Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 06:06 pm BST

PDB ID	:	2WCD
Title	:	Crystal structure of the assembled cytolysin A pore
Authors	:	Mueller, M.; Grauschopf, U.; Maier, T.; Glockshuber, R.; Ban, N.
Deposited on	:	2009-03-11
Resolution	:	3.29 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

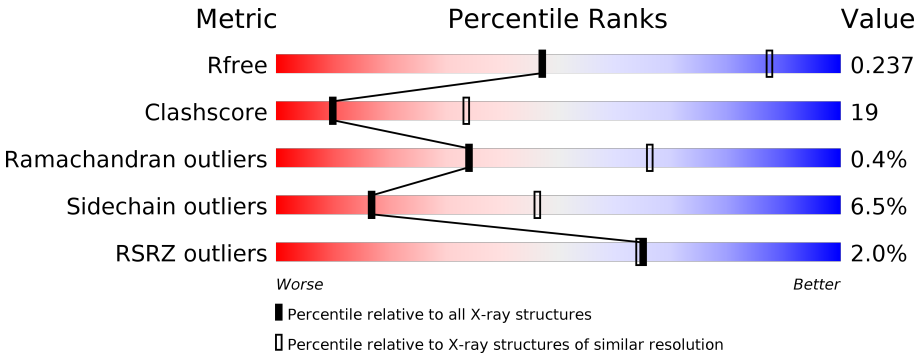
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.29 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	309	% 57% 32% • 8%
1	B	309	2% 56% 34% • 8%
1	C	309	% 58% 31% • 8%
1	D	309	% 56% 34% • 8%
1	E	309	3% 55% 34% • 8%
1	F	309	3% 58% 31% • 8%

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Mol	Chain	Length	Quality of chain
1	G	309	2% 57% 33% • 8%
1	H	309	3% 57% 33% • 8%
1	I	309	3% 57% 33% • 8%
1	J	309	2% 59% 30% • 8%
1	K	309	3% 56% 34% • 8%
1	L	309	2% 55% 35% • 8%
1	M	309	2% 57% 33% • 8%
1	N	309	% 59% 31% • 8%
1	O	309	2% 58% 31% • 8%
1	P	309	3% 59% 31% • 8%
1	Q	309	2% 58% 32% • 8%
1	R	309	58% 32% • 8%
1	S	309	2% 55% 35% • 8%
1	T	309	2% 57% 33% • 8%
1	U	309	2% 58% 31% • 8%
1	V	309	2% 59% 31% • 8%
1	W	309	2% 58% 32% • 8%
1	X	309	% 55% 34% • 8%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 53832 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 HEMOLYSIN E, CHROMOSOMAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	0	0	0
			2237	1427	360	445	5			
1	B	285	Total	C	N	O	S	0	0	0
			2237	1427	360	445	5			
1	C	285	Total	C	N	O	S	0	0	0
			2237	1427	360	445	5			
1	D	285	Total	C	N	O	S	0	0	0
			2237	1427	360	445	5			
1	E	285	Total	C	N	O	S	0	0	0
			2237	1427	360	445	5			
1	F	285	Total	C	N	O	S	0	0	0
			2237	1427	360	445	5			
1	G	285	Total	C	N	O	S	0	0	0
			2237	1427	360	445	5			
1	H	285	Total	C	N	O	S	0	0	0
			2237	1427	360	445	5			
1	I	285	Total	C	N	O	S	0	0	0
			2237	1427	360	445	5			
1	J	285	Total	C	N	O	S	0	0	0
			2237	1427	360	445	5			
1	K	285	Total	C	N	O	S	0	0	0
			2237	1427	360	445	5			
1	L	285	Total	C	N	O	S	0	0	0
			2237	1427	360	445	5			
1	M	285	Total	C	N	O	S	0	0	0
			2237	1427	360	445	5			
1	N	285	Total	C	N	O	S	0	0	0
			2237	1427	360	445	5			
1	O	285	Total	C	N	O	S	0	0	0
			2237	1427	360	445	5			
1	P	285	Total	C	N	O	S	0	0	0
			2237	1427	360	445	5			

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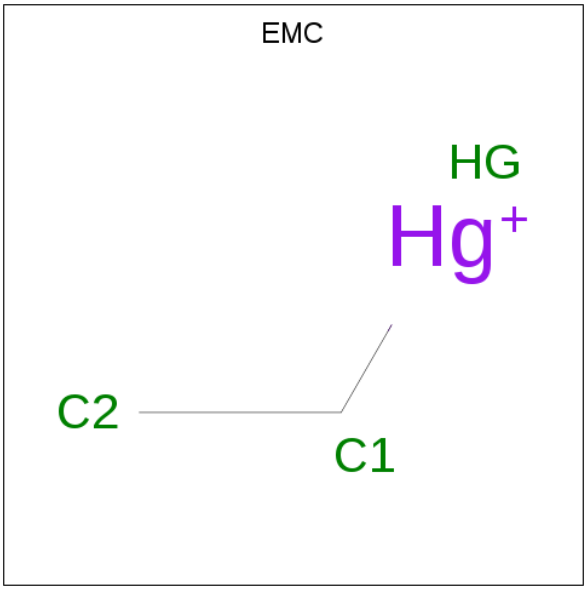
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	285	Total	C	N	O	S	0	0	0
			2237	1427	360	445	5			
1	R	285	Total	C	N	O	S	0	0	0
			2237	1427	360	445	5			
1	S	285	Total	C	N	O	S	0	0	0
			2237	1427	360	445	5			
1	T	285	Total	C	N	O	S	0	0	0
			2237	1427	360	445	5			
1	U	285	Total	C	N	O	S	0	0	0
			2237	1427	360	445	5			
1	V	285	Total	C	N	O	S	0	0	0
			2237	1427	360	445	5			
1	W	285	Total	C	N	O	S	0	0	0
			2237	1427	360	445	5			
1	X	285	Total	C	N	O	S	0	0	0
			2237	1427	360	445	5			

- Molecule 2 is ETHYL MERCURY ION (three-letter code: EMC) (formula: C_2H_5Hg).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	Hg	0	0
			3	2	1		
2	A	1	Total	C	Hg	0	0
			3	2	1		
2	B	1	Total	C	Hg	0	0
			3	2	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total 3	C 2	Hg 1	0	0
2	C	1	Total 3	C 2	Hg 1	0	0
2	C	1	Total 3	C 2	Hg 1	0	0
2	D	1	Total 3	C 2	Hg 1	0	0
2	D	1	Total 3	C 2	Hg 1	0	0
2	E	1	Total 3	C 2	Hg 1	0	0
2	E	1	Total 3	C 2	Hg 1	0	0
2	F	1	Total 3	C 2	Hg 1	0	0
2	F	1	Total 3	C 2	Hg 1	0	0
2	G	1	Total 3	C 2	Hg 1	0	0
2	G	1	Total 3	C 2	Hg 1	0	0
2	H	1	Total 3	C 2	Hg 1	0	0
2	H	1	Total 3	C 2	Hg 1	0	0
2	I	1	Total 3	C 2	Hg 1	0	0
2	I	1	Total 3	C 2	Hg 1	0	0
2	J	1	Total 3	C 2	Hg 1	0	0
2	J	1	Total 3	C 2	Hg 1	0	0
2	K	1	Total 3	C 2	Hg 1	0	0
2	K	1	Total 3	C 2	Hg 1	0	0
2	L	1	Total 3	C 2	Hg 1	0	0
2	L	1	Total 3	C 2	Hg 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	M	1	Total C Hg 3 2 1	0	0
2	M	1	Total C Hg 3 2 1	0	0
2	N	1	Total C Hg 3 2 1	0	0
2	N	1	Total C Hg 3 2 1	0	0
2	O	1	Total C Hg 3 2 1	0	0
2	O	1	Total C Hg 3 2 1	0	0
2	P	1	Total C Hg 3 2 1	0	0
2	P	1	Total C Hg 3 2 1	0	0
2	Q	1	Total C Hg 3 2 1	0	0
2	Q	1	Total C Hg 3 2 1	0	0
2	R	1	Total C Hg 3 2 1	0	0
2	R	1	Total C Hg 3 2 1	0	0
2	S	1	Total C Hg 3 2 1	0	0
2	S	1	Total C Hg 3 2 1	0	0
2	T	1	Total C Hg 3 2 1	0	0
2	T	1	Total C Hg 3 2 1	0	0
2	U	1	Total C Hg 3 2 1	0	0
2	U	1	Total C Hg 3 2 1	0	0
2	V	1	Total C Hg 3 2 1	0	0
2	V	1	Total C Hg 3 2 1	0	0
2	W	1	Total C Hg 3 2 1	0	0

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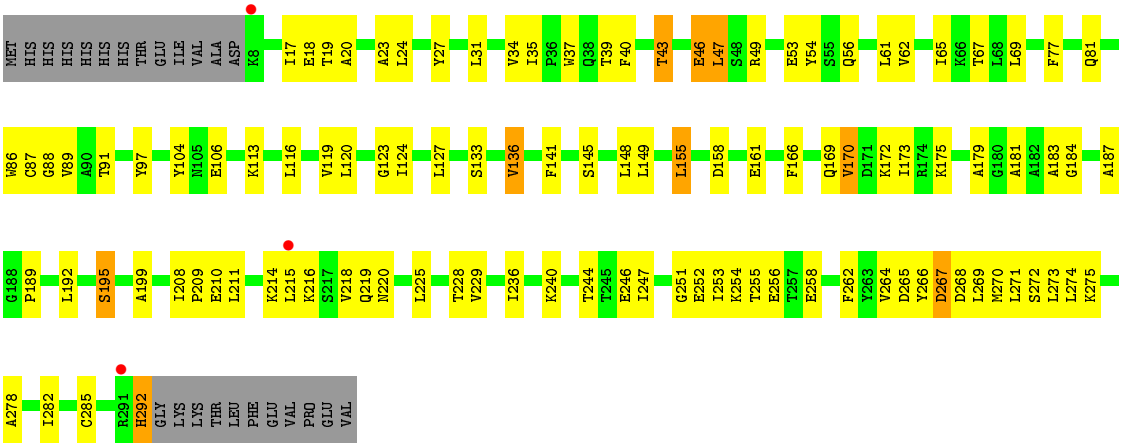
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	W	1	Total	C	Hg	0	0
			3	2	1		
2	X	1	Total	C	Hg	0	0
			3	2	1		
2	X	1	Total	C	Hg	0	0
			3	2	1		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

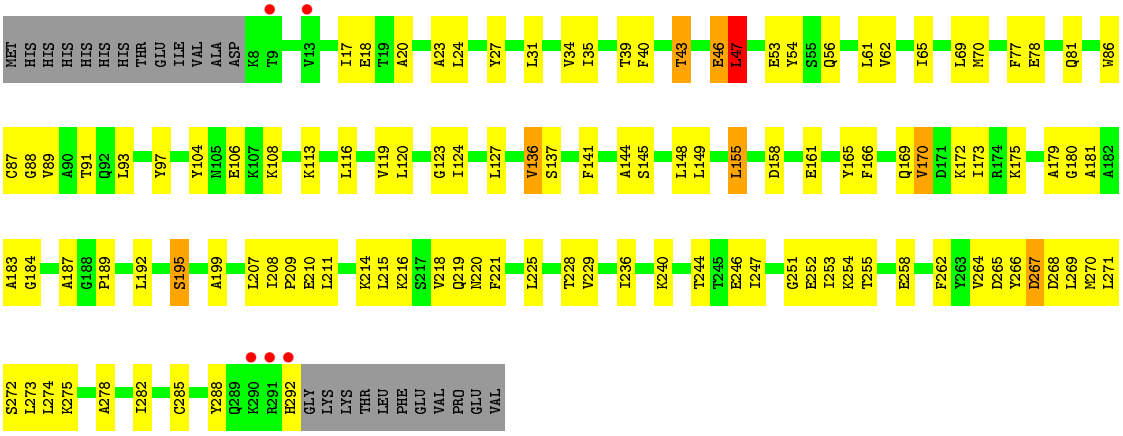
• Molecule 1: HEMOLYSIN E, CHROMOSOMAL

Chain A:



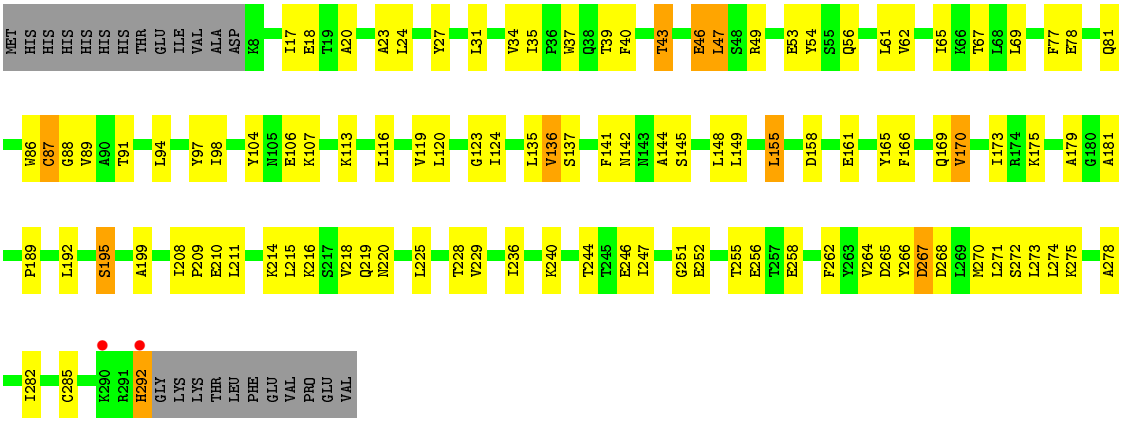
• Molecule 1: HEMOLYSIN E, CHROMOSOMAL

Chain B:



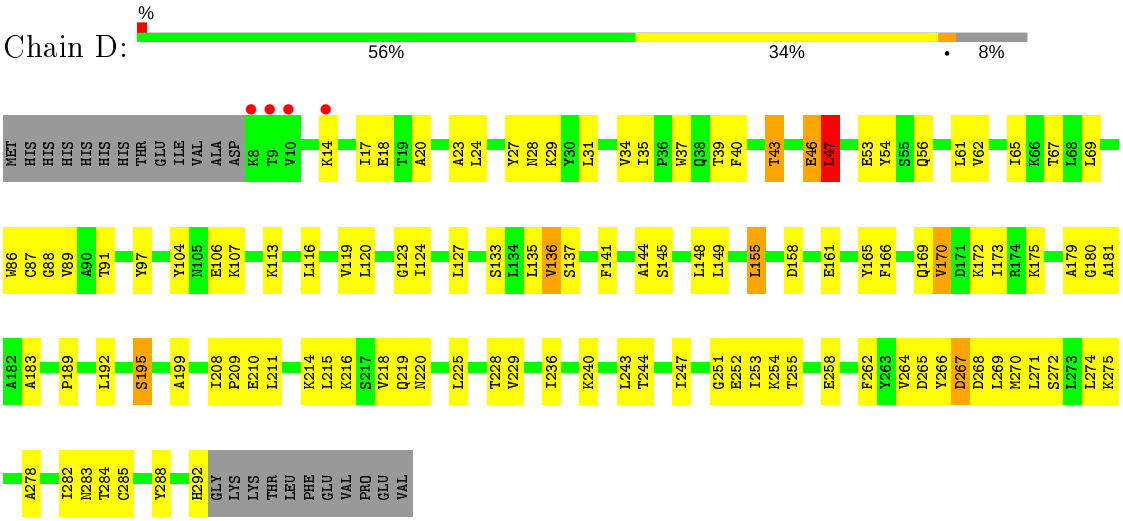
• Molecule 1: HEMOLYSIN E, CHROMOSOMAL

Chain C:



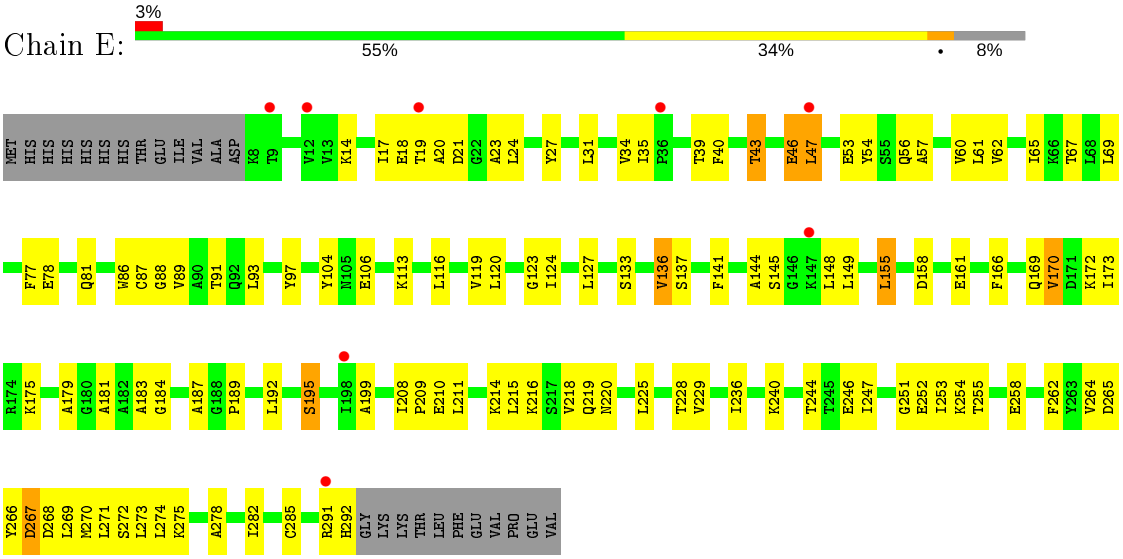
• Molecule 1: HEMOLYSIN E, CHROMOSOMAL

Chain D:

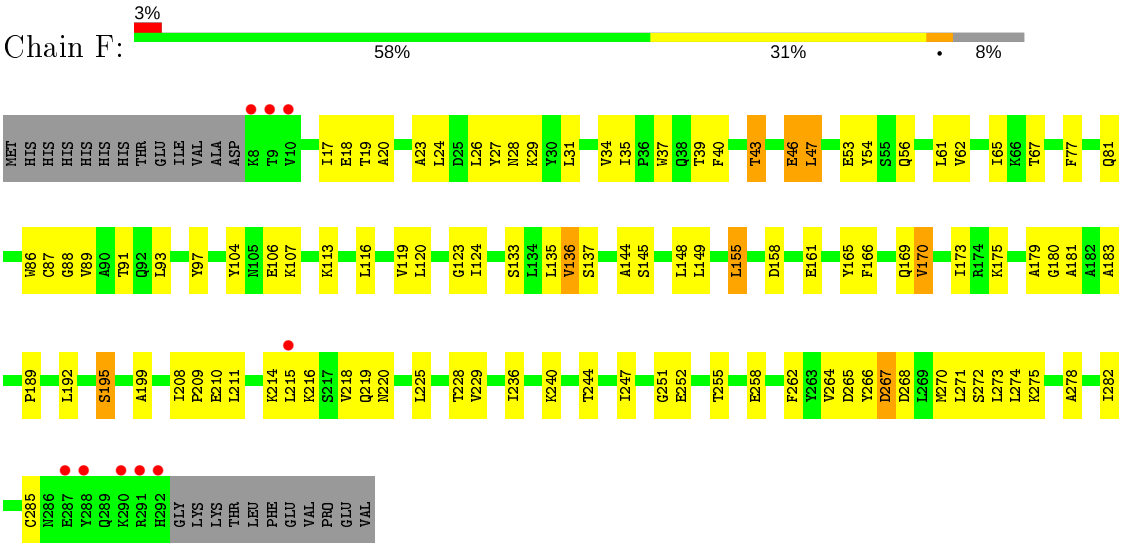


• Molecule 1: HEMOLYSIN E, CHROMOSOMAL

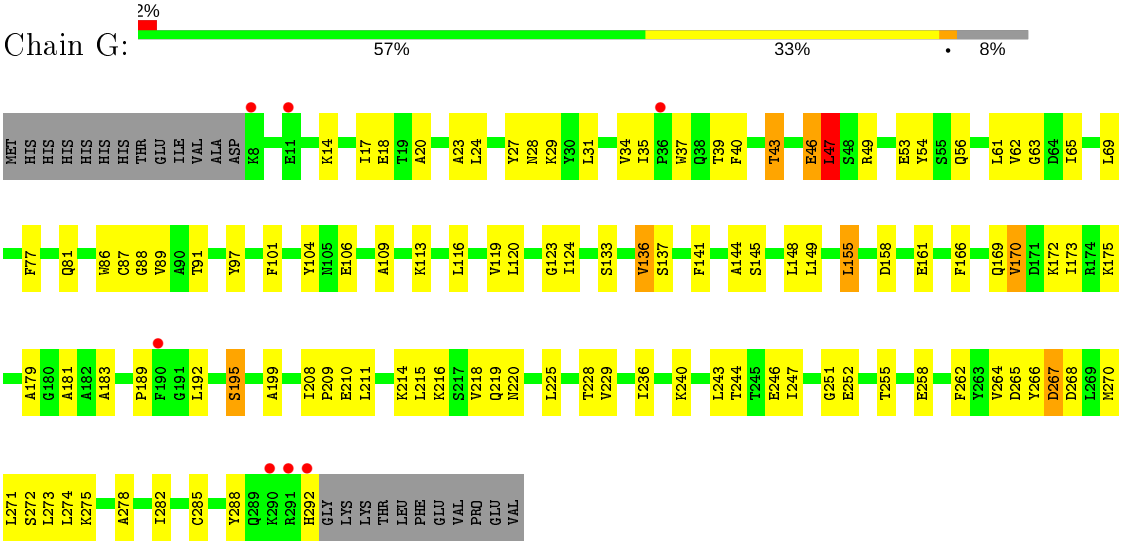
Chain E:



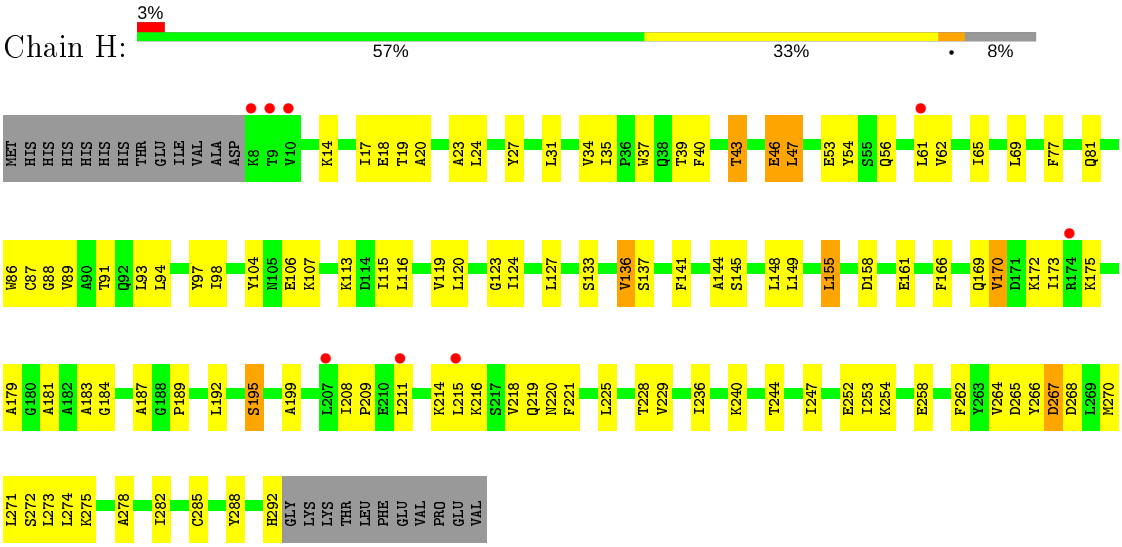
• Molecule 1: HEMOLYSIN E, CHROMOSOMAL



• Molecule 1: HEMOLYSIN E, CHROMOSOMAL

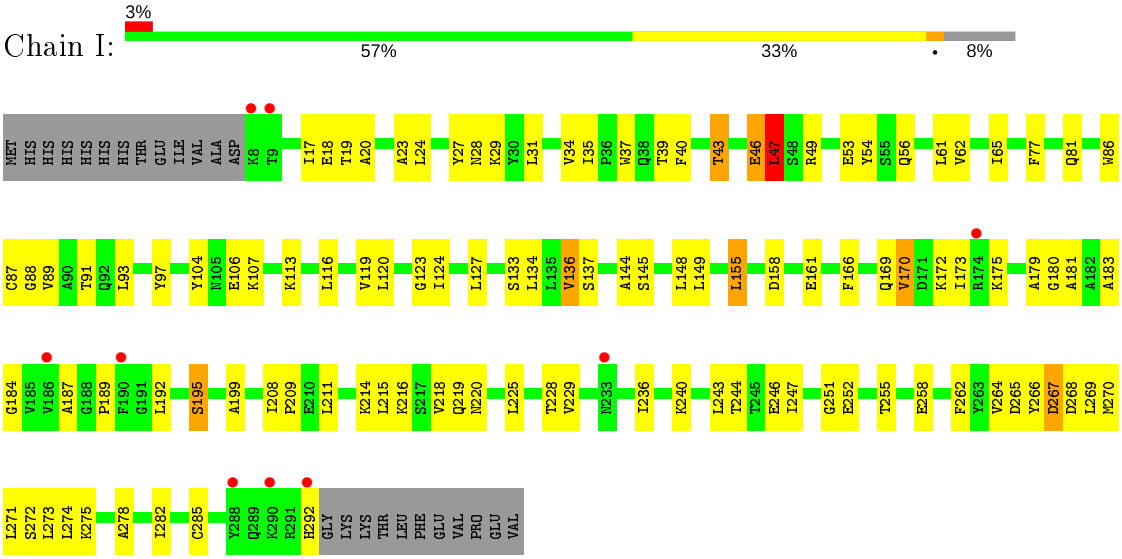


• Molecule 1: HEMOLYSIN E, CHROMOSOMAL



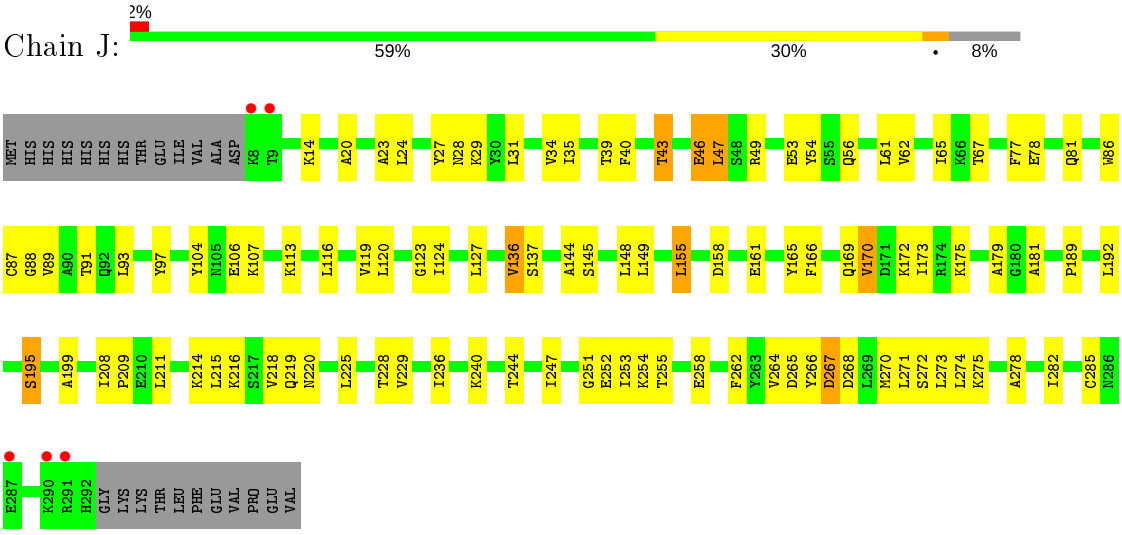
• Molecule 1: HEMOLYSIN E, CHROMOSOMAL

Chain I:



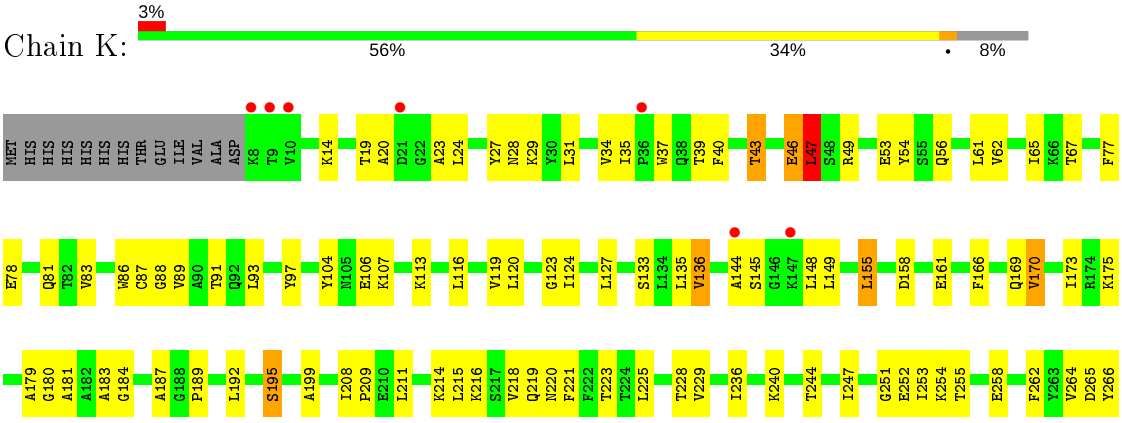
• Molecule 1: HEMOLYSIN E, CHROMOSOMAL

Chain J:

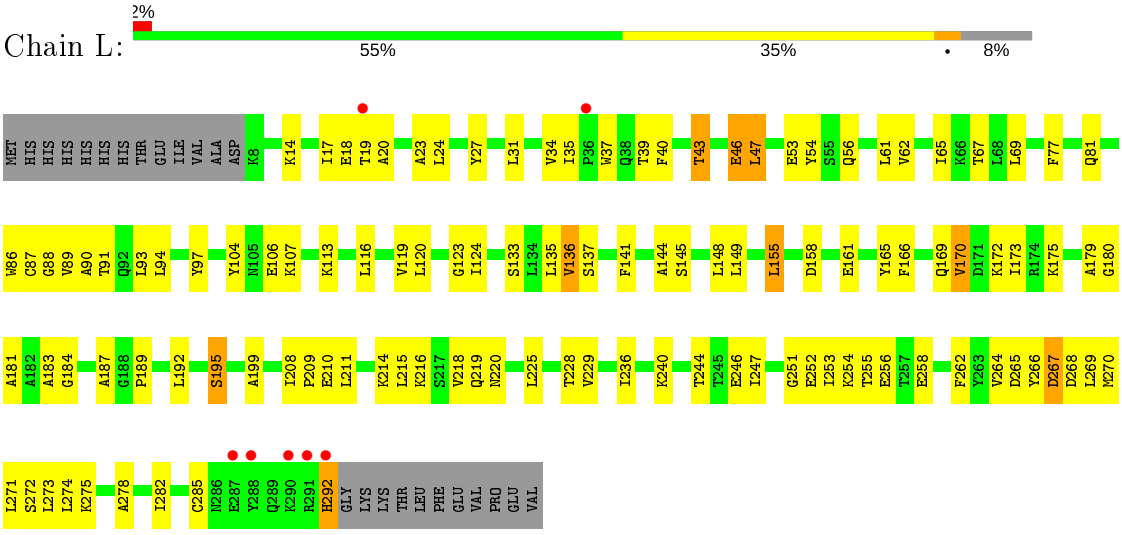


• Molecule 1: HEMOLYSIN E, CHROMOSOMAL

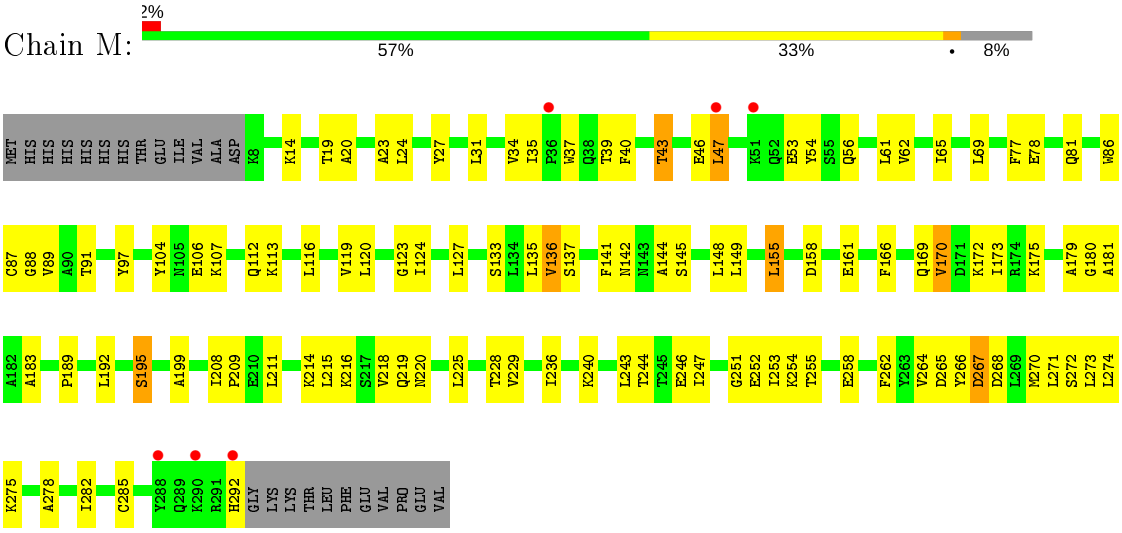
Chain K:



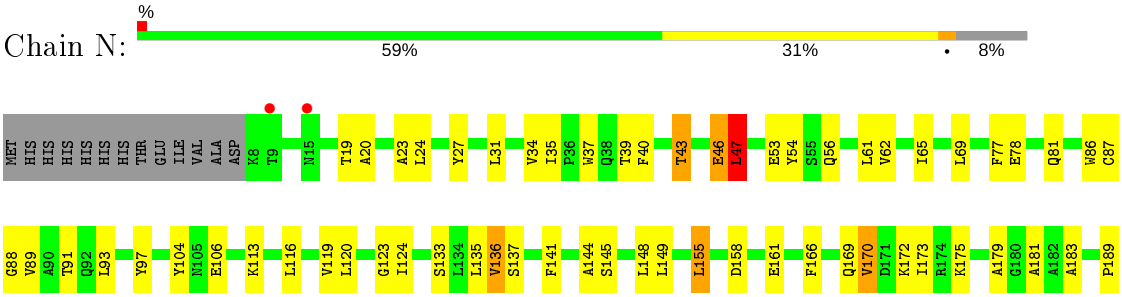
• Molecule 1: HEMOLYSIN E, CHROMOSOMAL

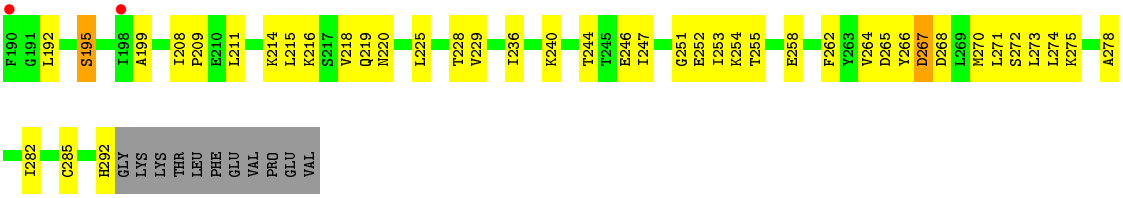


• Molecule 1: HEMOLYSIN E, CHROMOSOMAL



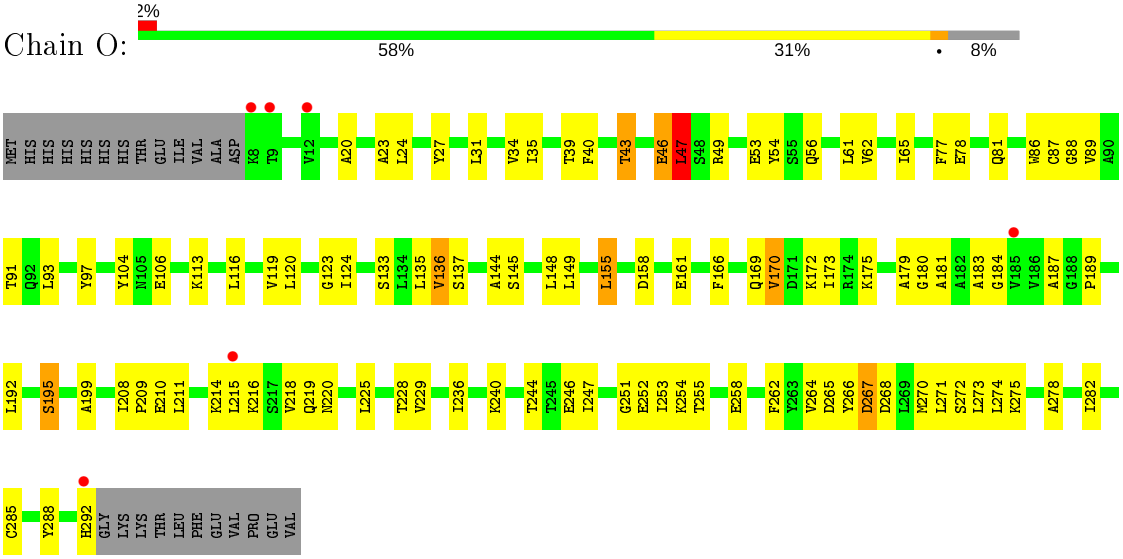
• Molecule 1: HEMOLYSIN E, CHROMOSOMAL





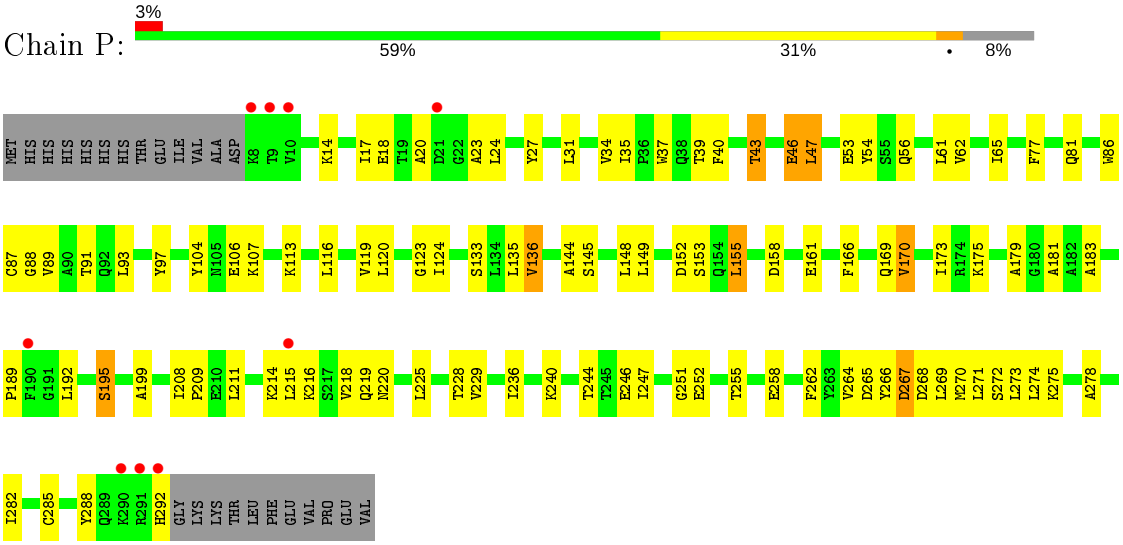
• Molecule 1: HEMOLYSIN E, CHROMOSOMAL

Chain O:



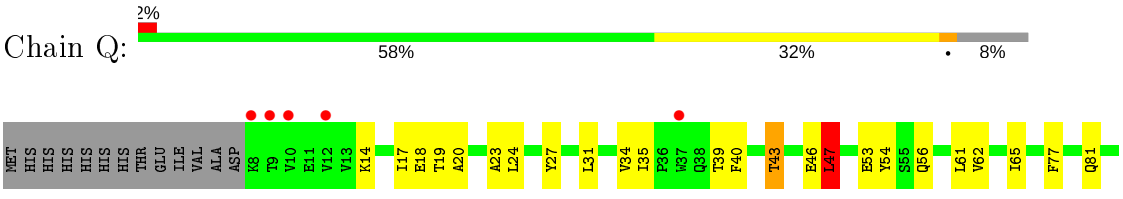
• Molecule 1: HEMOLYSIN E, CHROMOSOMAL

Chain P:



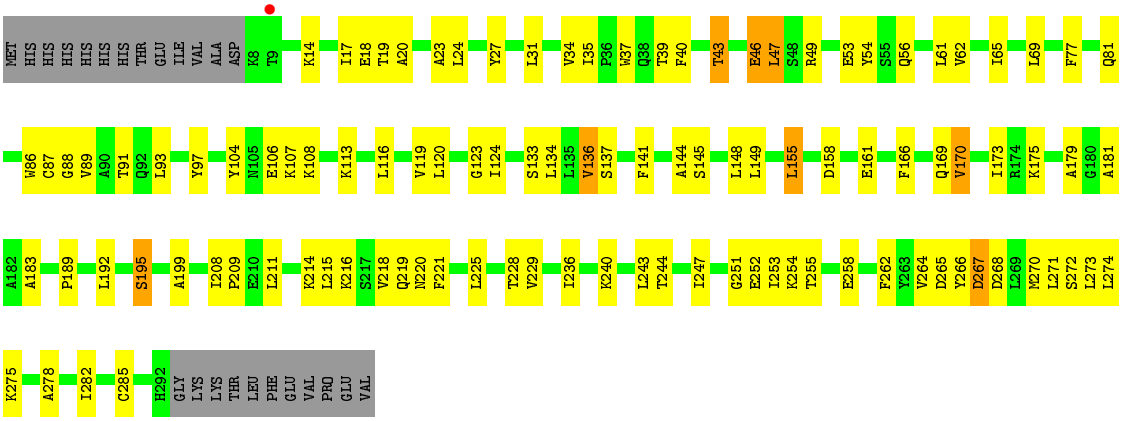
• Molecule 1: HEMOLYSIN E, CHROMOSOMAL

Chain Q:



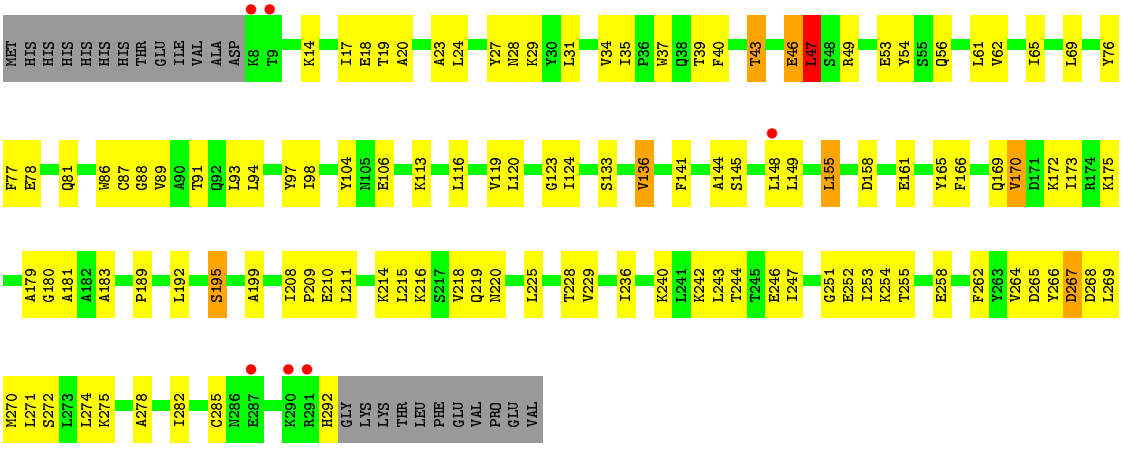
• Molecule 1: HEMOLYSIN E, CHROMOSOMAL

Chain R:



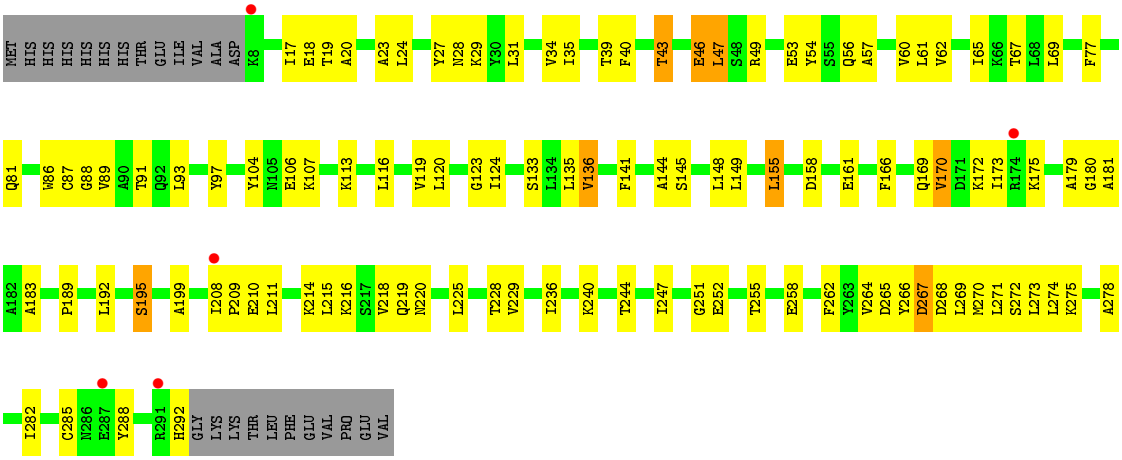
• Molecule 1: HEMOLYSIN E, CHROMOSOMAL

Chain S:



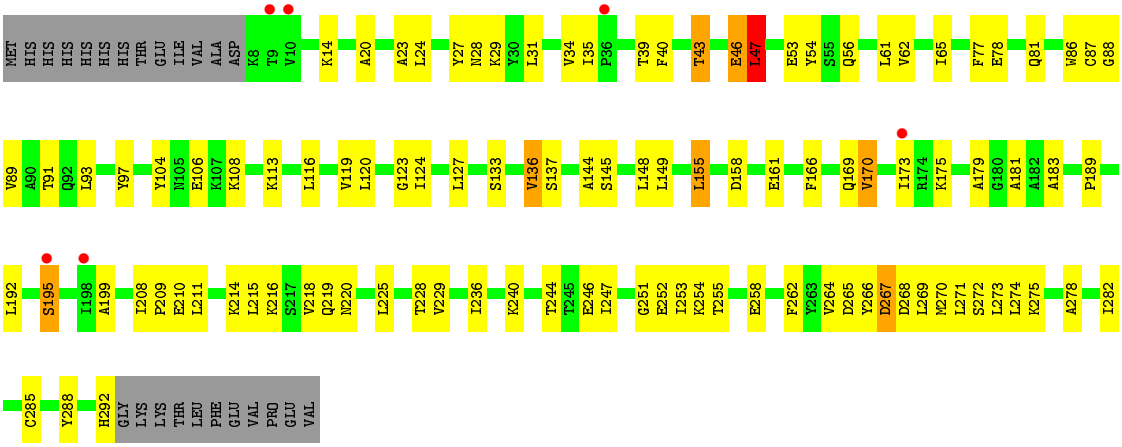
• Molecule 1: HEMOLYSIN E, CHROMOSOMAL

Chain T:



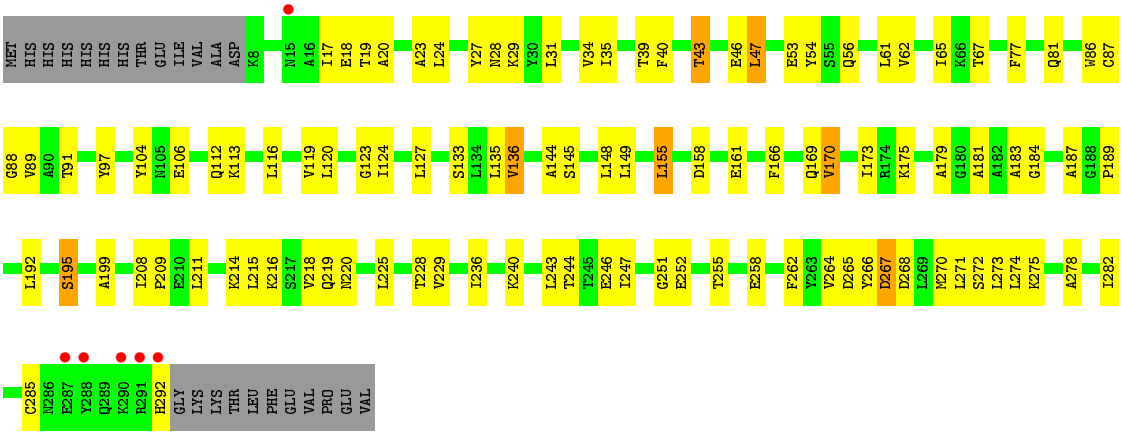
• Molecule 1: HEMOLYSIN E, CHROMOSOMAL

Chain U:



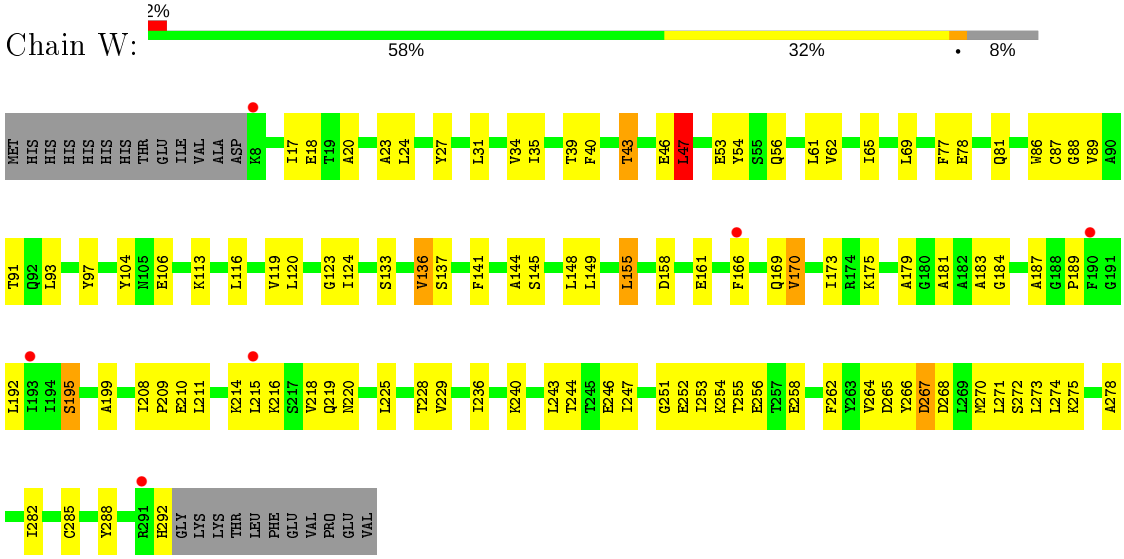
• Molecule 1: HEMOLYSIN E, CHROMOSOMAL

Chain V:



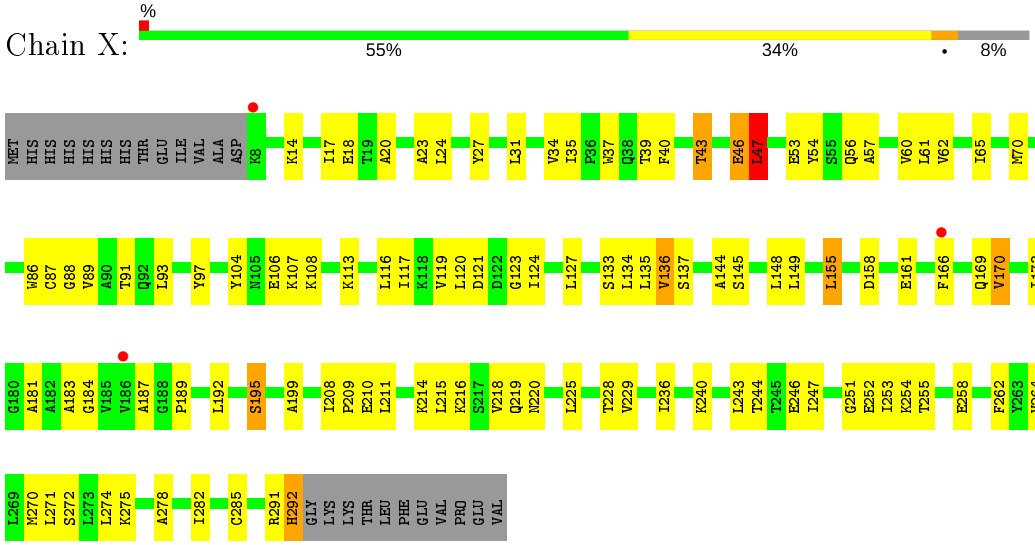
• Molecule 1: HEMOLYSIN E, CHROMOSOMAL

Chain W:



• Molecule 1: HEMOLYSIN E, CHROMOSOMAL

Chain X:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	111.43Å 114.41Å 270.55Å 94.44° 85.92° 102.55°	Depositor
Resolution (Å)	49.37 – 3.29 49.36 – 3.29	Depositor EDS
% Data completeness (in resolution range)	88.1 (49.37-3.29) 94.5 (49.36-3.29)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.03 (at 3.25Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.228 , 0.244 0.224 , 0.237	Depositor DCC
R_{free} test set	3745 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å^2)	98.8	Xtriage
Anisotropy	0.523	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 86.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.038 for k,h,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	53832	wwPDB-VP
Average B, all atoms (Å^2)	128.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.91% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EMC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.35	0/2268	0.47	0/3062
1	B	0.36	0/2268	0.48	1/3062 (0.0%)
1	C	0.35	0/2268	0.48	0/3062
1	D	0.37	0/2268	0.48	1/3062 (0.0%)
1	E	0.35	0/2268	0.48	0/3062
1	F	0.33	0/2268	0.48	0/3062
1	G	0.34	0/2268	0.47	1/3062 (0.0%)
1	H	0.34	0/2268	0.48	0/3062
1	I	0.35	0/2268	0.49	1/3062 (0.0%)
1	J	0.34	0/2268	0.48	0/3062
1	K	0.34	0/2268	0.48	1/3062 (0.0%)
1	L	0.35	0/2268	0.48	0/3062
1	M	0.34	0/2268	0.48	0/3062
1	N	0.35	0/2268	0.48	1/3062 (0.0%)
1	O	0.35	0/2268	0.48	1/3062 (0.0%)
1	P	0.33	0/2268	0.48	0/3062
1	Q	0.35	0/2268	0.49	1/3062 (0.0%)
1	R	0.35	0/2268	0.49	0/3062
1	S	0.35	0/2268	0.49	1/3062 (0.0%)
1	T	0.35	0/2268	0.48	0/3062
1	U	0.35	0/2268	0.49	1/3062 (0.0%)
1	V	0.35	0/2268	0.48	0/3062
1	W	0.35	0/2268	0.48	1/3062 (0.0%)
1	X	0.35	0/2268	0.49	1/3062 (0.0%)
All	All	0.35	0/54432	0.48	12/73488 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	S	47	LEU	CA-CB-CG	5.41	127.75	115.30
1	I	47	LEU	CA-CB-CG	5.22	127.30	115.30
1	D	47	LEU	CA-CB-CG	5.16	127.17	115.30
1	K	47	LEU	CA-CB-CG	5.16	127.17	115.30
1	B	47	LEU	CA-CB-CG	5.15	127.14	115.30
1	X	47	LEU	CA-CB-CG	5.09	127.00	115.30
1	G	47	LEU	CA-CB-CG	5.08	126.98	115.30
1	W	47	LEU	CA-CB-CG	5.07	126.97	115.30
1	N	47	LEU	CA-CB-CG	5.04	126.88	115.30
1	Q	47	LEU	CA-CB-CG	5.04	126.88	115.30
1	U	47	LEU	CA-CB-CG	5.02	126.84	115.30
1	O	47	LEU	CA-CB-CG	5.01	126.83	115.30

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	A	2237	0	2264	88	0
1	B	2237	0	2264	91	0
1	C	2237	0	2264	97	0
1	D	2237	0	2264	93	0
1	E	2237	0	2264	95	0
1	F	2237	0	2264	87	0
1	G	2237	0	2264	88	0
1	H	2237	0	2264	93	0
1	I	2237	0	2264	93	0
1	J	2237	0	2264	84	0
1	K	2237	0	2264	88	0
1	L	2237	0	2264	96	0
1	M	2237	0	2264	90	0
1	N	2237	0	2264	85	0
1	O	2237	0	2264	86	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	P	2237	0	2264	88	0
1	Q	2237	0	2264	92	0
1	R	2237	0	2264	93	0
1	S	2237	0	2264	91	0
1	T	2237	0	2264	85	0
1	U	2237	0	2264	88	0
1	V	2237	0	2264	85	0
1	W	2237	0	2264	90	0
1	X	2237	0	2264	96	0
2	A	6	0	0	2	0
2	B	6	0	0	2	0
2	C	6	0	0	2	0
2	D	6	0	0	2	0
2	E	6	0	0	2	0
2	F	6	0	0	2	0
2	G	6	0	0	2	0
2	H	6	0	0	2	0
2	I	6	0	0	2	0
2	J	6	0	0	2	0
2	K	6	0	0	2	0
2	L	6	0	0	2	0
2	M	6	0	0	2	0
2	N	6	0	0	2	0
2	O	6	0	0	2	0
2	P	6	0	0	2	0
2	Q	6	0	0	2	0
2	R	6	0	0	2	0
2	S	6	0	0	2	0
2	T	6	0	0	2	0
2	U	6	0	0	2	0
2	V	6	0	0	2	0
2	W	6	0	0	2	0
2	X	6	0	0	2	0
All	All	53832	0	54336	2050	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 19.

