



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Oct 29, 2017 – 12:07 AM EDT

PDB ID : 5MYU
EMDB ID: : EMD-3567
Title : VipA-N2/VipB contracted sheath of type VI secretion system
Authors : Wang, J.; Brackmann, B.; Castano-Diez, D.; Kudryashev, M.; Goldie, D.;
Maier, T.; Stahlberg, H.; Basler, M.
Deposited on : unknown
Resolution : 4.00 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

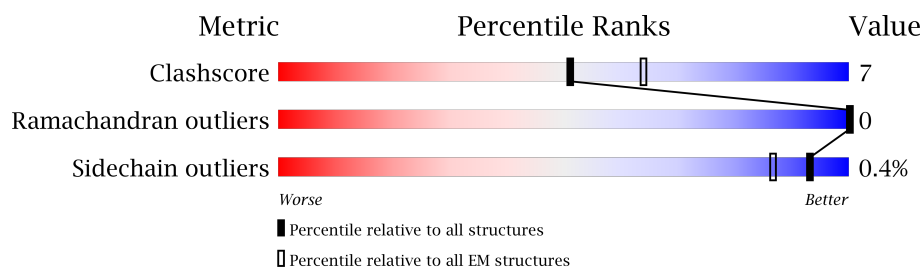
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 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.




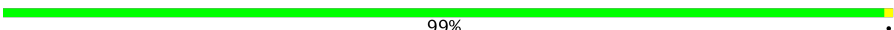
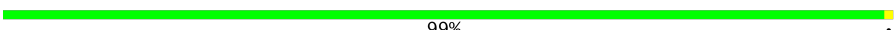
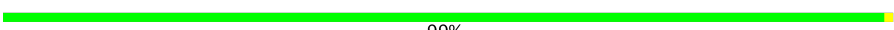
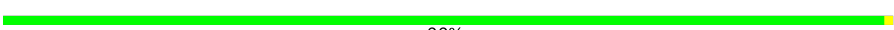















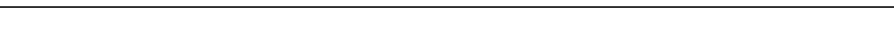

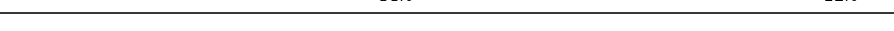


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	1-a	127	99% .
1	1-b	127	99% .
1	1-c	127	99% .
1	1-d	127	99% .
1	1-e	127	99% .
1	1-f	127	99% .
1	2-a	127	99% .
1	2-b	127	99% .
1	2-c	127	99% .



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Mol	Chain	Length	Quality of chain
1	2-d	127	 99%
1	2-e	127	 99%
1	2-f	127	 99%
1	3-a	127	 99%
1	3-b	127	 99%
1	3-c	127	 99%
1	3-d	127	 99%
1	3-e	127	 99%
1	3-f	127	 99%
2	1-A	430	 88% 12%
2	1-B	430	 88% 11%
2	1-C	430	 90% 10%
2	1-D	430	 89% 11%
2	1-E	430	 88% 11%
2	1-F	430	 89% 11%
2	2-A	430	 89% 11%
2	2-B	430	 88% 12%
2	2-C	430	 90% 10%
2	2-D	430	 88% 11%
2	2-E	430	 89% 11%
2	2-F	430	 89% 11%
2	3-A	430	 88% 12%
2	3-B	430	 89% 10%
2	3-C	430	 89% 11%
2	3-D	430	 89% 11%

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Mol	Chain	Length	Quality of chain
2	3-E	430	 90%10%
2	3-F	430	 88%12%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 79740 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1-a	127	Total	C	N	O	S	0	0
			977	616	162	198	1		
1	2-a	127	Total	C	N	O	S	0	0
			977	616	162	198	1		
1	3-a	127	Total	C	N	O	S	0	0
			977	616	162	198	1		
1	1-b	127	Total	C	N	O	S	0	0
			977	616	162	198	1		
1	2-b	127	Total	C	N	O	S	0	0
			977	616	162	198	1		
1	3-b	127	Total	C	N	O	S	0	0
			977	616	162	198	1		
1	1-c	127	Total	C	N	O	S	0	0
			977	616	162	198	1		
1	2-c	127	Total	C	N	O	S	0	0
			977	616	162	198	1		
1	3-c	127	Total	C	N	O	S	0	0
			977	616	162	198	1		
1	1-d	127	Total	C	N	O	S	0	0
			977	616	162	198	1		
1	2-d	127	Total	C	N	O	S	0	0
			977	616	162	198	1		
1	3-d	127	Total	C	N	O	S	0	0
			977	616	162	198	1		
1	1-e	127	Total	C	N	O	S	0	0
			977	616	162	198	1		
1	2-e	127	Total	C	N	O	S	0	0
			977	616	162	198	1		
1	3-e	127	Total	C	N	O	S	0	0
			977	616	162	198	1		
1	1-f	127	Total	C	N	O	S	0	0
			977	616	162	198	1		
1	2-f	127	Total	C	N	O	S	0	0
			977	616	162	198	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	3-f	127	Total	C	N	O	S	0	0
			977	616	162	198	1		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	26	ALA	-	insertion	UNP A0A023PRF3
a	27	GLU	-	insertion	UNP A0A023PRF3
b	26	ALA	-	insertion	UNP A0A023PRF3
b	27	GLU	-	insertion	UNP A0A023PRF3
c	26	ALA	-	insertion	UNP A0A023PRF3
c	27	GLU	-	insertion	UNP A0A023PRF3
d	26	ALA	-	insertion	UNP A0A023PRF3
d	27	GLU	-	insertion	UNP A0A023PRF3
e	26	ALA	-	insertion	UNP A0A023PRF3
e	27	GLU	-	insertion	UNP A0A023PRF3
f	26	ALA	-	insertion	UNP A0A023PRF3
f	27	GLU	-	insertion	UNP A0A023PRF3

- Molecule 2 is a protein called Type VI secretion system protein ImpC.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1-A	430	Total	C	N	O	S	0	0
			3453	2207	587	646	13		
2	2-A	430	Total	C	N	O	S	0	0
			3453	2207	587	646	13		
2	3-A	430	Total	C	N	O	S	0	0
			3453	2207	587	646	13		
2	1-B	430	Total	C	N	O	S	0	0
			3453	2207	587	646	13		
2	2-B	430	Total	C	N	O	S	0	0
			3453	2207	587	646	13		
2	3-B	430	Total	C	N	O	S	0	0
			3453	2207	587	646	13		
2	1-C	430	Total	C	N	O	S	0	0
			3453	2207	587	646	13		
2	2-C	430	Total	C	N	O	S	0	0
			3453	2207	587	646	13		
2	3-C	430	Total	C	N	O	S	0	0
			3453	2207	587	646	13		
2	1-D	430	Total	C	N	O	S	0	0
			3453	2207	587	646	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	2-D	430	Total	C	N	O	S	0	0
			3453	2207	587	646	13		
2	3-D	430	Total	C	N	O	S	0	0
			3453	2207	587	646	13		
2	1-E	430	Total	C	N	O	S	0	0
			3453	2207	587	646	13		
2	2-E	430	Total	C	N	O	S	0	0
			3453	2207	587	646	13		
2	3-E	430	Total	C	N	O	S	0	0
			3453	2207	587	646	13		
2	1-F	430	Total	C	N	O	S	0	0
			3453	2207	587	646	13		
2	2-F	430	Total	C	N	O	S	0	0
			3453	2207	587	646	13		
2	3-F	430	Total	C	N	O	S	0	0
			3453	2207	587	646	13		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Uncharacterized protein

Chain 1-a:  99%



- Molecule 1: Uncharacterized protein

Chain 1-b:  99%



- Molecule 1: Uncharacterized protein

Chain 1-c:  99%



- Molecule 1: Uncharacterized protein

Chain 1-d:  99%



- Molecule 1: Uncharacterized protein

Chain 1-e:  99%



- Molecule 1: Uncharacterized protein

Chain 1-f:  99%



- Molecule 1: Uncharacterized protein

Chain 2-a:  99%



- Molecule 1: Uncharacterized protein

Chain 2-b:  99%



- Molecule 1: Uncharacterized protein

Chain 2-c:  99%



- Molecule 1: Uncharacterized protein

Chain 2-d:  99%



- Molecule 1: Uncharacterized protein

Chain 2-e:  99%



- Molecule 1: Uncharacterized protein

Chain 2-f:  99%



- Molecule 1: Uncharacterized protein

Chain 3-a:  99%



- Molecule 1: Uncharacterized protein

Chain 3-b:  99%



- Molecule 1: Uncharacterized protein

Chain 3-c: 99%



- Molecule 1: Uncharacterized protein

Chain 3-d: 99%



- Molecule 1: Uncharacterized protein

Chain 3-e: 99%



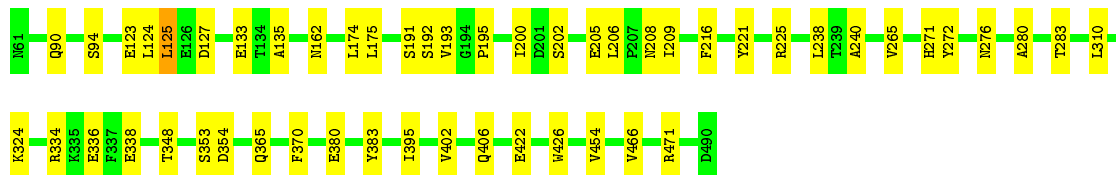
- Molecule 1: Uncharacterized protein

Chain 3-f:  99%



- Molecule 2: Type VI secretion system protein ImpC

Chain 1-A: 88% 12%



- Molecule 2: Type VI secretion system protein ImpC

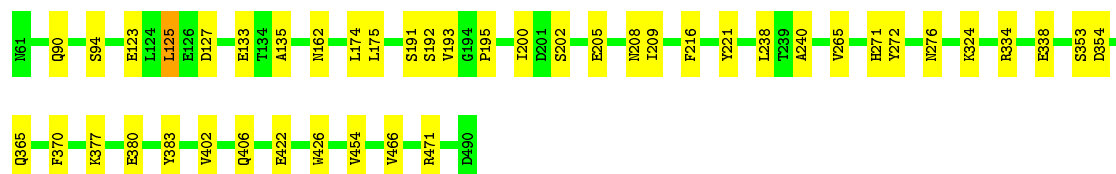
Chain 1-B: 88% 11%





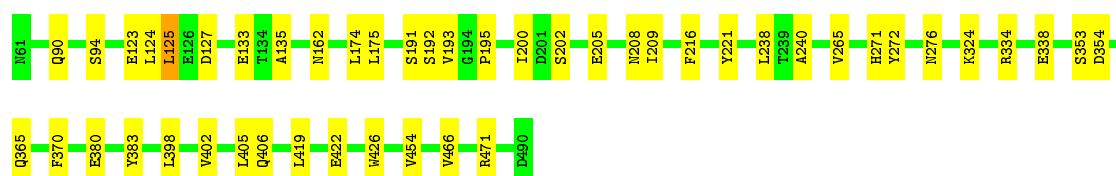
- Molecule 2: Type VI secretion system protein ImpC

