



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Aug 2, 2017 – 05:33 PM EDT

PDB ID : 5OJQ  
EMDB ID: : EMD-3566  
Title : The modeled structure of of wild type extended type VI secretion system sheath/tube complex in vibrio cholerae based on cryo-EM reconstruction of the non-contractile sheath/tube complex  
Authors : Wang, J.; Brackmann, M.; Castano-Diez, D.; Kudryashev, M.; Goldie, K.; Maier, T.; Stahlberg, H.; Basler, M.  
Deposited on : unknown  
Resolution : 3.70 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](mailto: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.

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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-20029824

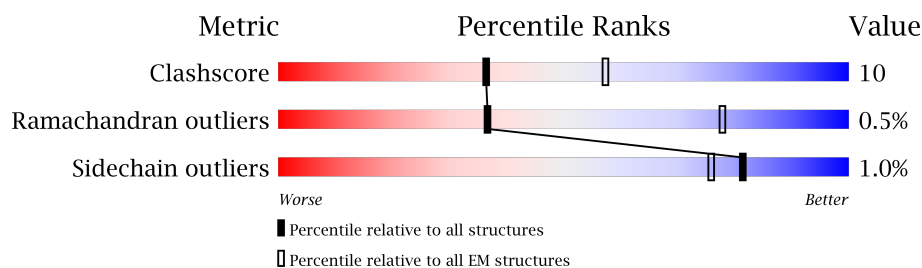
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.70 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.














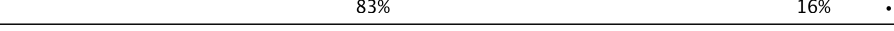






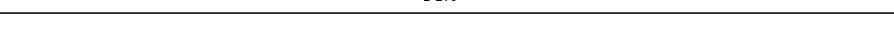
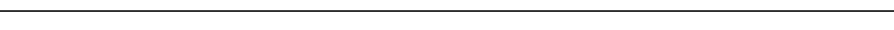

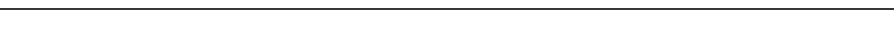
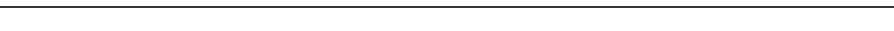


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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  $\geq 3$ , 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	170	85% 15%
1	2	170	82% 18%
1	3	170	83% 17%
1	4	170	84% 16%
1	5	170	85% 15%
1	6	170	84% 16%
1	L	170	83% 17%
1	M	170	84% 16%
1	N	170	83% 17%

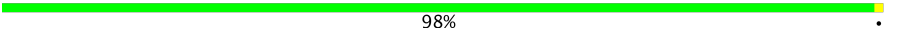
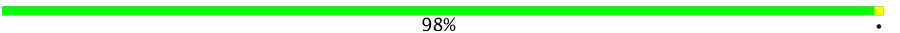













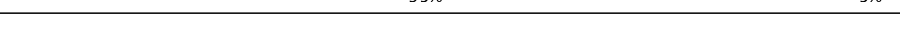
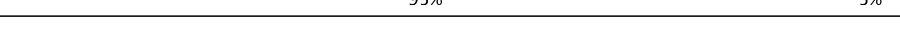
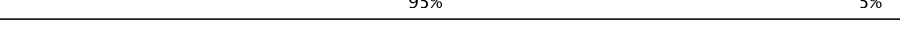
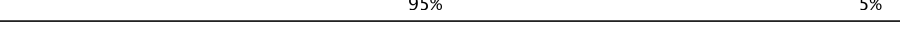
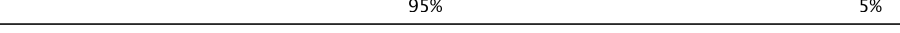
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Mol	Chain	Length	Quality of chain
1	O	170	 84% 16%
1	P	170	 83% 17%
1	Q	170	 85% 15%
1	R	170	 84% 16%
1	S	170	 82% 18%
1	T	170	 82% 18%
1	U	170	 82% 18%
1	V	170	 83% 17%
1	W	170	 84% 16%
2	A	473	 88% 12% .
2	B	473	 84% 15% .
2	C	473	 83% 16% .
2	D	473	 85% 15% .
2	E	473	 82% 17% .
2	F	473	 85% 14% .
2	X	473	 85% 14% .
2	Y	473	 87% 12% .
2	Z	473	 85% 14% .
2	b	473	 98% .
2	c	473	 98% .
2	d	473	 98% .
2	e	473	 98% .
2	f	473	 98% .
2	g	473	 98% .
2	h	473	 98% .

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Mol	Chain	Length	Quality of chain
2	i	473	 98% .
2	j	473	 98% .
3	G	155	 77% 19% .
3	H	155	 76% 20% .
3	I	155	 73% 23% .
3	J	155	 74% 22% .
3	K	155	 74% 22% .
3	a	155	 95% 5%
3	k	155	 95% 5%
3	l	155	 95% 5%
3	m	155	 95% 5%
3	n	155	 95% 5%
3	o	155	 95% 5%
3	p	155	 95% 5%
3	q	155	 95% 5%
3	r	155	 95% 5%
3	s	155	 95% 5%
3	t	155	 95% 5%
3	u	155	 95% 5%
3	v	155	 95% 5%

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 113346 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 Haemolysin co-regulated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	170	Total	C	N	O	S	0	0
			1326	833	224	263	6		
1	2	170	Total	C	N	O	S	0	0
			1326	833	224	263	6		
1	3	170	Total	C	N	O	S	0	0
			1326	833	224	263	6		
1	4	170	Total	C	N	O	S	0	0
			1326	833	224	263	6		
1	5	170	Total	C	N	O	S	0	0
			1326	833	224	263	6		
1	6	170	Total	C	N	O	S	0	0
			1326	833	224	263	6		
1	L	170	Total	C	N	O	S	0	0
			1326	833	224	263	6		
1	N	170	Total	C	N	O	S	0	0
			1326	833	224	263	6		
1	P	170	Total	C	N	O	S	0	0
			1326	833	224	263	6		
1	R	170	Total	C	N	O	S	0	0
			1326	833	224	263	6		
1	T	170	Total	C	N	O	S	0	0
			1326	833	224	263	6		
1	V	170	Total	C	N	O	S	0	0
			1326	833	224	263	6		
1	M	170	Total	C	N	O	S	0	0
			1326	833	224	263	6		
1	O	170	Total	C	N	O	S	0	0
			1326	833	224	263	6		
1	Q	170	Total	C	N	O	S	0	0
			1326	833	224	263	6		
1	S	170	Total	C	N	O	S	0	0
			1326	833	224	263	6		
1	U	170	Total	C	N	O	S	0	0
			1326	833	224	263	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	W	170	Total	C	N	O	S	0	0
			1326	833	224	263	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	473	Total	C	N	O	S	0	0
			3769	2403	640	710	16		
2	B	473	Total	C	N	O	S	0	0
			3769	2403	640	710	16		
2	C	473	Total	C	N	O	S	0	0
			3769	2403	640	710	16		
2	D	473	Total	C	N	O	S	0	0
			3769	2403	640	710	16		
2	E	473	Total	C	N	O	S	0	0
			3769	2403	640	710	16		
2	F	473	Total	C	N	O	S	0	0
			3769	2403	640	710	16		
2	X	473	Total	C	N	O	S	0	0
			3769	2403	640	710	16		
2	Z	473	Total	C	N	O	S	0	0
			3769	2403	640	710	16		
2	c	473	Total	C	N	O	S	0	0
			3769	2403	640	710	16		
2	e	473	Total	C	N	O	S	0	0
			3769	2403	640	710	16		
2	g	473	Total	C	N	O	S	0	0
			3769	2403	640	710	16		
2	i	473	Total	C	N	O	S	0	0
			3769	2403	640	710	16		
2	Y	473	Total	C	N	O	S	0	0
			3769	2403	640	710	16		
2	b	473	Total	C	N	O	S	0	0
			3769	2403	640	710	16		
2	d	473	Total	C	N	O	S	0	0
			3769	2403	640	710	16		
2	f	473	Total	C	N	O	S	0	0
			3769	2403	640	710	16		
2	h	473	Total	C	N	O	S	0	0
			3769	2403	640	710	16		
2	j	473	Total	C	N	O	S	0	0
			3769	2403	640	710	16		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	29	CYS	ILE	conflict	UNP A0A085SGI6
B	29	CYS	ILE	conflict	UNP A0A085SGI6
C	29	CYS	ILE	conflict	UNP A0A085SGI6
D	29	CYS	ILE	conflict	UNP A0A085SGI6
E	29	CYS	ILE	conflict	UNP A0A085SGI6
F	29	CYS	ILE	conflict	UNP A0A085SGI6
X	29	CYS	ILE	conflict	UNP A0A085SGI6
Z	29	CYS	ILE	conflict	UNP A0A085SGI6
c	29	CYS	ILE	conflict	UNP A0A085SGI6
e	29	CYS	ILE	conflict	UNP A0A085SGI6
g	29	CYS	ILE	conflict	UNP A0A085SGI6
i	29	CYS	ILE	conflict	UNP A0A085SGI6
Y	29	CYS	ILE	conflict	UNP A0A085SGI6
b	29	CYS	ILE	conflict	UNP A0A085SGI6
d	29	CYS	ILE	conflict	UNP A0A085SGI6
f	29	CYS	ILE	conflict	UNP A0A085SGI6
h	29	CYS	ILE	conflict	UNP A0A085SGI6
j	29	CYS	ILE	conflict	UNP A0A085SGI6

- Molecule 3 is a protein called VipA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	a	155	Total	C	N	O	S	0	0
			1202	756	204	241	1		
3	G	155	Total	C	N	O	S	0	0
			1202	756	204	241	1		
3	H	155	Total	C	N	O	S	0	0
			1202	756	204	241	1		
3	I	155	Total	C	N	O	S	0	0
			1202	756	204	241	1		
3	J	155	Total	C	N	O	S	0	0
			1202	756	204	241	1		
3	K	155	Total	C	N	O	S	0	0
			1202	756	204	241	1		
3	u	155	Total	C	N	O	S	0	0
			1202	756	204	241	1		
3	k	155	Total	C	N	O	S	0	0
			1202	756	204	241	1		
3	m	155	Total	C	N	O	S	0	0
			1202	756	204	241	1		
3	o	155	Total	C	N	O	S	0	0
			1202	756	204	241	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	q	155	Total	C	N	O	S	0	0
			1202	756	204	241	1		
3	s	155	Total	C	N	O	S	0	0
			1202	756	204	241	1		
3	v	155	Total	C	N	O	S	0	0
			1202	756	204	241	1		
3	l	155	Total	C	N	O	S	0	0
			1202	756	204	241	1		
3	n	155	Total	C	N	O	S	0	0
			1202	756	204	241	1		
3	p	155	Total	C	N	O	S	0	0
			1202	756	204	241	1		
3	r	155	Total	C	N	O	S	0	0
			1202	756	204	241	1		
3	t	155	Total	C	N	O	S	0	0
			1202	756	204	241	1		



### 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.

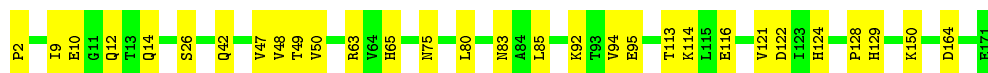
- Molecule 1: Haemolysin co-regulated protein

Chain 1: 




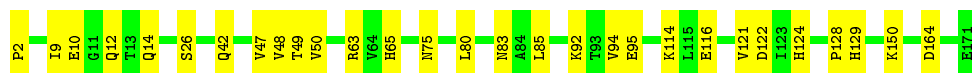
- Molecule 1: Haemolysin co-regulated protein

Chain 2: 




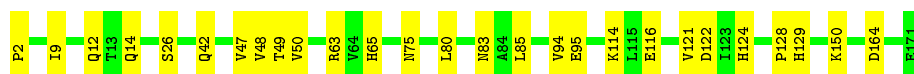
- Molecule 1: Haemolysin co-regulated protein

Chain 3: 




- Molecule 1: Haemolysin co-regulated protein

Chain 4: 




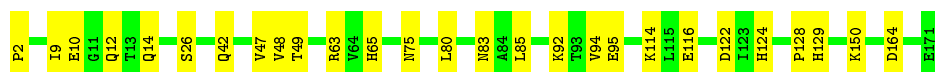
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Chain 5: 



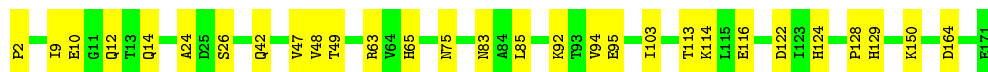
- Molecule 1: Haemolysin co-regulated protein

Chain 6: 



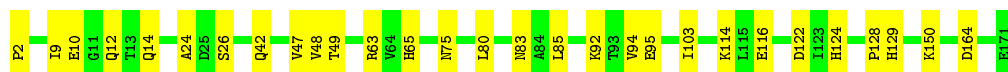
- Molecule 1: Haemolysin co-regulated protein

Chain L:   83% 17%



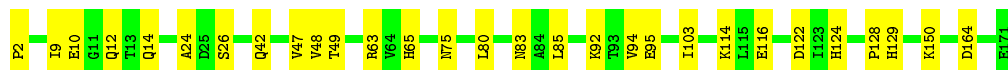
- Molecule 1: Haemolysin co-regulated protein

Chain N:   83% 17%



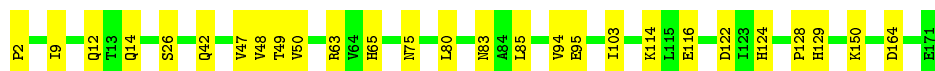
- Molecule 1: Haemolysin co-regulated protein

Chain P:   83% 17%



- Molecule 1: Haemolysin co-regulated protein

Chain R:   84% 16%



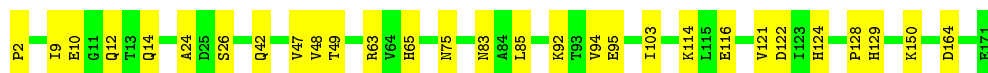
- Molecule 1: Haemolysin co-regulated protein

Chain T:   82% 18%



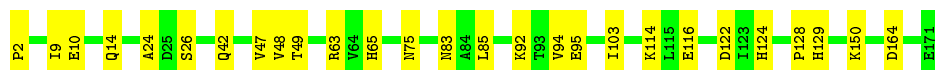
- Molecule 1: Haemolysin co-regulated protein

Chain V:   83% 17%

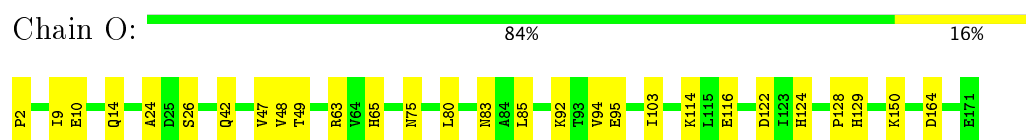


- Molecule 1: Haemolysin co-regulated protein

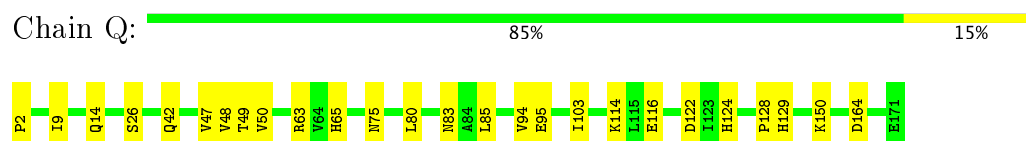
Chain M:   84% 16%



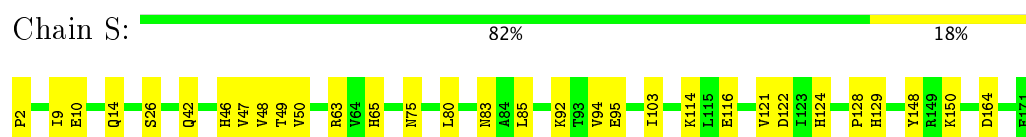
- Molecule 1: Haemolysin co-regulated protein



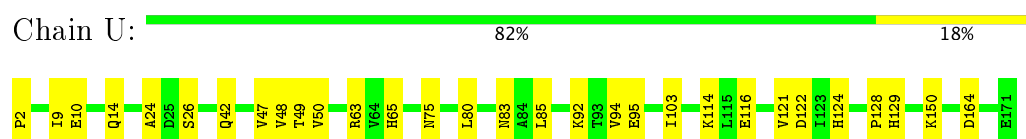
- Molecule 1: Haemolysin co-regulated protein



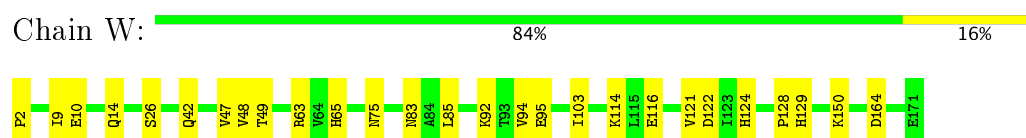
- Molecule 1: Haemolysin co-regulated protein



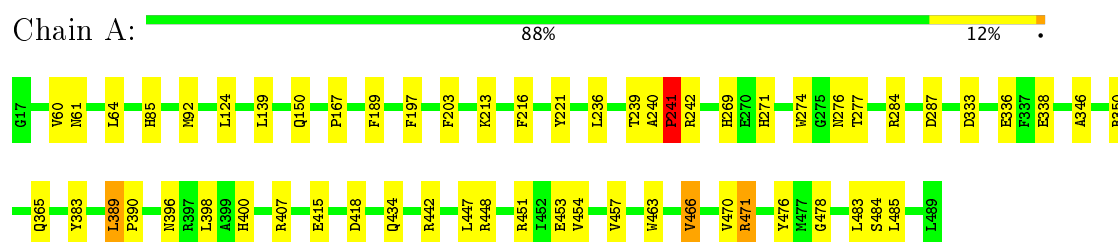
- Molecule 1: Haemolysin co-regulated protein



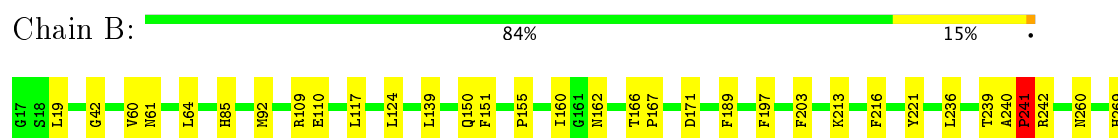
- Molecule 1: Haemolysin co-regulated protein

