2.19	0.42
1:D:150:GLU:O	1:D:153:LYS:HG2	2.20	0.42
1:D:168:ILE:HD13	1:D:188:ILE:HD13	2.01	0.42
1:A:57:MET:SD	1:A:57:MET:C	2.98	0.42
1:B:22:LEU:HD13	1:B:86:VAL:HG11	2.00	0.42
1:B:144:LEU:CD2	1:B:147:ILE:HG13	2.49	0.42
1:B:320:ILE:C	1:B:321:ILE:HD12	2.39	0.42
1:B:330:LYS:HB3	2:B:361:HOH:O	2.18	0.42
1:B:95:THR:HG21	1:B:112:SER:HG	1.84	0.42
1:C:184:GLU:O	1:C:185:ASN:HB2	2.19	0.42
1:C:48:THR:CG2	1:C:49:ALA:N	2.82	0.42
1:D:239:LYS:NZ	1:D:240:VAL:O	2.51	0.42
1:D:295:PRO:HD3	1:D:309:SER:CB	2.49	0.42
1:D:269:THR:HG21	1:D:312:PRO:CA	2.49	0.42
1:A:125:GLU:HG3	1:A:126:TRP:CD1	2.54	0.42
1:B:267:VAL:HG13	1:B:271:ASP:HB2	2.00	0.42
1:D:164:TYR:CE1	1:D:190:ALA:HB1	2.54	0.42
1:B:178:ALA:CB	1:B:275:GLN:HE21	2.32	0.42
1:C:103:PRO:O	1:C:105:ALA:N	2.51	0.42
1:B:239:LYS:HE3	2:B:474:HOH:O	2.20	0.42
1:B:251:MET:HE3	1:B:254:GLY:HA3	1.99	0.42
1:C:244:PHE:CZ	1:C:246:PRO:HG3	2.53	0.42
1:D:17:ILE:HB	1:D:42:PHE:CD1	2.54	0.42
1:D:204:ALA:O	1:D:210:ILE:HD11	2.18	0.42
1:B:269:THR:HG21	1:B:312:PRO:HB3	2.00	0.42
1:C:269:THR:HA	1:C:272:LEU:CG	2.47	0.42
1:B:220:THR:O	1:B:220:THR:HG22	2.18	0.42
1:C:22:LEU:HD11	1:C:80:PHE:HE2	1.81	0.42
1:C:120:ILE:HG22	1:C:121:ALA:N	2.33	0.42
1:B:50:ASP:HB2	2:B:416:HOH:O	2.19	0.42
1:C:52:LYS:HD3	1:C:60:VAL:HG22	2.00	0.42
1:C:96:GLN:O	1:C:100:LYS:HB2	2.19	0.42
1:D:46:LEU:HD23	1:D:46:LEU:C	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:300:VAL:HG21	1:D:325:ILE:HA	2.01	0.42
1:D:313:ASP:O	1:D:314:ARG:C	2.56	0.42
1:A:217:TYR:CE1	1:A:248:LEU:HB2	2.54	0.42
1:B:91:PRO:HD3	2:B:417:HOH:O	2.19	0.42
1:B:223:ARG:O	1:B:224:HIS:HD2	2.02	0.42
1:C:104:THR:O	1:C:156:ARG:HD2	2.19	0.42
1:C:36:LEU:HD12	1:C:44:VAL:CG2	2.48	0.42
1:D:46:LEU:HD21	1:D:78:ALA:HB1	2.00	0.42
1:A:20:GLY:O	1:A:86:VAL:HA	2.19	0.42
1:A:46:LEU:HD12	2:A:431:HOH:O	2.20	0.42
1:A:140:VAL:HG22	1:A:157:LEU:HD23	2.00	0.42
1:A:144:LEU:HD11	1:A:170:LEU:HG	2.00	0.42
1:B:190:ALA:C	1:B:191:LYS:HD2	2.40	0.42
1:C:124:GLU:CG	1:C:130:PRO:HA	2.41	0.42
1:C:354:HIS:CD2	1:C:354:HIS:H	2.36	0.42
1:D:48:THR:CB	1:D:75:VAL:HG22	2.50	0.42
1:D:124:GLU:O	1:D:128:GLY:N	2.53	0.42
1:B:58:GLU:OE1	1:B:65:ARG:HB2	2.19	0.42
1:B:204:ALA:O	1:B:210:ILE:HD11	2.20	0.42
1:D:115:PHE:HD1	1:D:137:GLN:OE1	2.01	0.42
1:A:167:THR:HG21	1:A:255:MET:HG2	2.02	0.42
1:B:33:VAL:HG12	1:B:67:GLN:HE22	1.83	0.42
1:B:173:VAL:HG22	1:B:235:VAL:HG21	2.01	0.42
1:D:195:SER:HB3	1:D:252:ILE:CG2	2.49	0.42
1:A:68:LYS:N	1:A:68:LYS:CD	2.81	0.42
1:B:186:ILE:C	1:B:187:ILE:HD12	2.39	0.42
1:B:244:PHE:CE2	1:B:246:PRO:HG3	2.53	0.42
1:A:351:GLY:O	1:A:354:HIS:HE1	2.02	0.42
1:A:191:LYS:N	1:A:191:LYS:CD	2.80	0.42
1:C:97:GLU:HG3	2:C:411:HOH:O	2.18	0.42
1:D:277:LYS:O	1:D:281:GLU:HG2	2.19	0.42
1:A:61:PHE:HB3	1:A:63:HIS:CE1	2.54	0.42
1:B:124:GLU:CG	1:B:130:PRO:HA	2.50	0.42
1:D:49:ALA:CB	1:D:52:LYS:HB2	2.50	0.42
1:D:114:ASP:OD2	2:D:546:HOH:O	2.21	0.42
1:A:52:LYS:HG2	1:A:55:GLN:NE2	2.33	0.42
1:B:153:LYS:HD2	2:B:554:HOH:O	2.20	0.42
1:B:217:TYR:O	1:B:246:PRO:HD2	2.19	0.42
1:D:190:ALA:C	1:D:191:LYS:HD2	2.40	0.42
1:A:36:LEU:HD12	1:A:44:VAL:CG2	2.49	0.42
1:A:125:GLU:HG3	1:A:126:TRP:CD1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:ALA:O	1:B:50:ASP:C	2.56	0.42
1:B:106:LEU:HD13	2:B:524:HOH:O	2.20	0.42
1:C:232:LEU:HD13	1:C:240:VAL:CG1	2.50	0.42
1:D:191:LYS:N	1:D:191:LYS:HD2	2.33	0.42
1:B:186:ILE:CG1	2:B:366:HOH:O	2.67	0.42
1:B:253:ARG:CZ	1:B:328:LEU:HD12	2.49	0.42
1:B:214:ILE:HG22	1:B:250:PRO:HD3	2.00	0.42
1:D:74:SER:OG	1:D:76:LYS:HB2	2.19	0.42
1:A:119:ASN:HB3	1:A:122:GLU:HB2	2.02	0.42
1:C:294:VAL:HG22	1:C:311:PHE:HE2	1.84	0.42
1:B:283:GLU:OE1	1:B:283:GLU:HA	2.20	0.42
1:C:107:LYS:HD3	1:C:343:MET:O	2.20	0.42
1:A:95:THR:HG21	1:A:110:ASP:CG	2.40	0.42
1:B:96:GLN:HG3	1:B:114:ASP:HB3	2.00	0.42
1:D:341:ASN:ND2	1:D:350:THR:HB	2.34	0.42
1:A:87:PHE:HA	1:A:109:VAL:O	2.18	0.42
1:C:142:TYR:HB3	1:C:148:LEU:CD1	2.49	0.42
1:C:149:ARG:NH1	1:C:348:GLU:OE1	2.51	0.42
1:D:144:LEU:CD2	1:D:147:ILE:HG13	2.49	0.42
1:A:351:GLY:O	1:A:354:HIS:HE1	2.03	0.42
1:C:301:ARG:HG3	2:C:505:HOH:O	2.19	0.42
1:B:51:ARG:C	1:B:53:ALA:H	2.23	0.42
1:B:301:ARG:NH1	1:C:212:GLU:O	2.51	0.42
1:D:144:LEU:HD23	1:D:147:ILE:HG13	2.01	0.42
1:D:146:GLU:HB3	1:D:280:TYR:HE1	1.82	0.42
1:D:216:SER:HA	1:D:247:HIS:HA	2.02	0.42
1:C:147:ILE:HB	1:C:148:LEU:HD12	2.02	0.42
1:B:17:ILE:HB	1:B:42:PHE:CD1	2.55	0.42
1:B:36:LEU:CD2	1:B:42:PHE:HB2	2.49	0.42
1:D:118:ARG:HG2	2:D:548:HOH:O	2.19	0.42
1:A:125:GLU:HG3	1:A:126:TRP:CD1	2.54	0.42
1:C:45:THR:O	1:C:70:PRO:HG2	2.20	0.42
1:C:256:GLN:HB2	1:C:297:THR:CG2	2.50	0.42
1:D:259:ILE:HG22	1:D:261:VAL:HG13	2.01	0.42
1:B:148:LEU:O	1:B:152:ILE:HG13	2.20	0.42
1:D:144:LEU:HD12	1:D:335:GLN:NE2	2.33	0.42
1:B:119:ASN:OD1	1:B:121:ALA:HB3	2.20	0.42
1:B:145:THR:HA	1:B:152:ILE:CD1	2.49	0.42
1:B:171:PRO:HG3	1:B:308:MET:CE	2.49	0.42
1:C:192:SER:HB2	1:C:255:MET:HE2	2.01	0.42
1:A:95:THR:HG22	1:A:99:ILE:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:LYS:HG3	1:A:235:VAL:CG2	2.49	0.42
1:D:52:LYS:HD3	1:D:60:VAL:HG22	2.01	0.42
1:B:46:LEU:HA	2:B:519:HOH:O	2.19	0.42
1:C:347:PRO:O	1:C:350:THR:OG1	2.36	0.42
1:D:326:ASP:O	1:D:328:LEU:N	2.53	0.42
1:B:295:PRO:HD3	1:B:309:SER:HB2	2.00	0.42
1:A:291:GLU:HG3	2:A:516:HOH:O	2.19	0.42
1:D:131:HIS:HB3	1:D:134:VAL:HG22	2.00	0.42
1:B:142:TYR:O	1:B:148:LEU:HD12	2.19	0.42
1:C:111:LEU:HD12	1:C:111:LEU:N	2.35	0.42
1:C:169:GLN:OE1	1:C:231:GLY:HA3	2.18	0.42
1:D:107:LYS:HG3	1:D:344:LEU:HD21	1.99	0.42
1:A:356:PRO:HB2	1:B:63:HIS:HD2	1.85	0.42
1:D:143:GLY:HA2	1:D:152:ILE:CD1	2.50	0.42
1:D:247:HIS:HB3	1:D:249:MET:HE3	2.02	0.42
1:B:36:LEU:HA	1:B:39:HIS:HB2	2.02	0.42
1:C:170:LEU:HB2	1:C:171:PRO:HD3	2.01	0.42
1:C:185:ASN:HB3	1:C:318:ARG:HH22	1.84	0.42
1:D:256:GLN:HB2	1:D:324:VAL:HG12	2.01	0.42
1:C:18:ARG:HD3	1:C:82:THR:O	2.18	0.42
1:C:36:LEU:HD22	1:C:42:PHE:HB2	2.01	0.42
1:C:54:GLY:C	2:C:526:HOH:O	2.57	0.42
1:D:57:MET:HE2	1:D:57:MET:HA	2.02	0.42
1:B:69:LEU:HB3	1:B:70:PRO:HD2	2.01	0.42
1:B:269:THR:HG21	1:B:312:PRO:CA	2.50	0.42
1:C:56:SER:O	1:C:60:VAL:HG23	2.20	0.42
1:C:249:MET:HB3	1:C:250:PRO:HD2	2.00	0.42
1:D:37:ALA:HB2	1:D:67:GLN:NE2	2.35	0.42
1:D:254:GLY:HA2	1:D:325:ILE:O	2.19	0.42
1:A:177:LYS:NZ	2:A:592:HOH:O	2.52	0.42
1:C:48:THR:HA	1:C:73:VAL:O	2.19	0.42
1:D:38:ASN:ND2	2:D:414:HOH:O	2.49	0.42
1:D:269:THR:HG21	1:D:312:PRO:CB	2.48	0.42
1:A:75:VAL:HG23	2:A:394:HOH:O	2.19	0.42
1:A:256:GLN:NE2	1:D:247:HIS:HD2	2.18	0.42
1:C:39:HIS:CE1	1:C:42:PHE:H	2.38	0.42
1:B:22:LEU:HB2	1:B:88:CYS:HA	2.01	0.42
1:D:244:PHE:CE2	1:D:246:PRO:HG3	2.54	0.42
1:C:48:THR:HG21	1:C:75:VAL:CG2	2.40	0.42
1:C:280:TYR:HD1	1:C:283:GLU:HG3	1.85	0.42
1:D:180:LEU:HB3	1:D:272:LEU:CD2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:HIS:CE1	1:C:213:GLY:HA3	2.54	0.42
1:C:36:LEU:HD12	1:C:44:VAL:CG2	2.50	0.42
1:D:28:THR:O	1:D:32:ILE:HG12	2.20	0.42
1:D:119:ASN:OD1	1:D:121:ALA:HB3	2.19	0.42
1:A:22:LEU:N	1:A:22:LEU:HD12	2.35	0.42
1:A:149:ARG:O	1:A:153:LYS:HG3	2.20	0.42
1:B:124:GLU:CD	2:B:433:HOH:O	2.58	0.42
1:C:358:PHE:HA	1:C:359:PRO:C	2.39	0.42
1:D:253:ARG:NH1	1:D:328:LEU:HD12	2.34	0.42
1:A:27:TYR:OH	1:C:208:SER:HB2	2.19	0.42
1:D:144:LEU:HD23	1:D:147:ILE:HG13	2.02	0.42
1:D:223:ARG:O	1:D:226:PRO:HD2	2.19	0.42
1:A:63:HIS:CG	1:A:64:LEU:N	2.87	0.42
1:A:262:GLU:HG2	2:A:394:HOH:O	2.19	0.42
1:B:140:VAL:HG22	1:B:157:LEU:HD23	2.02	0.42
1:D:190:ALA:C	1:D:191:LYS:HD2	2.40	0.42
1:D:311:PHE:CD1	1:D:311:PHE:N	2.87	0.42
1:B:339:ASN:O	1:B:342:ILE:HG12	2.19	0.42
1:B:35:LEU:HD13	1:B:334:GLY:HA2	2.02	0.42
1:B:95:THR:CG2	1:B:99:ILE:HD12	2.50	0.42
1:B:118:ARG:HB2	1:B:118:ARG:NH1	2.35	0.42
1:B:256:GLN:CB	1:B:324:VAL:HG12	2.50	0.42
1:C:18:ARG:HE	1:C:45:THR:HG21	1.85	0.42
1:C:74:SER:HB3	1:C:77:ASP:OD2	2.20	0.42
1:B:49:ALA:CB	1:B:72:LEU:HD13	2.41	0.42
1:B:168:ILE:C	1:B:171:PRO:HD2	2.39	0.42
1:A:228:ILE:O	1:A:232:LEU:HG	2.19	0.42
1:C:182:LYS:HE3	1:C:263:MET:O	2.19	0.42
1:D:303:SER:C	1:D:329:VAL:HG11	2.40	0.42
1:A:36:LEU:HD12	1:A:44:VAL:HG23	2.01	0.42
1:C:34:ARG:NH1	2:C:378:HOH:O	2.26	0.42
1:D:23:GLY:O	1:D:89:CYS:HB2	2.19	0.42
1:D:146:GLU:HG2	1:D:286:VAL:HG21	2.02	0.42
1:C:49:ALA:CB	1:C:72:LEU:HD13	2.49	0.42
1:A:27:TYR:O	1:A:30:ALA:HB3	2.19	0.42
1:A:295:PRO:HG2	1:A:322:ILE:CG2	2.49	0.42
1:D:244:PHE:CE2	1:D:246:PRO:HG3	2.55	0.42
1:D:255:MET:HB3	1:D:325:ILE:CD1	2.50	0.42
1:A:48:THR:HA	1:A:73:VAL:O	2.20	0.42
1:A:64:LEU:CD2	1:B:355:GLN:HB3	2.50	0.42
1:A:142:TYR:OH	1:A:161:PRO:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:ARG:HG3	1:A:314:ARG:HH11	1.84	0.42
1:B:22:LEU:HD13	1:B:86:VAL:HG13	2.02	0.42
1:D:187:ILE:HG12	1:D:243:SER:HB3	2.01	0.42
1:A:145:THR:HG21	1:A:338:GLN:CG	2.50	0.42
1:B:95:THR:HG21	1:B:112:SER:OG	2.20	0.42
1:B:99:ILE:HG21	1:B:157:LEU:HD22	2.01	0.42
1:B:104:THR:HA	1:B:156:ARG:NH1	2.35	0.42
1:C:102:LEU:HD12	1:C:108:ILE:HD13	2.02	0.42
1:C:149:ARG:HG3	1:C:342:ILE:HD12	2.01	0.42
1:D:46:LEU:HD12	1:D:47:MET:N	2.35	0.42
1:A:331:GLY:O	1:A:332:ALA:HB2	2.20	0.42
1:C:311:PHE:HB2	1:C:320:ILE:HB	2.02	0.42
1:D:306:CYS:HB2	1:D:325:ILE:HG22	2.01	0.42
1:A:217:TYR:CD1	1:A:248:LEU:HB2	2.55	0.42
1:C:311:PHE:CZ	1:C:322:ILE:HD12	2.54	0.42
1:D:341:ASN:ND2	1:D:350:THR:HB	2.35	0.42
1:A:170:LEU:N	1:A:171:PRO:HD2	2.35	0.42
1:C:277:LYS:O	1:C:281:GLU:HB3	2.19	0.42
1:D:214:ILE:CG2	1:D:250:PRO:HD3	2.49	0.42
1:A:48:THR:HA	1:A:73:VAL:O	2.20	0.42
1:A:162:GLY:O	1:A:165:PRO:HD2	2.20	0.42
1:B:153:LYS:HD2	2:B:553:HOH:O	2.20	0.42
1:B:277:LYS:O	1:B:281:GLU:HB3	2.20	0.42
1:B:326:ASP:HB3	1:B:329:VAL:HG23	2.02	0.42
1:D:88:CYS:SG	1:D:90:LEU:HD12	2.59	0.42
1:A:195:SER:HB2	1:A:252:ILE:O	2.20	0.42
1:B:18:ARG:HH12	1:B:82:THR:HB	1.82	0.42
1:B:194:VAL:CA	1:B:248:LEU:HD11	2.48	0.42
1:D:253:ARG:HG2	1:D:328:LEU:HD12	2.02	0.42
1:A:316:PRO:HG2	2:A:408:HOH:O	2.19	0.42
1:B:164:TYR:CE1	1:B:190:ALA:HB1	2.55	0.42
1:D:215:SER:OG	2:D:385:HOH:O	2.22	0.42
1:A:164:TYR:CE1	1:A:190:ALA:HB1	2.54	0.42
1:B:58:GLU:HG2	1:B:65:ARG:HA	2.01	0.42
1:B:164:TYR:CE1	1:B:190:ALA:HB1	2.55	0.42
1:B:245:THR:HA	1:B:246:PRO:HD3	1.89	0.42
1:C:49:ALA:O	1:C:53:ALA:N	2.53	0.42
1:A:56:SER:O	1:A:58:GLU:N	2.53	0.42
1:A:188:ILE:HG23	1:A:259:ILE:HG13	2.01	0.42
1:B:31:GLU:CD	1:B:34:ARG:HE	2.22	0.42
1:C:216:SER:HA	1:C:247:HIS:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:49:ALA:HB2	1:D:72:LEU:HD13	2.02	0.42
1:D:99:ILE:HG22	1:D:136:LEU:HD21	2.02	0.42
1:D:225:VAL:N	1:D:226:PRO:HD2	2.35	0.42
1:A:82:THR:HG21	2:A:559:HOH:O	2.19	0.42
1:C:353:LEU:HD12	2:D:456:HOH:O	2.20	0.42
1:D:58:GLU:HG2	1:D:65:ARG:HA	2.02	0.42
1:B:287:LYS:HB2	1:B:307:HIS:CD2	2.54	0.42
1:C:227:GLU:HB2	2:C:548:HOH:O	2.19	0.42
1:C:149:ARG:HD3	2:C:457:HOH:O	2.20	0.41
1:B:225:VAL:N	1:B:226:PRO:HD2	2.35	0.41
1:D:228:ILE:O	1:D:232:LEU:HG	2.20	0.41
1:D:239:LYS:NZ	1:D:240:VAL:O	2.52	0.41
1:D:303:SER:C	1:D:329:VAL:HG11	2.40	0.41
1:B:89:CYS:O	1:B:90:LEU:C	2.59	0.41
1:A:95:THR:HG21	1:A:110:ASP:OD2	2.20	0.41
1:A:168:ILE:O	1:A:171:PRO:HG2	2.20	0.41
1:B:37:ALA:HB2	1:B:67:GLN:NE2	2.34	0.41
1:B:216:SER:HA	1:B:247:HIS:HA	2.02	0.41
1:C:147:ILE:HD12	1:C:173:VAL:HG11	2.02	0.41
1:C:172:LEU:O	1:C:176:LEU:HD12	2.20	0.41
1:C:332:ALA:HB2	2:C:406:HOH:O	2.18	0.41
1:B:190:ALA:N	1:B:245:THR:O	2.52	0.41
1:D:186:ILE:HG22	1:D:188:ILE:HD11	2.02	0.41
1:B:42:PHE:HE2	1:B:340:LEU:HG	1.84	0.41
1:B:148:LEU:O	1:B:152:ILE:HG13	2.20	0.41
1:D:277:LYS:O	1:D:281:GLU:HG2	2.20	0.41
1:A:274:GLN:HE22	1:A:277:LYS:CE	2.32	0.41
1:D:55:GLN:HB3	1:D:59:SER:OG	2.19	0.41
1:A:147:ILE:HD11	1:A:280:TYR:OH	2.20	0.41
1:C:47:MET:HE3	1:C:57:MET:HB2	2.01	0.41
1:C:194:VAL:O	1:C:194:VAL:HG22	2.20	0.41
1:B:270:GLU:CD	1:B:270:GLU:H	2.24	0.41
1:C:104:THR:HA	1:C:156:ARG:NH1	2.34	0.41
1:C:326:ASP:OD1	1:C:326:ASP:C	2.59	0.41
1:D:140:VAL:HG22	1:D:157:LEU:HD23	2.01	0.41
1:A:125:GLU:HG3	1:A:126:TRP:CD1	2.55	0.41
1:A:195:SER:OG	1:A:328:LEU:HD11	2.19	0.41
1:B:140:VAL:HG22	1:B:157:LEU:CD2	2.45	0.41
1:B:199:ARG:O	1:B:199:ARG:HG2	2.20	0.41
1:C:126:TRP:CG	1:C:226:PRO:HG3	2.55	0.41
1:A:259:ILE:HG22	1:A:261:VAL:HG13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:GLY:N	1:B:326:ASP:OD2	2.38	0.41
1:D:51:ARG:HH11	1:D:51:ARG:HG2	1.85	0.41
1:D:214:ILE:HG22	1:D:250:PRO:HD3	2.01	0.41
1:A:103:PRO:HD2	1:A:106:LEU:HD12	2.01	0.41
1:B:96:GLN:HG3	2:B:429:HOH:O	2.19	0.41
1:B:186:ILE:HG12	1:B:261:VAL:HG12	2.01	0.41
1:D:146:GLU:HG2	1:D:286:VAL:CG2	2.49	0.41
1:A:65:ARG:NE	2:A:558:HOH:O	2.43	0.41
1:A:168:ILE:CD1	1:A:188:ILE:HG21	2.49	0.41
1:B:15:LYS:NZ	2:B:512:HOH:O	2.47	0.41
1:B:325:ILE:HD12	1:B:327:ASN:N	2.35	0.41
1:C:18:ARG:HH11	1:C:45:THR:HB	1.84	0.41
1:D:66:ALA:N	2:D:367:HOH:O	2.50	0.41
1:D:297:THR:CG2	2:D:360:HOH:O	2.60	0.41
1:A:256:GLN:HB2	1:A:324:VAL:HG12	2.02	0.41
1:B:27:TYR:OH	1:D:208:SER:HB2	2.19	0.41
1:B:222:HIS:C	1:B:224:HIS:H	2.22	0.41
1:B:280:TYR:HB3	1:B:286:VAL:HB	2.02	0.41
1:C:161:PRO:CG	1:C:335:GLN:HE21	2.31	0.41
1:D:164:TYR:CZ	1:D:192:SER:HB3	2.55	0.41
1:A:22:LEU:HD11	1:A:80:PHE:CZ	2.56	0.41
1:A:167:THR:HG21	1:A:255:MET:HG2	2.02	0.41
1:A:180:LEU:HB3	1:A:272:LEU:HD23	2.02	0.41
1:A:188:ILE:O	1:A:244:PHE:HA	2.20	0.41
1:A:330:LYS:NZ	1:A:338:GLN:OE1	2.52	0.41
1:B:173:VAL:HB	1:B:174:PRO:HD3	2.02	0.41
1:D:146:GLU:HG3	1:D:283:GLU:OE1	2.20	0.41
1:B:161:PRO:HG2	1:B:335:GLN:NE2	2.35	0.41
1:D:50:ASP:HB3	2:D:534:HOH:O	2.20	0.41
1:C:36:LEU:HD12	1:C:44:VAL:HG22	2.02	0.41
1:C:102:LEU:HD12	1:C:108:ILE:HD13	2.02	0.41
1:C:295:PRO:HG2	1:C:322:ILE:CG2	2.50	0.41
1:D:19:ILE:CD1	1:D:85:ALA:HB3	2.51	0.41
1:A:215:SER:OG	1:D:296:ARG:HG2	2.20	0.41
1:C:96:GLN:HG2	1:C:115:PHE:CE2	2.56	0.41
1:D:194:VAL:HG22	1:D:194:VAL:O	2.20	0.41
1:A:165:PRO:HD3	1:A:224:HIS:ND1	2.35	0.41
1:B:57:MET:HG3	1:B:64:LEU:HD12	2.02	0.41
1:B:273:HIS:HE1	1:B:277:LYS:HD3	1.84	0.41
1:C:42:PHE:N	1:C:42:PHE:CD1	2.88	0.41
1:C:89:CYS:SG	1:C:111:LEU:HD22	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:ASN:HB3	1:C:122:GLU:OE2	2.20	0.41
1:A:182:LYS:HB3	1:A:184:GLU:OE2	2.20	0.41
1:B:169:GLN:O	1:B:173:VAL:HG23	2.21	0.41
1:D:255:MET:HB3	1:D:325:ILE:CD1	2.50	0.41
1:B:52:LYS:HB3	1:B:55:GLN:OE1	2.20	0.41
1:B:175:LEU:HD22	1:B:272:LEU:HD22	2.01	0.41
1:C:75:VAL:O	1:C:78:ALA:HB3	2.21	0.41
1:D:131:HIS:O	1:D:134:VAL:HG23	2.20	0.41
1:D:146:GLU:HA	1:D:149:ARG:CZ	2.51	0.41
1:A:90:LEU:HB3	1:A:91:PRO:CD	2.50	0.41
1:A:125:GLU:HG3	1:A:126:TRP:CD1	2.55	0.41
1:A:183:HIS:HE1	2:A:604:HOH:O	2.02	0.41
1:B:120:ILE:HG22	2:B:434:HOH:O	2.20	0.41
1:C:83:VAL:HG12	1:C:84:ASP:N	2.35	0.41
1:D:94:THR:HA	2:D:537:HOH:O	2.21	0.41
1:A:68:LYS:HD2	1:A:68:LYS:N	2.35	0.41
1:A:119:ASN:HB3	1:A:122:GLU:HB2	2.02	0.41
1:C:58:GLU:CD	1:C:65:ARG:HA	2.40	0.41
1:B:110:ASP:CG	1:B:112:SER:HG	2.24	0.41
1:C:36:LEU:HD12	1:C:44:VAL:CG2	2.50	0.41
1:C:62:PRO:HD2	2:C:402:HOH:O	2.18	0.41
1:D:21:LEU:HD22	1:D:33:VAL:HG23	2.02	0.41
1:D:58:GLU:HG3	1:D:65:ARG:HA	2.02	0.41
1:A:215:SER:CB	1:D:296:ARG:HD2	2.51	0.41
1:C:49:ALA:O	1:C:53:ALA:N	2.53	0.41
1:C:95:THR:HG22	1:C:99:ILE:HD12	2.02	0.41
1:C:142:TYR:HB3	1:C:148:LEU:HD22	2.03	0.41
1:B:283:GLU:OE1	1:B:283:GLU:HA	2.20	0.41
1:C:214:ILE:HG22	1:C:250:PRO:HD3	2.01	0.41
1:D:106:LEU:O	1:D:156:ARG:HG2	2.20	0.41
1:A:183:HIS:CE1	2:A:599:HOH:O	2.72	0.41
1:B:31:GLU:HG3	1:B:328:LEU:HB3	2.02	0.41
1:B:124:GLU:CG	1:B:130:PRO:HA	2.50	0.41
1:B:280:TYR:HD1	1:B:283:GLU:HG3	1.85	0.41
1:C:168:ILE:CD1	1:C:188:ILE:HG21	2.50	0.41
1:D:311:PHE:CD1	1:D:311:PHE:N	2.88	0.41
1:C:306:CYS:HA	1:C:324:VAL:O	2.20	0.41
1:A:22:LEU:HD13	1:A:86:VAL:HG11	2.02	0.41
1:A:273:HIS:CD2	1:A:291:GLU:HG3	2.55	0.41
1:D:311:PHE:CD1	1:D:311:PHE:N	2.88	0.41
1:C:18:ARG:HB2	1:C:83:VAL:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:17:ILE:HB	1:D:42:PHE:CD1	2.55	0.41
1:B:120:ILE:HG22	2:B:433:HOH:O	2.21	0.41
1:B:170:LEU:CB	1:B:171:PRO:HD3	2.47	0.41
1:D:126:TRP:HZ3	1:D:221:ARG:HG3	1.85	0.41
1:D:342:ILE:O	1:D:344:LEU:N	2.53	0.41
1:A:65:ARG:NH1	1:B:287:LYS:HD2	2.34	0.41
1:C:22:LEU:HD11	1:C:80:PHE:HE2	1.85	0.41
1:C:193:GLY:HA3	1:C:252:ILE:O	2.20	0.41
