



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 24, 2026 – 09:29 pm BST

PDB ID : 2WCD / pdb_00002wcd
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 types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

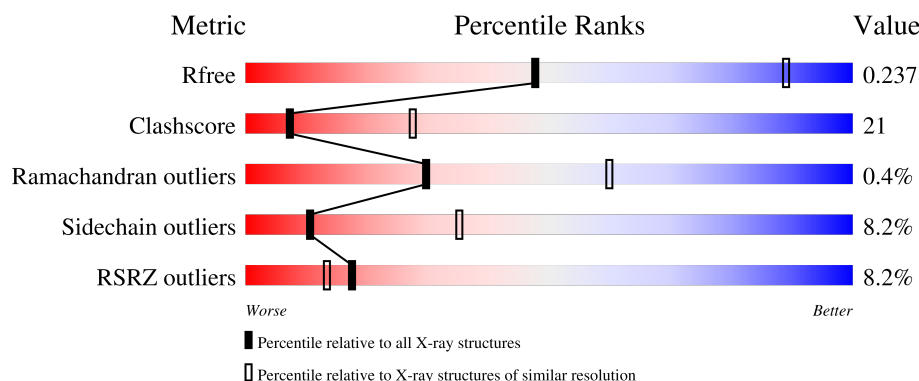
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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

Mol	Chain	Length	Quality of chain
1	A	309	4% 55% 33% • 8%
1	B	309	7% 51% 37% • 8%
1	C	309	7% 53% 34% 5% 8%
1	D	309	5% 53% 36% • 8%
1	E	309	8% 53% 35% 5% 8%

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Mol	Chain	Length	Quality of chain
1	F	309	
1	G	309	
1	H	309	
1	I	309	
1	J	309	
1	K	309	
1	L	309	
1	M	309	
1	N	309	
1	O	309	
1	P	309	
1	Q	309	
1	R	309	
1	S	309	
1	T	309	
1	U	309	
1	V	309	
1	W	309	
1	X	309	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EMC	A	305	-	-	-	X
2	EMC	B	305	-	-	-	X
2	EMC	C	304	-	-	X	-
2	EMC	C	305	-	-	-	X
2	EMC	F	305	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EMC	H	305	-	-	-	X
2	EMC	I	304	-	-	X	-
2	EMC	J	304	-	-	X	-
2	EMC	J	305	-	-	-	X
2	EMC	K	304	-	-	X	-
2	EMC	K	305	-	-	-	X
2	EMC	L	304	-	-	X	-
2	EMC	L	305	-	-	-	X
2	EMC	M	305	-	-	-	X
2	EMC	O	305	-	-	-	X
2	EMC	P	305	-	-	-	X
2	EMC	Q	304	-	-	X	-
2	EMC	R	304	-	-	X	-
2	EMC	V	304	-	-	X	-
2	EMC	V	305	-	-	-	X
2	EMC	X	305	-	-	-	X

2 Entry composition

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.

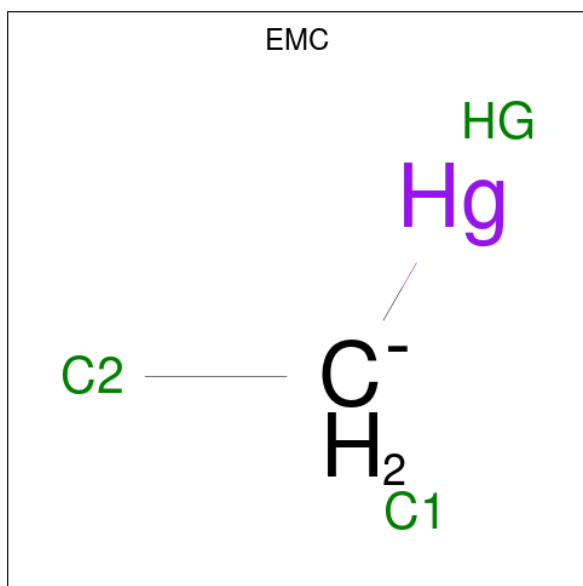
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	0	0	0
			2237	1427	360	445	5			
1	B	285	Total	C	N	O	S	0	0	0
			2237	1427	360	445	5			
1	C	285	Total	C	N	O	S	0	0	0
			2237	1427	360	445	5			
1	D	285	Total	C	N	O	S	0	0	0
			2237	1427	360	445	5			
1	E	285	Total	C	N	O	S	0	0	0
			2237	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 (CCD ID: 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 3	C 2	Hg 1	0	0
2	M	1	Total 3	C 2	Hg 1	0	0
2	N	1	Total 3	C 2	Hg 1	0	0
2	N	1	Total 3	C 2	Hg 1	0	0
2	O	1	Total 3	C 2	Hg 1	0	0
2	O	1	Total 3	C 2	Hg 1	0	0
2	P	1	Total 3	C 2	Hg 1	0	0
2	P	1	Total 3	C 2	Hg 1	0	0
2	Q	1	Total 3	C 2	Hg 1	0	0
2	Q	1	Total 3	C 2	Hg 1	0	0
2	R	1	Total 3	C 2	Hg 1	0	0
2	R	1	Total 3	C 2	Hg 1	0	0
2	S	1	Total 3	C 2	Hg 1	0	0
2	S	1	Total 3	C 2	Hg 1	0	0
2	T	1	Total 3	C 2	Hg 1	0	0
2	T	1	Total 3	C 2	Hg 1	0	0
2	U	1	Total 3	C 2	Hg 1	0	0
2	U	1	Total 3	C 2	Hg 1	0	0
2	V	1	Total 3	C 2	Hg 1	0	0
2	V	1	Total 3	C 2	Hg 1	0	0
2	W	1	Total 3	C 2	Hg 1	0	0

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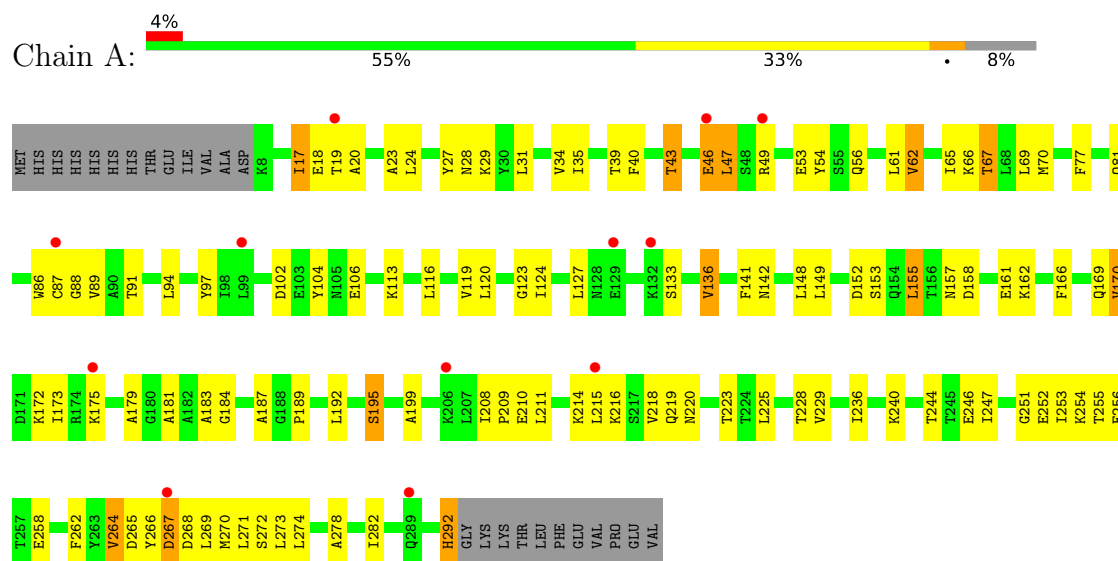
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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2	X	1	Total 3	C 2	Hg 1	0	0
2	X	1	Total 3	C 2	Hg 1	0	0

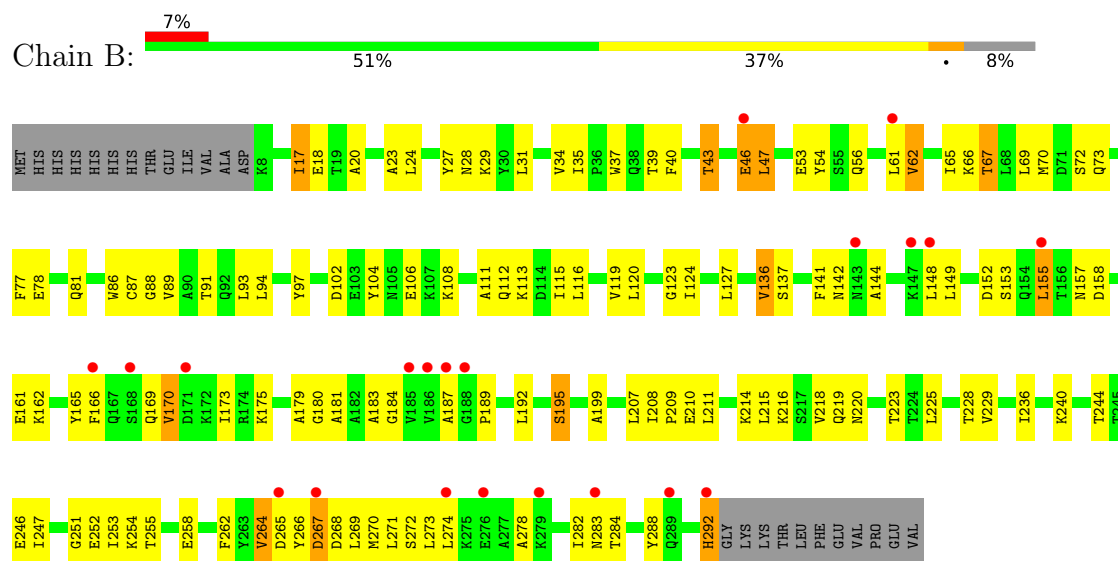
3 Residue-property plots

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

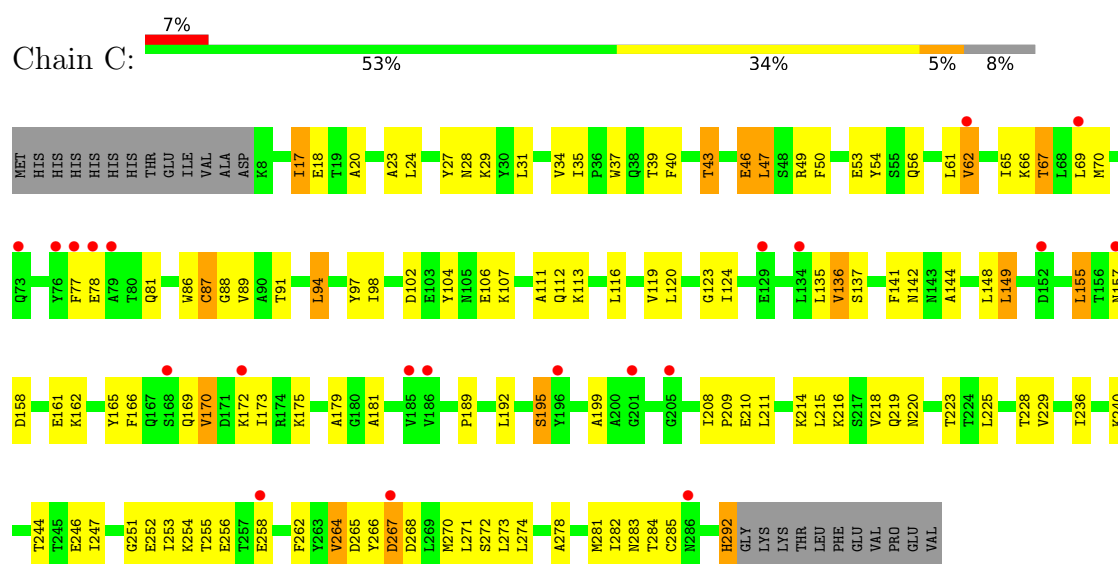
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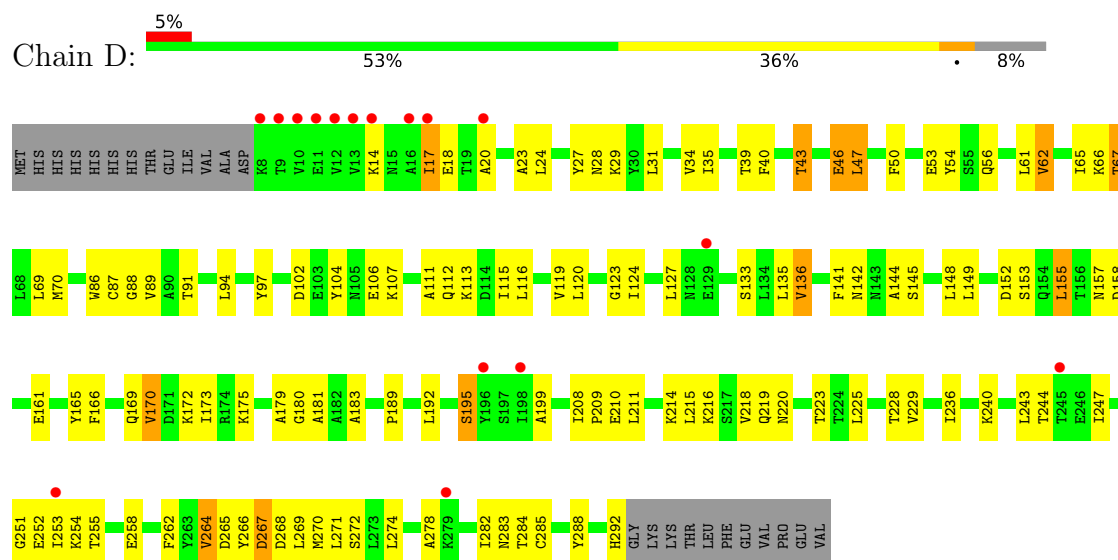
• Molecule 1: HEMOLYSIN E, CHROMOSOMAL



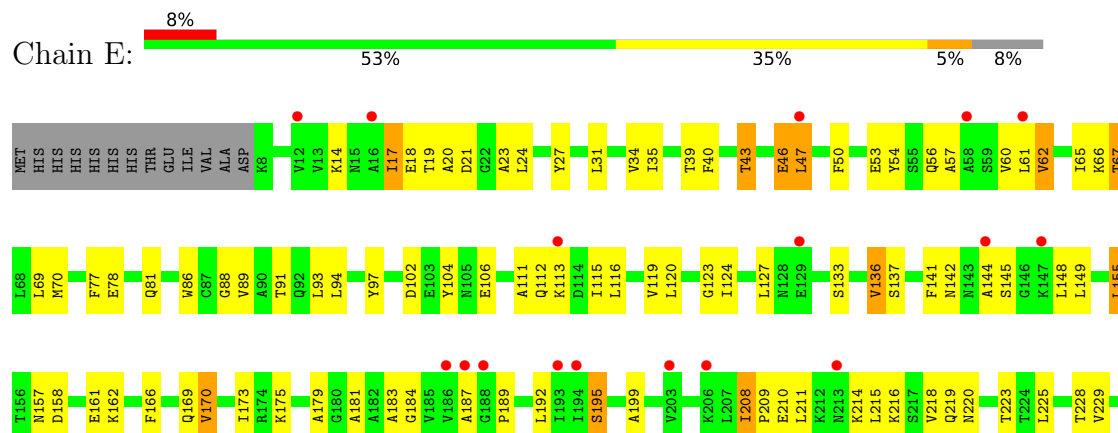
• Molecule 1: HEMOLYSIN E, CHROMOSOMAL

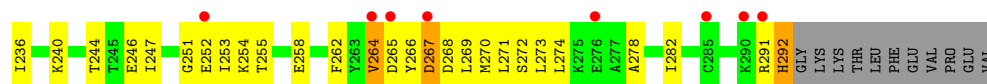


- Molecule 1: HEMOLYSIN E, CHROMOSOMAL

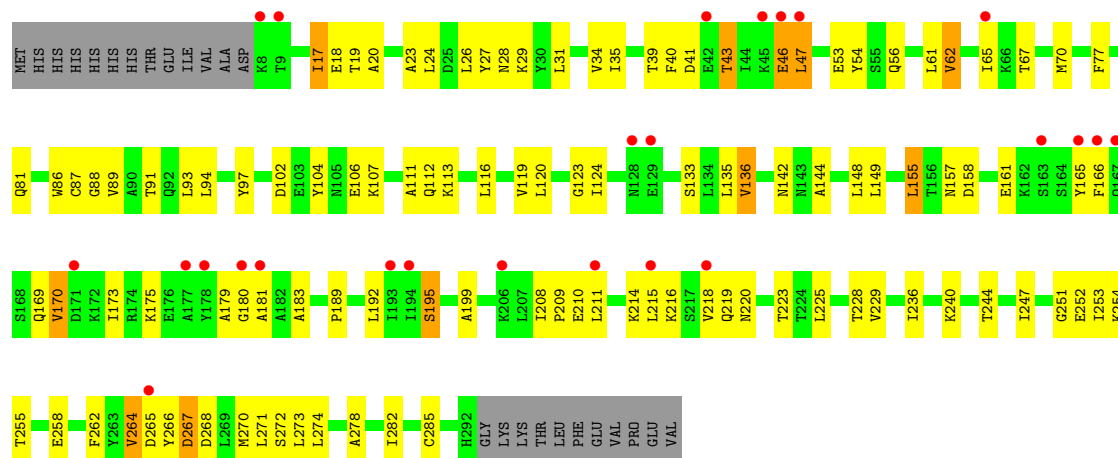


- Molecule 1: HEMOLYSIN E, CHROMOSOMAL

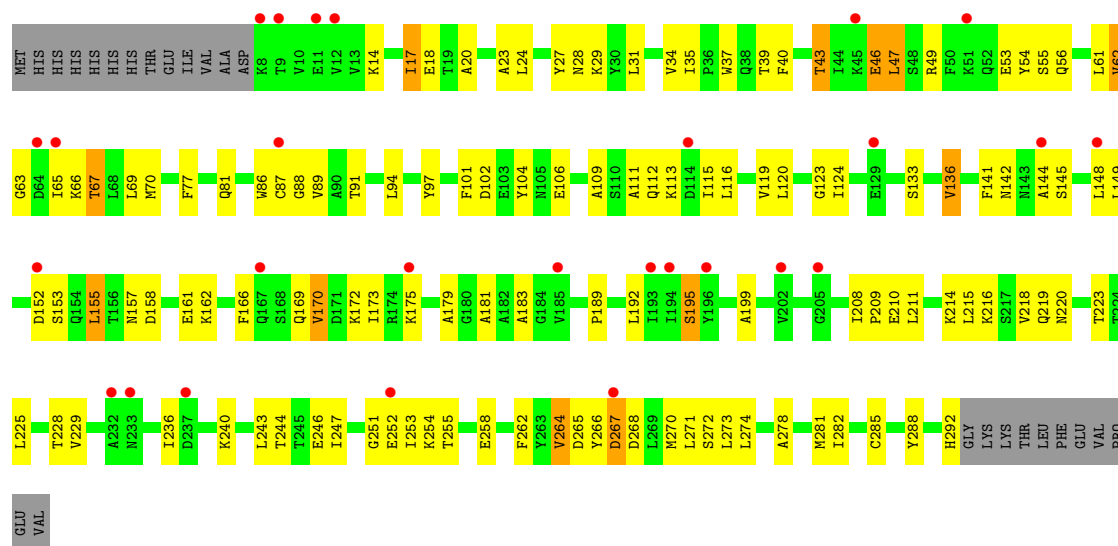




• Molecule 1: HEMOLYSIN E, CHROMOSOMAL

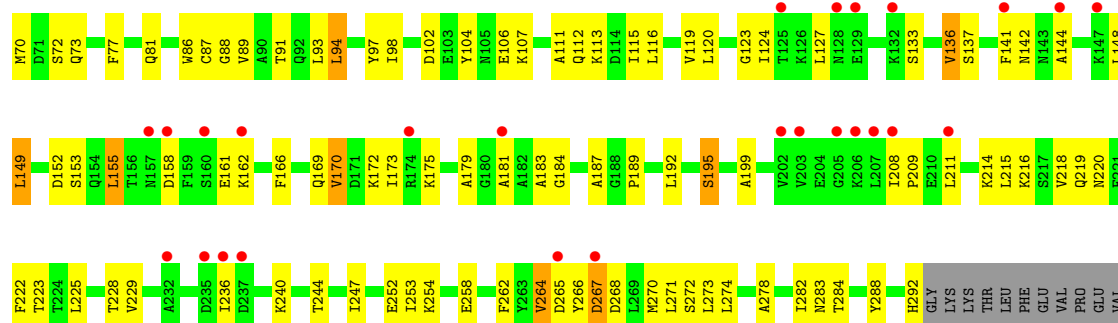


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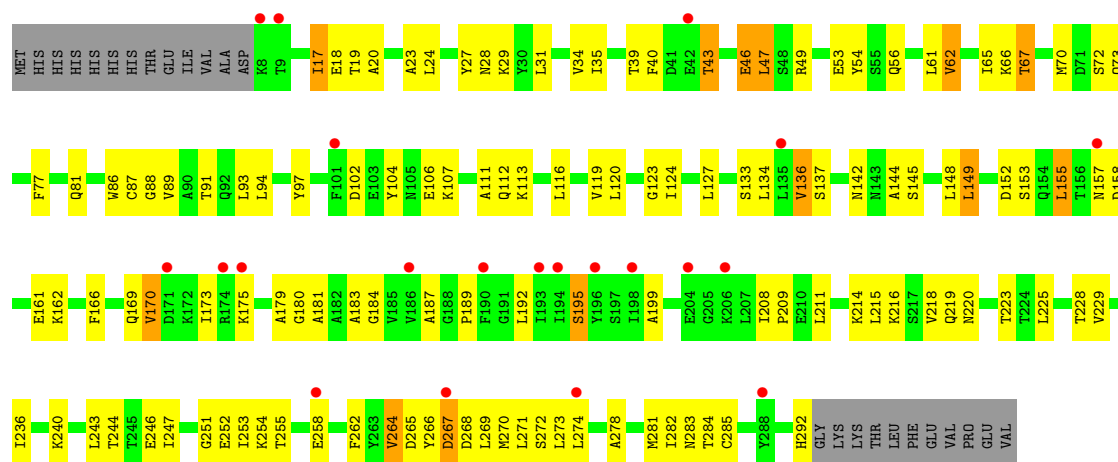