Chain 1-C: 90% 10%



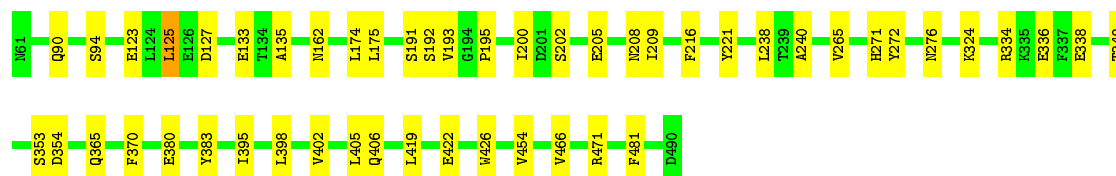
- Molecule 2: Type VI secretion system protein ImpC

Chain 1-D: 89% 11%



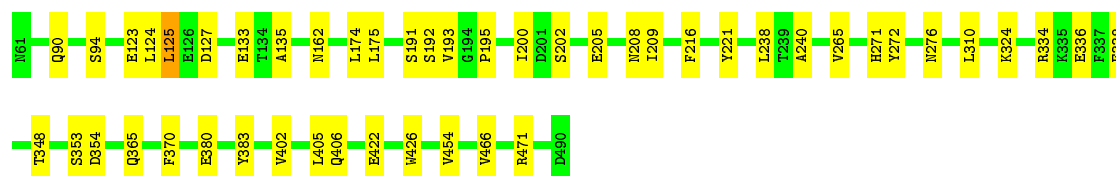
- Molecule 2: Type VI secretion system protein ImpC

Chain 1-E: 88% 11%



- Molecule 2: Type VI secretion system protein ImpC

Chain 1-F: 89% 11%



- Molecule 2: Type VI secretion system protein ImpC

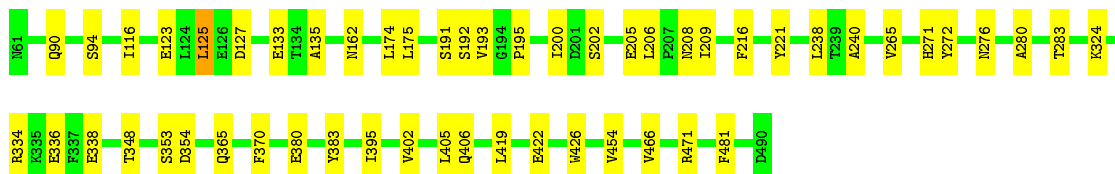
Chain 2-A: 89% 11%





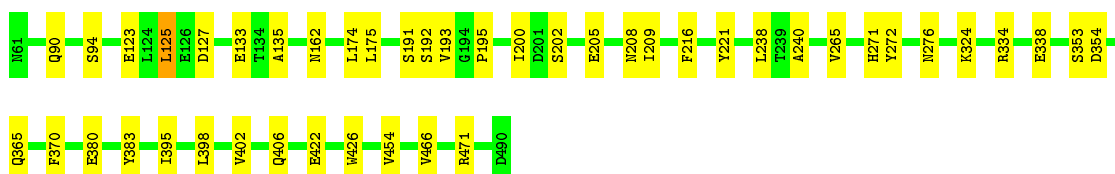
• Molecule 2: Type VI secretion system protein ImpC

Chain 2-B: 88% 12%



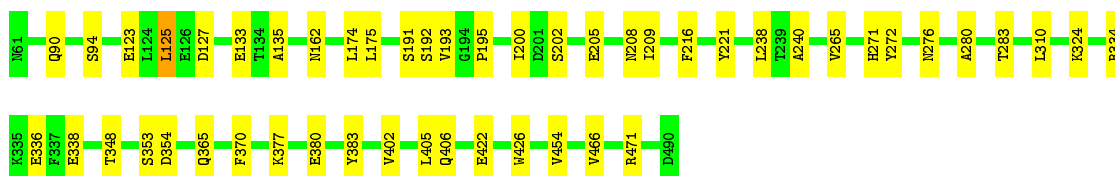
• Molecule 2: Type VI secretion system protein ImpC

Chain 2-C: 90% 10%



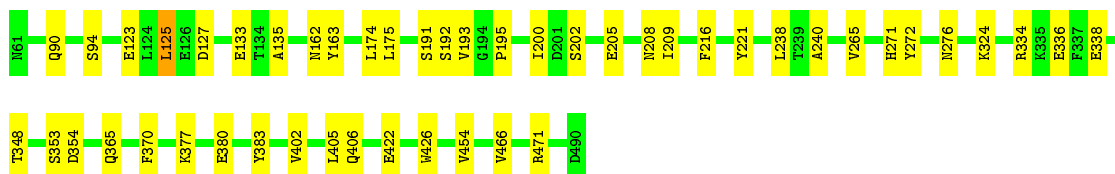
• Molecule 2: Type VI secretion system protein ImpC

Chain 2-D: 88% 11%



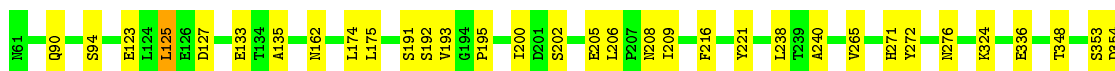
• Molecule 2: Type VI secretion system protein ImpC

Chain 2-E: 89% 11%



• Molecule 2: Type VI secretion system protein ImpC

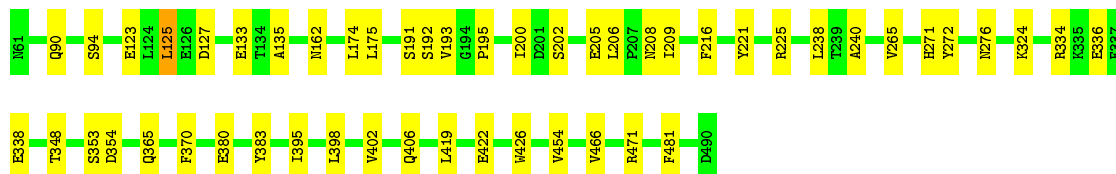
Chain 2-F: 89% 11%





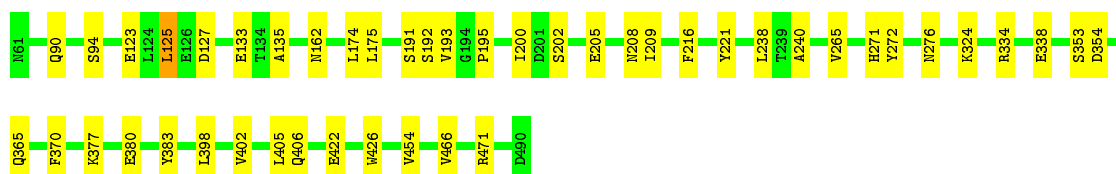
- Molecule 2: Type VI secretion system protein ImpC

Chain 3-A: 88% 12%



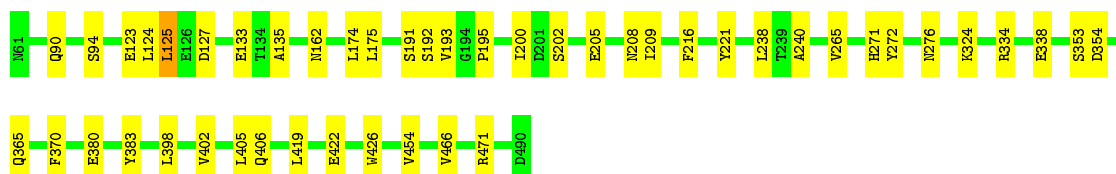
- Molecule 2: Type VI secretion system protein ImpC

Chain 3-B: 89% 10%



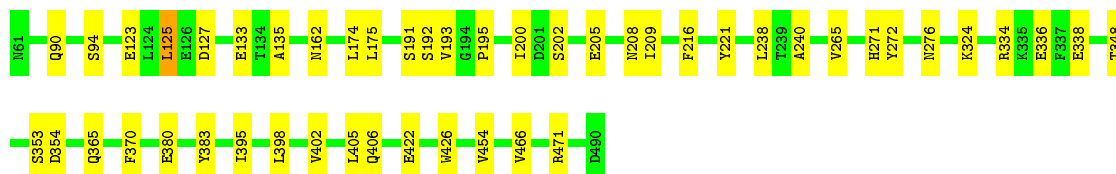
- Molecule 2: Type VI secretion system protein ImpC

Chain 3-C: 89% 11%



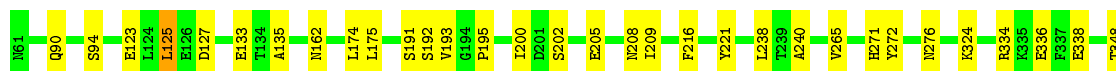
- Molecule 2: Type VI secretion system protein ImpC