1:D:106:LEU:O	1:D:156:ARG:HG2	2.21	0.41
1:A:214:ILE:HD13	1:D:251:MET:HE1	2.01	0.41
1:A:296:ARG:NH1	2:A:524:HOH:O	2.24	0.41
1:B:19:ILE:HG13	1:B:42:PHE:HB3	2.03	0.41
1:D:34:ARG:HH22	1:D:329:VAL:CG2	2.30	0.41
1:D:136:LEU:HD12	1:D:139:GLU:CG	2.51	0.41
1:A:95:THR:CG2	1:A:99:ILE:HD12	2.51	0.41
1:A:294:VAL:HG11	1:D:216:SER:O	2.21	0.41
1:B:218:GLY:HA3	1:B:222:HIS:HD2	1.84	0.41
1:B:237:GLN:O	1:B:238:SER:CB	2.68	0.41
1:B:274:GLN:HG3	2:B:483:HOH:O	2.19	0.41
1:A:39:HIS:HE1	1:A:41:HIS:HB2	1.85	0.41
1:B:97:GLU:OE1	1:B:132:LYS:HD3	2.20	0.41
1:B:148:LEU:O	1:B:152:ILE:HG13	2.21	0.41
1:C:24:ALA:HB1	1:C:57:MET:HE1	2.02	0.41
1:A:329:VAL:HG12	1:A:334:GLY:HA3	2.03	0.41
1:B:315:ILE:HD13	1:C:185:ASN:HA	2.02	0.41
1:D:160:ASN:ND2	2:D:370:HOH:O	2.53	0.41
1:D:191:LYS:HD2	1:D:191:LYS:N	2.35	0.41
1:A:57:MET:HG2	1:A:64:LEU:HD12	2.02	0.41
1:B:225:VAL:N	1:B:226:PRO:HD2	2.35	0.41
1:B:322:ILE:HG21	2:B:360:HOH:O	2.19	0.41
1:C:287:LYS:CB	1:D:65:ARG:HD2	2.51	0.41
1:C:293:VAL:O	1:C:295:PRO:HD3	2.20	0.41
1:B:36:LEU:HD12	1:B:44:VAL:CG2	2.51	0.41
1:C:23:GLY:HA3	1:C:90:LEU:HD23	2.02	0.41
1:C:262:GLU:CD	2:C:476:HOH:O	2.57	0.41
1:B:118:ARG:NH2	1:B:234:ASP:OD2	2.53	0.41
1:D:199:ARG:O	1:D:199:ARG:HG2	2.20	0.41
1:D:58:GLU:HG2	1:D:62:PRO:HA	2.03	0.41
1:C:204:ALA:O	1:C:210:ILE:HD11	2.20	0.41
1:A:153:LYS:HG2	1:A:342:ILE:HB	2.03	0.41
1:C:61:PHE:HB3	1:C:63:HIS:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:148:LEU:O	1:D:152:ILE:HG13	2.21	0.41
1:A:140:VAL:HG22	1:A:157:LEU:HD23	2.02	0.41
1:B:191:LYS:O	1:B:255:MET:HA	2.21	0.41
1:D:194:VAL:HA	1:D:248:LEU:HD11	2.03	0.41
1:A:22:LEU:N	1:A:22:LEU:HD12	2.36	0.41
1:A:97:GLU:CD	2:A:448:HOH:O	2.59	0.41
2:A:416:HOH:O	1:B:34:ARG:HD3	2.20	0.41
1:B:192:SER:HB2	1:B:255:MET:CE	2.49	0.41
1:B:277:LYS:O	1:B:281:GLU:HB3	2.21	0.41
1:C:99:ILE:HA	1:C:102:LEU:HG	2.02	0.41
1:C:160:ASN:HA	1:C:161:PRO:HD2	1.76	0.41
1:D:130:PRO:N	1:D:132:LYS:HZ2	2.19	0.41
1:B:337:LEU:HD23	1:B:352:LEU:HD21	2.03	0.41
1:B:98:ILE:O	1:B:102:LEU:HG	2.19	0.41
1:D:203:GLU:O	1:D:209:GLU:HG3	2.20	0.41
1:A:251:MET:CE	1:D:214:ILE:HG23	2.51	0.41
1:B:182:LYS:HD2	1:B:262:GLU:HG2	2.03	0.41
1:A:22:LEU:HD13	1:A:86:VAL:HG13	2.03	0.41
1:C:65:ARG:NH2	2:C:373:HOH:O	2.53	0.41
1:C:191:LYS:NZ	1:C:256:GLN:C	2.74	0.41
1:C:295:PRO:HG2	1:C:322:ILE:CG2	2.50	0.41
1:A:27:TYR:O	1:A:30:ALA:HB3	2.20	0.41
1:C:168:ILE:O	1:C:171:PRO:HD2	2.21	0.41
1:C:172:LEU:HD21	1:C:259:ILE:HG21	2.02	0.41
1:A:51:ARG:NE	2:A:555:HOH:O	2.45	0.41
1:A:156:ARG:NH2	2:A:405:HOH:O	2.54	0.41
1:B:219:VAL:CG1	1:B:220:THR:N	2.83	0.41
1:C:241:THR:O	2:C:365:HOH:O	2.21	0.41
1:A:219:VAL:HG11	1:D:311:PHE:CG	2.55	0.41
1:B:48:THR:HA	1:B:73:VAL:O	2.21	0.41
1:C:99:ILE:CD1	1:C:110:ASP:HB2	2.50	0.41
1:A:95:THR:HG21	1:A:110:ASP:CG	2.41	0.41
1:B:181:ILE:HA	1:B:263:MET:HA	2.02	0.41
1:D:52:LYS:NZ	2:D:521:HOH:O	2.50	0.41
1:D:268:ARG:HB3	1:D:270:GLU:OE1	2.20	0.41
1:A:16:ASP:HB2	1:A:41:HIS:HB3	2.01	0.41
1:C:69:LEU:HA	1:C:70:PRO:HD3	1.84	0.41
1:A:51:ARG:HG3	2:A:563:HOH:O	2.20	0.41
1:A:211:ALA:HB2	1:C:207:TYR:CE2	2.55	0.41
1:B:95:THR:HG21	1:B:110:ASP:OD2	2.20	0.41
1:C:328:LEU:O	1:C:332:ALA:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:96:GLN:HA	1:D:96:GLN:NE2	2.36	0.41
1:D:156:ARG:HG2	1:D:157:LEU:N	2.35	0.41
1:A:22:LEU:HA	1:A:48:THR:HB	2.03	0.41
1:C:211:ALA:O	1:C:212:GLU:HB2	2.21	0.41
1:B:247:HIS:HB3	1:B:249:MET:HE1	2.03	0.41
1:D:96:GLN:HG2	1:D:115:PHE:CZ	2.55	0.41
1:B:148:LEU:N	1:B:148:LEU:CD1	2.83	0.41
1:D:273:HIS:O	1:D:277:LYS:HB2	2.20	0.41
1:B:104:THR:O	1:B:156:ARG:HD2	2.21	0.41
1:B:137:GLN:HA	1:B:140:VAL:HG23	2.02	0.41
1:A:135:GLU:OE1	1:A:138:LYS:NZ	2.47	0.41
1:A:180:LEU:HB3	1:A:272:LEU:HD23	2.03	0.41
1:A:52:LYS:HG2	1:A:55:GLN:HE22	1.85	0.41
1:B:313:ASP:CB	1:B:318:ARG:O	2.69	0.41
1:C:152:ILE:HD13	1:C:339:ASN:OD1	2.20	0.41
1:C:194:VAL:O	1:C:194:VAL:HG22	2.20	0.41
1:D:296:ARG:NH1	2:D:427:HOH:O	2.54	0.41
1:D:353:LEU:HB2	2:D:458:HOH:O	2.19	0.41
1:B:49:ALA:O	1:B:50:ASP:C	2.59	0.41
1:C:168:ILE:O	1:C:171:PRO:HD2	2.21	0.41
1:D:239:LYS:HD2	1:D:240:VAL:H	1.84	0.41
1:A:36:LEU:HD12	1:A:44:VAL:CG2	2.51	0.41
1:A:88:CYS:HB3	1:A:110:ASP:CB	2.51	0.41
1:B:296:ARG:HB2	1:B:299:ASN:ND2	2.36	0.41
1:C:117:LEU:HD21	1:C:226:PRO:HB2	2.02	0.41
1:D:38:ASN:ND2	2:D:413:HOH:O	2.51	0.41
1:A:135:GLU:HB2	2:A:571:HOH:O	2.20	0.41
1:A:190:ALA:C	1:A:191:LYS:HD2	2.41	0.41
1:D:180:LEU:HB3	1:D:272:LEU:CD2	2.51	0.41
1:A:127:TYR:CE1	1:A:223:ARG:HD3	2.56	0.41
1:A:180:LEU:HB3	1:A:272:LEU:HD23	2.03	0.41
1:A:214:ILE:HD12	1:D:256:GLN:HB2	2.02	0.41
1:A:249:MET:SD	1:D:214:ILE:HG21	2.60	0.41
1:B:168:ILE:O	1:B:171:PRO:HD2	2.21	0.41
1:B:193:GLY:O	1:B:195:SER:N	2.53	0.41
1:B:301:ARG:NH2	1:B:359:PRO:OXT	2.51	0.41
1:C:268:ARG:HB3	1:C:270:GLU:OE1	2.21	0.41
1:D:306:CYS:HA	1:D:324:VAL:O	2.21	0.41
1:A:115:PHE:HA	1:A:137:GLN:OE1	2.21	0.41
1:A:178:ALA:HB2	1:A:275:GLN:HE21	1.85	0.41
1:B:300:VAL:HG12	1:B:307:HIS:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:SER:HB3	1:B:356:PRO:HG3	2.03	0.41
1:C:194:VAL:O	1:C:196:GLY:N	2.53	0.41
1:D:145:THR:HA	1:D:152:ILE:HD12	2.03	0.41
1:D:263:MET:N	1:D:317:GLY:O	2.42	0.41
1:D:357:LEU:HD12	1:D:357:LEU:HA	1.89	0.41
1:A:199:ARG:O	1:A:199:ARG:HG2	2.21	0.41
1:A:244:PHE:CZ	1:A:246:PRO:HG3	2.55	0.41
1:B:22:LEU:HD21	1:B:80:PHE:CZ	2.55	0.41
1:B:115:PHE:O	1:B:140:VAL:HG11	2.20	0.41
1:B:223:ARG:O	1:B:226:PRO:HD2	2.21	0.41
1:B:277:LYS:O	1:B:281:GLU:HB3	2.20	0.41
1:C:231:GLY:O	1:C:235:VAL:HG23	2.21	0.41
1:C:340:LEU:HD11	1:C:344:LEU:HD11	2.03	0.41
1:D:131:HIS:HB3	1:D:134:VAL:CG2	2.51	0.41
1:A:273:HIS:CG	1:A:291:GLU:HG3	2.56	0.41
1:B:96:GLN:CG	1:B:114:ASP:HB3	2.51	0.41
1:C:306:CYS:HB2	1:C:325:ILE:HG22	2.03	0.41
1:D:22:LEU:HD12	1:D:88:CYS:SG	2.60	0.41
1:D:77:ASP:O	1:D:78:ALA:C	2.59	0.41
1:D:347:PRO:O	1:D:350:THR:OG1	2.28	0.41
1:A:119:ASN:HB3	1:A:122:GLU:HB2	2.03	0.41
1:A:165:PRO:HD3	1:A:224:HIS:ND1	2.36	0.41
1:A:213:GLY:HA3	1:D:298:HIS:CD2	2.56	0.41
1:B:76:LYS:N	1:B:76:LYS:HD2	2.36	0.41
1:B:349:THR:O	1:B:350:THR:C	2.59	0.41
1:C:82:THR:O	1:C:82:THR:HG22	2.20	0.41
1:A:115:PHE:HB3	1:A:140:VAL:HG11	2.01	0.41
1:A:306:CYS:HB2	1:A:325:ILE:HG22	2.01	0.41
1:B:62:PRO:O	1:B:65:ARG:HG2	2.21	0.41
1:B:232:LEU:HA	1:B:235:VAL:HG23	2.03	0.41
1:B:267:VAL:HG13	1:B:271:ASP:HB2	2.03	0.41
1:C:21:LEU:HD11	1:C:89:CYS:SG	2.61	0.41
1:C:28:THR:CG2	1:C:111:LEU:HD22	2.51	0.41
1:C:83:VAL:HG12	1:C:85:ALA:H	1.85	0.41
1:C:96:GLN:HA	1:C:115:PHE:CZ	2.56	0.41
1:D:28:THR:HG21	1:D:111:LEU:HD22	2.03	0.41
1:B:97:GLU:HG2	1:B:132:LYS:HE3	2.02	0.41
1:B:268:ARG:HB3	1:B:270:GLU:OE2	2.21	0.41
1:D:132:LYS:HE3	1:D:132:LYS:HB2	1.88	0.41
1:D:324:VAL:O	1:D:325:ILE:HG23	2.21	0.41
1:A:48:THR:CB	1:A:75:VAL:HG22	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:VAL:HG23	2:A:561:HOH:O	2.19	0.41
1:A:152:ILE:HG23	1:A:158:VAL:HG21	2.02	0.41
1:B:69:LEU:HB3	1:B:70:PRO:HD2	2.01	0.41
1:B:182:LYS:HD2	1:B:262:GLU:CD	2.42	0.41
1:B:191:LYS:NZ	1:C:189:ASP:OD1	2.54	0.41
1:B:359:PRO:HB3	1:C:208:SER:O	2.21	0.41
1:A:126:TRP:CG	1:A:226:PRO:HG3	2.56	0.41
1:A:311:PHE:CD1	1:A:311:PHE:N	2.89	0.41
1:B:225:VAL:HG11	1:C:314:ARG:CZ	2.51	0.41
1:C:148:LEU:HD12	1:C:148:LEU:N	2.36	0.41
1:C:182:LYS:NZ	2:C:467:HOH:O	2.49	0.41
1:D:231:GLY:O	1:D:235:VAL:HG23	2.21	0.41
1:D:310:VAL:HG22	1:D:321:ILE:HG12	2.02	0.41
1:B:222:HIS:ND1	1:B:244:PHE:HE2	2.19	0.41
1:D:48:THR:CB	1:D:75:VAL:HG22	2.51	0.41
1:A:315:ILE:HD12	1:D:243:SER:HB2	2.03	0.41
1:B:117:LEU:HD13	1:B:122:GLU:CB	2.42	0.41
1:B:287:LYS:O	1:B:288:VAL:C	2.59	0.41
1:D:132:LYS:N	1:D:132:LYS:CD	2.83	0.41
1:D:225:VAL:N	1:D:226:PRO:HD2	2.36	0.41
1:D:225:VAL:O	1:D:229:GLU:HG3	2.21	0.41
1:A:17:ILE:HG23	1:A:84:ASP:HB2	2.03	0.41
1:A:156:ARG:NH2	2:A:405:HOH:O	2.54	0.41
1:A:180:LEU:HB3	1:A:272:LEU:HD23	2.03	0.41
1:D:307:HIS:O	1:D:324:VAL:HG22	2.21	0.41
1:B:52:LYS:HD3	1:B:60:VAL:HG22	2.03	0.40
1:B:357:LEU:HD12	1:B:357:LEU:HA	1.93	0.40
1:A:329:VAL:HG12	1:A:334:GLY:HA3	2.03	0.40
1:B:208:SER:HB2	1:D:27:TYR:OH	2.21	0.40
1:C:49:ALA:HB3	1:C:72:LEU:HD13	2.03	0.40
1:D:178:ALA:HB2	1:D:275:GLN:NE2	2.36	0.40
1:A:37:ALA:HB2	1:A:67:GLN:HE22	1.86	0.40
1:A:164:TYR:HB2	1:A:224:HIS:ND1	2.36	0.40
1:A:214:ILE:N	1:D:298:HIS:CE1	2.88	0.40
1:B:118:ARG:CB	1:B:118:ARG:NH1	2.84	0.40
1:D:141:VAL:HG21	1:D:155:ALA:HB2	2.03	0.40
1:B:86:VAL:HB	1:B:108:ILE:HA	2.03	0.40
1:B:237:GLN:O	1:B:238:SER:HB2	2.21	0.40
1:D:80:PHE:C	1:D:82:THR:H	2.24	0.40
1:D:132:LYS:HE2	2:D:545:HOH:O	2.21	0.40
1:A:259:ILE:HG22	1:A:261:VAL:HG13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:ARG:HG2	1:B:298:HIS:ND1	2.36	0.40
1:C:92:HIS:HE1	1:C:123:TYR:OH	2.05	0.40
1:D:281:GLU:HA	2:D:589:HOH:O	2.20	0.40
1:C:42:PHE:N	1:C:42:PHE:CD1	2.88	0.40
1:D:269:THR:HG21	1:D:312:PRO:CB	2.50	0.40
1:A:186:ILE:HB	1:A:242:VAL:HG12	2.02	0.40
1:A:206:LEU:HA	1:C:206:LEU:HA	2.03	0.40
1:A:216:SER:HA	1:A:246:PRO:O	2.21	0.40
1:B:207:TYR:HB2	1:D:207:TYR:HA	2.03	0.40
1:D:164:TYR:CE2	1:D:246:PRO:HB3	2.55	0.40
1:D:232:LEU:CD1	1:D:242:VAL:HG11	2.51	0.40
1:D:62:PRO:O	1:D:64:LEU:N	2.54	0.40
1:D:255:MET:HE3	1:D:327:ASN:CB	2.51	0.40
1:B:347:PRO:HB2	1:B:350:THR:OG1	2.21	0.40
1:D:22:LEU:HA	1:D:48:THR:OG1	2.22	0.40
1:A:95:THR:CG2	1:A:99:ILE:HD12	2.51	0.40
1:A:235:VAL:HG13	1:A:236:ALA:H	1.86	0.40
1:B:192:SER:HB2	1:B:255:MET:HE2	2.03	0.40
1:B:206:LEU:HD21	1:D:200:GLY:O	2.21	0.40
1:C:168:ILE:HD13	1:C:188:ILE:HD13	2.02	0.40
1:D:273:HIS:O	1:D:277:LYS:HB2	2.21	0.40
1:C:56:SER:C	1:C:58:GLU:H	2.24	0.40
1:C:214:ILE:HG22	1:C:249:MET:HG3	2.03	0.40
1:A:52:LYS:HG2	1:A:55:GLN:NE2	2.36	0.40
1:B:118:ARG:CB	1:B:118:ARG:HH11	2.35	0.40
1:C:20:GLY:HA2	1:C:46:LEU:O	2.21	0.40
1:D:180:LEU:HB3	1:D:272:LEU:CD2	2.51	0.40
1:B:96:GLN:HA	1:B:115:PHE:CZ	2.56	0.40
1:D:97:GLU:HG3	1:D:132:LYS:HZ2	1.86	0.40
1:D:136:LEU:C	1:D:138:LYS:N	2.75	0.40
1:A:189:ASP:CG	1:D:191:LYS:HZ1	2.25	0.40
1:B:82:THR:O	1:B:82:THR:HG22	2.21	0.40
1:B:107:LYS:HE3	1:B:343:MET:O	2.21	0.40
1:C:80:PHE:HB2	1:C:103:PRO:HG3	2.03	0.40
1:C:173:VAL:N	1:C:174:PRO:CD	2.84	0.40
1:D:50:ASP:HB3	2:D:533:HOH:O	2.21	0.40
1:A:65:ARG:C	1:A:67:GLN:H	2.24	0.40
1:A:75:VAL:HG23	2:A:560:HOH:O	2.21	0.40
1:A:355:GLN:HB2	1:B:34:ARG:HG3	2.04	0.40
1:C:65:ARG:NH2	2:C:374:HOH:O	2.51	0.40
1:C:23:GLY:O	1:C:89:CYS:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:ASN:HA	1:A:161:PRO:HD2	1.81	0.40
1:B:152:ILE:HD13	1:B:339:ASN:OD1	2.22	0.40
2:C:380:HOH:O	1:D:64:LEU:HD23	2.21	0.40
1:D:141:VAL:HG23	1:D:155:ALA:HB2	2.03	0.40
1:D:170:LEU:HA	1:D:170:LEU:HD23	1.89	0.40
1:D:256:GLN:O	1:D:257:SER:C	2.59	0.40
1:A:178:ALA:HB3	1:A:180:LEU:HG	2.02	0.40
1:B:120:ILE:HG22	2:B:434:HOH:O	2.21	0.40
1:A:119:ASN:HB3	1:A:122:GLU:HB2	2.04	0.40
1:A:255:MET:O	1:A:324:VAL:HA	2.21	0.40
1:A:256:GLN:CB	1:D:214:ILE:HD11	2.42	0.40
1:A:311:PHE:CE1	1:A:322:ILE:HD12	2.57	0.40
1:A:329:VAL:HA	1:A:333:SER:HG	1.87	0.40
1:B:173:VAL:CB	1:B:174:PRO:HD3	2.48	0.40
1:D:296:ARG:O	1:D:297:THR:C	2.60	0.40
1:A:165:PRO:HD3	1:A:224:HIS:ND1	2.36	0.40
1:B:61:PHE:HB3	1:B:63:HIS:CE1	2.55	0.40
1:B:167:THR:HG22	1:B:325:ILE:HG12	2.04	0.40
1:B:168:ILE:O	1:B:171:PRO:HD2	2.21	0.40
1:C:187:ILE:HG12	1:C:243:SER:HB3	2.03	0.40
1:D:300:VAL:HG21	1:D:325:ILE:CA	2.50	0.40
1:B:239:LYS:HG2	2:B:480:HOH:O	2.20	0.40
1:B:287:LYS:HB2	1:B:307:HIS:HD2	1.85	0.40
1:C:299:ASN:HB3	1:D:63:HIS:HA	2.02	0.40
1:D:141:VAL:HG11	1:D:151:ASP:HB3	2.04	0.40
1:A:46:LEU:HD21	1:A:78:ALA:HB1	2.02	0.40
1:A:298:HIS:HA	1:A:301:ARG:CD	2.39	0.40
1:B:117:LEU:HA	1:B:230:GLN:OE1	2.21	0.40
1:C:86:VAL:HB	1:C:108:ILE:HG12	2.02	0.40
1:D:144:LEU:CD2	1:D:169:GLN:HB3	2.49	0.40
1:C:52:LYS:HB3	1:C:55:GLN:OE1	2.21	0.40
1:A:52:LYS:HG2	1:A:55:GLN:HE22	1.86	0.40
1:B:22:LEU:HD21	1:B:80:PHE:CZ	2.56	0.40
1:D:306:CYS:HB2	1:D:325:ILE:CG2	2.52	0.40
1:A:199:ARG:O	1:A:199:ARG:HG2	2.22	0.40
1:B:15:LYS:HD3	1:B:40:PRO:C	2.41	0.40
1:B:148:LEU:O	1:B:152:ILE:HG13	2.22	0.40
1:B:154:LYS:H	1:B:154:LYS:HG2	1.70	0.40
1:C:223:ARG:HB2	2:C:396:HOH:O	2.21	0.40
1:C:270:GLU:CD	1:C:270:GLU:H	2.25	0.40
1:C:309:SER:O	1:C:321:ILE:HA	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:LYS:HG2	1:A:55:GLN:HE22	1.86	0.40
1:A:292:GLY:HA2	1:A:311:PHE:CD2	2.56	0.40
1:B:15:LYS:HB2	1:B:43:GLN:HB2	2.03	0.40
1:B:226:PRO:HA	2:B:406:HOH:O	2.21	0.40
1:C:125:GLU:C	1:C:127:TYR:N	2.75	0.40
1:D:119:ASN:OD1	1:D:121:ALA:HB3	2.21	0.40
1:A:65:ARG:HD2	1:B:307:HIS:CE1	2.56	0.40
1:A:86:VAL:HG12	1:A:87:PHE:N	2.36	0.40
1:B:306:CYS:HA	1:B:325:ILE:HG22	2.04	0.40
1:C:340:LEU:HD12	1:C:340:LEU:HA	1.87	0.40
1:A:48:THR:CG2	2:A:559:HOH:O	2.69	0.40
1:A:178:ALA:HB3	1:A:180:LEU:HG	2.02	0.40
1:C:108:ILE:HG22	1:C:109:VAL:N	2.36	0.40
1:C:237:GLN:CD	2:C:563:HOH:O	2.60	0.40
1:D:76:LYS:NZ	2:D:436:HOH:O	2.55	0.40
1:B:111:LEU:HA	1:B:160:ASN:HB3	2.02	0.40
1:D:304:ASN:HA	1:D:329:VAL:HG12	2.02	0.40
1:A:39:HIS:ND1	1:A:40:PRO:HD2	2.37	0.40
1:A:358:PHE:HA	1:A:359:PRO:HA	1.88	0.40
1:B:22:LEU:HD13	1:B:86:VAL:CG1	2.52	0.40
1:A:178:ALA:HB3	1:A:180:LEU:HG	2.02	0.40
1:C:127:TYR:HE1	1:C:223:ARG:HD3	1.87	0.40
1:D:84:ASP:O	1:D:106:LEU:HD22	2.22	0.40
1:A:115:PHE:HB3	1:A:140:VAL:HG11	2.04	0.40
1:C:285:PHE:CZ	1:C:353:LEU:HD23	2.57	0.40
1:A:213:GLY:HA3	1:D:298:HIS:NE2	2.37	0.40
1:B:110:ASP:OD2	2:B:367:HOH:O	2.22	0.40
1:D:228:ILE:O	1:D:232:LEU:HG	2.21	0.40
1:C:262:GLU:O	1:C:263:MET:O	2.40	0.40
1:B:194:VAL:O	1:B:194:VAL:CG2	2.69	0.40
1:B:220:THR:HG21	2:B:564:HOH:O	2.21	0.40
1:C:125:GLU:HG3	1:C:126:TRP:HD1	1.81	0.40
1:C:248:LEU:O	1:C:249:MET:HE1	2.21	0.40
2:C:378:HOH:O	1:D:64:LEU:HD23	2.22	0.40
1:D:38:ASN:ND2	2:D:409:HOH:O	2.45	0.40
1:B:104:THR:HG22	1:B:104:THR:O	2.21	0.40
1:B:117:LEU:HD21	1:B:226:PRO:HB2	2.04	0.40
1:B:214:ILE:HG22	1:B:250:PRO:HD3	2.03	0.40
1:C:103:PRO:O	1:C:105:ALA:N	2.54	0.40
1:A:303:SER:HB3	1:A:356:PRO:N	2.36	0.40
1:B:120:ILE:HG23	1:B:131:HIS:CB	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:287:LYS:HG3	1:D:65:ARG:HD2	2.04	0.40
1:A:42:PHE:CZ	1:A:344:LEU:HD12	2.56	0.40
1:B:67:GLN:NE2	1:B:69:LEU:HD21	2.35	0.40
1:C:214:ILE:HG22	1:C:250:PRO:HD3	2.03	0.40
1:C:285:PHE:HA	1:C:305:TYR:CD1	2.56	0.40
1:D:62:PRO:C	1:D:64:LEU:N	2.73	0.40
1:D:256:GLN:CB	1:D:324:VAL:HG12	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	1-A	343/359 (96%)	318 (93%)	22 (6%)	3 (1%)	17 16
1	1-B	343/359 (96%)	311 (91%)	25 (7%)	7 (2%)	7 4
1	1-C	343/359 (96%)	317 (92%)	24 (7%)	2 (1%)	25 26
1	1-D	343/359 (96%)	316 (92%)	19 (6%)	8 (2%)	6 3
1	2-A	343/359 (96%)	316 (92%)	24 (7%)	3 (1%)	17 16
1	2-B	343/359 (96%)	318 (93%)	16 (5%)	9 (3%)	5 3
1	2-C	343/359 (96%)	305 (89%)	30 (9%)	8 (2%)	6 3
1	2-D	343/359 (96%)	315 (92%)	21 (6%)	7 (2%)	7 4
1	3-A	343/359 (96%)	310 (90%)	29 (8%)	4 (1%)	13 10
1	3-B	343/359 (96%)	308 (90%)	26 (8%)	9 (3%)	5 3
1	3-C	343/359 (96%)	304 (89%)	33 (10%)	6 (2%)	9 6
1	3-D	343/359 (96%)	316 (92%)	25 (7%)	2 (1%)	25 26
1	4-A	343/359 (96%)	317 (92%)	22 (6%)	4 (1%)	13 10
1	4-B	343/359 (96%)	299 (87%)	34 (10%)	10 (3%)	4 2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	4-C	343/359 (96%)	310 (90%)	24 (7%)	9 (3%)	5	3
1	4-D	343/359 (96%)	312 (91%)	28 (8%)	3 (1%)	17	16
1	5-A	343/359 (96%)	318 (93%)	21 (6%)	4 (1%)	13	10
1	5-B	343/359 (96%)	313 (91%)	22 (6%)	8 (2%)	6	3
1	5-C	343/359 (96%)	311 (91%)	29 (8%)	3 (1%)	17	16
1	5-D	343/359 (96%)	310 (90%)	31 (9%)	2 (1%)	25	26
1	6-A	343/359 (96%)	320 (93%)	18 (5%)	5 (2%)	10	8
1	6-B	343/359 (96%)	301 (88%)	32 (9%)	10 (3%)	4	2
1	6-C	343/359 (96%)	310 (90%)	25 (7%)	8 (2%)	6	3
1	6-D	343/359 (96%)	312 (91%)	29 (8%)	2 (1%)	25	26
1	7-A	343/359 (96%)	316 (92%)	24 (7%)	3 (1%)	17	16
1	7-B	343/359 (96%)	304 (89%)	31 (9%)	8 (2%)	6	3
1	7-C	343/359 (96%)	311 (91%)	28 (8%)	4 (1%)	13	10
1	7-D	343/359 (96%)	309 (90%)	30 (9%)	4 (1%)	13	10
1	8-A	343/359 (96%)	317 (92%)	24 (7%)	2 (1%)	25	26
1	8-B	343/359 (96%)	310 (90%)	25 (7%)	8 (2%)	6	3
1	8-C	343/359 (96%)	308 (90%)	28 (8%)	7 (2%)	7	4
1	8-D	343/359 (96%)	309 (90%)	27 (8%)	7 (2%)	7	4
All	All	10976/11488 (96%)	9971 (91%)	826 (8%)	179 (2%)	9	7