All (2050) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:305:EMC:C1	2:C:305:EMC:C2	1.84	1.55
2:F:304:EMC:C1	2:F:304:EMC:C2	1.84	1.55
2:H:304:EMC:C1	2:H:304:EMC:C2	1.84	1.55
2:I:305:EMC:C1	2:I:305:EMC:C2	1.84	1.55
2:N:304:EMC:C2	2:N:304:EMC:C1	1.84	1.55
2:H:305:EMC:C1	2:H:305:EMC:C2	1.85	1.55
2:R:305:EMC:C1	2:R:305:EMC:C2	1.84	1.54
2:A:305:EMC:C1	2:A:305:EMC:C2	1.84	1.54
2:O:304:EMC:C1	2:O:304:EMC:C2	1.85	1.54
2:N:305:EMC:C2	2:N:305:EMC:C1	1.84	1.54
2:V:305:EMC:C1	2:V:305:EMC:C2	1.85	1.54
2:I:304:EMC:C2	2:I:304:EMC:C1	1.84	1.54
2:D:305:EMC:C2	2:D:305:EMC:C1	1.86	1.53
2:W:305:EMC:C2	2:W:305:EMC:C1	1.85	1.53
2:G:305:EMC:C1	2:G:305:EMC:C2	1.85	1.53
2:J:305:EMC:C2	2:J:305:EMC:C1	1.85	1.53
2:K:304:EMC:C1	2:K:304:EMC:C2	1.84	1.53
2:C:304:EMC:C1	2:C:304:EMC:C2	1.85	1.53
2:W:304:EMC:C1	2:W:304:EMC:C2	1.86	1.53
2:J:304:EMC:C1	2:J:304:EMC:C2	1.84	1.53
2:M:305:EMC:C2	2:M:305:EMC:C1	1.84	1.53
2:X:305:EMC:C1	2:X:305:EMC:C2	1.85	1.53
2:S:304:EMC:C1	2:S:304:EMC:C2	1.84	1.52
2:X:304:EMC:C1	2:X:304:EMC:C2	1.84	1.52
2:T:304:EMC:C1	2:T:304:EMC:C2	1.85	1.52
2:E:305:EMC:C2	2:E:305:EMC:C1	1.84	1.52
2:V:304:EMC:C1	2:V:304:EMC:C2	1.85	1.52
2:B:305:EMC:C1	2:B:305:EMC:C2	1.85	1.52
2:P:304:EMC:C1	2:P:304:EMC:C2	1.85	1.52
2:U:304:EMC:C2	2:U:304:EMC:C1	1.85	1.52
2:G:304:EMC:C1	2:G:304:EMC:C2	1.84	1.51
2:T:305:EMC:C1	2:T:305:EMC:C2	1.85	1.51
2:K:305:EMC:C2	2:K:305:EMC:C1	1.84	1.51
2:Q:305:EMC:C1	2:Q:305:EMC:C2	1.84	1.51
2:R:304:EMC:C2	2:R:304:EMC:C1	1.84	1.51
2:S:305:EMC:C2	2:S:305:EMC:C1	1.84	1.51
2:Q:304:EMC:C1	2:Q:304:EMC:C2	1.84	1.51
2:E:304:EMC:C1	2:E:304:EMC:C2	1.85	1.51
2:B:304:EMC:C1	2:B:304:EMC:C2	1.84	1.50
2:P:305:EMC:C2	2:P:305:EMC:C1	1.84	1.50
2:L:305:EMC:C2	2:L:305:EMC:C1	1.85	1.50
2:A:304:EMC:C2	2:A:304:EMC:C1	1.85	1.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:304:EMC:C1	2:L:304:EMC:C2	1.85	1.50
2:D:304:EMC:C2	2:D:304:EMC:C1	1.85	1.50
2:O:305:EMC:C1	2:O:305:EMC:C2	1.85	1.49
2:M:304:EMC:C1	2:M:304:EMC:C2	1.85	1.49
2:F:305:EMC:C1	2:F:305:EMC:C2	1.84	1.49
2:U:305:EMC:C1	2:U:305:EMC:C2	1.84	1.49
1:C:43:THR:OG1	1:C:169:GLN:HG2	1.59	1.03
1:I:43:THR:OG1	1:I:169:GLN:HG2	1.59	1.03
1:B:43:THR:OG1	1:B:169:GLN:HG2	1.59	1.02
1:G:43:THR:OG1	1:G:169:GLN:HG2	1.60	1.02
1:Q:43:THR:OG1	1:Q:169:GLN:HG2	1.61	1.01
1:A:43:THR:OG1	1:A:169:GLN:HG2	1.59	1.01
1:U:43:THR:OG1	1:U:169:GLN:HG2	1.61	1.01
1:V:43:THR:OG1	1:V:169:GLN:HG2	1.62	1.00
1:X:43:THR:OG1	1:X:169:GLN:HG2	1.61	1.00
1:L:43:THR:OG1	1:L:169:GLN:HG2	1.62	1.00
1:W:43:THR:OG1	1:W:169:GLN:HG2	1.62	0.99
1:E:43:THR:OG1	1:E:169:GLN:HG2	1.62	0.99
1:R:43:THR:OG1	1:R:169:GLN:HG2	1.61	0.99
1:M:43:THR:OG1	1:M:169:GLN:HG2	1.63	0.98
1:D:43:THR:OG1	1:D:169:GLN:HG2	1.63	0.98
1:O:43:THR:OG1	1:O:169:GLN:HG2	1.62	0.98
1:T:43:THR:OG1	1:T:169:GLN:HG2	1.63	0.98
1:N:43:THR:OG1	1:N:169:GLN:HG2	1.60	0.98
1:K:43:THR:OG1	1:K:169:GLN:HG2	1.63	0.97
1:S:43:THR:OG1	1:S:169:GLN:HG2	1.62	0.97
1:J:43:THR:OG1	1:J:169:GLN:HG2	1.63	0.97
1:H:43:THR:OG1	1:H:169:GLN:HG2	1.62	0.96
1:F:43:THR:OG1	1:F:169:GLN:HG2	1.64	0.95
1:P:43:THR:OG1	1:P:169:GLN:HG2	1.66	0.94
1:K:264:VAL:HG23	1:K:274:LEU:HD11	1.59	0.85
1:R:264:VAL:HG23	1:R:274:LEU:HD11	1.58	0.83
1:T:264:VAL:HG23	1:T:274:LEU:HD11	1.59	0.82
1:V:264:VAL:HG23	1:V:274:LEU:HD11	1.62	0.81
1:E:264:VAL:HG23	1:E:274:LEU:HD11	1.62	0.81
1:J:264:VAL:HG23	1:J:274:LEU:HD11	1.63	0.81
1:H:264:VAL:HG23	1:H:274:LEU:HD11	1.63	0.80
1:G:264:VAL:HG23	1:G:274:LEU:HD11	1.64	0.80
1:W:264:VAL:HG23	1:W:274:LEU:HD11	1.63	0.80
1:S:37:TRP:HE1	1:T:172:LYS:HZ3	1.30	0.79
1:A:264:VAL:HG23	1:A:274:LEU:HD11	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:264:VAL:HG23	1:U:274:LEU:HD11	1.65	0.79
1:F:264:VAL:HG23	1:F:274:LEU:HD11	1.65	0.78
1:M:264:VAL:HG23	1:M:274:LEU:HD11	1.64	0.78
1:N:264:VAL:HG23	1:N:274:LEU:HD11	1.66	0.78
1:L:264:VAL:HG23	1:L:274:LEU:HD11	1.65	0.78
1:D:288:TYR:O	1:D:292:HIS:HB3	1.83	0.78
1:X:266:TYR:O	1:X:267:ASP:HB2	1.82	0.78
1:M:266:TYR:O	1:M:267:ASP:HB2	1.82	0.78
1:B:264:VAL:HG23	1:B:274:LEU:HD11	1.63	0.78
1:P:264:VAL:HG23	1:P:274:LEU:HD11	1.66	0.78
1:S:264:VAL:HG23	1:S:274:LEU:HD11	1.66	0.77
1:A:172:LYS:HZ3	1:L:37:TRP:HE1	1.31	0.77
1:O:264:VAL:HG23	1:O:274:LEU:HD11	1.65	0.77
1:E:266:TYR:O	1:E:267:ASP:HB2	1.84	0.77
1:F:266:TYR:O	1:F:267:ASP:HB2	1.84	0.77
1:C:264:VAL:HG23	1:C:274:LEU:HD11	1.67	0.76
1:M:37:TRP:HE1	1:N:172:LYS:HZ3	1.35	0.75
1:C:62:VAL:HG12	1:D:149:LEU:HD21	1.69	0.75
1:N:266:TYR:O	1:N:267:ASP:HB2	1.87	0.75
1:Q:264:VAL:HG23	1:Q:274:LEU:HD11	1.68	0.75
1:B:266:TYR:O	1:B:267:ASP:HB2	1.85	0.74
1:G:62:VAL:HG12	1:H:149:LEU:HD21	1.67	0.74
1:D:264:VAL:HG23	1:D:274:LEU:HD11	1.70	0.74
1:K:266:TYR:O	1:K:267:ASP:HB2	1.84	0.74
1:F:86:TRP:CE2	1:F:123:GLY:HA3	2.23	0.74
1:M:86:TRP:CE2	1:M:123:GLY:HA3	2.23	0.74
1:O:266:TYR:O	1:O:267:ASP:HB2	1.87	0.73
1:X:264:VAL:HG23	1:X:274:LEU:HD11	1.70	0.73
1:J:266:TYR:O	1:J:267:ASP:HB2	1.89	0.73
1:R:266:TYR:O	1:R:267:ASP:HB2	1.87	0.73
1:I:264:VAL:HG23	1:I:274:LEU:HD11	1.67	0.73
1:W:266:TYR:O	1:W:267:ASP:HB2	1.89	0.73
1:W:62:VAL:HG12	1:X:149:LEU:HD21	1.70	0.73
1:R:86:TRP:CE2	1:R:123:GLY:HA3	2.24	0.73
1:Q:62:VAL:HG12	1:R:149:LEU:HD21	1.70	0.73
1:W:86:TRP:CE2	1:W:123:GLY:HA3	2.24	0.72
1:G:86:TRP:CE2	1:G:123:GLY:HA3	2.24	0.72
1:G:31:LEU:HD21	1:H:179:ALA:HB1	1.71	0.72
1:K:86:TRP:CE2	1:K:123:GLY:HA3	2.23	0.72
1:S:86:TRP:CE2	1:S:123:GLY:HA3	2.24	0.72
1:Q:86:TRP:CE2	1:Q:123:GLY:HA3	2.24	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:24:LEU:O	1:I:27:TYR:HB3	1.90	0.72
1:N:86:TRP:CE2	1:N:123:GLY:HA3	2.25	0.72
1:N:37:TRP:HE1	1:O:172:LYS:HZ3	1.35	0.72
1:T:266:TYR:O	1:T:267:ASP:HB2	1.86	0.72
1:U:86:TRP:CE2	1:U:123:GLY:HA3	2.25	0.72
1:P:266:TYR:O	1:P:267:ASP:HB2	1.88	0.72
1:T:86:TRP:CE2	1:T:123:GLY:HA3	2.24	0.72
1:H:86:TRP:CE2	1:H:123:GLY:HA3	2.25	0.72
1:I:86:TRP:CE2	1:I:123:GLY:HA3	2.25	0.71
1:D:266:TYR:O	1:D:267:ASP:HB2	1.89	0.71
1:H:62:VAL:HG12	1:I:149:LEU:HD21	1.73	0.71
1:A:86:TRP:CE2	1:A:123:GLY:HA3	2.24	0.71
1:W:97:TYR:OH	1:W:274:LEU:HD23	1.90	0.71
1:I:54:TYR:CE1	1:I:155:LEU:HB2	2.26	0.71
1:L:86:TRP:CE2	1:L:123:GLY:HA3	2.24	0.71
1:S:266:TYR:O	1:S:267:ASP:HB2	1.89	0.71
1:U:54:TYR:CE1	1:U:155:LEU:HB2	2.26	0.71
1:V:86:TRP:CE2	1:V:123:GLY:HA3	2.26	0.71
1:L:266:TYR:O	1:L:267:ASP:HB2	1.89	0.71
1:B:86:TRP:CE2	1:B:123:GLY:HA3	2.26	0.70
1:P:86:TRP:CE2	1:P:123:GLY:HA3	2.25	0.70
1:Q:266:TYR:O	1:Q:267:ASP:HB2	1.90	0.70
1:A:266:TYR:O	1:A:267:ASP:HB2	1.89	0.70
1:E:86:TRP:CE2	1:E:123:GLY:HA3	2.25	0.70
1:A:54:TYR:CE1	1:A:155:LEU:HB2	2.26	0.70
1:O:86:TRP:CE2	1:O:123:GLY:HA3	2.26	0.70
1:W:54:TYR:CE1	1:W:155:LEU:HB2	2.26	0.70
1:C:86:TRP:CE2	1:C:123:GLY:HA3	2.26	0.70
1:J:43:THR:HG1	1:J:169:GLN:HG2	1.55	0.70
1:X:54:TYR:CE1	1:X:155:LEU:HB2	2.27	0.70
1:D:62:VAL:HG12	1:E:149:LEU:HD21	1.74	0.70
1:H:54:TYR:CE1	1:H:155:LEU:HB2	2.26	0.70
1:M:54:TYR:CE1	1:M:155:LEU:HB2	2.27	0.70
1:G:266:TYR:O	1:G:267:ASP:HB2	1.92	0.69
1:R:97:TYR:OH	1:R:274:LEU:HD23	1.92	0.69
1:U:266:TYR:O	1:U:267:ASP:HB2	1.90	0.69
1:D:86:TRP:CE2	1:D:123:GLY:HA3	2.28	0.69
1:G:54:TYR:CE1	1:G:155:LEU:HB2	2.27	0.69
1:M:24:LEU:O	1:M:27:TYR:HB3	1.92	0.69
1:X:97:TYR:OH	1:X:274:LEU:HD23	1.93	0.69
1:D:54:TYR:CE1	1:D:155:LEU:HB2	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:86:TRP:CE2	1:J:123:GLY:HA3	2.28	0.69
1:O:62:VAL:HG12	1:P:149:LEU:HD21	1.74	0.69
1:H:266:TYR:O	1:H:267:ASP:HB2	1.92	0.69
1:T:54:TYR:CE1	1:T:155:LEU:HB2	2.28	0.69
1:U:288:TYR:O	1:U:292:HIS:HB3	1.93	0.69
1:S:24:LEU:O	1:S:27:TYR:HB3	1.94	0.68
1:V:266:TYR:O	1:V:267:ASP:HB2	1.93	0.68
1:V:97:TYR:OH	1:V:274:LEU:HD23	1.93	0.68
1:X:86:TRP:CE2	1:X:123:GLY:HA3	2.28	0.68
1:E:97:TYR:OH	1:E:274:LEU:HD23	1.94	0.68
1:G:24:LEU:O	1:G:27:TYR:HB3	1.94	0.68
1:C:54:TYR:CE1	1:C:155:LEU:HB2	2.29	0.68
1:Q:40:PHE:O	1:Q:43:THR:HG22	1.94	0.68
1:R:54:TYR:CE1	1:R:155:LEU:HB2	2.29	0.68
1:W:120:LEU:O	1:W:124:ILE:HG13	1.93	0.68
1:P:54:TYR:CE1	1:P:155:LEU:HB2	2.29	0.67
1:X:24:LEU:O	1:X:27:TYR:HB3	1.95	0.67
1:C:91:THR:HG23	1:C:282:ILE:HG23	1.76	0.67
1:X:120:LEU:O	1:X:124:ILE:HG13	1.93	0.67
1:C:24:LEU:O	1:C:27:TYR:HB3	1.95	0.67
1:I:62:VAL:HG12	1:J:149:LEU:HD21	1.75	0.67
1:J:97:TYR:OH	1:J:274:LEU:HD23	1.95	0.67
1:J:54:TYR:CE1	1:J:155:LEU:HB2	2.30	0.67
1:I:266:TYR:O	1:I:267:ASP:HB2	1.94	0.67
1:L:97:TYR:OH	1:L:274:LEU:HD23	1.95	0.67
1:Q:91:THR:HG23	1:Q:282:ILE:HG23	1.77	0.67
1:A:24:LEU:O	1:A:27:TYR:HB3	1.94	0.67
1:H:37:TRP:HE1	1:I:172:LYS:HZ3	1.43	0.67
1:A:149:LEU:HD21	1:L:62:VAL:HG12	1.77	0.67
1:J:91:THR:HG23	1:J:282:ILE:HG23	1.75	0.67
1:M:62:VAL:HG12	1:N:149:LEU:HD21	1.76	0.67
1:N:62:VAL:HG12	1:O:149:LEU:HD21	1.76	0.67
1:Q:54:TYR:CE1	1:Q:155:LEU:HB2	2.30	0.67
1:S:62:VAL:HG12	1:T:149:LEU:HD21	1.77	0.67
1:C:97:TYR:OH	1:C:274:LEU:HD23	1.95	0.67
1:F:54:TYR:CE1	1:F:155:LEU:HB2	2.29	0.67
1:H:120:LEU:O	1:H:124:ILE:HG13	1.94	0.67
1:U:24:LEU:O	1:U:27:TYR:HB3	1.94	0.67
1:J:24:LEU:O	1:J:27:TYR:HB3	1.94	0.66
1:K:97:TYR:OH	1:K:274:LEU:HD23	1.95	0.66
1:R:40:PHE:O	1:R:43:THR:HG22	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:VAL:HG12	1:B:149:LEU:HD21	1.76	0.66
1:L:54:TYR:CE1	1:L:155:LEU:HB2	2.30	0.66
1:N:54:TYR:CE1	1:N:155:LEU:HB2	2.30	0.66
1:P:91:THR:HG23	1:P:282:ILE:HG23	1.77	0.66
1:D:97:TYR:OH	1:D:274:LEU:HD23	1.96	0.66
1:E:54:TYR:CE1	1:E:155:LEU:HB2	2.31	0.66
1:I:40:PHE:O	1:I:43:THR:HG22	1.95	0.66
1:M:97:TYR:OH	1:M:274:LEU:HD23	1.95	0.66
1:N:40:PHE:O	1:N:43:THR:HG22	1.95	0.66
1:O:54:TYR:CE1	1:O:155:LEU:HB2	2.31	0.66
1:T:24:LEU:O	1:T:27:TYR:HB3	1.96	0.66
1:K:54:TYR:CE1	1:K:155:LEU:HB2	2.30	0.66
1:P:24:LEU:O	1:P:27:TYR:HB3	1.95	0.66
1:S:246:GLU:OE1	1:S:292:HIS:CD2	2.49	0.66
1:T:62:VAL:HG12	1:U:149:LEU:HD21	1.78	0.66
1:V:54:TYR:CE1	1:V:155:LEU:HB2	2.31	0.66
1:P:120:LEU:O	1:P:124:ILE:HG13	1.96	0.66
1:V:24:LEU:O	1:V:27:TYR:HB3	1.95	0.66
1:C:266:TYR:O	1:C:267:ASP:HB2	1.93	0.66
1:E:246:GLU:OE1	1:E:292:HIS:HD2	1.77	0.66
1:L:24:LEU:O	1:L:27:TYR:HB3	1.94	0.66
1:D:24:LEU:O	1:D:27:TYR:HB3	1.96	0.66
1:H:24:LEU:O	1:H:27:TYR:HB3	1.96	0.66
1:I:37:TRP:HE1	1:J:172:LYS:HZ3	1.43	0.66
1:K:24:LEU:O	1:K:27:TYR:HB3	1.96	0.66
1:P:40:PHE:O	1:P:43:THR:HG22	1.95	0.65
1:T:91:THR:HG23	1:T:282:ILE:HG23	1.78	0.65
1:V:62:VAL:HG12	1:W:149:LEU:HD21	1.77	0.65
1:F:62:VAL:HG12	1:G:149:LEU:HD21	1.77	0.65
1:O:24:LEU:O	1:O:27:TYR:HB3	1.96	0.65
1:Q:97:TYR:OH	1:Q:274:LEU:HD23	1.96	0.65
1:R:24:LEU:O	1:R:27:TYR:HB3	1.97	0.65
1:S:54:TYR:CE1	1:S:155:LEU:HB2	2.31	0.65
1:H:97:TYR:OH	1:H:274:LEU:HD23	1.97	0.65
1:B:40:PHE:O	1:B:43:THR:HG22	1.96	0.65
1:O:40:PHE:O	1:O:43:THR:HG22	1.97	0.65
1:P:97:TYR:OH	1:P:274:LEU:HD23	1.97	0.65
1:F:24:LEU:O	1:F:27:TYR:HB3	1.96	0.65
1:G:91:THR:HG23	1:G:282:ILE:HG23	1.78	0.65
1:V:91:THR:HG23	1:V:282:ILE:HG23	1.79	0.65
1:F:97:TYR:OH	1:F:274:LEU:HD23	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:91:THR:HG23	1:L:282:ILE:HG23	1.78	0.65
1:A:97:TYR:OH	1:A:274:LEU:HD23	1.97	0.64
1:B:91:THR:HG23	1:B:282:ILE:HG23	1.80	0.64
1:R:91:THR:HG23	1:R:282:ILE:HG23	1.80	0.64
1:B:54:TYR:CE1	1:B:155:LEU:HB2	2.32	0.64
1:H:40:PHE:O	1:H:43:THR:HG22	1.97	0.64
1:M:61:LEU:O	1:M:65:ILE:HG12	1.98	0.64
1:E:91:THR:HG23	1:E:282:ILE:HG23	1.79	0.64
1:N:24:LEU:O	1:N:27:TYR:HB3	1.96	0.64
1:S:97:TYR:OH	1:S:274:LEU:HD23	1.98	0.64
1:E:120:LEU:O	1:E:124:ILE:HG13	1.97	0.64
1:I:91:THR:HG23	1:I:282:ILE:HG23	1.78	0.64
1:O:120:LEU:O	1:O:124:ILE:HG13	1.97	0.64
1:S:91:THR:HG23	1:S:282:ILE:HG23	1.79	0.64
1:W:24:LEU:O	1:W:27:TYR:HB3	1.97	0.64
1:B:120:LEU:O	1:B:124:ILE:HG13	1.98	0.64
1:U:62:VAL:HG12	1:V:149:LEU:HD21	1.80	0.64
1:X:91:THR:HG23	1:X:282:ILE:HG23	1.80	0.63
1:K:91:THR:HG23	1:K:282:ILE:HG23	1.80	0.63
1:Q:24:LEU:O	1:Q:27:TYR:HB3	1.98	0.63
1:R:61:LEU:O	1:R:65:ILE:HG12	1.99	0.63
1:C:40:PHE:O	1:C:43:THR:HG22	1.97	0.63
1:P:62:VAL:HG12	1:Q:149:LEU:HD21	1.80	0.63
1:X:40:PHE:O	1:X:43:THR:HG22	1.99	0.63
1:E:24:LEU:O	1:E:27:TYR:HB3	1.98	0.63
1:M:31:LEU:HD21	1:N:179:ALA:HB1	1.81	0.63
1:S:40:PHE:O	1:S:43:THR:HG22	1.99	0.63
1:X:225:LEU:HD23	1:X:225:LEU:C	2.19	0.63
1:F:91:THR:HG23	1:F:282:ILE:HG23	1.80	0.63
1:M:91:THR:HG23	1:M:282:ILE:HG23	1.80	0.62
1:N:97:TYR:OH	1:N:274:LEU:HD23	1.97	0.62
1:H:31:LEU:HD21	1:I:179:ALA:HB1	1.80	0.62
1:A:91:THR:HG23	1:A:282:ILE:HG23	1.82	0.62
1:Q:31:LEU:HD21	1:R:179:ALA:HB1	1.81	0.62
1:B:97:TYR:OH	1:B:274:LEU:HD23	2.00	0.62
1:G:37:TRP:HE1	1:H:172:LYS:HZ3	1.47	0.62
1:G:97:TYR:OH	1:G:274:LEU:HD23	1.99	0.62
1:H:225:LEU:HD23	1:H:225:LEU:C	2.20	0.62
1:T:31:LEU:HD21	1:U:179:ALA:HB1	1.82	0.62
1:B:24:LEU:O	1:B:27:TYR:HB3	1.99	0.62
1:I:225:LEU:HD23	1:I:225:LEU:C	2.19	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:120:LEU:O	1:J:124:ILE:HG13	1.98	0.62
1:A:225:LEU:C	1:A:225:LEU:HD23	2.21	0.61
1:A:40:PHE:O	1:A:43:THR:HG22	1.99	0.61
1:G:40:PHE:O	1:G:43:THR:HG22	2.00	0.61
1:D:40:PHE:O	1:D:43:THR:HG22	2.00	0.61
1:D:91:THR:HG23	1:D:282:ILE:HG23	1.82	0.61
1:Q:225:LEU:HD23	1:Q:225:LEU:C	2.21	0.61
1:B:225:LEU:C	1:B:225:LEU:HD23	2.20	0.61
1:C:225:LEU:C	1:C:225:LEU:HD23	2.21	0.61
1:U:120:LEU:O	1:U:124:ILE:HG13	2.01	0.61
1:W:91:THR:HG23	1:W:282:ILE:HG23	1.82	0.61
1:G:61:LEU:O	1:G:65:ILE:HG12	2.01	0.61
1:C:246:GLU:OE1	1:C:292:HIS:CD2	2.54	0.61
1:M:40:PHE:O	1:M:43:THR:HG22	2.00	0.61
1:G:148:LEU:HD22	1:G:229:VAL:HG13	1.81	0.61
1:U:97:TYR:OH	1:U:274:LEU:HD23	2.00	0.61
1:D:120:LEU:O	1:D:124:ILE:HG13	2.00	0.61
1:I:120:LEU:O	1:I:124:ILE:HG13	2.00	0.61
1:N:148:LEU:HD22	1:N:229:VAL:HG13	1.83	0.61
1:T:225:LEU:C	1:T:225:LEU:HD23	2.21	0.61
1:K:31:LEU:HD21	1:L:179:ALA:HB1	1.83	0.61
1:Q:120:LEU:O	1:Q:124:ILE:HG13	2.01	0.61
1:Q:148:LEU:HD22	1:Q:229:VAL:HG13	1.83	0.61
1:D:225:LEU:HD23	1:D:225:LEU:C	2.20	0.60
1:R:120:LEU:O	1:R:124:ILE:HG13	2.01	0.60
1:G:225:LEU:C	1:G:225:LEU:HD23	2.21	0.60
1:J:62:VAL:HG12	1:K:149:LEU:HD21	1.83	0.60
1:O:148:LEU:HD22	1:O:229:VAL:HG13	1.83	0.60
1:L:40:PHE:O	1:L:43:THR:HG22	2.01	0.60
1:H:91:THR:HG23	1:H:282:ILE:HG23	1.81	0.60
1:N:225:LEU:HD23	1:N:225:LEU:C	2.22	0.60
1:R:225:LEU:C	1:R:225:LEU:HD23	2.22	0.60
1:G:120:LEU:O	1:G:124:ILE:HG13	2.01	0.60
1:R:62:VAL:HG12	1:S:149:LEU:HD21	1.83	0.60
1:W:27:TYR:CE2	1:X:183:ALA:HB2	2.36	0.60
1:I:97:TYR:OH	1:I:274:LEU:HD23	2.02	0.60
1:J:225:LEU:HD23	1:J:225:LEU:C	2.22	0.60
1:U:225:LEU:HD23	1:U:225:LEU:C	2.22	0.60
1:W:225:LEU:HD23	1:W:225:LEU:C	2.21	0.60
1:W:31:LEU:HD21	1:X:179:ALA:HB1	1.84	0.60
1:L:225:LEU:HD23	1:L:225:LEU:C	2.21	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:246:GLU:OE1	1:Q:292:HIS:CD2	2.55	0.60
1:U:61:LEU:O	1:U:65:ILE:HG12	2.02	0.60
1:D:34:VAL:HG13	1:D:199:ALA:HB2	1.83	0.60
1:A:37:TRP:HE1	1:B:172:LYS:HZ3	1.48	0.60
1:N:91:THR:HG23	1:N:282:ILE:HG23	1.84	0.60
1:O:225:LEU:C	1:O:225:LEU:HD23	2.22	0.60
1:R:148:LEU:HD22	1:R:229:VAL:HG13	1.84	0.60
1:I:34:VAL:HG13	1:I:199:ALA:HB2	1.84	0.60
1:T:97:TYR:OH	1:T:274:LEU:HD23	2.01	0.60
1:S:225:LEU:C	1:S:225:LEU:HD23	2.22	0.59
1:F:31:LEU:HD21	1:G:179:ALA:HB1	1.84	0.59
1:T:40:PHE:O	1:T:43:THR:HG22	2.02	0.59
1:F:225:LEU:C	1:F:225:LEU:HD23	2.23	0.59
1:S:34:VAL:HG13	1:S:199:ALA:HB2	1.84	0.59
1:U:91:THR:HG23	1:U:282:ILE:HG23	1.84	0.59
1:T:34:VAL:HG13	1:T:199:ALA:HB2	1.84	0.59
1:D:61:LEU:O	1:D:65:ILE:HG12	2.02	0.59
1:G:27:TYR:CE2	1:H:183:ALA:HB2	2.37	0.59
1:I:148:LEU:HD22	1:I:229:VAL:HG13	1.84	0.59
1:P:225:LEU:C	1:P:225:LEU:HD23	2.23	0.59
1:Q:61:LEU:O	1:Q:65:ILE:HG12	2.01	0.59
1:U:40:PHE:O	1:U:43:THR:HG22	2.02	0.59
1:V:148:LEU:HD22	1:V:229:VAL:HG13	1.83	0.59
1:H:34:VAL:HG13	1:H:199:ALA:HB2	1.85	0.59
1:X:34:VAL:HG13	1:X:199:ALA:HB2	1.85	0.59
1:E:225:LEU:C	1:E:225:LEU:HD23	2.22	0.59
1:K:225:LEU:HD23	1:K:225:LEU:C	2.23	0.59
1:F:148:LEU:HD22	1:F:229:VAL:HG13	1.83	0.59
1:J:40:PHE:O	1:J:43:THR:HG22	2.03	0.59
1:M:225:LEU:C	1:M:225:LEU:HD23	2.23	0.59
1:K:34:VAL:HG13	1:K:199:ALA:HB2	1.85	0.59
1:G:34:VAL:HG13	1:G:199:ALA:HB2	1.85	0.58
1:K:40:PHE:O	1:K:43:THR:HG22	2.02	0.58
1:U:148:LEU:HD22	1:U:229:VAL:HG13	1.83	0.58
1:C:34:VAL:HG13	1:C:199:ALA:HB2	1.85	0.58
1:J:240:LYS:O	1:J:244:THR:HG23	2.04	0.58
1:J:61:LEU:O	1:J:65:ILE:HG12	2.03	0.58
1:O:91:THR:HG23	1:O:282:ILE:HG23	1.83	0.58
1:V:225:LEU:C	1:V:225:LEU:HD23	2.23	0.58
1:L:258:GLU:O	1:L:262:PHE:HD2	1.85	0.58
1:P:61:LEU:O	1:P:65:ILE:HG12	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:288:TYR:O	1:T:292:HIS:HB3	2.03	0.58
1:X:61:LEU:O	1:X:65:ILE:HG12	2.03	0.58
1:A:31:LEU:HD21	1:B:179:ALA:HB1	1.85	0.58
1:T:258:GLU:O	1:T:262:PHE:HD2	1.86	0.58
1:C:61:LEU:O	1:C:65:ILE:HG12	2.03	0.58
1:H:148:LEU:HD22	1:H:229:VAL:HG13	1.85	0.58
1:W:34:VAL:HG13	1:W:199:ALA:HB2	1.86	0.58
1:B:61:LEU:O	1:B:65:ILE:HG12	2.04	0.58
1:S:61:LEU:O	1:S:65:ILE:HG12	2.04	0.58
1:V:34:VAL:HG13	1:V:199:ALA:HB2	1.86	0.58
1:W:40:PHE:O	1:W:43:THR:HG22	2.04	0.58
1:M:149:LEU:HD21	1:X:62:VAL:HG12	1.84	0.58
1:A:34:VAL:HG13	1:A:199:ALA:HB2	1.85	0.58
1:V:120:LEU:O	1:V:124:ILE:HG13	2.03	0.58
1:B:288:TYR:O	1:B:292:HIS:HB3	2.04	0.58
1:I:61:LEU:O	1:I:65:ILE:HG12	2.03	0.58
1:L:148:LEU:HD22	1:L:229:VAL:HG13	1.85	0.58
1:O:34:VAL:HG13	1:O:199:ALA:HB2	1.85	0.57
1:K:148:LEU:HD22	1:K:229:VAL:HG13	1.86	0.57
1:K:61:LEU:O	1:K:65:ILE:HG12	2.04	0.57
1:P:148:LEU:HD22	1:P:229:VAL:HG13	1.87	0.57
1:C:292:HIS:C	1:C:292:HIS:ND1	2.58	0.57
1:F:120:LEU:O	1:F:124:ILE:HG13	2.05	0.57
1:K:34:VAL:HG12	1:K:35:ILE:HG13	1.87	0.57
1:X:39:THR:CG2	1:X:173:ILE:HG12	2.34	0.57
1:B:62:VAL:HG12	1:C:149:LEU:HD21	1.85	0.57
1:F:34:VAL:HG13	1:F:199:ALA:HB2	1.86	0.57
1:J:258:GLU:O	1:J:262:PHE:HD2	1.88	0.57
1:W:61:LEU:O	1:W:65:ILE:HG12	2.03	0.57
1:M:262:PHE:CG	1:X:93:LEU:HD11	2.39	0.57
1:B:34:VAL:HG13	1:B:199:ALA:HB2	1.86	0.57
1:C:258:GLU:O	1:C:262:PHE:HD2	1.87	0.57
1:F:40:PHE:O	1:F:43:THR:HG22	2.04	0.57
1:T:120:LEU:O	1:T:124:ILE:HG13	2.05	0.57
1:T:166:PHE:O	1:T:170:VAL:HG13	2.05	0.57
1:V:40:PHE:O	1:V:43:THR:HG22	2.04	0.57
1:P:34:VAL:HG12	1:P:35:ILE:HG13	1.85	0.57
1:F:61:LEU:O	1:F:65:ILE:HG12	2.05	0.57
1:Q:166:PHE:CE1	1:Q:211:LEU:HB3	2.40	0.57
1:R:34:VAL:HG12	1:R:35:ILE:HG13	1.87	0.57
1:S:120:LEU:O	1:S:124:ILE:HG13	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:258:GLU:O	1:V:262:PHE:HD2	1.87	0.57
1:L:61:LEU:O	1:L:65:ILE:HG12	2.05	0.56
1:Q:216:LYS:O	1:Q:220:ASN:HB2	2.04	0.56
1:U:34:VAL:HG13	1:U:199:ALA:HB2	1.86	0.56
1:V:244:THR:HA	1:V:247:ILE:HD12	1.86	0.56
1:A:148:LEU:HD22	1:A:229:VAL:HG13	1.87	0.56
1:J:34:VAL:HG13	1:J:199:ALA:HB2	1.85	0.56
1:K:120:LEU:O	1:K:124:ILE:HG13	2.05	0.56
1:P:215:LEU:O	1:P:215:LEU:HD13	2.05	0.56
1:S:148:LEU:HD22	1:S:229:VAL:HG13	1.87	0.56
1:F:216:LYS:O	1:F:220:ASN:HB2	2.05	0.56
1:A:120:LEU:O	1:A:124:ILE:HG13	2.05	0.56
1:C:31:LEU:HD21	1:D:179:ALA:HB1	1.87	0.56
1:E:34:VAL:HG13	1:E:199:ALA:HB2	1.87	0.56
1:G:244:THR:HA	1:G:247:ILE:HD12	1.88	0.56
1:J:61:LEU:HD21	1:J:148:LEU:HG	1.88	0.56
1:A:179:ALA:HB1	1:L:31:LEU:HD21	1.88	0.56
1:S:216:LYS:O	1:S:220:ASN:HB2	2.06	0.56
1:T:244:THR:HA	1:T:247:ILE:HD12	1.88	0.56
1:M:120:LEU:O	1:M:124:ILE:HG13	2.05	0.56
1:N:34:VAL:HG13	1:N:199:ALA:HB2	1.87	0.56
1:R:34:VAL:HG13	1:R:199:ALA:HB2	1.86	0.56
1:X:148:LEU:HD22	1:X:229:VAL:HG13	1.88	0.56
1:E:39:THR:CG2	1:E:173:ILE:HG12	2.36	0.56
1:I:39:THR:CG2	1:I:173:ILE:HG12	2.36	0.56
1:U:244:THR:HA	1:U:247:ILE:HD12	1.87	0.56
1:V:61:LEU:O	1:V:65:ILE:HG12	2.05	0.56
1:A:61:LEU:O	1:A:65:ILE:HG12	2.06	0.56
1:V:34:VAL:HG12	1:V:35:ILE:HG13	1.87	0.56
1:K:78:GLU:HB2	1:L:135:LEU:HD21	1.88	0.56
1:Q:244:THR:HA	1:Q:247:ILE:HD12	1.86	0.56
1:R:39:THR:CG2	1:R:173:ILE:HG12	2.35	0.56
1:D:148:LEU:HD22	1:D:229:VAL:HG13	1.88	0.56
1:L:244:THR:HA	1:L:247:ILE:HD12	1.88	0.56
1:O:216:LYS:O	1:O:220:ASN:HB2	2.06	0.56
1:O:61:LEU:O	1:O:65:ILE:HG12	2.05	0.56
1:B:39:THR:CG2	1:B:173:ILE:HG12	2.36	0.56
1:E:148:LEU:HD22	1:E:229:VAL:HG13	1.88	0.56
1:I:61:LEU:HD21	1:I:148:LEU:HG	1.87	0.56
1:J:148:LEU:HD22	1:J:229:VAL:HG13	1.88	0.56
1:N:166:PHE:CE1	1:N:211:LEU:HB3	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:39:THR:CG2	1:S:173:ILE:HG12	2.36	0.56
1:V:189:PRO:HA	1:V:192:LEU:HD13	1.88	0.56
1:D:215:LEU:HD13	1:D:215:LEU:O	2.06	0.55
1:I:34:VAL:HG12	1:I:35:ILE:HG13	1.88	0.55
1:M:34:VAL:HG13	1:M:199:ALA:HB2	1.87	0.55
1:C:39:THR:CG2	1:C:173:ILE:HG12	2.36	0.55
1:E:216:LYS:O	1:E:220:ASN:HB2	2.07	0.55
1:H:39:THR:CG2	1:H:173:ILE:HG12	2.36	0.55
1:H:27:TYR:CE2	1:I:183:ALA:HB2	2.41	0.55
1:Q:215:LEU:HD13	1:Q:215:LEU:O	2.06	0.55
1:U:34:VAL:HG12	1:U:35:ILE:HG13	1.88	0.55
1:W:148:LEU:HD22	1:W:229:VAL:HG13	1.88	0.55
1:B:148:LEU:HD22	1:B:229:VAL:HG13	1.88	0.55
1:H:61:LEU:O	1:H:65:ILE:HG12	2.06	0.55
1:I:215:LEU:HD13	1:I:215:LEU:O	2.06	0.55
1:J:215:LEU:HD13	1:J:215:LEU:O	2.06	0.55
1:J:31:LEU:HD21	1:K:179:ALA:HB1	1.86	0.55
1:J:34:VAL:HG12	1:J:35:ILE:HG13	1.89	0.55
1:N:31:LEU:HD21	1:O:179:ALA:HB1	1.88	0.55
1:O:20:ALA:O	1:O:23:ALA:HB3	2.07	0.55
1:U:216:LYS:O	1:U:220:ASN:HB2	2.06	0.55
1:X:215:LEU:HD13	1:X:215:LEU:O	2.07	0.55
1:G:39:THR:CG2	1:G:173:ILE:HG12	2.37	0.55
1:J:166:PHE:CE1	1:J:211:LEU:HB3	2.42	0.55
1:T:166:PHE:CE1	1:T:211:LEU:HB3	2.42	0.55
1:T:148:LEU:HD22	1:T:229:VAL:HG13	1.88	0.55
1:C:216:LYS:O	1:C:220:ASN:HB2	2.07	0.55
1:K:244:THR:HA	1:K:247:ILE:HD12	1.89	0.55
1:P:216:LYS:O	1:P:220:ASN:HB2	2.07	0.55
1:A:27:TYR:CE2	1:B:183:ALA:HB2	2.42	0.55
1:C:34:VAL:HG12	1:C:35:ILE:HG13	1.89	0.55
1:N:120:LEU:O	1:N:124:ILE:HG13	2.05	0.55
1:P:244:THR:HA	1:P:247:ILE:HD12	1.88	0.55
1:U:240:LYS:O	1:U:244:THR:HG23	2.07	0.55
1:X:216:LYS:O	1:X:220:ASN:HB2	2.06	0.55
1:G:215:LEU:HD13	1:G:215:LEU:O	2.04	0.55
1:N:240:LYS:O	1:N:244:THR:HG23	2.07	0.55
1:Q:34:VAL:HG13	1:Q:199:ALA:HB2	1.88	0.55
1:R:216:LYS:O	1:R:220:ASN:HB2	2.06	0.55
1:V:39:THR:CG2	1:V:173:ILE:HG12	2.37	0.55
1:B:216:LYS:O	1:B:220:ASN:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:216:LYS:O	1:D:220:ASN:HB2	2.07	0.55
1:D:31:LEU:HD21	1:E:179:ALA:HB1	1.88	0.55
1:H:166:PHE:CE1	1:H:211:LEU:HB3	2.42	0.55
1:K:27:TYR:CE2	1:L:183:ALA:HB2	2.42	0.55
1:L:216:LYS:O	1:L:220:ASN:HB2	2.06	0.55
1:N:216:LYS:O	1:N:220:ASN:HB2	2.06	0.55
1:N:34:VAL:HG12	1:N:35:ILE:HG13	1.89	0.55
1:N:61:LEU:O	1:N:65:ILE:HG12	2.07	0.55
1:P:34:VAL:HG13	1:P:199:ALA:HB2	1.87	0.55
1:D:61:LEU:HD21	1:D:148:LEU:HG	1.89	0.55
1:I:258:GLU:O	1:I:262:PHE:HD2	1.90	0.55
1:K:216:LYS:O	1:K:220:ASN:HB2	2.06	0.55
1:W:216:LYS:O	1:W:220:ASN:HB2	2.06	0.55
1:K:39:THR:CG2	1:K:173:ILE:HG12	2.38	0.55
1:U:166:PHE:O	1:U:170:VAL:HG13	2.07	0.55
1:V:166:PHE:CE1	1:V:211:LEU:HB3	2.42	0.55
1:C:120:LEU:O	1:C:124:ILE:HG13	2.06	0.54
1:C:86:TRP:C	1:C:88:GLY:H	2.10	0.54
1:K:189:PRO:HA	1:K:192:LEU:HD13	1.89	0.54
1:L:34:VAL:HG13	1:L:199:ALA:HB2	1.87	0.54
1:M:216:LYS:O	1:M:220:ASN:HB2	2.07	0.54
1:O:97:TYR:OH	1:O:274:LEU:HD23	2.06	0.54
1:Q:189:PRO:HA	1:Q:192:LEU:HD13	1.88	0.54
1:T:216:LYS:O	1:T:220:ASN:HB2	2.06	0.54
1:E:40:PHE:O	1:E:43:THR:HG22	2.06	0.54
1:I:262:PHE:O	1:I:265:ASP:HB2	2.07	0.54
1:M:166:PHE:O	1:M:170:VAL:HG13	2.08	0.54
1:N:86:TRP:C	1:N:88:GLY:H	2.09	0.54
1:Q:39:THR:CG2	1:Q:173:ILE:HG12	2.36	0.54
1:A:216:LYS:O	1:A:220:ASN:HB2	2.07	0.54
1:M:166:PHE:CE1	1:M:211:LEU:HB3	2.42	0.54
1:Q:61:LEU:HD21	1:Q:148:LEU:HG	1.89	0.54
1:Q:262:PHE:O	1:Q:265:ASP:HB2	2.07	0.54
1:S:258:GLU:O	1:S:262:PHE:HD2	1.89	0.54
1:X:246:GLU:OE1	1:X:292:HIS:HD2	1.90	0.54
1:A:215:LEU:HD13	1:A:215:LEU:O	2.07	0.54
1:C:215:LEU:HD13	1:C:215:LEU:O	2.07	0.54
1:G:216:LYS:O	1:G:220:ASN:HB2	2.06	0.54
1:L:34:VAL:HG12	1:L:35:ILE:HG13	1.87	0.54
1:O:34:VAL:HG12	1:O:35:ILE:HG13	1.88	0.54
1:Q:34:VAL:HG12	1:Q:35:ILE:HG13	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:264:VAL:HG23	1:R:274:LEU:CD1	2.34	0.54
1:T:240:LYS:O	1:T:244:THR:HG23	2.08	0.54
1:T:61:LEU:O	1:T:65:ILE:HG12	2.08	0.54
1:C:244:THR:HA	1:C:247:ILE:HD12	1.88	0.54
1:F:252:GLU:HA	1:F:252:GLU:OE2	2.07	0.54
1:G:47:LEU:HD11	1:G:214:LYS:HB3	1.90	0.54
1:J:264:VAL:N	1:J:274:LEU:HD13	2.23	0.54
1:O:215:LEU:HD13	1:O:215:LEU:O	2.07	0.54
1:V:216:LYS:O	1:V:220:ASN:HB2	2.08	0.54
1:B:34:VAL:HG12	1:B:35:ILE:HG13	1.89	0.54
1:I:166:PHE:CE1	1:I:211:LEU:HB3	2.43	0.54
1:K:240:LYS:O	1:K:244:THR:HG23	2.07	0.54
1:M:258:GLU:O	1:M:262:PHE:HD2	1.90	0.54
1:S:61:LEU:HD21	1:S:148:LEU:HG	1.89	0.54
1:U:86:TRP:C	1:U:88:GLY:H	2.11	0.54
1:A:39:THR:CG2	1:A:173:ILE:HG12	2.38	0.54
1:F:39:THR:CG2	1:F:173:ILE:HG12	2.38	0.54
1:O:27:TYR:CE2	1:P:183:ALA:HB2	2.42	0.54
1:P:166:PHE:CE1	1:P:211:LEU:HB3	2.42	0.54
1:T:34:VAL:HG12	1:T:35:ILE:HG13	1.89	0.54
1:E:61:LEU:O	1:E:65:ILE:HG12	2.07	0.54
1:H:215:LEU:O	1:H:215:LEU:HD13	2.08	0.54
1:J:216:LYS:O	1:J:220:ASN:HB2	2.07	0.54
1:K:264:VAL:HG23	1:K:274:LEU:CD1	2.34	0.54
1:P:39:THR:CG2	1:P:173:ILE:HG12	2.37	0.54
1:Q:252:GLU:HA	1:Q:252:GLU:OE2	2.08	0.54
1:U:39:THR:CG2	1:U:173:ILE:HG12	2.38	0.54
1:X:34:VAL:HG12	1:X:35:ILE:HG13	1.89	0.54
1:A:244:THR:HA	1:A:247:ILE:HD12	1.90	0.54
1:B:244:THR:HA	1:B:247:ILE:HD12	1.90	0.54
1:F:34:VAL:HG12	1:F:35:ILE:HG13	1.89	0.54
1:G:166:PHE:CE1	1:G:211:LEU:HB3	2.43	0.54
1:H:189:PRO:HA	1:H:192:LEU:HD13	1.90	0.54
1:K:62:VAL:HG12	1:L:149:LEU:HD21	1.90	0.54
1:L:166:PHE:CE1	1:L:211:LEU:HB3	2.42	0.54
1:L:189:PRO:HA	1:L:192:LEU:HD13	1.90	0.54
1:M:39:THR:CG2	1:M:173:ILE:HG12	2.38	0.54
1:N:166:PHE:HE1	1:N:211:LEU:HB3	1.73	0.54
1:N:215:LEU:O	1:N:215:LEU:HD13	2.08	0.54
1:U:31:LEU:HD21	1:V:179:ALA:HB1	1.90	0.54
1:A:54:TYR:CD1	1:A:155:LEU:HB2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:216:LYS:O	1:H:220:ASN:HB2	2.07	0.54
1:K:252:GLU:HA	1:K:252:GLU:OE2	2.08	0.54
1:L:39:THR:CG2	1:L:173:ILE:HG12	2.37	0.54
1:M:148:LEU:HD22	1:M:229:VAL:HG13	1.90	0.54
1:S:34:VAL:HG12	1:S:35:ILE:HG13	1.90	0.54
1:A:34:VAL:HG12	1:A:35:ILE:HG13	1.90	0.53
1:B:215:LEU:HD13	1:B:215:LEU:O	2.08	0.53
1:U:93:LEU:HD11	1:V:262:PHE:CG	2.43	0.53
1:W:166:PHE:CE1	1:W:211:LEU:HB3	2.43	0.53
1:W:244:THR:HA	1:W:247:ILE:HD12	1.89	0.53
1:E:166:PHE:CE1	1:E:211:LEU:HB3	2.44	0.53
1:G:20:ALA:O	1:G:23:ALA:HB3	2.09	0.53
1:H:34:VAL:HG12	1:H:35:ILE:HG13	1.90	0.53
1:I:216:LYS:O	1:I:220:ASN:HB2	2.08	0.53
1:I:86:TRP:C	1:I:88:GLY:H	2.11	0.53
1:Q:264:VAL:N	1:Q:274:LEU:HD13	2.22	0.53
1:S:262:PHE:O	1:S:265:ASP:HB2	2.08	0.53
1:W:215:LEU:O	1:W:215:LEU:HD13	2.08	0.53
1:A:175:LYS:HD3	1:A:175:LYS:C	2.29	0.53
1:A:258:GLU:O	1:A:262:PHE:HD2	1.91	0.53
1:B:252:GLU:OE2	1:B:252:GLU:HA	2.09	0.53
1:G:252:GLU:HA	1:G:252:GLU:OE2	2.09	0.53
1:G:264:VAL:N	1:G:274:LEU:HD13	2.24	0.53
1:H:20:ALA:O	1:H:23:ALA:HB3	2.09	0.53
1:Q:251:GLY:O	1:Q:255:THR:HG23	2.08	0.53
1:R:61:LEU:HD21	1:R:148:LEU:HG	1.89	0.53
1:E:215:LEU:HD13	1:E:215:LEU:O	2.08	0.53
1:E:240:LYS:O	1:E:244:THR:HG23	2.09	0.53
1:O:31:LEU:HD21	1:P:179:ALA:HB1	1.90	0.53
1:R:166:PHE:CE1	1:R:211:LEU:HB3	2.43	0.53
1:A:262:PHE:O	1:A:265:ASP:HB2	2.09	0.53
1:A:86:TRP:C	1:A:88:GLY:H	2.11	0.53
1:B:166:PHE:CE1	1:B:211:LEU:HB3	2.44	0.53
1:I:65:ILE:HD12	1:I:236:ILE:HD11	1.91	0.53
1:J:166:PHE:O	1:J:170:VAL:HG13	2.08	0.53
1:L:252:GLU:OE2	1:L:252:GLU:HA	2.08	0.53
1:M:34:VAL:HG12	1:M:35:ILE:HG13	1.89	0.53
1:O:166:PHE:O	1:O:170:VAL:HG13	2.08	0.53
1:O:288:TYR:O	1:O:292:HIS:HB3	2.09	0.53
1:T:47:LEU:HD11	1:T:214:LYS:HB3	1.91	0.53
1:X:39:THR:HG22	1:X:173:ILE:HG12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:244:THR:HA	1:F:247:ILE:HD12	1.91	0.53
1:I:54:TYR:CD1	1:I:155:LEU:HB2	2.43	0.53
1:R:47:LEU:HD11	1:R:214:LYS:HB3	1.90	0.53
1:A:264:VAL:N	1:A:274:LEU:HD13	2.24	0.53
1:B:47:LEU:HD11	1:B:214:LYS:HB3	1.90	0.53
1:C:39:THR:HG22	1:C:173:ILE:HG12	1.91	0.53
1:J:189:PRO:HA	1:J:192:LEU:HD13	1.90	0.53
1:N:189:PRO:HA	1:N:192:LEU:HD13	1.91	0.53
1:Q:258:GLU:O	1:Q:262:PHE:HD2	1.91	0.53
1:S:166:PHE:CE1	1:S:211:LEU:HB3	2.43	0.53
1:B:20:ALA:O	1:B:23:ALA:HB3	2.09	0.53
1:H:166:PHE:HE1	1:H:211:LEU:HB3	1.74	0.53
1:H:252:GLU:HA	1:H:252:GLU:OE2	2.09	0.53
1:K:20:ALA:O	1:K:23:ALA:HB3	2.09	0.53
1:N:258:GLU:O	1:N:262:PHE:HD2	1.92	0.53
1:N:262:PHE:O	1:N:265:ASP:HB2	2.09	0.53
1:S:39:THR:HG22	1:S:173:ILE:HG12	1.90	0.53
1:T:215:LEU:O	1:T:215:LEU:HD13	2.09	0.53
1:F:175:LYS:HD3	1:F:175:LYS:C	2.29	0.53
1:Q:166:PHE:HE1	1:Q:211:LEU:HB3	1.72	0.53
1:Q:39:THR:HG22	1:Q:173:ILE:HG12	1.91	0.53
1:R:39:THR:HG22	1:R:173:ILE:HG12	1.90	0.53
1:T:166:PHE:HE1	1:T:211:LEU:HB3	1.74	0.53
1:B:189:PRO:HA	1:B:192:LEU:HD13	1.91	0.53
1:D:39:THR:CG2	1:D:173:ILE:HG12	2.38	0.53
1:D:86:TRP:C	1:D:88:GLY:H	2.11	0.53
1:K:166:PHE:CE1	1:K:211:LEU:HB3	2.43	0.53
1:P:262:PHE:O	1:P:265:ASP:HB2	2.09	0.53
1:U:54:TYR:CD1	1:U:155:LEU:HB2	2.44	0.53
1:W:34:VAL:HG12	1:W:35:ILE:HG13	1.90	0.53
1:B:93:LEU:HD11	1:C:262:PHE:CG	2.44	0.52
1:L:20:ALA:O	1:L:23:ALA:HB3	2.08	0.52
1:N:39:THR:CG2	1:N:173:ILE:HG12	2.38	0.52
1:P:252:GLU:HA	1:P:252:GLU:OE2	2.08	0.52
1:R:252:GLU:HA	1:R:252:GLU:OE2	2.10	0.52
1:U:166:PHE:CE1	1:U:211:LEU:HB3	2.44	0.52
1:U:215:LEU:HD13	1:U:215:LEU:O	2.09	0.52
1:G:14:LYS:HB2	1:H:19:THR:OG1	2.10	0.52
1:G:39:THR:HG22	1:G:173:ILE:HG12	1.91	0.52
1:J:264:VAL:HG23	1:J:274:LEU:CD1	2.38	0.52
1:Q:65:ILE:HD12	1:Q:236:ILE:HD11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:27:TYR:CE2	1:U:183:ALA:HB2	2.44	0.52
1:V:61:LEU:HD21	1:V:148:LEU:HG	1.90	0.52
1:W:175:LYS:C	1:W:175:LYS:HD3	2.30	0.52
1:M:179:ALA:HB1	1:X:31:LEU:HD21	1.91	0.52
1:A:252:GLU:HA	1:A:252:GLU:OE2	2.09	0.52
1:C:61:LEU:HD21	1:C:148:LEU:HG	1.92	0.52
1:E:39:THR:HG22	1:E:173:ILE:HG12	1.91	0.52
1:E:34:VAL:HG12	1:E:35:ILE:HG13	1.89	0.52
1:H:47:LEU:HD11	1:H:214:LYS:HB3	1.89	0.52
1:H:65:ILE:HD12	1:H:236:ILE:HD11	1.90	0.52
1:I:189:PRO:HA	1:I:192:LEU:HD13	1.90	0.52
1:I:20:ALA:O	1:I:23:ALA:HB3	2.10	0.52
1:K:215:LEU:O	1:K:215:LEU:HD13	2.10	0.52
1:L:47:LEU:HD11	1:L:214:LYS:HB3	1.90	0.52
1:M:166:PHE:HE1	1:M:211:LEU:HB3	1.75	0.52
1:M:262:PHE:O	1:M:265:ASP:HB2	2.08	0.52
1:P:240:LYS:O	1:P:244:THR:HG23	2.10	0.52
1:Q:27:TYR:CE2	1:R:183:ALA:HB2	2.44	0.52
1:T:39:THR:CG2	1:T:173:ILE:HG12	2.38	0.52
1:B:262:PHE:O	1:B:265:ASP:HB2	2.09	0.52
1:D:54:TYR:CD1	1:D:155:LEU:HB2	2.44	0.52
1:G:34:VAL:HG12	1:G:35:ILE:HG13	1.90	0.52
1:I:175:LYS:HD3	1:I:175:LYS:C	2.30	0.52
1:M:175:LYS:C	1:M:175:LYS:HD3	2.30	0.52
1:O:47:LEU:HD11	1:O:214:LYS:HB3	1.90	0.52
1:B:39:THR:HG22	1:B:173:ILE:HG12	1.91	0.52
1:C:252:GLU:OE2	1:C:252:GLU:HA	2.09	0.52
1:D:258:GLU:O	1:D:262:PHE:HD2	1.93	0.52
1:D:262:PHE:O	1:D:265:ASP:HB2	2.10	0.52