Chain 3-D: 89% 11%



- Molecule 2: Type VI secretion system protein ImpC

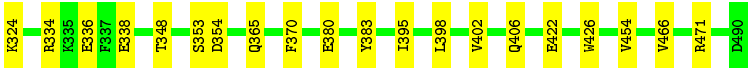
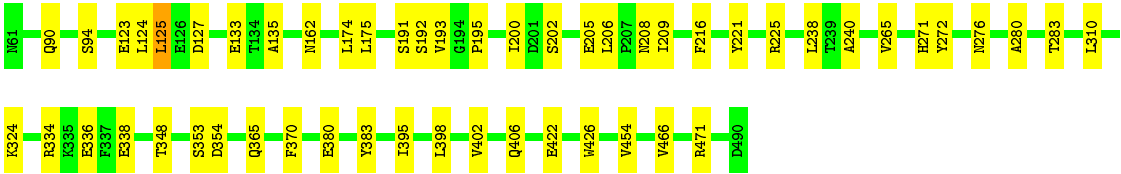
Chain 3-E: 90% 10%





● Molecule 2: Type VI secretion system protein ImpC

Chain 3-F: 88% 12%



4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=29.4°, rise=21.7 Å, axial sym=C6	Depositor
Number of segments used	7000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
1	1-a	0.40	0/989	0.54	0/1340
1	1-b	0.40	0/989	0.54	0/1340
1	1-c	0.40	0/989	0.54	0/1340
1	1-d	0.40	0/989	0.54	0/1340
1	1-e	0.40	0/989	0.54	0/1340
1	1-f	0.40	0/989	0.54	0/1340
1	2-a	0.40	0/989	0.54	0/1340
1	2-b	0.40	0/989	0.54	0/1340
1	2-c	0.40	0/989	0.54	0/1340
1	2-d	0.40	0/989	0.54	0/1340
1	2-e	0.40	0/989	0.54	0/1340
1	2-f	0.40	0/989	0.54	0/1340
1	3-a	0.40	0/989	0.54	0/1340
1	3-b	0.40	0/989	0.54	0/1340
1	3-c	0.40	0/989	0.54	0/1340
1	3-d	0.40	0/989	0.54	0/1340
1	3-e	0.40	0/989	0.54	0/1340
1	3-f	0.40	0/989	0.54	0/1340
2	1-A	0.53	0/3541	0.58	1/4792 (0.0%)
2	1-B	0.53	0/3541	0.58	1/4792 (0.0%)
2	1-C	0.53	0/3541	0.58	1/4792 (0.0%)
2	1-D	0.53	0/3541	0.58	1/4792 (0.0%)
2	1-E	0.53	0/3541	0.58	1/4792 (0.0%)
2	1-F	0.53	0/3541	0.58	1/4792 (0.0%)
2	2-A	0.53	0/3541	0.58	1/4792 (0.0%)
2	2-B	0.53	0/3541	0.58	1/4792 (0.0%)
2	2-C	0.53	0/3541	0.58	1/4792 (0.0%)
2	2-D	0.53	0/3541	0.58	1/4792 (0.0%)
2	2-E	0.53	0/3541	0.58	1/4792 (0.0%)
2	2-F	0.53	0/3541	0.58	1/4792 (0.0%)
2	3-A	0.53	0/3541	0.58	1/4792 (0.0%)
2	3-B	0.53	0/3541	0.58	1/4792 (0.0%)
2	3-C	0.53	0/3541	0.58	1/4792 (0.0%)
2	3-D	0.53	0/3541	0.58	1/4792 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
2	3-E	0.54	0/3541	0.58	1/4792 (0.0%)
2	3-F	0.53	0/3541	0.58	1/4792 (0.0%)
All	All	0.51	0/81540	0.57	18/110376 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	1-A	0	1
2	1-B	0	1
2	1-C	0	1
2	1-D	0	1
2	1-E	0	1
2	1-F	0	1
2	2-A	0	1
2	2-B	0	1
2	2-C	0	1
2	2-D	0	1
2	2-E	0	1
2	2-F	0	1
2	3-A	0	1
2	3-B	0	1
2	3-C	0	1
2	3-D	0	1
2	3-E	0	1
2	3-F	0	1
All	All	0	18

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3-A	125	LEU	CA-CB-CG	-5.15	103.45	115.30
2	2-B	125	LEU	CA-CB-CG	-5.14	103.48	115.30
2	2-F	125	LEU	CA-CB-CG	-5.14	103.48	115.30
2	1-C	125	LEU	CA-CB-CG	-5.14	103.49	115.30
2	1-F	125	LEU	CA-CB-CG	-5.13	103.50	115.30
2	2-C	125	LEU	CA-CB-CG	-5.13	103.50	115.30
2	1-A	125	LEU	CA-CB-CG	-5.12	103.51	115.30
2	3-D	125	LEU	CA-CB-CG	-5.12	103.51	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1-E	125	LEU	CA-CB-CG	-5.12	103.52	115.30
2	2-D	125	LEU	CA-CB-CG	-5.12	103.52	115.30
2	3-C	125	LEU	CA-CB-CG	-5.12	103.52	115.30
2	1-B	125	LEU	CA-CB-CG	-5.12	103.53	115.30
2	2-A	125	LEU	CA-CB-CG	-5.12	103.53	115.30
2	1-D	125	LEU	CA-CB-CG	-5.12	103.53	115.30
2	3-F	125	LEU	CA-CB-CG	-5.12	103.53	115.30
2	2-E	125	LEU	CA-CB-CG	-5.11	103.55	115.30
2	3-B	125	LEU	CA-CB-CG	-5.11	103.56	115.30
2	3-E	125	LEU	CA-CB-CG	-5.11	103.56	115.30

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1-A	240	ALA	Peptide
2	1-B	240	ALA	Peptide
2	1-C	240	ALA	Peptide
2	1-D	240	ALA	Peptide
2	1-E	240	ALA	Peptide
2	1-F	240	ALA	Peptide
2	2-A	240	ALA	Peptide
2	2-B	240	ALA	Peptide
2	2-C	240	ALA	Peptide
2	2-D	240	ALA	Peptide
2	2-E	240	ALA	Peptide
2	2-F	240	ALA	Peptide
2	3-A	240	ALA	Peptide
2	3-B	240	ALA	Peptide
2	3-C	240	ALA	Peptide
2	3-D	240	ALA	Peptide
2	3-E	240	ALA	Peptide
2	3-F	240	ALA	Peptide

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	1-a	977	0	997	0	0
1	1-b	977	0	997	0	0
1	1-c	977	0	997	0	0
1	1-d	977	0	997	0	0
1	1-e	977	0	997	0	0
1	1-f	977	0	997	0	0
1	2-a	977	0	997	0	0
1	2-b	977	0	997	0	0
1	2-c	977	0	997	0	0
1	2-d	977	0	997	0	0
1	2-e	977	0	997	0	0
1	2-f	977	0	997	0	0
1	3-a	977	0	997	0	0
1	3-b	977	0	997	0	0
1	3-c	977	0	997	0	0
1	3-d	977	0	997	0	0
1	3-e	977	0	997	0	0
1	3-f	977	0	997	0	0
2	1-A	3453	0	3372	31	0
2	1-B	3453	0	3372	31	0
2	1-C	3453	0	3372	26	0
2	1-D	3453	0	3372	29	0
2	1-E	3453	0	3372	31	0
2	1-F	3453	0	3372	28	0
2	2-A	3453	0	3372	29	0
2	2-B	3453	0	3372	32	0
2	2-C	3453	0	3372	26	0
2	2-D	3453	0	3372	30	0
2	2-E	3453	0	3372	28	0
2	2-F	3453	0	3372	28	0
2	3-A	3453	0	3372	32	0
2	3-B	3453	0	3372	28	0
2	3-C	3453	0	3372	28	0
2	3-D	3453	0	3372	28	0
2	3-E	3453	0	3372	25	0
2	3-F	3453	0	3372	32	0
All	All	79740	0	78642	522	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 7.

