



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

Aug 17, 2017 – 04:08 PM EDT

PDB ID : 4B2Q  
EMDB ID: : EMD-2161  
Title : Model of the yeast F1Fo-ATP synthase dimer based on subtomogram average  
Authors : Davies, K.M.; Kuehlbrandt, W.  
Deposited on : unknown  
Resolution : 37.00 Å(reported)  
Based on PDB ID : 2WPD

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  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
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

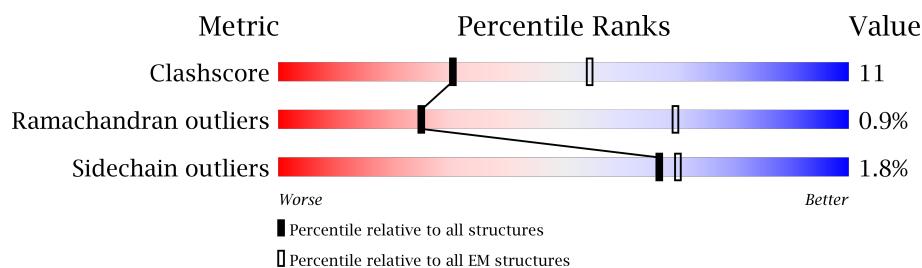
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 37.00 Å.

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




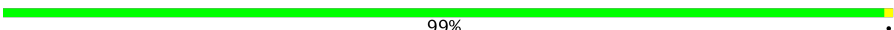
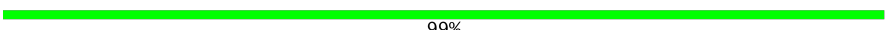

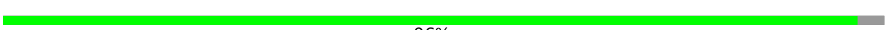





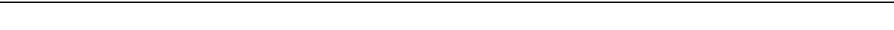

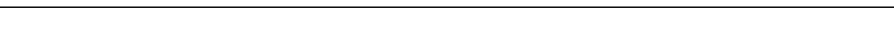
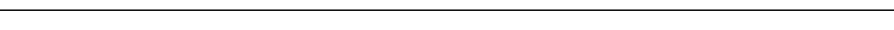






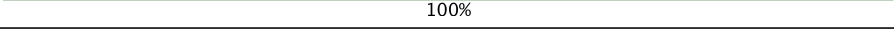
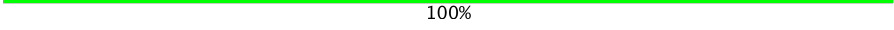
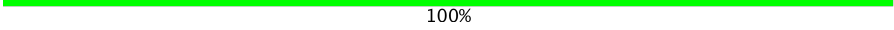
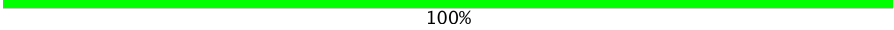
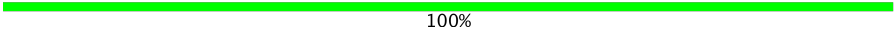
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	A	485	
1	C	485	
1	a	485	
1	c	485	
2	B	486	
2	b	486	
3	D	470	
3	d	470	
4	E	473	













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Mol	Chain	Length	Quality of chain
4	F	473	 59% 41%
4	e	473	 99%
4	f	473	 99%
5	G	278	 61% 35%
5	g	278	 96%
6	H	132	 51% 48%
6	h	132	 96%
7	I	59	 83% 17%
7	i	59	 100%
8	J	76	 71% 29%
8	K	76	 67% 33%
8	L	76	 70% 30%
8	M	76	 63% 37%
8	N	76	 63% 37%
8	O	76	 63% 37%
8	P	76	 64% 36%
8	Q	76	 68% 32%
8	R	76	 74% 26%
8	S	76	 74% 26%
8	j	76	 100%
8	k	76	 100%
8	l	76	 100%
8	m	76	 100%
8	n	76	 100%
8	o	76	 100%

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Mol	Chain	Length	Quality of chain
8	p	76	 100%
8	q	76	 100%
8	r	76	 100%
8	s	76	 100%
9	T	129	 39% 49% 11% .
9	t	129	 82% 16% .
10	U	120	 50% 38% 10% .
10	u	120	 84% 14% .
11	V	66	 48% 41% 9% .
11	v	66	 86% 12% .
12	W	120	 29% 43% 19% 8%
12	w	120	 64% 28% 8%

## 2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 70306 atoms, of which 1786 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 ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	485	Total	C	N	O	S	0	0
			3692	2334	651	704	3		
1	C	485	Total	C	N	O	S	0	0
			3692	2334	651	704	3		
1	a	485	Total	C	N	O	S	0	0
			3692	2334	651	704	3		
1	c	485	Total	C	N	O	S	0	0
			3692	2334	651	704	3		

- Molecule 2 is a protein called ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	485	Total	C	N	O	S	0	0
			3685	2328	651	703	3		
2	b	485	Total	C	N	O	S	0	0
			3685	2328	651	703	3		

- Molecule 3 is a protein called ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	470	Total	C	N	O	S	0	0
			3549	2250	604	689	6		
3	d	470	Total	C	N	O	S	0	0
			3549	2250	604	689	6		

- Molecule 4 is a protein called ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	473	Total	C	N	O	S	0	0
			3572	2262	608	696	6		
4	F	472	Total	C	N	O	S	0	0
			3566	2259	607	694	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	e	473	Total	C	N	O	S	0	0
			3572	2262	608	696	6		
4	f	472	Total	C	N	O	S	0	0
			3566	2259	607	694	6		

- Molecule 5 is a protein called ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	269	Total	C	N	O	S	0	0
			2086	1309	362	405	10		
5	g	269	Total	C	N	O	S	0	0
			2086	1309	362	405	10		

- Molecule 6 is a protein called ATP SYNTHASE SUBUNIT DELTA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	132	Total	C	N	O	S	0	0
			990	624	165	199	2		
6	h	132	Total	C	N	O	S	0	0
			990	624	165	199	2		

- Molecule 7 is a protein called ATP SYNTHASE SUBUNIT EPSILON, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	I	59	Total	C	N	O	0	0
			392	243	71	78		
7	i	59	Total	C	N	O	0	0
			392	243	71	78		