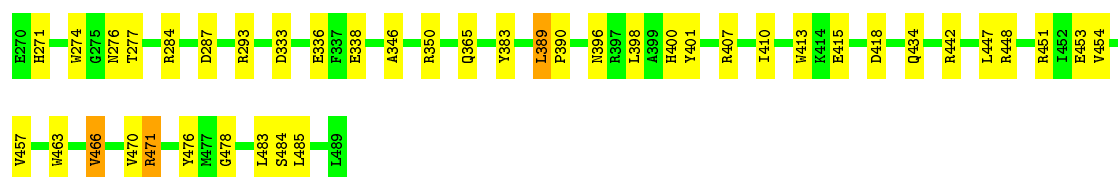


- Molecule 2: Type VI secretion protein

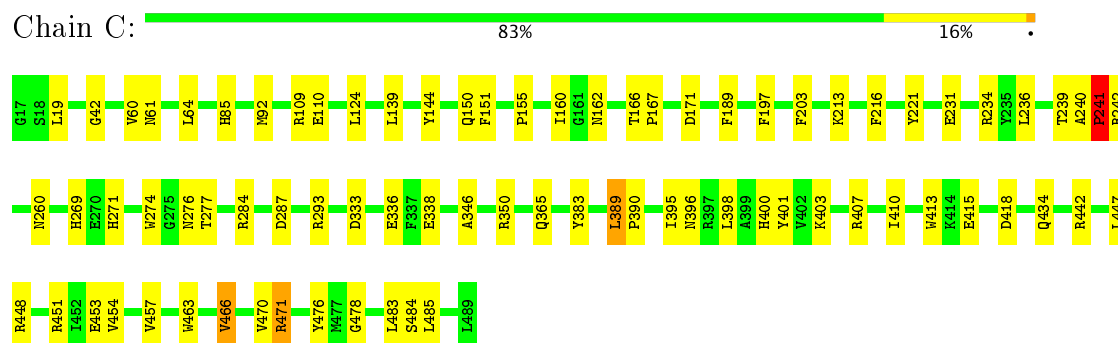


- Molecule 2: Type VI secretion protein

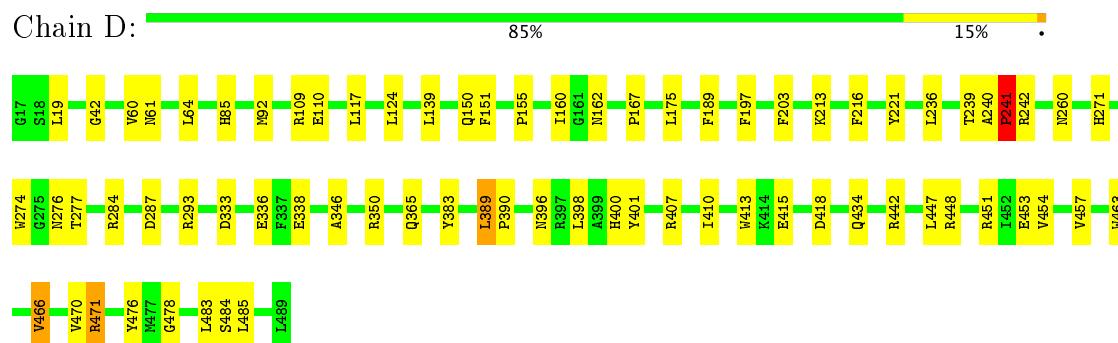




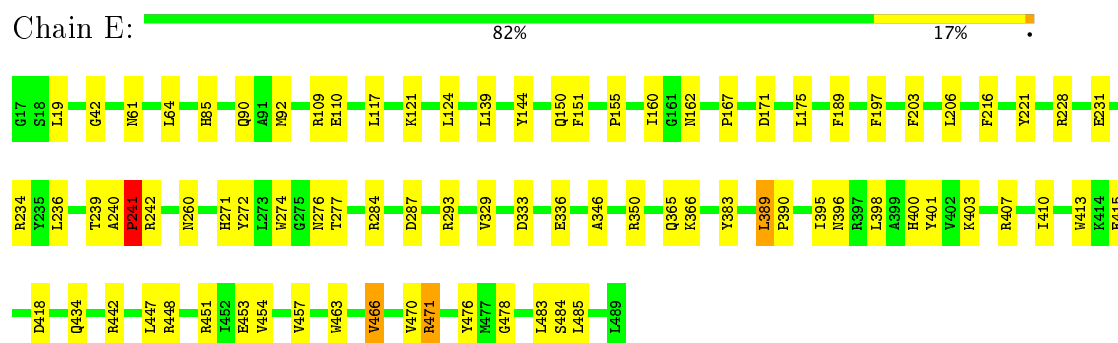
- Molecule 2: Type VI secretion protein



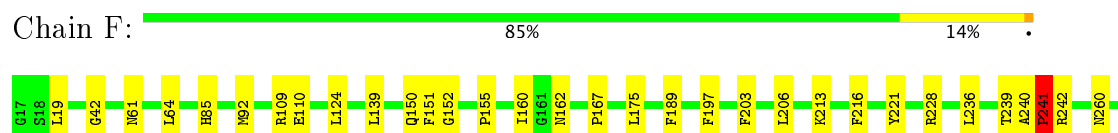
- Molecule 2: Type VI secretion protein

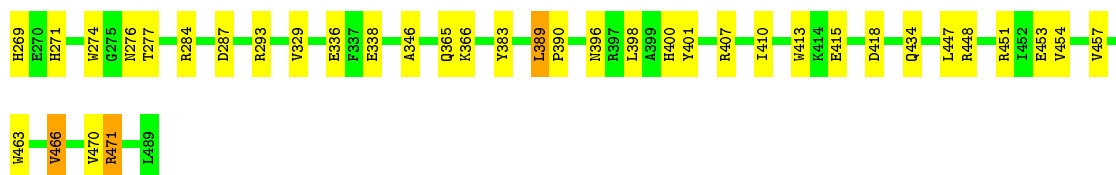


- Molecule 2: Type VI secretion protein

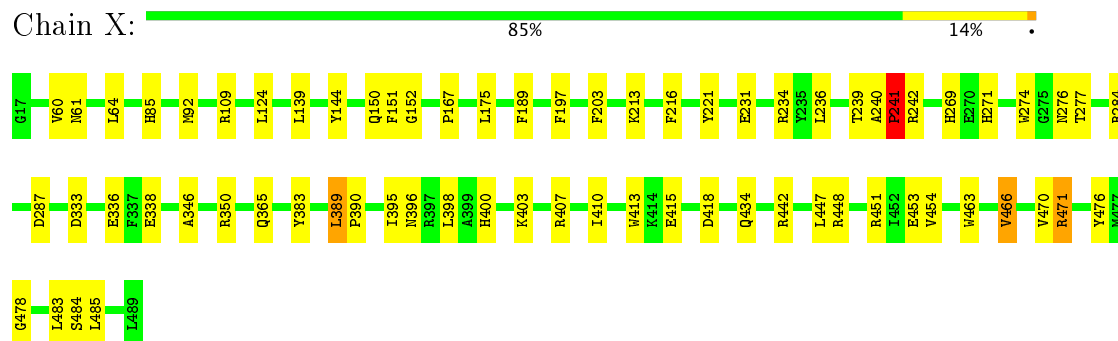


- Molecule 2: Type VI secretion protein

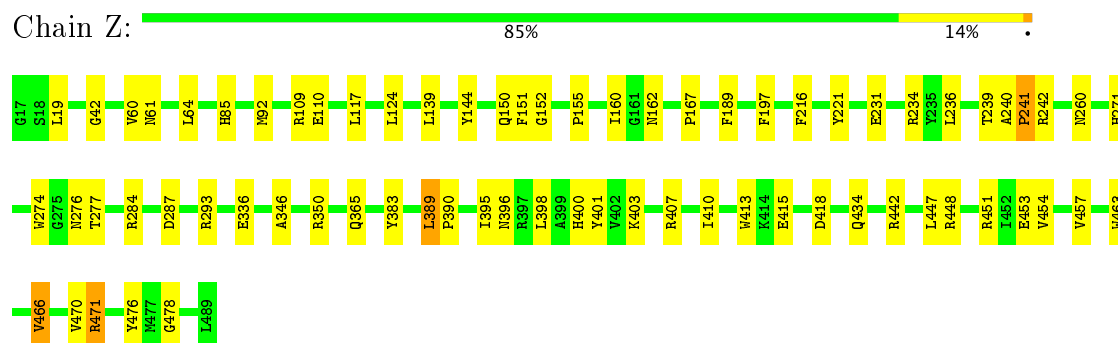




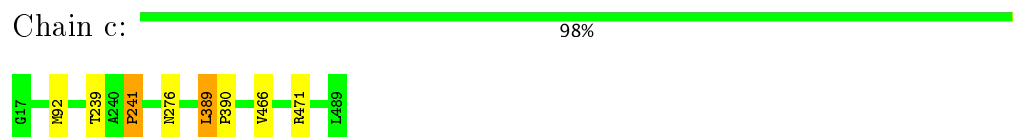
- Molecule 2: Type VI secretion protein



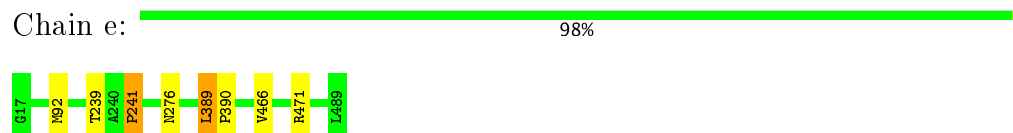
- Molecule 2: Type VI secretion protein



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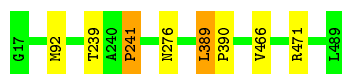


- Molecule 2: Type VI secretion protein



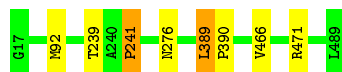
- Molecule 2: Type VI secretion protein





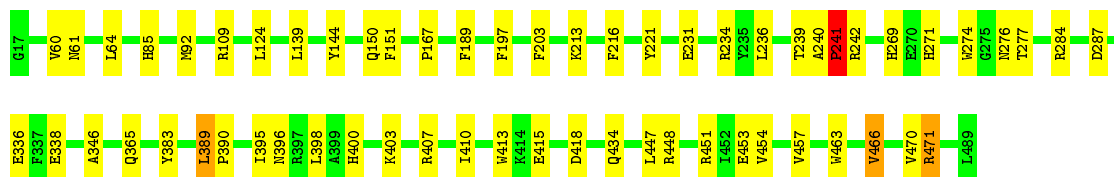
- Molecule 2: Type VI secretion protein

Chain i: 98%



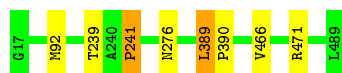
- Molecule 2: Type VI secretion protein

Chain Y: 87% 12%



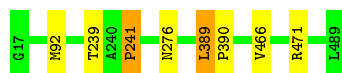
- Molecule 2: Type VI secretion protein

Chain b: 98%



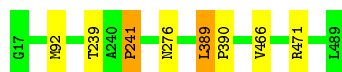
- Molecule 2: Type VI secretion protein

Chain d: 98%



- Molecule 2: Type VI secretion protein

Chain f: 98%



- Molecule 2: Type VI secretion protein

Chain h: 98%



- Molecule 2: Type VI secretion protein

Chain j: 98%



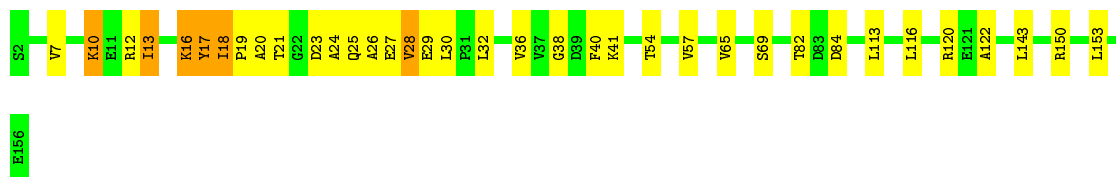
• Molecule 3: VipA

Chain a: 95% 5%



• Molecule 3: VipA

Chain G: 77% 19%



• Molecule 3: VipA

Chain H: 76% 20%



• Molecule 3: VipA

Chain I: 73% 23%

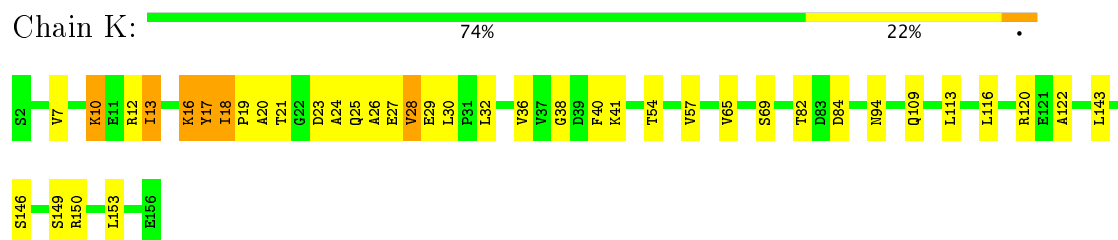


• Molecule 3: VipA

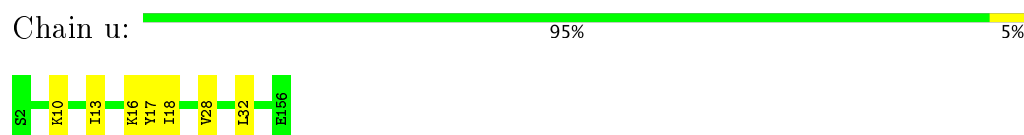
Chain J: 74% 22%



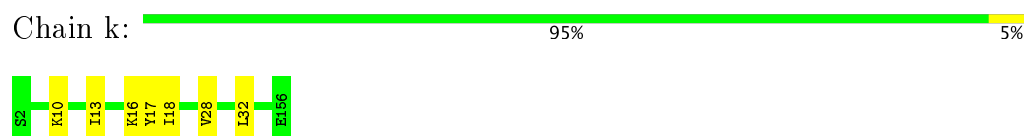
• Molecule 3: VipA



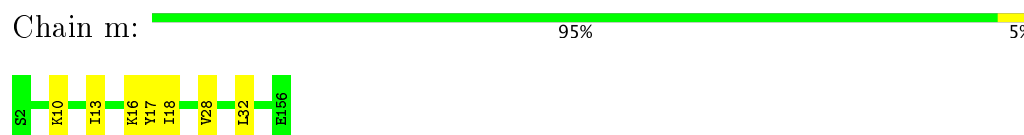
- Molecule 3: VipA



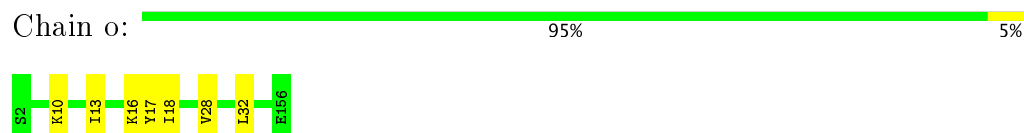
- Molecule 3: VipA



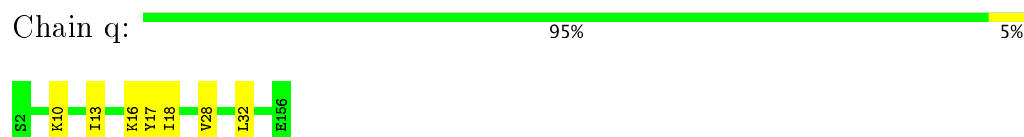
- Molecule 3: VipA



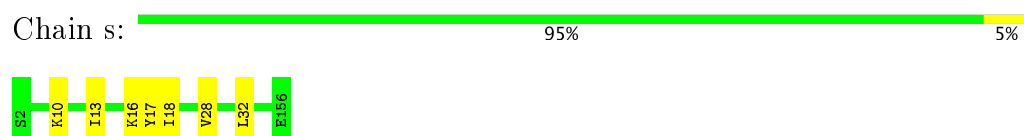
- Molecule 3: VipA



- Molecule 3: VipA



- Molecule 3: VipA



- Molecule 3: VipA



Chain v:  95% 5%



• Molecule 3: VipA

Chain l:  95% 5%



• Molecule 3: VipA

Chain n:  95% 5%



• Molecule 3: VipA

Chain p:  95% 5%



• Molecule 3: VipA

Chain r:  95% 5%



• Molecule 3: VipA

Chain t:  95% 5%



## 4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=23.5°, rise=37.8 Å, axial sym=C6	Depositor
Number of segments used	10000	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 ( $e^-/\text{\AA}^2$ )	1	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	0.57	0/1358	0.61	0/1846
1	2	0.57	0/1358	0.61	0/1846
1	3	0.57	0/1358	0.61	0/1846
1	4	0.57	0/1358	0.61	0/1846
1	5	0.57	0/1358	0.61	0/1846
1	6	0.57	0/1358	0.61	0/1846
1	L	0.57	0/1358	0.61	0/1846
1	M	0.57	0/1358	0.61	0/1846
1	N	0.57	0/1358	0.61	0/1846
1	O	0.57	0/1358	0.61	0/1846
1	P	0.57	0/1358	0.61	0/1846
1	Q	0.57	0/1358	0.61	0/1846
1	R	0.57	0/1358	0.61	0/1846
1	S	0.57	0/1358	0.61	0/1846
1	T	0.57	0/1358	0.61	0/1846
1	U	0.57	0/1358	0.61	0/1846
1	V	0.57	0/1358	0.61	0/1846
1	W	0.57	0/1358	0.61	0/1846
2	A	0.38	0/3862	0.56	2/5225 (0.0%)
2	B	0.38	0/3862	0.56	2/5225 (0.0%)
2	C	0.38	0/3862	0.56	2/5225 (0.0%)
2	D	0.38	0/3862	0.56	2/5225 (0.0%)
2	E	0.38	0/3862	0.56	2/5225 (0.0%)
2	F	0.38	0/3862	0.56	2/5225 (0.0%)
2	X	0.38	0/3862	0.56	2/5225 (0.0%)
2	Y	0.38	0/3862	0.56	2/5225 (0.0%)
2	Z	0.38	0/3862	0.56	2/5225 (0.0%)
2	b	0.38	0/3862	0.56	2/5225 (0.0%)
2	c	0.38	0/3862	0.56	2/5225 (0.0%)
2	d	0.38	0/3862	0.56	2/5225 (0.0%)
2	e	0.38	0/3862	0.56	2/5225 (0.0%)
2	f	0.38	0/3862	0.56	2/5225 (0.0%)
2	g	0.38	0/3862	0.56	2/5225 (0.0%)
2	h	0.38	0/3862	0.56	2/5225 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
2	i	0.38	0/3862	0.56	2/5225 (0.0%)
2	j	0.38	0/3862	0.56	2/5225 (0.0%)
3	G	0.41	0/1217	0.70	2/1644 (0.1%)
3	H	0.42	0/1217	0.70	2/1644 (0.1%)
3	I	0.41	0/1217	0.70	2/1644 (0.1%)
3	J	0.41	0/1217	0.70	2/1644 (0.1%)
3	K	0.41	0/1217	0.70	2/1644 (0.1%)
3	a	0.41	0/1217	0.70	2/1644 (0.1%)
3	k	0.42	0/1217	0.70	2/1644 (0.1%)
3	l	0.41	0/1217	0.70	2/1644 (0.1%)
3	m	0.41	0/1217	0.70	2/1644 (0.1%)
3	n	0.41	0/1217	0.70	2/1644 (0.1%)
3	o	0.42	0/1217	0.70	2/1644 (0.1%)
3	p	0.42	0/1217	0.70	2/1644 (0.1%)
3	q	0.41	0/1217	0.70	2/1644 (0.1%)
3	r	0.41	0/1217	0.70	2/1644 (0.1%)
3	s	0.42	0/1217	0.70	2/1644 (0.1%)
3	t	0.41	0/1217	0.70	2/1644 (0.1%)
3	u	0.41	0/1217	0.70	2/1644 (0.1%)
3	v	0.41	0/1217	0.70	2/1644 (0.1%)
All	All	0.44	0/115866	0.60	72/156870 (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	A	0	1
2	B	0	1
2	C	0	1
2	D	0	1
2	E	0	1
2	F	0	1
2	X	0	1
2	Y	0	1
2	Z	0	1
2	b	0	1
2	c	0	1
2	d	0	1
2	e	0	1
2	f	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	g	0	1
2	h	0	1
2	i	0	1
2	j	0	1
3	G	0	2
3	H	0	2
3	I	0	2
3	J	0	2
3	K	0	2
3	a	0	2
3	k	0	2
3	l	0	2
3	m	0	2
3	n	0	2
3	o	0	2
3	p	0	2
3	q	0	2
3	r	0	2
3	s	0	2
3	t	0	2
3	u	0	2
3	v	0	2
All	All	0	54

There are no bond length outliers.