All (522) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:365:GLN:NE2	2:C:383:TYR:OH	2.28	0.67
2:D:365:GLN:NE2	2:D:383:TYR:OH	2.28	0.67
2:D:365:GLN:NE2	2:D:383:TYR:OH	2.28	0.67
2:C:365:GLN:NE2	2:C:383:TYR:OH	2.28	0.67
2:B:365:GLN:NE2	2:B:383:TYR:OH	2.28	0.67
2:C:365:GLN:NE2	2:C:383:TYR:OH	2.28	0.67
2:B:365:GLN:NE2	2:B:383:TYR:OH	2.28	0.67
2:D:365:GLN:NE2	2:D:383:TYR:OH	2.28	0.67
2:E:365:GLN:NE2	2:E:383:TYR:OH	2.28	0.67
2:B:365:GLN:NE2	2:B:383:TYR:OH	2.28	0.67
2:E:365:GLN:NE2	2:E:383:TYR:OH	2.28	0.66
2:A:365:GLN:NE2	2:A:383:TYR:OH	2.28	0.66
2:A:365:GLN:NE2	2:A:383:TYR:OH	2.28	0.66
2:F:365:GLN:NE2	2:F:383:TYR:OH	2.28	0.66
2:E:365:GLN:NE2	2:E:383:TYR:OH	2.28	0.66
2:F:365:GLN:NE2	2:F:383:TYR:OH	2.28	0.66
2:A:365:GLN:NE2	2:A:383:TYR:OH	2.28	0.66
2:F:365:GLN:NE2	2:F:383:TYR:OH	2.28	0.66
2:B:133:GLU:HG3	2:B:135:ALA:H	1.63	0.64
2:B:133:GLU:HG3	2:B:135:ALA:H	1.63	0.64
2:C:133:GLU:HG3	2:C:135:ALA:H	1.63	0.64
2:A:133:GLU:HG3	2:A:135:ALA:H	1.63	0.64
2:A:133:GLU:HG3	2:A:135:ALA:H	1.63	0.64
2:B:133:GLU:HG3	2:B:135:ALA:H	1.63	0.64
2:A:133:GLU:HG3	2:A:135:ALA:H	1.63	0.64
2:C:133:GLU:HG3	2:C:135:ALA:H	1.63	0.64
2:D:133:GLU:HG3	2:D:135:ALA:H	1.63	0.63
2:F:133:GLU:HG3	2:F:135:ALA:H	1.63	0.63
2:F:133:GLU:HG3	2:F:135:ALA:H	1.63	0.63
2:C:133:GLU:HG3	2:C:135:ALA:H	1.63	0.63
2:D:133:GLU:HG3	2:D:135:ALA:H	1.63	0.63
2:E:133:GLU:HG3	2:E:135:ALA:H	1.63	0.63
2:F:133:GLU:HG3	2:F:135:ALA:H	1.63	0.63
2:D:133:GLU:HG3	2:D:135:ALA:H	1.63	0.62
2:E:133:GLU:HG3	2:E:135:ALA:H	1.63	0.62
2:E:133:GLU:HG3	2:E:135:ALA:H	1.63	0.62
2:D:370:PHE:HB2	2:D:380:GLU:HG3	1.83	0.61
2:C:370:PHE:HB2	2:C:380:GLU:HG3	1.83	0.61
2:D:370:PHE:HB2	2:D:380:GLU:HG3	1.83	0.61
2:C:370:PHE:HB2	2:C:380:GLU:HG3	1.83	0.61
2:C:370:PHE:HB2	2:C:380:GLU:HG3	1.83	0.61
2:E:370:PHE:HB2	2:E:380:GLU:HG3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:370:PHE:HB2	2:D:380:GLU:HG3	1.83	0.61
2:B:370:PHE:HB2	2:B:380:GLU:HG3	1.83	0.61
2:B:370:PHE:HB2	2:B:380:GLU:HG3	1.83	0.60
2:E:370:PHE:HB2	2:E:380:GLU:HG3	1.83	0.60
2:B:370:PHE:HB2	2:B:380:GLU:HG3	1.83	0.60
2:E:370:PHE:HB2	2:E:380:GLU:HG3	1.83	0.60
2:A:370:PHE:HB2	2:A:380:GLU:HG3	1.83	0.60
2:F:370:PHE:HB2	2:F:380:GLU:HG3	1.83	0.60
2:F:370:PHE:HB2	2:F:380:GLU:HG3	1.83	0.60
2:A:370:PHE:HB2	2:A:380:GLU:HG3	1.83	0.60
2:A:370:PHE:HB2	2:A:380:GLU:HG3	1.83	0.59
2:F:370:PHE:HB2	2:F:380:GLU:HG3	1.83	0.59
2:E:193:VAL:HG23	2:E:238:LEU:HB3	1.87	0.57
2:D:193:VAL:HG23	2:D:238:LEU:HB3	1.87	0.57
2:E:193:VAL:HG23	2:E:238:LEU:HB3	1.87	0.57
2:D:193:VAL:HG23	2:D:238:LEU:HB3	1.87	0.57
2:C:193:VAL:HG23	2:C:238:LEU:HB3	1.87	0.57
2:F:193:VAL:HG23	2:F:238:LEU:HB3	1.87	0.56
2:F:193:VAL:HG23	2:F:238:LEU:HB3	1.87	0.56
2:D:193:VAL:HG23	2:D:238:LEU:HB3	1.87	0.56
2:E:193:VAL:HG23	2:E:238:LEU:HB3	1.87	0.56
2:F:193:VAL:HG23	2:F:238:LEU:HB3	1.87	0.56
2:A:193:VAL:HG23	2:A:238:LEU:HB3	1.87	0.56
2:C:193:VAL:HG23	2:C:238:LEU:HB3	1.87	0.56
2:C:193:VAL:HG23	2:C:238:LEU:HB3	1.87	0.56
2:A:193:VAL:HG23	2:A:238:LEU:HB3	1.87	0.56
2:B:193:VAL:HG23	2:B:238:LEU:HB3	1.87	0.55
2:B:193:VAL:HG23	2:B:238:LEU:HB3	1.87	0.55
2:B:193:VAL:HG23	2:B:238:LEU:HB3	1.87	0.55
2:A:193:VAL:HG23	2:A:238:LEU:HB3	1.87	0.55
2:C:162:ASN:HA	2:C:276:ASN:HD22	1.72	0.55
2:D:162:ASN:HA	2:D:276:ASN:HD22	1.72	0.55
2:F:162:ASN:HA	2:F:276:ASN:HD22	1.72	0.55
2:A:162:ASN:HA	2:A:276:ASN:HD22	1.72	0.55
2:E:162:ASN:HA	2:E:276:ASN:HD22	1.72	0.55
2:F:402:VAL:O	2:F:406:GLN:HB2	2.07	0.55
2:A:162:ASN:HA	2:A:276:ASN:HD22	1.72	0.55
2:A:402:VAL:O	2:A:406:GLN:HB2	2.07	0.55
2:A:402:VAL:O	2:A:406:GLN:HB2	2.07	0.55
2:B:162:ASN:HA	2:B:276:ASN:HD22	1.72	0.55
2:B:402:VAL:O	2:B:406:GLN:HB2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:402:VAL:O	2:B:406:GLN:HB2	2.07	0.55
2:E:402:VAL:O	2:E:406:GLN:HB2	2.07	0.55
2:E:402:VAL:O	2:E:406:GLN:HB2	2.07	0.55
2:C:402:VAL:O	2:C:406:GLN:HB2	2.07	0.54
2:F:162:ASN:HA	2:F:276:ASN:HD22	1.72	0.54
2:F:402:VAL:O	2:F:406:GLN:HB2	2.07	0.54
2:E:402:VAL:O	2:E:406:GLN:HB2	2.07	0.54
2:B:162:ASN:HA	2:B:276:ASN:HD22	1.72	0.54
2:D:162:ASN:HA	2:D:276:ASN:HD22	1.72	0.54
2:A:402:VAL:O	2:A:406:GLN:HB2	2.07	0.54
2:C:162:ASN:HA	2:C:276:ASN:HD22	1.72	0.54
2:C:162:ASN:HA	2:C:276:ASN:HD22	1.72	0.54
2:C:402:VAL:O	2:C:406:GLN:HB2	2.07	0.54
2:E:162:ASN:HA	2:E:276:ASN:HD22	1.72	0.54
2:C:402:VAL:O	2:C:406:GLN:HB2	2.07	0.54
2:B:162:ASN:HA	2:B:276:ASN:HD22	1.72	0.54
2:B:402:VAL:O	2:B:406:GLN:HB2	2.07	0.54
2:D:162:ASN:HA	2:D:276:ASN:HD22	1.72	0.54
2:F:162:ASN:HA	2:F:276:ASN:HD22	1.72	0.54
2:F:402:VAL:O	2:F:406:GLN:HB2	2.07	0.54
2:A:162:ASN:HA	2:A:276:ASN:HD22	1.72	0.54
2:D:402:VAL:O	2:D:406:GLN:HB2	2.07	0.54
2:D:402:VAL:O	2:D:406:GLN:HB2	2.07	0.54
2:D:402:VAL:O	2:D:406:GLN:HB2	2.07	0.53
2:E:162:ASN:HA	2:E:276:ASN:HD22	1.72	0.53
2:E:200:ILE:HD13	2:E:209:ILE:HD11	1.93	0.51
2:E:200:ILE:HD13	2:E:209:ILE:HD11	1.93	0.51
2:A:200:ILE:HD13	2:A:209:ILE:HD11	1.93	0.51
2:C:200:ILE:HD13	2:C:209:ILE:HD11	1.93	0.51
2:F:200:ILE:HD13	2:F:209:ILE:HD11	1.93	0.51
2:A:200:ILE:HD13	2:A:209:ILE:HD11	1.93	0.51
2:A:200:ILE:HD13	2:A:209:ILE:HD11	1.93	0.51
2:B:200:ILE:HD13	2:B:209:ILE:HD11	1.93	0.51
2:F:200:ILE:HD13	2:F:209:ILE:HD11	1.93	0.51
2:D:200:ILE:HD13	2:D:209:ILE:HD11	1.93	0.51
2:E:200:ILE:HD13	2:E:209:ILE:HD11	1.93	0.51
2:C:200:ILE:HD13	2:C:209:ILE:HD11	1.93	0.51
2:B:200:ILE:HD13	2:B:209:ILE:HD11	1.93	0.51
2:C:200:ILE:HD13	2:C:209:ILE:HD11	1.93	0.51
2:F:200:ILE:HD13	2:F:209:ILE:HD11	1.93	0.51
2:B:200:ILE:HD13	2:B:209:ILE:HD11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:200:ILE:HD13	2:D:209:ILE:HD11	1.93	0.51
2:D:200:ILE:HD13	2:D:209:ILE:HD11	1.93	0.51
2:F:454:VAL:HG22	2:F:466:VAL:HG22	1.93	0.51
2:E:454:VAL:HG22	2:E:466:VAL:HG22	1.93	0.50
2:F:454:VAL:HG22	2:F:466:VAL:HG22	1.93	0.50
2:E:454:VAL:HG22	2:E:466:VAL:HG22	1.93	0.50
2:D:123:GLU:O	2:D:127:ASP:CB	2.60	0.50
2:E:123:GLU:O	2:E:127:ASP:CB	2.60	0.50
2:E:123:GLU:O	2:E:127:ASP:CB	2.60	0.50
2:F:454:VAL:HG22	2:F:466:VAL:HG22	1.93	0.50
2:D:123:GLU:O	2:D:127:ASP:CB	2.60	0.50
2:A:454:VAL:HG22	2:A:466:VAL:HG22	1.93	0.50
2:C:123:GLU:O	2:C:127:ASP:CB	2.60	0.50
2:B:265:VAL:HG13	2:B:271:HIS:HB2	1.94	0.50
2:E:454:VAL:HG22	2:E:466:VAL:HG22	1.93	0.50
2:F:123:GLU:O	2:F:127:ASP:CB	2.60	0.50
2:B:265:VAL:HG13	2:B:271:HIS:HB2	1.94	0.50
2:C:454:VAL:HG22	2:C:466:VAL:HG22	1.93	0.50
2:F:123:GLU:O	2:F:127:ASP:CB	2.60	0.50
2:B:265:VAL:HG13	2:B:271:HIS:HB2	1.94	0.50
2:D:454:VAL:HG22	2:D:466:VAL:HG22	1.93	0.50
2:C:265:VAL:HG13	2:C:271:HIS:HB2	1.94	0.49
2:C:454:VAL:HG22	2:C:466:VAL:HG22	1.93	0.49
2:D:123:GLU:O	2:D:127:ASP:CB	2.60	0.49
2:A:265:VAL:HG13	2:A:271:HIS:HB2	1.95	0.49
2:B:123:GLU:O	2:B:127:ASP:CB	2.60	0.49
2:A:265:VAL:HG13	2:A:271:HIS:HB2	1.94	0.49
2:A:454:VAL:HG22	2:A:466:VAL:HG22	1.93	0.49
2:B:123:GLU:O	2:B:127:ASP:CB	2.60	0.49
2:A:123:GLU:O	2:A:127:ASP:CB	2.60	0.49
2:C:265:VAL:HG13	2:C:271:HIS:HB2	1.94	0.49
2:E:123:GLU:O	2:E:127:ASP:CB	2.60	0.49
2:A:454:VAL:HG22	2:A:466:VAL:HG22	1.93	0.49
2:B:454:VAL:HG22	2:B:466:VAL:HG22	1.93	0.49
2:A:265:VAL:HG13	2:A:271:HIS:HB2	1.94	0.49
2:A:123:GLU:O	2:A:127:ASP:CB	2.60	0.49
2:C:123:GLU:O	2:C:127:ASP:CB	2.60	0.49
2:C:265:VAL:HG13	2:C:271:HIS:HB2	1.94	0.49
2:C:123:GLU:O	2:C:127:ASP:CB	2.60	0.49
2:D:265:VAL:HG13	2:D:271:HIS:HB2	1.94	0.49
2:D:454:VAL:HG22	2:D:466:VAL:HG22	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:123:GLU:O	2:B:127:ASP:CB	2.60	0.49
2:F:265:VAL:HG13	2:F:271:HIS:HB2	1.94	0.49
2:B:454:VAL:HG22	2:B:466:VAL:HG22	1.93	0.49
2:C:454:VAL:HG22	2:C:466:VAL:HG22	1.93	0.49
2:F:265:VAL:HG13	2:F:271:HIS:HB2	1.94	0.49
2:E:265:VAL:HG13	2:E:271:HIS:HB2	1.94	0.49
2:D:265:VAL:HG13	2:D:271:HIS:HB2	1.94	0.49
2:F:265:VAL:HG13	2:F:271:HIS:HB2	1.94	0.49
2:F:123:GLU:O	2:F:127:ASP:CB	2.60	0.49
2:E:265:VAL:HG13	2:E:271:HIS:HB2	1.94	0.49
2:A:123:GLU:O	2:A:127:ASP:CB	2.60	0.48
2:D:454:VAL:HG22	2:D:466:VAL:HG22	1.93	0.48
2:D:265:VAL:HG13	2:D:271:HIS:HB2	1.94	0.48
2:E:265:VAL:HG13	2:E:271:HIS:HB2	1.94	0.48
2:B:454:VAL:HG22	2:B:466:VAL:HG22	1.93	0.48
2:B:353:SER:OG	2:B:354:ASP:N	2.49	0.46
2:D:353:SER:OG	2:D:354:ASP:N	2.49	0.46
2:F:353:SER:OG	2:F:354:ASP:N	2.49	0.46
2:A:353:SER:OG	2:A:354:ASP:N	2.49	0.46
2:A:353:SER:OG	2:A:354:ASP:N	2.49	0.46
2:B:353:SER:OG	2:B:354:ASP:N	2.49	0.46
2:A:353:SER:OG	2:A:354:ASP:N	2.49	0.46