- Molecule 8 is a protein called ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	76	Total	C	N	O	S	0	0
			545	364	84	93	4		
8	K	76	Total	C	N	O	S	0	0
			545	364	84	93	4		
8	L	76	Total	C	N	O	S	0	0
			545	364	84	93	4		
8	M	76	Total	C	N	O	S	0	0
			545	364	84	93	4		
8	N	76	Total	C	N	O	S	0	0
			545	364	84	93	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	O	76	Total	C	N	O	S	0	0
			545	364	84	93	4		
8	P	76	Total	C	N	O	S	0	0
			545	364	84	93	4		
8	Q	76	Total	C	N	O	S	0	0
			545	364	84	93	4		
8	R	76	Total	C	N	O	S	0	0
			545	364	84	93	4		
8	S	76	Total	C	N	O	S	0	0
			545	364	84	93	4		
8	j	76	Total	C	N	O	S	0	0
			545	364	84	93	4		
8	k	76	Total	C	N	O	S	0	0
			545	364	84	93	4		
8	l	76	Total	C	N	O	S	0	0
			545	364	84	93	4		
8	m	76	Total	C	N	O	S	0	0
			545	364	84	93	4		
8	n	76	Total	C	N	O	S	0	0
			545	364	84	93	4		
8	o	76	Total	C	N	O	S	0	0
			545	364	84	93	4		
8	p	76	Total	C	N	O	S	0	0
			545	364	84	93	4		
8	q	76	Total	C	N	O	S	0	0
			545	364	84	93	4		
8	r	76	Total	C	N	O	S	0	0
			545	364	84	93	4		
8	s	76	Total	C	N	O	S	0	0
			545	364	84	93	4		

- Molecule 9 is a protein called ATP SYNTHASE SUBUNIT B, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	T	129	Total	C	N	O	S	0	0
			1077	671	200	200	6		
9	t	129	Total	C	N	O	S	0	0
			1077	671	200	200	6		

- Molecule 10 is a protein called ATP SYNTHASE SUBUNIT D, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	U	120	Total	C	N	O	S	0	0
			969	620	161	186	2		
10	u	120	Total	C	N	O	S	0	0
			969	620	161	186	2		

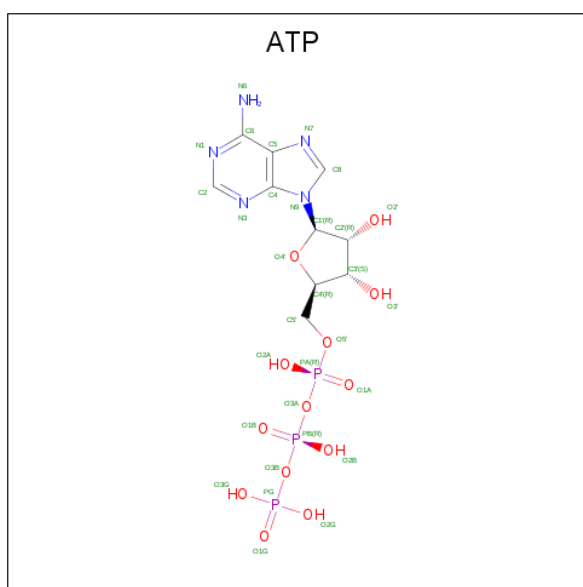
- Molecule 11 is a protein called ATP SYNTHASE-COUPPLING FACTOR 6, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	V	65	Total	C	N	O	S	0	0
			542	346	90	104	2		
11	v	65	Total	C	N	O	S	0	0
			542	346	90	104	2		

- Molecule 12 is a protein called ATP SYNTHASE SUBUNIT O, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	W	110	Total	C	H	N	O	S	0	0
			1739	535	893	146	160	5		
12	w	110	Total	C	H	N	O	S	0	0
			1739	535	893	146	160	5		

- Molecule 13 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).

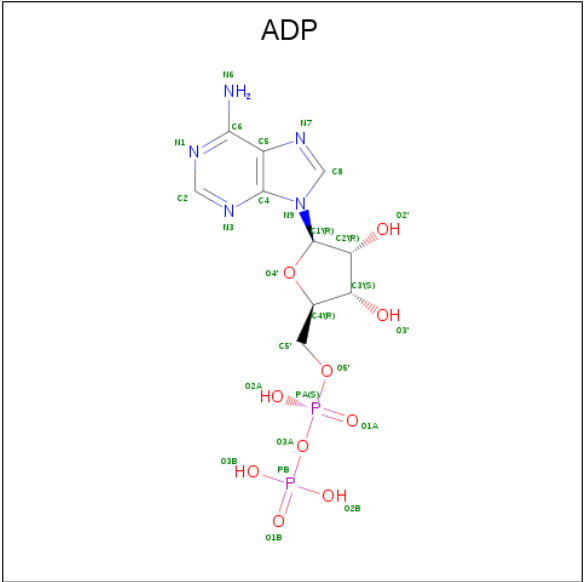


Mol	Chain	Residues	Atoms					AltConf
13	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
13	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
13	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
13	a	1	Total	C	N	O	P	0
			31	10	5	13	3	
13	b	1	Total	C	N	O	P	0
			31	10	5	13	3	
13	c	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 14 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
14	D	1	Total	Mg	0
			1	1	
14	B	1	Total	Mg	0
			1	1	
14	C	1	Total	Mg	0
			1	1	
14	c	1	Total	Mg	0
			1	1	
14	A	1	Total	Mg	0
			1	1	
14	a	1	Total	Mg	0
			1	1	
14	f	1	Total	Mg	0
			1	1	
14	d	1	Total	Mg	0
			1	1	
14	b	1	Total	Mg	0
			1	1	
14	F	1	Total	Mg	0
			1	1	

- Molecule 15 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).