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	s	18	ILE	CB-CA-C	7.12	125.83	111.60
3	k	18	ILE	CB-CA-C	7.11	125.82	111.60
3	q	18	ILE	CB-CA-C	7.11	125.82	111.60
3	m	18	ILE	CB-CA-C	7.11	125.82	111.60
3	a	18	ILE	CB-CA-C	7.10	125.80	111.60
3	I	18	ILE	CB-CA-C	7.10	125.80	111.60
3	r	18	ILE	CB-CA-C	7.10	125.80	111.60
3	o	18	ILE	CB-CA-C	7.10	125.79	111.60
3	l	18	ILE	CB-CA-C	7.09	125.79	111.60
3	J	18	ILE	CB-CA-C	7.09	125.78	111.60
3	v	18	ILE	CB-CA-C	7.09	125.78	111.60
3	t	18	ILE	CB-CA-C	7.09	125.78	111.60
3	n	18	ILE	CB-CA-C	7.08	125.76	111.60
3	p	18	ILE	CB-CA-C	7.08	125.76	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	u	18	ILE	CB-CA-C	7.07	125.74	111.60
3	H	18	ILE	CB-CA-C	7.07	125.74	111.60
3	K	18	ILE	CB-CA-C	7.07	125.74	111.60
3	G	18	ILE	CB-CA-C	7.07	125.73	111.60
2	c	389	LEU	CA-CB-CG	5.75	128.52	115.30
2	i	389	LEU	CA-CB-CG	5.75	128.52	115.30
2	d	389	LEU	CA-CB-CG	5.74	128.50	115.30
2	F	389	LEU	CA-CB-CG	5.74	128.50	115.30
2	C	389	LEU	CA-CB-CG	5.73	128.48	115.30
2	b	389	LEU	CA-CB-CG	5.73	128.48	115.30
2	D	389	LEU	CA-CB-CG	5.73	128.48	115.30
2	j	389	LEU	CA-CB-CG	5.73	128.47	115.30
2	e	389	LEU	CA-CB-CG	5.73	128.47	115.30
2	B	389	LEU	CA-CB-CG	5.72	128.46	115.30
2	f	389	LEU	CA-CB-CG	5.72	128.46	115.30
2	h	389	LEU	CA-CB-CG	5.72	128.46	115.30
2	A	389	LEU	CA-CB-CG	5.71	128.44	115.30
2	X	389	LEU	CA-CB-CG	5.71	128.44	115.30
2	Z	389	LEU	CA-CB-CG	5.71	128.43	115.30
2	Y	239	THR	C-N-CA	5.71	135.96	121.70
2	Y	389	LEU	CA-CB-CG	5.70	128.42	115.30
2	E	389	LEU	CA-CB-CG	5.70	128.41	115.30
2	g	389	LEU	CA-CB-CG	5.70	128.41	115.30
2	f	239	THR	C-N-CA	5.69	135.94	121.70
2	A	239	THR	C-N-CA	5.69	135.93	121.70
2	d	239	THR	C-N-CA	5.69	135.92	121.70
2	j	239	THR	C-N-CA	5.68	135.91	121.70
2	h	239	THR	C-N-CA	5.68	135.90	121.70
2	E	239	THR	C-N-CA	5.68	135.89	121.70
2	C	239	THR	C-N-CA	5.67	135.89	121.70
2	B	239	THR	C-N-CA	5.67	135.88	121.70
2	F	239	THR	C-N-CA	5.67	135.88	121.70
2	X	239	THR	C-N-CA	5.67	135.88	121.70
2	D	239	THR	C-N-CA	5.67	135.88	121.70
2	b	239	THR	C-N-CA	5.67	135.88	121.70
2	g	239	THR	C-N-CA	5.66	135.86	121.70
2	e	239	THR	C-N-CA	5.66	135.86	121.70
2	c	239	THR	C-N-CA	5.66	135.85	121.70
2	Z	239	THR	C-N-CA	5.66	135.84	121.70
2	i	239	THR	C-N-CA	5.65	135.83	121.70
3	o	13	ILE	CG1-CB-CG2	-5.53	99.23	111.40
3	s	13	ILE	CG1-CB-CG2	-5.53	99.24	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	13	ILE	CG1-CB-CG2	-5.52	99.25	111.40
3	n	13	ILE	CG1-CB-CG2	-5.52	99.25	111.40
3	u	13	ILE	CG1-CB-CG2	-5.52	99.25	111.40
3	H	13	ILE	CG1-CB-CG2	-5.52	99.26	111.40
3	K	13	ILE	CG1-CB-CG2	-5.52	99.26	111.40
3	q	13	ILE	CG1-CB-CG2	-5.52	99.26	111.40
3	I	13	ILE	CG1-CB-CG2	-5.52	99.26	111.40
3	t	13	ILE	CG1-CB-CG2	-5.52	99.26	111.40
3	m	13	ILE	CG1-CB-CG2	-5.51	99.27	111.40
3	v	13	ILE	CG1-CB-CG2	-5.51	99.27	111.40
3	k	13	ILE	CG1-CB-CG2	-5.51	99.28	111.40
3	l	13	ILE	CG1-CB-CG2	-5.51	99.27	111.40
3	a	13	ILE	CG1-CB-CG2	-5.51	99.28	111.40
3	r	13	ILE	CG1-CB-CG2	-5.50	99.29	111.40
3	p	13	ILE	CG1-CB-CG2	-5.50	99.30	111.40
3	G	13	ILE	CG1-CB-CG2	-5.50	99.30	111.40

There are no chirality outliers.

All (54) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	389	LEU	Peptide
2	B	389	LEU	Peptide
2	C	389	LEU	Peptide
2	D	389	LEU	Peptide
2	E	389	LEU	Peptide
2	F	389	LEU	Peptide
3	G	16	LYS	Mainchain
3	G	17	TYR	Mainchain
3	H	16	LYS	Mainchain
3	H	17	TYR	Mainchain
3	I	16	LYS	Mainchain
3	I	17	TYR	Mainchain
3	J	16	LYS	Mainchain
3	J	17	TYR	Mainchain
3	K	16	LYS	Mainchain
3	K	17	TYR	Mainchain
2	X	389	LEU	Peptide
2	Y	389	LEU	Peptide
2	Z	389	LEU	Peptide
3	a	16	LYS	Mainchain
3	a	17	TYR	Mainchain

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Mol	Chain	Res	Type	Group
2	b	389	LEU	Peptide
2	c	389	LEU	Peptide
2	d	389	LEU	Peptide
2	e	389	LEU	Peptide
2	f	389	LEU	Peptide
2	g	389	LEU	Peptide
2	h	389	LEU	Peptide
2	i	389	LEU	Peptide
2	j	389	LEU	Peptide
3	k	16	LYS	Mainchain
3	k	17	TYR	Mainchain
3	l	16	LYS	Mainchain
3	l	17	TYR	Mainchain
3	m	16	LYS	Mainchain
3	m	17	TYR	Mainchain
3	n	16	LYS	Mainchain
3	n	17	TYR	Mainchain
3	o	16	LYS	Mainchain
3	o	17	TYR	Mainchain
3	p	16	LYS	Mainchain
3	p	17	TYR	Mainchain
3	q	16	LYS	Mainchain
3	q	17	TYR	Mainchain
3	r	16	LYS	Mainchain
3	r	17	TYR	Mainchain
3	s	16	LYS	Mainchain
3	s	17	TYR	Mainchain
3	t	16	LYS	Mainchain
3	t	17	TYR	Mainchain
3	u	16	LYS	Mainchain
3	u	17	TYR	Mainchain
3	v	16	LYS	Mainchain
3	v	17	TYR	Mainchain

## 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	1326	0	1279	21	0
1	2	1326	0	1279	25	0
1	3	1326	0	1279	23	0
1	4	1326	0	1279	22	0
1	5	1326	0	1279	22	0
1	6	1326	0	1279	21	0
1	L	1326	0	1279	24	0
1	M	1326	0	1279	23	0
1	N	1326	0	1279	24	0
1	O	1326	0	1279	24	0
1	P	1326	0	1279	24	0
1	Q	1326	0	1279	22	0
1	R	1326	0	1279	22	0
1	S	1326	0	1279	25	0
1	T	1326	0	1279	25	0
1	U	1326	0	1279	26	0
1	V	1326	0	1279	25	0
1	W	1326	0	1279	22	0
2	A	3769	0	3681	40	0
2	B	3769	0	3681	95	0
2	C	3769	0	3681	113	0
2	D	3769	0	3681	93	0
2	E	3769	0	3681	115	0
2	F	3769	0	3681	83	0
2	X	3769	0	3681	64	0
2	Y	3769	0	3681	50	0
2	Z	3769	0	3681	98	0
2	b	3769	0	3681	0	0
2	c	3769	0	3681	0	0
2	d	3769	0	3681	0	0
2	e	3769	0	3681	0	0
2	f	3769	0	3681	0	0
2	g	3769	0	3681	0	0
2	h	3769	0	3681	0	0
2	i	3769	0	3681	0	0
2	j	3769	0	3681	0	0
3	G	1202	0	1231	88	0
3	H	1202	0	1231	89	0
3	I	1202	0	1231	90	0
3	J	1202	0	1231	91	0
3	K	1202	0	1231	152	0
3	a	1202	0	1231	0	0
3	k	1202	0	1231	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	l	1202	0	1231	0	0
3	m	1202	0	1231	0	0
3	n	1202	0	1231	0	0
3	o	1202	0	1231	0	0
3	p	1202	0	1231	0	0
3	q	1202	0	1231	0	0
3	r	1202	0	1231	0	0
3	s	1202	0	1231	0	0
3	t	1202	0	1231	0	0
3	u	1202	0	1231	0	0
3	v	1202	0	1231	0	0
All	All	113346	0	111438	1060	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 10.