1:D:47:LEU:HD11	1:D:214:LYS:HB3	1.91	0.52
1:E:47:LEU:HD11	1:E:214:LYS:HB3	1.91	0.52
1:F:258:GLU:O	1:F:262:PHE:HD2	1.92	0.52
1:O:252:GLU:HA	1:O:252:GLU:OE2	2.10	0.52
1:T:189:PRO:HA	1:T:192:LEU:HD13	1.91	0.52
1:D:20:ALA:O	1:D:23:ALA:HB3	2.09	0.52
1:F:264:VAL:HG23	1:F:274:LEU:CD1	2.39	0.52
1:G:258:GLU:O	1:G:262:PHE:HD2	1.92	0.52
1:H:39:THR:HG22	1:H:173:ILE:HG12	1.92	0.52
1:M:39:THR:HG22	1:M:173:ILE:HG12	1.91	0.52
1:M:27:TYR:CE2	1:N:183:ALA:HB2	2.44	0.52
1:V:166:PHE:O	1:V:170:VAL:HG13	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:252:GLU:HA	1:V:252:GLU:OE2	2.10	0.52
1:E:189:PRO:HA	1:E:192:LEU:HD13	1.92	0.52
1:J:244:THR:HA	1:J:247:ILE:HD12	1.91	0.52
1:O:166:PHE:CE1	1:O:211:LEU:HB3	2.45	0.52
1:R:189:PRO:HA	1:R:192:LEU:HD13	1.91	0.52
1:U:20:ALA:O	1:U:23:ALA:HB3	2.10	0.52
1:U:252:GLU:OE2	1:U:252:GLU:HA	2.10	0.52
1:V:215:LEU:O	1:V:215:LEU:HD13	2.10	0.52
1:C:175:LYS:HD3	1:C:175:LYS:C	2.29	0.52
1:E:14:LYS:HB2	1:F:19:THR:OG1	2.09	0.52
1:J:252:GLU:HA	1:J:252:GLU:OE2	2.10	0.52
1:M:252:GLU:OE2	1:M:252:GLU:HA	2.09	0.52
1:P:175:LYS:HD3	1:P:175:LYS:C	2.30	0.52
1:R:86:TRP:C	1:R:88:GLY:H	2.13	0.52
1:S:244:THR:HA	1:S:247:ILE:HD12	1.90	0.52
1:W:258:GLU:O	1:W:262:PHE:HD2	1.93	0.52
1:D:244:THR:HA	1:D:247:ILE:HD12	1.90	0.52
1:I:240:LYS:O	1:I:244:THR:HG23	2.10	0.52
1:I:47:LEU:HD11	1:I:214:LYS:HB3	1.91	0.52
1:K:175:LYS:HD3	1:K:175:LYS:C	2.31	0.52
1:Q:47:LEU:HD11	1:Q:214:LYS:HB3	1.91	0.52
1:R:215:LEU:O	1:R:215:LEU:HD13	2.10	0.52
1:U:175:LYS:C	1:U:175:LYS:HD3	2.30	0.52
1:X:189:PRO:HA	1:X:192:LEU:HD13	1.92	0.52
1:I:39:THR:HG22	1:I:173:ILE:HG12	1.91	0.52
1:T:20:ALA:O	1:T:23:ALA:HB3	2.10	0.52
1:U:47:LEU:HD11	1:U:214:LYS:HB3	1.92	0.52
1:J:262:PHE:O	1:J:265:ASP:HB2	2.10	0.51
1:K:47:LEU:HD11	1:K:214:LYS:HB3	1.92	0.51
1:L:166:PHE:HE1	1:L:211:LEU:HB3	1.75	0.51
1:N:278:ALA:O	1:N:282:ILE:HG13	2.10	0.51
1:P:61:LEU:HD21	1:P:148:LEU:HG	1.92	0.51
1:S:189:PRO:HA	1:S:192:LEU:HD13	1.92	0.51
1:V:262:PHE:O	1:V:265:ASP:HB2	2.10	0.51
1:X:166:PHE:CE1	1:X:211:LEU:HB3	2.44	0.51
1:C:166:PHE:CE1	1:C:211:LEU:HB3	2.45	0.51
1:C:148:LEU:HD22	1:C:229:VAL:HG13	1.91	0.51
1:H:54:TYR:CD1	1:H:155:LEU:HB2	2.44	0.51
1:O:39:THR:CG2	1:O:173:ILE:HG12	2.39	0.51
1:P:20:ALA:O	1:P:23:ALA:HB3	2.10	0.51
1:P:258:GLU:O	1:P:262:PHE:HD2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:175:LYS:HD3	1:R:175:LYS:C	2.30	0.51
1:R:31:LEU:HD21	1:S:179:ALA:HB1	1.93	0.51
1:S:47:LEU:HD11	1:S:214:LYS:HB3	1.91	0.51
1:T:262:PHE:O	1:T:265:ASP:HB2	2.10	0.51
1:W:54:TYR:CD1	1:W:155:LEU:HB2	2.44	0.51
1:X:175:LYS:HD3	1:X:175:LYS:C	2.30	0.51
1:A:166:PHE:CE1	1:A:211:LEU:HB3	2.46	0.51
1:F:65:ILE:HD12	1:F:236:ILE:HD11	1.91	0.51
1:J:166:PHE:HE1	1:J:211:LEU:HB3	1.76	0.51
1:I:31:LEU:HD21	1:J:179:ALA:HB1	1.92	0.51
1:M:54:TYR:CD1	1:M:155:LEU:HB2	2.44	0.51
1:V:166:PHE:HE1	1:V:211:LEU:HB3	1.74	0.51
1:V:240:LYS:O	1:V:244:THR:HG23	2.10	0.51
1:W:47:LEU:HD11	1:W:214:LYS:HB3	1.92	0.51
1:X:47:LEU:HD11	1:X:214:LYS:HB3	1.91	0.51
1:E:78:GLU:HB2	1:F:135:LEU:HD21	1.92	0.51
1:G:262:PHE:O	1:G:265:ASP:HB2	2.11	0.51
1:H:244:THR:HA	1:H:247:ILE:HD12	1.93	0.51
1:H:61:LEU:HD21	1:H:148:LEU:HG	1.92	0.51
1:J:175:LYS:C	1:J:175:LYS:HD3	2.31	0.51
1:L:175:LYS:HD3	1:L:175:LYS:C	2.30	0.51
1:N:175:LYS:C	1:N:175:LYS:HD3	2.31	0.51
1:O:278:ALA:O	1:O:282:ILE:HG13	2.11	0.51
1:P:39:THR:HG22	1:P:173:ILE:HG12	1.92	0.51
1:S:166:PHE:HE1	1:S:211:LEU:HB3	1.76	0.51
1:S:215:LEU:HD13	1:S:215:LEU:O	2.10	0.51
1:U:61:LEU:HD21	1:U:148:LEU:HG	1.92	0.51
1:V:86:TRP:C	1:V:88:GLY:H	2.13	0.51
1:X:65:ILE:HD12	1:X:236:ILE:HD11	1.93	0.51
1:A:183:ALA:HB2	1:L:27:TYR:CE2	2.45	0.51
1:A:20:ALA:O	1:A:23:ALA:HB3	2.10	0.51
1:A:47:LEU:HD11	1:A:214:LYS:HB3	1.92	0.51
1:E:262:PHE:O	1:E:265:ASP:HB2	2.11	0.51
1:G:166:PHE:O	1:G:170:VAL:HG13	2.11	0.51
1:G:225:LEU:HD23	1:G:225:LEU:O	2.11	0.51
1:G:54:TYR:CD1	1:G:155:LEU:HB2	2.44	0.51
1:M:135:LEU:HD21	1:X:78:GLU:HB2	1.93	0.51
1:U:189:PRO:HA	1:U:192:LEU:HD13	1.92	0.51
1:W:119:VAL:HG13	1:W:120:LEU:N	2.26	0.51
1:W:288:TYR:O	1:W:292:HIS:HB3	2.10	0.51
1:X:252:GLU:OE2	1:X:252:GLU:HA	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:PRO:HA	1:A:192:LEU:HD13	1.92	0.51
1:B:278:ALA:O	1:B:282:ILE:HG13	2.10	0.51
1:G:189:PRO:HA	1:G:192:LEU:HD13	1.92	0.51
1:J:39:THR:CG2	1:J:173:ILE:HG12	2.41	0.51
1:N:252:GLU:OE2	1:N:252:GLU:HA	2.10	0.51
1:O:189:PRO:HA	1:O:192:LEU:HD13	1.92	0.51
1:V:39:THR:HG22	1:V:173:ILE:HG12	1.93	0.51
1:D:34:VAL:HG12	1:D:35:ILE:HG13	1.92	0.51
1:J:20:ALA:O	1:J:23:ALA:HB3	2.11	0.51
1:M:19:THR:OG1	1:X:14:LYS:HB2	2.11	0.51
1:M:215:LEU:HD13	1:M:215:LEU:O	2.11	0.51
1:P:47:LEU:HD11	1:P:214:LYS:HB3	1.92	0.51
1:R:133:SER:O	1:R:136:VAL:HG12	2.11	0.51
1:S:252:GLU:HA	1:S:252:GLU:OE2	2.11	0.51
1:V:104:TYR:HE2	1:V:106:GLU:HA	1.75	0.51
1:W:252:GLU:OE2	1:W:252:GLU:HA	2.09	0.51
1:W:39:THR:CG2	1:W:173:ILE:HG12	2.39	0.51
1:C:278:ALA:O	1:C:282:ILE:HG13	2.11	0.51
1:C:47:LEU:HD11	1:C:214:LYS:HB3	1.92	0.51
1:F:189:PRO:HA	1:F:192:LEU:HD13	1.93	0.51
1:K:61:LEU:HD21	1:K:148:LEU:HG	1.91	0.51
1:M:183:ALA:HB2	1:X:27:TYR:CE2	2.45	0.51
1:M:240:LYS:O	1:M:244:THR:HG23	2.10	0.51
1:M:246:GLU:OE1	1:M:292:HIS:CD2	2.63	0.51
1:P:155:LEU:HD13	1:P:225:LEU:HD22	1.93	0.51
1:P:278:ALA:O	1:P:282:ILE:HG13	2.11	0.51
1:Q:278:ALA:O	1:Q:282:ILE:HG13	2.11	0.51
1:U:262:PHE:O	1:U:265:ASP:HB2	2.11	0.51
1:A:278:ALA:O	1:A:282:ILE:HG13	2.11	0.51
1:B:175:LYS:C	1:B:175:LYS:HD3	2.31	0.51
1:B:86:TRP:C	1:B:88:GLY:H	2.13	0.51
1:D:166:PHE:CE1	1:D:211:LEU:HB3	2.46	0.51
1:E:20:ALA:O	1:E:23:ALA:HB3	2.11	0.51
1:F:215:LEU:HD13	1:F:215:LEU:O	2.11	0.51
1:L:215:LEU:O	1:L:215:LEU:HD13	2.10	0.51
1:M:189:PRO:HA	1:M:192:LEU:HD13	1.93	0.51
1:M:244:THR:HA	1:M:247:ILE:HD12	1.91	0.51
1:M:264:VAL:HG23	1:M:274:LEU:CD1	2.39	0.51
1:M:86:TRP:C	1:M:88:GLY:H	2.14	0.51
1:O:262:PHE:O	1:O:265:ASP:HB2	2.11	0.51
1:R:20:ALA:O	1:R:23:ALA:HB3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:20:ALA:O	1:S:23:ALA:HB3	2.11	0.51
1:T:252:GLU:HA	1:T:252:GLU:OE2	2.10	0.51
1:D:189:PRO:HA	1:D:192:LEU:HD13	1.92	0.51
1:F:61:LEU:HD21	1:F:148:LEU:HG	1.92	0.51
1:K:119:VAL:HG13	1:K:120:LEU:N	2.25	0.51
1:T:61:LEU:HD21	1:T:148:LEU:HG	1.92	0.51
1:V:175:LYS:C	1:V:175:LYS:HD3	2.31	0.51
1:V:47:LEU:HD11	1:V:214:LYS:HB3	1.93	0.51
1:W:278:ALA:O	1:W:282:ILE:HG13	2.11	0.51
1:W:61:LEU:HD21	1:W:148:LEU:HG	1.93	0.51
1:X:20:ALA:O	1:X:23:ALA:HB3	2.11	0.51
1:F:166:PHE:O	1:F:170:VAL:HG13	2.10	0.50
1:F:240:LYS:O	1:F:244:THR:HG23	2.11	0.50
1:J:54:TYR:CD1	1:J:155:LEU:HB2	2.46	0.50
1:K:124:ILE:HD11	1:K:258:GLU:HA	1.93	0.50
1:L:61:LEU:HD21	1:L:148:LEU:HG	1.92	0.50
1:N:244:THR:HA	1:N:247:ILE:HD12	1.93	0.50
1:P:189:PRO:HA	1:P:192:LEU:HD13	1.92	0.50
1:P:166:PHE:HE1	1:P:211:LEU:HB3	1.74	0.50
1:P:31:LEU:HD21	1:Q:179:ALA:HB1	1.94	0.50
1:R:258:GLU:O	1:R:262:PHE:HD2	1.94	0.50
1:T:54:TYR:CD1	1:T:155:LEU:HB2	2.46	0.50
1:W:262:PHE:O	1:W:265:ASP:HB2	2.10	0.50
1:A:39:THR:HG22	1:A:173:ILE:HG12	1.93	0.50
1:B:240:LYS:O	1:B:244:THR:HG23	2.10	0.50
1:F:20:ALA:O	1:F:23:ALA:HB3	2.10	0.50
1:L:39:THR:HG22	1:L:173:ILE:HG12	1.93	0.50
1:M:61:LEU:HD21	1:M:148:LEU:HG	1.93	0.50
1:N:27:TYR:CE2	1:O:183:ALA:HB2	2.45	0.50
1:R:244:THR:HA	1:R:247:ILE:HD12	1.93	0.50
1:W:189:PRO:HA	1:W:192:LEU:HD13	1.93	0.50
1:X:262:PHE:O	1:X:265:ASP:HB2	2.11	0.50
1:X:54:TYR:CD1	1:X:155:LEU:HB2	2.45	0.50
1:D:116:LEU:O	1:D:120:LEU:HG	2.11	0.50
1:F:166:PHE:CE1	1:F:211:LEU:HB3	2.46	0.50
1:G:175:LYS:HD3	1:G:175:LYS:C	2.31	0.50
1:S:175:LYS:HD3	1:S:175:LYS:C	2.32	0.50
1:T:86:TRP:C	1:T:88:GLY:H	2.14	0.50
1:B:78:GLU:HB2	1:C:135:LEU:HD21	1.93	0.50
1:E:166:PHE:HE1	1:E:211:LEU:HB3	1.77	0.50
1:E:278:ALA:O	1:E:282:ILE:HG13	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:274:LEU:O	1:F:274:LEU:HG	2.12	0.50
1:I:166:PHE:HE1	1:I:211:LEU:HB3	1.76	0.50
1:K:278:ALA:O	1:K:282:ILE:HG13	2.11	0.50
1:O:240:LYS:O	1:O:244:THR:HG23	2.10	0.50
1:Q:166:PHE:O	1:Q:170:VAL:HG13	2.12	0.50
1:B:104:TYR:HE2	1:B:106:GLU:HA	1.77	0.50
1:D:240:LYS:O	1:D:244:THR:HG23	2.11	0.50
1:Q:119:VAL:HG13	1:Q:120:LEU:N	2.26	0.50
1:R:93:LEU:HD11	1:S:262:PHE:CG	2.46	0.50
1:T:181:ALA:HA	1:T:195:SER:OG	2.12	0.50
1:U:181:ALA:HA	1:U:195:SER:OG	2.11	0.50
1:X:166:PHE:O	1:X:170:VAL:HG13	2.11	0.50
1:D:252:GLU:OE2	1:D:252:GLU:HA	2.11	0.50
1:H:86:TRP:C	1:H:88:GLY:H	2.14	0.50
1:I:252:GLU:OE2	1:I:252:GLU:HA	2.11	0.50
1:K:166:PHE:HE1	1:K:211:LEU:HB3	1.76	0.50
1:K:258:GLU:O	1:K:262:PHE:HD2	1.94	0.50
1:M:14:LYS:HB2	1:N:19:THR:OG1	2.12	0.50
1:N:20:ALA:O	1:N:23:ALA:HB3	2.12	0.50
1:P:264:VAL:HG23	1:P:274:LEU:CD1	2.40	0.50
1:P:54:TYR:CD1	1:P:155:LEU:HB2	2.47	0.50
1:T:278:ALA:O	1:T:282:ILE:HG13	2.12	0.50
1:V:278:ALA:O	1:V:282:ILE:HG13	2.12	0.50
1:V:65:ILE:HD12	1:V:236:ILE:HD11	1.94	0.50
1:V:31:LEU:HD21	1:W:179:ALA:HB1	1.93	0.50
1:W:39:THR:HG22	1:W:173:ILE:HG12	1.93	0.50
1:C:119:VAL:HG13	1:C:120:LEU:N	2.27	0.50
1:C:65:ILE:HD12	1:C:236:ILE:HD11	1.94	0.50
1:E:244:THR:HA	1:E:247:ILE:HD12	1.94	0.50
1:H:258:GLU:O	1:H:262:PHE:HD2	1.94	0.50
1:H:264:VAL:N	1:H:274:LEU:HD13	2.26	0.50
1:L:166:PHE:O	1:L:170:VAL:HG13	2.11	0.50
1:E:119:VAL:HG13	1:E:120:LEU:N	2.27	0.50
1:N:54:TYR:CD1	1:N:155:LEU:HB2	2.47	0.50
1:N:47:LEU:HD11	1:N:214:LYS:HB3	1.93	0.50
1:O:39:THR:HG22	1:O:173:ILE:HG12	1.94	0.50
1:P:246:GLU:OE1	1:P:292:HIS:CD2	2.64	0.50
1:D:175:LYS:HD3	1:D:175:LYS:C	2.32	0.50
1:D:39:THR:HG22	1:D:173:ILE:HG12	1.94	0.50
1:E:264:VAL:HG23	1:E:274:LEU:CD1	2.36	0.50
1:F:77:PHE:O	1:F:81:GLN:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:116:LEU:O	1:I:120:LEU:HG	2.12	0.50
1:K:86:TRP:C	1:K:88:GLY:H	2.13	0.50
1:P:264:VAL:N	1:P:274:LEU:HD13	2.27	0.50
1:P:86:TRP:C	1:P:88:GLY:H	2.14	0.50
1:W:20:ALA:O	1:W:23:ALA:HB3	2.11	0.50
1:A:65:ILE:HD12	1:A:236:ILE:HD11	1.93	0.49
1:E:62:VAL:HG12	1:F:149:LEU:HD21	1.94	0.49
1:G:86:TRP:C	1:G:88:GLY:H	2.15	0.49
1:H:175:LYS:HD3	1:H:175:LYS:C	2.32	0.49
1:J:278:ALA:O	1:J:282:ILE:HG13	2.12	0.49
1:P:104:TYR:HE2	1:P:106:GLU:HA	1.75	0.49
1:Q:175:LYS:HD3	1:Q:175:LYS:C	2.32	0.49
1:B:258:GLU:O	1:B:262:PHE:HD2	1.94	0.49
1:C:262:PHE:O	1:C:265:ASP:HB2	2.12	0.49
1:I:225:LEU:HD23	1:I:225:LEU:O	2.11	0.49
1:L:246:GLU:OE1	1:L:292:HIS:CD2	2.65	0.49
1:N:39:THR:HG22	1:N:173:ILE:HG12	1.94	0.49
1:N:65:ILE:HD12	1:N:236:ILE:HD11	1.93	0.49
1:Q:155:LEU:HD13	1:Q:225:LEU:HD22	1.94	0.49
1:S:166:PHE:O	1:S:170:VAL:HG13	2.12	0.49
1:T:264:VAL:N	1:T:274:LEU:HD13	2.27	0.49
1:W:264:VAL:N	1:W:274:LEU:HD13	2.27	0.49
1:C:189:PRO:HA	1:C:192:LEU:HD13	1.94	0.49
1:C:20:ALA:O	1:C:23:ALA:HB3	2.12	0.49
1:E:175:LYS:HD3	1:E:175:LYS:C	2.33	0.49
1:E:252:GLU:HA	1:E:252:GLU:OE2	2.13	0.49
1:G:61:LEU:HD21	1:G:148:LEU:HG	1.95	0.49
1:J:86:TRP:C	1:J:88:GLY:H	2.15	0.49
1:K:39:THR:HG22	1:K:173:ILE:HG12	1.93	0.49
1:K:65:ILE:HD12	1:K:236:ILE:HD11	1.93	0.49
1:L:120:LEU:O	1:L:124:ILE:HG13	2.12	0.49
1:N:61:LEU:HD21	1:N:148:LEU:HG	1.94	0.49
1:O:181:ALA:HA	1:O:195:SER:OG	2.12	0.49
1:Q:20:ALA:O	1:Q:23:ALA:HB3	2.12	0.49
1:R:54:TYR:CD1	1:R:155:LEU:HB2	2.47	0.49
1:T:39:THR:HG22	1:T:173:ILE:HG12	1.94	0.49
1:D:86:TRP:C	1:D:88:GLY:N	2.65	0.49
1:F:104:TYR:HE2	1:F:106:GLU:HA	1.77	0.49
1:F:47:LEU:HD11	1:F:214:LYS:HB3	1.94	0.49
1:H:240:LYS:O	1:H:244:THR:HG23	2.12	0.49
1:K:161:GLU:OE1	1:K:161:GLU:HA	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:54:TYR:CD1	1:L:155:LEU:HB2	2.47	0.49
1:L:65:ILE:HD12	1:L:236:ILE:HD11	1.94	0.49
1:O:244:THR:HA	1:O:247:ILE:HD12	1.93	0.49
1:X:86:TRP:C	1:X:88:GLY:H	2.16	0.49
1:B:61:LEU:HD21	1:B:148:LEU:HG	1.95	0.49
1:E:292:HIS:C	1:E:292:HIS:ND1	2.65	0.49
1:G:161:GLU:HA	1:G:161:GLU:OE1	2.12	0.49
1:H:264:VAL:HG23	1:H:274:LEU:CD1	2.38	0.49
1:H:262:PHE:O	1:H:265:ASP:HB2	2.12	0.49
1:J:47:LEU:HD11	1:J:214:LYS:HB3	1.93	0.49
1:K:166:PHE:O	1:K:170:VAL:HG13	2.12	0.49
1:L:104:TYR:HE2	1:L:106:GLU:HA	1.77	0.49
1:U:14:LYS:HB2	1:V:19:THR:OG1	2.12	0.49
1:U:39:THR:HG22	1:U:173:ILE:HG12	1.93	0.49
1:B:86:TRP:C	1:B:88:GLY:N	2.66	0.49
1:H:104:TYR:HE2	1:H:106:GLU:HA	1.77	0.49
1:H:166:PHE:O	1:H:170:VAL:HG13	2.12	0.49
1:H:225:LEU:HD23	1:H:225:LEU:O	2.12	0.49
1:J:181:ALA:HA	1:J:195:SER:OG	2.12	0.49
1:K:181:ALA:HA	1:K:195:SER:OG	2.12	0.49
1:K:251:GLY:O	1:K:255:THR:HG23	2.13	0.49
1:L:278:ALA:O	1:L:282:ILE:HG13	2.12	0.49
1:M:181:ALA:HA	1:M:195:SER:OG	2.13	0.49
1:M:47:LEU:HD11	1:M:214:LYS:HB3	1.93	0.49
1:R:166:PHE:O	1:R:170:VAL:HG13	2.13	0.49
1:V:251:GLY:O	1:V:255:THR:HG23	2.12	0.49
1:W:104:TYR:HE2	1:W:106:GLU:HA	1.77	0.49
1:A:61:LEU:HD21	1:A:148:LEU:HG	1.95	0.49
1:B:170:VAL:HB	1:B:208:ILE:CD1	2.43	0.49
1:D:155:LEU:HD13	1:D:225:LEU:HD22	1.94	0.49
1:H:119:VAL:HG13	1:H:120:LEU:N	2.28	0.49
1:J:116:LEU:HB3	1:J:264:VAL:HG21	1.95	0.49
1:K:77:PHE:O	1:K:81:GLN:HB2	2.13	0.49
1:L:292:HIS:ND1	1:L:292:HIS:C	2.66	0.49
1:O:166:PHE:HE1	1:O:211:LEU:HB3	1.78	0.49
1:O:264:VAL:N	1:O:274:LEU:HD13	2.28	0.49
1:O:54:TYR:CD1	1:O:155:LEU:HB2	2.48	0.49
1:Q:54:TYR:CD1	1:Q:155:LEU:HB2	2.48	0.49
1:V:112:GLN:OE1	1:W:266:TYR:OH	2.28	0.49
1:V:264:VAL:N	1:V:274:LEU:HD13	2.27	0.49
1:W:166:PHE:HE1	1:W:211:LEU:HB3	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:218:VAL:HG12	1:W:219:GLN:N	2.28	0.49
1:C:86:TRP:C	1:C:88:GLY:N	2.64	0.49
1:D:278:ALA:O	1:D:282:ILE:HG13	2.12	0.49
1:F:124:ILE:HD11	1:F:258:GLU:HA	1.95	0.49
1:F:278:ALA:O	1:F:282:ILE:HG13	2.13	0.49
1:I:278:ALA:O	1:I:282:ILE:HG13	2.12	0.49
1:R:278:ALA:O	1:R:282:ILE:HG13	2.12	0.49
1:U:116:LEU:O	1:U:120:LEU:HG	2.13	0.49
1:W:225:LEU:HD23	1:W:225:LEU:O	2.12	0.49
1:A:86:TRP:C	1:A:88:GLY:N	2.65	0.49
1:F:39:THR:HG22	1:F:173:ILE:HG12	1.94	0.49
1:F:54:TYR:CD1	1:F:155:LEU:HB2	2.47	0.49
1:K:14:LYS:HB2	1:L:19:THR:OG1	2.13	0.49
1:M:218:VAL:HG12	1:M:219:GLN:N	2.28	0.49
1:O:93:LEU:HD11	1:P:262:PHE:CG	2.48	0.49
1:Q:86:TRP:C	1:Q:88:GLY:H	2.15	0.49
1:U:264:VAL:HG23	1:U:274:LEU:CD1	2.41	0.49
1:U:65:ILE:HD12	1:U:236:ILE:HD11	1.94	0.49
1:V:20:ALA:O	1:V:23:ALA:HB3	2.12	0.49
1:C:240:LYS:O	1:C:244:THR:HG23	2.13	0.49
1:D:65:ILE:HD12	1:D:236:ILE:HD11	1.95	0.49
1:E:54:TYR:CD1	1:E:155:LEU:HB2	2.48	0.49
1:H:86:TRP:C	1:H:88:GLY:N	2.66	0.49
1:I:181:ALA:HA	1:I:195:SER:OG	2.13	0.49
1:S:240:LYS:O	1:S:244:THR:HG23	2.13	0.49
1:S:278:ALA:O	1:S:282:ILE:HG13	2.13	0.49
1:S:86:TRP:C	1:S:88:GLY:H	2.15	0.49
1:X:244:THR:HA	1:X:247:ILE:HD12	1.94	0.49
1:C:54:TYR:CD1	1:C:155:LEU:HB2	2.48	0.48
1:L:225:LEU:HD23	1:L:225:LEU:O	2.13	0.48
1:L:262:PHE:O	1:L:265:ASP:HB2	2.13	0.48
1:N:104:TYR:HE2	1:N:106:GLU:HA	1.78	0.48
1:N:264:VAL:N	1:N:274:LEU:HD13	2.28	0.48
1:R:161:GLU:HA	1:R:161:GLU:OE1	2.13	0.48
1:W:170:VAL:HB	1:W:208:ILE:CD1	2.43	0.48
1:X:258:GLU:O	1:X:262:PHE:HD2	1.96	0.48
1:X:292:HIS:ND1	1:X:292:HIS:C	2.66	0.48
1:K:54:TYR:CD1	1:K:155:LEU:HB2	2.47	0.48
1:L:240:LYS:O	1:L:244:THR:HG23	2.13	0.48
1:L:86:TRP:C	1:L:88:GLY:H	2.14	0.48
1:O:175:LYS:HD3	1:O:175:LYS:C	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:104:TYR:CE2	1:P:106:GLU:HA	2.49	0.48
1:R:262:PHE:O	1:R:265:ASP:HB2	2.13	0.48
1:R:27:TYR:CE2	1:S:183:ALA:HB2	2.48	0.48
1:S:65:ILE:HD12	1:S:236:ILE:HD11	1.94	0.48
1:U:278:ALA:O	1:U:282:ILE:HG13	2.12	0.48
1:V:86:TRP:C	1:V:88:GLY:N	2.66	0.48
1:X:116:LEU:O	1:X:120:LEU:HG	2.14	0.48
1:B:166:PHE:HE1	1:B:211:LEU:HB3	1.78	0.48
1:B:65:ILE:HD12	1:B:236:ILE:HD11	1.95	0.48
1:E:116:LEU:O	1:E:120:LEU:HG	2.13	0.48
1:G:166:PHE:HE1	1:G:211:LEU:HB3	1.77	0.48
1:H:268:ASP:C	1:H:270:MET:H	2.16	0.48
1:J:251:GLY:O	1:J:255:THR:HG23	2.14	0.48
1:P:119:VAL:HG13	1:P:120:LEU:N	2.28	0.48
1:Q:133:SER:O	1:Q:136:VAL:HG12	2.14	0.48
1:R:166:PHE:HE1	1:R:211:LEU:HB3	1.76	0.48
1:X:61:LEU:HD21	1:X:148:LEU:HG	1.95	0.48
1:A:246:GLU:OE1	1:A:292:HIS:CD2	2.67	0.48
1:B:124:ILE:HD11	1:B:258:GLU:HA	1.95	0.48
1:C:274:LEU:HG	1:C:274:LEU:O	2.12	0.48
1:E:31:LEU:HD21	1:F:179:ALA:HB1	1.96	0.48
1:F:116:LEU:O	1:F:120:LEU:HG	2.13	0.48
1:F:181:ALA:HA	1:F:195:SER:OG	2.13	0.48
1:G:288:TYR:O	1:G:292:HIS:HB3	2.14	0.48
1:I:161:GLU:HA	1:I:161:GLU:OE1	2.14	0.48
1:I:86:TRP:C	1:I:88:GLY:N	2.65	0.48
1:J:104:TYR:HE2	1:J:106:GLU:HA	1.79	0.48
1:P:43:THR:HG1	1:P:169:GLN:HG2	1.73	0.48
1:P:181:ALA:HA	1:P:195:SER:OG	2.13	0.48
1:Q:288:TYR:O	1:Q:292:HIS:HB3	2.14	0.48
1:R:86:TRP:C	1:R:88:GLY:N	2.66	0.48
1:T:175:LYS:C	1:T:175:LYS:HD3	2.33	0.48
1:X:278:ALA:O	1:X:282:ILE:HG13	2.13	0.48
1:E:246:GLU:OE1	1:E:292:HIS:CD2	2.63	0.48
1:G:181:ALA:HA	1:G:195:SER:OG	2.13	0.48
1:G:268:ASP:C	1:G:270:MET:H	2.17	0.48
1:H:181:ALA:HA	1:H:195:SER:OG	2.13	0.48
1:H:278:ALA:O	1:H:282:ILE:HG13	2.13	0.48
1:I:244:THR:HA	1:I:247:ILE:HD12	1.94	0.48
1:O:124:ILE:HD11	1:O:258:GLU:HA	1.96	0.48
1:V:77:PHE:O	1:V:81:GLN:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:104:TYR:HE2	1:X:106:GLU:HA	1.78	0.48
1:A:225:LEU:O	1:A:225:LEU:HD23	2.14	0.48
1:B:268:ASP:C	1:B:270:MET:H	2.16	0.48
1:E:264:VAL:N	1:E:274:LEU:HD13	2.29	0.48
1:K:133:SER:O	1:K:136:VAL:HG12	2.13	0.48
1:K:264:VAL:N	1:K:274:LEU:HD13	2.29	0.48
1:N:86:TRP:C	1:N:88:GLY:N	2.65	0.48
1:S:181:ALA:HA	1:S:195:SER:OG	2.12	0.48
1:U:264:VAL:N	1:U:274:LEU:HD13	2.28	0.48
1:A:240:LYS:O	1:A:244:THR:HG23	2.14	0.48
1:C:166:PHE:HE1	1:C:211:LEU:HB3	1.78	0.48
1:D:264:VAL:N	1:D:274:LEU:HD13	2.28	0.48
1:L:251:GLY:O	1:L:255:THR:HG23	2.12	0.48
1:O:251:GLY:O	1:O:255:THR:HG23	2.14	0.48
1:Q:240:LYS:O	1:Q:244:THR:HG23	2.14	0.48
1:U:166:PHE:HE1	1:U:211:LEU:HB3	1.77	0.48
1:W:166:PHE:O	1:W:170:VAL:HG13	2.13	0.48
1:W:65:ILE:HD12	1:W:236:ILE:HD11	1.96	0.48
1:A:119:VAL:HG13	1:A:120:LEU:N	2.27	0.48
1:D:181:ALA:HA	1:D:195:SER:OG	2.14	0.48
1:D:218:VAL:HG12	1:D:219:GLN:N	2.28	0.48
1:E:65:ILE:HD12	1:E:236:ILE:HD11	1.94	0.48
1:L:77:PHE:O	1:L:81:GLN:HB2	2.14	0.48
1:P:170:VAL:HB	1:P:208:ILE:CD1	2.42	0.48
1:T:264:VAL:HG23	1:T:274:LEU:CD1	2.35	0.48
1:X:86:TRP:C	1:X:88:GLY:N	2.67	0.48
1:A:104:TYR:HE2	1:A:106:GLU:HA	1.79	0.48
1:C:268:ASP:C	1:C:270:MET:H	2.16	0.48
1:G:246:GLU:OE1	1:G:292:HIS:CD2	2.67	0.48
1:K:170:VAL:HB	1:K:208:ILE:CD1	2.43	0.48
1:L:86:TRP:C	1:L:88:GLY:N	2.67	0.48
1:M:112:GLN:OE1	1:N:266:TYR:OH	2.26	0.48
1:Q:104:TYR:HE2	1:Q:106:GLU:HA	1.79	0.48
1:S:155:LEU:HD13	1:S:225:LEU:HD22	1.95	0.48
1:T:65:ILE:HD12	1:T:236:ILE:HD11	1.94	0.48
1:V:54:TYR:CD1	1:V:155:LEU:HB2	2.48	0.48
1:V:264:VAL:HG23	1:V:274:LEU:CD1	2.39	0.48
1:V:268:ASP:C	1:V:270:MET:H	2.17	0.48
1:W:161:GLU:OE1	1:W:161:GLU:HA	2.14	0.48
1:C:218:VAL:HG12	1:C:219:GLN:N	2.28	0.48
1:G:65:ILE:HD12	1:G:236:ILE:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:116:LEU:O	1:J:120:LEU:HG	2.14	0.48
1:J:65:ILE:HD12	1:J:236:ILE:HD11	1.95	0.48
1:L:124:ILE:HD11	1:L:258:GLU:HA	1.96	0.48
1:M:86:TRP:C	1:M:88:GLY:N	2.66	0.48
1:N:181:ALA:HA	1:N:195:SER:OG	2.14	0.48
1:P:65:ILE:HD12	1:P:236:ILE:HD11	1.96	0.48
1:S:86:TRP:C	1:S:88:GLY:N	2.68	0.48
1:U:124:ILE:HD11	1:U:258:GLU:HA	1.96	0.48
1:W:181:ALA:HA	1:W:195:SER:OG	2.12	0.48
1:A:268:ASP:C	1:A:270:MET:H	2.17	0.47
1:B:119:VAL:HG13	1:B:120:LEU:N	2.29	0.47
1:C:181:ALA:HA	1:C:195:SER:OG	2.14	0.47
1:D:166:PHE:O	1:D:170:VAL:HG13	2.14	0.47
1:E:166:PHE:O	1:E:170:VAL:HG13	2.14	0.47
1:E:170:VAL:HB	1:E:208:ILE:CD1	2.44	0.47
1:F:104:TYR:CE2	1:F:106:GLU:HA	2.49	0.47
1:K:104:TYR:HE2	1:K:106:GLU:HA	1.79	0.47
1:K:262:PHE:O	1:K:265:ASP:HB2	2.13	0.47
1:A:19:THR:OG1	1:L:14:LYS:HB2	2.13	0.47
1:L:246:GLU:OE1	1:L:292:HIS:HD2	1.97	0.47
1:M:278:ALA:O	1:M:282:ILE:HG13	2.14	0.47
1:N:166:PHE:O	1:N:170:VAL:HG13	2.14	0.47
1:O:65:ILE:HD12	1:O:236:ILE:HD11	1.96	0.47
1:Q:107:LYS:HD3	1:Q:107:LYS:HA	1.71	0.47
1:T:86:TRP:C	1:T:88:GLY:N	2.67	0.47
1:U:274:LEU:O	1:U:274:LEU:HG	2.14	0.47
1:U:27:TYR:CE2	1:V:183:ALA:HB2	2.48	0.47
1:U:86:TRP:C	1:U:88:GLY:N	2.65	0.47
1:X:104:TYR:CE2	1:X:106:GLU:HA	2.49	0.47
1:X:161:GLU:HA	1:X:161:GLU:OE1	2.14	0.47
1:X:225:LEU:HD23	1:X:225:LEU:O	2.14	0.47
1:G:104:TYR:HE2	1:G:106:GLU:HA	1.78	0.47
1:G:278:ALA:O	1:G:282:ILE:HG13	2.14	0.47
1:H:133:SER:O	1:H:136:VAL:HG12	2.14	0.47
1:I:264:VAL:HG23	1:I:274:LEU:CD1	2.40	0.47
1:M:20:ALA:O	1:M:23:ALA:HB3	2.13	0.47
1:M:251:GLY:O	1:M:255:THR:HG23	2.14	0.47
1:O:86:TRP:C	1:O:88:GLY:H	2.17	0.47
1:R:116:LEU:HB3	1:R:264:VAL:HG21	1.96	0.47
1:S:54:TYR:CD1	1:S:155:LEU:HB2	2.49	0.47
1:S:31:LEU:HD21	1:T:179:ALA:HB1	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:258:GLU:O	1:U:262:PHE:HD2	1.97	0.47
1:X:166:PHE:HE1	1:X:211:LEU:HB3	1.79	0.47
1:X:246:GLU:OE1	1:X:292:HIS:CD2	2.67	0.47
1:E:86:TRP:C	1:E:88:GLY:H	2.16	0.47
1:L:181:ALA:HA	1:L:195:SER:OG	2.13	0.47
1:K:93:LEU:HD11	1:L:262:PHE:CG	2.48	0.47
1:N:116:LEU:O	1:N:120:LEU:HG	2.14	0.47
1:N:218:VAL:HG12	1:N:219:GLN:N	2.29	0.47
1:R:181:ALA:HA	1:R:195:SER:OG	2.14	0.47
1:R:251:GLY:O	1:R:255:THR:HG23	2.14	0.47
1:S:124:ILE:HD11	1:S:258:GLU:HA	1.97	0.47
1:B:161:GLU:OE1	1:B:161:GLU:HA	2.14	0.47
1:H:104:TYR:CE2	1:H:106:GLU:HA	2.50	0.47
1:I:264:VAL:N	1:I:274:LEU:HD13	2.29	0.47
1:K:86:TRP:C	1:K:88:GLY:N	2.67	0.47
1:N:62:VAL:CG1	1:O:149:LEU:HD21	2.45	0.47
1:O:155:LEU:HD13	1:O:225:LEU:HD22	1.96	0.47
1:O:116:LEU:HB3	1:O:264:VAL:HG21	1.96	0.47
1:O:61:LEU:HD21	1:O:148:LEU:HG	1.95	0.47
1:U:251:GLY:O	1:U:255:THR:HG23	2.14	0.47
1:W:253:ILE:O	1:W:254:LYS:C	2.53	0.47
1:B:264:VAL:N	1:B:274:LEU:HD13	2.29	0.47
1:C:124:ILE:HD11	1:C:258:GLU:HA	1.96	0.47
1:C:166:PHE:O	1:C:170:VAL:HG13	2.15	0.47
1:E:104:TYR:HE2	1:E:106:GLU:HA	1.79	0.47
1:E:61:LEU:HD21	1:E:148:LEU:HG	1.97	0.47
1:G:119:VAL:HG13	1:G:120:LEU:N	2.29	0.47
1:H:288:TYR:O	1:H:292:HIS:HB3	2.13	0.47
1:I:116:LEU:HB3	1:I:264:VAL:HG21	1.96	0.47
1:Q:181:ALA:HA	1:Q:195:SER:OG	2.13	0.47
1:Q:62:VAL:HG12	1:R:149:LEU:CD2	2.43	0.47
1:X:116:LEU:HB3	1:X:264:VAL:HG21	1.96	0.47
1:W:62:VAL:CG1	1:X:149:LEU:HD21	2.43	0.47
1:B:225:LEU:HD23	1:B:225:LEU:O	2.15	0.47
1:B:54:TYR:CD1	1:B:155:LEU:HB2	2.50	0.47
1:F:161:GLU:OE1	1:F:161:GLU:HA	2.14	0.47
1:N:133:SER:O	1:N:136:VAL:HG12	2.14	0.47
1:R:264:VAL:N	1:R:274:LEU:HD13	2.29	0.47
1:S:116:LEU:HB3	1:S:264:VAL:HG21	1.97	0.47
1:U:78:GLU:HB2	1:V:135:LEU:HD21	1.97	0.47
1:W:104:TYR:CE2	1:W:106:GLU:HA	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:TYR:HE2	1:C:106:GLU:HA	1.79	0.47
1:C:155:LEU:HD13	1:C:225:LEU:HD22	1.97	0.47
1:C:264:VAL:N	1:C:274:LEU:HD13	2.29	0.47
1:C:86:TRP:O	1:C:88:GLY:N	2.47	0.47
1:D:119:VAL:HG13	1:D:120:LEU:N	2.30	0.47
1:N:119:VAL:HG13	1:N:120:LEU:N	2.28	0.47
1:O:104:TYR:HE2	1:O:106:GLU:HA	1.79	0.47
1:Q:116:LEU:HB3	1:Q:264:VAL:HG21	1.97	0.47
1:Q:161:GLU:OE1	1:Q:161:GLU:HA	2.13	0.47
1:Q:53:GLU:O	1:Q:56:GLN:HB3	2.14	0.47
1:V:104:TYR:CE2	1:V:106:GLU:HA	2.50	0.47
1:A:181:ALA:HA	1:A:195:SER:OG	2.15	0.47
1:G:133:SER:O	1:G:136:VAL:HG12	2.15	0.47
1:I:119:VAL:HG13	1:I:120:LEU:N	2.29	0.47
1:L:170:VAL:HB	1:L:208:ILE:CD1	2.44	0.47
1:Q:268:ASP:C	1:Q:270:MET:H	2.18	0.47
1:R:218:VAL:HG12	1:R:219:GLN:N	2.30	0.47
1:S:274:LEU:HG	1:S:274:LEU:O	2.15	0.47
1:U:161:GLU:HA	1:U:161:GLU:OE1	2.15	0.47
1:D:133:SER:O	1:D:136:VAL:HG12	2.15	0.47
1:J:39:THR:HG22	1:J:173:ILE:HG12	1.97	0.47
1:J:218:VAL:HG12	1:J:219:GLN:N	2.29	0.47
1:N:104:TYR:CE2	1:N:106:GLU:HA	2.50	0.47
1:O:77:PHE:O	1:O:81:GLN:HB2	2.15	0.47
1:Q:104:TYR:CE2	1:Q:106:GLU:HA	2.50	0.47
1:X:240:LYS:O	1:X:244:THR:HG23	2.15	0.47
1:X:251:GLY:O	1:X:255:THR:HG23	2.15	0.47
1:A:166:PHE:HE1	1:A:211:LEU:HB3	1.79	0.47
1:B:251:GLY:O	1:B:255:THR:HG23	2.15	0.47
1:C:161:GLU:OE1	1:C:161:GLU:HA	2.15	0.47
1:F:119:VAL:HG13	1:F:120:LEU:N	2.29	0.47
1:F:37:TRP:HE1	1:G:172:LYS:HZ3	1.63	0.47
1:H:93:LEU:HD11	1:I:262:PHE:CG	2.50	0.47
1:N:161:GLU:HA	1:N:161:GLU:OE1	2.15	0.47
1:N:264:VAL:HG23	1:N:274:LEU:CD1	2.42	0.47
1:S:264:VAL:N	1:S:274:LEU:HD13	2.30	0.47
1:V:271:LEU:HD22	1:V:273:LEU:H	1.80	0.47
1:C:116:LEU:O	1:C:120:LEU:HG	2.14	0.47
1:G:264:VAL:HG23	1:G:274:LEU:CD1	2.41	0.47
1:G:86:TRP:C	1:G:88:GLY:N	2.68	0.47
1:I:246:GLU:OE1	1:I:292:HIS:CD2	2.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:116:LEU:O	1:L:120:LEU:HG	2.15	0.47
1:O:119:VAL:HG13	1:O:120:LEU:N	2.29	0.47
1:P:166:PHE:O	1:P:170:VAL:HG13	2.15	0.47
1:P:268:ASP:C	1:P:270:MET:H	2.17	0.47
1:Q:77:PHE:O	1:Q:81:GLN:HB2	2.14	0.47
1:W:240:LYS:O	1:W:244:THR:HG23	2.15	0.47
1:A:170:VAL:HB	1:A:208:ILE:CD1	2.45	0.46
1:C:116:LEU:HB3	1:C:264:VAL:HG21	1.97	0.46
1:E:181:ALA:HA	1:E:195:SER:OG	2.14	0.46
1:H:161:GLU:OE1	1:H:161:GLU:HA	2.15	0.46
1:H:274:LEU:HG	1:H:274:LEU:O	2.15	0.46
1:L:104:TYR:CE2	1:L:106:GLU:HA	2.50	0.46
1:M:104:TYR:HD1	1:M:270:MET:HG2	1.80	0.46
1:O:258:GLU:O	1:O:262:PHE:HD2	1.97	0.46
1:R:119:VAL:HG13	1:R:120:LEU:N	2.30	0.46
1:R:69:LEU:HD23	1:R:141:PHE:CZ	2.50	0.46
1:C:27:TYR:CE2	1:D:183:ALA:HB2	2.50	0.46
1:K:225:LEU:O	1:K:225:LEU:HD23	2.15	0.46
1:P:251:GLY:O	1:P:255:THR:HG23	2.15	0.46
1:H:116:LEU:HB3	1:H:264:VAL:HG21	1.97	0.46
1:K:116:LEU:O	1:K:120:LEU:HG	2.16	0.46
1:R:225:LEU:O	1:R:225:LEU:HD23	2.14	0.46
1:T:133:SER:O	1:T:136:VAL:HG12	2.15	0.46
1:V:155:LEU:HD13	1:V:225:LEU:HD22	1.96	0.46
1:X:181:ALA:HA	1:X:195:SER:OG	2.15	0.46
1:C:251:GLY:O	1:C:255:THR:HG23	2.15	0.46
1:F:166:PHE:HE1	1:F:211:LEU:HB3	1.80	0.46
1:G:124:ILE:HD11	1:G:258:GLU:HA	1.96	0.46
1:H:218:VAL:HG12	1:H:219:GLN:N	2.30	0.46
1:J:119:VAL:HG13	1:J:120:LEU:N	2.29	0.46
1:J:77:PHE:O	1:J:81:GLN:HB2	2.16	0.46
1:M:225:LEU:O	1:M:225:LEU:HD23	2.15	0.46
1:M:65:ILE:HD12	1:M:236:ILE:HD11	1.96	0.46
1:O:104:TYR:CE2	1:O:106:GLU:HA	2.51	0.46
1:Q:14:LYS:HB2	1:R:19:THR:OG1	2.15	0.46
1:S:170:VAL:HB	1:S:208:ILE:CD1	2.46	0.46
1:X:119:VAL:HG13	1:X:120:LEU:N	2.30	0.46
1:B:181:ALA:HA	1:B:195:SER:OG	2.16	0.46
1:G:104:TYR:CE2	1:G:106:GLU:HA	2.50	0.46
1:M:77:PHE:O	1:M:81:GLN:HB2	2.15	0.46
1:T:251:GLY:O	1:T:255:THR:HG23	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:104:TYR:HE2	1:U:106:GLU:HA	1.81	0.46
1:X:77:PHE:O	1:X:81:GLN:HB2	2.16	0.46
1:A:166:PHE:O	1:A:170:VAL:HG13	2.15	0.46
1:F:86:TRP:C	1:F:88:GLY:H	2.18	0.46
1:G:240:LYS:O	1:G:244:THR:HG23	2.16	0.46
1:I:170:VAL:HB	1:I:208:ILE:CD1	2.45	0.46
1:J:107:LYS:HA	1:J:107:LYS:HD3	1.73	0.46
1:J:268:ASP:C	1:J:270:MET:H	2.19	0.46
1:L:119:VAL:HG13	1:L:120:LEU:N	2.30	0.46
1:L:274:LEU:HG	1:L:274:LEU:O	2.15	0.46
1:O:225:LEU:O	1:O:225:LEU:HD23	2.15	0.46
1:P:288:TYR:O	1:P:292:HIS:HB3	2.15	0.46
1:Q:170:VAL:HB	1:Q:208:ILE:CD1	2.46	0.46
1:V:124:ILE:HD11	1:V:258:GLU:HA	1.96	0.46
1:V:181:ALA:HA	1:V:195:SER:OG	2.16	0.46
1:A:104:TYR:CE2	1:A:106:GLU:HA	2.50	0.46
1:A:251:GLY:O	1:A:255:THR:HG23	2.15	0.46
1:D:225:LEU:O	1:D:225:LEU:HD23	2.16	0.46
1:E:251:GLY:O	1:E:255:THR:HG23	2.15	0.46
1:K:116:LEU:HB3	1:K:264:VAL:HG21	1.98	0.46
1:L:264:VAL:N	1:L:274:LEU:HD13	2.30	0.46
1:M:116:LEU:HB3	1:M:264:VAL:HG21	1.97	0.46
1:P:116:LEU:O	1:P:120:LEU:HG	2.16	0.46
1:Q:225:LEU:HD23	1:Q:225:LEU:O	2.16	0.46
1:R:170:VAL:HB	1:R:208:ILE:CD1	2.46	0.46
1:T:116:LEU:O	1:T:120:LEU:HG	2.15	0.46
1:T:268:ASP:C	1:T:270:MET:H	2.19	0.46
1:W:133:SER:O	1:W:136:VAL:HG12	2.16	0.46
1:W:116:LEU:HB3	1:W:264:VAL:HG21	1.97	0.46
1:X:274:LEU:O	1:X:274:LEU:HG	2.16	0.46
1:N:116:LEU:HB3	1:N:264:VAL:HG21	1.96	0.46
1:O:116:LEU:O	1:O:120:LEU:HG	2.15	0.46
1:P:161:GLU:HA	1:P:161:GLU:OE1	2.16	0.46
1:R:274:LEU:HG	1:R:274:LEU:O	2.15	0.46
1:S:104:TYR:HE2	1:S:106:GLU:HA	1.80	0.46
1:U:225:LEU:HD23	1:U:225:LEU:O	2.15	0.46
1:X:218:VAL:HG12	1:X:219:GLN:N	2.31	0.46
1:X:268:ASP:C	1:X:270:MET:H	2.18	0.46
1:B:31:LEU:HD21	1:C:179:ALA:HB1	1.96	0.46
1:E:161:GLU:OE1	1:E:161:GLU:HA	2.15	0.46
1:F:155:LEU:HD13	1:F:225:LEU:HD22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:166:PHE:O	1:I:170:VAL:HG13	2.16	0.46
1:J:27:TYR:CE2	1:K:183:ALA:HB2	2.51	0.46
1:K:104:TYR:CE2	1:K:106:GLU:HA	2.51	0.46
1:L:161:GLU:HA	1:L:161:GLU:OE1	2.16	0.46
1:M:268:ASP:C	1:M:270:MET:H	2.17	0.46
1:Q:218:VAL:HG12	1:Q:219:GLN:N	2.31	0.46
1:Q:264:VAL:HG23	1:Q:274:LEU:CD1	2.43	0.46
1:X:107:LYS:HD3	1:X:107:LYS:HA	1.75	0.46
1:A:155:LEU:HD13	1:A:225:LEU:HD22	1.98	0.46
1:C:225:LEU:O	1:C:225:LEU:HD23	2.16	0.46
1:F:27:TYR:CE2	1:G:183:ALA:HB2	2.51	0.46
1:I:62:VAL:CG1	1:J:149:LEU:HD21	2.44	0.46
1:O:271:LEU:HD22	1:O:273:LEU:H	1.81	0.46
1:R:124:ILE:HD11	1:R:258:GLU:HA	1.98	0.46
1:V:127:LEU:HA	1:V:127:LEU:HD23	1.77	0.46
1:D:161:GLU:OE1	1:D:161:GLU:HA	2.16	0.45
1:D:251:GLY:O	1:D:255:THR:HG23	2.16	0.45
1:D:264:VAL:HG23	1:D:274:LEU:CD1	2.43	0.45
1:F:116:LEU:HB3	1:F:264:VAL:HG21	1.97	0.45
1:E:93:LEU:HD11	1:F:262:PHE:CG	2.51	0.45
1:F:264:VAL:N	1:F:274:LEU:HD13	2.30	0.45
1:M:104:TYR:CE2	1:M:106:GLU:HA	2.51	0.45
1:P:86:TRP:C	1:P:88:GLY:N	2.68	0.45
1:U:268:ASP:C	1:U:270:MET:H	2.20	0.45
1:U:77:PHE:O	1:U:81:GLN:HB2	2.16	0.45
1:W:124:ILE:HD11	1:W:258:GLU:HA	1.98	0.45
1:W:271:LEU:HD22	1:W:273:LEU:H	1.81	0.45
1:A:77:PHE:O	1:A:81:GLN:HB2	2.16	0.45
1:B:77:PHE:O	1:B:81:GLN:HB2	2.16	0.45
1:G:77:PHE:O	1:G:81:GLN:HB2	2.16	0.45
1:I:133:SER:O	1:I:136:VAL:HG12	2.15	0.45
1:J:104:TYR:CE2	1:J:106:GLU:HA	2.51	0.45
1:M:119:VAL:HG13	1:M:120:LEU:N	2.29	0.45
1:O:161:GLU:OE1	1:O:161:GLU:HA	2.15	0.45
1:O:86:TRP:C	1:O:88:GLY:N	2.69	0.45
1:P:93:LEU:HD11	1:Q:262:PHE:CG	2.52	0.45
1:R:104:TYR:CE2	1:R:106:GLU:HA	2.51	0.45
1:Q:62:VAL:CG1	1:R:149:LEU:HD21	2.44	0.45
1:R:104:TYR:HD1	1:R:270:MET:HG2	1.81	0.45
1:T:116:LEU:HB3	1:T:264:VAL:HG21	1.98	0.45
1:V:225:LEU:O	1:V:225:LEU:HD23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:86:TRP:C	1:W:88:GLY:H	2.19	0.45
1:A:161:GLU:OE1	1:A:161:GLU:HA	2.15	0.45
1:B:104:TYR:CE2	1:B:106:GLU:HA	2.49	0.45
1:B:264:VAL:HG23	1:B:274:LEU:CD1	2.40	0.45
1:E:155:LEU:HD13	1:E:225:LEU:HD22	1.98	0.45
1:E:27:TYR:CE2	1:F:183:ALA:HB2	2.52	0.45
1:H:170:VAL:HB	1:H:208:ILE:CD1	2.47	0.45
1:L:268:ASP:C	1:L:270:MET:H	2.18	0.45
1:R:107:LYS:HD3	1:R:107:LYS:HA	1.73	0.45
1:V:161:GLU:OE1	1:V:161:GLU:HA	2.16	0.45
1:D:104:TYR:HE2	1:D:106:GLU:HA	1.80	0.45
1:E:268:ASP:C	1:E:270:MET:H	2.20	0.45
1:I:251:GLY:O	1:I:255:THR:HG23	2.17	0.45
1:I:124:ILE:HD11	1:I:258:GLU:HA	1.97	0.45
1:I:271:LEU:HD23	1:I:272:SER:N	2.32	0.45
1:J:86:TRP:C	1:J:88:GLY:N	2.68	0.45
1:M:107:LYS:HA	1:M:107:LYS:HD3	1.72	0.45
1:R:268:ASP:C	1:R:270:MET:H	2.19	0.45
1:S:104:TYR:CE2	1:S:106:GLU:HA	2.51	0.45
1:T:161:GLU:HA	1:T:161:GLU:OE1	2.16	0.45
1:U:271:LEU:HD22	1:U:273:LEU:H	1.81	0.45
1:W:208:ILE:HA	1:W:208:ILE:HD13	1.81	0.45
1:X:264:VAL:HG23	1:X:274:LEU:CD1	2.45	0.45
1:A:116:LEU:HA	1:A:116:LEU:HD23	1.67	0.45
1:D:107:LYS:HA	1:D:107:LYS:HD3	1.74	0.45
1:D:274:LEU:O	1:D:274:LEU:HG	2.16	0.45