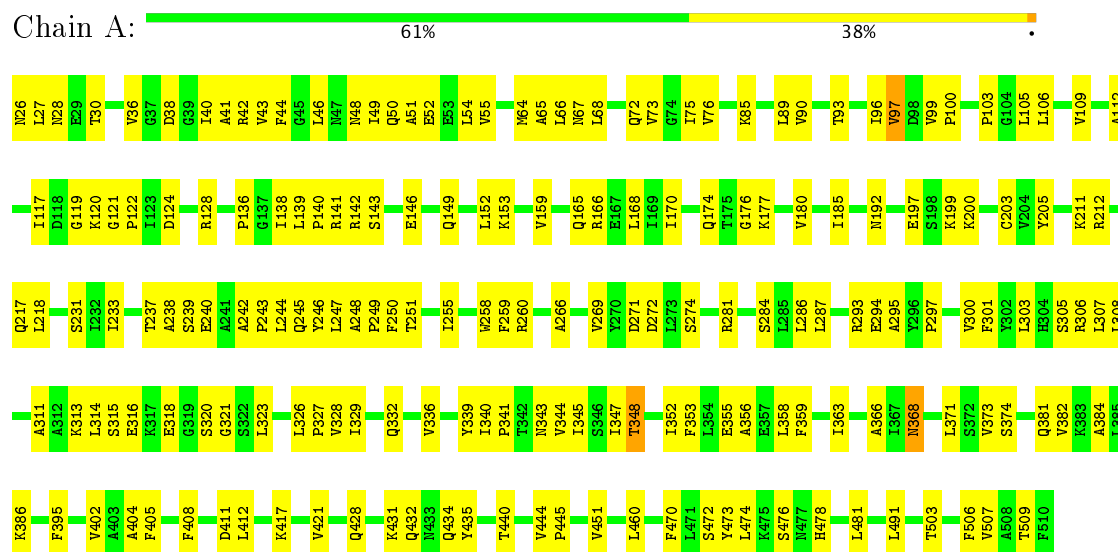


Mol	Chain	Residues	Atoms					AltConf
15	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
15	F	1	Total	C	N	O	P	0
			27	10	5	10	2	
15	d	1	Total	C	N	O	P	0
			27	10	5	10	2	
15	f	1	Total	C	N	O	P	0
			27	10	5	10	2	

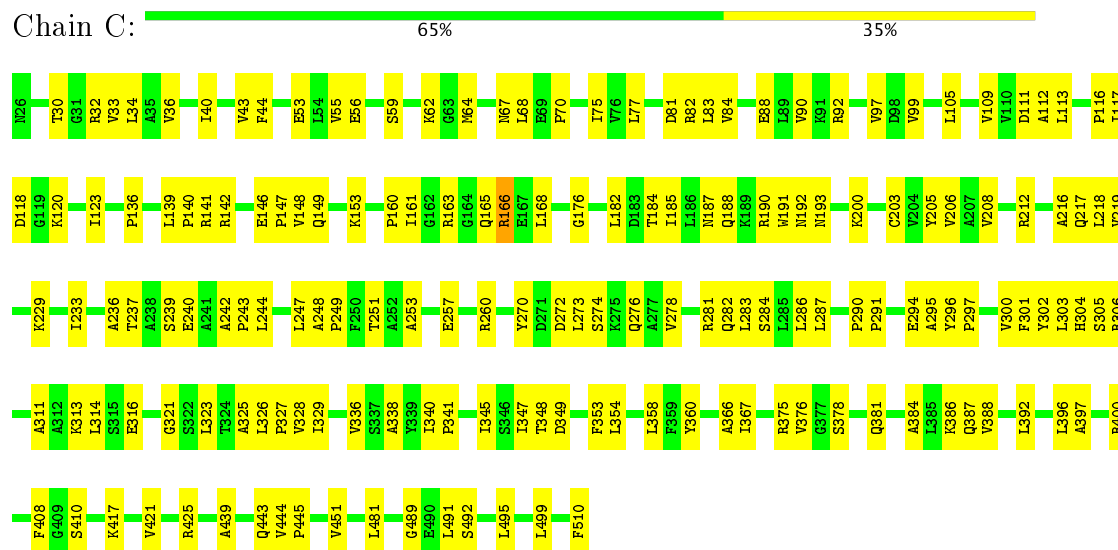
### 3 Residue-property plots

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: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL



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#### • Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

Chain a:  99%



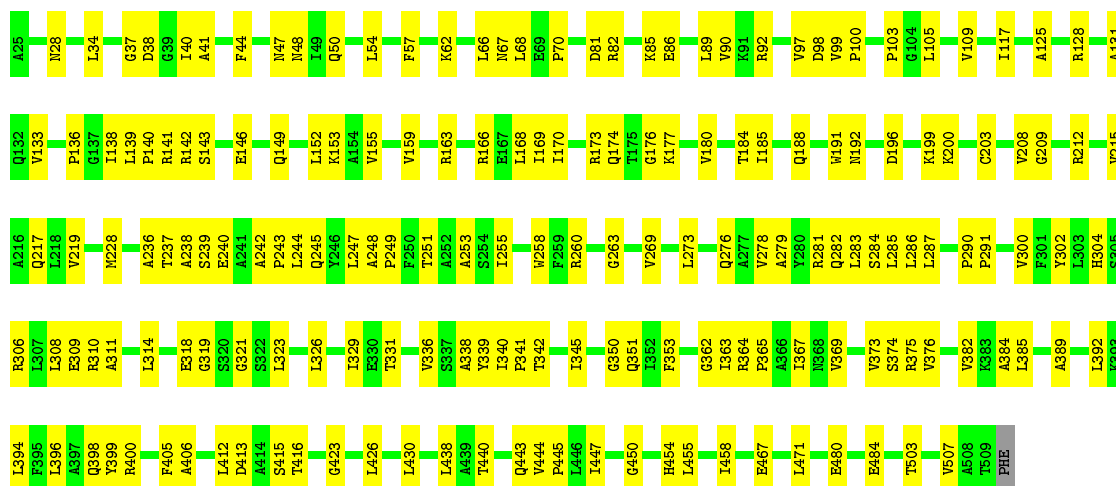
- Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