All (1060) 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:109:ARG:HD2	3:H:25:GLN:CB	1.53	1.38
2:D:109:ARG:HD2	3:I:25:GLN:CB	1.53	1.37
2:E:109:ARG:HD2	3:J:25:GLN:CB	1.53	1.37
2:B:109:ARG:HD2	3:G:25:GLN:CB	1.53	1.36
3:K:25:GLN:CB	2:Z:109:ARG:HD2	119.38	1.36
2:F:109:ARG:HD2	3:K:25:GLN:CB	1.53	1.35
2:C:483:LEU:O	3:I:18:ILE:CB	1.74	1.34
2:D:483:LEU:O	3:J:18:ILE:CB	1.75	1.34
2:B:483:LEU:O	3:H:18:ILE:CB	1.76	1.33
2:E:483:LEU:O	3:K:18:ILE:CB	1.75	1.33
2:A:483:LEU:O	3:G:18:ILE:CB	1.75	1.31
3:K:18:ILE:CB	2:X:483:LEU:O	122.74	1.31
2:F:293:ARG:HD2	3:K:28:VAL:CG1	1.62	1.29
2:E:293:ARG:HD2	3:J:28:VAL:CG1	1.62	1.28
2:B:293:ARG:HD2	3:G:28:VAL:CG1	1.62	1.27
3:K:28:VAL:CG1	2:Z:293:ARG:HD2	113.40	1.27
2:D:293:ARG:HD2	3:I:28:VAL:CG1	1.62	1.27
2:D:293:ARG:NH1	3:I:28:VAL:HG12	1.50	1.26
2:C:293:ARG:NH1	3:H:28:VAL:HG12	1.50	1.26
2:C:293:ARG:HD2	3:H:28:VAL:CG1	1.62	1.26
3:K:28:VAL:HG12	2:Z:293:ARG:NH1	111.11	1.24
2:C:293:ARG:NH2	3:H:27:GLU:O	1.72	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:109:ARG:CD	3:K:25:GLN:HB3	1.69	1.22
3:K:25:GLN:HB3	2:Z:109:ARG:CD	120.83	1.22
2:C:109:ARG:CD	3:H:25:GLN:HB3	1.69	1.22
2:F:293:ARG:NH1	3:K:28:VAL:HG12	1.50	1.22
2:E:109:ARG:CD	3:J:25:GLN:HB3	1.69	1.22
2:B:293:ARG:NH1	3:G:28:VAL:HG12	1.50	1.22
2:E:293:ARG:NH1	3:J:28:VAL:HG12	1.50	1.22
2:B:109:ARG:CD	3:G:25:GLN:HB3	1.69	1.22
3:K:27:GLU:O	2:Z:293:ARG:NH2	112.12	1.22
2:B:293:ARG:NH2	3:G:27:GLU:O	1.72	1.22
2:D:109:ARG:CD	3:I:25:GLN:HB3	1.69	1.20
2:D:293:ARG:NH2	3:I:27:GLU:O	1.72	1.20
2:E:333:ASP:HB2	3:K:12:ARG:HG3	1.23	1.20
2:B:333:ASP:HB2	3:H:12:ARG:HG3	1.23	1.20
2:E:293:ARG:NH2	3:J:27:GLU:O	1.72	1.19
2:F:293:ARG:NH2	3:K:27:GLU:O	1.72	1.18
2:B:109:ARG:HB3	3:G:25:GLN:HB2	1.26	1.18
2:C:293:ARG:CD	3:H:28:VAL:CG1	2.22	1.17
3:K:28:VAL:CG1	2:Z:293:ARG:CD	113.53	1.17
2:B:293:ARG:CD	3:G:28:VAL:CG1	2.22	1.17
2:E:293:ARG:CD	3:J:28:VAL:CG1	2.22	1.17
2:B:293:ARG:CZ	3:G:28:VAL:CG1	2.23	1.17
2:F:293:ARG:CZ	3:K:28:VAL:CG1	2.23	1.17
2:C:333:ASP:HB2	3:I:12:ARG:HG3	1.25	1.17
3:K:28:VAL:CG1	2:Z:293:ARG:CZ	112.73	1.16
2:F:293:ARG:CD	3:K:28:VAL:CG1	2.22	1.16
2:E:109:ARG:HB3	3:J:25:GLN:HB2	1.25	1.16
3:K:25:GLN:HB2	2:Z:109:ARG:HB3	119.37	1.16
2:D:293:ARG:CD	3:I:28:VAL:CG1	2.22	1.16
3:K:12:ARG:HG3	2:X:333:ASP:HB2	132.70	1.16
2:D:293:ARG:CZ	3:I:28:VAL:CG1	2.23	1.15
2:F:293:ARG:NH1	3:K:28:VAL:CG1	2.10	1.15
2:B:293:ARG:NH1	3:G:28:VAL:CG1	2.10	1.15
2:E:293:ARG:NH1	3:J:28:VAL:CG1	2.10	1.15
2:D:333:ASP:HB2	3:J:12:ARG:HG3	1.22	1.15
2:C:293:ARG:CZ	3:H:28:VAL:CG1	2.23	1.15
2:E:293:ARG:CZ	3:J:28:VAL:CG1	2.23	1.15
2:F:293:ARG:CZ	3:K:28:VAL:HG13	1.77	1.15
2:B:293:ARG:CZ	3:G:28:VAL:HG13	1.77	1.14
3:K:28:VAL:CG1	2:Z:293:ARG:NH1	111.94	1.14
2:C:293:ARG:NH1	3:H:28:VAL:CG1	2.10	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:333:ASP:HB2	3:G:12:ARG:HG3	1.23	1.14
3:K:28:VAL:HG13	2:Z:293:ARG:CZ	112.74	1.14
2:D:293:ARG:CZ	3:I:28:VAL:HG13	1.77	1.13
2:D:293:ARG:NH1	3:I:28:VAL:CG1	2.10	1.13
2:C:109:ARG:HB3	3:H:25:GLN:HB2	1.25	1.13
2:C:293:ARG:CZ	3:H:28:VAL:HG13	1.77	1.12
2:E:293:ARG:CZ	3:J:28:VAL:HG13	1.77	1.12
2:D:109:ARG:HB3	3:I:25:GLN:HB2	1.26	1.11
2:F:109:ARG:HB3	3:K:25:GLN:HB2	1.25	1.10
2:C:293:ARG:CD	3:H:28:VAL:HG12	1.84	1.07
2:B:293:ARG:CD	3:G:28:VAL:HG12	1.84	1.07
2:B:293:ARG:HD2	3:G:28:VAL:HG12	1.20	1.07
3:K:28:VAL:HG12	2:Z:293:ARG:HH11	111.08	1.07
2:D:293:ARG:CD	3:I:28:VAL:HG12	1.84	1.06
2:D:483:LEU:O	3:J:18:ILE:HB	0.87	1.05
3:K:28:VAL:HG12	2:Z:293:ARG:CD	112.69	1.05
2:B:483:LEU:O	3:H:18:ILE:HB	0.88	1.05
3:K:28:VAL:HG12	2:Z:293:ARG:HD2	112.56	1.05
2:A:483:LEU:O	3:G:18:ILE:HB	0.88	1.04
2:E:483:LEU:O	3:K:18:ILE:HB	0.87	1.04
2:C:483:LEU:O	3:I:18:ILE:HB	0.86	1.04
2:F:293:ARG:HH11	3:K:28:VAL:HG12	1.07	1.04
3:K:18:ILE:HB	2:X:483:LEU:O	121.87	1.04
2:C:485:LEU:O	3:I:21:THR:HG22	1.59	1.03
2:E:293:ARG:HH11	3:J:28:VAL:HG12	1.06	1.03
2:F:293:ARG:CD	3:K:28:VAL:HG12	1.84	1.03
2:C:293:ARG:HD2	3:H:28:VAL:HG12	1.20	1.03
2:E:293:ARG:HD2	3:J:28:VAL:HG12	1.20	1.03
2:E:293:ARG:CD	3:J:28:VAL:HG12	1.84	1.02
3:K:21:THR:HG22	2:X:485:LEU:O	117.28	1.02
2:B:485:LEU:O	3:H:21:THR:HG22	1.60	1.01
2:D:485:LEU:O	3:J:21:THR:HG22	1.59	1.01
2:A:485:LEU:O	3:G:21:THR:HG22	1.60	1.01
2:D:293:ARG:HH11	3:I:28:VAL:HG12	1.07	1.01
2:E:293:ARG:NE	3:J:28:VAL:CG1	2.24	1.00
2:C:293:ARG:NE	3:H:28:VAL:CG1	2.24	1.00
2:F:293:ARG:NE	3:K:28:VAL:CG1	2.24	1.00
2:D:293:ARG:HD2	3:I:28:VAL:HG12	1.20	1.00
2:D:293:ARG:NE	3:I:28:VAL:CG1	2.25	1.00
2:B:293:ARG:NE	3:G:28:VAL:CG1	2.24	0.99
2:E:485:LEU:O	3:K:21:THR:HG22	1.59	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:293:ARG:CZ	3:J:27:GLU:O	2.11	0.99
2:F:293:ARG:HD2	3:K:28:VAL:HG12	1.20	0.99
2:F:293:ARG:CZ	3:K:27:GLU:O	2.11	0.98
2:F:293:ARG:HD2	3:K:28:VAL:HG11	1.45	0.98
3:K:28:VAL:CG1	2:Z:293:ARG:NE	113.49	0.98
2:D:293:ARG:CZ	3:I:27:GLU:O	2.11	0.98
2:C:293:ARG:CZ	3:H:27:GLU:O	2.11	0.98
2:B:293:ARG:HD2	3:G:28:VAL:HG11	1.45	0.97
2:C:293:ARG:HH11	3:H:28:VAL:HG12	1.06	0.97
3:K:27:GLU:O	2:Z:293:ARG:CZ	112.05	0.97
2:B:293:ARG:CZ	3:G:27:GLU:O	2.11	0.97
3:K:28:VAL:HG11	2:Z:293:ARG:HD2	113.52	0.96
2:E:293:ARG:HD2	3:J:28:VAL:HG11	1.45	0.96
2:C:293:ARG:HD2	3:H:28:VAL:HG11	1.45	0.95
2:E:293:ARG:CZ	3:J:28:VAL:HG12	1.93	0.95
2:D:293:ARG:HD2	3:I:28:VAL:HG11	1.45	0.95
2:E:231:GLU:OE2	3:J:19:PRO:HG3	57.39	0.94
3:H:19:PRO:HG3	2:Z:231:GLU:OE2	1.68	0.94
2:D:293:ARG:CZ	3:I:28:VAL:HG12	1.93	0.93
3:K:27:GLU:O	2:Z:293:ARG:NH1	111.27	0.93
2:B:293:ARG:NH1	3:G:27:GLU:O	2.02	0.93
2:D:293:ARG:NH1	3:I:27:GLU:O	2.02	0.93
2:C:293:ARG:CZ	3:H:28:VAL:HG12	1.93	0.93
2:C:293:ARG:NH1	3:H:27:GLU:O	2.02	0.93
3:G:19:PRO:HG3	2:X:231:GLU:OE2	1.68	0.93
2:B:293:ARG:CZ	3:G:28:VAL:HG12	1.93	0.93
2:F:293:ARG:NH1	3:K:27:GLU:O	2.02	0.92
2:C:293:ARG:CD	3:H:28:VAL:HG11	1.98	0.92
2:B:293:ARG:HH11	3:G:28:VAL:HG12	1.06	0.92
2:F:293:ARG:CZ	3:K:28:VAL:HG12	1.93	0.91
2:E:293:ARG:NH1	3:J:27:GLU:O	2.02	0.91
2:C:231:GLU:OE2	3:I:19:PRO:HG3	45.90	0.91
3:K:28:VAL:HG12	2:Z:293:ARG:CZ	111.90	0.91
3:K:19:PRO:HG3	2:Y:231:GLU:OE2	134.87	0.91
2:D:293:ARG:CD	3:I:28:VAL:HG11	1.98	0.91
2:E:293:ARG:CD	3:J:28:VAL:HG11	1.98	0.91
2:F:293:ARG:CD	3:K:28:VAL:HG11	1.98	0.90
2:A:333:ASP:CB	3:G:12:ARG:HG3	2.02	0.90
2:B:333:ASP:CB	3:H:12:ARG:HG3	2.01	0.90
2:D:333:ASP:CB	3:J:12:ARG:HG3	2.01	0.89
3:K:12:ARG:HG3	2:X:333:ASP:CB	133.36	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:293:ARG:CD	3:G:28:VAL:HG11	1.98	0.88
2:E:333:ASP:CB	3:K:12:ARG:HG3	2.02	0.88
2:B:109:ARG:CD	3:G:25:GLN:CB	2.42	0.87
2:C:333:ASP:CB	3:I:12:ARG:HG3	2.03	0.86
2:F:109:ARG:CD	3:K:25:GLN:CB	2.42	0.84
2:F:109:ARG:CB	3:K:25:GLN:HB2	2.06	0.84
2:E:109:ARG:CB	3:J:25:GLN:HB2	2.06	0.83
2:F:155:PRO:HD3	3:K:30:LEU:HD13	1.60	0.83
2:D:155:PRO:HD3	3:I:30:LEU:HD13	1.60	0.83
2:E:155:PRO:HD3	3:J:30:LEU:HD13	1.60	0.83
3:K:30:LEU:HD13	2:Z:155:PRO:HD3	126.33	0.83
3:K:28:VAL:HG11	2:Z:293:ARG:CD	113.65	0.83
2:B:109:ARG:CB	3:G:25:GLN:HB2	2.06	0.83
2:C:155:PRO:HD3	3:H:30:LEU:HD13	1.60	0.83
2:B:155:PRO:HD3	3:G:30:LEU:HD13	1.60	0.83
2:C:109:ARG:CD	3:H:25:GLN:CB	2.42	0.83
2:D:109:ARG:CB	3:I:25:GLN:HB2	2.06	0.83
3:K:25:GLN:HB2	2:Z:109:ARG:CB	120.30	0.82
3:K:25:GLN:CB	2:Z:109:ARG:CD	120.32	0.82
2:D:109:ARG:CD	3:I:25:GLN:CB	2.42	0.82
2:B:293:ARG:NH1	3:G:28:VAL:HA	1.94	0.82
3:K:28:VAL:HA	2:Z:293:ARG:NH1	112.08	0.82
3:H:19:PRO:CG	2:Z:231:GLU:OE2	2.28	0.82
2:C:293:ARG:NH1	3:H:28:VAL:HA	1.94	0.82
2:E:231:GLU:OE2	3:J:19:PRO:CG	56.76	0.81
2:C:109:ARG:CB	3:H:25:GLN:HB2	2.06	0.81
2:D:293:ARG:NH1	3:I:28:VAL:HA	1.94	0.81
2:E:293:ARG:NH1	3:J:28:VAL:HA	1.94	0.81
2:F:293:ARG:NH1	3:K:28:VAL:HA	1.94	0.81
3:G:19:PRO:CG	2:X:231:GLU:OE2	2.28	0.80
3:K:19:PRO:CG	2:Y:231:GLU:OE2	134.06	0.80
2:C:231:GLU:OE2	3:I:19:PRO:CG	45.84	0.79
2:C:483:LEU:C	3:I:18:ILE:HB	1.99	0.79
2:E:109:ARG:CD	3:J:25:GLN:CB	2.42	0.79
2:D:483:LEU:C	3:J:18:ILE:HB	2.01	0.79
2:F:109:ARG:HB3	3:K:25:GLN:CB	2.11	0.78
2:C:109:ARG:HB3	3:H:25:GLN:CB	2.11	0.77
2:E:483:LEU:C	3:K:18:ILE:HB	2.00	0.77
3:K:12:ARG:CG	2:X:333:ASP:HB2	132.10	0.77
2:D:109:ARG:HB3	3:I:25:GLN:CB	2.12	0.77
2:B:333:ASP:HB2	3:H:12:ARG:CG	2.11	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:483:LEU:C	3:G:18:ILE:HB	2.01	0.76
3:K:12:ARG:HH22	2:Y:407:ARG:HB2	122.27	0.76
2:B:109:ARG:HB3	3:G:25:GLN:CB	2.12	0.76
3:K:25:GLN:CB	2:Z:109:ARG:HB3	118.88	0.76
2:A:333:ASP:HB2	3:G:12:ARG:CG	2.12	0.75
3:K:19:PRO:HB3	2:Y:234:ARG:CZ	132.36	0.75
2:C:407:ARG:HB2	3:I:12:ARG:HH22	46.01	0.74
2:A:478:GLY:HA3	2:X:463:TRP:CZ3	2.22	0.74
2:E:333:ASP:HB2	3:K:12:ARG:CG	2.11	0.74
2:E:109:ARG:HB3	3:J:25:GLN:CB	2.11	0.74
2:C:463:TRP:CZ3	2:C:478:GLY:HA3	46.17	0.74
2:E:234:ARG:CZ	3:J:19:PRO:HB3	55.05	0.74
2:B:478:GLY:HA3	2:Z:463:TRP:CZ3	2.22	0.73
2:D:333:ASP:HB2	3:J:12:ARG:CG	2.11	0.73
2:D:478:GLY:HA3	2:E:463:TRP:CZ3	56.10	0.73
3:K:13:ILE:HD11	2:Y:403:LYS:HA	120.68	0.73
3:H:19:PRO:HB3	2:Z:234:ARG:CZ	2.18	0.73
3:G:19:PRO:HB3	2:X:234:ARG:CZ	2.19	0.73
2:F:293:ARG:NE	3:K:28:VAL:HG13	1.99	0.73
2:F:109:ARG:HH12	1:P:24:ALA:N	97.29	0.73
2:B:483:LEU:C	3:H:18:ILE:HB	2.02	0.73
2:E:403:LYS:HA	3:J:13:ILE:HD11	52.33	0.73
2:E:109:ARG:HH12	3:J:24:ALA:N	1.86	0.73
2:C:234:ARG:CZ	3:I:19:PRO:HB3	45.64	0.72
2:C:333:ASP:HB2	3:I:12:ARG:CG	2.13	0.72
3:H:12:ARG:HH22	2:Z:407:ARG:HB2	1.55	0.72
2:D:109:ARG:HH12	3:I:24:ALA:N	1.86	0.72
3:K:24:ALA:N	2:Z:109:ARG:HH12	116.73	0.72
3:G:12:ARG:HH22	2:X:407:ARG:HB2	1.54	0.72
3:G:13:ILE:HD11	2:X:403:LYS:HA	1.71	0.72
2:E:407:ARG:HB2	3:J:12:ARG:HH22	53.02	0.72
2:X:109:ARG:HH12	1:U:24:ALA:N	86.23	0.72
3:H:13:ILE:HD11	2:Z:403:LYS:HA	1.70	0.72
2:B:109:ARG:HH12	3:G:24:ALA:N	1.86	0.71
2:C:478:GLY:HA3	2:D:463:TRP:CZ3	56.10	0.71
3:K:28:VAL:HG13	2:Z:293:ARG:NE	113.49	0.71
2:B:109:ARG:HH12	1:L:24:ALA:N	54.53	0.71
2:B:293:ARG:NE	3:G:28:VAL:HG13	1.99	0.71
2:C:403:LYS:HA	3:I:13:ILE:HD11	43.58	0.71
3:K:18:ILE:HB	2:X:483:LEU:C	120.91	0.71
2:E:478:GLY:HA3	2:F:463:TRP:CZ3	56.09	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:24:ALA:N	2:Y:109:ARG:HH12	104.49	0.71
2:B:463:TRP:CZ3	2:Z:478:GLY:HA3	91.10	0.70
2:X:478:GLY:HA3	2:Y:463:TRP:CZ3	2.26	0.70
2:C:293:ARG:NE	3:H:28:VAL:HG13	1.99	0.70
2:C:109:ARG:HH12	3:H:24:ALA:N	1.86	0.70
3:K:28:VAL:HG12	2:Z:293:ARG:NE	112.65	0.70
2:C:293:ARG:NE	3:H:28:VAL:HG12	2.02	0.69
3:K:12:ARG:HH12	2:Y:407:ARG:HA	120.59	0.69
3:K:12:ARG:NH2	2:Y:407:ARG:HB2	123.10	0.69
2:C:407:ARG:HB2	3:I:12:ARG:NH2	45.85	0.69
2:D:109:ARG:HD2	3:I:25:GLN:HB3	0.72	0.68
2:C:407:ARG:HA	3:I:12:ARG:HH12	45.64	0.68
2:E:109:ARG:HH12	1:O:24:ALA:N	106.28	0.68
2:D:109:ARG:HH12	1:N:24:ALA:N	86.24	0.68
2:F:109:ARG:HH12	3:K:24:ALA:N	1.86	0.68
2:C:109:ARG:HH12	1:M:24:ALA:N	88.58	0.68
2:F:109:ARG:HD2	3:K:25:GLN:HB3	0.72	0.68
2:D:293:ARG:NE	3:I:28:VAL:HG12	2.02	0.67
3:G:12:ARG:HH12	2:X:407:ARG:HA	1.61	0.66
2:E:407:ARG:HB2	3:J:12:ARG:NH2	53.03	0.66
2:E:109:ARG:HD2	3:J:25:GLN:HB3	0.72	0.66
3:H:12:ARG:HH12	2:Z:407:ARG:HA	1.61	0.66
2:C:484:SER:HB2	3:I:20:ALA:O	1.95	0.65
2:E:293:ARG:NE	3:J:28:VAL:HG12	2.02	0.65
2:E:407:ARG:HA	3:J:12:ARG:HH12	52.68	0.65
2:B:293:ARG:NE	3:G:28:VAL:HG12	2.02	0.65
2:D:484:SER:HB2	3:J:20:ALA:O	1.97	0.65
2:F:293:ARG:NE	3:K:28:VAL:HG12	2.02	0.65
3:G:12:ARG:NH2	2:X:407:ARG:HB2	2.10	0.65
3:H:12:ARG:NH2	2:Z:407:ARG:HB2	2.10	0.65
2:E:484:SER:HB2	3:K:20:ALA:O	1.96	0.65
2:B:484:SER:HB2	3:H:20:ALA:O	1.97	0.65
3:K:20:ALA:O	2:X:484:SER:HB2	120.53	0.64
2:X:109:ARG:HH22	1:U:24:ALA:H	87.66	0.64
2:F:109:ARG:HH22	3:K:24:ALA:H	1.45	0.64
1:R:49:THR:HA	1:T:122:ASP:HB3	1.80	0.64
2:A:484:SER:HB2	3:G:20:ALA:O	1.96	0.64
3:K:28:VAL:HA	2:Z:293:ARG:HH12	111.61	0.64
1:V:24:ALA:H	2:Y:109:ARG:HH22	106.23	0.64
2:C:293:ARG:HH12	3:H:28:VAL:HA	1.63	0.64
2:F:110:GLU:HA	3:K:26:ALA:C	2.19	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:49:THR:HA	1:6:122:ASP:HB3	1.80	0.64
2:B:293:ARG:HH12	3:G:28:VAL:HA	1.63	0.64
2:D:110:GLU:HA	3:I:26:ALA:C	2.19	0.63
2:D:293:ARG:HH12	3:I:28:VAL:HA	1.63	0.63
2:F:109:ARG:HH22	1:P:24:ALA:H	98.14	0.63
2:D:109:ARG:HH22	1:N:24:ALA:H	87.67	0.63
1:U:49:THR:HA	1:W:122:ASP:HB3	1.80	0.63
2:E:293:ARG:HH12	3:J:28:VAL:HA	1.63	0.63
2:C:109:ARG:HH22	1:M:24:ALA:H	89.52	0.63
3:I:16:LYS:HZ3	3:I:18:ILE:HD11	1.64	0.63
2:E:109:ARG:HH22	3:J:24:ALA:H	1.45	0.63
2:E:110:GLU:HA	3:J:26:ALA:C	2.19	0.63
1:S:49:THR:HA	1:U:122:ASP:HB3	1.80	0.63
2:E:293:ARG:NH1	3:J:28:VAL:CA	2.62	0.63
3:K:24:ALA:H	2:Z:109:ARG:HH22	117.89	0.63
2:C:110:GLU:HA	3:H:26:ALA:C	2.19	0.63
2:D:293:ARG:NH1	3:I:28:VAL:CA	2.62	0.63
1:4:49:THR:HA	1:5:122:ASP:HB3	1.80	0.63
3:K:26:ALA:C	2:Z:110:GLU:HA	116.41	0.63
2:B:109:ARG:HH22	1:L:24:ALA:H	55.88	0.63
2:C:109:ARG:HH22	3:H:24:ALA:H	1.45	0.63
2:B:109:ARG:HD2	3:G:25:GLN:HB3	0.72	0.62
2:B:109:ARG:HH22	3:G:24:ALA:H	1.45	0.62
2:D:109:ARG:HH22	3:I:24:ALA:H	1.45	0.62
2:B:110:GLU:HA	3:G:26:ALA:C	2.19	0.62
2:E:109:ARG:HH22	1:O:24:ALA:H	107.02	0.62
2:C:109:ARG:HD2	3:H:25:GLN:HB3	0.72	0.62
2:F:293:ARG:HH12	3:K:28:VAL:HA	1.63	0.62
3:K:25:GLN:HB3	2:Z:109:ARG:HD2	119.89	0.62
1:L:122:ASP:HB3	1:V:49:THR:HA	1.81	0.62
1:O:49:THR:HA	1:Q:122:ASP:HB3	1.81	0.62
1:Q:49:THR:HA	1:S:122:ASP:HB3	1.82	0.62
2:E:293:ARG:NE	3:J:28:VAL:HG13	1.99	0.62
1:T:49:THR:HA	1:V:122:ASP:HB3	1.80	0.62
2:Y:365:GLN:NE2	2:Y:383:TYR:OH	2.33	0.62
1:1:122:ASP:HB3	1:6:49:THR:HA	1.81	0.62
2:B:365:GLN:NE2	2:B:383:TYR:OH	2.33	0.62
2:C:293:ARG:NH1	3:H:28:VAL:CA	2.62	0.62
1:3:49:THR:HA	1:4:122:ASP:HB3	1.82	0.61
2:D:365:GLN:NE2	2:D:383:TYR:OH	2.33	0.61
2:C:365:GLN:NE2	2:C:383:TYR:OH	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:49:THR:HA	1:N:122:ASP:HB3	1.81	0.61
2:B:293:ARG:NH1	3:G:28:VAL:CA	2.62	0.61
3:K:28:VAL:CA	2:Z:293:ARG:NH1	113.01	0.61
2:X:365:GLN:NE2	2:X:383:TYR:OH	2.33	0.61
1:2:49:THR:HA	1:3:122:ASP:HB3	1.81	0.61
2:A:365:GLN:NE2	2:A:383:TYR:OH	2.33	0.61
2:F:293:ARG:NH1	3:K:28:VAL:CA	2.62	0.61
1:1:49:THR:HA	1:2:122:ASP:HB3	1.81	0.61
1:N:49:THR:HA	1:P:122:ASP:HB3	1.81	0.61
2:Z:365:GLN:NE2	2:Z:383:TYR:OH	2.33	0.61
2:F:365:GLN:NE2	2:F:383:TYR:OH	2.33	0.61
2:E:365:GLN:NE2	2:E:383:TYR:OH	2.33	0.61
1:M:49:THR:HA	1:O:122:ASP:HB3	1.81	0.60
1:P:116:GLU:HB2	1:P:150:LYS:HB3	1.83	0.60
1:P:49:THR:HA	1:R:122:ASP:HB3	1.82	0.60
1:L:116:GLU:HB2	1:L:150:LYS:HB3	1.83	0.60
1:Q:116:GLU:HB2	1:Q:150:LYS:HB3	1.84	0.60
1:1:116:GLU:HB2	1:1:150:LYS:HB3	1.84	0.60
1:4:116:GLU:HB2	1:4:150:LYS:HB3	1.84	0.60
1:W:116:GLU:HB2	1:W:150:LYS:HB3	1.83	0.60
1:M:122:ASP:HB3	1:W:49:THR:HA	1.81	0.60
3:K:16:LYS:NZ	3:K:18:ILE:HD11	2.17	0.60
1:3:116:GLU:HB2	1:3:150:LYS:HB3	1.83	0.60
2:D:293:ARG:NE	3:I:28:VAL:HG13	1.99	0.60
3:J:16:LYS:HZ3	3:J:18:ILE:HD11	1.67	0.60
1:R:116:GLU:HB2	1:R:150:LYS:HB3	1.84	0.60
1:V:116:GLU:HB2	1:V:150:LYS:HB3	1.84	0.60
1:2:116:GLU:HB2	1:2:150:LYS:HB3	1.83	0.60
1:O:116:GLU:HB2	1:O:150:LYS:HB3	1.84	0.60
1:M:116:GLU:HB2	1:M:150:LYS:HB3	1.84	0.60
1:U:116:GLU:HB2	1:U:150:LYS:HB3	1.83	0.59
1:6:116:GLU:HB2	1:6:150:LYS:HB3	1.84	0.59
3:H:16:LYS:NZ	3:H:18:ILE:HD11	2.17	0.59
3:J:16:LYS:NZ	3:J:18:ILE:HD11	2.17	0.59
3:G:16:LYS:NZ	3:G:18:ILE:HD11	2.17	0.59
1:5:116:GLU:HB2	1:5:150:LYS:HB3	1.83	0.59
3:K:12:ARG:NH2	2:Y:407:ARG:HD3	125.02	0.59
1:N:116:GLU:HB2	1:N:150:LYS:HB3	1.84	0.59
1:S:116:GLU:HB2	1:S:150:LYS:HB3	1.84	0.58
1:T:116:GLU:HB2	1:T:150:LYS:HB3	1.83	0.58
3:I:16:LYS:NZ	3:I:18:ILE:HD11	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:16:LYS:HZ3	3:K:18:ILE:HD11	1.71	0.58
2:B:155:PRO:HD3	3:G:30:LEU:CD1	2.33	0.58
2:B:109:ARG:HH22	3:G:23:ASP:HB3	1.69	0.58
3:K:23:ASP:HB3	2:Z:109:ARG:HH22	118.73	0.58
3:H:16:LYS:HZ3	3:H:18:ILE:HD11	1.69	0.58
2:F:61:ASN:HA	2:F:64:LEU:HB2	1.86	0.58
2:C:109:ARG:HH22	3:H:23:ASP:HB3	1.69	0.58
3:K:12:ARG:CZ	2:Y:407:ARG:HG3	124.06	0.57
2:A:61:ASN:HA	2:A:64:LEU:HB2	1.86	0.57
2:B:61:ASN:HA	2:B:64:LEU:HB2	1.86	0.57
2:E:442:ARG:HD3	2:F:413:TRP:CE3	48.89	0.57
2:A:442:ARG:HD3	2:X:413:TRP:CE3	2.39	0.57
2:B:442:ARG:HD3	2:Z:413:TRP:CE3	2.39	0.57
2:C:413:TRP:CE3	2:C:442:ARG:HD3	42.60	0.57
2:D:109:ARG:HH22	3:I:23:ASP:HB3	1.69	0.57
2:F:109:ARG:HH22	3:K:23:ASP:HB3	1.69	0.57
2:D:442:ARG:HD3	2:E:413:TRP:CE3	48.89	0.57
3:H:19:PRO:CB	2:Z:234:ARG:NH2	2.68	0.57
2:C:442:ARG:HD3	2:D:413:TRP:CE3	48.89	0.57
2:C:61:ASN:HA	2:C:64:LEU:HB2	1.86	0.57
2:E:61:ASN:HA	2:E:64:LEU:HB2	1.86	0.57
2:E:234:ARG:NH2	3:J:19:PRO:CB	55.32	0.57
2:X:61:ASN:HA	2:X:64:LEU:HB2	1.86	0.57
2:B:413:TRP:CE3	2:Z:442:ARG:HD3	85.10	0.56
2:D:61:ASN:HA	2:D:64:LEU:HB2	1.86	0.56