• Molecule 1: HEMOLYSIN E, CHROMOSOMAL

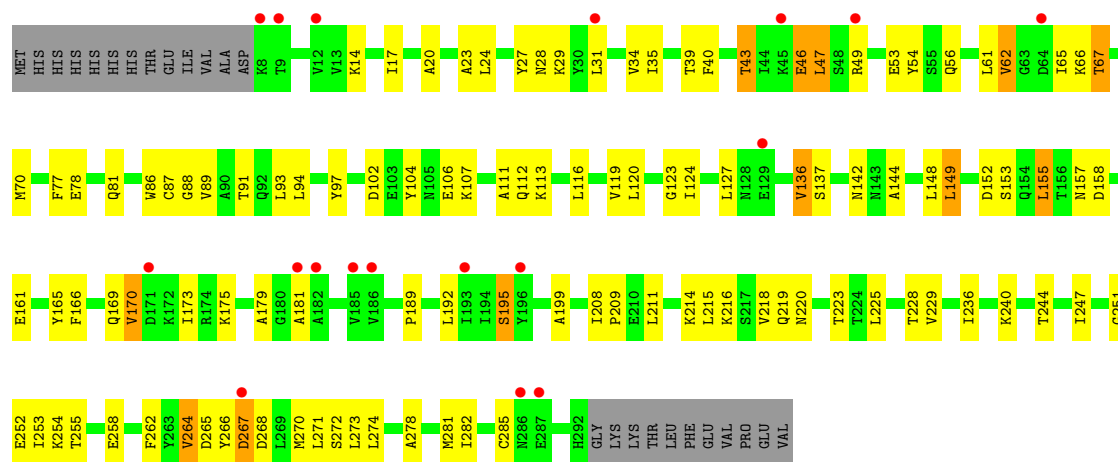




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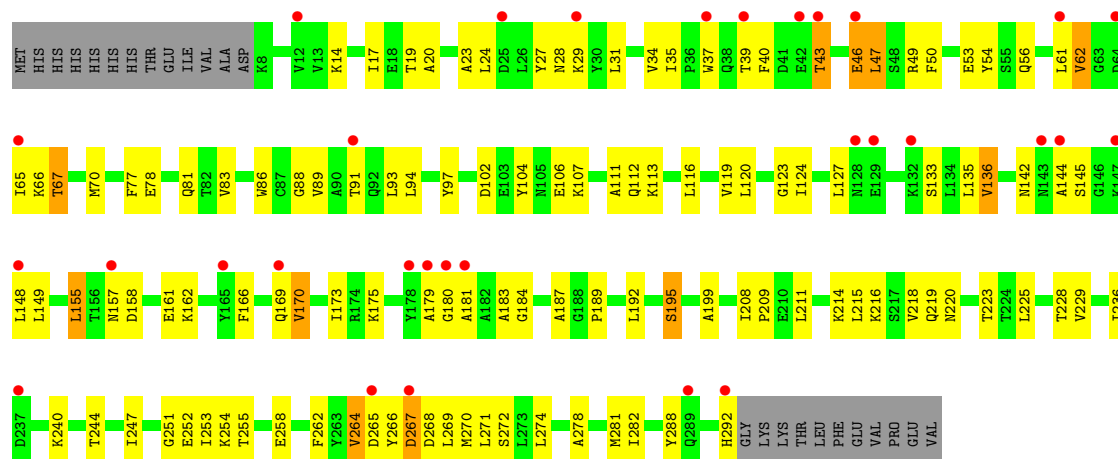


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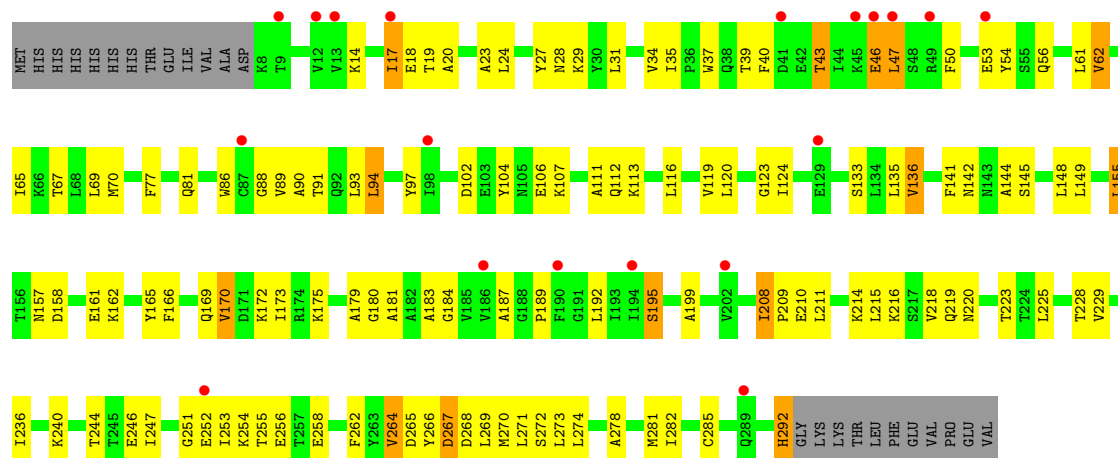


• Molecule 1: HEMOLYSIN E, CHROMOSOMAL

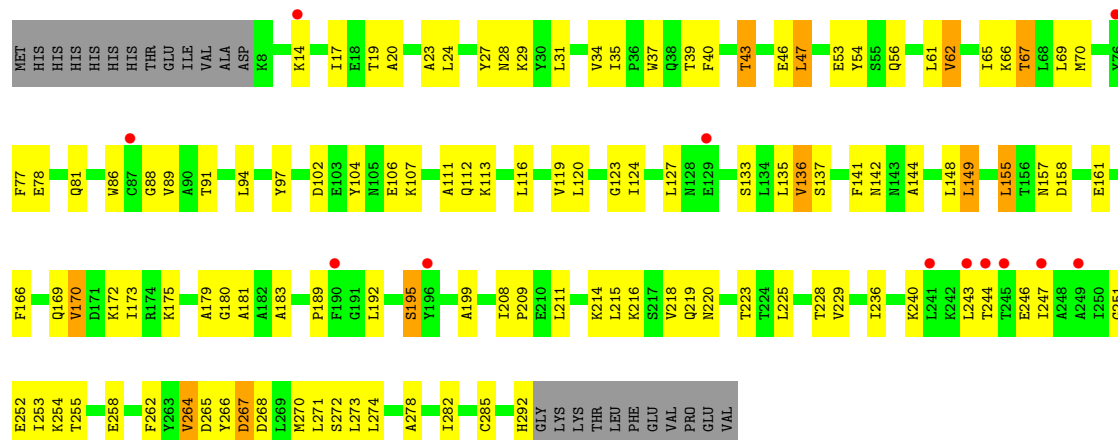




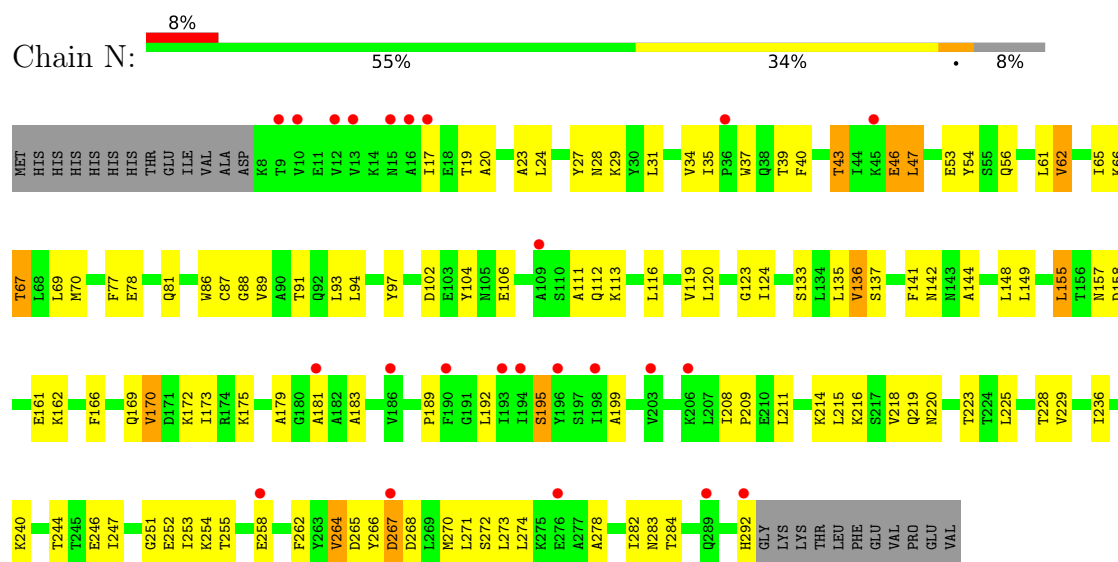
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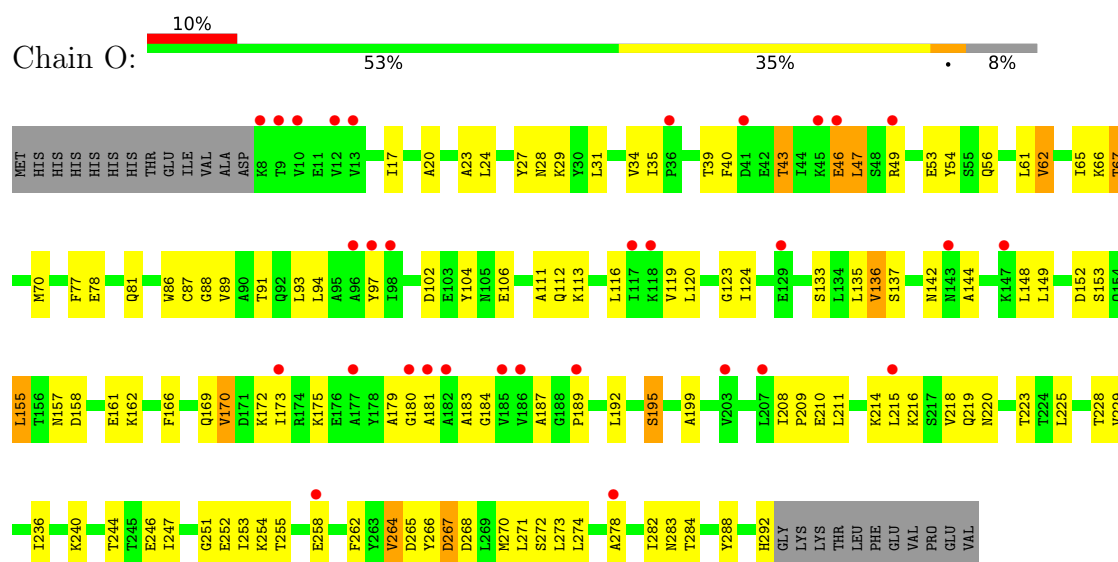
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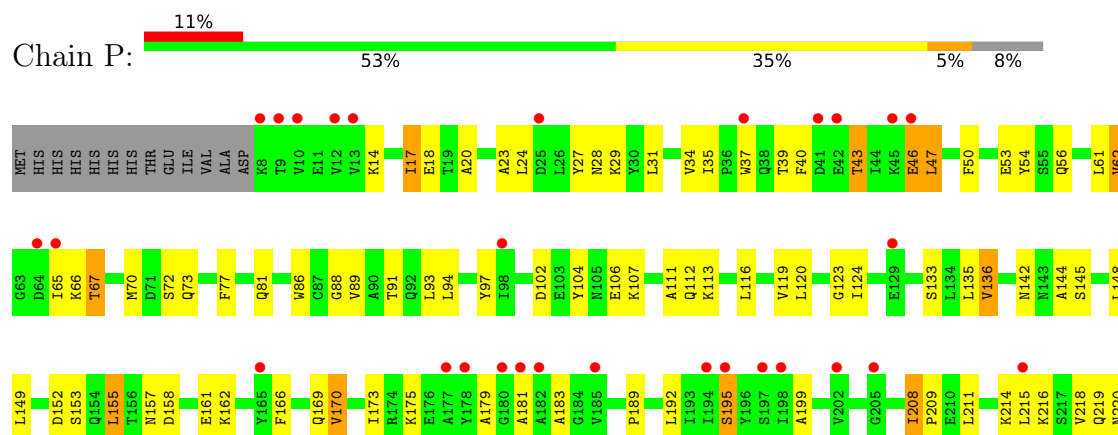
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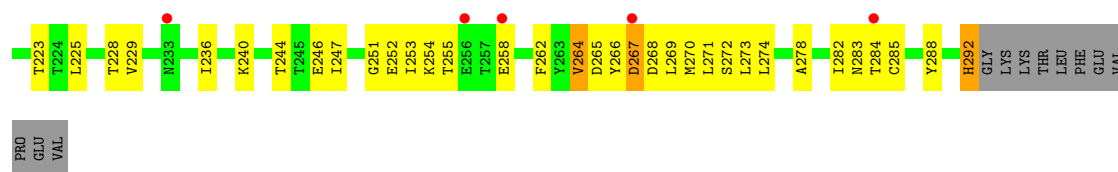


- Molecule 1: HEMOLYSIN E, CHROMOSOMAL

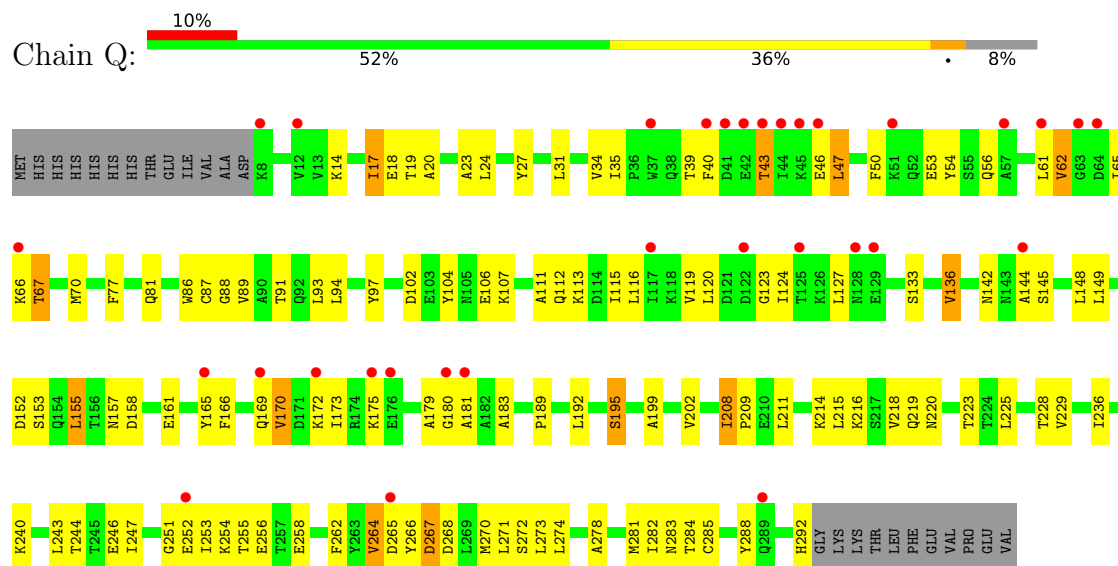


- Molecule 1: HEMOLYSIN E, CHROMOSOMAL

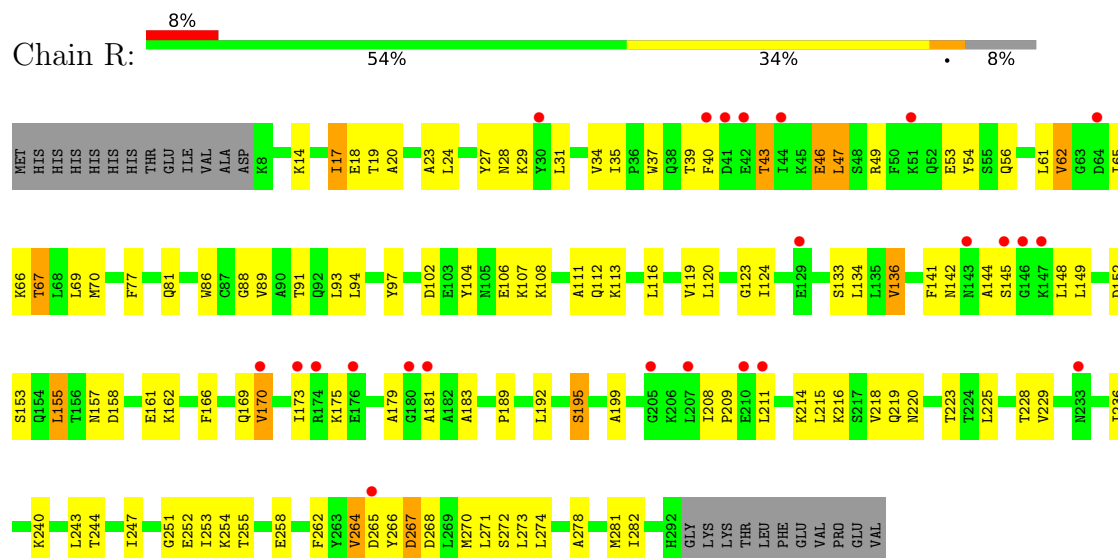




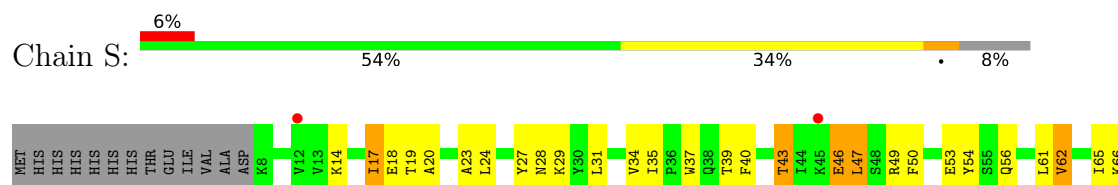
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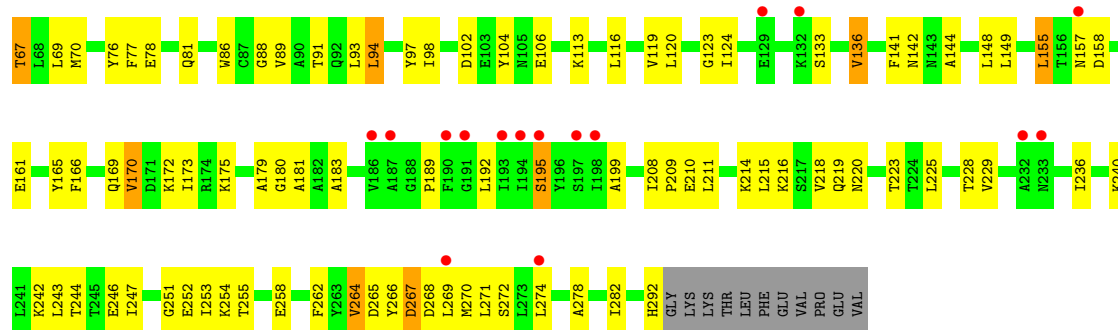