Chain c:  100%



- Molecule 2: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

Chain B:  63% 37%



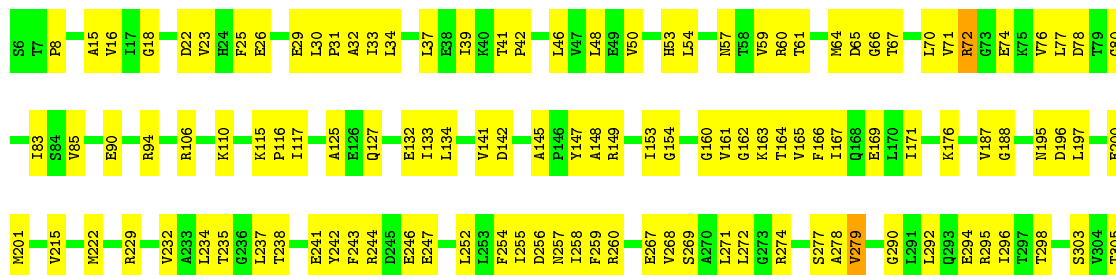
- Molecule 2: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

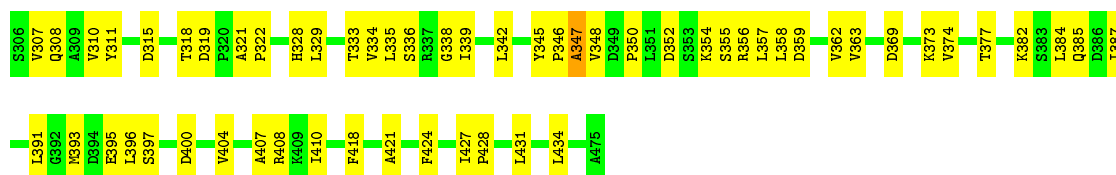
Chain b:  100%



- Molecule 3: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

Chain D:  63% 37%





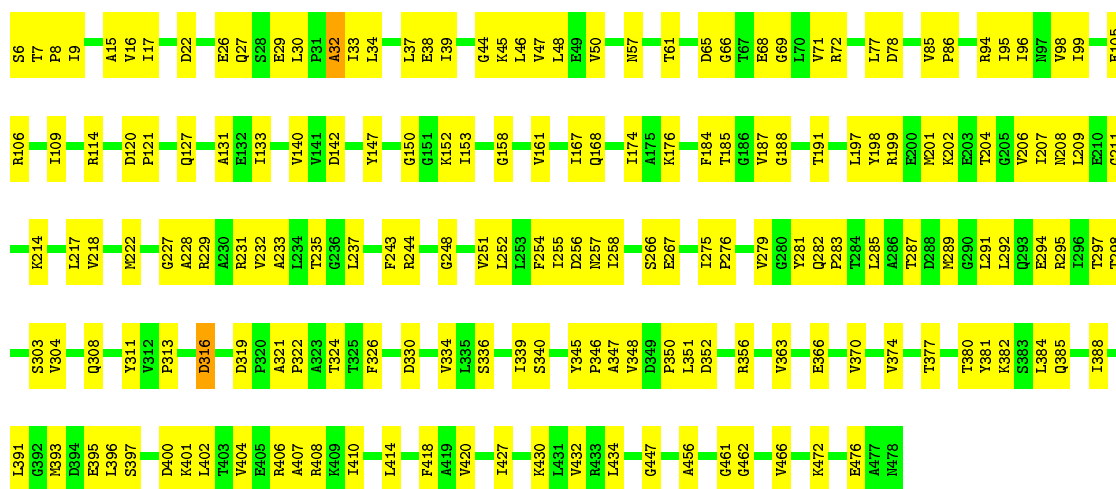
- Molecule 3: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

Chain d: 99%



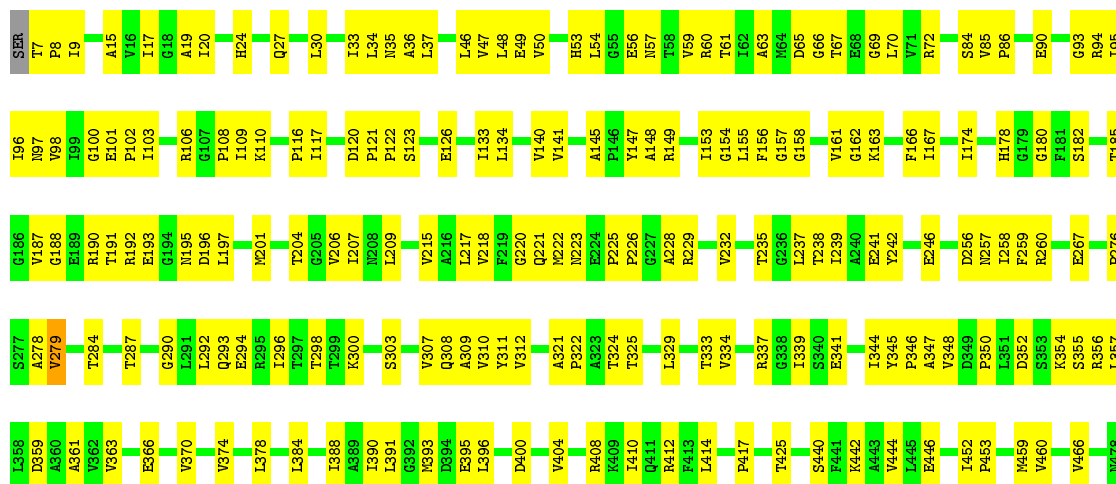
- Molecule 4: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

Chain E: 62% 37%

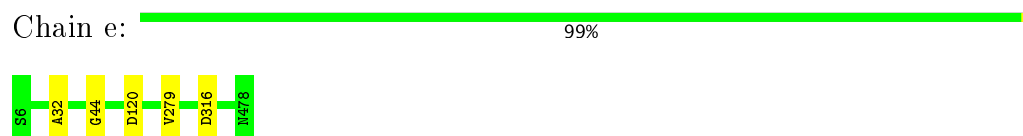


- Molecule 4: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

Chain F: 59% 41%



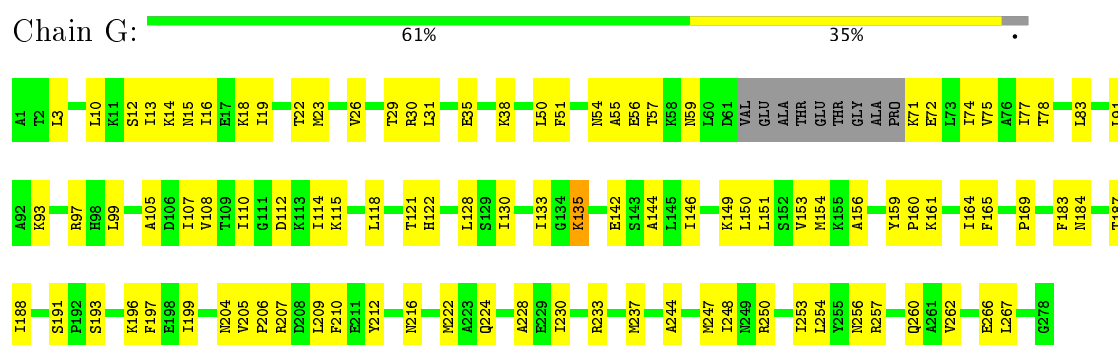
- Molecule 4: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL



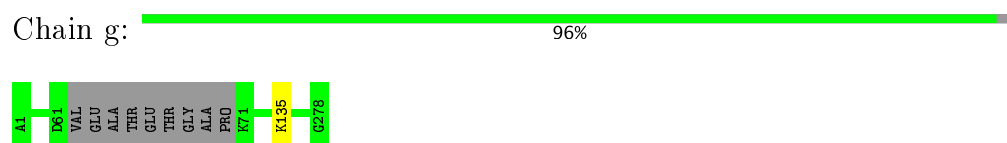
- Molecule 4: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL



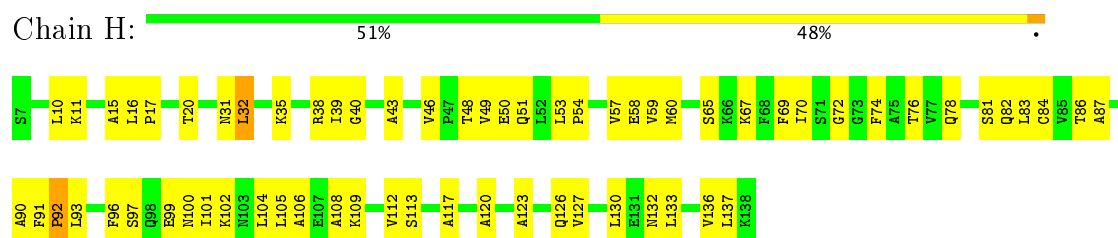
- Molecule 5: ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL



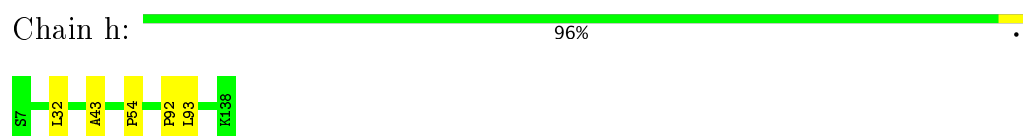
- Molecule 5: ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL



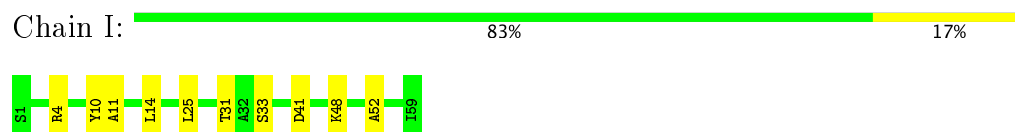
- Molecule 6: ATP SYNTHASE SUBUNIT DELTA, MITOCHONDRIAL



- Molecule 6: ATP SYNTHASE SUBUNIT DELTA, MITOCHONDRIAL



- Molecule 7: ATP SYNTHASE SUBUNIT EPSILON, MITOCHONDRIAL

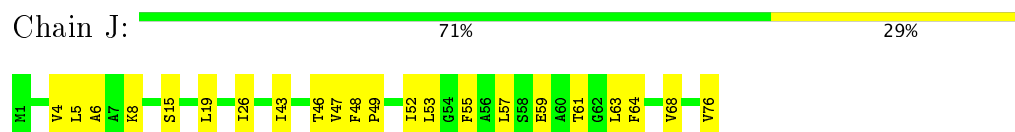


- Molecule 7: ATP SYNTHASE SUBUNIT EPSILON, MITOCHONDRIAL

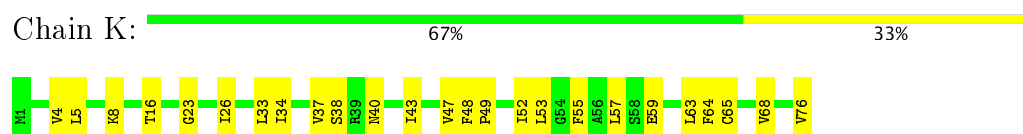


There are no outlier residues recorded for this chain.

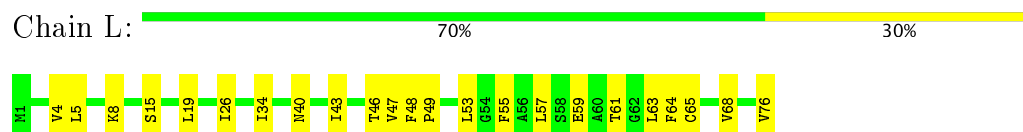
- Molecule 8: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL



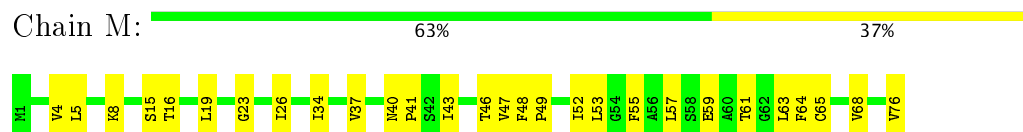
- Molecule 8: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL



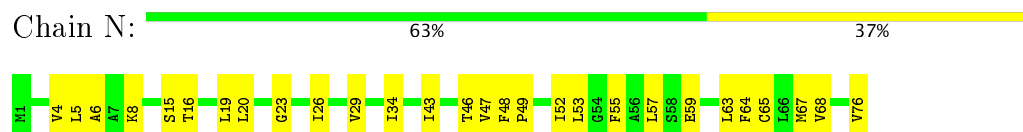
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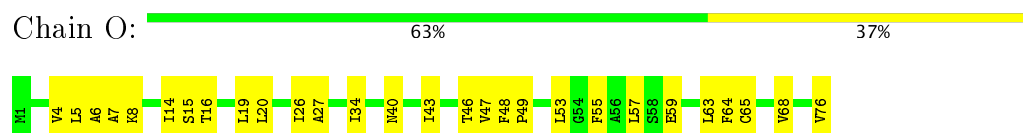
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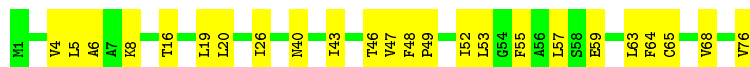
- Molecule 8: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