1:E:86:TRP:C	1:E:88:GLY:N	2.69	0.45
1:F:53:GLU:O	1:F:56:GLN:HB3	2.16	0.45
1:G:155:LEU:HD13	1:G:225:LEU:HD22	1.98	0.45
1:J:161:GLU:HA	1:J:161:GLU:OE1	2.17	0.45
1:K:288:TYR:O	1:K:292:HIS:HB3	2.17	0.45
1:M:104:TYR:HE2	1:M:106:GLU:HA	1.81	0.45
1:M:136:VAL:CG1	1:M:137:SER:N	2.79	0.45
1:N:246:GLU:OE1	1:N:292:HIS:CD2	2.70	0.45
1:R:116:LEU:O	1:R:120:LEU:HG	2.16	0.45
1:R:14:LYS:HB2	1:S:19:THR:OG1	2.15	0.45
1:S:251:GLY:O	1:S:255:THR:HG23	2.16	0.45
1:S:264:VAL:HG23	1:S:274:LEU:CD1	2.41	0.45
1:B:155:LEU:HD13	1:B:225:LEU:HD22	1.98	0.45
1:C:136:VAL:CG1	1:C:137:SER:N	2.79	0.45
1:D:166:PHE:HE1	1:D:211:LEU:HB3	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:124:ILE:HD11	1:D:258:GLU:HA	1.98	0.45
1:E:77:PHE:O	1:E:81:GLN:HB2	2.16	0.45
1:I:218:VAL:HG12	1:I:219:GLN:N	2.31	0.45
1:I:77:PHE:O	1:I:81:GLN:HB2	2.16	0.45
1:I:93:LEU:HD11	1:J:262:PHE:CG	2.52	0.45
1:N:86:TRP:O	1:N:88:GLY:N	2.49	0.45
1:P:53:GLU:O	1:P:56:GLN:HB3	2.17	0.45
1:S:246:GLU:OE1	1:S:292:HIS:HD2	1.97	0.45
1:S:77:PHE:O	1:S:81:GLN:HB2	2.17	0.45
1:T:104:TYR:HD1	1:T:270:MET:HG2	1.81	0.45
1:U:208:ILE:HD13	1:U:208:ILE:HA	1.83	0.45
1:C:104:TYR:CE2	1:C:106:GLU:HA	2.51	0.45
1:F:262:PHE:O	1:F:265:ASP:HB2	2.16	0.45
1:G:116:LEU:HB3	1:G:264:VAL:HG21	1.98	0.45
1:H:77:PHE:O	1:H:81:GLN:HB2	2.17	0.45
1:I:268:ASP:C	1:I:270:MET:H	2.19	0.45
1:L:264:VAL:HG23	1:L:274:LEU:CD1	2.39	0.45
1:M:116:LEU:O	1:M:120:LEU:HG	2.16	0.45
1:P:225:LEU:HD23	1:P:225:LEU:O	2.15	0.45
1:Q:274:LEU:HG	1:Q:274:LEU:O	2.16	0.45
1:R:104:TYR:HE2	1:R:106:GLU:HA	1.80	0.45
1:C:271:LEU:HD23	1:C:272:SER:N	2.32	0.45
1:G:104:TYR:HD1	1:G:270:MET:HG2	1.82	0.45
1:J:155:LEU:HD13	1:J:225:LEU:HD22	1.97	0.45
1:N:268:ASP:C	1:N:270:MET:H	2.18	0.45
1:P:77:PHE:O	1:P:81:GLN:HB2	2.17	0.45
1:W:62:VAL:HG12	1:X:149:LEU:CD2	2.44	0.45
1:W:86:TRP:C	1:W:88:GLY:N	2.70	0.45
1:F:251:GLY:O	1:F:255:THR:HG23	2.16	0.45
1:H:107:LYS:HA	1:H:107:LYS:HD3	1.73	0.45
1:H:104:TYR:HD1	1:H:270:MET:HG2	1.82	0.45
1:I:104:TYR:HE2	1:I:106:GLU:HA	1.81	0.45
1:K:274:LEU:O	1:K:274:LEU:HG	2.16	0.45
1:L:116:LEU:HB3	1:L:264:VAL:HG21	1.98	0.45
1:M:127:LEU:HD23	1:M:127:LEU:HA	1.76	0.45
1:M:124:ILE:HD11	1:M:258:GLU:HA	1.99	0.45
1:Q:271:LEU:HD23	1:Q:272:SER:N	2.32	0.45
1:T:155:LEU:HD13	1:T:225:LEU:HD22	1.99	0.45
1:U:108:LYS:HE3	1:V:268:ASP:HB2	1.99	0.45
1:W:104:TYR:HD1	1:W:270:MET:HG2	1.81	0.45
1:D:170:VAL:HB	1:D:208:ILE:CD1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:116:LEU:HB3	1:E:264:VAL:HG21	1.99	0.45
1:F:268:ASP:C	1:F:270:MET:H	2.19	0.45
1:H:116:LEU:O	1:H:120:LEU:HG	2.17	0.45
1:N:225:LEU:HD23	1:N:225:LEU:O	2.16	0.45
1:N:271:LEU:HD22	1:N:273:LEU:H	1.81	0.45
1:P:116:LEU:HB3	1:P:264:VAL:HG21	1.98	0.45
1:Q:86:TRP:C	1:Q:88:GLY:N	2.68	0.45
1:S:93:LEU:HD11	1:T:262:PHE:CG	2.52	0.45
1:U:104:TYR:HD1	1:U:270:MET:HG2	1.82	0.45
1:V:133:SER:O	1:V:136:VAL:HG12	2.17	0.45
1:W:251:GLY:O	1:W:255:THR:HG23	2.16	0.45
1:X:136:VAL:CG1	1:X:137:SER:N	2.80	0.45
1:B:116:LEU:O	1:B:120:LEU:HG	2.17	0.44
1:B:253:ILE:O	1:B:254:LYS:C	2.56	0.44
1:E:104:TYR:CE2	1:E:106:GLU:HA	2.52	0.44
1:F:170:VAL:HB	1:F:208:ILE:CD1	2.47	0.44
1:J:104:TYR:HD1	1:J:270:MET:HG2	1.82	0.44
1:M:161:GLU:OE1	1:M:161:GLU:HA	2.17	0.44
1:P:218:VAL:HG12	1:P:219:GLN:N	2.31	0.44
1:Q:93:LEU:HD11	1:R:262:PHE:CG	2.52	0.44
1:R:65:ILE:HD12	1:R:236:ILE:HD11	1.98	0.44
1:S:119:VAL:HG13	1:S:120:LEU:N	2.32	0.44
1:S:161:GLU:HA	1:S:161:GLU:OE1	2.16	0.44
1:X:264:VAL:N	1:X:274:LEU:HD13	2.32	0.44
1:B:46:GLU:O	1:B:46:GLU:HG3	2.17	0.44
1:D:268:ASP:C	1:D:270:MET:H	2.20	0.44
1:H:271:LEU:HD23	1:H:272:SER:N	2.32	0.44
1:K:218:VAL:HG12	1:K:219:GLN:N	2.31	0.44
1:O:218:VAL:HG12	1:O:219:GLN:N	2.31	0.44
1:P:124:ILE:HD11	1:P:258:GLU:HA	1.98	0.44
1:V:116:LEU:O	1:V:120:LEU:HG	2.17	0.44
1:V:119:VAL:HG13	1:V:120:LEU:N	2.32	0.44
1:V:274:LEU:O	1:V:274:LEU:HG	2.16	0.44
1:X:53:GLU:O	1:X:56:GLN:HB3	2.17	0.44
1:A:86:TRP:O	1:A:88:GLY:N	2.50	0.44
1:B:218:VAL:HG12	1:B:219:GLN:N	2.32	0.44
1:D:116:LEU:HB3	1:D:264:VAL:HG21	1.99	0.44
1:E:258:GLU:O	1:E:262:PHE:HD2	2.00	0.44
1:F:86:TRP:C	1:F:88:GLY:N	2.69	0.44
1:G:116:LEU:O	1:G:120:LEU:HG	2.17	0.44
1:H:69:LEU:HD23	1:H:141:PHE:CZ	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:104:TYR:CE2	1:I:106:GLU:HA	2.52	0.44
1:I:116:LEU:HD23	1:I:116:LEU:HA	1.71	0.44
1:J:28:ASN:O	1:J:29:LYS:C	2.56	0.44
1:K:37:TRP:HE1	1:L:172:LYS:HZ3	1.66	0.44
1:N:124:ILE:HD11	1:N:258:GLU:HA	1.99	0.44
1:A:274:LEU:HG	1:A:274:LEU:O	2.18	0.44
1:A:292:HIS:ND1	1:A:292:HIS:C	2.70	0.44
1:B:116:LEU:HB3	1:B:264:VAL:HG21	2.00	0.44
1:C:170:VAL:HB	1:C:208:ILE:CD1	2.48	0.44
1:E:274:LEU:O	1:E:274:LEU:HG	2.16	0.44
1:I:43:THR:HG1	1:I:169:GLN:HG2	1.77	0.44
1:J:127:LEU:HA	1:J:127:LEU:HD23	1.74	0.44
1:M:264:VAL:N	1:M:274:LEU:HD13	2.32	0.44
1:R:53:GLU:O	1:R:56:GLN:HB3	2.17	0.44
1:S:116:LEU:O	1:S:120:LEU:HG	2.16	0.44
1:S:268:ASP:C	1:S:270:MET:H	2.21	0.44
1:S:65:ILE:CD1	1:S:144:ALA:HB1	2.48	0.44
1:S:76:TYR:CE2	1:S:242:LYS:HE2	2.52	0.44
1:T:53:GLU:O	1:T:56:GLN:HB3	2.17	0.44
1:V:271:LEU:HD23	1:V:272:SER:N	2.32	0.44
1:W:116:LEU:O	1:W:120:LEU:HG	2.17	0.44
1:A:116:LEU:HB3	1:A:264:VAL:HG21	1.98	0.44
1:A:17:ILE:CG2	1:A:18:GLU:N	2.81	0.44
1:C:62:VAL:HG12	1:D:149:LEU:CD2	2.45	0.44
1:D:104:TYR:CE2	1:D:106:GLU:HA	2.53	0.44
1:I:127:LEU:HA	1:I:127:LEU:HD23	1.76	0.44
1:I:53:GLU:O	1:I:56:GLN:HB3	2.18	0.44
1:L:116:LEU:HA	1:L:116:LEU:HD23	1.72	0.44
1:L:271:LEU:HD23	1:L:272:SER:N	2.33	0.44
1:T:119:VAL:HG13	1:T:120:LEU:N	2.33	0.44
1:U:86:TRP:O	1:U:88:GLY:N	2.50	0.44
1:W:268:ASP:C	1:W:270:MET:H	2.19	0.44
1:C:264:VAL:HG23	1:C:274:LEU:CD1	2.43	0.44
1:C:37:TRP:HE1	1:D:172:LYS:HZ3	1.66	0.44
1:I:86:TRP:O	1:I:88:GLY:N	2.51	0.44
1:J:170:VAL:HB	1:J:208:ILE:CD1	2.47	0.44
1:N:77:PHE:O	1:N:81:GLN:HB2	2.18	0.44
1:P:269:LEU:HA	1:P:269:LEU:HD23	1.86	0.44
1:R:240:LYS:O	1:R:244:THR:HG23	2.17	0.44
1:G:271:LEU:HD22	1:G:273:LEU:H	1.82	0.44
1:H:253:ILE:O	1:H:254:LYS:C	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:271:LEU:HD22	1:H:273:LEU:H	1.83	0.44
1:O:170:VAL:HB	1:O:208:ILE:CD1	2.47	0.44
1:O:246:GLU:OE1	1:O:292:HIS:CD2	2.71	0.44
1:P:14:LYS:HB2	1:Q:19:THR:OG1	2.17	0.44
1:P:208:ILE:N	1:P:209:PRO:CD	2.81	0.44
1:P:37:TRP:HE1	1:Q:172:LYS:HZ3	1.65	0.44
1:Q:116:LEU:HD23	1:Q:116:LEU:HA	1.66	0.44
1:T:77:PHE:O	1:T:81:GLN:HB2	2.17	0.44
1:V:208:ILE:HD13	1:V:208:ILE:HA	1.83	0.44
1:W:208:ILE:N	1:W:209:PRO:CD	2.81	0.44
1:W:271:LEU:HD23	1:W:272:SER:N	2.33	0.44
1:W:78:GLU:HB2	1:X:135:LEU:HD21	2.00	0.44
1:M:172:LYS:HZ3	1:X:37:TRP:HE1	1.65	0.44
1:B:108:LYS:HE3	1:C:268:ASP:HB2	2.00	0.44
1:D:253:ILE:O	1:D:254:LYS:C	2.53	0.44
1:I:107:LYS:HD3	1:I:107:LYS:HA	1.73	0.44
1:M:142:ASN:HA	1:X:70:MET:HE2	2.00	0.44
1:M:53:GLU:O	1:M:56:GLN:HB3	2.17	0.44
1:N:155:LEU:HD13	1:N:225:LEU:HD22	1.99	0.44
1:N:65:ILE:HD13	1:N:144:ALA:HB1	1.99	0.44
1:O:78:GLU:HB2	1:P:135:LEU:HD21	1.99	0.44
1:R:77:PHE:O	1:R:81:GLN:HB2	2.17	0.44
1:U:119:VAL:HG13	1:U:120:LEU:N	2.32	0.44
1:W:77:PHE:O	1:W:81:GLN:HB2	2.18	0.44
1:D:14:LYS:HB2	1:E:19:THR:OG1	2.18	0.44
1:G:251:GLY:O	1:G:255:THR:HG23	2.18	0.44
1:F:93:LEU:HD11	1:G:262:PHE:CG	2.52	0.44
1:G:274:LEU:HG	1:G:274:LEU:O	2.18	0.44
1:I:271:LEU:HD22	1:I:273:LEU:H	1.83	0.44
1:J:93:LEU:HD11	1:K:262:PHE:CG	2.53	0.44
1:L:107:LYS:HA	1:L:107:LYS:HD3	1.74	0.44
1:K:37:TRP:CZ3	1:L:175:LYS:HG3	2.53	0.44
1:L:271:LEU:HD22	1:L:273:LEU:H	1.83	0.44
1:P:271:LEU:HD23	1:P:272:SER:N	2.33	0.44
1:S:225:LEU:HD23	1:S:225:LEU:O	2.18	0.44
1:U:116:LEU:HB3	1:U:264:VAL:HG21	1.98	0.44
1:B:246:GLU:OE1	1:B:292:HIS:CD2	2.71	0.43
1:C:77:PHE:O	1:C:81:GLN:HB2	2.18	0.43
1:J:225:LEU:HD23	1:J:225:LEU:O	2.17	0.43
1:O:268:ASP:C	1:O:270:MET:H	2.21	0.43
1:T:218:VAL:HG12	1:T:219:GLN:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:78:GLU:CG	1:V:135:LEU:HD21	2.48	0.43
1:V:86:TRP:O	1:V:88:GLY:N	2.50	0.43
1:M:262:PHE:CD1	1:X:93:LEU:HD11	2.53	0.43
1:A:124:ILE:HD11	1:A:258:GLU:HA	1.99	0.43
1:B:17:ILE:CG2	1:B:18:GLU:N	2.81	0.43
1:F:271:LEU:HD22	1:F:273:LEU:H	1.82	0.43
1:F:28:ASN:O	1:F:29:LYS:C	2.55	0.43
1:J:208:ILE:N	1:J:209:PRO:CD	2.81	0.43
1:L:104:TYR:HD1	1:L:270:MET:HG2	1.82	0.43
1:L:218:VAL:HG12	1:L:219:GLN:N	2.32	0.43
1:M:170:VAL:HB	1:M:208:ILE:CD1	2.48	0.43
1:N:78:GLU:HB2	1:O:135:LEU:HD21	2.01	0.43
1:O:264:VAL:HG23	1:O:274:LEU:CD1	2.42	0.43
1:S:78:GLU:HB2	1:T:135:LEU:HD21	1.99	0.43
1:T:225:LEU:O	1:T:225:LEU:HD23	2.17	0.43
1:V:116:LEU:HB3	1:V:264:VAL:HG21	2.00	0.43
1:X:127:LEU:HA	1:X:127:LEU:HD23	1.77	0.43
1:I:155:LEU:HD13	1:I:225:LEU:HD22	1.99	0.43
1:J:124:ILE:HD11	1:J:258:GLU:HA	1.99	0.43
1:P:133:SER:O	1:P:136:VAL:HG12	2.18	0.43
1:O:62:VAL:CG1	1:P:149:LEU:HD21	2.45	0.43
1:S:218:VAL:HG12	1:S:219:GLN:N	2.33	0.43
1:U:170:VAL:HB	1:U:208:ILE:CD1	2.48	0.43
1:X:208:ILE:N	1:X:209:PRO:CD	2.80	0.43
1:A:104:TYR:HD1	1:A:270:MET:HG2	1.84	0.43
1:A:17:ILE:HG22	1:A:18:GLU:N	2.34	0.43
1:A:46:GLU:O	1:A:46:GLU:HG3	2.18	0.43
1:D:116:LEU:HA	1:D:116:LEU:HD23	1.69	0.43
1:G:170:VAL:HB	1:G:208:ILE:CD1	2.48	0.43
1:G:62:VAL:CG1	1:H:149:LEU:HD21	2.43	0.43
1:H:17:ILE:CG2	1:H:18:GLU:N	2.81	0.43
1:K:208:ILE:N	1:K:209:PRO:CD	2.82	0.43
1:P:208:ILE:HA	1:P:208:ILE:HD13	1.82	0.43
1:S:104:TYR:HD1	1:S:270:MET:HG2	1.83	0.43
1:S:65:ILE:HD13	1:S:144:ALA:HB1	2.00	0.43
1:T:93:LEU:HD11	1:U:262:PHE:CG	2.54	0.43
1:U:271:LEU:HD23	1:U:272:SER:N	2.34	0.43
1:W:53:GLU:O	1:W:56:GLN:HB3	2.18	0.43
1:B:86:TRP:O	1:B:88:GLY:N	2.51	0.43
1:C:208:ILE:N	1:C:209:PRO:CD	2.82	0.43
1:E:46:GLU:O	1:E:46:GLU:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:46:GLU:O	1:F:46:GLU:HG3	2.19	0.43
1:I:104:TYR:HD1	1:I:270:MET:HG2	1.83	0.43
1:I:208:ILE:HB	1:I:209:PRO:HD3	2.00	0.43
1:J:271:LEU:HD22	1:J:273:LEU:H	1.84	0.43
1:K:155:LEU:HD13	1:K:225:LEU:HD22	2.00	0.43
1:M:62:VAL:CG1	1:N:149:LEU:HD21	2.47	0.43
1:N:170:VAL:HB	1:N:208:ILE:CD1	2.49	0.43
1:O:53:GLU:O	1:O:56:GLN:HB3	2.18	0.43
1:P:46:GLU:HG3	1:P:46:GLU:O	2.19	0.43
1:Q:124:ILE:HD11	1:Q:258:GLU:HA	2.01	0.43
1:V:218:VAL:HG12	1:V:219:GLN:N	2.33	0.43
1:X:155:LEU:HD13	1:X:225:LEU:HD22	2.00	0.43
1:A:271:LEU:HD23	1:A:272:SER:N	2.33	0.43
1:E:127:LEU:HA	1:E:127:LEU:HD23	1.78	0.43
1:E:104:TYR:HD1	1:E:270:MET:HG2	1.83	0.43
1:K:107:LYS:HD3	1:K:107:LYS:HA	1.72	0.43
1:K:253:ILE:O	1:K:254:LYS:C	2.57	0.43
1:R:155:LEU:HD13	1:R:225:LEU:HD22	2.01	0.43
1:U:104:TYR:CE2	1:U:106:GLU:HA	2.54	0.43
1:A:116:LEU:O	1:A:120:LEU:HG	2.18	0.43
1:C:246:GLU:OE1	1:C:292:HIS:HD2	1.98	0.43
1:D:269:LEU:HD23	1:D:269:LEU:HA	1.87	0.43
1:D:27:TYR:CE2	1:E:183:ALA:HB2	2.54	0.43
1:O:104:TYR:HD1	1:O:270:MET:HG2	1.83	0.43
1:P:104:TYR:HD1	1:P:270:MET:HG2	1.84	0.43
1:T:17:ILE:CG2	1:T:18:GLU:N	2.81	0.43
1:A:53:GLU:O	1:A:56:GLN:HB3	2.19	0.43
1:G:53:GLU:O	1:G:56:GLN:HB3	2.18	0.43
1:I:136:VAL:CG1	1:I:137:SER:N	2.82	0.43
1:N:271:LEU:HD23	1:N:272:SER:N	2.34	0.43
1:P:271:LEU:HD22	1:P:273:LEU:H	1.84	0.43
1:E:218:VAL:HG12	1:E:219:GLN:N	2.34	0.43
1:F:17:ILE:CG2	1:F:18:GLU:N	2.82	0.43
1:G:17:ILE:CG2	1:G:18:GLU:N	2.82	0.43
1:G:208:ILE:N	1:G:209:PRO:CD	2.82	0.43
1:G:218:VAL:HG12	1:G:219:GLN:N	2.32	0.43
1:I:274:LEU:O	1:I:274:LEU:HG	2.18	0.43
1:J:53:GLU:O	1:J:56:GLN:HB3	2.19	0.43
1:K:269:LEU:HD23	1:K:269:LEU:HA	1.85	0.43
1:R:17:ILE:CG2	1:R:18:GLU:N	2.81	0.43
1:R:46:GLU:HG3	1:R:46:GLU:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:104:TYR:HE2	1:T:106:GLU:HA	1.83	0.43
1:T:17:ILE:HG22	1:T:18:GLU:N	2.34	0.43
1:V:246:GLU:OE1	1:V:292:HIS:CD2	2.72	0.43
1:M:268:ASP:HB2	1:X:108:LYS:HE3	2.00	0.43
1:C:69:LEU:HD23	1:C:141:PHE:CZ	2.54	0.43
1:E:184:GLY:O	1:E:187:ALA:O	2.37	0.43
1:F:225:LEU:O	1:F:225:LEU:HD23	2.19	0.43
1:F:124:ILE:CD1	1:F:258:GLU:HA	2.49	0.43
1:J:78:GLU:HB2	1:K:135:LEU:HD21	2.01	0.43
1:N:251:GLY:O	1:N:255:THR:HG23	2.19	0.43
1:O:253:ILE:O	1:O:254:LYS:C	2.58	0.43
1:O:46:GLU:O	1:O:46:GLU:HG3	2.17	0.43
1:R:208:ILE:HD13	1:R:208:ILE:HA	1.78	0.43
1:S:17:ILE:CG2	1:S:18:GLU:N	2.82	0.43
1:X:170:VAL:HB	1:X:208:ILE:CD1	2.49	0.43
1:B:269:LEU:HD23	1:B:269:LEU:HA	1.85	0.42
1:B:271:LEU:HD22	1:B:273:LEU:H	1.84	0.42
1:N:65:ILE:CD1	1:N:144:ALA:HB1	2.49	0.42
1:Q:253:ILE:O	1:Q:254:LYS:C	2.57	0.42
1:R:208:ILE:N	1:R:209:PRO:CD	2.81	0.42
1:U:46:GLU:O	1:U:46:GLU:HG3	2.19	0.42
1:B:136:VAL:CG1	1:B:137:SER:N	2.81	0.42
1:E:253:ILE:O	1:E:254:LYS:C	2.55	0.42
1:E:53:GLU:O	1:E:56:GLN:HB3	2.19	0.42
1:K:28:ASN:O	1:K:29:LYS:C	2.57	0.42
1:L:53:GLU:O	1:L:56:GLN:HB3	2.19	0.42
1:T:104:TYR:CE2	1:T:106:GLU:HA	2.54	0.42
1:W:17:ILE:CG2	1:W:18:GLU:N	2.82	0.42
1:W:17:ILE:HG22	1:W:18:GLU:N	2.34	0.42
1:W:264:VAL:HG23	1:W:274:LEU:CD1	2.42	0.42
1:A:218:VAL:HG12	1:A:219:GLN:N	2.33	0.42
1:B:17:ILE:HG22	1:B:18:GLU:N	2.34	0.42
1:B:70:MET:HE1	1:C:142:ASN:HA	2.01	0.42
1:C:46:GLU:O	1:C:46:GLU:HG3	2.19	0.42
1:D:283:ASN:O	1:D:284:THR:C	2.58	0.42
1:D:53:GLU:O	1:D:56:GLN:HB3	2.19	0.42
1:E:65:ILE:HD13	1:E:144:ALA:HB1	2.02	0.42
1:G:17:ILE:HG22	1:G:18:GLU:N	2.34	0.42
1:G:271:LEU:HD23	1:G:272:SER:N	2.35	0.42
1:I:65:ILE:HD13	1:I:144:ALA:HB1	2.01	0.42
1:J:65:ILE:HD13	1:J:144:ALA:HB1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:116:LEU:HD23	1:P:116:LEU:HA	1.67	0.42
1:R:108:LYS:HE3	1:S:268:ASP:HB2	2.02	0.42
1:W:119:VAL:CG1	1:W:120:LEU:N	2.83	0.42
1:F:208:ILE:HB	1:F:209:PRO:HD3	2.00	0.42
1:M:65:ILE:HD13	1:M:144:ALA:HB1	2.00	0.42
1:O:116:LEU:HD23	1:O:116:LEU:HA	1.69	0.42
1:Q:208:ILE:N	1:Q:209:PRO:CD	2.83	0.42
1:R:69:LEU:HD23	1:R:141:PHE:CE1	2.54	0.42
1:R:37:TRP:CZ3	1:S:175:LYS:HG3	2.55	0.42
1:U:65:ILE:HD13	1:U:144:ALA:HB1	2.01	0.42
1:C:104:TYR:HD1	1:C:270:MET:HG2	1.84	0.42
1:D:86:TRP:O	1:D:88:GLY:N	2.53	0.42
1:E:78:GLU:CG	1:F:135:LEU:HD21	2.50	0.42
1:F:47:LEU:C	1:F:47:LEU:HD12	2.39	0.42
1:G:136:VAL:CG1	1:G:137:SER:N	2.83	0.42
1:L:17:ILE:CG2	1:L:18:GLU:N	2.82	0.42
1:O:271:LEU:HD23	1:O:272:SER:N	2.35	0.42
1:R:17:ILE:HG22	1:R:18:GLU:N	2.35	0.42
1:R:208:ILE:HB	1:R:209:PRO:HD3	2.00	0.42
1:R:271:LEU:HD22	1:R:273:LEU:H	1.84	0.42
1:S:165:TYR:O	1:S:169:GLN:HB2	2.20	0.42
1:S:271:LEU:HD23	1:S:272:SER:N	2.35	0.42
1:S:53:GLU:O	1:S:56:GLN:HB3	2.19	0.42
1:W:116:LEU:HD23	1:W:116:LEU:HA	1.72	0.42
1:W:69:LEU:HD23	1:W:141:PHE:CZ	2.54	0.42
1:X:133:SER:O	1:X:136:VAL:HG12	2.19	0.42
1:A:127:LEU:HA	1:A:127:LEU:HD23	1.82	0.42
1:C:119:VAL:CG1	1:C:120:LEU:N	2.82	0.42
1:D:104:TYR:HD1	1:D:270:MET:HG2	1.83	0.42
1:D:127:LEU:HD23	1:D:127:LEU:HA	1.80	0.42
1:K:271:LEU:HD23	1:K:272:SER:N	2.34	0.42
1:N:93:LEU:HD11	1:O:262:PHE:CG	2.54	0.42
1:P:107:LYS:HD3	1:P:107:LYS:HA	1.73	0.42
1:Q:116:LEU:O	1:Q:120:LEU:HG	2.19	0.42
1:R:271:LEU:HD23	1:R:272:SER:N	2.34	0.42
1:S:210:GLU:HA	1:S:210:GLU:OE2	2.20	0.42
1:S:269:LEU:HA	1:S:269:LEU:HD23	1.86	0.42
1:T:170:VAL:HB	1:T:208:ILE:CD1	2.50	0.42
1:U:218:VAL:HG12	1:U:219:GLN:N	2.33	0.42
1:U:124:ILE:CD1	1:U:258:GLU:HA	2.49	0.42
1:X:39:THR:HG21	1:X:173:ILE:HG12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:LEU:HA	1:A:269:LEU:HD23	1.89	0.42
1:B:271:LEU:HD23	1:B:272:SER:N	2.35	0.42
1:B:53:GLU:O	1:B:56:GLN:HB3	2.20	0.42
1:C:65:ILE:HD13	1:C:144:ALA:HB1	2.02	0.42
1:I:208:ILE:HA	1:I:208:ILE:HD13	1.81	0.42
1:K:268:ASP:C	1:K:270:MET:H	2.22	0.42
1:N:69:LEU:HD23	1:N:141:PHE:CZ	2.55	0.42
1:O:62:VAL:HG12	1:P:149:LEU:CD2	2.46	0.42
1:S:69:LEU:HD23	1:S:141:PHE:CZ	2.55	0.42
1:U:133:SER:O	1:U:136:VAL:HG12	2.20	0.42
1:U:53:GLU:O	1:U:56:GLN:HB3	2.20	0.42
1:X:184:GLY:O	1:X:187:ALA:O	2.38	0.42
1:X:17:ILE:CG2	1:X:18:GLU:N	2.82	0.42
1:A:208:ILE:N	1:A:209:PRO:CD	2.82	0.42
1:D:62:VAL:HG12	1:E:149:LEU:CD2	2.47	0.42
1:J:271:LEU:HD23	1:J:272:SER:N	2.35	0.42
1:K:184:GLY:O	1:K:187:ALA:O	2.38	0.42
1:K:46:GLU:HG3	1:K:46:GLU:O	2.18	0.42
1:M:65:ILE:CD1	1:M:144:ALA:HB1	2.50	0.42
1:N:274:LEU:O	1:N:274:LEU:HG	2.19	0.42
1:O:208:ILE:N	1:O:209:PRO:CD	2.82	0.42
1:R:37:TRP:HE1	1:S:172:LYS:HZ3	1.66	0.42
1:T:180:GLY:O	1:T:183:ALA:HB3	2.19	0.42
1:T:124:ILE:HD11	1:T:258:GLU:HA	2.02	0.42
1:U:208:ILE:N	1:U:209:PRO:CD	2.82	0.42
1:B:127:LEU:HA	1:B:127:LEU:HD23	1.81	0.42
1:C:256:GLU:HA	1:C:256:GLU:OE1	2.20	0.42
1:E:225:LEU:O	1:E:225:LEU:HD23	2.19	0.42
1:H:136:VAL:CG1	1:H:137:SER:N	2.83	0.42
1:J:274:LEU:O	1:J:274:LEU:HG	2.19	0.42
1:K:78:GLU:CG	1:L:135:LEU:HD21	2.50	0.42
1:L:184:GLY:O	1:L:187:ALA:O	2.37	0.42
1:M:271:LEU:HD23	1:M:272:SER:N	2.35	0.42
1:Q:180:GLY:O	1:Q:183:ALA:HB3	2.20	0.42
1:R:136:VAL:CG1	1:R:137:SER:N	2.83	0.42
1:T:107:LYS:HA	1:T:107:LYS:HD3	1.75	0.42
1:T:208:ILE:N	1:T:209:PRO:CD	2.82	0.42
1:V:170:VAL:HB	1:V:208:ILE:CD1	2.50	0.42
1:W:136:VAL:CG1	1:W:137:SER:N	2.82	0.42
1:X:65:ILE:HD13	1:X:144:ALA:HB1	2.02	0.42
1:C:208:ILE:HB	1:C:209:PRO:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:GLU:HB2	1:D:135:LEU:HD21	2.02	0.42
1:D:208:ILE:N	1:D:209:PRO:CD	2.83	0.42
1:F:104:TYR:HD1	1:F:270:MET:HG2	1.85	0.42
1:H:127:LEU:HA	1:H:127:LEU:HD23	1.79	0.42
1:I:208:ILE:N	1:I:209:PRO:CD	2.82	0.42
1:K:65:ILE:HD13	1:K:144:ALA:HB1	2.02	0.42
1:L:133:SER:O	1:L:136:VAL:HG12	2.19	0.42
1:N:136:VAL:CG1	1:N:137:SER:N	2.82	0.42
1:P:86:TRP:O	1:P:88:GLY:N	2.53	0.42
1:S:133:SER:O	1:S:136:VAL:HG12	2.19	0.42
1:U:246:GLU:OE1	1:U:292:HIS:CD2	2.73	0.42
1:U:28:ASN:O	1:U:29:LYS:C	2.57	0.42
1:W:292:HIS:ND1	1:W:292:HIS:C	2.73	0.42
1:W:65:ILE:HD13	1:W:144:ALA:HB1	2.01	0.42
1:B:208:ILE:N	1:B:209:PRO:CD	2.83	0.41
1:D:208:ILE:HB	1:D:209:PRO:HD3	2.02	0.41
1:D:65:ILE:HD13	1:D:144:ALA:HB1	2.02	0.41
1:G:208:ILE:HB	1:G:209:PRO:HD3	2.03	0.41
1:H:17:ILE:HG22	1:H:18:GLU:N	2.35	0.41
1:H:124:ILE:HD11	1:H:258:GLU:HA	2.01	0.41
1:H:53:GLU:O	1:H:56:GLN:HB3	2.20	0.41
1:I:184:GLY:O	1:I:187:ALA:O	2.38	0.41
1:I:28:ASN:O	1:I:29:LYS:C	2.57	0.41
1:M:243:LEU:HD23	1:M:243:LEU:HA	1.91	0.41
1:S:208:ILE:N	1:S:209:PRO:CD	2.82	0.41
1:V:65:ILE:HD13	1:V:144:ALA:HB1	2.02	0.41
1:B:69:LEU:HD23	1:B:141:PHE:CZ	2.55	0.41
1:C:17:ILE:CG2	1:C:18:GLU:N	2.82	0.41
1:E:65:ILE:CD1	1:E:144:ALA:HB1	2.51	0.41
1:F:271:LEU:HD23	1:F:272:SER:N	2.35	0.41
1:G:243:LEU:HA	1:G:243:LEU:HD23	1.93	0.41
1:H:46:GLU:HG3	1:H:46:GLU:O	2.20	0.41
1:I:134:LEU:HD22	1:I:243:LEU:CD2	2.51	0.41
1:I:62:VAL:HG12	1:J:149:LEU:CD2	2.45	0.41
1:I:65:ILE:CD1	1:I:144:ALA:HB1	2.50	0.41
1:L:90:ALA:O	1:L:94:LEU:HD22	2.20	0.41
1:P:65:ILE:HD13	1:P:144:ALA:HB1	2.02	0.41
1:S:46:GLU:O	1:S:46:GLU:HG3	2.19	0.41
1:X:134:LEU:HD22	1:X:243:LEU:CD2	2.50	0.41
1:W:93:LEU:HD11	1:X:262:PHE:CG	2.55	0.41
1:A:184:GLY:O	1:A:187:ALA:O	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:GLU:OE2	1:A:210:GLU:HA	2.21	0.41
1:C:17:ILE:HG22	1:C:18:GLU:N	2.35	0.41
1:C:271:LEU:HD22	1:C:273:LEU:H	1.84	0.41
1:E:21:ASP:HA	1:F:26:LEU:HD13	2.02	0.41
1:G:65:ILE:CD1	1:G:144:ALA:HB1	2.50	0.41
1:H:155:LEU:HD13	1:H:225:LEU:HD22	2.01	0.41
1:I:17:ILE:CG2	1:I:18:GLU:N	2.83	0.41
1:J:46:GLU:HA	1:J:49:ARG:NH1	2.35	0.41
1:K:53:GLU:O	1:K:56:GLN:HB3	2.20	0.41
1:L:46:GLU:HG3	1:L:46:GLU:O	2.18	0.41
1:M:86:TRP:O	1:M:88:GLY:N	2.54	0.41
1:N:208:ILE:N	1:N:209:PRO:CD	2.83	0.41
1:N:253:ILE:O	1:N:254:LYS:C	2.59	0.41
1:P:208:ILE:HB	1:P:209:PRO:HD3	2.03	0.41
1:V:184:GLY:O	1:V:187:ALA:O	2.38	0.41
1:V:124:ILE:CD1	1:V:258:GLU:HA	2.50	0.41
1:B:166:PHE:O	1:B:170:VAL:HG13	2.20	0.41
1:B:184:GLY:O	1:B:187:ALA:O	2.39	0.41
1:B:39:THR:O	1:B:43:THR:HB	2.21	0.41
1:B:78:GLU:CG	1:C:135:LEU:HD21	2.50	0.41
1:C:107:LYS:HD3	1:C:107:LYS:HA	1.74	0.41
1:E:124:ILE:HD11	1:E:258:GLU:HA	2.02	0.41
1:G:46:GLU:O	1:G:46:GLU:HG3	2.19	0.41
1:H:39:THR:HG21	1:H:173:ILE:HG12	2.02	0.41
1:L:65:ILE:HD13	1:L:144:ALA:HB1	2.03	0.41
1:M:69:LEU:HD23	1:M:141:PHE:CZ	2.55	0.41
1:O:133:SER:O	1:O:136:VAL:HG12	2.20	0.41
1:P:124:ILE:CD1	1:P:258:GLU:HA	2.49	0.41
1:P:27:TYR:CE2	1:Q:183:ALA:HB2	2.55	0.41
1:Q:104:TYR:HD1	1:Q:270:MET:HG2	1.85	0.41
1:Q:165:TYR:O	1:Q:169:GLN:HB2	2.20	0.41
1:S:28:ASN:O	1:S:29:LYS:C	2.58	0.41
1:T:271:LEU:HD22	1:T:273:LEU:H	1.84	0.41
1:U:155:LEU:HD13	1:U:225:LEU:HD22	2.03	0.41
1:V:17:ILE:HG22	1:V:18:GLU:N	2.36	0.41
1:X:17:ILE:HG22	1:X:18:GLU:N	2.35	0.41
1:C:210:GLU:OE2	1:C:210:GLU:HA	2.21	0.41
1:C:53:GLU:O	1:C:56:GLN:HB3	2.20	0.41
1:C:65:ILE:CD1	1:C:144:ALA:HB1	2.50	0.41
1:E:271:LEU:HD23	1:E:272:SER:N	2.34	0.41
1:F:107:LYS:HA	1:F:107:LYS:HD3	1.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:46:GLU:HA	1:G:49:ARG:NH1	2.36	0.41
1:H:208:ILE:N	1:H:209:PRO:CD	2.83	0.41
1:H:86:TRP:O	1:H:88:GLY:N	2.53	0.41
1:J:116:LEU:HA	1:J:116:LEU:HD23	1.70	0.41
1:K:180:GLY:O	1:K:183:ALA:HB3	2.20	0.41
1:N:53:GLU:O	1:N:56:GLN:HB3	2.20	0.41
1:O:184:GLY:O	1:O:187:ALA:O	2.38	0.41
1:P:152:ASP:O	1:P:153:SER:C	2.59	0.41
1:P:17:ILE:HG22	1:P:18:GLU:N	2.35	0.41
1:R:253:ILE:O	1:R:254:LYS:C	2.58	0.41
1:S:94:LEU:O	1:S:98:ILE:HG12	2.21	0.41
1:X:117:ILE:O	1:X:121:ASP:HB2	2.21	0.41
1:X:104:TYR:HD1	1:X:270:MET:HG2	1.84	0.41
1:A:106:GLU:HG2	1:A:106:GLU:O	2.20	0.41
1:A:271:LEU:HD22	1:A:273:LEU:H	1.85	0.41
1:B:165:TYR:O	1:B:169:GLN:HB2	2.20	0.41
1:B:104:TYR:HD1	1:B:270:MET:HG2	1.86	0.41
1:D:210:GLU:OE2	1:D:210:GLU:HA	2.21	0.41
1:E:57:ALA:O	1:E:60:VAL:HG12	2.21	0.41
1:F:208:ILE:N	1:F:209:PRO:CD	2.83	0.41
1:H:14:LYS:HB2	1:I:19:THR:OG1	2.21	0.41
1:I:269:LEU:HD23	1:I:269:LEU:HA	1.88	0.41
1:J:136:VAL:CG1	1:J:137:SER:N	2.81	0.41
1:J:14:LYS:HB2	1:K:19:THR:OG1	2.20	0.41
1:K:37:TRP:HE1	1:L:172:LYS:NZ	2.19	0.41
1:L:180:GLY:O	1:L:183:ALA:HB3	2.20	0.41
1:L:17:ILE:HG22	1:L:18:GLU:N	2.35	0.41
1:M:208:ILE:N	1:M:209:PRO:CD	2.83	0.41
1:T:69:LEU:HD23	1:T:141:PHE:CZ	2.55	0.41
1:V:208:ILE:N	1:V:209:PRO:CD	2.84	0.41
1:V:208:ILE:HB	1:V:209:PRO:HD3	2.03	0.41
1:X:124:ILE:HD11	1:X:258:GLU:HA	2.02	0.41
1:A:208:ILE:HB	1:A:209:PRO:HD3	2.03	0.41
1:C:208:ILE:HA	1:C:208:ILE:HD13	1.79	0.41
1:D:28:ASN:O	1:D:29:LYS:C	2.58	0.41
1:G:101:PHE:HZ	1:G:109:ALA:HA	1.86	0.41
1:H:116:LEU:HD23	1:H:116:LEU:HA	1.69	0.41
1:H:208:ILE:HA	1:H:208:ILE:HD13	1.81	0.41
1:L:208:ILE:N	1:L:209:PRO:CD	2.83	0.41
1:S:180:GLY:O	1:S:183:ALA:HB3	2.20	0.41
1:U:253:ILE:O	1:U:254:LYS:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:39:THR:HG21	1:V:173:ILE:HG12	2.02	0.41
1:V:53:GLU:O	1:V:56:GLN:HB3	2.20	0.41
1:X:46:GLU:HG3	1:X:46:GLU:O	2.20	0.41
1:A:253:ILE:O	1:A:254:LYS:C	2.58	0.41
1:C:47:LEU:C	1:C:47:LEU:HD12	2.42	0.41
1:D:180:GLY:O	1:D:183:ALA:HB3	2.21	0.41
1:D:62:VAL:CG1	1:E:149:LEU:HD21	2.47	0.41
1:F:17:ILE:HG22	1:F:18:GLU:N	2.35	0.41
1:G:210:GLU:HA	1:G:210:GLU:OE2	2.21	0.41
1:J:47:LEU:HD12	1:J:47:LEU:C	2.40	0.41
1:K:119:VAL:CG1	1:K:120:LEU:N	2.84	0.41
1:M:133:SER:O	1:M:136:VAL:HG12	2.20	0.41
1:O:210:GLU:HA	1:O:210:GLU:OE2	2.21	0.41
1:Q:39:THR:HG21	1:Q:173:ILE:HG12	2.02	0.41
1:R:243:LEU:O	1:R:247:ILE:HG13	2.21	0.41
1:S:14:LYS:HB2	1:T:19:THR:OG1	2.20	0.41
1:A:262:PHE:CG	1:L:93:LEU:HD11	2.56	0.41
1:B:210:GLU:HA	1:B:210:GLU:OE2	2.21	0.41
1:D:243:LEU:HD23	1:D:243:LEU:HA	1.93	0.41
1:D:271:LEU:HD23	1:D:272:SER:N	2.35	0.41
1:H:65:ILE:HD13	1:H:144:ALA:HB1	2.02	0.41
1:H:184:GLY:O	1:H:187:ALA:O	2.38	0.41
1:J:165:TYR:O	1:J:169:GLN:HB2	2.21	0.41
1:L:136:VAL:CG1	1:L:137:SER:N	2.84	0.41
1:N:46:GLU:HG3	1:N:46:GLU:O	2.19	0.41
1:Q:119:VAL:CG1	1:Q:120:LEU:N	2.84	0.41
1:R:104:TYR:HD1	1:R:270:MET:CG	2.34	0.41
1:T:271:LEU:HD23	1:T:272:SER:N	2.35	0.41
1:T:46:GLU:O	1:T:46:GLU:HG3	2.20	0.41
1:T:65:ILE:HD13	1:T:144:ALA:HB1	2.02	0.41
1:W:274:LEU:HG	1:W:274:LEU:O	2.19	0.41
1:X:243:LEU:HA	1:X:243:LEU:HD23	1.90	0.41
1:A:133:SER:O	1:A:136:VAL:HG12	2.21	0.41
1:D:136:VAL:CG1	1:D:137:SER:N	2.82	0.41
1:D:165:TYR:O	1:D:169:GLN:HB2	2.21	0.41
1:E:208:ILE:HB	1:E:209:PRO:HD3	2.03	0.41
1:E:208:ILE:N	1:E:209:PRO:CD	2.84	0.41
1:F:210:GLU:HA	1:F:210:GLU:OE2	2.21	0.41
1:G:69:LEU:HD23	1:G:141:PHE:CZ	2.55	0.41
1:G:63:GLY:HA2	1:H:149:LEU:HD22	2.01	0.41
1:H:94:LEU:O	1:H:98:ILE:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:46:GLU:HA	1:K:49:ARG:NH1	2.36	0.41
1:M:180:GLY:O	1:M:183:ALA:HB3	2.21	0.41
1:Q:271:LEU:HD22	1:Q:273:LEU:H	1.85	0.41
1:R:65:ILE:HD13	1:R:144:ALA:HB1	2.03	0.41
1:T:46:GLU:HA	1:T:49:ARG:NH1	2.36	0.41
1:U:210:GLU:OE2	1:U:210:GLU:HA	2.21	0.41
1:U:269:LEU:HA	1:U:269:LEU:HD23	1.86	0.41
1:V:243:LEU:HA	1:V:243:LEU:HD23	1.94	0.41
1:W:184:GLY:O	1:W:187:ALA:O	2.39	0.41
1:B:39:THR:HG21	1:B:173:ILE:HG12	2.03	0.41
1:C:116:LEU:HD23	1:C:116:LEU:HA	1.73	0.41
1:C:94:LEU:O	1:C:98:ILE:HG12	2.21	0.41
1:D:17:ILE:CG2	1:D:18:GLU:N	2.84	0.41
1:D:46:GLU:HG3	1:D:46:GLU:O	2.21	0.41
1:E:133:SER:O	1:E:136:VAL:HG12	2.21	0.41
1:E:210:GLU:OE2	1:E:210:GLU:HA	2.21	0.41
1:E:269:LEU:HA	1:E:269:LEU:HD23	1.84	0.41
1:F:136:VAL:CG1	1:F:137:SER:N	2.84	0.41
1:F:218:VAL:HG12	1:F:219:GLN:N	2.36	0.41
1:I:39:THR:HG21	1:I:173:ILE:HG12	2.02	0.41
1:I:180:GLY:O	1:I:183:ALA:HB3	2.20	0.41
1:J:253:ILE:O	1:J:254:LYS:C	2.59	0.41
1:J:65:ILE:CD1	1:J:144:ALA:HB1	2.51	0.41
1:L:124:ILE:CD1	1:L:258:GLU:HA	2.50	0.41
1:M:253:ILE:O	1:M:254:LYS:C	2.60	0.41
1:O:65:ILE:HD13	1:O:144:ALA:HB1	2.02	0.41
1:Q:65:ILE:CD1	1:Q:144:ALA:HB1	2.51	0.41
1:T:57:ALA:O	1:T:60:VAL:HG12	2.21	0.41
1:U:136:VAL:CG1	1:U:137:SER:N	2.82	0.41
1:V:17:ILE:CG2	1:V:18:GLU:N	2.83	0.41
1:V:28:ASN:O	1:V:29:LYS:C	2.59	0.41
1:X:57:ALA:O	1:X:60:VAL:HG12	2.20	0.41
1:B:274:LEU:O	1:B:274:LEU:HG	2.21	0.40
1:B:65:ILE:CD1	1:B:144:ALA:HB1	2.50	0.40
1:B:65:ILE:HD13	1:B:144:ALA:HB1	2.01	0.40
1:D:17:ILE:HG22	1:D:18:GLU:N	2.36	0.40
1:E:271:LEU:HD22	1:E:273:LEU:H	1.85	0.40
1:E:69:LEU:HD23	1:E:141:PHE:CZ	2.56	0.40
1:F:180:GLY:O	1:F:183:ALA:HB3	2.21	0.40
1:F:65:ILE:HD13	1:F:144:ALA:HB1	2.03	0.40
1:H:268:ASP:C	1:H:270:MET:N	2.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:46:GLU:HA	1:I:49:ARG:NH1	2.36	0.40
1:N:47:LEU:HD12	1:N:47:LEU:C	2.42	0.40
1:P:17:ILE:CG2	1:P:18:GLU:N	2.83	0.40
1:Q:127:LEU:HA	1:Q:127:LEU:HD23	1.78	0.40
1:Q:243:LEU:HA	1:Q:243:LEU:HD23	1.94	0.40
1:S:46:GLU:HA	1:S:49:ARG:NH1	2.37	0.40
1:T:210:GLU:OE2	1:T:210:GLU:HA	2.21	0.40
1:T:28:ASN:O	1:T:29:LYS:C	2.59	0.40
1:U:127:LEU:HA	1:U:127:LEU:HD23	1.79	0.40
1:U:39:THR:HG21	1:U:173:ILE:HG12	2.03	0.40
1:W:210:GLU:HA	1:W:210:GLU:OE2	2.21	0.40
1:W:256:GLU:OE1	1:W:256:GLU:HA	2.19	0.40
1:X:210:GLU:OE2	1:X:210:GLU:HA	2.21	0.40
1:A:119:VAL:CG1	1:A:120:LEU:N	2.84	0.40
1:D:69:LEU:HD23	1:D:141:PHE:CZ	2.56	0.40
1:G:65:ILE:HD13	1:G:144:ALA:HB1	2.02	0.40
1:K:124:ILE:CD1	1:K:258:GLU:HA	2.50	0.40
1:L:165:TYR:O	1:L:169:GLN:HB2	2.21	0.40
1:Q:208:ILE:HB	1:Q:209:PRO:HD3	2.03	0.40
1:R:134:LEU:HD22	1:R:243:LEU:CD2	2.51	0.40
1:S:253:ILE:O	1:S:254:LYS:C	2.60	0.40
1:T:104:TYR:HD1	1:T:270:MET:CG	2.34	0.40
1:T:269:LEU:HD23	1:T:269:LEU:HA	1.87	0.40
1:W:208:ILE:HB	1:W:209:PRO:HD3	2.04	0.40
1:W:243:LEU:HD23	1:W:243:LEU:HA	1.92	0.40
1:W:246:GLU:OE1	1:W:292:HIS:CD2	2.74	0.40
1:A:256:GLU:OE1	1:A:256:GLU:HA	2.22	0.40
1:B:124:ILE:CD1	1:B:258:GLU:HA	2.51	0.40
1:C:268:ASP:C	1:C:270:MET:N	2.75	0.40
1:C:46:GLU:HA	1:C:49:ARG:NH1	2.37	0.40
1:D:65:ILE:CD1	1:D:144:ALA:HB1	2.51	0.40
1:E:119:VAL:CG1	1:E:120:LEU:N	2.84	0.40
1:E:136:VAL:CG1	1:E:137:SER:N	2.83	0.40
1:E:39:THR:HG21	1:E:173:ILE:HG12	2.02	0.40
1:H:115:ILE:O	1:H:116:LEU:C	2.60	0.40
1:H:208:ILE:HB	1:H:209:PRO:HD3	2.02	0.40
1:L:256:GLU:OE1	1:L:256:GLU:HA	2.21	0.40
1:M:274:LEU:O	1:M:274:LEU:HG	2.20	0.40
1:M:78:GLU:CG	1:N:135:LEU:HD21	2.51	0.40
1:W:124:ILE:CD1	1:W:258:GLU:HA	2.52	0.40
1:A:46:GLU:HA	1:A:49:ARG:NH1	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:GLY:O	1:B:183:ALA:HB3	2.22	0.40
1:C:124:ILE:CD1	1:C:258:GLU:HA	2.51	0.40
1:D:37:TRP:HE1	1:E:172:LYS:HZ3	1.68	0.40
1:F:165:TYR:O	1:F:169:GLN:HB2	2.21	0.40
1:G:28:ASN:O	1:G:29:LYS:C	2.59	0.40
1:I:17:ILE:HG22	1:I:18:GLU:N	2.36	0.40
1:K:83:VAL:HG22	1:K:127:LEU:CD2	2.52	0.40
1:L:210:GLU:OE2	1:L:210:GLU:HA	2.22	0.40
1:M:155:LEU:HD13	1:M:225:LEU:HD22	2.04	0.40
1:O:180:GLY:O	1:O:183:ALA:HB3	2.21	0.40
1:Q:65:ILE:HD13	1:Q:144:ALA:HB1	2.02	0.40
1:R:46:GLU:HA	1:R:49:ARG:NH1	2.36	0.40
1:R:86:TRP:O	1:R:88:GLY:N	2.55	0.40
1:S:243:LEU:HD23	1:S:243:LEU:HA	1.93	0.40
1:X:253:ILE:O	1:X:254:LYS:C	2.58	0.40
1:X:271:LEU:HD23	1:X:272:SER:N	2.37	0.40
1:X:65:ILE:CD1	1:X:144:ALA:HB1	2.51	0.40
1:A:69:LEU:HD23	1:A:141:PHE:CZ	2.56	0.40
1:C:165:TYR:O	1:C:169:GLN:HB2	2.22	0.40
1:E:17:ILE:HG22	1:E:18:GLU:N	2.36	0.40
1:E:104:TYR:HD1	1:E:270:MET:CG	2.34	0.40
1:F:133:SER:O	1:F:136:VAL:HG12	2.22	0.40
1:H:65:ILE:CD1	1:H:144:ALA:HB1	2.52	0.40
1:L:253:ILE:O	1:L:254:LYS:C	2.58	0.40
1:L:269:LEU:HD23	1:L:269:LEU:HA	1.90	0.40
1:L:69:LEU:HD23	1:L:141:PHE:CZ	2.56	0.40
1:M:271:LEU:HD22	1:M:273:LEU:H	1.87	0.40
1:N:208:ILE:HD13	1:N:208:ILE:HA	1.81	0.40
1:O:136:VAL:CG1	1:O:137:SER:N	2.82	0.40
1:O:274:LEU:O	1:O:274:LEU:HG	2.20	0.40
1:O:46:GLU:HA	1:O:49:ARG:NH1	2.37	0.40
1:Q:17:ILE:HG22	1:Q:18:GLU:N	2.37	0.40
1:Q:256:GLU:HA	1:Q:256:GLU:OE1	2.22	0.40
1:Q:268:ASP:C	1:Q:270:MET:N	2.75	0.40
1:Q:39:THR:O	1:Q:43:THR:HB	2.21	0.40
1:R:116:LEU:HA	1:R:116:LEU:HD23	1.66	0.40
1:T:39:THR:HG21	1:T:173:ILE:HG12	2.03	0.40
1:U:116:LEU:HD23	1:U:116:LEU:HA	1.71	0.40
1:V:27:TYR:CE2	1:W:183:ALA:HB2	2.57	0.40
1:W:155:LEU:HD13	1:W:225:LEU:HD22	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	283/309 (92%)	242 (86%)	40 (14%)	1 (0%)	34	66
1	B	283/309 (92%)	247 (87%)	34 (12%)	2 (1%)	22	54
1	C	283/309 (92%)	246 (87%)	35 (12%)	2 (1%)	22	54
1	D	283/309 (92%)	243 (86%)	39 (14%)	1 (0%)	34	66
1	E	283/309 (92%)	243 (86%)	38 (13%)	2 (1%)	22	54
1	F	283/309 (92%)	248 (88%)	34 (12%)	1 (0%)	34	66
1	G	283/309 (92%)	241 (85%)	41 (14%)	1 (0%)	34	66
1	H	283/309 (92%)	244 (86%)	38 (13%)	1 (0%)	34	66
1	I	283/309 (92%)	241 (85%)	41 (14%)	1 (0%)	34	66
1	J	283/309 (92%)	243 (86%)	39 (14%)	1 (0%)	34	66
1	K	283/309 (92%)	243 (86%)	39 (14%)	1 (0%)	34	66
1	L	283/309 (92%)	243 (86%)	39 (14%)	1 (0%)	34	66
1	M	283/309 (92%)	242 (86%)	40 (14%)	1 (0%)	34	66
1	N	283/309 (92%)	243 (86%)	39 (14%)	1 (0%)	34	66
1	O	283/309 (92%)	242 (86%)	40 (14%)	1 (0%)	34	66
1	P	283/309 (92%)	246 (87%)	36 (13%)	1 (0%)	34	66
1	Q	283/309 (92%)	243 (86%)	39 (14%)	1 (0%)	34	66
1	R	283/309 (92%)	240 (85%)	42 (15%)	1 (0%)	34	66
1	S	283/309 (92%)	242 (86%)	40 (14%)	1 (0%)	34	66
1	T	283/309 (92%)	245 (87%)	37 (13%)	1 (0%)	34	66
1	U	283/309 (92%)	244 (86%)	38 (13%)	1 (0%)	34	66
1	V	283/309 (92%)	240 (85%)	42 (15%)	1 (0%)	34	66
1	W	283/309 (92%)	241 (85%)	41 (14%)	1 (0%)	34	66
1	X	283/309 (92%)	243 (86%)	38 (13%)	2 (1%)	22	54
All	All	6792/7416 (92%)	5835 (86%)	929 (14%)	28 (0%)	34	66