• Molecule 1: HEMOLYSIN E, CHROMOSOMAL

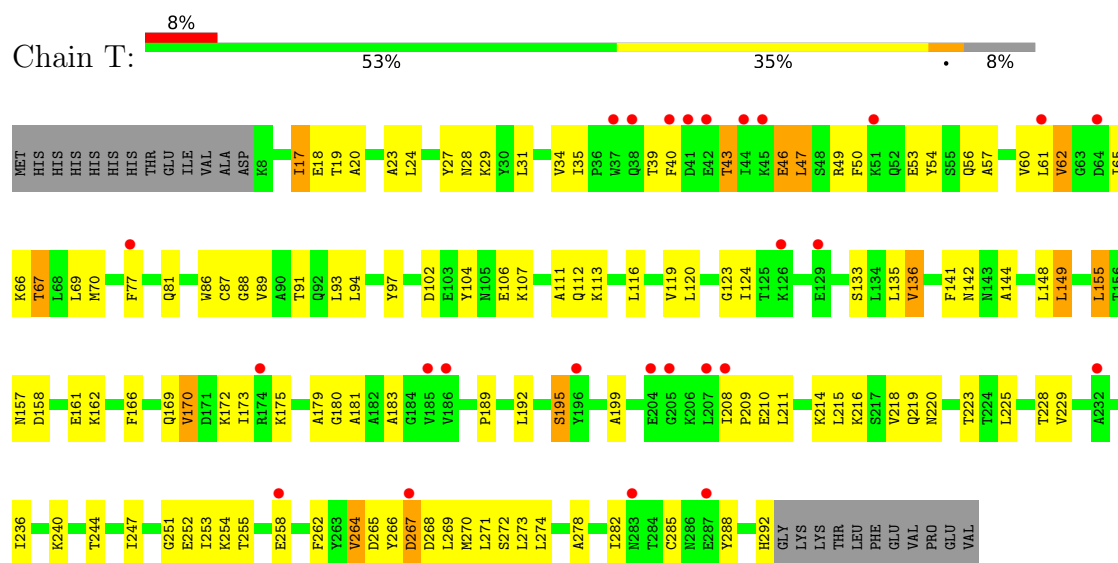


• Molecule 1: HEMOLYSIN E, CHROMOSOMAL

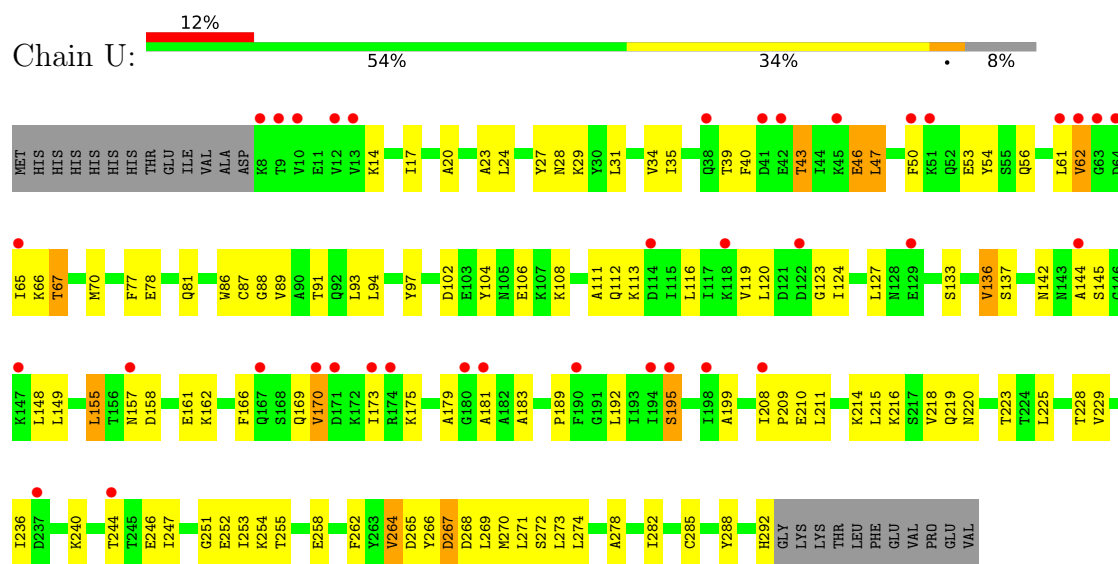




• Molecule 1: HEMOLYSIN E, CHROMOSOMAL



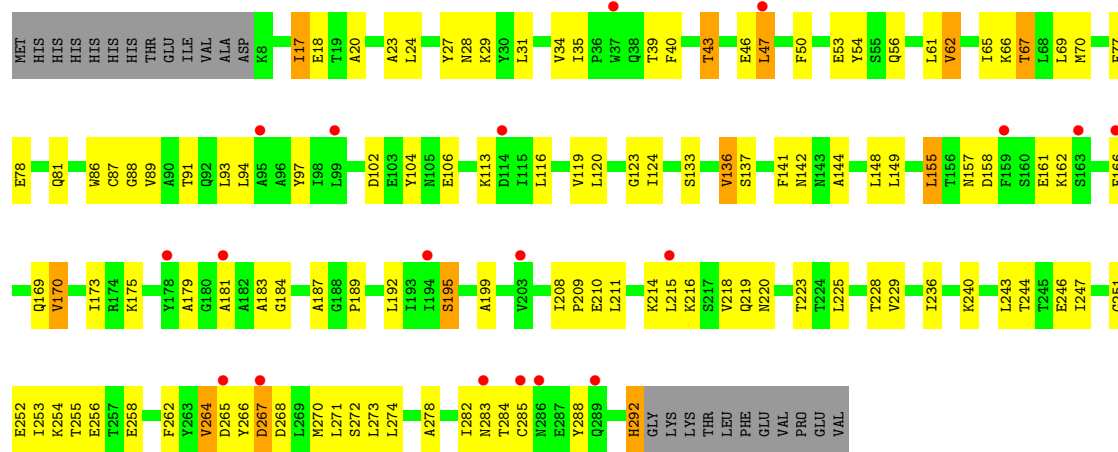
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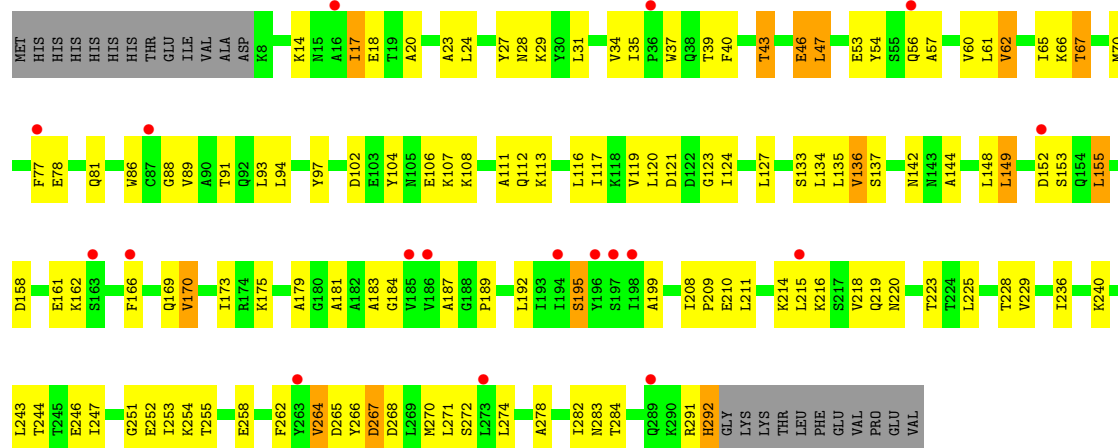
• Molecule 1: HEMOLYSIN E, CHROMOSOMAL



- Molecule 1: HEMOLYSIN E, CHROMOSOMAL



- Molecule 1: HEMOLYSIN E, CHROMOSOMAL



4 Data and refinement statistics

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 49.37 – 3.29	Depositor EDS
% Data completeness (in resolution range)	88.1 (49.37-3.29) 94.6 (49.37-3.29)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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)	0.27 , 135.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.038 for k,h,-l	Xtriage
F_o, F_c correlation	0.92	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.48	0/2268	0.75	1/3062 (0.0%)
1	B	0.51	0/2268	0.75	1/3062 (0.0%)
1	C	0.49	0/2268	0.75	1/3062 (0.0%)
1	D	0.51	0/2268	0.75	1/3062 (0.0%)
1	E	0.47	0/2268	0.75	2/3062 (0.1%)
1	F	0.45	0/2268	0.75	1/3062 (0.0%)
1	G	0.44	0/2268	0.74	1/3062 (0.0%)
1	H	0.45	0/2268	0.74	1/3062 (0.0%)
1	I	0.44	0/2268	0.76	1/3062 (0.0%)
1	J	0.44	0/2268	0.75	1/3062 (0.0%)
1	K	0.44	0/2268	0.75	1/3062 (0.0%)
1	L	0.46	0/2268	0.75	2/3062 (0.1%)
1	M	0.45	0/2268	0.75	1/3062 (0.0%)
1	N	0.46	0/2268	0.76	1/3062 (0.0%)
1	O	0.45	0/2268	0.75	1/3062 (0.0%)
1	P	0.43	0/2268	0.76	2/3062 (0.1%)
1	Q	0.43	0/2268	0.76	2/3062 (0.1%)
1	R	0.45	0/2268	0.75	1/3062 (0.0%)
1	S	0.44	0/2268	0.75	1/3062 (0.0%)
1	T	0.45	0/2268	0.75	1/3062 (0.0%)
1	U	0.45	0/2268	0.75	1/3062 (0.0%)
1	V	0.44	0/2268	0.75	1/3062 (0.0%)
1	W	0.47	0/2268	0.76	1/3062 (0.0%)
1	X	0.45	0/2268	0.76	1/3062 (0.0%)
All	All	0.46	0/54432	0.75	28/73488 (0.0%)

There are no bond length outliers.

All (28) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	102	ASP	N-CA-C	-7.29	103.02	110.97
1	B	102	ASP	N-CA-C	-7.03	103.31	110.97
1	D	102	ASP	N-CA-C	-6.81	103.54	110.97
1	O	102	ASP	N-CA-C	-6.75	103.61	110.97
1	R	102	ASP	N-CA-C	-6.72	103.64	110.97
1	T	102	ASP	N-CA-C	-6.70	103.67	110.97
1	I	102	ASP	N-CA-C	-6.66	103.71	110.97
1	K	102	ASP	N-CA-C	-6.65	103.72	110.97
1	S	102	ASP	N-CA-C	-6.56	103.82	110.97
1	W	102	ASP	N-CA-C	-6.43	103.96	110.97
1	A	102	ASP	N-CA-C	-6.40	104.00	110.97
1	Q	102	ASP	N-CA-C	-6.36	104.04	110.97
1	L	102	ASP	N-CA-C	-6.35	104.04	110.97
1	P	102	ASP	N-CA-C	-6.31	104.09	110.97
1	H	102	ASP	N-CA-C	-6.24	104.17	110.97
1	M	102	ASP	N-CA-C	-6.19	104.22	110.97
1	J	102	ASP	N-CA-C	-6.06	104.37	110.97
1	E	102	ASP	N-CA-C	-5.89	104.55	110.97
1	G	102	ASP	N-CA-C	-5.86	104.58	110.97
1	X	102	ASP	N-CA-C	-5.80	104.65	110.97
1	C	102	ASP	N-CA-C	-5.74	104.71	110.97
1	V	102	ASP	N-CA-C	-5.69	104.77	110.97
1	F	102	ASP	N-CA-C	-5.45	105.03	110.97
1	E	208	ILE	CB-CA-C	-5.17	108.79	113.70
1	L	208	ILE	CB-CA-C	-5.12	108.83	113.70
1	Q	208	ILE	CB-CA-C	-5.08	108.87	113.70
1	P	208	ILE	CB-CA-C	-5.04	108.91	113.70
1	U	102	ASP	N-CA-C	-5.03	105.49	110.97

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2237	0	2264	97	0
1	B	2237	0	2264	104	0
1	C	2237	0	2264	108	0
1	D	2237	0	2264	101	0
1	E	2237	0	2264	102	0
1	F	2237	0	2264	93	0
1	G	2237	0	2264	100	0
1	H	2237	0	2264	103	0
1	I	2237	0	2264	104	0
1	J	2237	0	2264	92	0
1	K	2237	0	2264	96	0
1	L	2237	0	2264	104	0
1	M	2237	0	2264	96	0
1	N	2237	0	2264	94	0
1	O	2237	0	2264	95	0
1	P	2237	0	2264	100	0
1	Q	2237	0	2264	105	0
1	R	2237	0	2264	102	0
1	S	2237	0	2264	98	0
1	T	2237	0	2264	95	0
1	U	2237	0	2264	96	0
1	V	2237	0	2264	96	0
1	W	2237	0	2264	99	0
1	X	2237	0	2264	105	0
2	A	6	0	0	1	0
2	B	6	0	0	1	0
2	C	6	0	0	2	0
2	D	6	0	0	1	0
2	E	6	0	0	1	0
2	F	6	0	0	1	0
2	G	6	0	0	1	0
2	H	6	0	0	1	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	1	0
2	N	6	0	0	1	0
2	O	6	0	0	1	0
2	P	6	0	0	1	0
2	Q	6	0	0	2	0
2	R	6	0	0	2	0
2	S	6	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	T	6	0	0	1	0
2	U	6	0	0	1	0
2	V	6	0	0	2	0
2	W	6	0	0	1	0
2	X	6	0	0	1	0
All	All	53832	0	54336	2230	0