All (179) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-C	332	ALA
1	1-D	105	ALA
1	1-D	212	GLU
1	2-A	161	PRO
1	2-C	145	THR
1	2-D	197	ALA
1	3-A	327	ASN
1	3-D	332	ALA
1	4-A	145	THR
1	4-B	238	SER
1	4-B	329	VAL
1	4-C	128	GLY
1	4-C	263	MET

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Mol	Chain	Res	Type
1	4-D	172	LEU
1	4-D	173	VAL
1	5-A	332	ALA
1	5-B	50	ASP
1	6-B	223	ARG
1	7-A	303	SER
1	7-D	115	PHE
1	7-D	145	THR
1	8-A	103	PRO
1	8-B	142	TYR
1	1-B	145	THR
1	1-B	146	GLU
1	1-D	332	ALA
1	2-C	49	ALA
1	2-D	25	SER
1	2-D	133	ALA
1	2-D	194	VAL
1	2-D	220	THR
1	3-A	145	THR
1	3-B	194	VAL
1	3-B	332	ALA
1	3-C	115	PHE
1	3-C	119	ASN
1	3-C	120	ILE
1	3-D	327	ASN
1	4-B	285	PHE
1	4-C	125	GLU
1	4-C	332	ALA
1	4-D	332	ALA
1	5-B	112	SER
1	5-C	104	THR
1	6-A	222	HIS
1	6-B	49	ALA
1	6-C	46	LEU
1	6-C	104	THR
1	7-B	145	THR
1	7-B	201	ALA
1	7-C	104	THR
1	8-B	144	LEU
1	8-C	41	HIS
1	8-D	82	THR
1	1-A	332	ALA