2:C:353:SER:OG	2:C:354:ASP:N	2.49	0.46
2:D:175:LEU:HD23	2:D:175:LEU:HA	1.83	0.46
2:D:353:SER:OG	2:D:354:ASP:N	2.49	0.46
2:B:353:SER:OG	2:B:354:ASP:N	2.49	0.46
2:D:175:LEU:HD23	2:D:175:LEU:HA	1.83	0.46
2:E:175:LEU:HD23	2:E:175:LEU:HA	1.83	0.46
2:C:353:SER:OG	2:C:354:ASP:N	2.49	0.46
2:F:353:SER:OG	2:F:354:ASP:N	2.49	0.46
2:C:123:GLU:O	2:C:127:ASP:HB2	2.17	0.45
2:D:123:GLU:O	2:D:127:ASP:HB2	2.17	0.45
2:C:123:GLU:O	2:C:127:ASP:HB2	2.17	0.45
2:D:123:GLU:O	2:D:127:ASP:HB2	2.17	0.45
2:D:123:GLU:O	2:D:127:ASP:HB2	2.17	0.45
2:E:123:GLU:O	2:E:127:ASP:HB2	2.17	0.45
2:E:353:SER:OG	2:E:354:ASP:N	2.49	0.45
2:E:353:SER:OG	2:E:354:ASP:N	2.49	0.45
2:C:123:GLU:O	2:C:127:ASP:HB2	2.17	0.45
2:E:123:GLU:O	2:E:127:ASP:HB2	2.17	0.45
2:E:191:SER:OG	2:E:192:SER:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:191:SER:OG	2:F:192:SER:N	2.50	0.45
2:C:125:LEU:HD21	2:C:174:LEU:HB2	1.99	0.45
2:E:123:GLU:O	2:E:127:ASP:HB2	2.17	0.45
2:B:191:SER:OG	2:B:192:SER:N	2.50	0.45
2:B:272:TYR:HE2	2:B:324:LYS:HE2	1.82	0.45
2:B:123:GLU:O	2:B:127:ASP:HB2	2.17	0.45
2:D:191:SER:OG	2:D:192:SER:N	2.49	0.45
2:E:191:SER:OG	2:E:192:SER:N	2.50	0.45
2:B:123:GLU:O	2:B:127:ASP:HB2	2.17	0.45
2:C:175:LEU:HA	2:C:175:LEU:HD23	1.83	0.45
2:D:191:SER:OG	2:D:192:SER:N	2.50	0.45
2:A:191:SER:OG	2:A:192:SER:N	2.50	0.45
2:B:123:GLU:O	2:B:127:ASP:HB2	2.17	0.45
2:C:353:SER:OG	2:C:354:ASP:N	2.49	0.45
2:F:123:GLU:O	2:F:127:ASP:HB2	2.17	0.45
2:F:353:SER:OG	2:F:354:ASP:N	2.49	0.45
2:B:125:LEU:HD21	2:B:174:LEU:HB2	1.99	0.45
2:E:191:SER:OG	2:E:192:SER:N	2.49	0.45
2:A:123:GLU:O	2:A:127:ASP:HB2	2.17	0.45
2:A:272:TYR:HE2	2:A:324:LYS:HE2	1.82	0.45
2:D:175:LEU:HD23	2:D:175:LEU:HA	1.83	0.45
2:F:272:TYR:HE2	2:F:324:LYS:HE2	1.82	0.45
2:B:272:TYR:HE2	2:B:324:LYS:HE2	1.82	0.45
2:E:272:TYR:HE2	2:E:324:LYS:HE2	1.82	0.45
2:F:191:SER:OG	2:F:192:SER:N	2.50	0.45
2:F:272:TYR:HE2	2:F:324:LYS:HE2	1.82	0.45
2:C:125:LEU:HD21	2:C:174:LEU:HB2	1.99	0.45
2:C:191:SER:OG	2:C:192:SER:N	2.50	0.45
2:D:353:SER:OG	2:D:354:ASP:N	2.49	0.45
2:F:123:GLU:O	2:F:127:ASP:HB2	2.17	0.45
2:C:125:LEU:HD21	2:C:174:LEU:HB2	1.99	0.45
2:D:125:LEU:HD21	2:D:174:LEU:HB2	1.99	0.45
2:E:272:TYR:HE2	2:E:324:LYS:HE2	1.82	0.45
2:A:191:SER:OG	2:A:192:SER:N	2.50	0.45
2:A:272:TYR:HE2	2:A:324:LYS:HE2	1.82	0.45
2:D:125:LEU:HD21	2:D:174:LEU:HB2	1.99	0.45
2:E:353:SER:OG	2:E:354:ASP:N	2.49	0.45
2:A:272:TYR:HE2	2:A:324:LYS:HE2	1.82	0.45
2:D:272:TYR:HE2	2:D:324:LYS:HE2	1.82	0.45
2:F:280:ALA:O	2:F:283:THR:OG1	2.30	0.45
2:F:272:TYR:HE2	2:F:324:LYS:HE2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:125:LEU:HD21	2:B:174:LEU:HB2	1.99	0.45
2:A:123:GLU:O	2:A:127:ASP:HB2	2.17	0.45
2:A:191:SER:OG	2:A:192:SER:N	2.50	0.45
2:E:272:TYR:HE2	2:E:324:LYS:HE2	1.82	0.45
2:C:272:TYR:HE2	2:C:324:LYS:HE2	1.82	0.44
2:B:191:SER:OG	2:B:192:SER:N	2.50	0.44
2:C:398:LEU:HD23	2:C:398:LEU:HA	1.86	0.44
2:D:272:TYR:HE2	2:D:324:LYS:HE2	1.82	0.44
2:B:272:TYR:HE2	2:B:324:LYS:HE2	1.82	0.44
2:C:272:TYR:HE2	2:C:324:LYS:HE2	1.82	0.44
2:D:125:LEU:HD21	2:D:174:LEU:HB2	1.99	0.44
2:F:191:SER:OG	2:F:192:SER:N	2.50	0.44
2:C:272:TYR:HE2	2:C:324:LYS:HE2	1.82	0.44
2:F:123:GLU:O	2:F:127:ASP:HB2	2.17	0.44
2:A:125:LEU:HD21	2:A:174:LEU:HB2	1.99	0.44
2:B:125:LEU:HD21	2:B:174:LEU:HB2	1.99	0.44
2:D:272:TYR:HE2	2:D:324:LYS:HE2	1.82	0.44
2:E:125:LEU:HD21	2:E:174:LEU:HB2	1.99	0.44
2:E:175:LEU:HA	2:E:175:LEU:HD23	1.83	0.44
2:B:175:LEU:HA	2:B:175:LEU:HD23	1.83	0.44
2:C:124:LEU:HA	2:C:124:LEU:HD23	1.88	0.44
2:A:280:ALA:O	2:A:283:THR:OG1	2.30	0.44
2:C:191:SER:OG	2:C:192:SER:N	2.50	0.44
2:E:405:LEU:HD23	2:E:405:LEU:HA	1.86	0.44
2:A:123:GLU:O	2:A:127:ASP:HB2	2.16	0.44
2:B:419:LEU:HD23	2:B:419:LEU:HA	1.86	0.44
2:A:125:LEU:HD21	2:A:174:LEU:HB2	1.99	0.44
2:E:125:LEU:HD21	2:E:174:LEU:HB2	1.99	0.44
2:F:125:LEU:HD21	2:F:174:LEU:HB2	1.99	0.44
2:D:398:LEU:HA	2:D:398:LEU:HD23	1.86	0.44
2:F:125:LEU:HD21	2:F:174:LEU:HB2	1.99	0.44
2:D:125:LEU:HA	2:D:125:LEU:HD23	1.86	0.44
2:A:125:LEU:HD21	2:A:174:LEU:HB2	1.99	0.44
2:D:405:LEU:HA	2:D:405:LEU:HD23	1.86	0.43
2:F:405:LEU:HA	2:F:405:LEU:HD23	1.86	0.43
2:B:191:SER:OG	2:B:192:SER:N	2.49	0.43
2:D:205:GLU:HG3	2:D:208:ASN:HD22	1.83	0.43
2:E:205:GLU:HG3	2:E:208:ASN:HD22	1.83	0.43
2:E:195:PRO:HB3	2:E:202:SER:HA	2.00	0.43
2:A:205:GLU:HG3	2:A:208:ASN:HD22	1.83	0.43
2:B:125:LEU:HD23	2:B:125:LEU:HA	1.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:205:GLU:HG3	2:B:208:ASN:HD22	1.83	0.43
2:E:195:PRO:HB3	2:E:202:SER:HA	2.00	0.43
2:F:125:LEU:HD21	2:F:174:LEU:HB2	1.99	0.43
2:F:195:PRO:HB3	2:F:202:SER:HA	2.00	0.43
2:B:124:LEU:HA	2:B:124:LEU:HD23	1.88	0.43
2:F:205:GLU:HG3	2:F:208:ASN:HD22	1.84	0.43
2:C:205:GLU:HG3	2:C:208:ASN:HD22	1.83	0.43
2:C:205:GLU:HG3	2:C:208:ASN:HD22	1.83	0.43
2:D:195:PRO:HB3	2:D:202:SER:HA	2.00	0.43
2:A:195:PRO:HB3	2:A:202:SER:HA	2.00	0.43
2:D:195:PRO:HB3	2:D:202:SER:HA	2.00	0.43
2:E:125:LEU:HD21	2:E:174:LEU:HB2	1.99	0.43
2:E:195:PRO:HB3	2:E:202:SER:HA	2.00	0.43
2:B:195:PRO:HB3	2:B:202:SER:HA	2.00	0.43
2:D:191:SER:OG	2:D:192:SER:N	2.50	0.43
2:D:419:LEU:HA	2:D:419:LEU:HD23	1.86	0.43
2:C:175:LEU:HD23	2:C:175:LEU:HA	1.83	0.43
2:F:205:GLU:HG3	2:F:208:ASN:HD22	1.83	0.43
2:D:124:LEU:HD23	2:D:124:LEU:HA	1.89	0.43
2:F:205:GLU:HG3	2:F:208:ASN:HD22	1.83	0.43
2:A:205:GLU:HG3	2:A:208:ASN:HD22	1.83	0.43
2:B:195:PRO:HB3	2:B:202:SER:HA	2.00	0.43
2:C:195:PRO:HB3	2:C:202:SER:HA	2.00	0.43
2:E:205:GLU:HG3	2:E:208:ASN:HD22	1.84	0.43
2:D:195:PRO:HB3	2:D:202:SER:HA	2.00	0.43
2:C:191:SER:OG	2:C:192:SER:N	2.50	0.43
2:B:205:GLU:HG3	2:B:208:ASN:HD22	1.83	0.43
2:D:395:ILE:HA	2:D:395:ILE:HD13	1.83	0.43
2:F:175:LEU:HA	2:F:175:LEU:HD23	1.83	0.43
2:A:195:PRO:HB3	2:A:202:SER:HA	2.00	0.43
2:D:205:GLU:HG3	2:D:208:ASN:HD22	1.83	0.43
2:E:205:GLU:HG3	2:E:208:ASN:HD22	1.83	0.43
2:F:195:PRO:HB3	2:F:202:SER:HA	2.00	0.43
2:C:195:PRO:HB3	2:C:202:SER:HA	2.00	0.43
2:E:163:TYR:O	2:E:192:SER:OG	2.30	0.43
2:A:398:LEU:HD23	2:A:398:LEU:HA	1.86	0.43
2:B:195:PRO:HB3	2:B:202:SER:HA	2.00	0.42
2:E:175:LEU:HA	2:E:175:LEU:HD23	1.83	0.42
2:A:205:GLU:HG3	2:A:208:ASN:HD22	1.83	0.42
2:C:195:PRO:HB3	2:C:202:SER:HA	2.00	0.42
2:F:377:LYS:HA	2:F:377:LYS:HD2	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:398:LEU:HA	2:E:398:LEU:HD23	1.86	0.42
2:E:377:LYS:HD2	2:E:377:LYS:HA	1.88	0.42
2:A:125:LEU:HD23	2:A:125:LEU:HA	1.86	0.42
2:B:175:LEU:HA	2:B:175:LEU:HD23	1.83	0.42
2:A:195:PRO:HB3	2:A:202:SER:HA	2.00	0.42
2:A:124:LEU:HA	2:A:124:LEU:HD23	1.88	0.42
2:B:205:GLU:HG3	2:B:208:ASN:HD22	1.83	0.42
2:E:125:LEU:HD23	2:E:125:LEU:HA	1.86	0.42
2:A:175:LEU:HA	2:A:175:LEU:HD23	1.83	0.42
2:C:205:GLU:HG3	2:C:208:ASN:HD22	1.83	0.42
2:F:195:PRO:HB3	2:F:202:SER:HA	2.00	0.42
2:C:216:PHE:HA	2:C:221:TYR:HD2	1.85	0.42
2:B:377:LYS:HA	2:B:377:LYS:HD2	1.88	0.42
2:C:125:LEU:HA	2:C:125:LEU:HD23	1.86	0.42
2:A:395:ILE:HA	2:A:395:ILE:HD13	1.83	0.42
2:B:419:LEU:HD23	2:B:419:LEU:HA	1.86	0.42
2:C:216:PHE:HA	2:C:221:TYR:HD2	1.85	0.42
2:C:419:LEU:HD23	2:C:419:LEU:HA	1.86	0.42
2:B:265:VAL:HG11	2:B:272:TYR:CE1	2.55	0.42
2:C:90:GLN:O	2:C:94:SER:HB3	2.20	0.42
2:D:216:PHE:HA	2:D:221:TYR:HD2	1.85	0.42
2:B:216:PHE:HA	2:B:221:TYR:HD2	1.85	0.42
2:C:422:GLU:O	2:C:426:TRP:HB2	2.20	0.42
2:E:265:VAL:HG11	2:E:272:TYR:CE1	2.55	0.42
2:B:216:PHE:HA	2:B:221:TYR:HD2	1.85	0.42
2:C:395:ILE:HA	2:C:395:ILE:HD13	1.83	0.42
2:F:216:PHE:HA	2:F:221:TYR:HD2	1.85	0.42
2:A:265:VAL:HG11	2:A:272:TYR:CE1	2.55	0.42
2:A:395:ILE:HD13	2:A:395:ILE:HA	1.83	0.42
2:A:422:GLU:O	2:A:426:TRP:HB2	2.20	0.42
2:B:90:GLN:O	2:B:94:SER:HB3	2.20	0.42
2:B:216:PHE:HA	2:B:221:TYR:HD2	1.85	0.41
2:B:422:GLU:O	2:B:426:TRP:HB2	2.20	0.41
2:C:265:VAL:HG11	2:C:272:TYR:CE1	2.55	0.41
2:D:205:GLU:HG3	2:D:208:ASN:HD22	1.84	0.41
2:A:395:ILE:HA	2:A:395:ILE:HD13	1.83	0.41
2:B:206:LEU:HD23	2:B:206:LEU:HA	1.92	0.41
2:C:265:VAL:HG11	2:C:272:TYR:CE1	2.55	0.41
2:D:90:GLN:O	2:D:94:SER:HB3	2.20	0.41
2:F:422:GLU:O	2:F:426:TRP:HB2	2.20	0.41
2:B:280:ALA:O	2:B:283:THR:OG1	2.30	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:216:PHE:HA	2:D:221:TYR:HD2	1.85	0.41
2:D:265:VAL:HG11	2:D:272:TYR:CE1	2.55	0.41
2:E:422:GLU:O	2:E:426:TRP:HB2	2.20	0.41
2:A:216:PHE:HA	2:A:221:TYR:HD2	1.85	0.41
2:C:216:PHE:HA	2:C:221:TYR:HD2	1.85	0.41
2:E:422:GLU:O	2:E:426:TRP:HB2	2.20	0.41