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

All (2230) 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:F:304:EMC:C1	2:F:304:EMC:C2	1.84	1.55
2:H:304:EMC:C2	2:H:304:EMC:C1	1.84	1.55
2:N:304:EMC:C1	2:N:304:EMC:C2	1.84	1.55
2:O:304:EMC:C1	2:O:304:EMC:C2	1.85	1.54
2:I:304:EMC:C1	2:I:304:EMC:C2	1.84	1.54
2:C:304:EMC:C2	2:C:304:EMC:C1	1.85	1.53
2:K:304:EMC:C2	2:K:304:EMC:C1	1.84	1.53
2:J:304:EMC:C1	2:J:304:EMC:C2	1.84	1.53
2:W:304:EMC:C1	2:W:304:EMC:C2	1.86	1.53
2:S:304:EMC:C2	2:S:304:EMC:C1	1.84	1.52
2:X:304:EMC:C2	2:X:304:EMC:C1	1.84	1.52
2:T:304:EMC:C1	2:T:304:EMC:C2	1.85	1.52
2:V:304:EMC:C1	2:V:304:EMC:C2	1.85	1.52
2:P:304:EMC:C2	2:P:304:EMC:C1	1.85	1.52
2:U:304:EMC:C1	2:U:304:EMC:C2	1.85	1.52
2:G:304:EMC:C1	2:G:304:EMC:C2	1.84	1.51
2:R:304:EMC:C1	2:R:304:EMC:C2	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:A:304:EMC:C1	2:A:304:EMC:C2	1.85	1.50
2:L:304:EMC:C1	2:L:304:EMC:C2	1.85	1.50
2:D:304:EMC:C1	2:D:304:EMC:C2	1.85	1.50
2:M:304:EMC:C1	2:M:304:EMC:C2	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:264:VAL:HG23	1:A:274:LEU:HD11	1.65	0.79
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:62:VAL:HG12	1:X:149:LEU:HD21	1.70	0.73
1:W:266:TYR:O	1:W:267:ASP:HB2	1.89	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:31:LEU:HD21	1:H:179:ALA:HB1	1.71	0.72
1:G:86:TRP:CE2	1:G:123:GLY:HA3	2.24	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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:266:TYR:O	1:D:267:ASP:HB2	1.89	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
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:97:TYR:OH	1:V:274:LEU:HD23	1.93	0.68
1:V:266:TYR:O	1:V:267:ASP:HB2	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:X:225:LEU:HD23	1:X:225:LEU:C	2.19	0.68
1:Q:40:PHE:O	1:Q:43:THR:HG22	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:H:225:LEU:HD23	1:H:225:LEU:C	2.20	0.66
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
1:A:62:VAL:HG12	1:B:149:LEU:HD21	1.76	0.66
1:I:225:LEU:HD23	1:I:225:LEU:C	2.19	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:A:225:LEU:HD23	1:A:225:LEU:C	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:225:LEU:HD23	1:B:225:LEU:C	2.20	0.66
1:C:225:LEU:C	1:C:225:LEU:HD23	2.21	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:K:24:LEU:O	1:K:27:TYR:HB3	1.96	0.66
1:D:225:LEU:HD23	1:D:225:LEU:C	2.20	0.65
1:T:225:LEU:HD23	1:T:225:LEU:C	2.21	0.65
1:P:40:PHE:O	1:P:43:THR:HG22	1.95	0.65
1:Q:225:LEU:HD23	1:Q:225:LEU:C	2.21	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:G:225:LEU:HD23	1:G:225:LEU:C	2.21	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:U:225:LEU:HD23	1:U:225:LEU:C	2.22	0.65
1:H:97:TYR:OH	1:H:274:LEU:HD23	1.97	0.65
1:N:225:LEU:C	1:N:225:LEU:HD23	2.22	0.65
1:R:225:LEU:HD23	1:R:225:LEU:C	2.22	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
1:J:225:LEU:HD23	1:J:225:LEU:C	2.22	0.65
1:W:225:LEU:HD23	1:W:225:LEU:C	2.21	0.65
1:L:91:THR:HG23	1:L:282:ILE:HG23	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:225:LEU:HD23	1:L:225:LEU:C	2.21	0.64
1:O:225:LEU:HD23	1:O:225:LEU:C	2.22	0.64
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:S:225:LEU:C	1:S:225:LEU:HD23	2.22	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:P:225:LEU:HD23	1:P:225:LEU:C	2.23	0.64
1:E:225:LEU:HD23	1:E:225:LEU:C	2.22	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:F:225:LEU:C	1:F:225:LEU:HD23	2.23	0.64
1:K:225:LEU:C	1:K:225:LEU:HD23	2.23	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:M:225:LEU:HD23	1:M:225:LEU:C	2.23	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:V:225:LEU:C	1:V:225:LEU:HD23	2.23	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:TYR:OH	1:B:274:LEU:HD23	2.00	0.62
1:C:292:HIS:C	1:C:292:HIS:ND1	2.58	0.62
1:G:97:TYR:OH	1:G:274:LEU:HD23	1.99	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:J:120:LEU:O	1:J:124:ILE:HG13	1.98	0.62
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: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: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:R:120:LEU:O	1:R:124:ILE:HG13	2.01	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: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:W:31:LEU:HD21	1:X:179:ALA:HB1	1.84	0.60
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:N:91:THR:HG23	1:N:282:ILE:HG23	1.84	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:N:86:TRP:C	1:N:88:GLY:H	2.09	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:C:86:TRP:C	1:C:88:GLY:H	2.10	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: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: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:61:LEU:O	1:J:65:ILE:HG12	2.03	0.58
1:J:240:LYS:O	1:J:244:THR:HG23	2.04	0.58
1:O:91:THR:HG23	1:O:282:ILE:HG23	1.83	0.58
1:D:86:TRP:C	1:D:88:GLY:H	2.11	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
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:A:175:LYS:C	1:A:175:LYS:HD3	2.29	0.58
1:B:61:LEU:O	1:B:65:ILE:HG12	2.04	0.58
1:M:149:LEU:HD21	1:X:62:VAL:HG12	1.84	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:A:34:VAL:HG13	1:A:199:ALA:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:K:70:MET:HE2	1:L:142:ASN:OD1	2.04	0.58
1:A:86:TRP:C	1:A:88:GLY:H	2.11	0.57
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:F:175:LYS:C	1:F:175:LYS:HD3	2.29	0.57
1:K:61:LEU:O	1:K:65:ILE:HG12	2.04	0.57
1:U:86:TRP:C	1:U:88:GLY:H	2.11	0.57
1:C:175:LYS:C	1:C:175:LYS:HD3	2.29	0.57
1:M:175:LYS:HD3	1:M:175:LYS:C	2.30	0.57
1:P:148:LEU:HD22	1:P:229:VAL:HG13	1.87	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:I:86:TRP:C	1:I:88:GLY:H	2.11	0.57
1:J:258:GLU:O	1:J:262:PHE:HD2	1.88	0.57
1:M:262:PHE:CG	1:X:93:LEU:HD11	2.39	0.57
1:W:61:LEU:O	1:W:65:ILE:HG12	2.03	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:I:175:LYS:C	1:I:175:LYS:HD3	2.30	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:175:LYS:HD3	1:P:175:LYS:C	2.30	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:V:86:TRP:C	1:V:88:GLY:H	2.13	0.56
1:A:120:LEU:O	1:A:124:ILE:HG13	2.05	0.56
1:A:179:ALA:HB1	1:L:31:LEU:HD21	1.88	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:F:216:LYS:O	1:F:220:ASN:HB2	2.05	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:K:175:LYS:C	1:K:175:LYS:HD3	2.31	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:B:70:MET:HE2	1:C:142:ASN:OD1	2.06	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:L:175:LYS:C	1:L:175:LYS:HD3	2.30	0.56
1:R:175:LYS:HD3	1:R:175:LYS:C	2.30	0.56
1:T:86:TRP:C	1:T:88:GLY:H	2.14	0.56
1:U:175:LYS:HD3	1:U:175:LYS:C	2.30	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:K:86:TRP:C	1:K:88:GLY:H	2.13	0.56
1:V:34:VAL:HG12	1:V:35:ILE:HG13	1.87	0.56
1:W:175:LYS:C	1:W:175:LYS:HD3	2.30	0.56
1:J:175:LYS:HD3	1:J:175:LYS:C	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:X:175:LYS:HD3	1:X:175:LYS:C	2.30	0.56
1:B:175:LYS:HD3	1:B:175:LYS:C	2.31	0.55
1:D:215:LEU:O	1:D:215:LEU:HD13	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:M:142:ASN:OD1	1:X:70:MET:HE2	2.06	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:27:TYR:CE2	1:I:183:ALA:HB2	2.41	0.55
1:H:39:THR:CG2	1:H:173:ILE:HG12	2.36	0.55
1:Q:215:LEU:O	1:Q:215:LEU:HD13	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:O	1:I:215:LEU:HD13	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:J:215:LEU:O	1:J:215:LEU:HD13	2.06	0.55
1:M:86:TRP:C	1:M:88:GLY:H	2.14	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:O	1:X:215:LEU:HD13	2.07	0.55
1:B:86:TRP:C	1:B:88:GLY:H	2.13	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:148:LEU:HD22	1:T:229:VAL:HG13	1.88	0.55
1:T:166:PHE:CE1	1:T:211:LEU:HB3	2.42	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:Q:175:LYS:C	1:Q:175:LYS:HD3	2.32	0.55
1:R:86:TRP:C	1:R:88:GLY:H	2.13	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:175:LYS:C	1:G:175:LYS:HD3	2.31	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:S:175:LYS:C	1:S:175:LYS:HD3	2.32	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:O	1:G:215:LEU:HD13	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
1:D:31:LEU:HD21	1:E:179:ALA:HB1	1.88	0.55
1:D:216:LYS:O	1:D:220:ASN:HB2	2.07	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: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:N:216:LYS:O	1:N:220:ASN:HB2	2.06	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:N:175:LYS:C	1:N:175:LYS:HD3	2.31	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:D:175:LYS:C	1:D:175:LYS:HD3	2.32	0.54
1:H:175:LYS:C	1:H:175:LYS:HD3	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:86:TRP:C	1:G:88:GLY:H	2.15	0.54
1:H:86:TRP:C	1:H:88:GLY:H	2.14	0.54
1:I:262:PHE:O	1:I:265:ASP:HB2	2.07	0.54
1:L:86:TRP:C	1:L:88:GLY:H	2.14	0.54
1:M:166:PHE:O	1:M:170:VAL:HG13	2.08	0.54
1:Q:39:THR:CG2	1:Q:173:ILE:HG12	2.36	0.54
1:Q:86:TRP:C	1:Q:88:GLY:H	2.15	0.54
1:V:175:LYS:C	1:V:175:LYS:HD3	2.31	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:O	1:A:215:LEU:HD13	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
1:R:264:VAL:HG23	1:R:274:LEU:CD1	2.34	0.54
1:T:61:LEU:O	1:T:65:ILE:HG12	2.08	0.54
1:T:240:LYS:O	1:T:244:THR:HG23	2.08	0.54
1:C:244:THR:HA	1:C:247:ILE:HD12	1.88	0.54
1:E:175:LYS:HD3	1:E:175:LYS:C	2.33	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:86:TRP:C	1:J:88:GLY:H	2.15	0.54
1:J:264:VAL:N	1:J:274:LEU:HD13	2.23	0.54
1:O:215:LEU:O	1:O:215:LEU:HD13	2.07	0.54
1:P:86:TRP:C	1:P:88:GLY:H	2.14	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:X:86:TRP:C	1:X:88:GLY:H	2.16	0.54
1:A:39:THR:CG2	1:A:173:ILE:HG12	2.38	0.54
1:D:86:TRP:C	1:D:88:GLY:N	2.65	0.54
1:E:292:HIS:ND1	1:E:292:HIS:C	2.65	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD13	1:H:215:LEU:O	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:N:70:MET:HE2	1:O:142:ASN:OD1	2.07	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:L:292:HIS:C	1:L:292:HIS:ND1	2.66	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
1:C:86:TRP:C	1:C:88:GLY:N	2.64	0.54
1:H:216:LYS:O	1:H:220:ASN:HB2	2.07	0.54
1:K:252:GLU:OE2	1:K:252:GLU:HA	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:O	1:B:215:LEU:HD13	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:A:86:TRP:C	1:A:88:GLY:N	2.65	0.53
1:B:86:TRP:C	1:B:88:GLY:N	2.66	0.53
1:E:166:PHE:CE1	1:E:211:LEU:HB3	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:258:GLU:O	1:A:262:PHE:HD2	1.91	0.53
1:B:252:GLU:HA	1:B:252:GLU:OE2	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:O:70:MET:HE2	1:P:142:ASN:OD1	2.08	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:X:292:HIS:ND1	1:X:292:HIS:C	2.66	0.53
1:E:215:LEU:O	1:E:215:LEU:HD13	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:O:175:LYS:C	1:O:175:LYS:HD3	2.32	0.53
1:R:166:PHE:CE1	1:R:211:LEU:HB3	2.43	0.53
1:V:86:TRP:C	1:V:88:GLY:N	2.66	0.53
1:A:262:PHE:O	1:A:265:ASP:HB2	2.09	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:HA	1:L:252:GLU:OE2	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
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:I:86:TRP:C	1:I:88:GLY:N	2.65	0.53
1:R:47:LEU:HD11	1:R:214:LYS:HB3	1.90	0.53
1:T:175:LYS:C	1:T:175:LYS:HD3	2.33	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:B:268:ASP:C	1:B:270:MET:H	2.16	0.53
1:C:39:THR:HG22	1:C:173:ILE:HG12	1.91	0.53
1:G:268:ASP:C	1:G:270:MET:H	2.17	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:R:86:TRP:C	1:R:88:GLY:N	2.66	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:OE2	1:H:252:GLU:HA	2.09	0.53
1:H:268:ASP:C	1:H:270:MET:H	2.16	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:Q:39:THR:HG22	1:Q:173:ILE:HG12	1.91	0.53
1:Q:166:PHE:HE1	1:Q:211:LEU:HB3	1.72	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:K:166:PHE:CE1	1:K:211:LEU:HB3	2.43	0.53
1:N:86:TRP:C	1:N:88:GLY:N	2.65	0.53
1:P:262:PHE:O	1:P:265:ASP:HB2	2.09	0.53
1:S:86:TRP:C	1:S:88:GLY:H	2.15	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:C:268:ASP:C	1:C:270:MET:H	2.16	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:OE2	1:P:252:GLU:HA	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:O	1:U:215:LEU:HD13	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:M:179:ALA:HB1	1:X:31:LEU:HD21	1.91	0.52
1:Q:65:ILE:HD12	1:Q:236:ILE:HD11	1.92	0.52
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:86:TRP:C	1:X:88:GLY:N	2.67	0.52
1:A:268:ASP:C	1:A:270:MET:H	2.17	0.52
1:C:61:LEU:HD21	1:C:148:LEU:HG	1.92	0.52
1:E:34:VAL:HG12	1:E:35:ILE:HG13	1.89	0.52
1:E:39:THR:HG22	1:E:173:ILE:HG12	1.91	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:20:ALA:O	1:I:23:ALA:HB3	2.10	0.52
1:I:189:PRO:HA	1:I:192:LEU:HD13	1.90	0.52
1:K:215:LEU:HD13	1:K:215:LEU:O	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:E:86:TRP:C	1:E:88:GLY:H	2.16	0.52
1:G:34:VAL:HG12	1:G:35:ILE:HG13	1.90	0.52
1:O:47:LEU:HD11	1:O:214:LYS:HB3	1.90	0.52
1:V:268:ASP:C	1:V:270:MET:H	2.17	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:47:LEU:HD11	1:D:214:LYS:HB3	1.91	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: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:A:252:GLU:HA	1:A:252:GLU:OE2	2.09	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:27:TYR:CE2	1:N:183:ALA:HB2	2.44	0.52
1:M:39:THR:HG22	1:M:173:ILE:HG12	1.91	0.52
1:P:268:ASP:C	1:P:270:MET:H	2.17	0.52
1:V:166:PHE:O	1:V:170:VAL:HG13	2.10	0.52
1:V:252:GLU:HA	1:V:252:GLU:OE2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:253:ILE:O	1:W:254:LYS:C	2.53	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:HA	1:U:252:GLU:OE2	2.10	0.52
1:V:215:LEU:O	1:V:215:LEU:HD13	2.10	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:HA	1:M:252:GLU:OE2	2.09	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:47:LEU:HD11	1:I:214:LYS:HB3	1.91	0.52
1:I:240:LYS:O	1:I:244:THR:HG23	2.10	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: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:H:86:TRP:C	1:H:88:GLY:N	2.66	0.51
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:O:86:TRP:C	1:O:88:GLY:H	2.17	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:148:LEU:HD22	1:C:229:VAL:HG13	1.91	0.51
1:C:166:PHE:CE1	1:C:211:LEU:HB3	2.45	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:86:TRP:C	1:P:88:GLY:N	2.68	0.51
1:P:258:GLU:O	1:P:262:PHE:HD2	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:I:31:LEU:HD21	1:J:179:ALA:HB1	1.92	0.51
1:J:166:PHE:HE1	1:J:211:LEU:HB3	1.76	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:86:TRP:C	1:G:88:GLY:N	2.68	0.51
1:G:262:PHE:O	1:G:265:ASP:HB2	2.11	0.51
1:H:61:LEU:HD21	1:H:148:LEU:HG	1.92	0.51
1:H:244:THR:HA	1:H:247:ILE:HD12	1.93	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:X:65:ILE:HD12	1:X:236:ILE:HD11	1.93	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:A:183:ALA:HB2	1:L:27:TYR:CE2	2.45	0.51
1:E:262:PHE:O	1:E:265:ASP:HB2	2.11	0.51
1:G:54:TYR:CD1	1:G:155:LEU:HB2	2.44	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:M:135:LEU:HD21	1:X:78:GLU:HB2	1.93	0.51
1:U:86:TRP:C	1:U:88:GLY:N	2.65	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:HA	1:X:252:GLU:OE2	2.10	0.51
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:HA	1:N:252:GLU:OE2	2.10	0.51
1:O:189:PRO:HA	1:O:192:LEU:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	1:M:215:LEU:HD13	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:OE2	1:S:252:GLU:HA	2.11	0.51
1:T:86:TRP:C	1:T:88:GLY:N	2.67	0.51
1:V:104:TYR:HE2	1:V:106:GLU:HA	1.75	0.51
1:W:39:THR:CG2	1:W:173:ILE:HG12	2.39	0.51
1:W:252:GLU:HA	1:W:252:GLU:OE2	2.09	0.51
1:C:47:LEU:HD11	1:C:214:LYS:HB3	1.92	0.51
1:C:278:ALA:O	1:C:282:ILE:HG13	2.11	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: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:86:TRP:C	1:F:88:GLY:H	2.18	0.51
1:F:215:LEU:O	1:F:215:LEU:HD13	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: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
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:T:268:ASP:C	1:T:270:MET:H	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:47:LEU:HD11	1:V:214:LYS:HB3	1.93	0.51
1:W:61:LEU:HD21	1:W:148:LEU:HG	1.93	0.51
1:W:278:ALA:O	1:W:282:ILE:HG13	2.11	0.51
1:X:20:ALA:O	1:X:23:ALA:HB3	2.11	0.51
1:A:142:ASN:OD1	1:L:70:MET:HE2	2.11	0.50
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:86:TRP:C	1:K:88:GLY:N	2.67	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:31:LEU:HD21	1:Q:179:ALA:HB1	1.94	0.50
1:P:166:PHE:HE1	1:P:211:LEU:HB3	1.74	0.50
1:P:189:PRO:HA	1:P:192:LEU:HD13	1.92	0.50
1:R:258:GLU:O	1:R:262:PHE:HD2	1.94	0.50
1:S:86:TRP:C	1:S:88:GLY:N	2.68	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:54:TYR:CD1	1:X:155:LEU:HB2	2.45	0.50
1:X:262:PHE:O	1:X:265:ASP:HB2	2.11	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:I:70:MET:HE2	1:J:142:ASN:OD1	2.10	0.50
1:M:268:ASP:C	1:M:270:MET:H	2.17	0.50
1:Q:268:ASP:C	1:Q:270:MET:H	2.18	0.50
1:X:268:ASP:C	1:X:270:MET:H	2.18	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
1:F:274:LEU:HG	1:F:274:LEU:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:U:268:ASP:C	1:U:270:MET:H	2.20	0.50
1:V:70:MET:HE2	1:W:142:ASN:OD1	2.12	0.50
1:W:70:MET:HE2	1:X:142:ASN:OD1	2.11	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:D:268:ASP:C	1:D:270:MET:H	2.20	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:HA	1:D:252:GLU:OE2	2.11	0.50
1:I:252:GLU:HA	1:I:252:GLU:OE2	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:M:86:TRP:C	1:M:88:GLY:N	2.66	0.50
1:N:20:ALA:O	1:N:23:ALA:HB3	2.12	0.50
1:P:54:TYR:CD1	1:P:155:LEU:HB2	2.47	0.50
1:P:264:VAL:HG23	1:P:274:LEU:CD1	2.40	0.50
1:T:278:ALA:O	1:T:282:ILE:HG13	2.12	0.50
1:V:31:LEU:HD21	1:W:179:ALA:HB1	1.93	0.50
1:V:65:ILE:HD12	1:V:236:ILE:HD11	1.94	0.50
1:V:278:ALA:O	1:V:282:ILE:HG13	2.12	0.50
1:W:39:THR:HG22	1:W:173:ILE:HG12	1.93	0.50
1:W:86:TRP:C	1:W:88:GLY:H	2.19	0.50
1:C:65:ILE:HD12	1:C:236:ILE:HD11	1.94	0.50
1:C:119:VAL:HG13	1:C:120:LEU:N	2.27	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:86:TRP:C	1:E:88:GLY:N	2.69	0.50
1:E:119:VAL:HG13	1:E:120:LEU:N	2.27	0.50
1:J:86:TRP:C	1:J:88:GLY:N	2.68	0.50
1:N:47:LEU:HD11	1:N:214:LYS:HB3	1.93	0.50
1:N:54:TYR:CD1	1:N:155:LEU:HB2	2.47	0.50
1:N:268:ASP:C	1:N:270:MET:H	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:119:VAL:HG13	1:Q:120:LEU:N	2.26	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
1:I:116:LEU:O	1:I:120:LEU:HG	2.12	0.50
1:L:86:TRP:C	1:L:88:GLY:N	2.67	0.50
1:O:86:TRP:C	1:O:88:GLY:N	2.69	0.50
1:P:264:VAL:N	1:P:274:LEU:HD13	2.27	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:H:70:MET:HE2	1:I:142:ASN:OD1	2.11	0.49
1:J:278:ALA:O	1:J:282:ILE:HG13	2.12	0.49
1:L:268:ASP:C	1:L:270:MET:H	2.18	0.49
1:P:104:TYR:HE2	1:P:106:GLU:HA	1.75	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:R:70:MET:HE2	1:S:142:ASN:OD1	2.12	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:A:70:MET:HE2	1:B:142:ASN:OD1	2.12	0.49
1:C:20:ALA:O	1:C:23:ALA:HB3	2.12	0.49
1:C:189:PRO:HA	1:C:192:LEU:HD13	1.94	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:268:ASP:C	1:J:270:MET:H	2.19	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:F:47:LEU:HD11	1:F:214:LYS:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:104:TYR:HE2	1:F:106:GLU:HA	1.77	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