2:E:109:ARG:HH22	3:J:23:ASP:HB3	1.69	0.56
2:F:155:PRO:HD3	3:K:30:LEU:CD1	2.33	0.56
3:K:19:PRO:CB	2:Y:234:ARG:NH2	132.76	0.56
2:Y:61:ASN:HA	2:Y:64:LEU:HB2	1.86	0.56
2:X:442:ARG:HD3	2:Y:413:TRP:CE3	2.40	0.56
2:D:396:ASN:O	2:D:400:HIS:ND1	2.39	0.56
2:F:396:ASN:O	2:F:400:HIS:ND1	2.39	0.56
2:B:396:ASN:O	2:B:400:HIS:ND1	2.39	0.56
2:D:167:PRO:HD3	2:D:197:PHE:HA	1.88	0.56
3:G:19:PRO:CB	2:X:234:ARG:NH2	2.69	0.56
2:C:167:PRO:HD3	2:C:197:PHE:HA	1.88	0.56
2:C:396:ASN:O	2:C:400:HIS:ND1	2.39	0.56
2:E:155:PRO:HD3	3:J:30:LEU:CD1	2.33	0.56
2:E:167:PRO:HD3	2:E:197:PHE:HA	1.88	0.56
3:I:143:LEU:HB3	3:I:150:ARG:HD3	1.87	0.56
2:Y:396:ASN:O	2:Y:400:HIS:ND1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:396:ASN:O	2:Z:400:HIS:ND1	2.39	0.56
2:B:260:ASN:H	3:G:120:ARG:HH12	1.54	0.56
2:C:234:ARG:NH2	3:I:19:PRO:CB	45.08	0.56
3:K:120:ARG:HH12	2:Z:260:ASN:H	170.30	0.56
2:E:396:ASN:O	2:E:400:HIS:ND1	2.39	0.56
2:Y:150:GLN:O	2:Y:407:ARG:NH1	2.39	0.56
2:X:150:GLN:O	2:X:407:ARG:NH1	2.39	0.55
2:A:396:ASN:O	2:A:400:HIS:ND1	2.39	0.55
2:F:167:PRO:HD3	2:F:197:PHE:HA	1.88	0.55
2:X:396:ASN:O	2:X:400:HIS:ND1	2.39	0.55
2:Z:150:GLN:O	2:Z:407:ARG:NH1	2.39	0.55
2:Z:61:ASN:HA	2:Z:64:LEU:HB2	1.86	0.55
2:D:150:GLN:O	2:D:407:ARG:NH1	2.39	0.55
2:E:150:GLN:O	2:E:407:ARG:NH1	2.39	0.55
2:A:150:GLN:O	2:A:407:ARG:NH1	2.39	0.55
2:B:167:PRO:HD3	2:B:197:PHE:HA	1.88	0.55
3:H:143:LEU:HB3	3:H:150:ARG:HD3	1.87	0.55
3:J:143:LEU:HB3	3:J:150:ARG:HD3	1.87	0.55
2:B:150:GLN:O	2:B:407:ARG:NH1	2.39	0.55
2:F:260:ASN:H	3:K:120:ARG:HH12	1.54	0.55
3:K:143:LEU:HB3	3:K:150:ARG:HD3	1.87	0.55
2:X:167:PRO:HD3	2:X:197:PHE:HA	1.88	0.55
2:A:167:PRO:HD3	2:A:197:PHE:HA	1.88	0.55
3:K:13:ILE:HG13	2:Y:403:LYS:HD2	123.77	0.55
2:Z:167:PRO:HD3	2:Z:197:PHE:HA	1.88	0.55
2:F:150:GLN:O	2:F:407:ARG:NH1	2.39	0.55
3:H:10:LYS:HE2	3:H:12:ARG:HB2	1.89	0.55
2:C:407:ARG:HD3	3:I:12:ARG:NH2	45.99	0.55
2:C:407:ARG:HG3	3:I:12:ARG:CZ	46.80	0.55
2:C:150:GLN:O	2:C:407:ARG:NH1	2.39	0.55
2:C:260:ASN:H	3:H:120:ARG:HH12	1.54	0.55
1:5:65:HIS:NE2	1:5:164:ASP:OD2	2.39	0.55
2:D:155:PRO:HD3	3:I:30:LEU:CD1	2.33	0.55
1:O:65:HIS:NE2	1:O:164:ASP:OD2	2.39	0.55
3:H:12:ARG:NH2	2:Z:407:ARG:HD3	2.22	0.54
1:1:65:HIS:NE2	1:1:164:ASP:OD2	2.39	0.54
3:G:143:LEU:HB3	3:G:150:ARG:HD3	1.87	0.54
2:D:260:ASN:H	3:I:120:ARG:HH12	1.54	0.54
2:E:407:ARG:HG3	3:J:12:ARG:CZ	52.79	0.54
2:F:109:ARG:CB	3:K:25:GLN:CB	2.81	0.54
3:G:16:LYS:HZ3	3:G:18:ILE:HD11	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:10:LYS:HE2	3:K:12:ARG:HB2	1.89	0.54
3:G:12:ARG:CZ	2:X:407:ARG:HG3	2.38	0.54
2:Y:167:PRO:HD3	2:Y:197:PHE:HA	1.88	0.54
3:J:10:LYS:HE2	3:J:12:ARG:HB2	1.89	0.54
2:E:407:ARG:HD3	3:J:12:ARG:NH2	52.62	0.54
2:B:410:ILE:HA	2:Z:476:TYR:HD2	88.52	0.54
3:I:10:LYS:HE2	3:I:12:ARG:HB2	1.89	0.54
2:X:476:TYR:HD2	2:Y:410:ILE:HA	1.72	0.54
1:3:65:HIS:NE2	1:3:164:ASP:OD2	2.39	0.54
1:T:65:HIS:NE2	1:T:164:ASP:OD2	2.39	0.54
2:C:155:PRO:HD3	3:H:30:LEU:CD1	2.33	0.53
2:E:260:ASN:H	3:J:120:ARG:HH12	1.54	0.53
3:K:30:LEU:CD1	2:Z:155:PRO:HD3	125.60	0.53
2:C:484:SER:HA	3:I:18:ILE:O	2.08	0.53
3:G:12:ARG:NH2	2:X:407:ARG:HD3	2.22	0.53
2:A:484:SER:HA	3:G:18:ILE:O	2.09	0.53
2:C:124:LEU:HD11	2:C:139:LEU:HD22	1.91	0.53
2:D:124:LEU:HD11	2:D:139:LEU:HD22	1.91	0.53
2:F:124:LEU:HD11	2:F:139:LEU:HD22	1.91	0.53
3:H:12:ARG:CZ	2:Z:407:ARG:HG3	2.38	0.53
3:G:10:LYS:HE2	3:G:12:ARG:HB2	1.89	0.53
1:L:65:HIS:NE2	1:L:164:ASP:OD2	2.39	0.53
3:K:18:ILE:O	2:X:484:SER:HA	121.76	0.53
2:E:124:LEU:HD11	2:E:139:LEU:HD22	1.91	0.53
2:B:124:LEU:HD11	2:B:139:LEU:HD22	1.91	0.53
1:P:65:HIS:NE2	1:P:164:ASP:OD2	2.39	0.53
2:C:476:TYR:HD2	2:D:410:ILE:HA	50.77	0.52
2:E:484:SER:HA	3:K:18:ILE:O	2.09	0.52
2:B:484:SER:HA	3:H:18:ILE:O	2.09	0.52
2:D:484:SER:HA	3:J:18:ILE:O	2.09	0.52
2:A:124:LEU:HD11	2:A:139:LEU:HD22	1.91	0.52
1:U:65:HIS:NE2	1:U:164:ASP:OD2	2.39	0.52
1:6:9:ILE:HG12	1:6:94:VAL:HG22	1.92	0.52
2:Z:124:LEU:HD11	2:Z:139:LEU:HD22	1.91	0.52
2:F:434:GLN:HG3	1:U:80:LEU:HD21	88.14	0.52
1:1:9:ILE:HG12	1:1:94:VAL:HG22	1.92	0.52
2:E:109:ARG:CB	3:J:25:GLN:CB	2.81	0.52
1:W:9:ILE:HG12	1:W:94:VAL:HG22	1.92	0.52
2:X:124:LEU:HD11	2:X:139:LEU:HD22	1.91	0.52
2:Y:124:LEU:HD11	2:Y:139:LEU:HD22	1.91	0.52
3:H:13:ILE:HG13	2:Z:403:LYS:HD2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:85:HIS:HB3	2:E:271:HIS:HD2	1.75	0.52
2:E:234:ARG:NH2	3:J:19:PRO:HB3	56.28	0.52
1:T:9:ILE:HG12	1:T:94:VAL:HG22	1.92	0.52
3:K:28:VAL:CG1	2:Z:293:ARG:HH11	111.92	0.52
2:Z:434:GLN:HG3	1:P:80:LEU:HD21	1.92	0.52
2:E:434:GLN:HG3	1:T:80:LEU:HD21	44.49	0.52
2:E:476:TYR:HD2	2:F:410:ILE:HA	50.77	0.52
1:U:9:ILE:HG12	1:U:94:VAL:HG22	1.92	0.52
3:K:7:VAL:HG11	2:Y:144:TYR:CZ	137.52	0.52
2:E:434:GLN:HG3	1:6:80:LEU:HD21	1.92	0.52
2:B:434:GLN:HG3	1:3:80:LEU:HD21	1.92	0.52
2:B:434:GLN:HG3	1:Q:80:LEU:HD21	81.28	0.52
2:D:85:HIS:HB3	2:D:271:HIS:HD2	1.75	0.52
2:D:415:GLU:H	2:D:418:ASP:HB3	1.75	0.52
1:Q:65:HIS:NE2	1:Q:164:ASP:OD2	2.39	0.52
2:X:85:HIS:HB3	2:X:271:HIS:HD2	1.75	0.52
2:A:85:HIS:HB3	2:A:271:HIS:HD2	1.75	0.51
2:F:85:HIS:HB3	2:F:271:HIS:HD2	1.75	0.51
2:B:85:HIS:HB3	2:B:271:HIS:HD2	1.75	0.51
3:G:13:ILE:HG13	2:X:403:LYS:HD2	1.92	0.51
3:H:19:PRO:HB3	2:Z:234:ARG:NH2	2.24	0.51
2:B:415:GLU:H	2:B:418:ASP:HB3	1.75	0.51
2:B:476:TYR:HD2	2:Z:410:ILE:HA	1.75	0.51
2:D:109:ARG:CB	3:I:25:GLN:CB	2.81	0.51
1:M:65:HIS:NE2	1:M:164:ASP:OD2	2.39	0.51
2:Y:85:HIS:HB3	2:Y:271:HIS:HD2	1.75	0.51
1:5:9:ILE:HG12	1:5:94:VAL:HG22	1.92	0.51
2:C:407:ARG:HA	3:I:12:ARG:NH1	45.49	0.51
2:C:109:ARG:CB	3:H:25:GLN:CB	2.81	0.51
2:E:403:LYS:HD2	3:J:13:ILE:HG13	52.58	0.51
3:K:25:GLN:CB	2:Z:109:ARG:CB	119.80	0.51
1:L:9:ILE:HG12	1:L:94:VAL:HG22	1.92	0.51
1:R:9:ILE:HG12	1:R:94:VAL:HG22	1.92	0.51
3:G:19:PRO:HB3	2:X:234:ARG:NH2	2.25	0.51
2:C:403:LYS:HD2	3:I:13:ILE:HG13	44.74	0.51
2:C:85:HIS:HB3	2:C:271:HIS:HD2	1.75	0.51
3:K:82:THR:HG23	3:K:84:ASP:H	1.76	0.51
2:A:476:TYR:HD2	2:X:410:ILE:HA	1.76	0.51
2:Z:85:HIS:HB3	2:Z:271:HIS:HD2	1.75	0.51
2:E:415:GLU:H	2:E:418:ASP:HB3	1.75	0.51
2:A:415:GLU:H	2:A:418:ASP:HB3	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:415:GLU:H	2:C:418:ASP:HB3	1.75	0.51
2:F:415:GLU:H	2:F:418:ASP:HB3	1.75	0.51
1:M:9:ILE:HG12	1:M:94:VAL:HG22	1.92	0.51
2:Y:434:GLN:HG3	1:O:80:LEU:HD21	1.93	0.51
2:D:434:GLN:HG3	1:5:80:LEU:HD21	1.92	0.51
1:V:9:ILE:HG12	1:V:94:VAL:HG22	1.92	0.51
2:X:415:GLU:H	2:X:418:ASP:HB3	1.75	0.51
3:K:19:PRO:HB3	2:Y:234:ARG:NH2	132.85	0.51
2:Z:415:GLU:H	2:Z:418:ASP:HB3	1.75	0.51
2:C:410:ILE:HA	2:C:476:TYR:HD2	44.70	0.51
3:J:82:THR:HG23	3:J:84:ASP:H	1.76	0.51
1:Q:9:ILE:HG12	1:Q:94:VAL:HG22	1.92	0.51
1:1:80:LEU:HD21	2:F:434:GLN:HG3	1.92	0.50
1:N:9:ILE:HG12	1:N:94:VAL:HG22	1.92	0.50
2:Y:415:GLU:H	2:Y:418:ASP:HB3	1.75	0.50
1:6:65:HIS:NE2	1:6:164:ASP:OD2	2.39	0.50
1:P:9:ILE:HG12	1:P:94:VAL:HG22	1.92	0.50
2:X:434:GLN:HG3	1:N:80:LEU:HD21	1.93	0.50
1:3:9:ILE:HG12	1:3:94:VAL:HG22	1.92	0.50
2:E:398:LEU:HD11	2:E:447:LEU:HD11	1.93	0.50
2:F:398:LEU:HD11	2:F:447:LEU:HD11	1.93	0.50
3:G:82:THR:HG23	3:G:84:ASP:H	1.76	0.50
3:I:146:SER:HG	3:I:149:SER:HG	1.57	0.50
1:O:9:ILE:HG12	1:O:94:VAL:HG22	1.92	0.50
3:I:41:LYS:HE2	3:I:69:SER:HB2	1.93	0.50
3:H:82:THR:HG23	3:H:84:ASP:H	1.76	0.50
1:4:9:ILE:HG12	1:4:94:VAL:HG22	1.92	0.50
2:C:434:GLN:HG3	1:4:80:LEU:HD21	1.94	0.50
1:S:9:ILE:HG12	1:S:94:VAL:HG22	1.92	0.50
1:4:65:HIS:NE2	1:4:164:ASP:OD2	2.39	0.50
2:D:398:LEU:HD11	2:D:447:LEU:HD11	1.93	0.50
3:H:41:LYS:HE2	3:H:69:SER:HB2	1.93	0.50
3:I:82:THR:HG23	3:I:84:ASP:H	1.76	0.50
2:A:434:GLN:HG3	1:2:80:LEU:HD21	1.93	0.50
2:C:234:ARG:NH2	3:I:19:PRO:HB3	45.36	0.50
2:X:398:LEU:HD11	2:X:447:LEU:HD11	1.93	0.50
2:A:398:LEU:HD11	2:A:447:LEU:HD11	1.93	0.49
3:H:146:SER:HG	3:H:149:SER:HG	1.59	0.49
3:K:12:ARG:NH1	2:Y:407:ARG:HA	121.42	0.49
1:U:95:GLU:HG3	1:U:114:LYS:HG2	1.94	0.49
1:2:9:ILE:HG12	1:2:94:VAL:HG22	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:109:ARG:CB	3:G:25:GLN:CB	2.81	0.49
2:B:447:LEU:HD22	2:B:470:VAL:HB	1.95	0.49
3:K:41:LYS:HE2	3:K:69:SER:HB2	1.93	0.49
1:2:65:HIS:NE2	1:2:164:ASP:OD2	2.39	0.49
2:E:407:ARG:HA	3:J:12:ARG:NH1	52.69	0.49
2:Z:447:LEU:HD22	2:Z:470:VAL:HB	1.95	0.49
2:B:398:LEU:HD11	2:B:447:LEU:HD11	1.93	0.49
2:C:447:LEU:HD22	2:C:470:VAL:HB	1.95	0.49
2:D:447:LEU:HD22	2:D:470:VAL:HB	1.95	0.49
2:D:434:GLN:HG3	1:S:80:LEU:HD21	75.61	0.49
1:1:95:GLU:HG3	1:1:114:LYS:HG2	1.94	0.49
2:F:454:VAL:HG13	2:F:466:VAL:HG12	1.95	0.49
2:X:454:VAL:HG13	2:X:466:VAL:HG12	1.95	0.49
2:Y:398:LEU:HD11	2:Y:447:LEU:HD11	1.93	0.49
2:A:448:ARG:HB3	2:A:471:ARG:HD3	1.95	0.49
1:S:95:GLU:HG3	1:S:114:LYS:HG2	1.94	0.49
2:Z:454:VAL:HG13	2:Z:466:VAL:HG12	1.95	0.49
2:C:434:GLN:HG3	1:R:80:LEU:HD21	40.52	0.49
1:T:95:GLU:HG3	1:T:114:LYS:HG2	1.94	0.49
3:G:41:LYS:HE2	3:G:69:SER:HB2	1.93	0.49
1:N:65:HIS:NE2	1:N:164:ASP:OD2	2.39	0.49
1:W:95:GLU:HG3	1:W:114:LYS:HG2	1.95	0.49
2:X:447:LEU:HD22	2:X:470:VAL:HB	1.95	0.49
2:C:398:LEU:HD11	2:C:447:LEU:HD11	1.93	0.49
2:D:476:TYR:HD2	2:E:410:ILE:HA	50.77	0.49
3:J:41:LYS:HE2	3:J:69:SER:HB2	1.93	0.49
1:V:65:HIS:NE2	1:V:164:ASP:OD2	2.39	0.49
2:C:454:VAL:HG13	2:C:466:VAL:HG12	1.95	0.48
2:Y:447:LEU:HD22	2:Y:470:VAL:HB	1.95	0.48
2:Z:398:LEU:HD11	2:Z:447:LEU:HD11	1.93	0.48
2:E:454:VAL:HG13	2:E:466:VAL:HG12	1.95	0.48
3:G:57:VAL:HG22	3:G:65:VAL:HG21	1.95	0.48
3:H:10:LYS:HG2	3:H:12:ARG:H	1.78	0.48
2:A:454:VAL:HG13	2:A:466:VAL:HG12	1.95	0.48
2:E:448:ARG:HB3	2:E:471:ARG:HD3	1.95	0.48
3:K:10:LYS:HG2	3:K:12:ARG:H	1.78	0.48
1:R:65:HIS:NE2	1:R:164:ASP:OD2	2.39	0.48
2:X:448:ARG:HB3	2:X:471:ARG:HD3	1.95	0.48
2:Y:454:VAL:HG13	2:Y:466:VAL:HG12	1.95	0.48
1:6:95:GLU:HG3	1:6:114:LYS:HG2	1.94	0.48
2:B:454:VAL:HG13	2:B:466:VAL:HG12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:454:VAL:HG13	2:D:466:VAL:HG12	1.95	0.48
2:E:110:GLU:HA	3:J:26:ALA:HB3	1.96	0.48
3:J:10:LYS:HG2	3:J:12:ARG:H	1.79	0.48
3:K:26:ALA:HB3	2:Z:110:GLU:CA	115.95	0.48
1:2:95:GLU:HG3	1:2:114:LYS:HG2	1.94	0.48
2:A:447:LEU:HD22	2:A:470:VAL:HB	1.95	0.48
2:D:110:GLU:HA	3:I:26:ALA:HB3	1.96	0.48
2:F:448:ARG:HB3	2:F:471:ARG:HD3	1.95	0.48
2:C:110:GLU:HA	3:H:26:ALA:HB3	1.96	0.48
2:F:336:GLU:HG2	2:F:346:ALA:HB3	1.95	0.48
2:F:447:LEU:HD22	2:F:470:VAL:HB	1.95	0.48
3:H:57:VAL:HG22	3:H:65:VAL:HG21	1.95	0.48
3:K:57:VAL:HG22	3:K:65:VAL:HG21	1.95	0.48
1:R:95:GLU:HG3	1:R:114:LYS:HG2	1.94	0.48
1:V:95:GLU:HG3	1:V:114:LYS:HG2	1.94	0.48
2:B:336:GLU:HG2	2:B:346:ALA:HB3	1.95	0.48
2:E:336:GLU:HG2	2:E:346:ALA:HB3	1.95	0.48
2:E:447:LEU:HD22	2:E:470:VAL:HB	1.95	0.48
1:M:95:GLU:HG3	1:M:114:LYS:HG2	1.94	0.48
1:W:65:HIS:NE2	1:W:164:ASP:OD2	2.39	0.48
2:Z:336:GLU:HG2	2:Z:346:ALA:HB3	1.95	0.48
2:F:110:GLU:HA	3:K:26:ALA:HB3	1.96	0.48
1:O:95:GLU:HG3	1:O:114:LYS:HG2	1.94	0.48
1:P:95:GLU:HG3	1:P:114:LYS:HG2	1.94	0.48
1:Q:95:GLU:HG3	1:Q:114:LYS:HG2	1.94	0.48
1:S:65:HIS:NE2	1:S:164:ASP:OD2	2.39	0.48
2:Y:336:GLU:HG2	2:Y:346:ALA:HB3	1.95	0.48
1:3:95:GLU:HG3	1:3:114:LYS:HG2	1.94	0.48
2:C:448:ARG:HB3	2:C:471:ARG:HD3	1.95	0.48
2:D:448:ARG:HB3	2:D:471:ARG:HD3	1.95	0.48
3:G:10:LYS:HG2	3:G:12:ARG:H	1.79	0.48
2:C:144:TYR:CZ	3:I:7:VAL:HG11	48.24	0.48
3:J:146:SER:HG	3:J:149:SER:HG	1.59	0.48
1:L:95:GLU:HG3	1:L:114:LYS:HG2	1.94	0.48
1:4:95:GLU:HG3	1:4:114:LYS:HG2	1.94	0.47
1:5:95:GLU:HG3	1:5:114:LYS:HG2	1.94	0.47
2:E:110:GLU:CA	3:J:26:ALA:HB3	2.35	0.47
2:B:110:GLU:CA	3:G:26:ALA:HB3	2.35	0.47
1:N:95:GLU:HG3	1:N:114:LYS:HG2	1.94	0.47
2:B:448:ARG:HB3	2:B:471:ARG:HD3	1.95	0.47
2:D:336:GLU:HG2	2:D:346:ALA:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:350:ARG:NH2	2:X:151:PHE:HZ	2.12	0.47
3:K:122:ALA:HB1	2:Z:42:GLY:HA2	190.79	0.47
2:Z:448:ARG:HB3	2:Z:471:ARG:HD3	1.95	0.47
3:K:17:TYR:CD1	2:Y:395:ILE:HD12	122.56	0.47
3:I:57:VAL:HG22	3:I:65:VAL:HG21	1.95	0.47
2:X:336:GLU:HG2	2:X:346:ALA:HB3	1.95	0.47
2:Y:448:ARG:HB3	2:Y:471:ARG:HD3	1.95	0.47
3:G:113:LEU:HD23	3:G:116:LEU:HD12	1.97	0.47
2:B:42:GLY:HA2	3:G:122:ALA:HB1	1.97	0.47
2:F:42:GLY:HA2	3:K:122:ALA:HB1	1.97	0.47
2:C:151:PHE:HZ	2:C:350:ARG:NH2	45.74	0.47
2:C:336:GLU:HG2	2:C:346:ALA:HB3	1.95	0.47
3:K:146:SER:HG	3:K:149:SER:HG	1.62	0.47
2:C:155:PRO:CD	3:H:30:LEU:HD13	2.40	0.47
3:G:12:ARG:NH1	2:X:407:ARG:HA	2.28	0.47
3:K:113:LEU:HD23	3:K:116:LEU:HD12	1.97	0.47
3:J:57:VAL:HG22	3:J:65:VAL:HG21	1.95	0.47
2:E:42:GLY:HA2	3:J:122:ALA:HB1	1.96	0.47
3:H:23:ASP:HB3	3:H:24:ALA:H	1.52	0.47
2:D:350:ARG:NH2	2:E:151:PHE:HZ	55.73	0.46
2:C:42:GLY:HA2	3:H:122:ALA:HB1	1.96	0.46
2:B:350:ARG:NH2	2:Z:151:PHE:HZ	2.13	0.46
2:B:401:TYR:HE1	3:G:29:GLU:HG3	1.80	0.46
3:H:113:LEU:HD23	3:H:116:LEU:HD12	1.97	0.46
2:C:401:TYR:HE1	3:H:29:GLU:HG3	1.81	0.46
2:D:42:GLY:HA2	3:I:122:ALA:HB1	1.96	0.46
3:H:7:VAL:HG11	2:Z:144:TYR:CZ	2.51	0.46
3:I:10:LYS:HG2	3:I:12:ARG:H	1.79	0.46
2:A:336:GLU:HG2	2:A:346:ALA:HB3	1.95	0.46
2:F:401:TYR:HE1	3:K:29:GLU:HG3	1.81	0.46
2:B:110:GLU:HA	3:G:26:ALA:HB3	1.96	0.46
3:H:12:ARG:NH1	2:Z:407:ARG:HA	2.28	0.46
1:R:42:GLN:HB3	1:T:129:HIS:CD2	2.51	0.46
3:J:113:LEU:HD23	3:J:116:LEU:HD12	1.97	0.46
2:F:109:ARG:CG	3:K:25:GLN:HB2	2.46	0.46
3:K:26:ALA:HB3	2:Z:110:GLU:HA	115.04	0.46
1:S:42:GLN:HB3	1:U:129:HIS:CD2	2.51	0.46
3:G:7:VAL:HG11	2:X:144:TYR:CZ	2.50	0.46
1:2:42:GLN:HB3	1:3:129:HIS:CD2	2.51	0.46
2:E:401:TYR:HE1	3:J:29:GLU:HG3	1.81	0.46
3:K:29:GLU:HG3	2:Z:401:TYR:HE1	111.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:42:GLN:HB3	1:5:129:HIS:CD2	2.51	0.46
2:D:109:ARG:HD2	3:I:25:GLN:CA	2.39	0.46
3:I:113:LEU:HD23	3:I:116:LEU:HD12	1.97	0.46
3:K:25:GLN:HB2	2:Z:109:ARG:CG	121.18	0.46
2:C:109:ARG:CG	3:H:25:GLN:HB2	2.46	0.46
2:E:144:TYR:CZ	3:J:7:VAL:HG11	55.69	0.46
1:S:47:VAL:HG22	1:U:124:HIS:CD2	2.51	0.45
1:1:42:GLN:HB3	1:2:129:HIS:CD2	2.52	0.45
1:6:116:GLU:HG3	1:6:150:LYS:HD3	1.99	0.45
2:B:109:ARG:CG	3:G:25:GLN:HB2	2.46	0.45
2:F:293:ARG:NH2	3:K:27:GLU:C	2.62	0.45
1:R:47:VAL:HG22	1:T:124:HIS:CD2	2.51	0.45
1:U:116:GLU:HG3	1:U:150:LYS:HD3	1.99	0.45
1:4:47:VAL:HG22	1:5:124:HIS:CD2	2.51	0.45
2:C:395:ILE:HD12	3:I:17:TYR:CD1	44.91	0.45
1:N:42:GLN:HB3	1:P:129:HIS:CD2	2.51	0.45
1:S:2:PRO:HG3	1:U:128:PRO:HG2	1.99	0.45
1:T:116:GLU:HG3	1:T:150:LYS:HD3	1.99	0.45
3:G:16:LYS:HZ2	3:G:18:ILE:CG1	2.29	0.45
3:G:23:ASP:HB3	3:G:24:ALA:H	1.52	0.45
1:L:42:GLN:HB3	1:N:129:HIS:CD2	2.52	0.45
1:R:2:PRO:HG3	1:T:128:PRO:HG2	1.99	0.45
1:V:116:GLU:HG3	1:V:150:LYS:HD3	1.99	0.45
3:K:12:ARG:CZ	2:Y:407:ARG:CG	123.88	0.45
1:5:116:GLU:HG3	1:5:150:LYS:HD3	1.99	0.45
1:5:42:GLN:HB3	1:6:129:HIS:CD2	2.52	0.45
1:S:116:GLU:HG3	1:S:150:LYS:HD3	1.99	0.45
2:D:110:GLU:CA	3:I:26:ALA:HB3	2.35	0.45
2:D:284:ARG:NH2	2:D:287:ASP:OD2	2.50	0.45
2:E:109:ARG:CG	3:J:25:GLN:HB2	2.46	0.45
2:F:110:GLU:CA	3:K:26:ALA:HB3	2.36	0.45
1:O:42:GLN:HB3	1:Q:129:HIS:CD2	2.51	0.45
1:U:47:VAL:HG22	1:W:124:HIS:CD2	2.52	0.45
1:5:2:PRO:HG3	1:6:128:PRO:HG2	1.99	0.45
2:E:395:ILE:HD12	3:J:17:TYR:CD1	51.78	0.45
1:T:42:GLN:HB3	1:V:129:HIS:CD2	2.52	0.45
1:L:129:HIS:CD2	1:V:42:GLN:HB3	2.52	0.45
1:U:42:GLN:HB3	1:W:129:HIS:CD2	2.52	0.45
1:1:116:GLU:HG3	1:1:150:LYS:HD3	1.99	0.45
2:C:166:THR:OG1	2:C:171:ASP:OD2	2.34	0.45
2:C:284:ARG:NH2	2:C:287:ASP:OD2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:401:TYR:HE1	3:I:29:GLU:HG3	1.81	0.45
2:E:160:ILE:HB	3:J:36:VAL:HA	1.99	0.45
3:K:12:ARG:NH1	2:Y:407:ARG:HG3	123.45	0.45
1:N:116:GLU:HG3	1:N:150:LYS:HD3	1.99	0.45
1:2:47:VAL:HG22	1:3:124:HIS:CD2	2.52	0.45
1:3:116:GLU:HG3	1:3:150:LYS:HD3	1.99	0.45
1:4:2:PRO:HG3	1:5:128:PRO:HG2	1.99	0.45
2:A:284:ARG:NH2	2:A:287:ASP:OD2	2.50	0.45
2:B:284:ARG:NH2	2:B:287:ASP:OD2	2.50	0.45
2:D:60:VAL:O	2:D:64:LEU:N	2.48	0.45
2:E:284:ARG:NH2	2:E:287:ASP:OD2	2.50	0.45
2:D:109:ARG:CG	3:I:25:GLN:HB2	2.46	0.45
1:M:116:GLU:HG3	1:M:150:LYS:HD3	1.98	0.45
1:O:116:GLU:HG3	1:O:150:LYS:HD3	1.99	0.45
1:T:2:PRO:HG3	1:V:128:PRO:HG2	1.99	0.45
1:W:116:GLU:HG3	1:W:150:LYS:HD3	1.99	0.45
2:X:284:ARG:NH2	2:X:287:ASP:OD2	2.50	0.45
2:X:60:VAL:O	2:X:64:LEU:N	2.48	0.45
1:1:47:VAL:HG22	1:2:124:HIS:CD2	2.52	0.45
1:5:47:VAL:HG22	1:6:124:HIS:CD2	2.52	0.45
2:A:240:ALA:HB3	2:A:277:THR:HG21	1.99	0.45
2:E:350:ARG:NH2	2:F:151:PHE:HZ	55.73	0.45
3:J:94:ASN:O	3:J:109:GLN:NE2	2.40	0.45
1:U:2:PRO:HG3	1:W:128:PRO:HG2	1.99	0.45
2:Y:284:ARG:NH2	2:Y:287:ASP:OD2	2.50	0.45
2:Z:284:ARG:NH2	2:Z:287:ASP:OD2	2.50	0.45
2:F:160:ILE:HB	3:K:36:VAL:HA	1.99	0.44
2:F:284:ARG:NH2	2:F:287:ASP:OD2	2.50	0.44
3:J:18:ILE:HD13	3:J:18:ILE:HA	1.90	0.44
1:M:42:GLN:HB3	1:O:129:HIS:CD2	2.52	0.44