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Mol	Chain	Res	Type
1	1-B	106	LEU
1	1-D	145	THR
1	1-D	327	ASN
1	2-B	49	ALA
1	2-B	106	LEU
1	2-B	145	THR
1	2-B	146	GLU
1	2-C	104	THR
1	2-C	133	ALA
1	2-C	146	GLU
1	2-D	211	ALA
1	3-A	114	ASP
1	3-B	76	LYS
1	4-B	75	VAL
1	5-A	114	ASP
1	5-B	145	THR
1	5-B	201	ALA
1	6-B	115	PHE
1	6-C	16	ASP
1	6-C	161	PRO
1	6-C	179	ASN
1	6-D	217	TYR
1	7-A	114	ASP
1	7-A	332	ALA
1	7-B	49	ALA
1	8-B	50	ASP
1	8-B	146	GLU
1	8-B	258	THR
1	8-D	63	HIS
1	1-C	134	VAL
1	1-D	146	GLU
1	1-D	230	GLN
1	1-D	343	MET
1	2-B	300	VAL
1	2-C	183	HIS
1	3-A	216	SER
1	3-B	51	ARG
1	3-B	52	LYS
1	3-C	329	VAL
1	3-C	332	ALA
1	4-A	80	PHE
1	4-A	133	ALA