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:S:37:TRP:HE1	1:T:172:LYS:HZ3	1.59	0.49
1:B:61:LEU:HD21	1:B:148:LEU:HG	1.95	0.49
1:B:253:ILE:O	1:B:254:LYS:C	2.56	0.49
1:G:161:GLU:HA	1:G:161:GLU:OE1	2.12	0.49
1:H:262:PHE:O	1:H:265:ASP:HB2	2.12	0.49
1:H:264:VAL:HG23	1:H:274:LEU:CD1	2.38	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:E:268:ASP:C	1:E:270:MET:H	2.20	0.49
1:F:268:ASP:C	1:F:270:MET:H	2.19	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:47:LEU:HD11	1:M:214:LYS:HB3	1.93	0.49
1:M:181:ALA:HA	1:M:195:SER:OG	2.13	0.49
1:Q:86:TRP:C	1:Q:88:GLY:N	2.68	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:C:70:MET:HE2	1:D:142:ASN:OD1	2.11	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:I:268:ASP:C	1:I:270:MET:H	2.19	0.49
1:J:28:ASN:O	1:J:29:LYS:C	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:54:TYR:CD1	1:O:155:LEU:HB2	2.48	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:P:70:MET:HE2	1:Q:142:ASN:OD1	2.12	0.49
1:Q:54:TYR:CD1	1:Q:155:LEU:HB2	2.48	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
1:W:218:VAL:HG12	1:W:219:GLN:N	2.28	0.49
1:A:292:HIS:C	1:A:292:HIS:ND1	2.70	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: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:U:65:ILE:HD12	1:U:236:ILE:HD11	1.94	0.49
1:U:264:VAL:HG23	1:U:274:LEU:CD1	2.41	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: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:268:ASP:C	1:S:270:MET:H	2.21	0.49
1:S:278:ALA:O	1:S:282:ILE:HG13	2.13	0.49
1:W:86:TRP:C	1:W:88:GLY:N	2.70	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:H:253:ILE:O	1:H:254:LYS:C	2.56	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:R:268:ASP:C	1:R:270:MET:H	2.19	0.48
1:W:170:VAL:HB	1:W:208:ILE:CD1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:258:GLU:O	1:X:262:PHE:HD2	1.96	0.48
1:A:172:LYS:HZ3	1:L:37:TRP:HE1	1.61	0.48
1:D:253:ILE:O	1:D:254:LYS:C	2.53	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:P:104:TYR:CE2	1:P:106:GLU:HA	2.49	0.48
1:R:27:TYR:CE2	1:S:183:ALA:HB2	2.48	0.48
1:R:262:PHE:O	1:R:265:ASP:HB2	2.13	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:X:116:LEU:O	1:X:120:LEU:HG	2.14	0.48
1:B:65:ILE:HD12	1:B:236:ILE:HD11	1.95	0.48
1:B:166:PHE:HE1	1:B:211:LEU:HB3	1.78	0.48
1:E:116:LEU:O	1:E:120:LEU:HG	2.13	0.48
1:F:86:TRP:C	1:F:88:GLY:N	2.69	0.48
1:G:166:PHE:HE1	1:G:211:LEU:HB3	1.77	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:W:268:ASP:C	1:W:270:MET:H	2.19	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:O	1:C:274:LEU:HG	2.12	0.48
1:E:31:LEU:HD21	1:F:179:ALA:HB1	1.96	0.48
1:F:28:ASN:O	1:F:29:LYS:C	2.55	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:OE1	1:I:161:GLU:HA	2.14	0.48
1:J:70:MET:HE2	1:K:142:ASN:OD1	2.12	0.48
1:J:104:TYR:HE2	1:J:106:GLU:HA	1.79	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:37:TRP:HE1	1:N:172:LYS:HZ3	1.61	0.48
1:O:124:ILE:HD11	1:O:258:GLU:HA	1.96	0.48
1:O:268:ASP:C	1:O:270:MET:H	2.21	0.48
1:V:77:PHE:O	1:V:81:GLN:HB2	2.14	0.48
1:X:104:TYR:HE2	1:X:106:GLU:HA	1.78	0.48
1:A:225:LEU:HD23	1:A:225:LEU:O	2.14	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: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:N:37:TRP:HE1	1:O:172:LYS:HZ3	1.61	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:65:ILE:HD12	1:W:236:ILE:HD11	1.96	0.48
1:W:166:PHE:O	1:W:170:VAL:HG13	2.13	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:K:253:ILE:O	1:K:254:LYS:C	2.57	0.48
1:L:77:PHE:O	1:L:81:GLN:HB2	2.14	0.48
1:L:225:LEU:HD23	1:L:225:LEU:O	2.13	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:A:104:TYR:HE2	1:A:106:GLU:HA	1.79	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:65:ILE:HD12	1:G:236:ILE:HD11	1.95	0.48
1:J:65:ILE:HD12	1:J:236:ILE:HD11	1.95	0.48
1:J:116:LEU:O	1:J:120:LEU:HG	2.14	0.48
1:L:124:ILE:HD11	1:L:258:GLU:HA	1.96	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: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:19:THR:OG1	1:L:14:LYS:HB2	2.13	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: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:HA	1:Q:107:LYS:HD3	1.71	0.47
1:U:27:TYR:CE2	1:V:183:ALA:HB2	2.48	0.47
1:U:274:LEU:O	1:U:274:LEU:HG	2.14	0.47
1:X:104:TYR:CE2	1:X:106:GLU:HA	2.49	0.47
1:X:161:GLU:OE1	1:X:161:GLU:HA	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:253:ILE:O	1:O:254:LYS:C	2.58	0.47
1:R:116:LEU:HB3	1:R:264:VAL:HG21	1.96	0.47
1:S:31:LEU:HD21	1:T:179:ALA:HB1	1.95	0.47
1:S:54:TYR:CD1	1:S:155:LEU:HB2	2.49	0.47
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:K:93:LEU:HD11	1:L:262:PHE:CG	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:181:ALA:HA	1:L:195:SER:OG	2.13	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:HA	1:B:161:GLU:OE1	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:N:62:VAL:CG1	1:O:149:LEU:HD21	2.45	0.47
1:O:61:LEU:HD21	1:O:148:LEU:HG	1.95	0.47
1:O:116:LEU:HB3	1:O:264:VAL:HG21	1.96	0.47
1:O:155:LEU:HD13	1:O:225:LEU:HD22	1.96	0.47
1:U:251:GLY:O	1:U:255:THR:HG23	2.14	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:61:LEU:HD21	1:E:148:LEU:HG	1.97	0.47
1:E:104:TYR:HE2	1:E:106:GLU:HA	1.79	0.47
1:E:253:ILE:O	1:E:254:LYS:C	2.55	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:K:28:ASN:O	1:K:29:LYS:C	2.57	0.47
1:Q:62:VAL:HG12	1:R:149:LEU:CD2	2.43	0.47
1:Q:181:ALA:HA	1:Q:195:SER:OG	2.13	0.47
1:W:62:VAL:CG1	1:X:149:LEU:HD21	2.43	0.47
1:X:116:LEU:HB3	1:X:264:VAL:HG21	1.96	0.47
1:B:54:TYR:CD1	1:B:155:LEU:HB2	2.50	0.47
1:D:283:ASN:O	1:D:284:THR:C	2.58	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
1:A:181:ALA:HA	1:A:195:SER:OG	2.15	0.47
1:C:86:TRP:O	1:C:88:GLY:N	2.47	0.47
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:70:MET:HE2	1:E:142:ASN:OD1	2.14	0.47
1:D:119:VAL:HG13	1:D:120:LEU:N	2.30	0.47
1:F:47:LEU:HD12	1:F:47:LEU:C	2.39	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:K:268:ASP:C	1:K:270:MET:H	2.22	0.47
1:L:170:VAL:HB	1:L:208:ILE:CD1	2.44	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:53:GLU:O	1:Q:56:GLN:HB3	2.14	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:R:218:VAL:HG12	1:R:219:GLN:N	2.30	0.47
1:S:274:LEU:O	1:S:274:LEU:HG	2.15	0.47
1:U:161:GLU:OE1	1:U:161:GLU:HA	2.15	0.47
1:V:104:TYR:CE2	1:V:106:GLU:HA	2.50	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:Q:253:ILE:O	1:Q:254:LYS:C	2.57	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:H:93:LEU:HD11	1:I:262:PHE:CG	2.50	0.47
1:N:161:GLU:OE1	1:N:161:GLU:HA	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:I:246:GLU:OE1	1:I:292:HIS:CD2	2.68	0.47
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:Q:77:PHE:O	1:Q:81:GLN:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:70:MET:HE2	1:U:142:ASN:OD1	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:O	1:H:274:LEU:HG	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:69:LEU:HD23	1:R:141:PHE:CZ	2.50	0.46
1:R:119:VAL:HG13	1:R:120:LEU:N	2.30	0.46
1:C:27:TYR:CE2	1:D:183:ALA:HB2	2.50	0.46
1:P:251:GLY:O	1:P:255:THR:HG23	2.15	0.46
1:W:292:HIS:C	1:W:292:HIS:ND1	2.73	0.46
1:H:116:LEU:HB3	1:H:264:VAL:HG21	1.97	0.46
1:I:28:ASN:O	1:I:29:LYS:C	2.57	0.46
1:K:116:LEU:O	1:K:120:LEU:HG	2.16	0.46
1:R:225:LEU:HD23	1:R:225:LEU:O	2.14	0.46
1:T:133:SER:O	1:T:136:VAL:HG12	2.15	0.46
1:U:28:ASN:O	1:U:29:LYS:C	2.57	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:77:PHE:O	1:J:81:GLN:HB2	2.16	0.46
1:J:119:VAL:HG13	1:J:120:LEU:N	2.29	0.46
1:M:65:ILE:HD12	1:M:236:ILE:HD11	1.96	0.46
1:M:172:LYS:HZ3	1:X:37:TRP:HE1	1.62	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:N:253:ILE:O	1:N:254:LYS:C	2.59	0.46
1:S:70:MET:HE2	1:T:142:ASN:OD1	2.14	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: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:L:119:VAL:HG13	1:L:120:LEU:N	2.30	0.46
1:L:274:LEU:O	1:L:274:LEU:HG	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:HD23	1:D:225:LEU:O	2.16	0.46
1:E:251:GLY:O	1:E:255:THR:HG23	2.15	0.46
1:F:41:ASP:OD2	1:G:172:LYS:NZ	2.48	0.46
1:I:281:MET:HE2	2:I:304:EMC:C1	2.46	0.46
1:K:116:LEU:HB3	1:K:264:VAL:HG21	1.98	0.46
1:K:225:LEU:HD23	1:K:225:LEU:O	2.15	0.46
1:L:264:VAL:N	1:L:274:LEU:HD13	2.30	0.46
1:M:70:MET:HE2	1:N:142:ASN:OD1	2.16	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:P:152:ASP:O	1:P:153:SER:C	2.59	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:R:253:ILE:O	1:R:254:LYS:C	2.58	0.46
1:T:116:LEU:O	1:T:120:LEU:HG	2.15	0.46
1:W:116:LEU:HB3	1:W:264:VAL:HG21	1.97	0.46
1:W:133:SER:O	1:W:136:VAL:HG12	2.16	0.46
1:X:274:LEU:O	1:X:274:LEU:HG	2.16	0.46
1:J:47:LEU:C	1:J:47:LEU:HD12	2.40	0.46
1:M:225:LEU:HD23	1:M:225:LEU:O	2.15	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:OE1	1:P:161:GLU:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:70:MET:HE2	1:G:142:ASN:OD1	2.16	0.46
1:F:155:LEU:HD13	1:F:225:LEU:HD22	1.97	0.46
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:OE1	1:L:161:GLU:HA	2.16	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:U:253:ILE:O	1:U:254:LYS:C	2.59	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:A:253:ILE:O	1:A:254:LYS:C	2.58	0.46
1:B:225:LEU:HD23	1:B:225:LEU:O	2.15	0.46
1:B:268:ASP:C	1:B:270:MET:N	2.74	0.46
1:C:47:LEU:C	1:C:47:LEU:HD12	2.42	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:225:LEU:HD23	1:O:225:LEU:O	2.15	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:HD23	1:V:127:LEU:HA	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:E:93:LEU:HD11	1:F:262:PHE:CG	2.51	0.45
1:F:116:LEU:HB3	1:F:264:VAL:HG21	1.97	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:S:28:ASN:O	1:S:29:LYS:C	2.58	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:J:281:MET:HE2	2:J:304:EMC:C1	2.45	0.45
1:M:119:VAL:HG13	1:M:120:LEU:N	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:161:GLU:OE1	1:O:161:GLU:HA	2.15	0.45
1:P:93:LEU:HD11	1:Q:262:PHE:CG	2.52	0.45
1:Q:62:VAL:CG1	1:R:149:LEU:HD21	2.44	0.45
1:Q:70:MET:HE2	1:R:142:ASN:OD1	2.16	0.45
1:R:104:TYR:CE2	1:R:106:GLU:HA	2.51	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:HD23	1:V:225:LEU:O	2.16	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:27:TYR:CE2	1:F:183:ALA:HB2	2.52	0.45
1:E:155:LEU:HD13	1:E:225:LEU:HD22	1.98	0.45
1:H:170:VAL:HB	1:H:208:ILE:CD1	2.47	0.45
1:J:253:ILE:O	1:J:254:LYS:C	2.59	0.45
1:M:253:ILE:O	1:M:254:LYS:C	2.60	0.45
1:R:107:LYS:HA	1:R:107:LYS:HD3	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:I:124:ILE:HD11	1:I:258:GLU:HA	1.97	0.45
1:I:251:GLY:O	1:I:255:THR:HG23	2.17	0.45
1:I:271:LEU:HD23	1:I:272:SER:N	2.32	0.45
1:M:107:LYS:HD3	1:M:107:LYS:HA	1.72	0.45
1:N:47:LEU:HD12	1:N:47:LEU:C	2.42	0.45
1:S:104:TYR:CE2	1:S:106:GLU:HA	2.51	0.45
1:T:28:ASN:O	1:T:29:LYS:C	2.59	0.45
1:T:161:GLU:OE1	1:T:161:GLU:HA	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:HD23	1:A:116:LEU:HA	1.67	0.45
1:D:28:ASN:O	1:D:29:LYS:C	2.58	0.45
1:D:107:LYS:HD3	1:D:107:LYS:HA	1.74	0.45
1:D:274:LEU:O	1:D:274:LEU:HG	2.16	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:N:246:GLU:OE1	1:N:292:HIS:CD2	2.70	0.45
1:R:14:LYS:HB2	1:S:19:THR:OG1	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:116:LEU:O	1:R:120:LEU:HG	2.16	0.45
1:S:251:GLY:O	1:S:255:THR:HG23	2.16	0.45
1:S:253:ILE:O	1:S:254:LYS:C	2.60	0.45
1:S:264:VAL:HG23	1:S:274:LEU:CD1	2.41	0.45
1:V:28:ASN:O	1:V:29:LYS:C	2.59	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:124:ILE:HD11	1:D:258:GLU:HA	1.98	0.45
1:D:166:PHE:HE1	1:D:211:LEU:HB3	1.80	0.45
1:E:77:PHE:O	1:E:81:GLN:HB2	2.16	0.45
1:H:115:ILE:O	1:H:116:LEU:C	2.60	0.45
1:H:268:ASP:C	1:H:270:MET:N	2.74	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:I:218:VAL:HG12	1:I:219:GLN:N	2.31	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:77:PHE:O	1:S:81:GLN:HB2	2.17	0.45
1:S:246:GLU:OE1	1:S:292:HIS:HD2	1.97	0.45
1:T:104:TYR:HD1	1:T:270:MET:HG2	1.81	0.45
1:U:70:MET:HE2	1:V:142:ASN:OD1	2.16	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:E:70:MET:HE2	1:F:142:ASN:OD1	2.17	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: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:O	1:Q:274:LEU:HG	2.16	0.45
1:R:104:TYR:HE2	1:R:106:GLU:HA	1.80	0.45
1:X:253:ILE:O	1:X:254:LYS:C	2.58	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:L:253:ILE:O	1:L:254:LYS:C	2.58	0.45
1:P:77:PHE:O	1:P:81:GLN:HB2	2.17	0.45
1:V:47:LEU:C	1:V:47:LEU:HD12	2.42	0.45
1:W:62:VAL:HG12	1:X:149:LEU:CD2	2.44	0.45
1:B:283:ASN:O	1:B:284:THR:C	2.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:47:LEU:C	1:E:47:LEU:HD12	2.42	0.45
1:F:251:GLY:O	1:F:255:THR:HG23	2.16	0.45
1:H:104:TYR:HD1	1:H:270:MET:HG2	1.82	0.45
1:H:107:LYS:HA	1:H:107:LYS:HD3	1.73	0.45
1:I:104:TYR:HE2	1:I:106:GLU:HA	1.81	0.45
1:J:111:ALA:O	1:J:112:GLN:C	2.60	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:124:ILE:HD11	1:M:258:GLU:HA	1.99	0.45
1:M:127:LEU:HD23	1:M:127:LEU:HA	1.76	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:X:283:ASN:O	1:X:284:THR:C	2.60	0.45
1:D:157:ASN:OD1	1:D:157:ASN:C	2.60	0.45
1:D:170:VAL:HB	1:D:208:ILE:CD1	2.47	0.45
1:E:116:LEU:HB3	1:E:264:VAL:HG21	1.99	0.45
1:H:28:ASN:O	1:H:29:LYS:C	2.60	0.45
1:H:116:LEU:O	1:H:120:LEU:HG	2.17	0.45
1:M:47:LEU:C	1:M:47:LEU:HD12	2.42	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:47:LEU:C	1:P:47:LEU:HD12	2.41	0.45
1:P:116:LEU:HB3	1:P:264:VAL:HG21	1.98	0.45
1:P:268:ASP:C	1:P:270:MET:N	2.75	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: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:H:66:LYS:O	1:H:67:THR:C	2.61	0.44
1:J:104:TYR:HD1	1:J:270:MET:HG2	1.82	0.44
1:L:28:ASN:O	1:L:29:LYS:C	2.60	0.44
1:M:161:GLU:OE1	1:M:161:GLU:HA	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:161:GLU:OE1	1:S:161:GLU:HA	2.16	0.44
1:T:253:ILE:O	1:T:254:LYS:C	2.59	0.44
1:X:264:VAL:N	1:X:274:LEU:HD13	2.32	0.44
1:A:268:ASP:C	1:A:270:MET:N	2.75	0.44
1:B:46:GLU:O	1:B:46:GLU:HG3	2.17	0.44
1:C:66:LYS:O	1:C:67:THR:C	2.60	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:111:ALA:O	1:B:112:GLN:C	2.61	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: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
1:I:104:TYR:CE2	1:I:106:GLU:HA	2.52	0.44
1:I:116:LEU:HA	1:I:116:LEU:HD23	1.71	0.44
1:K:111:ALA:O	1:K:112:GLN:C	2.61	0.44
1:N:124:ILE:HD11	1:N:258:GLU:HA	1.99	0.44
1:X:28:ASN:O	1:X:29:LYS:C	2.60	0.44
1:A:274:LEU:O	1:A:274:LEU:HG	2.18	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:J:127:LEU:HD23	1:J:127:LEU:HA	1.74	0.44
1:M:264:VAL:N	1:M:274:LEU:HD13	2.32	0.44
1:M:268:ASP:C	1:M:270:MET:N	2.76	0.44
1:O:47:LEU:C	1:O:47:LEU:HD12	2.43	0.44
1:P:28:ASN:O	1:P:29:LYS:C	2.60	0.44
1:R:53:GLU:O	1:R:56:GLN:HB3	2.17	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:S:116:LEU:O	1:S:120:LEU:HG	2.16	0.44
1:T:53:GLU:O	1:T:56:GLN:HB3	2.17	0.44
1:V:268:ASP:C	1:V:270:MET:N	2.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:W:225:LEU:C	1:W:225:LEU:CD2	2.91	0.44
1:X:225:LEU:C	1:X:225:LEU:CD2	2.89	0.44
1:A:17:ILE:CG2	1:A:18:GLU:N	2.81	0.44
1:A:116:LEU:HB3	1:A:264:VAL:HG21	1.98	0.44
1:C:62:VAL:HG12	1:D:149:LEU:CD2	2.45	0.44
1:C:225:LEU:HD23	1:C:225:LEU:O	2.16	0.44
1:C:253:ILE:O	1:C:254:LYS:C	2.59	0.44
1:D:104:TYR:CE2	1:D:106:GLU:HA	2.53	0.44
1:G:268:ASP:C	1:G:270:MET:N	2.75	0.44
1:I:53:GLU:O	1:I:56:GLN:HB3	2.18	0.44
1:I:127:LEU:HD23	1:I:127:LEU:HA	1.76	0.44
1:L:116:LEU:HD23	1:L:116:LEU:HA	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:C:264:VAL:HG23	1:C:274:LEU:CD1	2.43	0.44
1:D:152:ASP:O	1:D:153:SER:C	2.58	0.44
1:G:115:ILE:O	1:G:116:LEU:C	2.60	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:218:VAL:HG12	1:P:219:GLN:N	2.31	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:28:ASN:O	1:G:29:LYS:C	2.59	0.44
1:G:111:ALA:O	1:G:112:GLN:C	2.61	0.44
1:G:271:LEU:HD22	1:G:273:LEU:H	1.82	0.44
1:H:152:ASP:O	1:H:153:SER:C	2.59	0.44
1:H:271:LEU:HD22	1:H:273:LEU:H	1.83	0.44
1:N:268:ASP:C	1:N:270:MET:N	2.76	0.44
1:O:157:ASN:OD1	1:O:157:ASN:C	2.61	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:37:TRP:HE1	1:Q:172:LYS:HZ3	1.65	0.44
1:P:208:ILE:N	1:P:209:PRO:CD	2.81	0.44
1:Q:116:LEU:HD23	1:Q:116:LEU:HA	1.66	0.44
1:T:66:LYS:O	1:T:67:THR:C	2.60	0.44
1:T:77:PHE:O	1:T:81:GLN:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:208:ILE:HD13	1:V:208:ILE:HA	1.83	0.44
1:W:78:GLU:HB2	1:X:135:LEU:HD21	2.00	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:283:ASN:O	1:W:284:THR:C	2.61	0.44
1:B:108:LYS:HE3	1:C:268:ASP:HB2	2.00	0.44
1:B:157:ASN:OD1	1:B:157:ASN:C	2.61	0.44
1:I:107:LYS:HD3	1:I:107:LYS:HA	1.73	0.44
1:I:253:ILE:O	1:I:254:LYS:C	2.60	0.44
1:M:53:GLU:O	1:M:56:GLN:HB3	2.17	0.44
1:N:65:ILE:HD13	1:N:144:ALA:HB1	1.99	0.44
1:N:155:LEU:HD13	1:N:225:LEU:HD22	1.99	0.44
1:O:66:LYS:O	1:O:67:THR:C	2.60	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:F:93:LEU:HD11	1:G:262:PHE:CG	2.52	0.44
1:G:251:GLY:O	1:G:255:THR:HG23	2.18	0.44
1:G:274:LEU:O	1:G:274:LEU:HG	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:K:37:TRP:CZ3	1:L:175:LYS:HG3	2.53	0.44
1:L:107:LYS:HD3	1:L:107:LYS:HA	1.74	0.44
1:L:271:LEU:HD22	1:L:273:LEU:H	1.83	0.44
1:M:66:LYS:O	1:M:67:THR:C	2.60	0.44
1:P:253:ILE:O	1:P:254:LYS:C	2.60	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:X:66:LYS:O	1:X:67:THR:C	2.60	0.44
1:B:246:GLU:OE1	1:B:292:HIS:CD2	2.71	0.43
1:C:28:ASN:O	1:C:29:LYS:C	2.61	0.43
1:C:77:PHE:O	1:C:81:GLN:HB2	2.18	0.43
1:E:66:LYS:O	1:E:67:THR:C	2.61	0.43
1:E:111:ALA:O	1:E:112:GLN:C	2.60	0.43
1:M:262:PHE:CD1	1:X:93:LEU:HD11	2.53	0.43
1:R:268:ASP:C	1:R:270:MET:N	2.76	0.43
1:T:218:VAL:HG12	1:T:219:GLN:N	2.33	0.43
1:U:47:LEU:C	1:U:47:LEU:HD12	2.43	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:A:124:ILE:HD11	1:A:258:GLU:HA	1.99	0.43
1:B:37:TRP:HE1	1:C:172:LYS:HZ3	1.65	0.43
1:F:271:LEU:HD22	1:F:273:LEU:H	1.82	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:HD23	1:T:225:LEU:O	2.17	0.43
1:V:116:LEU:HB3	1:V:264:VAL:HG21	2.00	0.43
1:V:157:ASN:OD1	1:V:157:ASN:C	2.61	0.43
1:W:268:ASP:C	1:W:270:MET:N	2.76	0.43
1:X:127:LEU:HD23	1:X:127:LEU:HA	1.77	0.43
1:C:268:ASP:C	1:C:270:MET:N	2.75	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:O:62:VAL:CG1	1:P:149:LEU:HD21	2.45	0.43
1:P:133:SER:O	1:P:136:VAL:HG12	2.18	0.43
1:Q:157:ASN:C	1:Q:157:ASN:OD1	2.61	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: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:A:104:TYR:HD1	1:A:270:MET:HG2	1.84	0.43
1:B:292:HIS:C	1:B:292:HIS:ND1	2.76	0.43
1:D:116:LEU:HD23	1:D:116:LEU:HA	1.69	0.43
1:F:268:ASP:C	1:F:270:MET:N	2.77	0.43
1:G:62:VAL:CG1	1:H:149:LEU:HD21	2.43	0.43
1:G:170:VAL:HB	1:G:208:ILE:CD1	2.48	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:M:136:VAL:CG1	1:M:137:SER:N	2.79	0.43
1:P:111:ALA:O	1:P:112:GLN:C	2.60	0.43
1:P:208:ILE:HD13	1:P:208:ILE:HA	1.82	0.43
1:S:65:ILE:HD13	1:S:144:ALA:HB1	2.00	0.43
1:S:104:TYR:HD1	1:S:270:MET:HG2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:268:ASP:C	1:J:270:MET:N	2.76	0.43
1:J:271:LEU:HD22	1:J:273:LEU:H	1.84	0.43
1:K:66:LYS:O	1:K:67:THR:C	2.62	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:O	1:P:46:GLU:HG3	2.19	0.43