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	267	ASP
1	B	267	ASP
1	C	267	ASP
1	D	267	ASP
1	E	267	ASP
1	F	267	ASP
1	G	267	ASP
1	H	267	ASP
1	I	267	ASP
1	J	267	ASP
1	K	267	ASP
1	L	267	ASP
1	M	267	ASP
1	N	267	ASP
1	O	267	ASP
1	P	267	ASP
1	Q	267	ASP
1	R	267	ASP
1	S	267	ASP
1	T	267	ASP
1	U	267	ASP
1	W	267	ASP
1	X	267	ASP
1	X	291	ARG
1	E	291	ARG
1	V	267	ASP
1	B	207	LEU
1	C	87	CYS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	244/266 (92%)	227 (93%)	17 (7%)	15 43
1	B	244/266 (92%)	228 (93%)	16 (7%)	16 46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	244/266 (92%)	227 (93%)	17 (7%)	15	43
1	D	244/266 (92%)	228 (93%)	16 (7%)	16	46
1	E	244/266 (92%)	228 (93%)	16 (7%)	16	46
1	F	244/266 (92%)	228 (93%)	16 (7%)	16	46
1	G	244/266 (92%)	229 (94%)	15 (6%)	18	48
1	H	244/266 (92%)	228 (93%)	16 (7%)	16	46
1	I	244/266 (92%)	229 (94%)	15 (6%)	18	48
1	J	244/266 (92%)	228 (93%)	16 (7%)	16	46
1	K	244/266 (92%)	226 (93%)	18 (7%)	13	40
1	L	244/266 (92%)	227 (93%)	17 (7%)	15	43
1	M	244/266 (92%)	229 (94%)	15 (6%)	18	48
1	N	244/266 (92%)	229 (94%)	15 (6%)	18	48
1	O	244/266 (92%)	229 (94%)	15 (6%)	18	48
1	P	244/266 (92%)	229 (94%)	15 (6%)	18	48
1	Q	244/266 (92%)	229 (94%)	15 (6%)	18	48
1	R	244/266 (92%)	228 (93%)	16 (7%)	16	46
1	S	244/266 (92%)	229 (94%)	15 (6%)	18	48
1	T	244/266 (92%)	228 (93%)	16 (7%)	16	46
1	U	244/266 (92%)	229 (94%)	15 (6%)	18	48
1	V	244/266 (92%)	228 (93%)	16 (7%)	16	46
1	W	244/266 (92%)	229 (94%)	15 (6%)	18	48
1	X	244/266 (92%)	228 (93%)	16 (7%)	16	46
All	All	5856/6384 (92%)	5477 (94%)	379 (6%)	17	46