1:M:47:VAL:HG22	1:O:124:HIS:CD2	2.52	0.44
1:N:47:VAL:HG22	1:P:124:HIS:CD2	2.52	0.44
1:2:116:GLU:HG3	1:2:150:LYS:HD3	1.99	0.44
1:1:124:HIS:CD2	1:6:47:VAL:HG22	2.53	0.44
2:F:240:ALA:HB3	2:F:277:THR:HG21	1.99	0.44
2:D:160:ILE:HB	3:I:36:VAL:HA	1.99	0.44
1:L:47:VAL:HG22	1:N:124:HIS:CD2	2.52	0.44
1:O:47:VAL:HG22	1:Q:124:HIS:CD2	2.52	0.44
1:R:116:GLU:HG3	1:R:150:LYS:HD3	1.99	0.44
1:1:129:HIS:CD2	1:6:42:GLN:HB3	2.52	0.44
2:E:189:PHE:HB3	2:E:236:LEU:HD23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:189:PHE:HB3	2:F:236:LEU:HD23	1.99	0.44
1:M:124:HIS:CD2	1:W:47:VAL:HG22	2.53	0.44
1:P:116:GLU:HG3	1:P:150:LYS:HD3	1.99	0.44
1:1:128:PRO:HG2	1:6:2:PRO:HG3	1.99	0.44
2:E:240:ALA:HB3	2:E:277:THR:HG21	1.99	0.44
1:T:47:VAL:HG22	1:V:124:HIS:CD2	2.52	0.44
3:K:16:LYS:HZ2	3:K:18:ILE:CG1	2.30	0.44
1:L:128:PRO:HG2	1:V:2:PRO:HG3	1.99	0.44
1:L:124:HIS:CD2	1:V:47:VAL:HG22	2.53	0.44
2:A:269:HIS:O	2:A:274:TRP:NE1	2.36	0.44
3:G:17:TYR:CD1	2:X:395:ILE:HD12	2.53	0.44
1:M:129:HIS:CD2	1:W:42:GLN:HB3	2.52	0.44
1:P:47:VAL:HG22	1:R:124:HIS:CD2	2.53	0.44
2:Y:60:VAL:O	2:Y:64:LEU:N	2.48	0.44
1:3:47:VAL:HG22	1:4:124:HIS:CD2	2.53	0.44
2:D:240:ALA:HB3	2:D:277:THR:HG21	1.99	0.44
1:R:12:GLN:HG3	1:Q:103:ILE:HG22	2.00	0.44
1:Q:47:VAL:HG22	1:S:124:HIS:CD2	2.53	0.44
1:M:128:PRO:HG2	1:W:2:PRO:HG3	1.99	0.44
1:4:116:GLU:HG3	1:4:150:LYS:HD3	1.99	0.44
2:C:160:ILE:HB	3:H:36:VAL:HA	1.99	0.44
2:C:350:ARG:NH2	2:D:151:PHE:HZ	55.73	0.44
3:J:23:ASP:HB3	3:J:24:ALA:H	1.52	0.44
2:E:109:ARG:CG	3:J:25:GLN:CB	2.96	0.44
1:Q:116:GLU:HG3	1:Q:150:LYS:HD3	1.99	0.44
1:O:2:PRO:HG3	1:Q:128:PRO:HG2	1.99	0.44
2:X:240:ALA:HB3	2:X:277:THR:HG21	1.99	0.44
1:1:2:PRO:HG3	1:2:128:PRO:HG2	1.99	0.44
2:B:151:PHE:HZ	2:Z:350:ARG:NH2	90.60	0.44
3:G:18:ILE:HA	3:G:18:ILE:HD13	1.90	0.44
1:L:116:GLU:HG3	1:L:150:LYS:HD3	1.99	0.44
2:A:189:PHE:HB3	2:A:236:LEU:HD23	1.99	0.43
2:B:189:PHE:HB3	2:B:236:LEU:HD23	1.99	0.43
1:N:2:PRO:HG3	1:P:128:PRO:HG2	1.99	0.43
3:H:17:TYR:CD1	2:Z:395:ILE:HD12	2.53	0.43
1:2:2:PRO:HG3	1:3:128:PRO:HG2	1.99	0.43
1:3:42:GLN:HB3	1:4:129:HIS:CD2	2.53	0.43
2:C:240:ALA:HB3	2:C:277:THR:HG21	1.99	0.43
3:H:16:LYS:HZ2	3:H:18:ILE:CG1	2.31	0.43
1:Q:2:PRO:HG3	1:S:128:PRO:HG2	2.00	0.43
2:X:269:HIS:O	2:X:274:TRP:NE1	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:48:VAL:HB	1:5:85:LEU:HD21	2.01	0.43
2:A:60:VAL:O	2:A:64:LEU:N	2.48	0.43
2:B:160:ILE:HB	3:G:36:VAL:HA	1.99	0.43
2:C:109:ARG:CG	3:H:25:GLN:CB	2.96	0.43
1:L:2:PRO:HG3	1:N:128:PRO:HG2	1.99	0.43
1:T:12:GLN:HG3	1:S:103:ILE:HG22	2.01	0.43
2:Y:189:PHE:HB3	2:Y:236:LEU:HD23	1.99	0.43
2:Z:189:PHE:HB3	2:Z:236:LEU:HD23	1.99	0.43
1:5:48:VAL:HB	1:6:85:LEU:HD21	2.01	0.43
3:I:94:ASN:O	3:I:109:GLN:NE2	2.40	0.43
2:F:109:ARG:CG	3:K:25:GLN:CB	2.96	0.43
1:M:2:PRO:HG3	1:O:128:PRO:HG2	1.99	0.43
1:R:48:VAL:HB	1:T:85:LEU:HD21	2.01	0.43
2:X:189:PHE:HB3	2:X:236:LEU:HD23	1.99	0.43
3:K:36:VAL:HA	2:Z:160:ILE:HB	146.95	0.43
1:4:12:GLN:HG3	1:P:103:ILE:HG22	2.01	0.43
1:5:12:GLN:HG3	1:R:103:ILE:HG22	2.01	0.43
2:B:60:VAL:O	2:B:64:LEU:N	2.48	0.43
2:C:60:VAL:O	2:C:64:LEU:N	2.49	0.43
2:B:109:ARG:CG	3:G:25:GLN:CB	2.96	0.43
1:Q:48:VAL:HB	1:S:85:LEU:HD21	2.01	0.43
3:K:18:ILE:CG1	2:X:483:LEU:O	123.99	0.43
2:B:240:ALA:HB3	2:B:277:THR:HG21	1.99	0.43
2:F:269:HIS:O	2:F:274:TRP:NE1	2.37	0.43
1:Q:42:GLN:HB3	1:S:129:HIS:CD2	2.53	0.43
1:S:48:VAL:HB	1:U:85:LEU:HD21	2.01	0.43
1:V:12:GLN:HG3	1:U:103:ILE:HG22	2.01	0.43
1:V:26:SER:HB3	1:V:75:ASN:HB2	2.01	0.43
1:1:48:VAL:HB	1:2:85:LEU:HD21	2.01	0.43
2:B:166:THR:OG1	2:B:171:ASP:OD2	2.34	0.43
3:K:25:GLN:CB	2:Z:109:ARG:CG	120.68	0.43
1:L:48:VAL:HB	1:N:85:LEU:HD21	2.01	0.43
1:P:2:PRO:HG3	1:R:128:PRO:HG2	2.00	0.43
2:Z:60:VAL:O	2:Z:64:LEU:N	2.48	0.43
1:2:14:GLN:HE22	1:2:83:ASN:HB2	1.84	0.43
1:4:26:SER:HB3	1:4:75:ASN:HB2	2.01	0.43
2:C:483:LEU:O	3:I:18:ILE:CG1	2.58	0.43
2:D:189:PHE:HB3	2:D:236:LEU:HD23	1.99	0.43
1:M:14:GLN:HE22	1:M:83:ASN:HB2	1.84	0.43
1:N:26:SER:HB3	1:N:75:ASN:HB2	2.01	0.43
1:P:48:VAL:HB	1:R:85:LEU:HD21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:26:SER:HB3	1:Q:75:ASN:HB2	2.01	0.43
1:T:48:VAL:HB	1:V:85:LEU:HD21	2.01	0.43
1:U:48:VAL:HB	1:W:85:LEU:HD21	2.01	0.43
1:3:2:PRO:HG3	1:4:128:PRO:HG2	2.00	0.43
1:4:47:VAL:HG22	1:5:124:HIS:HD2	1.84	0.43
2:A:483:LEU:O	3:G:18:ILE:CG1	2.60	0.43
2:C:189:PHE:HB3	2:C:236:LEU:HD23	1.99	0.43
1:L:14:GLN:HE22	1:L:83:ASN:HB2	1.84	0.43
1:M:26:SER:HB3	1:M:75:ASN:HB2	2.01	0.43
1:M:85:LEU:HD21	1:W:48:VAL:HB	2.01	0.43
1:P:42:GLN:HB3	1:R:129:HIS:CD2	2.53	0.43
1:1:14:GLN:HE22	1:1:83:ASN:HB2	1.84	0.43
1:1:26:SER:HB3	1:1:75:ASN:HB2	2.01	0.43
2:C:110:GLU:CA	3:H:26:ALA:HB3	2.35	0.43
2:E:175:LEU:HA	2:E:175:LEU:HD23	1.90	0.43
2:D:109:ARG:CG	3:I:25:GLN:CB	2.96	0.43
1:S:26:SER:HB3	1:S:75:ASN:HB2	2.01	0.43
1:W:14:GLN:HE22	1:W:83:ASN:HB2	1.84	0.43
2:Y:240:ALA:HB3	2:Y:277:THR:HG21	1.99	0.43
1:3:26:SER:HB3	1:3:75:ASN:HB2	2.01	0.42
2:C:109:ARG:HD2	3:H:25:GLN:CA	2.39	0.42
2:E:485:LEU:O	3:K:21:THR:CG2	2.49	0.42
2:F:242:ARG:HD2	2:F:274:TRP:HB3	2.01	0.42
3:K:94:ASN:O	3:K:109:GLN:NE2	2.40	0.42
1:L:85:LEU:HD21	1:V:48:VAL:HB	2.01	0.42
1:M:48:VAL:HB	1:O:85:LEU:HD21	2.01	0.42
1:P:26:SER:HB3	1:P:75:ASN:HB2	2.01	0.42
2:Z:240:ALA:HB3	2:Z:277:THR:HG21	1.99	0.42
1:2:26:SER:HB3	1:2:75:ASN:HB2	2.01	0.42
1:3:48:VAL:HB	1:4:85:LEU:HD21	2.01	0.42
2:E:162:ASN:HB3	3:J:38:GLY:HA3	2.01	0.42
1:P:12:GLN:HG3	1:O:103:ILE:HG22	2.01	0.42
1:6:12:GLN:HG3	1:T:103:ILE:HG22	2.01	0.42
2:A:242:ARG:HD2	2:A:274:TRP:HB3	2.01	0.42
2:E:216:PHE:HA	2:E:221:TYR:HD2	1.85	0.42
1:T:26:SER:HB3	1:T:75:ASN:HB2	2.01	0.42
1:U:26:SER:HB3	1:U:75:ASN:HB2	2.01	0.42
1:1:85:LEU:HD21	1:6:48:VAL:HB	2.01	0.42
1:5:26:SER:HB3	1:5:75:ASN:HB2	2.01	0.42
2:D:160:ILE:HD13	3:I:36:VAL:HG22	2.01	0.42
2:E:242:ARG:HD2	2:E:274:TRP:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:160:ILE:HD13	3:K:36:VAL:HG22	2.01	0.42
2:F:162:ASN:HB3	3:K:38:GLY:HA3	2.01	0.42
3:K:23:ASP:HB3	3:K:24:ALA:H	1.52	0.42
1:N:14:GLN:HE22	1:N:83:ASN:HB2	1.84	0.42
1:2:48:VAL:HB	1:3:85:LEU:HD21	2.02	0.42
2:B:483:LEU:O	3:H:18:ILE:CG1	2.60	0.42
2:D:162:ASN:HB3	3:I:38:GLY:HA3	2.01	0.42
1:U:47:VAL:HG22	1:W:124:HIS:HD2	1.85	0.42
2:X:350:ARG:NH2	2:Y:151:PHE:HZ	2.16	0.42
2:Y:269:HIS:O	2:Y:274:TRP:NE1	2.37	0.42
2:C:216:PHE:HA	2:C:221:TYR:HD2	1.85	0.42
1:R:47:VAL:HG22	1:T:124:HIS:HD2	1.84	0.42
1:V:14:GLN:HE22	1:V:83:ASN:HB2	1.84	0.42
2:Z:216:PHE:HA	2:Z:221:TYR:HD2	1.85	0.42
1:O:48:VAL:HB	1:Q:85:LEU:HD21	2.02	0.42
1:U:10:GLU:O	1:U:92:LYS:N	2.53	0.42
1:W:26:SER:HB3	1:W:75:ASN:HB2	2.01	0.42
2:X:216:PHE:HA	2:X:221:TYR:HD2	1.85	0.42
2:X:242:ARG:HD2	2:X:274:TRP:HB3	2.02	0.42
2:F:216:PHE:HA	2:F:221:TYR:HD2	1.85	0.42
1:L:26:SER:HB3	1:L:75:ASN:HB2	2.01	0.42
1:S:47:VAL:HG22	1:U:124:HIS:HD2	1.84	0.42
2:A:216:PHE:HA	2:A:221:TYR:HD2	1.85	0.42
2:B:242:ARG:HD2	2:B:274:TRP:HB3	2.01	0.42
2:D:216:PHE:HA	2:D:221:TYR:HD2	1.85	0.42
2:D:242:ARG:HD2	2:D:274:TRP:HB3	2.01	0.42
2:C:160:ILE:HD13	3:H:36:VAL:HG22	2.01	0.42
1:R:14:GLN:HE22	1:R:83:ASN:HB2	1.84	0.42
1:6:26:SER:HB3	1:6:75:ASN:HB2	2.01	0.42
2:B:162:ASN:HB3	3:G:38:GLY:HA3	2.01	0.42
2:B:19:LEU:HG	3:G:153:LEU:HD13	2.02	0.42
2:E:160:ILE:HD13	3:J:36:VAL:HG22	2.01	0.42
2:C:407:ARG:CG	3:I:12:ARG:CZ	46.30	0.42
3:J:16:LYS:HZ2	3:J:18:ILE:CG1	2.32	0.42
1:N:12:GLN:HG3	1:M:103:ILE:HG22	2.01	0.42
1:M:47:VAL:HG22	1:O:124:HIS:HD2	1.85	0.42
1:N:48:VAL:HB	1:P:85:LEU:HD21	2.02	0.42
1:O:14:GLN:HE22	1:O:83:ASN:HB2	1.84	0.42
1:R:26:SER:HB3	1:R:75:ASN:HB2	2.01	0.42
1:V:10:GLU:O	1:V:92:LYS:N	2.53	0.42
1:T:47:VAL:HG22	1:V:124:HIS:HD2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:153:LEU:HD13	2:Z:19:LEU:HG	211.28	0.42
1:1:47:VAL:HG22	1:2:124:HIS:HD2	1.85	0.41
2:B:216:PHE:HA	2:B:221:TYR:HD2	1.85	0.41
2:Y:242:ARG:HD2	2:Y:274:TRP:HB3	2.01	0.41
1:3:14:GLN:HE22	1:3:83:ASN:HB2	1.84	0.41
1:5:47:VAL:HG22	1:6:124:HIS:HD2	1.85	0.41
2:E:293:ARG:NH2	3:J:27:GLU:C	2.62	0.41
2:C:162:ASN:HB3	3:H:38:GLY:HA3	2.01	0.41
1:O:26:SER:HB3	1:O:75:ASN:HB2	2.01	0.41
1:U:14:GLN:HE22	1:U:83:ASN:HB2	1.84	0.41
3:K:17:TYR:CD1	2:Y:395:ILE:CD1	122.98	0.41
2:Z:242:ARG:HD2	2:Z:274:TRP:HB3	2.01	0.41
3:K:27:GLU:C	2:Z:293:ARG:NH2	113.34	0.41
1:2:47:VAL:HG22	1:3:124:HIS:HD2	1.85	0.41
2:E:121:LYS:NZ	2:E:171:ASP:OD1	2.49	0.41
2:F:457:VAL:HB	2:F:463:TRP:HB2	2.03	0.41
1:L:12:GLN:HG3	1:W:103:ILE:HG22	2.02	0.41
1:6:14:GLN:HE22	1:6:83:ASN:HB2	1.84	0.41
2:E:109:ARG:HD2	3:J:25:GLN:CA	2.39	0.41
2:F:175:LEU:HD23	2:F:175:LEU:HA	1.90	0.41
3:I:18:ILE:HA	3:I:18:ILE:HD13	1.90	0.41
1:O:10:GLU:O	1:O:92:LYS:N	2.53	0.41
1:T:14:GLN:HE22	1:T:83:ASN:HB2	1.84	0.41
1:4:14:GLN:HE22	1:4:83:ASN:HB2	1.84	0.41
2:C:242:ARG:HD2	2:C:274:TRP:HB3	2.02	0.41
2:C:457:VAL:HB	2:C:463:TRP:HB2	2.02	0.41
2:D:451:ARG:NH2	2:D:453:GLU:OE1	2.54	0.41
2:E:407:ARG:CG	3:J:12:ARG:CZ	51.89	0.41
3:K:36:VAL:HG12	3:K:40:PHE:HZ	1.86	0.41
3:K:38:GLY:HA3	2:Z:162:ASN:HB3	158.59	0.41
1:N:47:VAL:HG22	1:P:124:HIS:HD2	1.85	0.41
1:T:50:VAL:N	1:V:121:VAL:O	2.54	0.41
2:B:457:VAL:HB	2:B:463:TRP:HB2	2.03	0.41
2:D:203:PHE:CE2	2:D:241:PRO:HB3	2.56	0.41
2:E:451:ARG:NH2	2:E:453:GLU:OE1	2.54	0.41
2:F:19:LEU:HG	3:K:153:LEU:HD13	2.02	0.41
1:3:12:GLN:HG3	1:N:103:ILE:HG22	2.01	0.41
1:P:14:GLN:HE22	1:P:83:ASN:HB2	1.84	0.41
1:S:10:GLU:O	1:S:92:LYS:N	2.53	0.41
1:3:10:GLU:O	1:3:92:LYS:N	2.53	0.41
2:A:451:ARG:NH2	2:A:453:GLU:OE1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:160:ILE:HD13	3:G:36:VAL:HG22	2.01	0.41
2:B:293:ARG:NH2	3:G:27:GLU:C	2.62	0.41
2:D:457:VAL:HB	2:D:463:TRP:HB2	2.03	0.41
2:E:203:PHE:CE2	2:E:241:PRO:HB3	2.56	0.41
2:F:162:ASN:HD22	3:K:40:PHE:HE1	1.68	0.41
2:F:451:ARG:NH2	2:F:453:GLU:OE1	2.54	0.41
3:G:36:VAL:HG12	3:G:40:PHE:HZ	1.86	0.41
3:H:18:ILE:HD13	3:H:18:ILE:HA	1.90	0.41
3:H:36:VAL:HG12	3:H:40:PHE:HZ	1.86	0.41
1:M:124:HIS:HD2	1:W:47:VAL:HG22	1.86	0.41
2:Y:216:PHE:HA	2:Y:221:TYR:HD2	1.85	0.41
1:2:10:GLU:O	1:2:92:LYS:N	2.53	0.41
2:C:203:PHE:CE2	2:C:241:PRO:HB3	2.56	0.41
2:C:269:HIS:O	2:C:274:TRP:NE1	2.36	0.41
2:C:19:LEU:HG	3:H:153:LEU:HD13	2.02	0.41
3:I:16:LYS:HZ2	3:I:18:ILE:CG1	2.34	0.41
2:E:407:ARG:HG3	3:J:12:ARG:NH1	52.13	0.41
2:E:19:LEU:HG	3:J:153:LEU:HD13	2.02	0.41
1:O:47:VAL:HG22	1:Q:124:HIS:HD2	1.85	0.41
1:P:10:GLU:O	1:P:92:LYS:N	2.53	0.41
1:T:10:GLU:O	1:T:92:LYS:N	2.53	0.41
3:K:25:GLN:CA	2:Z:109:ARG:HD2	118.02	0.41
3:K:36:VAL:HG22	2:Z:160:ILE:HD13	143.02	0.41
2:Z:451:ARG:NH2	2:Z:453:GLU:OE1	2.54	0.41
2:Z:457:VAL:HB	2:Z:463:TRP:HB2	2.02	0.41
1:1:12:GLN:HG3	1:V:103:ILE:HG22	2.02	0.41
1:5:10:GLU:O	1:5:92:LYS:N	2.53	0.41
2:X:175:LEU:HA	2:X:175:LEU:HD23	1.90	0.41
2:F:213:LYS:N	2:F:338:GLU:OE2	2.54	0.41
2:B:451:ARG:NH2	2:B:453:GLU:OE1	2.54	0.41
2:C:451:ARG:NH2	2:C:453:GLU:OE1	2.54	0.41
2:E:162:ASN:HD22	3:J:40:PHE:HE1	1.68	0.41
2:F:203:PHE:CE2	2:F:241:PRO:HB3	2.56	0.41
2:D:19:LEU:HG	3:I:153:LEU:HD13	2.02	0.41
1:S:50:VAL:N	1:U:121:VAL:O	2.54	0.41
2:X:203:PHE:CE2	2:X:241:PRO:HB3	2.56	0.41
2:B:213:LYS:N	2:B:338:GLU:OE2	2.54	0.41
2:B:269:HIS:O	2:B:274:TRP:NE1	2.37	0.41
2:C:213:LYS:N	2:C:338:GLU:OE2	2.54	0.41
2:E:457:VAL:HB	2:E:463:TRP:HB2	2.03	0.41
3:I:36:VAL:HG12	3:I:40:PHE:HZ	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:113:THR:O	1:L:113:THR:OG1	2.35	0.41
1:S:14:GLN:HE22	1:S:83:ASN:HB2	1.84	0.41
2:X:213:LYS:N	2:X:338:GLU:OE2	2.54	0.41
2:Y:451:ARG:NH2	2:Y:453:GLU:OE1	2.54	0.41
3:J:36:VAL:HG12	3:J:40:PHE:HZ	1.86	0.41
1:R:50:VAL:N	1:T:121:VAL:O	2.54	0.41
1:6:10:GLU:O	1:6:92:LYS:N	2.53	0.40
2:A:213:LYS:N	2:A:338:GLU:OE2	2.54	0.40
3:G:12:ARG:CZ	2:X:407:ARG:CG	2.99	0.40
3:H:12:ARG:CZ	2:Z:407:ARG:CG	2.99	0.40
1:2:12:GLN:HG3	1:L:103:ILE:HG22	2.02	0.40
1:4:50:VAL:N	1:5:121:VAL:O	2.54	0.40
2:A:457:VAL:HB	2:A:463:TRP:HB2	2.03	0.40
2:B:203:PHE:CE2	2:B:241:PRO:HB3	2.56	0.40
2:C:162:ASN:HD22	3:H:40:PHE:HE1	1.68	0.40
2:E:117:LEU:HD13	3:J:54:THR:HG22	2.04	0.40
2:E:206:LEU:HB3	2:E:329:VAL:HG11	2.03	0.40
2:F:228:ARG:HB3	2:F:366:LYS:HG3	2.03	0.40
1:U:50:VAL:N	1:W:121:VAL:O	2.54	0.40
1:L:124:HIS:HD2	1:V:47:VAL:HG22	1.85	0.40
1:W:10:GLU:O	1:W:92:LYS:N	2.53	0.40
1:Q:14:GLN:HE22	1:Q:83:ASN:HB2	1.84	0.40
3:K:7:VAL:HG11	2:Y:144:TYR:CE1	137.91	0.40
2:Y:457:VAL:HB	2:Y:463:TRP:HB2	2.03	0.40
1:Q:50:VAL:N	1:S:121:VAL:O	2.54	0.40
1:1:50:VAL:N	1:2:121:VAL:O	2.54	0.40
1:2:113:THR:O	1:2:113:THR:OG1	2.35	0.40
2:C:407:ARG:HG3	3:I:12:ARG:NH1	45.90	0.40
2:F:152:GLY:H	2:F:407:ARG:NH2	2.20	0.40
3:G:12:ARG:NH1	2:X:407:ARG:HG3	2.36	0.40
2:B:117:LEU:HD13	3:G:54:THR:HG22	2.04	0.40
1:N:10:GLU:O	1:N:92:LYS:N	2.53	0.40
2:X:451:ARG:NH2	2:X:453:GLU:OE1	2.54	0.40
2:Y:213:LYS:N	2:Y:338:GLU:OE2	2.54	0.40
1:3:50:VAL:N	1:4:121:VAL:O	2.54	0.40
2:A:350:ARG:NH2	2:X:151:PHE:CZ	2.90	0.40
2:D:117:LEU:HD13	3:I:54:THR:HG22	2.04	0.40
2:E:228:ARG:HB3	2:E:366:LYS:HG3	2.03	0.40
2:F:206:LEU:HB3	2:F:329:VAL:HG11	2.03	0.40
3:K:40:PHE:HE1	2:Z:162:ASN:HD22	157.22	0.40
1:L:10:GLU:O	1:L:92:LYS:N	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:10:GLU:O	1:M:92:LYS:N	2.53	0.40
1:Q:47:VAL:HG22	1:S:124:HIS:HD2	1.86	0.40
1:S:46:HIS:NE2	1:S:148:TYR:OH	2.54	0.40
2:Y:203:PHE:CE2	2:Y:241:PRO:HB3	2.56	0.40
2:D:213:LYS:N	2:D:338:GLU:OE2	2.54	0.40
2:A:203:PHE:CE2	2:A:241:PRO:HB3	2.56	0.40
2:D:175:LEU:HA	2:D:175:LEU:HD23	1.90	0.40
2:E:90:GLN:NE2	2:E:272:TYR:O	2.55	0.40
3:I:128:GLY:O	3:I:132:ASN:ND2	2.55	0.40
3:K:54:THR:HG22	2:Z:117:LEU:HD13	154.89	0.40
2:X:152:GLY:H	2:X:407:ARG:NH2	2.20	0.40
1:2:50:VAL:N	1:3:121:VAL:O	2.55	0.40
2:Z:152:GLY:H	2:Z:407:ARG:NH2	2.20	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	168/170 (99%)	154 (92%)	14 (8%)	0	100	100
1	2	168/170 (99%)	154 (92%)	14 (8%)	0	100	100
1	3	168/170 (99%)	154 (92%)	14 (8%)	0	100	100
1	4	168/170 (99%)	154 (92%)	14 (8%)	0	100	100
1	5	168/170 (99%)	154 (92%)	14 (8%)	0	100	100
1	6	168/170 (99%)	154 (92%)	14 (8%)	0	100	100
1	L	168/170 (99%)	154 (92%)	14 (8%)	0	100	100
1	M	168/170 (99%)	154 (92%)	14 (8%)	0	100	100
1	N	168/170 (99%)	154 (92%)	14 (8%)	0	100	100
1	O	168/170 (99%)	154 (92%)	14 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	P	168/170 (99%)	154 (92%)	14 (8%)	0	100	100
1	Q	168/170 (99%)	154 (92%)	14 (8%)	0	100	100
1	R	168/170 (99%)	154 (92%)	14 (8%)	0	100	100
1	S	168/170 (99%)	154 (92%)	14 (8%)	0	100	100
1	T	168/170 (99%)	154 (92%)	14 (8%)	0	100	100
1	U	168/170 (99%)	154 (92%)	14 (8%)	0	100	100
1	V	168/170 (99%)	154 (92%)	14 (8%)	0	100	100
1	W	168/170 (99%)	154 (92%)	14 (8%)	0	100	100
2	A	471/473 (100%)	437 (93%)	32 (7%)	2 (0%)	38	77
2	B	471/473 (100%)	437 (93%)	32 (7%)	2 (0%)	38	77
2	C	471/473 (100%)	437 (93%)	32 (7%)	2 (0%)	38	77
2	D	471/473 (100%)	437 (93%)	32 (7%)	2 (0%)	38	77
2	E	471/473 (100%)	437 (93%)	32 (7%)	2 (0%)	38	77
2	F	471/473 (100%)	437 (93%)	32 (7%)	2 (0%)	38	77
2	X	471/473 (100%)	437 (93%)	32 (7%)	2 (0%)	38	77
2	Y	471/473 (100%)	437 (93%)	32 (7%)	2 (0%)	38	77
2	Z	471/473 (100%)	437 (93%)	32 (7%)	2 (0%)	38	77
2	b	471/473 (100%)	436 (93%)	33 (7%)	2 (0%)	38	77
2	c	471/473 (100%)	437 (93%)	32 (7%)	2 (0%)	38	77
2	d	471/473 (100%)	437 (93%)	32 (7%)	2 (0%)	38	77
2	e	471/473 (100%)	437 (93%)	32 (7%)	2 (0%)	38	77
2	f	471/473 (100%)	437 (93%)	32 (7%)	2 (0%)	38	77
2	g	471/473 (100%)	437 (93%)	32 (7%)	2 (0%)	38	77
2	h	471/473 (100%)	439 (93%)	30 (6%)	2 (0%)	38	77
2	i	471/473 (100%)	437 (93%)	32 (7%)	2 (0%)	38	77
2	j	471/473 (100%)	436 (93%)	33 (7%)	2 (0%)	38	77
3	G	153/155 (99%)	141 (92%)	10 (6%)	2 (1%)	14	57
3	H	153/155 (99%)	141 (92%)	10 (6%)	2 (1%)	14	57
3	I	153/155 (99%)	141 (92%)	10 (6%)	2 (1%)	14	57
3	J	153/155 (99%)	141 (92%)	10 (6%)	2 (1%)	14	57
3	K	153/155 (99%)	141 (92%)	10 (6%)	2 (1%)	14	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	a	153/155 (99%)	141 (92%)	10 (6%)	2 (1%)	14	57
3	k	153/155 (99%)	141 (92%)	10 (6%)	2 (1%)	14	57
3	l	153/155 (99%)	141 (92%)	10 (6%)	2 (1%)	14	57
3	m	153/155 (99%)	141 (92%)	10 (6%)	2 (1%)	14	57
3	n	153/155 (99%)	141 (92%)	10 (6%)	2 (1%)	14	57
3	o	153/155 (99%)	141 (92%)	10 (6%)	2 (1%)	14	57
3	p	153/155 (99%)	141 (92%)	10 (6%)	2 (1%)	14	57
3	q	153/155 (99%)	141 (92%)	10 (6%)	2 (1%)	14	57
3	r	153/155 (99%)	141 (92%)	10 (6%)	2 (1%)	14	57
3	s	153/155 (99%)	141 (92%)	10 (6%)	2 (1%)	14	57
3	t	153/155 (99%)	141 (92%)	10 (6%)	2 (1%)	14	57
3	u	153/155 (99%)	141 (92%)	10 (6%)	2 (1%)	14	57
3	v	153/155 (99%)	141 (92%)	10 (6%)	2 (1%)	14	57
All	All	14256/14364 (99%)	13176 (92%)	1008 (7%)	72 (0%)	37	73