1:Q:124:ILE:HD11	1:Q:258:GLU:HA	2.01	0.43
1:T:47:LEU:C	1:T:47:LEU:HD12	2.43	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:B:47:LEU:C	1:B:47:LEU:HD12	2.44	0.43
1:E:104:TYR:HD1	1:E:270:MET:HG2	1.83	0.43
1:E:127:LEU:HD23	1:E:127:LEU:HA	1.78	0.43
1:J:225:LEU:HD23	1:J:225:LEU:O	2.17	0.43
1:K:107:LYS:HA	1:K:107:LYS:HD3	1.72	0.43
1:Q:66:LYS:O	1:Q:67:THR:C	2.61	0.43
1:Q:268:ASP:C	1:Q:270:MET:N	2.75	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:27:TYR:CE2	1:E:183:ALA:HB2	2.54	0.43
1:D:269:LEU:HD23	1:D:269:LEU:HA	1.87	0.43
1:F:253:ILE:O	1:F:254:LYS:C	2.61	0.43
1:I:43:THR:HG1	1:I:169:GLN:HG2	1.78	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:Q:152:ASP:O	1:Q:153:SER:C	2.62	0.43
1:T:17:ILE:CG2	1:T:18:GLU:N	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:157:ASN:OD1	1:W:157:ASN:C	2.62	0.43
1:A:53:GLU:O	1:A:56:GLN:HB3	2.19	0.43
1:C:225:LEU:C	1:C:225:LEU:CD2	2.91	0.43
1:G:53:GLU:O	1:G:56:GLN:HB3	2.18	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:T:111:ALA:O	1:T:112:GLN:C	2.62	0.43
1:X:47:LEU:C	1:X:47:LEU:HD12	2.44	0.43
1:E:157:ASN:OD1	1:E:157:ASN:C	2.61	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: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:152:ASP:O	1:I:153:SER:C	2.62	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:HA	1:K:269:LEU:HD23	1.85	0.43
1:M:268:ASP:HB2	1:X:108:LYS:HE3	2.00	0.43
1:R:17:ILE:CG2	1:R:18:GLU:N	2.81	0.43
1:R:46:GLU:O	1:R:46:GLU:HG3	2.19	0.43
1:T:17:ILE:HG22	1:T:18:GLU:N	2.34	0.43
1:T:104:TYR:HE2	1:T:106:GLU:HA	1.83	0.43
1:V:246:GLU:OE1	1:V:292:HIS:CD2	2.72	0.43
1:V:253:ILE:O	1:V:254:LYS:C	2.62	0.43
1:B:28:ASN:O	1:B:29:LYS:C	2.60	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:124:ILE:CD1	1:F:258:GLU:HA	2.49	0.43
1:F:225:LEU:HD23	1:F:225:LEU:O	2.19	0.43
1:G:47:LEU:C	1:G:47:LEU:HD12	2.44	0.43
1:J:78:GLU:HB2	1:K:135:LEU:HD21	2.01	0.43
1:K:281:MET:HE2	2:K:304:EMC:C1	2.49	0.43
1:N:157:ASN:OD1	1:N:157:ASN:C	2.62	0.43
1:N:251:GLY:O	1:N:255:THR:HG23	2.19	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:T:268:ASP:C	1:T:270:MET:N	2.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:111:ALA:O	1:D:112:GLN:C	2.60	0.42
1:K:47:LEU:C	1:K:47:LEU:HD12	2.44	0.42
1:M:28:ASN:O	1:M:29:LYS:C	2.61	0.42
1:N:65:ILE:CD1	1:N:144:ALA:HB1	2.49	0.42
1:P:225:LEU:C	1:P:225:LEU:CD2	2.92	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:66:LYS:O	1:B:67:THR:C	2.61	0.42
1:C:157:ASN:C	1:C:157:ASN:OD1	2.61	0.42
1:D:47:LEU:C	1:D:47:LEU:HD12	2.44	0.42
1:E:53:GLU:O	1:E:56:GLN:HB3	2.19	0.42
1:G:225:LEU:C	1:G:225:LEU:CD2	2.90	0.42
1:L:53:GLU:O	1:L:56:GLN:HB3	2.19	0.42
1:P:157:ASN:OD1	1:P:157:ASN:C	2.62	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:X:268:ASP:C	1:X:270:MET:N	2.76	0.42
1:A:152:ASP:O	1:A:153:SER:C	2.63	0.42
1:B:17:ILE:HG22	1:B:18:GLU:N	2.34	0.42
1:C:46:GLU:O	1:C:46:GLU:HG3	2.19	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
1:N:225:LEU:C	1:N:225:LEU:CD2	2.92	0.42
1:P:116:LEU:HD23	1:P:116:LEU:HA	1.67	0.42
1:Q:225:LEU:C	1:Q:225:LEU:CD2	2.91	0.42
1:R:108:LYS:HE3	1:S:268:ASP:HB2	2.02	0.42
1:T:157:ASN:OD1	1:T:157:ASN:C	2.63	0.42
1:W:119:VAL:CG1	1:W:120:LEU:N	2.83	0.42
1:E:115:ILE:O	1:E:116:LEU:C	2.63	0.42
1:F:157:ASN:OD1	1:F:157:ASN:C	2.62	0.42
1:F:208:ILE:HB	1:F:209:PRO:HD3	2.00	0.42
1:J:66:LYS:O	1:J:67:THR:C	2.61	0.42
1:J:157:ASN:OD1	1:J:157:ASN:C	2.61	0.42
1:L:47:LEU:C	1:L:47:LEU:HD12	2.44	0.42
1:M:65:ILE:HD13	1:M:144:ALA:HB1	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:116:LEU:HA	1:O:116:LEU:HD23	1.69	0.42
1:Q:115:ILE:O	1:Q:116:LEU:C	2.62	0.42
1:Q:208:ILE:N	1:Q:209:PRO:CD	2.83	0.42
1:R:37:TRP:CZ3	1:S:175:LYS:HG3	2.55	0.42
1:R:69:LEU:HD23	1:R:141:PHE:CE1	2.54	0.42
1:U:65:ILE:HD13	1:U:144:ALA:HB1	2.01	0.42
1:V:281:MET:HE2	2:V:304:EMC:C1	2.49	0.42
1:W:47:LEU:C	1:W:47:LEU:HD12	2.44	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:G:70:MET:HE2	1:H:142:ASN:OD1	2.19	0.42
1:H:47:LEU:C	1:H:47:LEU:HD12	2.44	0.42
1:H:111:ALA:O	1:H:112:GLN:C	2.63	0.42
1:I:47:LEU:C	1:I:47:LEU:HD12	2.45	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:28:ASN:O	1:R:29:LYS:C	2.62	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:53:GLU:O	1:S:56:GLN:HB3	2.19	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:W:69:LEU:HD23	1:W:141:PHE:CZ	2.54	0.42
1:W:116:LEU:HA	1:W:116:LEU:HD23	1.72	0.42
1:X:133:SER:O	1:X:136:VAL:HG12	2.19	0.42
1:A:127:LEU:HD23	1:A:127:LEU:HA	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:O:152:ASP:O	1:O:153:SER:C	2.62	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:66:LYS:O	1:R:67:THR:C	2.62	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:HD23	1:S:269:LEU:HA	1.86	0.42
1:T:170:VAL:HB	1:T:208:ILE:CD1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:124:ILE:CD1	1:U:258:GLU:HA	2.49	0.42
1:U:218:VAL:HG12	1:U:219:GLN:N	2.33	0.42
1:W:66:LYS:O	1:W:67:THR:C	2.63	0.42
1:X:39:THR:HG21	1:X:173:ILE:HG12	2.00	0.42
1:A:269:LEU:HD23	1:A:269:LEU:HA	1.89	0.42
1:B:53:GLU:O	1:B:56:GLN:HB3	2.20	0.42
1:B:271:LEU:HD23	1:B:272:SER:N	2.35	0.42
1:C:65:ILE:HD13	1:C:144:ALA:HB1	2.02	0.42
1:G:66:LYS:O	1:G:67:THR:C	2.63	0.42
1:H:225:LEU:C	1:H:225:LEU:CD2	2.89	0.42
1:I:208:ILE:HD13	1:I:208:ILE:HA	1.81	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:P:283:ASN:O	1:P:284:THR:C	2.62	0.42
1:S:69:LEU:HD23	1:S:141:PHE:CZ	2.55	0.42
1:U:53:GLU:O	1:U:56:GLN:HB3	2.20	0.42
1:U:133:SER:O	1:U:136:VAL:HG12	2.20	0.42
1:V:50:PHE:C	1:V:50:PHE:CD2	2.98	0.42
1:X:17:ILE:CG2	1:X:18:GLU:N	2.82	0.42
1:X:184:GLY:O	1:X:187:ALA:O	2.38	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: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:R:47:LEU:C	1:R:47:LEU:HD12	2.44	0.42
1:T:50:PHE:C	1:T:50:PHE:CD2	2.97	0.42
1:T:124:ILE:HD11	1:T:258:GLU:HA	2.02	0.42
1:T:180:GLY:O	1:T:183:ALA:HB3	2.19	0.42
1:U:208:ILE:N	1:U:209:PRO:CD	2.82	0.42
1:A:218:VAL:HG12	1:A:219:GLN:N	2.33	0.42
1:B:127:LEU:HD23	1:B:127:LEU:HA	1.81	0.42
1:C:256:GLU:HA	1:C:256:GLU:OE1	2.20	0.42
1:D:115:ILE:O	1:D:116:LEU:C	2.63	0.42
1:E:225:LEU:HD23	1:E:225:LEU:O	2.19	0.42
1:H:136:VAL:CG1	1:H:137:SER:N	2.83	0.42
1:I:66:LYS:O	1:I:67:THR:C	2.62	0.42
1:J:225:LEU:C	1:J:225:LEU:CD2	2.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:P:66:LYS:O	1:P:67:THR:C	2.62	0.42
1:Q:180:GLY:O	1:Q:183:ALA:HB3	2.20	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:111:ALA:O	1:V:112:GLN:C	2.62	0.42
1:V:170:VAL:HB	1:V:208:ILE:CD1	2.50	0.42
1:W:28:ASN:O	1:W:29:LYS:C	2.62	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:B:136:VAL:CG1	1:B:137:SER:N	2.81	0.42
1:C:78:GLU:HB2	1:D:135:LEU:HD21	2.02	0.42
1:C:208:ILE:HB	1:C:209:PRO:HD3	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:HD23	1:H:127:LEU:HA	1.79	0.42
1:I:208:ILE:N	1:I:209:PRO:CD	2.82	0.42
1:I:225:LEU:C	1:I:225:LEU:CD2	2.88	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:L:157:ASN:OD1	1:L:157:ASN:C	2.62	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:111:ALA:O	1:U:112:GLN:C	2.62	0.42
1:U:246:GLU:OE1	1:U:292:HIS:CD2	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:65:ILE:HD13	1:D:144:ALA:HB1	2.02	0.41
1:D:66:LYS:O	1:D:67:THR:C	2.63	0.41
1:D:208:ILE:HB	1:D:209:PRO:HD3	2.02	0.41
1:F:225:LEU:C	1:F:225:LEU:CD2	2.93	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:53:GLU:O	1:H:56:GLN:HB3	2.20	0.41
1:H:124:ILE:HD11	1:H:258:GLU:HA	2.01	0.41
1:I:184:GLY:O	1:I:187:ALA:O	2.38	0.41
1:M:243:LEU:HD23	1:M:243:LEU:HA	1.91	0.41
1:N:136:VAL:CG1	1:N:137:SER:N	2.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:157:ASN:OD1	1:R:157:ASN:C	2.63	0.41
1:S:66:LYS:O	1:S:67:THR:C	2.61	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:C:283:ASN:O	1:C:284:THR:C	2.63	0.41
1:D:50:PHE:CD2	1:D:50:PHE:C	2.98	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:HD23	1:G:243:LEU:HA	1.93	0.41
1:H:46:GLU:O	1:H:46:GLU:HG3	2.20	0.41
1:H:72:SER:O	1:H:73:GLN:C	2.64	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:I:134:LEU:HD22	1:I:243:LEU:CD2	2.51	0.41
1:L:90:ALA:O	1:L:94:LEU:HD22	2.20	0.41
1:L:268:ASP:C	1:L:270:MET:N	2.76	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:W:93:LEU:HD11	1:X:262:PHE:CG	2.55	0.41
1:X:134:LEU:HD22	1:X:243:LEU:CD2	2.50	0.41
1:A:184:GLY:O	1:A:187:ALA:O	2.39	0.41
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:37:TRP:HE1	1:D:172:LYS:HZ3	1.68	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:E:50:PHE:CD2	1:E:50:PHE:C	2.99	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: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:O	1:L:46:GLU:HG3	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:P:208:ILE:HB	1:P:209:PRO:HD3	2.03	0.41
1:Q:111:ALA:O	1:Q:112:GLN:C	2.62	0.41
1:S:268:ASP:C	1:S:270:MET:N	2.78	0.41
1:V:124:ILE:CD1	1:V:258:GLU:HA	2.50	0.41
1:V:184:GLY:O	1:V:187:ALA:O	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:107:LYS:HD3	1:C:107:LYS:HA	1.74	0.41
1:C:111:ALA:O	1:C:112:GLN:C	2.64	0.41
1:D:268:ASP:C	1:D:270:MET:N	2.77	0.41
1:E:124:ILE:HD11	1:E:258:GLU:HA	2.02	0.41
1:G:37:TRP:HE1	1:H:172:LYS:HZ3	1.68	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:I:23:ALA:O	1:I:24:LEU:C	2.63	0.41
1:I:157:ASN:OD1	1:I:157:ASN:C	2.63	0.41
1:K:157:ASN:OD1	1:K:157:ASN:C	2.63	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:N:283:ASN:O	1:N:284:THR:C	2.63	0.41
1:O:133:SER:O	1:O:136:VAL:HG12	2.20	0.41
1:P:27:TYR:CE2	1:Q:183:ALA:HB2	2.55	0.41
1:P:50:PHE:CD2	1:P:50:PHE:C	2.98	0.41
1:P:124:ILE:CD1	1:P:258:GLU:HA	2.49	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: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:A:66:LYS:O	1:A:67:THR:C	2.63	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:C:210:GLU:HA	1:C:210:GLU:OE2	2.21	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
1:F:111:ALA:O	1:F:112:GLN:C	2.64	0.41
1:G:46:GLU:HA	1:G:49:ARG:NH1	2.36	0.41
1:G:157:ASN:OD1	1:G:157:ASN:C	2.63	0.41
1:H:86:TRP:O	1:H:88:GLY:N	2.53	0.41
1:H:208:ILE:N	1:H:209:PRO:CD	2.83	0.41
1:J:116:LEU:HD23	1:J:116:LEU:HA	1.70	0.41
1:K:46:GLU:O	1:K:46:GLU:HG3	2.18	0.41
1:K:180:GLY:O	1:K:183:ALA:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:17:ILE:HG22	1:P:18:GLU:N	2.35	0.41
1:Q:283:ASN:O	1:Q:284:THR:C	2.63	0.41
1:S:50:PHE:CD2	1:S:50:PHE:C	2.99	0.41
1:S:94:LEU:O	1:S:98:ILE:HG12	2.21	0.41
1:U:157:ASN:OD1	1:U:157:ASN:C	2.63	0.41
1:W:50:PHE:CD2	1:W:50:PHE:C	2.99	0.41
1:X:104:TYR:HD1	1:X:270:MET:HG2	1.84	0.41
1:X:117:ILE:O	1:X:121:ASP:HB2	2.21	0.41
1:A:106:GLU:O	1:A:106:GLU:HG2	2.20	0.41
1:A:271:LEU:HD22	1:A:273:LEU:H	1.85	0.41
1:B:104:TYR:HD1	1:B:270:MET:HG2	1.86	0.41
1:B:165:TYR:O	1:B:169:GLN:HB2	2.20	0.41
1:D:210:GLU:HA	1:D:210:GLU:OE2	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:111:ALA:O	1:I:112:GLN:C	2.63	0.41
1:I:269:LEU:HD23	1:I:269:LEU:HA	1.88	0.41
1:J:14:LYS:HB2	1:K:19:THR:OG1	2.20	0.41
1:J:136:VAL:CG1	1:J:137:SER:N	2.81	0.41
1:K:37:TRP:HE1	1:L:172:LYS:NZ	2.19	0.41
1:K:225:LEU:C	1:K:225:LEU:CD2	2.92	0.41
1:L:17:ILE:HG22	1:L:18:GLU:N	2.35	0.41
1:L:50:PHE:CD2	1:L:50:PHE:C	2.98	0.41
1:L:180:GLY:O	1:L:183:ALA:HB3	2.20	0.41
1:M:111:ALA:O	1:M:112:GLN:C	2.63	0.41
1:M:208:ILE:N	1:M:209:PRO:CD	2.83	0.41
1:O:111:ALA:O	1:O:112:GLN:C	2.63	0.41
1:Q:50:PHE:CD2	1:Q:50:PHE:C	2.98	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:V:225:LEU:C	1:V:225:LEU:CD2	2.92	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:A:225:LEU:C	1:A:225:LEU:CD2	2.90	0.41
1:B:72:SER:O	1:B:73:GLN:C	2.63	0.41
1:B:225:LEU:C	1:B:225:LEU:CD2	2.91	0.41
1:C:208:ILE:HD13	1:C:208:ILE:HA	1.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD13	1:H:208:ILE:HA	1.81	0.41
1:H:283:ASN:O	1:H:284:THR:C	2.64	0.41
1:K:50:PHE:CD2	1:K:50:PHE:C	2.98	0.41
1:L:208:ILE:N	1:L:209:PRO:CD	2.83	0.41
1:O:28:ASN:O	1:O:29:LYS:C	2.62	0.41
1:R:111:ALA:O	1:R:112:GLN:C	2.64	0.41
1:S:157:ASN:OD1	1:S:157:ASN:C	2.64	0.41
1:S:180:GLY:O	1:S:183:ALA:HB3	2.20	0.41
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:O	1:X:46:GLU:HG3	2.20	0.41
1:D:62:VAL:CG1	1:E:149:LEU:HD21	2.47	0.41
1:D:180:GLY:O	1:D:183:ALA:HB3	2.21	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: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:N:28:ASN:O	1:N:29:LYS:C	2.64	0.41
1:N:66:LYS:O	1:N:67:THR:C	2.62	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:152:ASP:O	1:R:153:SER:C	2.63	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:47:LEU:C	1:A:47:LEU:HD12	2.45	0.41
1:A:133:SER:O	1:A:136:VAL:HG12	2.21	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:C:281:MET:HE2	2:C:304:EMC:C1	2.51	0.41
1:D:165:TYR:O	1:D:169:GLN:HB2	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: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:63:GLY:HA2	1:H:149:LEU:HD22	2.01	0.41
1:G:69:LEU:HD23	1:G:141:PHE:CZ	2.55	0.41
1:H:65:ILE:HD13	1:H:144:ALA:HB1	2.02	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:H:184:GLY:O	1:H:187:ALA:O	2.38	0.41
1:I:283:ASN:O	1:I:284:THR:C	2.64	0.41
1:J:165:TYR:O	1:J:169:GLN:HB2	2.21	0.41
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:119:VAL:CG1	1:Q:120:LEU:N	2.84	0.41
1:Q:271:LEU:HD22	1:Q:273:LEU:H	1.85	0.41
1:Q:281:MET:HE2	2:Q:304:EMC:C1	2.51	0.41
1:Q:292:HIS:ND1	1:Q:292:HIS:C	2.78	0.41
1:R:65:ILE:HD13	1:R:144:ALA:HB1	2.03	0.41
1:R:104:TYR:HD1	1:R:270:MET:CG	2.34	0.41
1:R:281:MET:HE2	2:R:304:EMC:C1	2.50	0.41
1:T:46:GLU:O	1:T:46:GLU:HG3	2.20	0.41
1:T:46:GLU:HA	1:T:49:ARG:NH1	2.36	0.41
1:T:65:ILE:HD13	1:T:144:ALA:HB1	2.02	0.41
1:T:271:LEU:HD23	1:T:272:SER:N	2.35	0.41
1:U:66:LYS:O	1:U:67:THR:C	2.63	0.41
1:U:210:GLU:HA	1:U:210:GLU:OE2	2.21	0.41
1:U:268:ASP:C	1:U:270:MET:N	2.78	0.41
1:U:269:LEU:HD23	1:U:269:LEU:HA	1.86	0.41
1:V:243:LEU:HD23	1:V:243:LEU:HA	1.94	0.41
1:W:184:GLY:O	1:W:187:ALA:O	2.39	0.41
1:W:274:LEU:O	1:W:274:LEU:HG	2.19	0.41
1:X:243:LEU:HD23	1:X:243:LEU:HA	1.90	0.41
1:B:39:THR:HG21	1:B:173:ILE:HG12	2.03	0.41
1:C:94:LEU:O	1:C:98:ILE:HG12	2.21	0.41
1:C:116:LEU:HD23	1:C:116:LEU:HA	1.73	0.41
1:D:17:ILE:CG2	1:D:18:GLU:N	2.84	0.41
1:D:46:GLU:O	1:D:46:GLU:HG3	2.21	0.41
1:E:133:SER:O	1:E:136:VAL:HG12	2.21	0.41
1:E:210:GLU:HA	1:E:210:GLU:OE2	2.21	0.41
1:E:269:LEU:HA	1:E:269:LEU:HD23	1.84	0.41
1:F:218:VAL:HG12	1:F:219:GLN:N	2.36	0.41
1:G:152:ASP:O	1:G:153:SER:C	2.62	0.41
1:I:39:THR:HG21	1:I:173:ILE:HG12	2.02	0.41
1:I:136:VAL:CG1	1:I:137:SER:N	2.82	0.41
1:I:180:GLY:O	1:I:183:ALA:HB3	2.20	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:O:65:ILE:HD13	1:O:144:ALA:HB1	2.02	0.41
1:P:72:SER:O	1:P:73:GLN:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:X:57:ALA:O	1:X:60:VAL:HG12	2.20	0.41
1:X:152:ASP:O	1:X:153:SER:C	2.64	0.41
1:B:17:ILE:CG2	1:B:18:GLU:N	2.81	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:B:274:LEU:O	1:B:274:LEU:HG	2.21	0.40
1:D:17:ILE:HG22	1:D:18:GLU:N	2.36	0.40
1:E:69:LEU:HD23	1:E:141:PHE:CZ	2.56	0.40
1:E:271:LEU:HD22	1:E:273:LEU:H	1.85	0.40
1:F:65:ILE:HD13	1:F:144:ALA:HB1	2.03	0.40
1:F:180:GLY:O	1:F:183:ALA:HB3	2.21	0.40
1:G:54:TYR:O	1:G:55:SER:C	2.64	0.40
1:G:253:ILE:O	1:G:254:LYS:C	2.62	0.40
1:I:46:GLU:HA	1:I:49:ARG:NH1	2.36	0.40
1:I:268:ASP:C	1:I:270:MET:N	2.77	0.40
1:L:111:ALA:O	1:L:112:GLN:C	2.64	0.40
1:P:17:ILE:CG2	1:P:18:GLU:N	2.83	0.40
1:Q:127:LEU:HD23	1:Q:127:LEU:HA	1.78	0.40
1:Q:243:LEU:HD23	1:Q:243:LEU:HA	1.94	0.40
1:S:46:GLU:HA	1:S:49:ARG:NH1	2.37	0.40
1:T:210:GLU:HA	1:T:210:GLU:OE2	2.21	0.40
1:U:39:THR:HG21	1:U:173:ILE:HG12	2.03	0.40
1:U:127:LEU:HD23	1:U:127:LEU:HA	1.79	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:A:172:LYS:NZ	1:L:37:TRP:HE1	2.19	0.40
1:D:69:LEU:HD23	1:D:141:PHE:CZ	2.56	0.40
1:G:17:ILE:CG2	1:G:18:GLU:N	2.82	0.40
1:G:65:ILE:HD13	1:G:144:ALA:HB1	2.02	0.40
1:J:152:ASP:O	1:J:153:SER:C	2.64	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:M:157:ASN:OD1	1:M:157:ASN:C	2.64	0.40
1:Q:47:LEU:C	1:Q:47:LEU:HD12	2.46	0.40
1:Q:208:ILE:HB	1:Q:209:PRO:HD3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:134:LEU:HD22	1:R:243:LEU:CD2	2.51	0.40
1:S:37:TRP:HE1	1:T:172:LYS:NZ	2.19	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:V:152:ASP:O	1:V:153:SER:C	2.63	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:B:152:ASP:O	1:B:153:SER:C	2.64	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:39:THR:HG21	1:E:173:ILE:HG12	2.02	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:H:208:ILE:HB	1:H:209:PRO:HD3	2.02	0.40
1:H:222:PHE:CD2	1:H:222:PHE:C	2.98	0.40
1:I:72:SER:O	1:I:73:GLN:C	2.64	0.40
1:L:256:GLU:OE1	1:L:256:GLU:HA	2.21	0.40
1:M:78:GLU:CG	1:N:135:LEU:HD21	2.51	0.40
1:O:283:ASN:O	1:O:284:THR:C	2.63	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
1:A:157:ASN:OD1	1:A:157:ASN:C	2.64	0.40
1:B:115:ILE:O	1:B:116:LEU:C	2.63	0.40
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:F:165:TYR:O	1:F:169:GLN:HB2	2.21	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:N:111:ALA:O	1:N:112:GLN:C	2.64	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:U:50:PHE:CD2	1:U:50:PHE:C	2.99	0.40
1:V:241:LEU:O	1:V:242:LYS:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:65:ILE:CD1	1:X:144:ALA:HB1	2.51	0.40
1:X:271:LEU:HD23	1:X:272:SER:N	2.37	0.40
1:A:28:ASN:O	1:A:29:LYS:C	2.65	0.40
1:A:69:LEU:HD23	1:A:141:PHE:CZ	2.56	0.40
1:C:50:PHE:CD2	1:C:50:PHE:C	3.00	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:G:281:MET:HE2	1:G:281:MET:HB3	2.00	0.40
1:H:65:ILE:CD1	1:H:144:ALA:HB1	2.52	0.40
1:L:69:LEU:HD23	1:L:141:PHE:CZ	2.56	0.40
1:L:269:LEU:HA	1:L:269:LEU:HD23	1.90	0.40
1:L:281:MET:HE2	2:L:304:EMC:C1	2.52	0.40
1:M:271:LEU:HD22	1:M:273:LEU:H	1.87	0.40
1:N:46:GLU:O	1:N:46:GLU:HG3	2.19	0.40
1:N:208:ILE:HD13	1:N:208:ILE:HA	1.81	0.40
1:O:46:GLU:HA	1:O:49:ARG:NH1	2.37	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:Q:17:ILE:HG22	1:Q:18:GLU:N	2.37	0.40
1:Q:39:THR:O	1:Q:43:THR:HB	2.21	0.40
1:Q:256:GLU:OE1	1:Q:256:GLU:HA	2.22	0.40
1:R:116:LEU:HD23	1:R:116:LEU:HA	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
1:X:111:ALA:O	1:X:112:GLN:C	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	283/309 (92%)	242 (86%)	40 (14%)	1 (0%)	30	60
1	B	283/309 (92%)	247 (87%)	34 (12%)	2 (1%)	18	49
1	C	283/309 (92%)	246 (87%)	35 (12%)	2 (1%)	18	49
1	D	283/309 (92%)	243 (86%)	39 (14%)	1 (0%)	30	60
1	E	283/309 (92%)	243 (86%)	38 (13%)	2 (1%)	18	49
1	F	283/309 (92%)	248 (88%)	34 (12%)	1 (0%)	30	60
1	G	283/309 (92%)	241 (85%)	41 (14%)	1 (0%)	30	60
1	H	283/309 (92%)	244 (86%)	38 (13%)	1 (0%)	30	60
1	I	283/309 (92%)	241 (85%)	41 (14%)	1 (0%)	30	60
1	J	283/309 (92%)	243 (86%)	39 (14%)	1 (0%)	30	60
1	K	283/309 (92%)	243 (86%)	39 (14%)	1 (0%)	30	60
1	L	283/309 (92%)	243 (86%)	39 (14%)	1 (0%)	30	60
1	M	283/309 (92%)	242 (86%)	40 (14%)	1 (0%)	30	60
1	N	283/309 (92%)	243 (86%)	39 (14%)	1 (0%)	30	60
1	O	283/309 (92%)	242 (86%)	40 (14%)	1 (0%)	30	60
1	P	283/309 (92%)	246 (87%)	36 (13%)	1 (0%)	30	60
1	Q	283/309 (92%)	243 (86%)	39 (14%)	1 (0%)	30	60
1	R	283/309 (92%)	240 (85%)	42 (15%)	1 (0%)	30	60
1	S	283/309 (92%)	242 (86%)	40 (14%)	1 (0%)	30	60
1	T	283/309 (92%)	245 (87%)	37 (13%)	1 (0%)	30	60
1	U	283/309 (92%)	244 (86%)	38 (13%)	1 (0%)	30	60
1	V	283/309 (92%)	240 (85%)	42 (15%)	1 (0%)	30	60
1	W	283/309 (92%)	241 (85%)	41 (14%)	1 (0%)	30	60
1	X	283/309 (92%)	243 (86%)	38 (13%)	2 (1%)	18	49
All	All	6792/7416 (92%)	5835 (86%)	929 (14%)	28 (0%)	30	60