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Mol	Chain	Res	Type
1	4-B	119	ASN
1	4-B	301	ARG
1	4-C	103	PRO
1	4-C	329	VAL
1	5-B	332	ALA
1	5-D	145	THR
1	6-A	133	ALA
1	6-A	332	ALA
1	6-B	50	ASP
1	6-B	51	ARG
1	6-B	96	GLN
1	6-C	313	ASP
1	7-B	119	ASN
1	7-B	313	ASP
1	7-C	281	GLU
1	7-D	238	SER
1	8-C	104	THR
1	8-D	332	ALA
1	1-A	220	THR
1	1-B	49	ALA
1	1-B	80	PHE
1	1-B	332	ALA
1	2-A	112	SER
1	2-B	104	THR
1	2-C	332	ALA
1	3-B	49	ALA
1	3-B	50	ASP
1	3-C	104	THR
1	4-B	76	LYS
1	4-B	332	ALA
1	4-C	173	VAL
1	5-A	133	ALA
1	5-D	332	ALA
1	6-A	134	VAL
1	6-C	49	ALA
1	7-B	50	ASP
1	7-B	332	ALA
1	7-B	348	GLU
1	7-C	49	ALA
1	7-C	332	ALA
1	7-D	290	ASP
1	8-A	133	ALA