All (72) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	a	32	LEU
3	G	32	LEU
3	H	32	LEU
3	I	32	LEU
3	J	32	LEU
3	K	32	LEU
3	u	32	LEU
3	k	32	LEU
3	m	32	LEU
3	o	32	LEU
3	q	32	LEU
3	s	32	LEU
3	v	32	LEU
3	l	32	LEU
3	n	32	LEU
3	p	32	LEU
3	r	32	LEU
3	t	32	LEU
2	A	241	PRO

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Mol	Chain	Res	Type
2	B	241	PRO
2	C	241	PRO
2	D	241	PRO
2	E	241	PRO
2	F	241	PRO
2	X	241	PRO
2	Z	241	PRO
2	c	241	PRO
2	e	241	PRO
2	g	241	PRO
2	i	241	PRO
2	Y	241	PRO
2	b	241	PRO
2	d	241	PRO
2	f	241	PRO
2	h	241	PRO
2	j	241	PRO
2	A	390	PRO
2	B	390	PRO
2	C	390	PRO
2	D	390	PRO
2	E	390	PRO
2	F	390	PRO
2	X	390	PRO
2	Z	390	PRO
2	c	390	PRO
2	e	390	PRO
2	g	390	PRO
2	i	390	PRO
2	Y	390	PRO
2	b	390	PRO
2	d	390	PRO
2	f	390	PRO
2	h	390	PRO
2	j	390	PRO
3	a	28	VAL
3	G	28	VAL
3	H	28	VAL
3	I	28	VAL
3	J	28	VAL
3	K	28	VAL
3	u	28	VAL