Chain P:  64% 36%



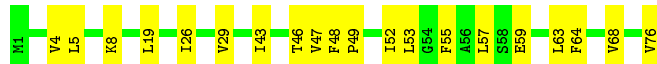
- Molecule 8: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

Chain Q:  68% 32%



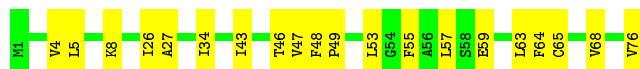
- Molecule 8: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

Chain R:  74% 26%



- Molecule 8: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

Chain S:  74% 26%



- Molecule 8: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

Chain j:  100%

There are no outlier residues recorded for this chain.

- Molecule 8: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

Chain k:  100%

There are no outlier residues recorded for this chain.

- Molecule 8: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

Chain l:  100%

There are no outlier residues recorded for this chain.

- Molecule 8: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

Chain m:  100%

There are no outlier residues recorded for this chain.

- Molecule 8: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

Chain n:  100%

There are no outlier residues recorded for this chain.

- Molecule 8: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

Chain o:  100%

There are no outlier residues recorded for this chain.

- Molecule 8: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

Chain p:  100%

There are no outlier residues recorded for this chain.

- Molecule 8: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

Chain q:  100%

There are no outlier residues recorded for this chain.

- Molecule 8: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

Chain r:  100%

There are no outlier residues recorded for this chain.

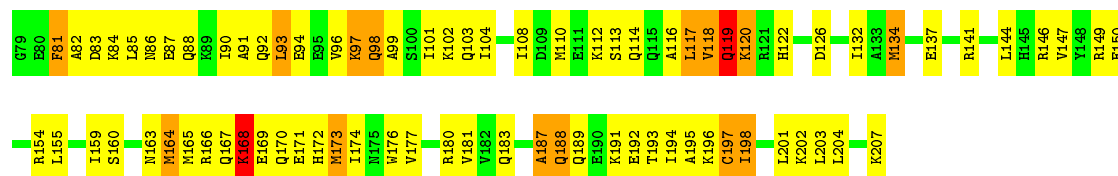
- Molecule 8: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

Chain s:  100%


There are no outlier residues recorded for this chain.

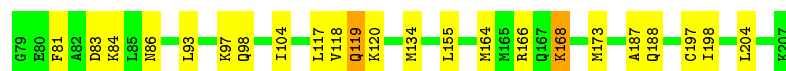
- Molecule 9: ATP SYNTHASE SUBUNIT B, MITOCHONDRIAL

Chain T:  39% 49% 11%

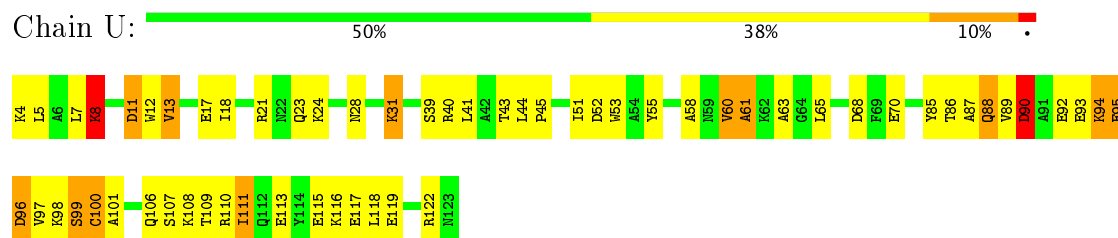


- Molecule 9: ATP SYNTHASE SUBUNIT B, MITOCHONDRIAL

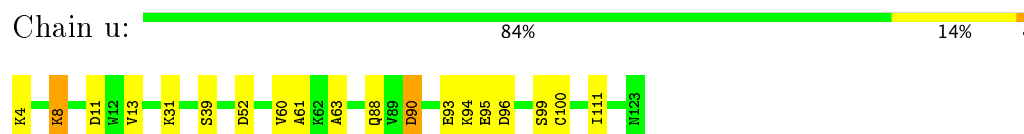
Chain t:  82% 16%



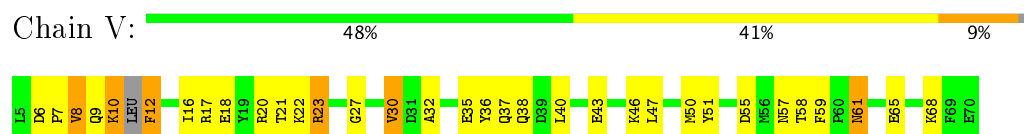
- Molecule 10: ATP SYNTHASE SUBUNIT D, MITOCHONDRIAL



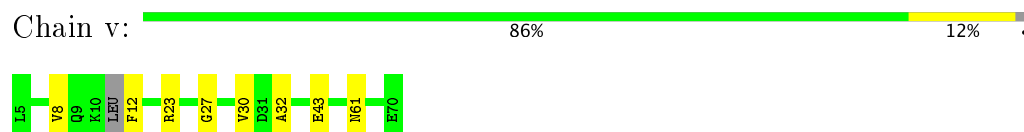
• Molecule 10: ATP SYNTHASE SUBUNIT D, MITOCHONDRIAL



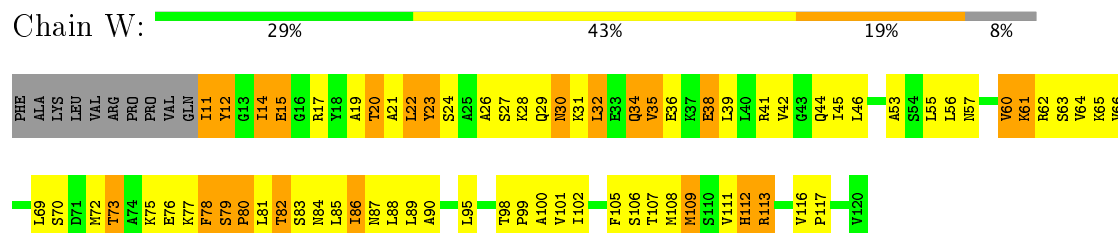
• Molecule 11: ATP SYNTHASE-COUPLING FACTOR 6, MITOCHONDRIAL