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

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Mol	Chain	Res	Type
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 ⓘ

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%)	224 (92%)	20 (8%)	10	35
1	B	244/266 (92%)	224 (92%)	20 (8%)	10	35
1	C	244/266 (92%)	222 (91%)	22 (9%)	9	31
1	D	244/266 (92%)	224 (92%)	20 (8%)	10	35
1	E	244/266 (92%)	224 (92%)	20 (8%)	10	35
1	F	244/266 (92%)	225 (92%)	19 (8%)	11	36
1	G	244/266 (92%)	223 (91%)	21 (9%)	10	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	244/266 (92%)	224 (92%)	20 (8%)	10	35
1	I	244/266 (92%)	222 (91%)	22 (9%)	9	31
1	J	244/266 (92%)	224 (92%)	20 (8%)	10	35
1	K	244/266 (92%)	225 (92%)	19 (8%)	11	36
1	L	244/266 (92%)	223 (91%)	21 (9%)	10	33
1	M	244/266 (92%)	225 (92%)	19 (8%)	11	36
1	N	244/266 (92%)	225 (92%)	19 (8%)	11	36
1	O	244/266 (92%)	225 (92%)	19 (8%)	11	36
1	P	244/266 (92%)	223 (91%)	21 (9%)	10	33
1	Q	244/266 (92%)	223 (91%)	21 (9%)	10	33
1	R	244/266 (92%)	225 (92%)	19 (8%)	11	36
1	S	244/266 (92%)	227 (93%)	17 (7%)	14	41
1	T	244/266 (92%)	223 (91%)	21 (9%)	10	33
1	U	244/266 (92%)	223 (91%)	21 (9%)	10	33
1	V	244/266 (92%)	224 (92%)	20 (8%)	10	35
1	W	244/266 (92%)	223 (91%)	21 (9%)	10	33
1	X	244/266 (92%)	224 (92%)	20 (8%)	10	35
All	All	5856/6384 (92%)	5374 (92%)	482 (8%)	10	35

All (482) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ILE
1	A	43	THR
1	A	46	GLU
1	A	47	LEU
1	A	62	VAL
1	A	67	THR
1	A	87	CYS
1	A	89	VAL
1	A	94	LEU
1	A	113	LYS
1	A	136	VAL
1	A	155	LEU
1	A	158	ASP
1	A	162	LYS

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Mol	Chain	Res	Type
1	A	170	VAL
1	A	195	SER
1	A	223	THR
1	A	228	THR
1	A	264	VAL
1	A	292	HIS
1	B	17	ILE
1	B	43	THR
1	B	46	GLU
1	B	47	LEU
1	B	62	VAL
1	B	67	THR
1	B	87	CYS
1	B	89	VAL
1	B	94	LEU
1	B	113	LYS
1	B	136	VAL
1	B	155	LEU
1	B	158	ASP
1	B	162	LYS
1	B	170	VAL
1	B	195	SER
1	B	223	THR
1	B	228	THR
1	B	264	VAL
1	B	292	HIS
1	C	17	ILE
1	C	43	THR
1	C	46	GLU
1	C	47	LEU
1	C	62	VAL
1	C	67	THR
1	C	87	CYS
1	C	89	VAL
1	C	94	LEU
1	C	113	LYS
1	C	136	VAL
1	C	149	LEU
1	C	155	LEU
1	C	158	ASP
1	C	162	LYS
1	C	170	VAL

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Mol	Chain	Res	Type
1	C	195	SER
1	C	223	THR
1	C	228	THR
1	C	264	VAL
1	C	285	CYS
1	C	292	HIS
1	D	17	ILE
1	D	43	THR
1	D	46	GLU
1	D	47	LEU
1	D	62	VAL
1	D	67	THR
1	D	87	CYS
1	D	89	VAL
1	D	94	LEU
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	223	THR
1	D	228	THR
1	D	264	VAL
1	D	285	CYS
1	E	17	ILE
1	E	43	THR
1	E	46	GLU
1	E	47	LEU
1	E	62	VAL
1	E	67	THR
1	E	89	VAL
1	E	94	LEU
1	E	113	LYS
1	E	136	VAL
1	E	145	SER
1	E	155	LEU
1	E	158	ASP
1	E	162	LYS
1	E	170	VAL
1	E	195	SER

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Mol	Chain	Res	Type
1	E	223	THR
1	E	228	THR
1	E	264	VAL
1	E	292	HIS
1	F	17	ILE
1	F	43	THR
1	F	46	GLU
1	F	47	LEU
1	F	62	VAL
1	F	67	THR
1	F	87	CYS
1	F	89	VAL
1	F	94	LEU
1	F	113	LYS
1	F	136	VAL
1	F	155	LEU
1	F	158	ASP
1	F	170	VAL
1	F	195	SER
1	F	223	THR
1	F	228	THR
1	F	264	VAL
1	F	285	CYS
1	G	17	ILE
1	G	43	THR
1	G	46	GLU
1	G	47	LEU
1	G	62	VAL
1	G	67	THR
1	G	87	CYS
1	G	89	VAL
1	G	94	LEU
1	G	113	LYS
1	G	136	VAL
1	G	145	SER
1	G	155	LEU
1	G	158	ASP
1	G	162	LYS
1	G	170	VAL
1	G	195	SER
1	G	223	THR
1	G	228	THR

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Mol	Chain	Res	Type
1	G	264	VAL
1	G	285	CYS
1	H	17	ILE
1	H	43	THR
1	H	46	GLU
1	H	47	LEU
1	H	62	VAL
1	H	67	THR
1	H	87	CYS
1	H	89	VAL
1	H	94	LEU
1	H	113	LYS
1	H	136	VAL
1	H	149	LEU
1	H	155	LEU
1	H	158	ASP
1	H	162	LYS
1	H	170	VAL
1	H	195	SER
1	H	223	THR
1	H	228	THR
1	H	264	VAL
1	I	17	ILE
1	I	43	THR
1	I	46	GLU
1	I	47	LEU
1	I	62	VAL
1	I	67	THR
1	I	87	CYS
1	I	89	VAL
1	I	94	LEU
1	I	113	LYS
1	I	136	VAL
1	I	145	SER
1	I	149	LEU
1	I	155	LEU
1	I	158	ASP
1	I	162	LYS
1	I	170	VAL
1	I	195	SER
1	I	223	THR
1	I	228	THR

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Mol	Chain	Res	Type
1	I	264	VAL
1	I	285	CYS
1	J	17	ILE
1	J	43	THR
1	J	46	GLU
1	J	47	LEU
1	J	62	VAL
1	J	67	THR
1	J	87	CYS
1	J	89	VAL
1	J	94	LEU
1	J	113	LYS
1	J	136	VAL
1	J	149	LEU
1	J	155	LEU
1	J	158	ASP
1	J	170	VAL
1	J	195	SER
1	J	223	THR
1	J	228	THR
1	J	264	VAL
1	J	285	CYS
1	K	17	ILE
1	K	43	THR
1	K	46	GLU
1	K	47	LEU
1	K	62	VAL
1	K	67	THR
1	K	89	VAL
1	K	94	LEU
1	K	113	LYS
1	K	136	VAL
1	K	145	SER
1	K	155	LEU
1	K	158	ASP
1	K	162	LYS
1	K	170	VAL
1	K	195	SER
1	K	223	THR
1	K	228	THR
1	K	264	VAL
1	L	17	ILE

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Mol	Chain	Res	Type
1	L	43	THR
1	L	46	GLU
1	L	47	LEU
1	L	62	VAL
1	L	67	THR
1	L	89	VAL
1	L	94	LEU
1	L	113	LYS
1	L	136	VAL
1	L	145	SER
1	L	155	LEU
1	L	158	ASP
1	L	162	LYS
1	L	170	VAL
1	L	195	SER
1	L	223	THR
1	L	228	THR
1	L	264	VAL
1	L	285	CYS
1	L	292	HIS
1	M	17	ILE
1	M	43	THR
1	M	46	GLU
1	M	47	LEU
1	M	62	VAL
1	M	67	THR
1	M	89	VAL
1	M	94	LEU
1	M	113	LYS
1	M	136	VAL
1	M	149	LEU
1	M	155	LEU
1	M	158	ASP
1	M	170	VAL
1	M	195	SER
1	M	223	THR
1	M	228	THR
1	M	264	VAL
1	M	285	CYS
1	N	17	ILE
1	N	43	THR
1	N	46	GLU

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Mol	Chain	Res	Type
1	N	47	LEU
1	N	62	VAL
1	N	67	THR
1	N	87	CYS
1	N	89	VAL
1	N	94	LEU
1	N	113	LYS
1	N	136	VAL
1	N	155	LEU
1	N	158	ASP
1	N	162	LYS
1	N	170	VAL
1	N	195	SER
1	N	223	THR
1	N	228	THR
1	N	264	VAL
1	O	17	ILE
1	O	43	THR
1	O	46	GLU
1	O	47	LEU
1	O	62	VAL
1	O	67	THR
1	O	87	CYS
1	O	89	VAL
1	O	94	LEU
1	O	113	LYS
1	O	136	VAL
1	O	155	LEU
1	O	158	ASP
1	O	162	LYS
1	O	170	VAL
1	O	195	SER
1	O	223	THR
1	O	228	THR
1	O	264	VAL
1	P	17	ILE
1	P	43	THR
1	P	46	GLU
1	P	47	LEU
1	P	62	VAL
1	P	67	THR
1	P	89	VAL

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Mol	Chain	Res	Type
1	P	94	LEU
1	P	113	LYS
1	P	136	VAL
1	P	145	SER
1	P	155	LEU
1	P	158	ASP
1	P	162	LYS
1	P	170	VAL
1	P	195	SER
1	P	223	THR
1	P	228	THR
1	P	264	VAL
1	P	285	CYS
1	P	292	HIS
1	Q	17	ILE
1	Q	43	THR
1	Q	46	GLU
1	Q	47	LEU
1	Q	62	VAL
1	Q	67	THR
1	Q	87	CYS
1	Q	89	VAL
1	Q	94	LEU
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	202	VAL
1	Q	223	THR
1	Q	228	THR
1	Q	264	VAL
1	Q	285	CYS
1	R	17	ILE
1	R	43	THR
1	R	46	GLU
1	R	47	LEU
1	R	62	VAL
1	R	67	THR
1	R	89	VAL

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Mol	Chain	Res	Type
1	R	94	LEU
1	R	113	LYS
1	R	136	VAL
1	R	145	SER
1	R	155	LEU
1	R	158	ASP
1	R	162	LYS
1	R	170	VAL
1	R	195	SER
1	R	223	THR
1	R	228	THR
1	R	264	VAL
1	S	17	ILE
1	S	43	THR
1	S	46	GLU
1	S	47	LEU
1	S	62	VAL
1	S	67	THR
1	S	89	VAL
1	S	94	LEU
1	S	113	LYS
1	S	136	VAL
1	S	155	LEU
1	S	158	ASP
1	S	170	VAL
1	S	195	SER
1	S	223	THR
1	S	228	THR
1	S	264	VAL
1	T	17	ILE
1	T	43	THR
1	T	46	GLU
1	T	47	LEU
1	T	62	VAL
1	T	67	THR
1	T	87	CYS
1	T	89	VAL
1	T	94	LEU
1	T	113	LYS
1	T	136	VAL
1	T	149	LEU
1	T	155	LEU

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Mol	Chain	Res	Type
1	T	158	ASP
1	T	162	LYS
1	T	170	VAL
1	T	195	SER
1	T	223	THR
1	T	228	THR
1	T	264	VAL
1	T	285	CYS
1	U	17	ILE
1	U	43	THR
1	U	46	GLU
1	U	47	LEU
1	U	62	VAL
1	U	67	THR
1	U	87	CYS
1	U	89	VAL
1	U	94	LEU
1	U	113	LYS
1	U	136	VAL
1	U	145	SER
1	U	155	LEU
1	U	158	ASP
1	U	162	LYS
1	U	170	VAL
1	U	195	SER
1	U	223	THR
1	U	228	THR
1	U	264	VAL
1	U	285	CYS
1	V	17	ILE
1	V	43	THR
1	V	46	GLU
1	V	47	LEU
1	V	62	VAL
1	V	67	THR
1	V	89	VAL
1	V	94	LEU
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	162	LYS
1	V	170	VAL
1	V	195	SER
1	V	223	THR
1	V	228	THR
1	V	264	VAL
1	V	285	CYS
1	W	17	ILE
1	W	43	THR
1	W	46	GLU
1	W	47	LEU
1	W	62	VAL
1	W	67	THR
1	W	87	CYS
1	W	89	VAL
1	W	94	LEU
1	W	113	LYS
1	W	136	VAL
1	W	155	LEU
1	W	158	ASP
1	W	162	LYS
1	W	170	VAL
1	W	195	SER
1	W	223	THR
1	W	228	THR
1	W	264	VAL
1	W	285	CYS
1	W	292	HIS
1	X	17	ILE
1	X	43	THR
1	X	46	GLU
1	X	47	LEU
1	X	62	VAL
1	X	67	THR
1	X	89	VAL
1	X	94	LEU
1	X	113	LYS
1	X	136	VAL
1	X	149	LEU
1	X	155	LEU
1	X	158	ASP
1	X	162	LYS

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Mol	Chain	Res	Type
1	X	170	VAL
1	X	195	SER
1	X	223	THR
1	X	228	THR
1	X	264	VAL
1	X	292	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	227	ASN
1	B	227	ASN
1	B	233	ASN
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	73	GLN
1	J	227	ASN
1	K	227	ASN
1	L	227	ASN
1	L	292	HIS
1	M	227	ASN
1	M	292	HIS
1	N	227	ASN
1	N	292	HIS
1	O	227	ASN
1	P	73	GLN
1	P	227	ASN
1	Q	227	ASN
1	Q	233	ASN
1	R	227	ASN
1	R	292	HIS
1	S	28	ASN
1	S	227	ASN
1	S	292	HIS
1	T	33	GLN

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Mol	Chain	Res	Type
1	T	227	ASN
1	U	28	ASN
1	U	227	ASN
1	U	233	ASN
1	U	286	ASN
1	V	33	GLN
1	V	227	ASN
1	W	227	ASN
1	X	227	ASN
1	X	233	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	S	304	1	1,2,2	6.68	1 (100%)	-		
2	EMC	T	305	1	1,2,2	6.79	1 (100%)	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EMC	I	305	1	1,2,2	6.77	1 (100%)	-		
2	EMC	F	304	1	1,2,2	6.76	1 (100%)	-		
2	EMC	G	305	1	1,2,2	6.79	1 (100%)	-		
2	EMC	J	305	1	1,2,2	6.78	1 (100%)	-		
2	EMC	Q	304	1	1,2,2	6.74	1 (100%)	-		
2	EMC	H	304	1	1,2,2	6.70	1 (100%)	-		
2	EMC	L	304	1	1,2,2	6.86	1 (100%)	-		
2	EMC	E	304	1	1,2,2	6.82	1 (100%)	-		
2	EMC	K	305	1	1,2,2	6.76	1 (100%)	-		
2	EMC	P	304	1	1,2,2	6.82	1 (100%)	-		
2	EMC	T	304	1	1,2,2	6.84	1 (100%)	-		
2	EMC	N	304	1	1,2,2	6.76	1 (100%)	-		
2	EMC	U	304	1	1,2,2	6.81	1 (100%)	-		
2	EMC	A	304	1	1,2,2	6.90	1 (100%)	-		
2	EMC	E	305	1	1,2,2	6.76	1 (100%)	-		
2	EMC	R	304	1	1,2,2	6.69	1 (100%)	-		
2	EMC	B	305	1	1,2,2	6.80	1 (100%)	-		
2	EMC	N	305	1	1,2,2	6.75	1 (100%)	-		
2	EMC	X	304	1	1,2,2	6.75	1 (100%)	-		
2	EMC	O	305	1	1,2,2	6.81	1 (100%)	-		
2	EMC	F	305	1	1,2,2	6.74	1 (100%)	-		
2	EMC	O	304	1	1,2,2	6.78	1 (100%)	-		
2	EMC	S	305	1	1,2,2	6.75	1 (100%)	-		
2	EMC	P	305	1	1,2,2	6.75	1 (100%)	-		
2	EMC	V	304	1	1,2,2	6.83	1 (100%)	-		
2	EMC	W	304	1	1,2,2	7.05	1 (100%)	-		
2	EMC	H	305	1	1,2,2	6.78	1 (100%)	-		
2	EMC	L	305	1	1,2,2	6.80	1 (100%)	-		
2	EMC	X	305	1	1,2,2	6.84	1 (100%)	-		
2	EMC	C	304	1	1,2,2	6.93	1 (100%)	-		
2	EMC	M	305	1	1,2,2	6.71	1 (100%)	-		
2	EMC	A	305	1	1,2,2	6.74	1 (100%)	-		
2	EMC	M	304	1	1,2,2	6.88	1 (100%)	-		
2	EMC	K	304	1	1,2,2	6.64	1 (100%)	-		
2	EMC	D	304	1	1,2,2	6.92	1 (100%)	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EMC	D	305	1	1,2,2	6.97	1 (100%)	-		
2	EMC	G	304	1	1,2,2	6.74	1 (100%)	-		
2	EMC	I	304	1	1,2,2	6.72	1 (100%)	-		
2	EMC	Q	305	1	1,2,2	6.74	1 (100%)	-		
2	EMC	R	305	1	1,2,2	6.77	1 (100%)	-		
2	EMC	V	305	1	1,2,2	6.78	1 (100%)	-		
2	EMC	B	304	1	1,2,2	6.75	1 (100%)	-		
2	EMC	J	304	1	1,2,2	6.76	1 (100%)	-		
2	EMC	C	305	1	1,2,2	6.73	1 (100%)	-		
2	EMC	U	305	1	1,2,2	6.74	1 (100%)	-		
2	EMC	W	305	1	1,2,2	6.83	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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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	E	305	EMC	C2-C1	6.76	1.84	1.49
2	J	304	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	A	305	EMC	C2-C1	6.74	1.84	1.49
2	Q	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.

24 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	S	304	EMC	1	0
2	F	304	EMC	1	0
2	Q	304	EMC	2	0
2	H	304	EMC	1	0
2	L	304	EMC	2	0
2	E	304	EMC	1	0
2	P	304	EMC	1	0
2	T	304	EMC	1	0
2	N	304	EMC	1	0
2	U	304	EMC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	304	EMC	1	0
2	R	304	EMC	2	0
2	X	304	EMC	1	0
2	O	304	EMC	1	0
2	V	304	EMC	2	0
2	W	304	EMC	1	0
2	C	304	EMC	2	0
2	M	304	EMC	1	0
2	K	304	EMC	2	0
2	D	304	EMC	1	0
2	G	304	EMC	1	0
2	I	304	EMC	2	0
2	B	304	EMC	1	0
2	J	304	EMC	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	285/309 (92%)	0.17	12 (4%)	40	26	62, 123, 190, 270	0
1	B	285/309 (92%)	0.41	21 (7%)	20	15	61, 124, 190, 270	0
1	C	285/309 (92%)	0.39	21 (7%)	20	15	63, 123, 189, 270	0
1	D	285/309 (92%)	0.29	16 (5%)	30	20	64, 122, 189, 270	0
1	E	285/309 (92%)	0.36	25 (8%)	15	12	64, 124, 190, 270	0
1	F	285/309 (92%)	0.47	25 (8%)	15	12	64, 125, 193, 270	0
1	G	285/309 (92%)	0.37	27 (9%)	14	11	64, 125, 190, 270	0
1	H	285/309 (92%)	0.39	32 (11%)	10	9	63, 124, 190, 270	0
1	I	285/309 (92%)	0.29	21 (7%)	20	15	63, 127, 190, 270	0
1	J	285/309 (92%)	0.25	18 (6%)	26	17	64, 126, 191, 270	0
1	K	285/309 (92%)	0.47	31 (10%)	10	9	62, 125, 192, 270	0
1	L	285/309 (92%)	0.29	19 (6%)	24	16	63, 124, 190, 270	0
1	M	285/309 (92%)	0.10	12 (4%)	40	26	65, 125, 190, 270	0
1	N	285/309 (92%)	0.36	24 (8%)	17	13	63, 123, 194, 272	0
1	O	285/309 (92%)	0.51	31 (10%)	10	9	62, 124, 191, 270	0
1	P	285/309 (92%)	0.51	34 (11%)	9	7	66, 125, 190, 270	0
1	Q	285/309 (92%)	0.57	32 (11%)	10	9	66, 125, 191, 270	0
1	R	285/309 (92%)	0.38	24 (8%)	17	13	64, 125, 191, 270	0
1	S	285/309 (92%)	0.29	18 (6%)	26	17	63, 126, 190, 270	0
1	T	285/309 (92%)	0.40	26 (9%)	15	11	62, 125, 191, 270	0
1	U	285/309 (92%)	0.53	37 (12%)	7	6	64, 124, 192, 270	0
1	V	285/309 (92%)	0.21	19 (6%)	24	16	65, 125, 191, 270	0
1	W	285/309 (92%)	0.22	19 (6%)	24	16	64, 123, 190, 270	0
1	X	285/309 (92%)	0.15	18 (6%)	26	17	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%)	0.35	562 (8%) 17 13	61, 125, 193, 272	0