2:F:265:VAL:HG11	2:F:272:TYR:CE1	2.55	0.41
2:E:125:LEU:HA	2:E:125:LEU:HD23	1.86	0.41
2:E:265:VAL:HG11	2:E:272:TYR:CE1	2.55	0.41
2:E:422:GLU:O	2:E:426:TRP:HB2	2.20	0.41
2:F:216:PHE:HA	2:F:221:TYR:HD2	1.85	0.41
2:A:422:GLU:O	2:A:426:TRP:HB2	2.20	0.41
2:F:265:VAL:HG11	2:F:272:TYR:CE1	2.55	0.41
2:D:422:GLU:O	2:D:426:TRP:HB2	2.20	0.41
2:F:124:LEU:HA	2:F:124:LEU:HD23	1.89	0.41
2:F:216:PHE:HA	2:F:221:TYR:HD2	1.85	0.41
2:F:398:LEU:HA	2:F:398:LEU:HD23	1.86	0.41
2:A:216:PHE:HA	2:A:221:TYR:HD2	1.85	0.41
2:E:216:PHE:HA	2:E:221:TYR:HD2	1.85	0.41
2:E:419:LEU:HA	2:E:419:LEU:HD23	1.86	0.41
2:E:90:GLN:O	2:E:94:SER:CB	2.69	0.41
2:F:175:LEU:HA	2:F:175:LEU:HD23	1.83	0.41
2:A:265:VAL:HG11	2:A:272:TYR:CE1	2.55	0.41
2:C:422:GLU:O	2:C:426:TRP:HB2	2.20	0.41
2:D:265:VAL:HG11	2:D:272:TYR:CE1	2.55	0.41
2:D:334:ARG:NH1	2:D:338:GLU:HB2	2.36	0.41
2:B:90:GLN:O	2:B:94:SER:HB3	2.20	0.41
2:C:334:ARG:NH1	2:C:338:GLU:HB2	2.36	0.41
2:D:405:LEU:HA	2:D:405:LEU:HD23	1.86	0.41
2:F:422:GLU:O	2:F:426:TRP:HB2	2.20	0.41
2:C:422:GLU:O	2:C:426:TRP:HB2	2.20	0.41
2:E:265:VAL:HG11	2:E:272:TYR:CE1	2.55	0.41
2:F:124:LEU:HD23	2:F:124:LEU:HA	1.88	0.41
2:F:90:GLN:O	2:F:94:SER:HB3	2.20	0.41
2:A:216:PHE:HA	2:A:221:TYR:HD2	1.85	0.41
2:A:90:GLN:O	2:A:94:SER:HB3	2.20	0.41
2:C:90:GLN:O	2:C:94:SER:HB3	2.21	0.41
2:D:280:ALA:O	2:D:283:THR:OG1	2.30	0.41
2:D:334:ARG:NH1	2:D:338:GLU:HB2	2.36	0.41
2:B:175:LEU:HA	2:B:175:LEU:HD23	1.83	0.41
2:B:265:VAL:HG11	2:B:272:TYR:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:334:ARG:NH1	2:C:338:GLU:HB2	2.36	0.41
2:C:405:LEU:HD23	2:C:405:LEU:HA	1.86	0.41
2:E:216:PHE:HA	2:E:221:TYR:HD2	1.85	0.41
2:F:90:GLN:O	2:F:94:SER:CB	2.69	0.41
2:C:90:GLN:O	2:C:94:SER:CB	2.69	0.41
2:D:422:GLU:O	2:D:426:TRP:HB2	2.20	0.41
2:E:395:ILE:HA	2:E:395:ILE:HD13	1.83	0.41
2:A:175:LEU:HA	2:A:175:LEU:HD23	1.83	0.41
2:B:90:GLN:O	2:B:94:SER:CB	2.69	0.41
2:D:422:GLU:O	2:D:426:TRP:HB2	2.20	0.41
2:F:90:GLN:O	2:F:94:SER:CB	2.69	0.41
2:B:422:GLU:O	2:B:426:TRP:HB2	2.20	0.41
2:C:265:VAL:HG11	2:C:272:TYR:CE1	2.55	0.41
2:D:265:VAL:HG11	2:D:272:TYR:CE1	2.55	0.41
2:D:405:LEU:HD23	2:D:405:LEU:HA	1.86	0.41
2:D:90:GLN:O	2:D:94:SER:HB3	2.20	0.41
2:E:90:GLN:O	2:E:94:SER:HB3	2.20	0.41
2:A:422:GLU:O	2:A:426:TRP:HB2	2.20	0.41
2:A:90:GLN:O	2:A:94:SER:CB	2.69	0.41
2:B:398:LEU:HA	2:B:398:LEU:HD23	1.86	0.41
2:C:175:LEU:HA	2:C:175:LEU:HD23	1.83	0.41
2:C:334:ARG:NH1	2:C:338:GLU:HB2	2.36	0.41
2:E:90:GLN:O	2:E:94:SER:CB	2.69	0.41
2:A:265:VAL:HG11	2:A:272:TYR:CE1	2.55	0.41
2:B:405:LEU:HD23	2:B:405:LEU:HA	1.86	0.41
2:B:422:GLU:O	2:B:426:TRP:HB2	2.20	0.41
2:B:481:PHE:HD1	2:B:481:PHE:HA	1.75	0.41
2:D:216:PHE:HA	2:D:221:TYR:HD2	1.85	0.41
2:D:334:ARG:NH1	2:D:338:GLU:HB2	2.36	0.41
2:E:334:ARG:NH1	2:E:338:GLU:HB2	2.36	0.41
2:F:422:GLU:O	2:F:426:TRP:HB2	2.20	0.41
2:E:334:ARG:NH1	2:E:338:GLU:HB2	2.36	0.41
2:A:216:PHE:O	2:A:225:ARG:NH1	2.53	0.41
2:B:334:ARG:NH1	2:B:338:GLU:HB2	2.36	0.41
2:C:377:LYS:HA	2:C:377:LYS:HD2	1.88	0.41
2:D:90:GLN:O	2:D:94:SER:HB3	2.20	0.41
2:E:481:PHE:HD1	2:E:481:PHE:HA	1.75	0.41
2:E:90:GLN:O	2:E:94:SER:HB3	2.20	0.41
2:F:265:VAL:HG11	2:F:272:TYR:CE1	2.55	0.41
2:F:334:ARG:NH1	2:F:338:GLU:HB2	2.36	0.41
2:F:90:GLN:O	2:F:94:SER:CB	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:336:GLU:HG3	2:A:348:THR:HG21	2.03	0.41
2:B:334:ARG:NH1	2:B:338:GLU:HB2	2.36	0.41
2:E:216:PHE:HA	2:E:221:TYR:HD2	1.85	0.41
2:E:336:GLU:HG3	2:E:348:THR:HG21	2.03	0.41
2:E:405:LEU:HD23	2:E:405:LEU:HA	1.86	0.41
2:F:206:LEU:HA	2:F:206:LEU:HD23	1.92	0.41
2:A:163:TYR:O	2:A:192:SER:OG	2.30	0.41
2:B:265:VAL:HG11	2:B:272:TYR:CE1	2.55	0.41
2:D:125:LEU:HA	2:D:125:LEU:HD23	1.86	0.41
2:A:481:PHE:HA	2:A:481:PHE:HD1	1.75	0.41
2:B:90:GLN:O	2:B:94:SER:CB	2.69	0.41
2:E:90:GLN:O	2:E:94:SER:CB	2.69	0.41
2:A:90:GLN:O	2:A:94:SER:HB3	2.21	0.41
2:B:398:LEU:HD23	2:B:398:LEU:HA	1.86	0.41
2:C:398:LEU:HD23	2:C:398:LEU:HA	1.86	0.41
2:F:175:LEU:HA	2:F:175:LEU:HD23	1.83	0.41
2:A:175:LEU:HA	2:A:175:LEU:HD23	1.83	0.41
2:B:206:LEU:HA	2:B:206:LEU:HD23	1.92	0.41
2:B:336:GLU:HG3	2:B:348:THR:HG21	2.03	0.41
2:B:90:GLN:O	2:B:94:SER:HB3	2.20	0.41
2:F:310:LEU:HA	2:F:310:LEU:HD23	1.91	0.41
2:F:336:GLU:HG3	2:F:348:THR:HG21	2.03	0.41
2:B:395:ILE:HD13	2:B:395:ILE:HA	1.83	0.41
2:A:419:LEU:HD23	2:A:419:LEU:HA	1.86	0.41
2:B:334:ARG:NH1	2:B:338:GLU:HB2	2.36	0.41
2:D:90:GLN:O	2:D:94:SER:CB	2.69	0.41
2:F:310:LEU:HA	2:F:310:LEU:HD23	1.91	0.41
2:F:336:GLU:HG3	2:F:348:THR:HG21	2.03	0.41
2:A:90:GLN:O	2:A:94:SER:HB3	2.20	0.40
2:B:125:LEU:HD23	2:B:125:LEU:HA	1.86	0.40
2:E:336:GLU:HG3	2:E:348:THR:HG21	2.03	0.40
2:A:125:LEU:HD23	2:A:125:LEU:HA	1.86	0.40
2:F:405:LEU:HD23	2:F:405:LEU:HA	1.86	0.40
2:F:90:GLN:O	2:F:94:SER:HB3	2.20	0.40
2:A:336:GLU:HG3	2:A:348:THR:HG21	2.03	0.40
2:A:90:GLN:O	2:A:94:SER:CB	2.69	0.40
2:D:336:GLU:HG3	2:D:348:THR:HG21	2.03	0.40
2:E:336:GLU:HG3	2:E:348:THR:HG21	2.03	0.40
2:F:206:LEU:HA	2:F:206:LEU:HD23	1.92	0.40
2:F:216:PHE:O	2:F:225:ARG:NH1	2.54	0.40
2:A:336:GLU:HG3	2:A:348:THR:HG21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:334:ARG:NH1	2:A:338:GLU:HB2	2.36	0.40
2:B:90:GLN:O	2:B:94:SER:CB	2.69	0.40
2:A:310:LEU:HD23	2:A:310:LEU:HA	1.91	0.40
2:A:405:LEU:HA	2:A:405:LEU:HD23	1.86	0.40
2:A:206:LEU:HD23	2:A:206:LEU:HA	1.92	0.40
2:A:334:ARG:NH1	2:A:338:GLU:HB2	2.36	0.40
2:F:334:ARG:NH1	2:F:338:GLU:HB2	2.36	0.40
2:F:90:GLN:O	2:F:94:SER:HB3	2.20	0.40
2:A:124:LEU:HA	2:A:124:LEU:HD23	1.88	0.40
2:A:206:LEU:HA	2:A:206:LEU:HD23	1.92	0.40
2:C:90:GLN:O	2:C:94:SER:CB	2.69	0.40
2:D:377:LYS:HD2	2:D:377:LYS:HA	1.88	0.40
2:E:334:ARG:NH1	2:E:338:GLU:HB2	2.36	0.40
2:F:336:GLU:HG3	2:F:348:THR:HG21	2.03	0.40
2:F:398:LEU:HA	2:F:398:LEU:HD23	1.86	0.40
2:A:310:LEU:HD23	2:A:310:LEU:HA	1.91	0.40
2:D:90:GLN:O	2:D:94:SER:CB	2.69	0.40
2:B:336:GLU:HG3	2:B:348:THR:HG21	2.03	0.40
2:D:310:LEU:HD23	2:D:310:LEU:HA	1.91	0.40
2:A:216:PHE:O	2:A:225:ARG:NH1	2.54	0.40
2:B:405:LEU:HA	2:B:405:LEU:HD23	1.86	0.40
2:C:90:GLN:O	2:C:94:SER:CB	2.69	0.40
2:C:90:GLN:O	2:C:94:SER:HB3	2.21	0.40
2:F:395:ILE:HD13	2:F:395:ILE:HA	1.83	0.40
2:B:216:PHE:O	2:B:225:ARG:NH1	2.54	0.40
2:D:398:LEU:HD23	2:D:398:LEU:HA	1.86	0.40
2:B:116:ILE:HA	2:B:116:ILE:HD13	1.94	0.40
2:D:336:GLU:HG3	2:D:348:THR:HG21	2.03	0.40
2:D:90:GLN:O	2:D:94:SER:CB	2.69	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 PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1-a	125/127 (98%)	120 (96%)	5 (4%)	0	100	100
1	1-b	125/127 (98%)	120 (96%)	5 (4%)	0	100	100
1	1-c	125/127 (98%)	120 (96%)	5 (4%)	0	100	100
1	1-d	125/127 (98%)	120 (96%)	5 (4%)	0	100	100
1	1-e	125/127 (98%)	120 (96%)	5 (4%)	0	100	100
1	1-f	125/127 (98%)	120 (96%)	5 (4%)	0	100	100
1	2-a	125/127 (98%)	120 (96%)	5 (4%)	0	100	100
1	2-b	125/127 (98%)	120 (96%)	5 (4%)	0	100	100
1	2-c	125/127 (98%)	120 (96%)	5 (4%)	0	100	100
1	2-d	125/127 (98%)	120 (96%)	5 (4%)	0	100	100
1	2-e	125/127 (98%)	120 (96%)	5 (4%)	0	100	100
1	2-f	125/127 (98%)	120 (96%)	5 (4%)	0	100	100
1	3-a	125/127 (98%)	120 (96%)	5 (4%)	0	100	100
1	3-b	125/127 (98%)	120 (96%)	5 (4%)	0	100	100
1	3-c	125/127 (98%)	120 (96%)	5 (4%)	0	100	100
1	3-d	125/127 (98%)	120 (96%)	5 (4%)	0	100	100
1	3-e	125/127 (98%)	120 (96%)	5 (4%)	0	100	100
1	3-f	125/127 (98%)	120 (96%)	5 (4%)	0	100	100
2	1-A	428/430 (100%)	400 (94%)	28 (6%)	0	100	100
2	1-B	428/430 (100%)	401 (94%)	27 (6%)	0	100	100
2	1-C	428/430 (100%)	400 (94%)	28 (6%)	0	100	100
2	1-D	428/430 (100%)	400 (94%)	28 (6%)	0	100	100
2	1-E	428/430 (100%)	400 (94%)	28 (6%)	0	100	100
2	1-F	428/430 (100%)	400 (94%)	28 (6%)	0	100	100
2	2-A	428/430 (100%)	400 (94%)	28 (6%)	0	100	100
2	2-B	428/430 (100%)	400 (94%)	28 (6%)	0	100	100
2	2-C	428/430 (100%)	400 (94%)	28 (6%)	0	100	100
2	2-D	428/430 (100%)	401 (94%)	27 (6%)	0	100	100
2	2-E	428/430 (100%)	400 (94%)	28 (6%)	0	100	100
2	2-F	428/430 (100%)	400 (94%)	28 (6%)	0	100	100
2	3-A	428/430 (100%)	401 (94%)	27 (6%)	0	100	100
2	3-B	428/430 (100%)	400 (94%)	28 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	3-C	428/430 (100%)	401 (94%)	27 (6%)	0	100	100
2	3-D	428/430 (100%)	401 (94%)	27 (6%)	0	100	100
2	3-E	428/430 (100%)	400 (94%)	28 (6%)	0	100	100
2	3-F	428/430 (100%)	401 (94%)	27 (6%)	0	100	100
All	All	9954/10026 (99%)	9366 (94%)	588 (6%)	0	100	100