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Mol	Chain	Res	Type
1	8-B	332	ALA
1	8-C	49	ALA
1	8-C	124	GLU
1	8-D	103	PRO
1	8-D	171	PRO
1	8-D	238	SER
1	1-A	210	ILE
1	2-D	252	ILE
1	3-B	252	ILE
1	4-C	126	TRP
1	5-B	171	PRO
1	5-C	49	ALA
1	5-C	80	PHE
1	6-B	37	ALA
1	6-B	332	ALA
1	8-B	51	ARG
1	8-C	134	VAL
1	8-C	318	ARG
1	4-A	329	VAL
1	6-A	171	PRO
1	6-D	329	VAL
1	8-B	143	GLY
1	1-B	103	PRO
1	2-A	325	ILE
1	2-B	252	ILE
1	2-B	356	PRO
1	2-C	300	VAL
1	4-B	171	PRO
1	5-A	329	VAL
1	6-B	171	PRO
1	8-D	73	VAL
1	4-C	252	ILE
1	5-B	134	VAL
1	5-B	242	VAL
1	6-C	171	PRO
1	2-B	171	PRO
1	3-B	171	PRO
1	4-B	40	PRO
1	6-B	342	ILE
1	8-C	40	PRO

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	1-A	295/308 (96%)	291 (99%)	4 (1%)	67	80
1	1-B	295/308 (96%)	292 (99%)	3 (1%)	76	86
1	1-C	295/308 (96%)	290 (98%)	5 (2%)	60	74
1	1-D	295/308 (96%)	288 (98%)	7 (2%)	49	62
1	2-A	295/308 (96%)	292 (99%)	3 (1%)	76	86
1	2-B	295/308 (96%)	290 (98%)	5 (2%)	60	74
1	2-C	295/308 (96%)	287 (97%)	8 (3%)	44	57
1	2-D	295/308 (96%)	289 (98%)	6 (2%)	55	69
1	3-A	295/308 (96%)	290 (98%)	5 (2%)	60	74
1	3-B	295/308 (96%)	288 (98%)	7 (2%)	49	62
1	3-C	295/308 (96%)	286 (97%)	9 (3%)	40	51
1	3-D	295/308 (96%)	290 (98%)	5 (2%)	60	74
1	4-A	295/308 (96%)	290 (98%)	5 (2%)	60	74
1	4-B	295/308 (96%)	291 (99%)	4 (1%)	67	80
1	4-C	295/308 (96%)	287 (97%)	8 (3%)	44	57
1	4-D	295/308 (96%)	291 (99%)	4 (1%)	67	80
1	5-A	295/308 (96%)	287 (97%)	8 (3%)	44	57
1	5-B	295/308 (96%)	289 (98%)	6 (2%)	55	69
1	5-C	295/308 (96%)	286 (97%)	9 (3%)	40	51
1	5-D	295/308 (96%)	290 (98%)	5 (2%)	60	74
1	6-A	295/308 (96%)	290 (98%)	5 (2%)	60	74
1	6-B	295/308 (96%)	290 (98%)	5 (2%)	60	74
1	6-C	295/308 (96%)	282 (96%)	13 (4%)	28	35
1	6-D	295/308 (96%)	286 (97%)	9 (3%)	40	51
1	7-A	295/308 (96%)	289 (98%)	6 (2%)	55	69
1	7-B	295/308 (96%)	287 (97%)	8 (3%)	44	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	7-C	295/308 (96%)	289 (98%)	6 (2%)	55	69
1	7-D	295/308 (96%)	287 (97%)	8 (3%)	44	57
1	8-A	295/308 (96%)	292 (99%)	3 (1%)	76	86
1	8-B	295/308 (96%)	286 (97%)	9 (3%)	40	51
1	8-C	295/308 (96%)	291 (99%)	4 (1%)	67	80
1	8-D	295/308 (96%)	286 (97%)	9 (3%)	40	51
All	All	9440/9856 (96%)	9239 (98%)	201 (2%)	53	67

All (201) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	16	ASP
1	1-A	145	THR
1	1-A	191	LYS
1	1-A	298	HIS
1	1-B	57	MET
1	1-B	65	ARG
1	1-B	112	SER
1	1-C	25	SER
1	1-C	51	ARG
1	1-C	65	ARG
1	1-C	82	THR
1	1-C	298	HIS
1	1-D	96	GLN
1	1-D	114	ASP
1	1-D	145	THR
1	1-D	154	LYS
1	1-D	179	ASN
1	1-D	202	LYS
1	1-D	298	HIS
1	2-A	65	ARG
1	2-A	145	THR
1	2-A	354	HIS
1	2-B	65	ARG
1	2-B	92	HIS
1	2-B	125	GLU
1	2-B	151	ASP
1	2-B	354	HIS
1	2-C	51	ARG
1	2-C	65	ARG

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Mol	Chain	Res	Type
1	2-C	117	LEU
1	2-C	179	ASN
1	2-C	191	LYS
1	2-C	301	ARG
1	2-C	311	PHE
1	2-C	344	LEU
1	2-D	16	ASP
1	2-D	57	MET
1	2-D	58	GLU
1	2-D	65	ARG
1	2-D	86	VAL
1	2-D	145	THR
1	3-A	65	ARG
1	3-A	77	ASP
1	3-A	169	GLN
1	3-A	183	HIS
1	3-A	184	GLU
1	3-B	16	ASP
1	3-B	57	MET
1	3-B	65	ARG
1	3-B	88	CYS
1	3-B	106	LEU
1	3-B	125	GLU
1	3-B	311	PHE
1	3-C	51	ARG
1	3-C	112	SER
1	3-C	167	THR
1	3-C	191	LYS
1	3-C	223	ARG
1	3-C	234	ASP
1	3-C	249	MET
1	3-C	298	HIS
1	3-C	311	PHE
1	3-D	16	ASP
1	3-D	65	ARG
1	3-D	145	THR
1	3-D	256	GLN
1	3-D	311	PHE
1	4-A	28	THR
1	4-A	65	ARG
1	4-A	151	ASP
1	4-A	298	HIS

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Mol	Chain	Res	Type
1	4-A	354	HIS
1	4-B	51	ARG
1	4-B	57	MET
1	4-B	65	ARG
1	4-B	185	ASN
1	4-C	51	ARG
1	4-C	65	ARG
1	4-C	82	THR
1	4-C	151	ASP
1	4-C	156	ARG
1	4-C	169	GLN
1	4-C	184	GLU
1	4-C	298	HIS
1	4-D	65	ARG
1	4-D	145	THR
1	4-D	179	ASN
1	4-D	306	CYS
1	5-A	48	THR
1	5-A	65	ARG
1	5-A	145	THR
1	5-A	257	SER
1	5-A	282	ASP
1	5-A	290	ASP
1	5-A	298	HIS
1	5-A	354	HIS
1	5-B	65	ARG
1	5-B	106	LEU
1	5-B	112	SER
1	5-B	167	THR
1	5-B	169	GLN
1	5-B	290	ASP
1	5-C	16	ASP
1	5-C	43	GLN
1	5-C	51	ARG
1	5-C	57	MET
1	5-C	117	LEU
1	5-C	184	GLU
1	5-C	270	GLU
1	5-C	298	HIS
1	5-C	335	GLN
1	5-D	112	SER
1	5-D	122	GLU

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Mol	Chain	Res	Type
1	5-D	145	THR
1	5-D	235	VAL
1	5-D	311	PHE
1	6-A	48	THR
1	6-A	65	ARG
1	6-A	145	THR
1	6-A	184	GLU
1	6-A	298	HIS
1	6-B	32	ILE
1	6-B	65	ARG
1	6-B	106	LEU
1	6-B	112	SER
1	6-B	270	GLU
1	6-C	16	ASP
1	6-C	43	GLN
1	6-C	51	ARG
1	6-C	57	MET
1	6-C	79	ASP
1	6-C	112	SER
1	6-C	163	CYS
1	6-C	169	GLN
1	6-C	179	ASN
1	6-C	203	GLU
1	6-C	257	SER
1	6-C	298	HIS
1	6-C	310	VAL
1	6-D	57	MET
1	6-D	65	ARG
1	6-D	112	SER
1	6-D	114	ASP
1	6-D	145	THR
1	6-D	194	VAL
1	6-D	234	ASP
1	6-D	298	HIS
1	6-D	325	ILE
1	7-A	65	ARG
1	7-A	145	THR
1	7-A	185	ASN
1	7-A	191	LYS
1	7-A	256	GLN
1	7-A	306	CYS
1	7-B	57	MET

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Mol	Chain	Res	Type
1	7-B	65	ARG
1	7-B	92	HIS
1	7-B	112	SER
1	7-B	234	ASP
1	7-B	310	VAL
1	7-B	341	ASN
1	7-B	354	HIS
1	7-C	42	PHE
1	7-C	51	ARG
1	7-C	125	GLU
1	7-C	154	LYS
1	7-C	284	GLU
1	7-C	311	PHE
1	7-D	16	ASP
1	7-D	57	MET
1	7-D	65	ARG
1	7-D	112	SER
1	7-D	151	ASP
1	7-D	223	ARG
1	7-D	282	ASP
1	7-D	306	CYS
1	8-A	65	ARG
1	8-A	111	LEU
1	8-A	145	THR
1	8-B	50	ASP
1	8-B	65	ARG
1	8-B	92	HIS
1	8-B	150	GLU
1	8-B	239	LYS
1	8-B	297	THR
1	8-B	298	HIS
1	8-B	311	PHE
1	8-B	354	HIS
1	8-C	51	ARG
1	8-C	298	HIS
1	8-C	344	LEU
1	8-C	354	HIS
1	8-D	57	MET
1	8-D	67	GLN
1	8-D	76	LYS
1	8-D	82	THR
1	8-D	86	VAL

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Mol	Chain	Res	Type
1	8-D	112	SER
1	8-D	145	THR
1	8-D	223	ARG
1	8-D	296	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (154) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	55	GLN
1	1-A	63	HIS
1	1-A	67	GLN
1	1-A	129	GLN
1	1-A	185	ASN
1	1-A	237	GLN
1	1-A	273	HIS
1	1-B	55	GLN
1	1-B	237	GLN
1	1-B	275	GLN
1	1-B	307	HIS
1	1-B	355	GLN
1	1-C	63	HIS
1	1-C	92	HIS
1	1-C	129	GLN
1	1-C	205	ASN
1	1-C	307	HIS
1	1-D	55	GLN
1	1-D	63	HIS
1	1-D	96	GLN
1	1-D	205	ASN
1	1-D	256	GLN
1	1-D	275	GLN
1	2-A	67	GLN
1	2-A	185	ASN
1	2-A	237	GLN
1	2-A	275	GLN
1	2-B	55	GLN
1	2-B	237	GLN
1	2-B	275	GLN
1	2-C	63	HIS
1	2-C	67	GLN
1	2-C	129	GLN
1	2-C	341	ASN

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Mol	Chain	Res	Type
1	2-C	354	HIS
1	2-D	129	GLN
1	2-D	205	ASN
1	3-A	63	HIS
1	3-A	67	GLN
1	3-A	129	GLN
1	3-A	169	GLN
1	3-A	237	GLN
1	3-B	55	GLN
1	3-B	179	ASN
1	3-B	205	ASN
1	3-B	237	GLN
1	3-B	256	GLN
1	3-B	275	GLN
1	3-B	299	ASN
1	3-C	205	ASN
1	3-C	230	GLN
1	3-D	63	HIS
1	3-D	92	HIS
1	3-D	205	ASN
1	3-D	256	GLN
1	4-A	67	GLN
1	4-A	237	GLN
1	4-A	275	GLN
1	4-B	38	ASN
1	4-B	55	GLN
1	4-B	224	HIS
1	4-B	237	GLN
1	4-B	273	HIS
1	4-B	274	GLN
1	4-B	275	GLN
1	4-B	299	ASN
1	4-B	339	ASN
1	4-B	354	HIS
1	4-C	43	GLN
1	4-C	55	GLN
1	4-C	63	HIS
1	4-C	169	GLN
1	4-C	183	HIS
1	4-D	129	GLN
1	4-D	205	ASN
1	4-D	274	GLN