All (562) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	186	VAL	10.2
1	P	9	THR	9.1
1	Q	129	GLU	8.1
1	N	9	THR	8.1
1	I	193	ILE	8.0
1	K	129	GLU	8.0
1	F	215	LEU	7.4
1	O	185	VAL	7.4
1	S	194	ILE	7.3
1	P	45	LYS	7.1
1	O	9	THR	7.1
1	C	73	GLN	7.0
1	K	144	ALA	7.0
1	O	12	VAL	6.9
1	J	129	GLU	6.7
1	P	12	VAL	6.7
1	D	196	TYR	6.6
1	F	194	ILE	6.6
1	K	147	LYS	6.5
1	Q	64	ASP	6.3
1	O	129	GLU	6.3
1	S	193	ILE	6.3
1	N	13	VAL	6.2
1	U	194	ILE	6.2
1	S	191	GLY	6.1
1	I	194	ILE	6.0
1	P	13	VAL	6.0
1	L	13	VAL	5.9
1	Q	175	LYS	5.9
1	R	147	LYS	5.8
1	D	9	THR	5.8
1	U	147	LYS	5.7
1	J	186	VAL	5.7
1	T	174	ARG	5.6
1	P	41	ASP	5.5
1	A	129	GLU	5.5
1	F	9	THR	5.4

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Mol	Chain	Res	Type	RSRZ
1	N	276	GLU	5.3
1	D	16	ALA	5.3
1	V	15	ASN	5.3
1	F	8	LYS	5.3
1	H	64	ASP	5.2
1	I	174	ARG	5.2
1	Q	176	GLU	5.2
1	C	196	TYR	5.2
1	T	185	VAL	5.2
1	L	53	GLU	5.2
1	B	276	GLU	5.1
1	H	61	LEU	5.1
1	T	42	GLU	5.1
1	X	163	SER	5.0
1	Q	172	LYS	5.0
1	H	174	ARG	5.0
1	U	64	ASP	4.9
1	B	185	VAL	4.9
1	U	12	VAL	4.9
1	Q	61	LEU	4.9
1	G	185	VAL	4.8
1	G	9	THR	4.8
1	E	47	LEU	4.8
1	S	12	VAL	4.8
1	A	215	LEU	4.7
1	W	166	PHE	4.7
1	N	12	VAL	4.7
1	U	41	ASP	4.6
1	Q	46	GLU	4.6
1	P	10	VAL	4.6
1	R	176	GLU	4.5
1	F	166	PHE	4.5
1	M	245	THR	4.5
1	C	76	TYR	4.5
1	E	267	ASP	4.4
1	X	166	PHE	4.4
1	N	16	ALA	4.4
1	U	61	LEU	4.4
1	W	215	LEU	4.4
1	W	114	ASP	4.3
1	W	265	ASP	4.3
1	N	193	ILE	4.3

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Mol	Chain	Res	Type	RSRZ
1	J	45	LYS	4.3
1	G	233	ASN	4.3
1	U	62	VAL	4.3
1	O	186	VAL	4.2
1	I	258	GLU	4.2
1	U	129	GLU	4.2
1	U	9	THR	4.2
1	G	8	LYS	4.2
1	F	46	GLU	4.2
1	G	129	GLU	4.2
1	E	186	VAL	4.2
1	R	64	ASP	4.2
1	V	129	GLU	4.2
1	U	65	ILE	4.2
1	C	62	VAL	4.1
1	K	265	ASP	4.1
1	S	198	ILE	4.1
1	Q	125	THR	4.1
1	K	12	VAL	4.1
1	P	181	ALA	4.1
1	K	128	ASN	4.1
1	Q	42	GLU	4.1
1	H	205	GLY	4.0
1	R	205	GLY	4.0
1	X	185	VAL	4.0
1	O	177	ALA	4.0
1	P	8	LYS	4.0
1	C	185	VAL	3.9
1	D	10	VAL	3.9
1	R	174	ARG	3.9
1	Q	66	LYS	3.9
1	I	204	GLU	3.9
1	W	267	ASP	3.9
1	K	42	GLU	3.9
1	Q	37	TRP	3.9
1	G	194	ILE	3.8
1	K	65	ILE	3.8
1	U	144	ALA	3.8
1	C	205	GLY	3.8
1	T	208	ILE	3.8
1	P	215	LEU	3.8
1	O	45	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
1	K	165	TYR	3.7
1	G	232	ALA	3.7
1	J	12	VAL	3.7
1	P	46	GLU	3.7
1	K	143	ASN	3.7
1	X	215	LEU	3.7
1	C	77	PHE	3.7
1	T	64	ASP	3.7
1	H	132	LYS	3.7
1	F	181	ALA	3.6
1	F	178	TYR	3.6
1	F	193	ILE	3.6
1	J	49	ARG	3.6
1	C	152	ASP	3.6
1	V	167	GLN	3.6
1	D	13	VAL	3.6
1	A	132	LYS	3.6
1	G	202	VAL	3.6
1	Q	144	ALA	3.6
1	R	173	ILE	3.6
1	W	178	TYR	3.6
1	O	180	GLY	3.5
1	K	61	LEU	3.5
1	H	129	GLU	3.5
1	U	237	ASP	3.5
1	E	265	ASP	3.5
1	S	186	VAL	3.5
1	F	165	TYR	3.5
1	J	185	VAL	3.5
1	P	185	VAL	3.5
1	H	267	ASP	3.5
1	U	114	ASP	3.5
1	S	129	GLU	3.4
1	X	197	SER	3.4
1	W	99	LEU	3.4
1	P	197	SER	3.4
1	H	237	ASP	3.4
1	L	46	GLU	3.4
1	X	196	TYR	3.4
1	C	201	GLY	3.4
1	B	187	ALA	3.4
1	R	181	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	H	65	ILE	3.4
1	B	147	LYS	3.4
1	F	171	ASP	3.4
1	E	12	VAL	3.4
1	X	263	TYR	3.4
1	O	49	ARG	3.4
1	R	40	PHE	3.4
1	O	215	LEU	3.4
1	J	196	TYR	3.4
1	N	198	ILE	3.4
1	D	12	VAL	3.3
1	U	208	ILE	3.3
1	V	190	PHE	3.3
1	Q	45	LYS	3.3
1	L	41	ASP	3.3
1	F	45	LYS	3.3
1	P	129	GLU	3.3
1	R	180	GLY	3.3
1	N	267	ASP	3.3
1	U	10	VAL	3.3
1	T	204	GLU	3.3
1	B	274	LEU	3.3
1	H	157	ASN	3.3
1	H	158	ASP	3.2
1	R	207	LEU	3.2
1	C	186	VAL	3.2
1	N	203	VAL	3.2
1	V	196	TYR	3.2
1	N	186	VAL	3.2
1	T	41	ASP	3.2
1	U	198	ILE	3.2
1	C	258	GLU	3.2
1	H	207	LEU	3.2
1	O	278	ALA	3.2
1	O	8	LYS	3.2
1	R	211	LEU	3.2
1	M	196	TYR	3.2
1	M	244	THR	3.2
1	P	205	GLY	3.2
1	F	47	LEU	3.2
1	G	11	GLU	3.2
1	L	129	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	Q	169	GLN	3.2
1	A	99	LEU	3.1
1	K	148	LEU	3.1
1	N	10	VAL	3.1
1	G	45	LYS	3.1
1	H	144	ALA	3.1
1	I	267	ASP	3.1
1	P	37	TRP	3.1
1	D	198	ILE	3.1
1	P	198	ILE	3.1
1	J	287	GLU	3.1
1	O	118	LYS	3.1
1	S	132	LYS	3.1
1	U	118	LYS	3.1
1	K	43	THR	3.1
1	H	202	VAL	3.1
1	R	44	ILE	3.1
1	X	198	ILE	3.1
1	J	181	ALA	3.0
1	P	202	VAL	3.0
1	D	279	LYS	3.0
1	N	258	GLU	3.0
1	O	36	PRO	3.0
1	J	182	ALA	3.0
1	U	167	GLN	3.0
1	O	13	VAL	3.0
1	T	77	PHE	3.0
1	E	194	ILE	3.0
1	A	175	LYS	3.0
1	T	40	PHE	3.0
1	V	19	THR	3.0
1	O	258	GLU	3.0
1	B	188	GLY	3.0
1	C	157	ASN	3.0
1	W	194	ILE	3.0
1	O	189	PRO	2.9
1	T	287	GLU	2.9
1	K	289	GLN	2.9
1	N	17	ILE	2.9
1	E	129	GLU	2.9
1	V	18	GLU	2.9
1	F	218	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	L	194	ILE	2.9
1	C	69	LEU	2.9
1	P	42	GLU	2.9
1	G	64	ASP	2.9
1	I	8	LYS	2.9
1	R	42	GLU	2.9
1	R	170	VAL	2.9
1	G	205	GLY	2.9
1	N	190	PHE	2.9
1	F	211	LEU	2.9
1	H	208	ILE	2.9
1	K	179	ALA	2.9
1	O	10	VAL	2.9
1	D	8	LYS	2.9
1	H	162	LYS	2.9
1	U	51	LYS	2.9
1	P	258	GLU	2.8
1	U	170	VAL	2.8
1	K	267	ASP	2.8
1	N	206	LYS	2.8
1	U	181	ALA	2.8
1	U	42	GLU	2.8
1	X	77	PHE	2.8
1	S	232	ALA	2.8
1	G	12	VAL	2.8
1	U	13	VAL	2.8
1	K	39	THR	2.8
1	T	44	ILE	2.8
1	D	129	GLU	2.8
1	P	64	ASP	2.7
1	I	157	ASN	2.7
1	C	79	ALA	2.7
1	W	181	ALA	2.7
1	E	203	VAL	2.7
1	L	186	VAL	2.7
1	X	186	VAL	2.7
1	H	160	SER	2.7
1	S	195	SER	2.7
1	Q	63	GLY	2.7
1	C	267	ASP	2.7
1	U	122	ASP	2.7
1	L	49	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	O	147	LYS	2.7
1	P	194	ILE	2.7
1	V	163	SER	2.7
1	I	101	PHE	2.7
1	Q	8	LYS	2.7
1	I	171	ASP	2.7
1	T	267	ASP	2.7
1	I	135	LEU	2.7
1	S	157	ASN	2.7
1	H	235	ASP	2.7
1	K	169	GLN	2.6
1	V	193	ILE	2.6
1	E	147	LYS	2.6
1	L	45	LYS	2.6
1	A	46	GLU	2.6
1	H	236	ILE	2.6
1	P	25	ASP	2.6
1	A	206	LYS	2.6
1	F	128	ASN	2.6
1	T	129	GLU	2.6
1	I	274	LEU	2.6
1	N	109	ALA	2.6
1	P	182	ALA	2.6
1	G	152	ASP	2.6
1	G	167	GLN	2.6
1	P	256	GLU	2.6
1	H	51	LYS	2.6
1	M	14	LYS	2.6
1	U	173	ILE	2.6
1	L	190	PHE	2.6
1	E	213	ASN	2.6
1	H	181	ALA	2.6
1	B	279	LYS	2.6
1	G	175	LYS	2.6
1	N	196	TYR	2.6
1	Q	40	PHE	2.6
1	P	267	ASP	2.6
1	U	63	GLY	2.6
1	M	241	LEU	2.6
1	W	47	LEU	2.6
1	I	186	VAL	2.6
1	W	159	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	M	243	LEU	2.5
1	F	265	ASP	2.5
1	U	174	ARG	2.5
1	K	181	ALA	2.5
1	M	129	GLU	2.5
1	Q	252	GLU	2.5
1	L	9	THR	2.5
1	P	284	THR	2.5
1	C	168	SER	2.5
1	F	180	GLY	2.5
1	U	38	GLN	2.5
1	V	289	GLN	2.5
1	J	267	ASP	2.5
1	O	182	ALA	2.5
1	H	141	PHE	2.5
1	S	190	PHE	2.5
1	J	31	LEU	2.5
1	O	41	ASP	2.5
1	R	143	ASN	2.5
1	W	203	VAL	2.5
1	W	289	GLN	2.5
1	O	96	ALA	2.5
1	K	46	GLU	2.5
1	J	286	ASN	2.5
1	W	283	ASN	2.5
1	D	245	THR	2.5
1	K	178	TYR	2.5
1	M	76	TYR	2.5
1	X	56	GLN	2.5
1	H	232	ALA	2.4
1	V	17	ILE	2.4
1	K	132	LYS	2.4
1	T	37	TRP	2.4
1	K	180	GLY	2.4
1	M	190	PHE	2.4
1	R	51	LYS	2.4
1	K	157	ASN	2.4
1	W	37	TRP	2.4
1	Q	265	ASP	2.4
1	V	152	ASP	2.4
1	H	203	VAL	2.4
1	Q	165	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	206	LYS	2.4
1	D	11	GLU	2.4
1	R	210	GLU	2.4
1	E	285	CYS	2.4
1	C	286	ASN	2.4
1	H	125	THR	2.4
1	Q	12	VAL	2.4
1	Q	122	ASP	2.4
1	V	13	VAL	2.4
1	Q	180	GLY	2.4
1	Q	181	ALA	2.4
1	I	175	LYS	2.4
1	Q	289	GLN	2.4
1	E	276	GLU	2.4
1	F	129	GLU	2.4
1	P	195	SER	2.4
1	X	87	CYS	2.4
1	H	37	TRP	2.4
1	O	203	VAL	2.4
1	E	188	GLY	2.4
1	X	194	ILE	2.4
1	I	206	LYS	2.4
1	X	289	GLN	2.4
1	R	145	SER	2.4
1	U	195	SER	2.4
1	L	12	VAL	2.4
1	G	87	CYS	2.4
1	N	36	PRO	2.4
1	W	285	CYS	2.4
1	H	206	LYS	2.3
1	B	171	ASP	2.3
1	G	196	TYR	2.3
1	L	47	LEU	2.3
1	O	207	LEU	2.3
1	C	78	GLU	2.3
1	T	258	GLU	2.3
1	F	206	LYS	2.3
1	Q	51	LYS	2.3
1	G	193	ILE	2.3
1	J	193	ILE	2.3
1	N	194	ILE	2.3
1	P	178	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	R	233	ASN	2.3
1	U	171	ASP	2.3
1	T	207	LEU	2.3
1	B	46	GLU	2.3
1	G	252	GLU	2.3
1	L	202	VAL	2.3
1	Q	43	THR	2.3
1	S	187	ALA	2.3
1	K	292	HIS	2.3
1	B	166	PHE	2.3
1	U	190	PHE	2.3
1	G	237	ASP	2.3
1	J	64	ASP	2.3
1	K	29	LYS	2.3
1	P	65	ILE	2.3
1	X	36	PRO	2.3
1	A	19	THR	2.3
1	B	168	SER	2.3
1	X	273	LEU	2.3
1	H	265	ASP	2.3
1	J	171	ASP	2.3
1	R	41	ASP	2.3
1	O	173	ILE	2.3
1	E	58	ALA	2.3
1	O	181	ALA	2.3
1	F	163	SER	2.3
1	W	163	SER	2.3
1	I	196	TYR	2.3
1	W	286	ASN	2.3
1	A	267	ASP	2.3
1	R	129	GLU	2.2
1	Q	44	ILE	2.2
1	N	292	HIS	2.2
1	J	8	LYS	2.2
1	T	45	LYS	2.2
1	U	8	LYS	2.2
1	G	267	ASP	2.2
1	X	152	ASP	2.2
1	L	17	ILE	2.2
1	E	144	ALA	2.2
1	D	14	LYS	2.2
1	H	147	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	U	45	LYS	2.2
1	O	97	TYR	2.2
1	L	289	GLN	2.2
1	F	65	ILE	2.2
1	I	42	GLU	2.2
1	Q	117	ILE	2.2
1	R	265	ASP	2.2
1	G	144	ALA	2.2
1	U	180	GLY	2.2
1	L	98	ILE	2.2
1	B	283	ASN	2.2
1	S	269	LEU	2.2
1	T	61	LEU	2.2
1	F	177	ALA	2.2
1	G	51	LYS	2.2
1	G	114	ASP	2.2
1	J	9	THR	2.2
1	I	288	TYR	2.2
1	D	17	ILE	2.2
1	F	167	GLN	2.2
1	V	194	ILE	2.2
1	B	155	LEU	2.2
1	N	15	ASN	2.2
1	P	177	ALA	2.2
1	P	180	GLY	2.2
1	R	146	GLY	2.2
1	S	45	LYS	2.2
1	S	233	ASN	2.2
1	T	283	ASN	2.2
1	B	292	HIS	2.2
1	K	91	THR	2.1
1	P	165	TYR	2.1
1	G	65	ILE	2.1
1	O	117	ILE	2.1
1	N	289	GLN	2.1
1	E	16	ALA	2.1
1	B	265	ASP	2.1
1	K	25	ASP	2.1
1	M	87	CYS	2.1
1	T	186	VAL	2.1
1	U	244	THR	2.1
1	I	198	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	O	98	ILE	2.1
1	E	61	LEU	2.1
1	H	211	LEU	2.1
1	S	274	LEU	2.1
1	T	232	ALA	2.1
1	T	205	GLY	2.1
1	H	128	ASN	2.1
1	L	87	CYS	2.1
1	B	148	LEU	2.1
1	R	30	TYR	2.1
1	T	126	LYS	2.1
1	A	49	ARG	2.1
1	M	249	ALA	2.1
1	Q	57	ALA	2.1
1	T	38	GLN	2.1
1	E	252	GLU	2.1
1	S	197	SER	2.1
1	V	14	LYS	2.1
1	G	148	LEU	2.1
1	P	98	ILE	2.1
1	T	196	TYR	2.1
1	A	289	GLN	2.1
1	C	129	GLU	2.1
1	U	50	PHE	2.1
1	B	143	ASN	2.1
1	E	113	LYS	2.1
1	H	8	LYS	2.1
1	B	61	LEU	2.1
1	C	134	LEU	2.1
1	B	267	ASP	2.1
1	K	64	ASP	2.1
1	I	9	THR	2.1
1	D	20	ALA	2.1
1	W	95	ALA	2.1
1	X	16	ALA	2.1
1	V	251	GLY	2.1
1	F	42	GLU	2.1
1	I	190	PHE	2.1
1	E	290	LYS	2.0
1	O	143	ASN	2.0
1	P	233	ASN	2.0
1	Q	128	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	V	117	ILE	2.0
1	K	37	TRP	2.0
1	E	187	ALA	2.0
1	V	288	TYR	2.0
1	T	51	LYS	2.0
1	E	264	VAL	2.0
1	E	291	ARG	2.0
1	M	247	ILE	2.0
1	U	157	ASN	2.0
1	N	181	ALA	2.0
1	K	237	ASP	2.0
1	Q	41	ASP	2.0
1	A	87	CYS	2.0
1	B	289	GLN	2.0
1	C	172	LYS	2.0
1	N	45	LYS	2.0
1	L	252	GLU	2.0
1	O	46	GLU	2.0
1	V	186	VAL	2.0
1	D	253	ILE	2.0
1	E	193	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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, 95th 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($\text{\AA}^2$)	Q<0.9
2	EMC	M	305	3/3	0.56	0.51	52,52,57,140	3
2	EMC	C	305	3/3	0.61	0.46	62,62,63,136	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	EMC	L	305	3/3	0.64	0.56	64,64,65,146	3
2	EMC	P	305	3/3	0.65	0.44	57,57,57,136	3
2	EMC	F	305	3/3	0.69	0.54	76,76,78,143	3
2	EMC	A	305	3/3	0.72	0.46	55,55,60,144	3
2	EMC	V	305	3/3	0.73	0.47	67,67,68,139	3
2	EMC	H	305	3/3	0.75	0.46	57,57,62,133	3
2	EMC	J	305	3/3	0.76	0.54	73,73,74,136	3
2	EMC	X	305	3/3	0.76	0.55	56,56,61,126	3
2	EMC	I	305	3/3	0.77	0.35	56,56,58,144	3
2	EMC	N	305	3/3	0.77	0.40	56,56,62,139	3
2	EMC	O	305	3/3	0.77	0.50	73,73,73,141	3
2	EMC	K	305	3/3	0.79	0.66	75,75,76,141	3
2	EMC	S	305	3/3	0.80	0.37	54,54,55,138	3
2	EMC	G	305	3/3	0.80	0.48	54,54,57,133	3
2	EMC	B	305	3/3	0.80	0.45	56,56,60,134	3
2	EMC	D	305	3/3	0.81	0.54	70,70,72,115	3
2	EMC	Q	305	3/3	0.83	0.49	70,70,71,138	3
2	EMC	E	305	3/3	0.83	0.41	57,57,59,139	3
2	EMC	W	305	3/3	0.84	0.55	57,57,58,125	3
2	EMC	U	305	3/3	0.85	0.41	57,57,59,133	3
2	EMC	T	305	3/3	0.89	0.40	53,53,60,133	3
2	EMC	R	305	3/3	0.90	0.33	79,79,79,149	3
2	EMC	X	304	3/3	0.96	0.19	45,45,90,119	3
2	EMC	J	304	3/3	0.96	0.20	59,59,91,137	3
2	EMC	B	304	3/3	0.97	0.18	29,29,91,104	3
2	EMC	Q	304	3/3	0.97	0.12	52,52,91,125	3
2	EMC	F	304	3/3	0.97	0.21	57,57,88,123	3
2	EMC	R	304	3/3	0.97	0.13	61,61,93,127	3
2	EMC	K	304	3/3	0.97	0.17	61,61,86,119	3
2	EMC	C	304	3/3	0.97	0.22	42,42,90,119	3
2	EMC	M	304	3/3	0.98	0.18	32,32,95,116	3
2	EMC	E	304	3/3	0.98	0.14	45,45,87,106	3
2	EMC	S	304	3/3	0.98	0.12	36,36,88,135	3
2	EMC	H	304	3/3	0.98	0.14	36,36,92,121	3
2	EMC	T	304	3/3	0.98	0.14	30,30,96,118	3
2	EMC	O	304	3/3	0.98	0.17	55,55,89,120	3
2	EMC	U	304	3/3	0.98	0.18	31,31,89,118	3
2	EMC	D	304	3/3	0.98	0.16	51,51,93,102	3
2	EMC	V	304	3/3	0.98	0.19	49,49,88,122	3
2	EMC	P	304	3/3	0.98	0.12	39,39,94,125	3
2	EMC	I	304	3/3	0.98	0.10	41,41,92,127	3
2	EMC	L	304	3/3	0.98	0.18	51,51,90,123	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	EMC	G	304	3/3	0.98	0.18	30,30,85,119	3
2	EMC	N	304	3/3	0.99	0.15	37,37,90,113	3
2	EMC	A	304	3/3	0.99	0.18	40,40,88,105	3
2	EMC	W	304	3/3	0.99	0.14	40,40,92,103	3

6.5 Other polymers [i](#)

There are no such residues in this entry.