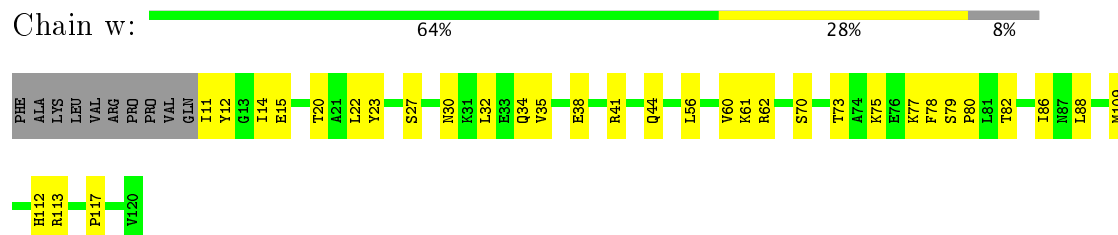
• Molecule 11: ATP SYNTHASE-COUPLING FACTOR 6, MITOCHONDRIAL



• Molecule 12: ATP SYNTHASE SUBUNIT O, MITOCHONDRIAL



• Molecule 12: ATP SYNTHASE SUBUNIT O, MITOCHONDRIAL



## 4 Experimental information

Property	Value	Source
Reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of tilted images used	121	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	160	Depositor
Minimum defocus (nm)	6500	Depositor
Maximum defocus (nm)	7500	Depositor
Magnification	24500	Depositor
Image detector	GATAN ULTRASCAN 1000 (2k x 2k)	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ATP, ADP

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	A	0.28	0/3749	0.43	0/5073
1	C	0.27	0/3749	0.43	0/5073
1	a	0.28	0/3749	0.43	0/5073
1	c	0.27	0/3749	0.43	0/5073
10	U	0.61	0/988	0.76	1/1335 (0.1%)
10	u	0.61	0/988	0.76	1/1335 (0.1%)
11	V	19.73	1/553 (0.2%)	0.82	1/738 (0.1%)
11	v	0.58	0/554	0.71	0/741
12	W	0.26	0/857	0.36	0/1154
12	w	0.26	0/857	0.36	0/1154
2	B	0.24	0/3741	0.39	0/5064
2	b	0.25	0/3741	0.39	0/5064
3	D	0.28	0/3605	0.44	0/4889
3	d	0.28	0/3605	0.44	0/4889
4	E	0.24	0/3628	0.41	0/4919
4	F	0.26	0/3622	0.43	0/4911
4	e	0.24	0/3628	0.41	0/4919
4	f	0.27	0/3622	0.43	0/4911
5	G	0.25	0/2111	0.39	0/2838
5	g	0.24	0/2111	0.39	0/2838
6	H	0.24	0/1004	0.39	0/1359
6	h	0.24	0/1004	0.39	0/1359
7	I	0.23	0/398	0.34	0/547
7	i	0.23	0/398	0.34	0/547
8	J	0.23	0/553	0.35	0/747
8	K	0.24	0/553	0.37	0/747
8	L	0.22	0/553	0.35	0/747
8	M	0.23	0/553	0.36	0/747
8	N	0.23	0/553	0.35	0/747
8	O	0.23	0/553	0.35	0/747
8	P	0.23	0/553	0.35	0/747
8	Q	0.23	0/553	0.34	0/747

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
8	R	0.23	0/553	0.34	0/747
8	S	0.23	0/553	0.35	0/747
8	j	0.23	0/553	0.35	0/747
8	k	0.23	0/553	0.37	0/747
8	l	0.23	0/553	0.35	0/747
8	m	0.23	0/553	0.36	0/747
8	n	0.22	0/553	0.35	0/747
8	o	0.23	0/553	0.35	0/747
8	p	0.23	0/553	0.35	0/747
8	q	0.23	0/553	0.34	0/747
8	r	0.23	0/553	0.34	0/747
8	s	0.23	0/553	0.35	0/747
9	T	0.72	2/1088 (0.2%)	0.69	1/1453 (0.1%)
9	t	0.72	2/1088 (0.2%)	0.69	1/1453 (0.1%)
All	All	1.79	5/69247 (0.0%)	0.44	5/93649 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	V	10	LYS	N-CA	463.87	10.74	1.46
9	T	168	LYS	C-N	-14.85	0.99	1.34
9	t	168	LYS	C-N	-14.84	0.99	1.34
9	T	173	MET	CG-SD	5.98	1.96	1.81
9	t	173	MET	CG-SD	5.97	1.96	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	V	10	LYS	N-CA-CB	-11.15	90.52	110.60
9	t	173	MET	CG-SD-CE	6.80	111.08	100.20
9	T	173	MET	CG-SD-CE	6.79	111.06	100.20
10	U	90	ASP	CB-CG-OD1	6.38	124.05	118.30
10	u	90	ASP	CB-CG-OD1	6.37	124.03	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3692	0	3769	241	0
1	C	3692	0	3772	134	0
1	a	3692	0	3769	0	0
1	c	3692	0	3772	0	0
2	B	3685	0	3768	139	0
2	b	3685	0	3768	0	0
3	D	3549	0	3621	138	0
3	d	3549	0	3621	0	0
4	E	3572	0	3638	160	0
4	F	3566	0	3633	175	0
4	e	3572	0	3638	0	0
4	f	3566	0	3633	0	0
5	G	2086	0	2156	87	0
5	g	2086	0	2156	0	0
6	H	990	0	999	64	0
6	h	990	0	999	0	0
7	I	392	0	306	10	0
7	i	392	0	306	0	0
8	J	545	0	591	17	0
8	K	545	0	591	25	0
8	L	545	0	591	28	0
8	M	545	0	591	33	0
8	N	545	0	591	30	0
8	O	545	0	591	29	0
8	P	545	0	591	28	0
8	Q	545	0	591	25	0
8	R	545	0	591	20	0
8	S	545	0	591	18	0
8	j	545	0	591	0	0
8	k	545	0	591	0	0
8	l	545	0	591	0	0
8	m	545	0	591	0	0
8	n	545	0	591	0	0
8	o	545	0	591	0	0
8	p	545	0	591	0	0
8	q	545	0	591	0	0
8	r	545	0	591	0	0
8	s	545	0	591	0	0
9	T	1077	0	1104	166	0
9	t	1077	0	1104	0	0
10	U	969	0	980	82	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	u	969	0	980	0	0
11	V	542	0	520	94	0
11	v	542	0	521	0	0
12	W	846	893	889	146	0
12	w	846	893	889	0	0
13	A	31	0	12	5	0
13	B	31	0	12	1	0
13	C	31	0	12	1	0
13	a	31	0	12	0	0
13	b	31	0	12	0	0
13	c	31	0	12	0	0
14	A	1	0	0	0	0
14	B	1	0	0	0	0
14	C	1	0	0	0	0
14	D	1	0	0	0	0
14	F	1	0	0	0	0
14	a	1	0	0	0	0
14	b	1	0	0	0	0
14	c	1	0	0	0	0
14	d	1	0	0	0	0
14	f	1	0	0	0	0
15	D	27	0	12	2	0
15	F	27	0	12	2	0
15	d	27	0	12	0	0
15	f	27	0	12	0	0
All	All	68520	1786	70251	1554	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 11.