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Mol	Chain	Res	Type
1	4-D	275	GLN
1	4-D	355	GLN
1	5-A	185	ASN
1	5-A	237	GLN
1	5-A	256	GLN
1	5-A	274	GLN
1	5-B	55	GLN
1	5-B	237	GLN
1	5-B	274	GLN
1	5-B	307	HIS
1	5-C	55	GLN
1	5-C	92	HIS
1	5-C	129	GLN
1	5-C	185	ASN
1	5-C	275	GLN
1	5-C	354	HIS
1	5-D	41	HIS
1	5-D	183	HIS
1	5-D	299	ASN
1	6-A	55	GLN
1	6-A	67	GLN
1	6-A	169	GLN
1	6-A	237	GLN
1	6-A	273	HIS
1	6-A	307	HIS
1	6-B	237	GLN
1	6-B	256	GLN
1	6-B	273	HIS
1	6-B	275	GLN
1	6-C	169	GLN
1	6-C	256	GLN
1	6-C	354	HIS
1	6-D	129	GLN
1	6-D	205	ASN
1	6-D	275	GLN
1	6-D	354	HIS
1	7-A	41	HIS
1	7-A	55	GLN
1	7-A	185	ASN
1	7-A	237	GLN
1	7-A	274	GLN
1	7-A	307	HIS

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Mol	Chain	Res	Type
1	7-B	38	ASN
1	7-B	67	GLN
1	7-B	237	GLN
1	7-B	256	GLN
1	7-B	275	GLN
1	7-B	307	HIS
1	7-B	354	HIS
1	7-C	92	HIS
1	7-C	129	GLN
1	7-C	307	HIS
1	7-D	92	HIS
1	7-D	183	HIS
1	7-D	275	GLN
1	7-D	307	HIS
1	8-A	41	HIS
1	8-A	67	GLN
1	8-A	237	GLN
1	8-A	273	HIS
1	8-B	67	GLN
1	8-B	185	ASN
1	8-B	237	GLN
1	8-B	256	GLN
1	8-B	274	GLN
1	8-B	275	GLN
1	8-B	307	HIS
1	8-C	43	GLN
1	8-C	55	GLN
1	8-C	63	HIS
1	8-C	67	GLN
1	8-C	354	HIS
1	8-D	92	HIS
1	8-D	129	GLN
1	8-D	169	GLN
1	8-D	307	HIS
1	8-D	335	GLN
1	8-D	354	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	1-A	345/359 (96%)	-0.06	6 (1%)	70	68	17, 30, 56, 67	345 (100%)
1	1-B	345/359 (96%)	0.18	20 (5%)	23	22	14, 31, 60, 98	345 (100%)
1	1-C	345/359 (96%)	0.27	25 (7%)	15	14	16, 31, 65, 88	345 (100%)
1	1-D	345/359 (96%)	0.02	12 (3%)	44	42	16, 30, 57, 94	345 (100%)
1	2-A	345/359 (96%)	-0.06	6 (1%)	70	68	17, 30, 56, 67	345 (100%)
1	2-B	345/359 (96%)	0.18	20 (5%)	23	22	14, 31, 60, 98	345 (100%)
1	2-C	345/359 (96%)	0.27	25 (7%)	15	14	16, 31, 65, 88	345 (100%)
1	2-D	345/359 (96%)	0.02	12 (3%)	44	42	16, 30, 57, 94	345 (100%)
1	3-A	345/359 (96%)	-0.06	6 (1%)	70	68	17, 30, 56, 67	345 (100%)
1	3-B	345/359 (96%)	0.18	20 (5%)	23	22	14, 31, 60, 98	345 (100%)
1	3-C	345/359 (96%)	0.27	25 (7%)	15	14	16, 31, 65, 88	345 (100%)
1	3-D	345/359 (96%)	0.02	12 (3%)	44	42	16, 30, 57, 94	345 (100%)
1	4-A	345/359 (96%)	-0.06	6 (1%)	70	68	17, 30, 56, 67	345 (100%)
1	4-B	345/359 (96%)	0.18	20 (5%)	23	22	14, 31, 60, 98	345 (100%)
1	4-C	345/359 (96%)	0.27	25 (7%)	15	14	16, 31, 65, 88	345 (100%)
1	4-D	345/359 (96%)	0.02	12 (3%)	44	42	16, 30, 57, 94	345 (100%)
1	5-A	345/359 (96%)	-0.06	6 (1%)	70	68	17, 30, 56, 67	345 (100%)
1	5-B	345/359 (96%)	0.18	20 (5%)	23	22	14, 31, 60, 98	345 (100%)
1	5-C	345/359 (96%)	0.27	25 (7%)	15	14	16, 31, 65, 88	345 (100%)
1	5-D	345/359 (96%)	0.02	12 (3%)	44	42	16, 30, 57, 94	345 (100%)
1	6-A	345/359 (96%)	-0.06	6 (1%)	70	68	17, 30, 56, 67	345 (100%)
1	6-B	345/359 (96%)	0.18	20 (5%)	23	22	14, 31, 60, 98	345 (100%)
1	6-C	345/359 (96%)	0.27	25 (7%)	15	14	16, 31, 65, 88	345 (100%)
1	6-D	345/359 (96%)	0.02	12 (3%)	44	42	16, 30, 57, 94	345 (100%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	7-A	345/359 (96%)	-0.06	6 (1%)	70	68	17, 30, 56, 67	345 (100%)
1	7-B	345/359 (96%)	0.18	20 (5%)	23	22	14, 31, 60, 98	345 (100%)
1	7-C	345/359 (96%)	0.27	25 (7%)	15	14	16, 31, 65, 88	345 (100%)
1	7-D	345/359 (96%)	0.02	12 (3%)	44	42	16, 30, 57, 94	345 (100%)
1	8-A	345/359 (96%)	-0.06	6 (1%)	70	68	17, 30, 56, 67	345 (100%)
1	8-B	345/359 (96%)	0.18	20 (5%)	23	22	14, 31, 60, 98	345 (100%)
1	8-C	345/359 (96%)	0.27	25 (7%)	15	14	16, 31, 65, 88	345 (100%)
1	8-D	345/359 (96%)	0.02	12 (3%)	44	42	16, 30, 57, 94	345 (100%)
All	All	11040/11488 (96%)	0.10	504 (4%)	36	31	14, 30, 60, 98	11040 (100%)