All (379) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	THR
1	A	46	GLU
1	A	47	LEU
1	A	67	THR
1	A	87	CYS
1	A	89	VAL
1	A	113	LYS

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Mol	Chain	Res	Type
1	A	136	VAL
1	A	145	SER
1	A	155	LEU
1	A	158	ASP
1	A	170	VAL
1	A	195	SER
1	A	228	THR
1	A	275	LYS
1	A	285	CYS
1	A	292	HIS
1	B	43	THR
1	B	46	GLU
1	B	47	LEU
1	B	87	CYS
1	B	89	VAL
1	B	113	LYS
1	B	136	VAL
1	B	145	SER
1	B	155	LEU
1	B	158	ASP
1	B	170	VAL
1	B	195	SER
1	B	221	PHE
1	B	228	THR
1	B	275	LYS
1	B	285	CYS
1	C	43	THR
1	C	46	GLU
1	C	47	LEU
1	C	67	THR
1	C	87	CYS
1	C	89	VAL
1	C	113	LYS
1	C	136	VAL
1	C	145	SER
1	C	155	LEU
1	C	158	ASP
1	C	170	VAL
1	C	195	SER
1	C	228	THR
1	C	275	LYS
1	C	285	CYS

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Mol	Chain	Res	Type
1	C	292	HIS
1	D	43	THR
1	D	46	GLU
1	D	47	LEU
1	D	67	THR
1	D	87	CYS
1	D	89	VAL
1	D	113	LYS
1	D	136	VAL
1	D	145	SER
1	D	155	LEU
1	D	158	ASP
1	D	170	VAL
1	D	195	SER
1	D	228	THR
1	D	275	LYS
1	D	285	CYS
1	E	43	THR
1	E	46	GLU
1	E	47	LEU
1	E	67	THR
1	E	87	CYS
1	E	89	VAL
1	E	113	LYS
1	E	136	VAL
1	E	145	SER
1	E	155	LEU
1	E	158	ASP
1	E	170	VAL
1	E	195	SER
1	E	228	THR
1	E	275	LYS
1	E	285	CYS
1	F	43	THR
1	F	46	GLU
1	F	47	LEU
1	F	67	THR
1	F	87	CYS
1	F	89	VAL
1	F	113	LYS
1	F	136	VAL
1	F	145	SER