There are no Ramachandran outliers to report.

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 PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1-a	107/107 (100%)	106 (99%)	1 (1%)	82	92
1	1-b	107/107 (100%)	106 (99%)	1 (1%)	82	92
1	1-c	107/107 (100%)	106 (99%)	1 (1%)	82	92
1	1-d	107/107 (100%)	106 (99%)	1 (1%)	82	92
1	1-e	107/107 (100%)	106 (99%)	1 (1%)	82	92
1	1-f	107/107 (100%)	106 (99%)	1 (1%)	82	92
1	2-a	107/107 (100%)	106 (99%)	1 (1%)	82	92
1	2-b	107/107 (100%)	106 (99%)	1 (1%)	82	92
1	2-c	107/107 (100%)	106 (99%)	1 (1%)	82	92
1	2-d	107/107 (100%)	106 (99%)	1 (1%)	82	92
1	2-e	107/107 (100%)	106 (99%)	1 (1%)	82	92
1	2-f	107/107 (100%)	106 (99%)	1 (1%)	82	92
1	3-a	107/107 (100%)	106 (99%)	1 (1%)	82	92
1	3-b	107/107 (100%)	106 (99%)	1 (1%)	82	92
1	3-c	107/107 (100%)	106 (99%)	1 (1%)	82	92
1	3-d	107/107 (100%)	106 (99%)	1 (1%)	82	92
1	3-e	107/107 (100%)	106 (99%)	1 (1%)	82	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	3-f	107/107 (100%)	106 (99%)	1 (1%)	82	92
2	1-A	368/368 (100%)	367 (100%)	1 (0%)	94	97
2	1-B	368/368 (100%)	367 (100%)	1 (0%)	94	97
2	1-C	368/368 (100%)	367 (100%)	1 (0%)	94	97
2	1-D	368/368 (100%)	367 (100%)	1 (0%)	94	97
2	1-E	368/368 (100%)	367 (100%)	1 (0%)	94	97
2	1-F	368/368 (100%)	367 (100%)	1 (0%)	94	97
2	2-A	368/368 (100%)	367 (100%)	1 (0%)	94	97
2	2-B	368/368 (100%)	367 (100%)	1 (0%)	94	97
2	2-C	368/368 (100%)	367 (100%)	1 (0%)	94	97
2	2-D	368/368 (100%)	367 (100%)	1 (0%)	94	97
2	2-E	368/368 (100%)	367 (100%)	1 (0%)	94	97
2	2-F	368/368 (100%)	367 (100%)	1 (0%)	94	97
2	3-A	368/368 (100%)	367 (100%)	1 (0%)	94	97
2	3-B	368/368 (100%)	367 (100%)	1 (0%)	94	97
2	3-C	368/368 (100%)	367 (100%)	1 (0%)	94	97
2	3-D	368/368 (100%)	367 (100%)	1 (0%)	94	97
2	3-E	368/368 (100%)	367 (100%)	1 (0%)	94	97
2	3-F	368/368 (100%)	367 (100%)	1 (0%)	94	97
All	All	8550/8550 (100%)	8514 (100%)	36 (0%)	93	96