All (504) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	93	GLY	6.6
1	2-A	93	GLY	6.6
1	3-A	93	GLY	6.6
1	4-A	93	GLY	6.6
1	5-A	93	GLY	6.6
1	6-A	93	GLY	6.6
1	7-A	93	GLY	6.6
1	8-A	93	GLY	6.6
1	1-B	76	LYS	4.5
1	2-B	76	LYS	4.5
1	3-B	76	LYS	4.5
1	4-B	76	LYS	4.5
1	5-B	76	LYS	4.5
1	6-B	76	LYS	4.5
1	7-B	76	LYS	4.5
1	8-B	76	LYS	4.5
1	1-A	104	THR	3.8
1	2-A	104	THR	3.8
1	3-A	104	THR	3.8
1	4-A	104	THR	3.8
1	5-A	104	THR	3.8
1	6-A	104	THR	3.8
1	7-A	104	THR	3.8
1	8-A	104	THR	3.8
1	1-C	135	GLU	3.8
1	2-C	135	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
1	3-C	135	GLU	3.8
1	4-C	135	GLU	3.8
1	5-C	135	GLU	3.8
1	6-C	135	GLU	3.8
1	7-C	135	GLU	3.8
1	8-C	135	GLU	3.8
1	1-B	78	ALA	3.7
1	2-B	78	ALA	3.7
1	3-B	78	ALA	3.7
1	4-B	78	ALA	3.7
1	5-B	78	ALA	3.7
1	6-B	78	ALA	3.7
1	7-B	78	ALA	3.7
1	8-B	78	ALA	3.7
1	1-B	278	THR	3.6
1	2-B	278	THR	3.6
1	3-B	278	THR	3.6
1	4-B	278	THR	3.6
1	5-B	278	THR	3.6
1	6-B	278	THR	3.6
1	7-B	278	THR	3.6
1	8-B	278	THR	3.6
1	1-D	51	ARG	3.6
1	2-D	51	ARG	3.6
1	3-D	51	ARG	3.6
1	4-D	51	ARG	3.6
1	5-D	51	ARG	3.6
1	6-D	51	ARG	3.6
1	7-D	51	ARG	3.6
1	8-D	51	ARG	3.6
1	1-C	53	ALA	3.6
1	2-C	53	ALA	3.6
1	3-C	53	ALA	3.6
1	4-C	53	ALA	3.6
1	5-C	53	ALA	3.6
1	6-C	53	ALA	3.6
1	7-C	53	ALA	3.6
1	8-C	53	ALA	3.6
1	1-D	329	VAL	3.6
1	2-D	329	VAL	3.6
1	3-D	329	VAL	3.6
1	4-D	329	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	5-D	329	VAL	3.6
1	6-D	329	VAL	3.6
1	7-D	329	VAL	3.6
1	8-D	329	VAL	3.6
1	1-C	78	ALA	3.4
1	1-D	292	GLY	3.4
1	2-C	78	ALA	3.4
1	2-D	292	GLY	3.4
1	3-C	78	ALA	3.4
1	3-D	292	GLY	3.4
1	4-C	78	ALA	3.4
1	4-D	292	GLY	3.4
1	5-C	78	ALA	3.4
1	5-D	292	GLY	3.4
1	6-C	78	ALA	3.4
1	6-D	292	GLY	3.4
1	7-C	78	ALA	3.4
1	7-D	292	GLY	3.4
1	8-C	78	ALA	3.4
1	8-D	292	GLY	3.4
1	1-C	18	ARG	3.4
1	2-C	18	ARG	3.4
1	3-C	18	ARG	3.4
1	4-C	18	ARG	3.4
1	5-C	18	ARG	3.4
1	6-C	18	ARG	3.4
1	7-C	18	ARG	3.4
1	8-C	18	ARG	3.4
1	1-C	54	GLY	3.4
1	2-C	54	GLY	3.4
1	3-C	54	GLY	3.4
1	4-C	54	GLY	3.4
1	5-C	54	GLY	3.4
1	6-C	54	GLY	3.4
1	7-C	54	GLY	3.4
1	8-C	54	GLY	3.4
1	1-C	129	GLN	3.3
1	2-C	129	GLN	3.3
1	3-C	129	GLN	3.3
1	4-C	129	GLN	3.3
1	5-C	129	GLN	3.3
1	6-C	129	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
1	7-C	129	GLN	3.3
1	8-C	129	GLN	3.3
1	1-B	80	PHE	3.3
1	2-B	80	PHE	3.3
1	3-B	80	PHE	3.3
1	4-B	80	PHE	3.3
1	5-B	80	PHE	3.3
1	6-B	80	PHE	3.3
1	7-B	80	PHE	3.3
1	8-B	80	PHE	3.3
1	1-A	259	ILE	3.2
1	2-A	259	ILE	3.2
1	3-A	259	ILE	3.2
1	4-A	259	ILE	3.2
1	5-A	259	ILE	3.2
1	6-A	259	ILE	3.2
1	7-A	259	ILE	3.2
1	8-A	259	ILE	3.2
1	1-A	120	ILE	3.2
1	2-A	120	ILE	3.2
1	3-A	120	ILE	3.2
1	4-A	120	ILE	3.2
1	5-A	120	ILE	3.2
1	6-A	120	ILE	3.2
1	7-A	120	ILE	3.2
1	8-A	120	ILE	3.2
1	1-D	93	GLY	3.2
1	2-D	93	GLY	3.2
1	3-D	93	GLY	3.2
1	4-D	93	GLY	3.2
1	5-D	93	GLY	3.2
1	6-D	93	GLY	3.2
1	7-D	93	GLY	3.2
1	8-D	93	GLY	3.2
1	1-B	82	THR	3.1
1	2-B	82	THR	3.1
1	3-B	82	THR	3.1
1	4-B	82	THR	3.1
1	5-B	82	THR	3.1
1	6-B	82	THR	3.1
1	7-B	82	THR	3.1
1	8-B	82	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	1-C	76	LYS	3.1
1	2-C	76	LYS	3.1
1	3-C	76	LYS	3.1
1	4-C	76	LYS	3.1
1	5-C	76	LYS	3.1
1	6-C	76	LYS	3.1
1	7-C	76	LYS	3.1
1	8-C	76	LYS	3.1
1	1-C	16	ASP	3.1
1	2-C	16	ASP	3.1
1	3-C	16	ASP	3.1
1	4-C	16	ASP	3.1
1	5-C	16	ASP	3.1
1	6-C	16	ASP	3.1
1	7-C	16	ASP	3.1
1	8-C	16	ASP	3.1
1	1-B	121	ALA	3.1
1	2-B	121	ALA	3.1
1	3-B	121	ALA	3.1
1	4-B	121	ALA	3.1
1	5-B	121	ALA	3.1
1	6-B	121	ALA	3.1
1	7-B	121	ALA	3.1
1	8-B	121	ALA	3.1
1	1-C	121	ALA	3.0
1	2-C	121	ALA	3.0
1	3-C	121	ALA	3.0
1	4-C	121	ALA	3.0
1	5-C	121	ALA	3.0
1	6-C	121	ALA	3.0
1	7-C	121	ALA	3.0
1	8-C	121	ALA	3.0
1	1-B	291	GLU	2.9
1	2-B	291	GLU	2.9
1	3-B	291	GLU	2.9
1	4-B	291	GLU	2.9
1	5-B	291	GLU	2.9
1	6-B	291	GLU	2.9
1	7-B	291	GLU	2.9
1	8-B	291	GLU	2.9
1	1-C	41	HIS	2.9
1	2-C	41	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
1	3-C	41	HIS	2.9
1	4-C	41	HIS	2.9
1	5-C	41	HIS	2.9
1	6-C	41	HIS	2.9
1	7-C	41	HIS	2.9
1	8-C	41	HIS	2.9
1	1-D	16	ASP	2.9
1	2-D	16	ASP	2.9
1	3-D	16	ASP	2.9
1	4-D	16	ASP	2.9
1	5-D	16	ASP	2.9
1	6-D	16	ASP	2.9
1	7-D	16	ASP	2.9
1	8-D	16	ASP	2.9
1	1-B	259	ILE	2.8
1	2-B	259	ILE	2.8
1	3-B	259	ILE	2.8
1	4-B	259	ILE	2.8
1	5-B	259	ILE	2.8
1	6-B	259	ILE	2.8
1	7-B	259	ILE	2.8
1	8-B	259	ILE	2.8
1	1-C	346	TYR	2.8
1	2-C	346	TYR	2.8
1	3-C	346	TYR	2.8
1	4-C	346	TYR	2.8
1	5-C	346	TYR	2.8
1	6-C	346	TYR	2.8
1	7-C	346	TYR	2.8
1	8-C	346	TYR	2.8
1	1-B	91	PRO	2.8
1	2-B	91	PRO	2.8
1	3-B	91	PRO	2.8
1	4-B	91	PRO	2.8
1	5-B	91	PRO	2.8
1	6-B	91	PRO	2.8
1	7-B	91	PRO	2.8
1	8-B	91	PRO	2.8
1	1-C	268	ARG	2.8
1	2-C	268	ARG	2.8
1	3-C	268	ARG	2.8
1	4-C	268	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	5-C	268	ARG	2.8
1	6-C	268	ARG	2.8
1	7-C	268	ARG	2.8
1	8-C	268	ARG	2.8
1	1-D	238	SER	2.8
1	2-D	238	SER	2.8
1	3-D	238	SER	2.8
1	4-D	238	SER	2.8
1	5-D	238	SER	2.8
1	6-D	238	SER	2.8
1	7-D	238	SER	2.8
1	8-D	238	SER	2.8
1	1-C	125	GLU	2.7
1	2-C	125	GLU	2.7
1	3-C	125	GLU	2.7
1	4-C	125	GLU	2.7
1	5-C	125	GLU	2.7
1	6-C	125	GLU	2.7
1	7-C	125	GLU	2.7
1	8-C	125	GLU	2.7
1	1-B	75	VAL	2.7
1	2-B	75	VAL	2.7
1	3-B	75	VAL	2.7
1	4-B	75	VAL	2.7
1	5-B	75	VAL	2.7
1	6-B	75	VAL	2.7
1	7-B	75	VAL	2.7
1	8-B	75	VAL	2.7
1	1-D	32	ILE	2.6
1	2-D	32	ILE	2.6
1	3-D	32	ILE	2.6
1	4-D	32	ILE	2.6
1	5-D	32	ILE	2.6
1	6-D	32	ILE	2.6
1	7-D	32	ILE	2.6
1	8-D	32	ILE	2.6
1	1-C	266	GLY	2.6
1	2-C	266	GLY	2.6
1	3-C	266	GLY	2.6
1	4-C	266	GLY	2.6
1	5-C	266	GLY	2.6
1	6-C	266	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	7-C	266	GLY	2.6
1	8-C	266	GLY	2.6
1	1-C	264	ALA	2.6
1	2-C	264	ALA	2.6
1	3-C	264	ALA	2.6
1	4-C	264	ALA	2.6
1	5-C	264	ALA	2.6
1	6-C	264	ALA	2.6
1	7-C	264	ALA	2.6
1	8-C	264	ALA	2.6
1	1-C	51	ARG	2.5
1	2-C	51	ARG	2.5
1	3-C	51	ARG	2.5
1	4-C	51	ARG	2.5
1	5-C	51	ARG	2.5
1	6-C	51	ARG	2.5
1	7-C	51	ARG	2.5
1	8-C	51	ARG	2.5
1	1-C	72	LEU	2.5
1	2-C	72	LEU	2.5
1	3-C	72	LEU	2.5
1	4-C	72	LEU	2.5
1	5-C	72	LEU	2.5
1	6-C	72	LEU	2.5
1	7-C	72	LEU	2.5
1	8-C	72	LEU	2.5
1	1-C	105	ALA	2.4
1	2-C	105	ALA	2.4
1	3-C	105	ALA	2.4
1	4-C	105	ALA	2.4
1	5-C	105	ALA	2.4
1	6-C	105	ALA	2.4
1	7-C	105	ALA	2.4
1	8-C	105	ALA	2.4
1	1-B	79	ASP	2.4
1	2-B	79	ASP	2.4
1	3-B	79	ASP	2.4
1	4-B	79	ASP	2.4
1	5-B	79	ASP	2.4
1	6-B	79	ASP	2.4
1	7-B	79	ASP	2.4
1	8-B	79	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	1-C	40	PRO	2.4
1	2-C	40	PRO	2.4
1	3-C	40	PRO	2.4
1	4-C	40	PRO	2.4
1	5-C	40	PRO	2.4
1	6-C	40	PRO	2.4
1	7-C	40	PRO	2.4
1	8-C	40	PRO	2.4
1	1-D	345	GLY	2.4
1	2-D	345	GLY	2.4
1	3-D	345	GLY	2.4
1	4-D	345	GLY	2.4
1	5-D	345	GLY	2.4
1	6-D	345	GLY	2.4
1	7-D	345	GLY	2.4
1	8-D	345	GLY	2.4
1	1-D	281	GLU	2.3
1	2-D	281	GLU	2.3
1	3-D	281	GLU	2.3
1	4-D	281	GLU	2.3
1	5-D	281	GLU	2.3
1	6-D	281	GLU	2.3
1	7-D	281	GLU	2.3
1	8-D	281	GLU	2.3
1	1-D	237	GLN	2.3
1	2-D	237	GLN	2.3
1	3-D	237	GLN	2.3
1	4-D	237	GLN	2.3
1	5-D	237	GLN	2.3
1	6-D	237	GLN	2.3
1	7-D	237	GLN	2.3
1	8-D	237	GLN	2.3
1	1-B	16	ASP	2.2
1	2-B	16	ASP	2.2
1	3-B	16	ASP	2.2
1	4-B	16	ASP	2.2
1	5-B	16	ASP	2.2
1	6-B	16	ASP	2.2
1	7-B	16	ASP	2.2
1	8-B	16	ASP	2.2
1	1-B	292	GLY	2.2
1	2-B	292	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	3-B	292	GLY	2.2
1	4-B	292	GLY	2.2
1	5-B	292	GLY	2.2
1	6-B	292	GLY	2.2
1	7-B	292	GLY	2.2
1	8-B	292	GLY	2.2
1	1-B	123	TYR	2.2
1	2-B	123	TYR	2.2
1	3-B	123	TYR	2.2
1	4-B	123	TYR	2.2
1	5-B	123	TYR	2.2
1	6-B	123	TYR	2.2
1	7-B	123	TYR	2.2
1	8-B	123	TYR	2.2
1	1-B	274	GLN	2.2
1	2-B	274	GLN	2.2
1	3-B	274	GLN	2.2
1	4-B	274	GLN	2.2
1	5-B	274	GLN	2.2
1	6-B	274	GLN	2.2
1	7-B	274	GLN	2.2
1	8-B	274	GLN	2.2
1	1-B	129	GLN	2.1
1	2-B	129	GLN	2.1
1	3-B	129	GLN	2.1
1	4-B	129	GLN	2.1
1	5-B	129	GLN	2.1
1	6-B	129	GLN	2.1
1	7-B	129	GLN	2.1
1	8-B	129	GLN	2.1
1	1-D	306	CYS	2.1
1	2-D	306	CYS	2.1
1	3-D	306	CYS	2.1
1	4-D	306	CYS	2.1
1	5-D	306	CYS	2.1
1	6-D	306	CYS	2.1
1	7-D	306	CYS	2.1
1	8-D	306	CYS	2.1
1	1-C	278	THR	2.1
1	2-C	278	THR	2.1
1	3-C	278	THR	2.1
1	4-C	278	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	5-C	278	THR	2.1
1	6-C	278	THR	2.1
1	7-C	278	THR	2.1
1	8-C	278	THR	2.1
1	1-C	100	LYS	2.1
1	2-C	100	LYS	2.1
1	3-C	100	LYS	2.1
1	4-C	100	LYS	2.1
1	5-C	100	LYS	2.1
1	6-C	100	LYS	2.1
1	7-C	100	LYS	2.1
1	8-C	100	LYS	2.1
1	1-C	259	ILE	2.1
1	2-C	259	ILE	2.1
1	3-C	259	ILE	2.1
1	4-C	259	ILE	2.1
1	5-C	259	ILE	2.1
1	6-C	259	ILE	2.1
1	7-C	259	ILE	2.1
1	8-C	259	ILE	2.1
1	1-C	267	VAL	2.1
1	2-C	267	VAL	2.1
1	3-C	267	VAL	2.1
1	4-C	267	VAL	2.1
1	5-C	267	VAL	2.1
1	6-C	267	VAL	2.1
1	7-C	267	VAL	2.1
1	8-C	267	VAL	2.1
1	1-B	49	ALA	2.1
1	2-B	49	ALA	2.1
1	3-B	49	ALA	2.1
1	4-B	49	ALA	2.1
1	5-B	49	ALA	2.1
1	6-B	49	ALA	2.1
1	7-B	49	ALA	2.1
1	8-B	49	ALA	2.1
1	1-B	128	GLY	2.1
1	2-B	128	GLY	2.1
1	3-B	128	GLY	2.1
1	4-B	128	GLY	2.1
1	5-B	128	GLY	2.1
1	6-B	128	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	7-B	128	GLY	2.1
1	8-B	128	GLY	2.1
1	1-C	188	ILE	2.0
1	2-C	188	ILE	2.0
1	3-C	188	ILE	2.0
1	4-C	188	ILE	2.0
1	5-C	188	ILE	2.0
1	6-C	188	ILE	2.0
1	7-C	188	ILE	2.0
1	8-C	188	ILE	2.0
1	1-B	77	ASP	2.0
1	2-B	77	ASP	2.0
1	3-B	77	ASP	2.0
1	4-B	77	ASP	2.0
1	5-B	77	ASP	2.0
1	6-B	77	ASP	2.0
1	7-B	77	ASP	2.0
1	8-B	77	ASP	2.0
1	1-B	120	ILE	2.0
1	2-B	120	ILE	2.0
1	3-B	120	ILE	2.0
1	4-B	120	ILE	2.0
1	5-B	120	ILE	2.0
1	6-B	120	ILE	2.0
1	7-B	120	ILE	2.0
1	8-B	120	ILE	2.0
1	1-C	109	VAL	2.0
1	2-C	109	VAL	2.0
1	3-C	109	VAL	2.0
1	4-C	109	VAL	2.0
1	5-C	109	VAL	2.0
1	6-C	109	VAL	2.0
1	7-C	109	VAL	2.0
1	8-C	109	VAL	2.0
1	1-D	92	HIS	2.0
1	2-D	92	HIS	2.0
1	3-D	92	HIS	2.0
1	4-D	92	HIS	2.0
1	5-D	92	HIS	2.0
1	6-D	92	HIS	2.0
1	7-D	92	HIS	2.0
1	8-D	92	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
1	1-A	52	LYS	2.0
1	1-A	274	GLN	2.0
1	2-A	52	LYS	2.0
1	2-A	274	GLN	2.0
1	3-A	52	LYS	2.0
1	3-A	274	GLN	2.0
1	4-A	52	LYS	2.0
1	4-A	274	GLN	2.0
1	5-A	52	LYS	2.0
1	5-A	274	GLN	2.0
1	6-A	52	LYS	2.0
1	6-A	274	GLN	2.0
1	7-A	52	LYS	2.0
1	7-A	274	GLN	2.0
1	8-A	52	LYS	2.0
1	8-A	274	GLN	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.