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Mol	Chain	Res	Type
1	F	155	LEU
1	F	158	ASP
1	F	170	VAL
1	F	195	SER
1	F	228	THR
1	F	275	LYS
1	F	285	CYS
1	G	43	THR
1	G	46	GLU
1	G	47	LEU
1	G	87	CYS
1	G	89	VAL
1	G	113	LYS
1	G	136	VAL
1	G	145	SER
1	G	155	LEU
1	G	158	ASP
1	G	170	VAL
1	G	195	SER
1	G	228	THR
1	G	275	LYS
1	G	285	CYS
1	H	43	THR
1	H	46	GLU
1	H	47	LEU
1	H	87	CYS
1	H	89	VAL
1	H	113	LYS
1	H	136	VAL
1	H	145	SER
1	H	155	LEU
1	H	158	ASP
1	H	170	VAL
1	H	195	SER
1	H	221	PHE
1	H	228	THR
1	H	275	LYS
1	H	285	CYS
1	I	43	THR
1	I	46	GLU
1	I	47	LEU
1	I	87	CYS

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Mol	Chain	Res	Type
1	I	89	VAL
1	I	113	LYS
1	I	136	VAL
1	I	145	SER
1	I	155	LEU
1	I	158	ASP
1	I	170	VAL
1	I	195	SER
1	I	228	THR
1	I	275	LYS
1	I	285	CYS
1	J	43	THR
1	J	46	GLU
1	J	47	LEU
1	J	67	THR
1	J	87	CYS
1	J	89	VAL
1	J	113	LYS
1	J	136	VAL
1	J	145	SER
1	J	155	LEU
1	J	158	ASP
1	J	170	VAL
1	J	195	SER
1	J	228	THR
1	J	275	LYS
1	J	285	CYS
1	K	43	THR
1	K	46	GLU
1	K	47	LEU
1	K	67	THR
1	K	87	CYS
1	K	89	VAL
1	K	113	LYS
1	K	136	VAL
1	K	145	SER
1	K	155	LEU
1	K	158	ASP
1	K	170	VAL
1	K	195	SER
1	K	221	PHE
1	K	223	THR

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Mol	Chain	Res	Type
1	K	228	THR
1	K	275	LYS
1	K	285	CYS
1	L	43	THR
1	L	46	GLU
1	L	47	LEU
1	L	67	THR
1	L	87	CYS
1	L	89	VAL
1	L	113	LYS
1	L	136	VAL
1	L	145	SER
1	L	155	LEU
1	L	158	ASP
1	L	170	VAL
1	L	195	SER
1	L	228	THR
1	L	275	LYS
1	L	285	CYS
1	L	292	HIS
1	M	43	THR
1	M	46	GLU
1	M	47	LEU
1	M	87	CYS
1	M	89	VAL
1	M	113	LYS
1	M	136	VAL
1	M	145	SER
1	M	155	LEU
1	M	158	ASP
1	M	170	VAL
1	M	195	SER
1	M	228	THR
1	M	275	LYS
1	M	285	CYS
1	N	43	THR
1	N	46	GLU
1	N	47	LEU
1	N	87	CYS
1	N	89	VAL
1	N	113	LYS
1	N	136	VAL

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Mol	Chain	Res	Type
1	N	145	SER
1	N	155	LEU
1	N	158	ASP
1	N	170	VAL
1	N	195	SER
1	N	228	THR
1	N	275	LYS
1	N	285	CYS
1	O	43	THR
1	O	46	GLU
1	O	47	LEU
1	O	87	CYS
1	O	89	VAL
1	O	113	LYS
1	O	136	VAL
1	O	145	SER
1	O	155	LEU
1	O	158	ASP
1	O	170	VAL
1	O	195	SER
1	O	228	THR
1	O	275	LYS
1	O	285	CYS
1	P	43	THR
1	P	46	GLU
1	P	47	LEU
1	P	87	CYS
1	P	89	VAL
1	P	113	LYS
1	P	136	VAL
1	P	145	SER
1	P	155	LEU
1	P	158	ASP
1	P	170	VAL
1	P	195	SER
1	P	228	THR
1	P	275	LYS
1	P	285	CYS
1	Q	43	THR
1	Q	46	GLU
1	Q	47	LEU
1	Q	87	CYS

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Mol	Chain	Res	Type
1	Q	89	VAL
1	Q	113	LYS
1	Q	136	VAL
1	Q	145	SER
1	Q	155	LEU
1	Q	158	ASP
1	Q	170	VAL
1	Q	195	SER
1	Q	228	THR
1	Q	275	LYS
1	Q	285	CYS
1	R	43	THR
1	R	46	GLU
1	R	47	LEU
1	R	87	CYS
1	R	89	VAL
1	R	113	LYS
1	R	136	VAL
1	R	145	SER
1	R	155	LEU
1	R	158	ASP
1	R	170	VAL
1	R	195	SER
1	R	221	PHE
1	R	228	THR
1	R	275	LYS
1	R	285	CYS
1	S	43	THR
1	S	46	GLU
1	S	47	LEU
1	S	87	CYS
1	S	89	VAL
1	S	113	LYS
1	S	136	VAL
1	S	145	SER
1	S	155	LEU
1	S	158	ASP
1	S	170	VAL
1	S	195	SER
1	S	228	THR
1	S	275	LYS
1	S	285	CYS

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Mol	Chain	Res	Type
1	T	43	THR
1	T	46	GLU
1	T	47	LEU
1	T	67	THR
1	T	87	CYS
1	T	89	VAL
1	T	113	LYS
1	T	136	VAL
1	T	145	SER
1	T	155	LEU
1	T	158	ASP
1	T	170	VAL
1	T	195	SER
1	T	228	THR
1	T	275	LYS
1	T	285	CYS
1	U	43	THR
1	U	46	GLU
1	U	47	LEU
1	U	87	CYS
1	U	89	VAL
1	U	113	LYS
1	U	136	VAL
1	U	145	SER
1	U	155	LEU
1	U	158	ASP
1	U	170	VAL
1	U	195	SER
1	U	228	THR
1	U	275	LYS
1	U	285	CYS
1	V	43	THR
1	V	46	GLU
1	V	47	LEU
1	V	67	THR
1	V	87	CYS
1	V	89	VAL
1	V	113	LYS
1	V	136	VAL
1	V	145	SER
1	V	155	LEU
1	V	158	ASP

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Mol	Chain	Res	Type
1	V	170	VAL
1	V	195	SER
1	V	228	THR
1	V	275	LYS
1	V	285	CYS
1	W	43	THR
1	W	46	GLU
1	W	47	LEU
1	W	87	CYS
1	W	89	VAL
1	W	113	LYS
1	W	136	VAL
1	W	145	SER
1	W	155	LEU
1	W	158	ASP
1	W	170	VAL
1	W	195	SER
1	W	228	THR
1	W	275	LYS
1	W	285	CYS
1	X	43	THR
1	X	46	GLU
1	X	47	LEU
1	X	87	CYS
1	X	89	VAL
1	X	113	LYS
1	X	136	VAL
1	X	145	SER
1	X	155	LEU
1	X	158	ASP
1	X	170	VAL
1	X	195	SER
1	X	228	THR
1	X	275	LYS
1	X	285	CYS
1	X	292	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	227	ASN
1	B	227	ASN

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Mol	Chain	Res	Type
1	C	227	ASN
1	D	227	ASN
1	E	227	ASN
1	E	292	HIS
1	F	227	ASN
1	F	292	HIS
1	G	227	ASN
1	H	227	ASN
1	I	227	ASN
1	J	227	ASN
1	K	227	ASN
1	L	227	ASN
1	L	292	HIS
1	M	227	ASN
1	N	227	ASN
1	O	227	ASN
1	P	227	ASN
1	Q	227	ASN
1	R	227	ASN
1	S	227	ASN
1	T	227	ASN
1	U	227	ASN
1	V	227	ASN
1	W	227	ASN
1	X	227	ASN
1	X	292	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

48 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	EMC	G	304	1	1,2,2	6.74	1 (100%)	-		
2	EMC	F	304	1	1,2,2	6.76	1 (100%)	-		
2	EMC	C	305	1	1,2,2	6.73	1 (100%)	-		
2	EMC	V	305	1	1,2,2	6.78	1 (100%)	-		
2	EMC	T	305	1	1,2,2	6.79	1 (100%)	-		
2	EMC	N	304	1	1,2,2	6.76	1 (100%)	-		
2	EMC	J	305	1	1,2,2	6.78	1 (100%)	-		
2	EMC	L	304	1	1,2,2	6.86	1 (100%)	-		
2	EMC	X	305	1	1,2,2	6.84	1 (100%)	-		
2	EMC	U	304	1	1,2,2	6.81	1 (100%)	-		
2	EMC	T	304	1	1,2,2	6.84	1 (100%)	-		
2	EMC	Q	305	1	1,2,2	6.74	1 (100%)	-		
2	EMC	H	305	1	1,2,2	6.78	1 (100%)	-		
2	EMC	E	304	1	1,2,2	6.82	1 (100%)	-		
2	EMC	D	304	1	1,2,2	6.92	1 (100%)	-		
2	EMC	P	305	1	1,2,2	6.75	1 (100%)	-		
2	EMC	O	304	1	1,2,2	6.78	1 (100%)	-		
2	EMC	H	304	1	1,2,2	6.70	1 (100%)	-		
2	EMC	M	304	1	1,2,2	6.88	1 (100%)	-		
2	EMC	W	304	1	1,2,2	7.05	1 (100%)	-		
2	EMC	V	304	1	1,2,2	6.83	1 (100%)	-		
2	EMC	R	305	1	1,2,2	6.77	1 (100%)	-		
2	EMC	M	305	1	1,2,2	6.71	1 (100%)	-		
2	EMC	W	305	1	1,2,2	6.83	1 (100%)	-		
2	EMC	U	305	1	1,2,2	6.74	1 (100%)	-		
2	EMC	N	305	1	1,2,2	6.75	1 (100%)	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	EMC	B	305	1	1,2,2	6.80	1 (100%)	-		
2	EMC	I	304	1	1,2,2	6.72	1 (100%)	-		
2	EMC	J	304	1	1,2,2	6.76	1 (100%)	-		
2	EMC	G	305	1	1,2,2	6.79	1 (100%)	-		
2	EMC	C	304	1	1,2,2	6.93	1 (100%)	-		
2	EMC	E	305	1	1,2,2	6.76	1 (100%)	-		
2	EMC	Q	304	1	1,2,2	6.74	1 (100%)	-		
2	EMC	R	304	1	1,2,2	6.69	1 (100%)	-		
2	EMC	P	304	1	1,2,2	6.82	1 (100%)	-		
2	EMC	O	305	1	1,2,2	6.81	1 (100%)	-		
2	EMC	K	304	1	1,2,2	6.64	1 (100%)	-		
2	EMC	F	305	1	1,2,2	6.74	1 (100%)	-		
2	EMC	X	304	1	1,2,2	6.75	1 (100%)	-		
2	EMC	D	305	1	1,2,2	6.97	1 (100%)	-		
2	EMC	A	304	1	1,2,2	6.90	1 (100%)	-		
2	EMC	B	304	1	1,2,2	6.75	1 (100%)	-		
2	EMC	L	305	1	1,2,2	6.80	1 (100%)	-		
2	EMC	A	305	1	1,2,2	6.74	1 (100%)	-		
2	EMC	K	305	1	1,2,2	6.76	1 (100%)	-		
2	EMC	I	305	1	1,2,2	6.77	1 (100%)	-		
2	EMC	S	305	1	1,2,2	6.75	1 (100%)	-		
2	EMC	S	304	1	1,2,2	6.68	1 (100%)	-		

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	W	304	EMC	C2-C1	7.05	1.86	1.49
2	D	305	EMC	C2-C1	6.97	1.86	1.49
2	C	304	EMC	C2-C1	6.93	1.85	1.49
2	D	304	EMC	C2-C1	6.92	1.85	1.49
2	A	304	EMC	C2-C1	6.90	1.85	1.49
2	M	304	EMC	C2-C1	6.88	1.85	1.49
2	L	304	EMC	C2-C1	6.86	1.85	1.49
2	T	304	EMC	C2-C1	6.84	1.85	1.49
2	X	305	EMC	C2-C1	6.84	1.85	1.49
2	W	305	EMC	C2-C1	6.83	1.85	1.49
2	V	304	EMC	C2-C1	6.83	1.85	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	304	EMC	C2-C1	6.82	1.85	1.49
2	P	304	EMC	C2-C1	6.82	1.85	1.49
2	O	305	EMC	C2-C1	6.81	1.85	1.49
2	U	304	EMC	C2-C1	6.81	1.85	1.49
2	L	305	EMC	C2-C1	6.80	1.85	1.49
2	B	305	EMC	C2-C1	6.80	1.85	1.49
2	T	305	EMC	C2-C1	6.79	1.85	1.49
2	G	305	EMC	C2-C1	6.79	1.85	1.49
2	V	305	EMC	C2-C1	6.78	1.85	1.49
2	J	305	EMC	C2-C1	6.78	1.85	1.49
2	O	304	EMC	C2-C1	6.78	1.85	1.49
2	H	305	EMC	C2-C1	6.78	1.85	1.49
2	R	305	EMC	C2-C1	6.77	1.84	1.49
2	I	305	EMC	C2-C1	6.77	1.84	1.49
2	F	304	EMC	C2-C1	6.76	1.84	1.49
2	N	304	EMC	C2-C1	6.76	1.84	1.49
2	K	305	EMC	C2-C1	6.76	1.84	1.49
2	J	304	EMC	C2-C1	6.76	1.84	1.49
2	E	305	EMC	C2-C1	6.76	1.84	1.49
2	X	304	EMC	C2-C1	6.75	1.84	1.49
2	B	304	EMC	C2-C1	6.75	1.84	1.49
2	S	305	EMC	C2-C1	6.75	1.84	1.49
2	P	305	EMC	C2-C1	6.75	1.84	1.49
2	N	305	EMC	C2-C1	6.75	1.84	1.49
2	U	305	EMC	C2-C1	6.74	1.84	1.49
2	G	304	EMC	C2-C1	6.74	1.84	1.49
2	F	305	EMC	C2-C1	6.74	1.84	1.49
2	Q	305	EMC	C2-C1	6.74	1.84	1.49
2	A	305	EMC	C2-C1	6.74	1.84	1.49
2	Q	304	EMC	C2-C1	6.74	1.84	1.49
2	C	305	EMC	C2-C1	6.73	1.84	1.49
2	I	304	EMC	C2-C1	6.72	1.84	1.49
2	M	305	EMC	C2-C1	6.71	1.84	1.49
2	H	304	EMC	C2-C1	6.70	1.84	1.49
2	R	304	EMC	C2-C1	6.69	1.84	1.49
2	S	304	EMC	C2-C1	6.68	1.84	1.49
2	K	304	EMC	C2-C1	6.64	1.84	1.49

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

48 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	304	EMC	1	0
2	F	304	EMC	1	0
2	C	305	EMC	1	0
2	V	305	EMC	1	0
2	T	305	EMC	1	0
2	N	304	EMC	1	0
2	J	305	EMC	1	0
2	L	304	EMC	1	0
2	X	305	EMC	1	0
2	U	304	EMC	1	0
2	T	304	EMC	1	0
2	Q	305	EMC	1	0
2	H	305	EMC	1	0
2	E	304	EMC	1	0
2	D	304	EMC	1	0
2	P	305	EMC	1	0
2	O	304	EMC	1	0
2	H	304	EMC	1	0
2	M	304	EMC	1	0
2	W	304	EMC	1	0
2	V	304	EMC	1	0
2	R	305	EMC	1	0
2	M	305	EMC	1	0
2	W	305	EMC	1	0
2	U	305	EMC	1	0
2	N	305	EMC	1	0
2	B	305	EMC	1	0
2	I	304	EMC	1	0
2	J	304	EMC	1	0
2	G	305	EMC	1	0
2	C	304	EMC	1	0
2	E	305	EMC	1	0
2	Q	304	EMC	1	0
2	R	304	EMC	1	0
2	P	304	EMC	1	0
2	O	305	EMC	1	0
2	K	304	EMC	1	0
2	F	305	EMC	1	0
2	X	304	EMC	1	0
2	D	305	EMC	1	0
2	A	304	EMC	1	0
2	B	304	EMC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	305	EMC	1	0
2	A	305	EMC	1	0
2	K	305	EMC	1	0
2	I	305	EMC	1	0
2	S	305	EMC	1	0
2	S	304	EMC	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	285/309 (92%)	-0.38	3 (1%)	80	81	62, 123, 190, 270	0
1	B	285/309 (92%)	-0.20	5 (1%)	68	67	61, 124, 190, 270	0
1	C	285/309 (92%)	-0.26	2 (0%)	87	88	63, 123, 189, 270	0
1	D	285/309 (92%)	-0.25	4 (1%)	75	75	64, 122, 189, 270	0
1	E	285/309 (92%)	-0.17	8 (2%)	53	51	64, 124, 190, 270	0
1	F	285/309 (92%)	-0.21	9 (3%)	47	46	64, 125, 193, 270	0
1	G	285/309 (92%)	-0.24	7 (2%)	57	54	64, 125, 190, 270	0
1	H	285/309 (92%)	-0.16	8 (2%)	53	51	63, 124, 190, 270	0
1	I	285/309 (92%)	-0.23	9 (3%)	47	46	63, 127, 190, 270	0
1	J	285/309 (92%)	-0.31	5 (1%)	68	67	64, 126, 191, 270	0
1	K	285/309 (92%)	-0.20	8 (2%)	53	51	62, 125, 192, 270	0
1	L	285/309 (92%)	-0.21	7 (2%)	57	54	63, 124, 190, 270	0
1	M	285/309 (92%)	-0.22	6 (2%)	63	62	65, 125, 190, 270	0
1	N	285/309 (92%)	-0.28	4 (1%)	75	75	63, 123, 194, 272	0
1	O	285/309 (92%)	-0.31	6 (2%)	63	62	62, 124, 191, 270	0
1	P	285/309 (92%)	-0.20	9 (3%)	47	46	66, 125, 190, 270	0
1	Q	285/309 (92%)	-0.21	7 (2%)	57	54	66, 125, 191, 270	0
1	R	285/309 (92%)	-0.33	1 (0%)	92	93	64, 125, 191, 270	0
1	S	285/309 (92%)	-0.26	6 (2%)	63	62	63, 126, 190, 270	0
1	T	285/309 (92%)	-0.30	5 (1%)	68	67	62, 125, 191, 270	0
1	U	285/309 (92%)	-0.23	6 (2%)	63	62	64, 124, 192, 270	0
1	V	285/309 (92%)	-0.26	6 (2%)	63	62	65, 125, 191, 270	0
1	W	285/309 (92%)	-0.24	6 (2%)	63	62	64, 123, 190, 270	0
1	X	285/309 (92%)	-0.29	3 (1%)	80	81	64, 125, 191, 270	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
All	All	6840/7416 (92%)	-0.25	140 (2%) 65 64	61, 125, 193, 272	0

All (140) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	291	ARG	8.2
1	H	8	LYS	7.4
1	L	291	ARG	6.7
1	I	8	LYS	6.0
1	M	292	HIS	5.7
1	V	291	ARG	5.7
1	P	9	THR	5.7
1	Q	8	LYS	5.6
1	Q	9	THR	5.6
1	F	290	LYS	5.3
1	V	290	LYS	5.3
1	F	9	THR	5.1
1	F	292	HIS	4.9
1	O	9	THR	4.8
1	H	9	THR	4.6
1	N	9	THR	4.6
1	W	8	LYS	4.5
1	C	290	LYS	4.5
1	I	288	TYR	4.3
1	S	290	LYS	4.2
1	G	290	LYS	4.1
1	W	190	PHE	4.0
1	L	292	HIS	4.0
1	G	292	HIS	3.9
1	B	291	ARG	3.9
1	D	8	LYS	3.9
1	U	36	PRO	3.8
1	U	9	THR	3.8
1	O	8	LYS	3.8
1	F	215	LEU	3.7
1	I	9	THR	3.7
1	F	8	LYS	3.7
1	G	8	LYS	3.7
1	S	291	ARG	3.7
1	S	287	GLU	3.6
1	Q	10	VAL	3.6
1	E	47	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	L	290	LYS	3.6
1	P	290	LYS	3.6
1	L	287	GLU	3.5
1	S	8	LYS	3.5
1	J	290	LYS	3.5
1	D	9	THR	3.5
1	T	287	GLU	3.4
1	J	8	LYS	3.4
1	K	144	ALA	3.2
1	P	215	LEU	3.2
1	P	8	LYS	3.2
1	I	292	HIS	3.2
1	E	36	PRO	3.1
1	J	287	GLU	3.0
1	T	291	ARG	3.0
1	W	291	ARG	3.0
1	Q	175	LYS	3.0
1	J	9	THR	3.0
1	V	288	TYR	3.0
1	O	12	VAL	3.0
1	G	291	ARG	2.9
1	P	291	ARG	2.9
1	J	291	ARG	2.9
1	A	215	LEU	2.9
1	V	292	HIS	2.9
1	B	9	THR	2.9
1	Q	37	TRP	2.9
1	D	10	VAL	2.9
1	U	10	VAL	2.9
1	L	36	PRO	2.9
1	M	290	LYS	2.8
1	K	9	THR	2.8
1	V	287	GLU	2.8
1	A	8	LYS	2.8
1	I	190	PHE	2.8
1	E	19	THR	2.7
1	K	36	PRO	2.7
1	M	47	LEU	2.7
1	C	292	HIS	2.7
1	F	287	GLU	2.7
1	E	291	ARG	2.7
1	K	291	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	W	215	LEU	2.7
1	U	198	ILE	2.6
1	E	147	LYS	2.6
1	U	173	ILE	2.6
1	T	8	LYS	2.5
1	G	36	PRO	2.5
1	H	10	VAL	2.5
1	P	292	HIS	2.5
1	W	166	PHE	2.5
1	M	288	TYR	2.5
1	G	190	PHE	2.4
1	H	207	LEU	2.4
1	K	8	LYS	2.4
1	S	9	THR	2.4
1	B	290	LYS	2.4
1	X	186	VAL	2.4
1	I	233	ASN	2.4
1	H	174	ARG	2.4
1	I	290	LYS	2.3
1	O	292	HIS	2.3
1	P	190	PHE	2.3
1	M	51	LYS	2.3
1	T	174	ARG	2.3
1	E	198	ILE	2.3
1	X	8	LYS	2.3
1	E	9	THR	2.2
1	F	288	TYR	2.2
1	B	292	HIS	2.2
1	G	11	GLU	2.2
1	Q	155	LEU	2.2
1	R	9	THR	2.2
1	N	198	ILE	2.2
1	X	166	PHE	2.2
1	W	193	ILE	2.2
1	M	36	PRO	2.2
1	P	10	VAL	2.2
1	Q	12	VAL	2.2
1	H	211	LEU	2.2
1	K	21	ASP	2.1
1	D	14	LYS	2.1
1	U	195	SER	2.1
1	V	15	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	291	ARG	2.1
1	B	13	VAL	2.1
1	F	10	VAL	2.1
1	N	15	ASN	2.1
1	O	215	LEU	2.1
1	K	147	LYS	2.1
1	T	208	ILE	2.1
1	I	174	ARG	2.1
1	I	186	VAL	2.1
1	H	215	LEU	2.1
1	S	148	LEU	2.1
1	N	190	PHE	2.1
1	E	12	VAL	2.1
1	O	185	VAL	2.1
1	K	10	VAL	2.0
1	L	19	THR	2.0
1	H	61	LEU	2.0
1	P	21	ASP	2.0
1	L	288	TYR	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 carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	EMC	M	305	3/3	0.91	0.25	52,52,57,140	3
2	EMC	D	305	3/3	0.94	0.25	70,70,72,115	3
2	EMC	C	305	3/3	0.95	0.14	62,62,63,136	3
2	EMC	W	305	3/3	0.95	0.26	57,57,58,125	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	EMC	P	305	3/3	0.95	0.16	57,57,57,136	3
2	EMC	S	305	3/3	0.95	0.17	54,54,55,138	3
2	EMC	E	305	3/3	0.96	0.23	57,57,59,139	3
2	EMC	O	305	3/3	0.96	0.15	73,73,73,141	3
2	EMC	K	304	3/3	0.96	0.16	61,61,86,119	3
2	EMC	F	305	3/3	0.96	0.16	76,76,78,143	3
2	EMC	V	305	3/3	0.96	0.17	67,67,68,139	3
2	EMC	I	305	3/3	0.96	0.20	56,56,58,144	3
2	EMC	N	305	3/3	0.96	0.15	56,56,62,139	3
2	EMC	J	305	3/3	0.97	0.12	73,73,74,136	3
2	EMC	B	305	3/3	0.97	0.25	56,56,60,134	3
2	EMC	G	305	3/3	0.97	0.12	54,54,57,133	3
2	EMC	B	304	3/3	0.97	0.16	29,29,91,104	3
2	EMC	L	305	3/3	0.97	0.11	64,64,65,146	3
2	EMC	A	305	3/3	0.97	0.13	55,55,60,144	3
2	EMC	X	305	3/3	0.97	0.18	56,56,61,126	3
2	EMC	Q	305	3/3	0.97	0.15	70,70,71,138	3
2	EMC	U	305	3/3	0.98	0.15	57,57,59,133	3
2	EMC	T	304	3/3	0.98	0.14	30,30,96,118	3
2	EMC	X	304	3/3	0.98	0.11	45,45,90,119	3
2	EMC	H	304	3/3	0.98	0.15	36,36,92,121	3
2	EMC	I	304	3/3	0.98	0.16	41,41,92,127	3
2	EMC	R	305	3/3	0.98	0.21	79,79,79,149	3
2	EMC	T	305	3/3	0.98	0.12	53,53,60,133	3
2	EMC	K	305	3/3	0.98	0.10	75,75,76,141	3
2	EMC	Q	304	3/3	0.98	0.10	52,52,91,125	3
2	EMC	H	305	3/3	0.98	0.18	57,57,62,133	3
2	EMC	S	304	3/3	0.98	0.16	36,36,88,135	3
2	EMC	W	304	3/3	0.99	0.12	40,40,92,103	3
2	EMC	R	304	3/3	0.99	0.10	61,61,93,127	3
2	EMC	V	304	3/3	0.99	0.11	49,49,88,122	3
2	EMC	N	304	3/3	0.99	0.14	37,37,90,113	3
2	EMC	F	304	3/3	0.99	0.13	57,57,88,123	3
2	EMC	L	304	3/3	0.99	0.14	51,51,90,123	3
2	EMC	E	304	3/3	0.99	0.13	45,45,87,106	3
2	EMC	A	304	3/3	0.99	0.13	40,40,88,105	3
2	EMC	D	304	3/3	0.99	0.11	51,51,93,102	3
2	EMC	G	304	3/3	0.99	0.13	30,30,85,119	3
2	EMC	O	304	3/3	0.99	0.13	55,55,89,120	3
2	EMC	J	304	3/3	0.99	0.14	59,59,91,137	3
2	EMC	U	304	3/3	0.99	0.14	31,31,89,118	3
2	EMC	C	304	3/3	0.99	0.16	42,42,90,119	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	EMC	M	304	3/3	0.99	0.14	32,32,95,116	3
2	EMC	P	304	3/3	1.00	0.14	39,39,94,125	3

6.5 Other polymers (i)

There are no such residues in this entry.