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-a	10	LYS
2	1-A	471	ARG
1	1-b	10	LYS
2	1-B	471	ARG
1	1-c	10	LYS
2	1-C	471	ARG
1	1-d	10	LYS
2	1-D	471	ARG
1	1-e	10	LYS
2	1-E	471	ARG
1	1-f	10	LYS

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Mol	Chain	Res	Type
2	1-F	471	ARG
1	2-a	10	LYS
2	2-A	471	ARG
1	2-b	10	LYS
2	2-B	471	ARG
1	2-c	10	LYS
2	2-C	471	ARG
1	2-d	10	LYS
2	2-D	471	ARG
1	2-e	10	LYS
2	2-E	471	ARG
1	2-f	10	LYS
2	2-F	471	ARG
1	3-a	10	LYS
2	3-A	471	ARG
1	3-b	10	LYS
2	3-B	471	ARG
1	3-c	10	LYS
2	3-C	471	ARG
1	3-d	10	LYS
2	3-D	471	ARG
1	3-e	10	LYS
2	3-E	471	ARG
1	3-f	10	LYS
2	3-F	471	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
2	1-A	208	ASN
2	1-A	269	HIS
2	1-A	355	ASN
2	1-A	365	GLN
2	1-B	208	ASN
2	1-B	269	HIS
2	1-B	355	ASN
2	1-B	365	GLN
2	1-C	208	ASN
2	1-C	269	HIS
2	1-C	355	ASN
2	1-C	365	GLN
2	1-D	208	ASN

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Mol	Chain	Res	Type
2	1-D	269	HIS
2	1-D	355	ASN
2	1-D	365	GLN
2	1-E	208	ASN
2	1-E	269	HIS
2	1-E	355	ASN
2	1-E	365	GLN
2	1-F	208	ASN
2	1-F	269	HIS
2	1-F	355	ASN
2	1-F	365	GLN
2	2-A	208	ASN
2	2-A	269	HIS
2	2-A	355	ASN
2	2-A	365	GLN
2	2-B	208	ASN
2	2-B	269	HIS
2	2-B	355	ASN
2	2-B	365	GLN
2	2-C	208	ASN
2	2-C	269	HIS
2	2-C	355	ASN
2	2-C	365	GLN
2	2-D	208	ASN
2	2-D	269	HIS
2	2-D	355	ASN
2	2-D	365	GLN
2	2-E	208	ASN
2	2-E	269	HIS
2	2-E	355	ASN
2	2-E	365	GLN
2	2-F	208	ASN
2	2-F	269	HIS
2	2-F	355	ASN
2	2-F	365	GLN
2	3-A	208	ASN
2	3-A	269	HIS
2	3-A	355	ASN
2	3-A	365	GLN
2	3-B	208	ASN
2	3-B	269	HIS
2	3-B	355	ASN

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Mol	Chain	Res	Type
2	3-B	365	GLN
2	3-C	208	ASN
2	3-C	269	HIS
2	3-C	355	ASN
2	3-C	365	GLN
2	3-D	208	ASN
2	3-D	269	HIS
2	3-D	355	ASN
2	3-D	365	GLN
2	3-E	208	ASN
2	3-E	269	HIS
2	3-E	355	ASN
2	3-E	365	GLN
2	3-F	208	ASN
2	3-F	269	HIS
2	3-F	355	ASN
2	3-F	365	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.