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Mol	Chain	Res	Type
3	k	28	VAL
3	m	28	VAL
3	o	28	VAL
3	q	28	VAL
3	s	28	VAL
3	v	28	VAL
3	l	28	VAL
3	n	28	VAL
3	p	28	VAL
3	r	28	VAL
3	t	28	VAL

### 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	150/150 (100%)	149 (99%)	1 (1%)	87	94
1	2	150/150 (100%)	149 (99%)	1 (1%)	87	94
1	3	150/150 (100%)	149 (99%)	1 (1%)	87	94
1	4	150/150 (100%)	149 (99%)	1 (1%)	87	94
1	5	150/150 (100%)	149 (99%)	1 (1%)	87	94
1	6	150/150 (100%)	149 (99%)	1 (1%)	87	94
1	L	150/150 (100%)	149 (99%)	1 (1%)	87	94
1	M	150/150 (100%)	149 (99%)	1 (1%)	87	94
1	N	150/150 (100%)	149 (99%)	1 (1%)	87	94
1	O	150/150 (100%)	149 (99%)	1 (1%)	87	94
1	P	150/150 (100%)	149 (99%)	1 (1%)	87	94
1	Q	150/150 (100%)	149 (99%)	1 (1%)	87	94
1	R	150/150 (100%)	149 (99%)	1 (1%)	87	94
1	S	150/150 (100%)	149 (99%)	1 (1%)	87	94
1	T	150/150 (100%)	149 (99%)	1 (1%)	87	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	U	150/150 (100%)	149 (99%)	1 (1%)	87	94
1	V	150/150 (100%)	149 (99%)	1 (1%)	87	94
1	W	150/150 (100%)	149 (99%)	1 (1%)	87	94
2	A	401/401 (100%)	396 (99%)	5 (1%)	75	90
2	B	401/401 (100%)	396 (99%)	5 (1%)	75	90
2	C	401/401 (100%)	396 (99%)	5 (1%)	75	90
2	D	401/401 (100%)	396 (99%)	5 (1%)	75	90
2	E	401/401 (100%)	396 (99%)	5 (1%)	75	90
2	F	401/401 (100%)	396 (99%)	5 (1%)	75	90
2	X	401/401 (100%)	396 (99%)	5 (1%)	75	90
2	Y	401/401 (100%)	396 (99%)	5 (1%)	75	90
2	Z	401/401 (100%)	396 (99%)	5 (1%)	75	90
2	b	401/401 (100%)	396 (99%)	5 (1%)	75	90
2	c	401/401 (100%)	396 (99%)	5 (1%)	75	90
2	d	401/401 (100%)	396 (99%)	5 (1%)	75	90
2	e	401/401 (100%)	396 (99%)	5 (1%)	75	90
2	f	401/401 (100%)	396 (99%)	5 (1%)	75	90
2	g	401/401 (100%)	396 (99%)	5 (1%)	75	90
2	h	401/401 (100%)	396 (99%)	5 (1%)	75	90
2	i	401/401 (100%)	396 (99%)	5 (1%)	75	90
2	j	401/401 (100%)	396 (99%)	5 (1%)	75	90
3	G	132/132 (100%)	131 (99%)	1 (1%)	85	93
3	H	132/132 (100%)	131 (99%)	1 (1%)	85	93
3	I	132/132 (100%)	131 (99%)	1 (1%)	85	93
3	J	132/132 (100%)	131 (99%)	1 (1%)	85	93
3	K	132/132 (100%)	131 (99%)	1 (1%)	85	93
3	a	132/132 (100%)	131 (99%)	1 (1%)	85	93
3	k	132/132 (100%)	131 (99%)	1 (1%)	85	93
3	l	132/132 (100%)	131 (99%)	1 (1%)	85	93
3	m	132/132 (100%)	131 (99%)	1 (1%)	85	93
3	n	132/132 (100%)	131 (99%)	1 (1%)	85	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	o	132/132 (100%)	131 (99%)	1 (1%)	85	93
3	p	132/132 (100%)	131 (99%)	1 (1%)	85	93
3	q	132/132 (100%)	131 (99%)	1 (1%)	85	93
3	r	132/132 (100%)	131 (99%)	1 (1%)	85	93
3	s	132/132 (100%)	131 (99%)	1 (1%)	85	93
3	t	132/132 (100%)	131 (99%)	1 (1%)	85	93
3	u	132/132 (100%)	131 (99%)	1 (1%)	85	93
3	v	132/132 (100%)	131 (99%)	1 (1%)	85	93
All	All	12294/12294 (100%)	12168 (99%)	126 (1%)	81	91

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	63	ARG
2	A	92	MET
2	A	241	PRO
2	A	276	ASN
2	A	466	VAL
2	A	471	ARG
1	2	63	ARG
2	B	92	MET
2	B	241	PRO
2	B	276	ASN
2	B	466	VAL
2	B	471	ARG
1	3	63	ARG
2	C	92	MET
2	C	241	PRO
2	C	276	ASN
2	C	466	VAL
2	C	471	ARG
1	4	63	ARG
2	D	92	MET
2	D	241	PRO
2	D	276	ASN
2	D	466	VAL
2	D	471	ARG
1	5	63	ARG
2	E	92	MET

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Mol	Chain	Res	Type
2	E	241	PRO
2	E	276	ASN
2	E	466	VAL
2	E	471	ARG
1	6	63	ARG
2	F	92	MET
2	F	241	PRO
2	F	276	ASN
2	F	466	VAL
2	F	471	ARG
3	a	10	LYS
3	G	10	LYS
3	H	10	LYS
3	I	10	LYS
3	J	10	LYS
3	K	10	LYS
1	L	63	ARG
2	X	92	MET
2	X	241	PRO
2	X	276	ASN
2	X	466	VAL
2	X	471	ARG
1	N	63	ARG
2	Z	92	MET
2	Z	241	PRO
2	Z	276	ASN
2	Z	466	VAL
2	Z	471	ARG
1	P	63	ARG
2	c	92	MET
2	c	241	PRO
2	c	276	ASN
2	c	466	VAL
2	c	471	ARG
1	R	63	ARG
2	e	92	MET
2	e	241	PRO
2	e	276	ASN
2	e	466	VAL
2	e	471	ARG
1	T	63	ARG
2	g	92	MET

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Mol	Chain	Res	Type
2	g	241	PRO
2	g	276	ASN
2	g	466	VAL
2	g	471	ARG
1	V	63	ARG
2	i	92	MET
2	i	241	PRO
2	i	276	ASN
2	i	466	VAL
2	i	471	ARG
3	u	10	LYS
3	k	10	LYS
3	m	10	LYS
3	o	10	LYS
3	q	10	LYS
3	s	10	LYS
1	M	63	ARG
2	Y	92	MET
2	Y	241	PRO
2	Y	276	ASN
2	Y	466	VAL
2	Y	471	ARG
1	O	63	ARG
2	b	92	MET
2	b	241	PRO
2	b	276	ASN
2	b	466	VAL
2	b	471	ARG
1	Q	63	ARG
2	d	92	MET
2	d	241	PRO
2	d	276	ASN
2	d	466	VAL
2	d	471	ARG
1	S	63	ARG
2	f	92	MET
2	f	241	PRO
2	f	276	ASN
2	f	466	VAL
2	f	471	ARG
1	U	63	ARG
2	h	92	MET

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Mol	Chain	Res	Type
2	h	241	PRO
2	h	276	ASN
2	h	466	VAL
2	h	471	ARG
1	W	63	ARG
2	j	92	MET
2	j	241	PRO
2	j	276	ASN
2	j	466	VAL
2	j	471	ARG
3	v	10	LYS
3	l	10	LYS
3	n	10	LYS
3	p	10	LYS
3	r	10	LYS
3	t	10	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (153) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	35	HIS
1	1	129	HIS
2	A	26	GLN
2	A	271	HIS
2	A	276	ASN
2	A	365	GLN
1	2	14	GLN
1	2	35	HIS
1	2	129	HIS
2	B	26	GLN
2	B	271	HIS
2	B	276	ASN
2	B	365	GLN
1	3	14	GLN
1	3	35	HIS
1	3	129	HIS
2	C	26	GLN
2	C	271	HIS
2	C	276	ASN
2	C	365	GLN
1	4	14	GLN
1	4	35	HIS

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Mol	Chain	Res	Type
1	4	129	HIS
2	D	26	GLN
2	D	271	HIS
2	D	276	ASN
2	D	365	GLN
1	5	14	GLN
1	5	35	HIS
1	5	129	HIS
2	E	26	GLN
2	E	271	HIS
2	E	276	ASN
2	E	365	GLN
1	6	35	HIS
1	6	129	HIS
2	F	26	GLN
2	F	271	HIS
2	F	276	ASN
2	F	365	GLN
3	a	132	ASN
3	G	132	ASN
3	H	132	ASN
3	I	132	ASN
3	J	132	ASN
3	K	132	ASN
1	L	14	GLN
1	L	35	HIS
1	L	129	HIS
1	L	131	GLN
2	X	26	GLN
2	X	271	HIS
2	X	276	ASN
2	X	365	GLN
1	N	35	HIS
1	N	129	HIS
1	N	131	GLN
2	Z	26	GLN
2	Z	271	HIS
2	Z	276	ASN
2	Z	365	GLN
1	P	14	GLN
1	P	35	HIS
1	P	129	HIS

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Mol	Chain	Res	Type
1	P	131	GLN
2	c	26	GLN
2	c	271	HIS
2	c	276	ASN
2	c	365	GLN
1	R	14	GLN
1	R	35	HIS
1	R	129	HIS
1	R	131	GLN
2	e	26	GLN
2	e	271	HIS
2	e	276	ASN
2	e	365	GLN
1	T	14	GLN
1	T	35	HIS
1	T	129	HIS
1	T	131	GLN
2	g	26	GLN
2	g	271	HIS
2	g	276	ASN
2	g	365	GLN
1	V	14	GLN
1	V	35	HIS
1	V	129	HIS
1	V	131	GLN
2	i	26	GLN
2	i	271	HIS
2	i	276	ASN
2	i	365	GLN
3	u	132	ASN
3	k	132	ASN
3	m	132	ASN
3	o	132	ASN
3	q	132	ASN
3	s	132	ASN
1	M	14	GLN
1	M	35	HIS
1	M	129	HIS
1	M	131	GLN
2	Y	26	GLN
2	Y	271	HIS
2	Y	276	ASN

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Mol	Chain	Res	Type
2	Y	365	GLN
1	O	14	GLN
1	O	35	HIS
1	O	129	HIS
1	O	131	GLN
2	b	26	GLN
2	b	271	HIS
2	b	276	ASN
2	b	365	GLN
1	Q	14	GLN
1	Q	35	HIS
1	Q	129	HIS
1	Q	131	GLN
2	d	26	GLN
2	d	271	HIS
2	d	276	ASN
2	d	365	GLN
1	S	14	GLN
1	S	35	HIS
1	S	129	HIS
1	S	131	GLN
2	f	26	GLN
2	f	271	HIS
2	f	276	ASN
2	f	365	GLN
1	U	14	GLN
1	U	35	HIS
1	U	129	HIS
1	U	131	GLN
2	h	26	GLN
2	h	271	HIS
2	h	276	ASN
2	h	365	GLN
1	W	14	GLN
1	W	35	HIS
1	W	129	HIS
1	W	131	GLN
2	j	26	GLN
2	j	271	HIS
2	j	276	ASN
2	j	365	GLN
3	v	132	ASN

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Mol	Chain	Res	Type
3	l	132	ASN
3	n	132	ASN
3	p	132	ASN
3	r	132	ASN
3	t	132	ASN

### 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 [i](#)

There are no chain breaks in this entry.