All (1554) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:PRO:CD	9:T:159:ILE:CG2	1.78	1.59
1:A:27:LEU:CD2	9:T:202:LYS:HE2	1.35	1.56
4:F:56:GLU:CD	12:W:53:ALA:HB2	1.25	1.55
9:T:203:LEU:HD21	12:W:84:ASN:CB	1.45	1.47
9:T:201:LEU:HD13	11:V:7:PRO:CG	1.01	1.47
9:T:201:LEU:CD1	11:V:7:PRO:HG3	0.98	1.46
1:A:119:GLY:O	11:V:51:TYR:CZ	1.67	1.46
4:F:56:GLU:OE1	12:W:53:ALA:CB	1.63	1.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:PRO:CD	9:T:159:ILE:HG22	1.37	1.44
1:A:122:PRO:CG	9:T:159:ILE:HG21	1.49	1.41
1:A:119:GLY:HA3	11:V:50:MET:CE	1.51	1.41
1:A:472:SER:CB	10:U:31:LYS:HE3	1.55	1.36
9:T:203:LEU:CD2	12:W:84:ASN:HB2	1.60	1.32
9:T:116:ALA:O	9:T:120:LYS:HB2	1.27	1.28
1:A:122:PRO:CG	9:T:159:ILE:CG2	2.09	1.28
1:A:476:SER:CB	10:U:12:TRP:H	1.48	1.27
1:A:27:LEU:CD2	9:T:202:LYS:CE	2.12	1.25
1:A:28:ASN:HD22	11:V:8:VAL:HG11	1.01	1.18
1:A:119:GLY:HA3	11:V:50:MET:SD	1.84	1.18
8:N:4:VAL:HG21	8:O:5:LEU:HD23	1.19	1.17
1:A:119:GLY:CA	11:V:50:MET:CE	2.21	1.17
8:O:4:VAL:HG21	8:P:5:LEU:HD23	1.25	1.16
9:T:176:TRP:CZ3	11:V:22:LYS:HB2	1.80	1.15
1:A:122:PRO:CD	9:T:159:ILE:HG21	1.55	1.15
8:M:4:VAL:HG21	8:N:5:LEU:HD23	1.28	1.14
8:K:4:VAL:HG21	8:L:5:LEU:HD23	1.15	1.13
1:A:27:LEU:HD22	9:T:202:LYS:CE	1.79	1.12
9:T:116:ALA:HB1	9:T:120:LYS:NZ	1.64	1.12
8:Q:4:VAL:HG21	8:R:5:LEU:HD23	1.16	1.11
1:A:27:LEU:HD21	9:T:202:LYS:HE2	1.16	1.10
1:A:476:SER:HB3	10:U:12:TRP:H	0.94	1.10
1:A:472:SER:HB2	10:U:31:LYS:HE3	1.12	1.10
1:A:122:PRO:HD2	9:T:159:ILE:CG2	1.58	1.10
1:A:28:ASN:ND2	11:V:8:VAL:HG11	1.70	1.07
1:A:122:PRO:HG3	9:T:159:ILE:CG2	1.83	1.07
1:A:476:SER:HB3	10:U:12:TRP:N	1.69	1.07
1:A:122:PRO:HB3	9:T:163:ASN:HD21	1.13	1.06
9:T:120:LYS:HD3	10:U:18:ILE:HG22	1.38	1.06
9:T:173:MET:HG3	11:V:22:LYS:HE2	1.33	1.04
4:F:56:GLU:OE1	12:W:53:ALA:HB2	0.86	1.03
8:L:4:VAL:HG21	8:M:5:LEU:HD23	1.03	1.02
4:E:50:VAL:HA	4:E:61:THR:HG22	1.41	1.02
1:A:119:GLY:HA3	11:V:50:MET:HE2	1.41	1.01
9:T:201:LEU:CD1	11:V:7:PRO:CB	2.39	1.01
9:T:180:ARG:NH2	11:V:21:THR:HG21	1.75	1.00
9:T:176:TRP:HZ3	11:V:22:LYS:HB2	1.19	1.00
8:P:4:VAL:HG21	8:Q:5:LEU:HD23	1.02	1.00
1:C:212:ARG:HG2	1:C:237:THR:HG21	1.43	1.00
9:T:201:LEU:CD1	11:V:7:PRO:CG	1.80	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:4:VAL:HG21	8:M:5:LEU:CD2	1.92	0.99
6:H:10:LEU:HD21	6:H:83:LEU:H	1.28	0.99
9:T:116:ALA:HB1	9:T:120:LYS:CE	1.92	0.99
1:A:119:GLY:O	11:V:51:TYR:CE1	2.16	0.99
9:T:176:TRP:HZ3	11:V:22:LYS:CB	1.76	0.99
8:J:4:VAL:HG21	8:K:5:LEU:HD23	1.41	0.98
4:F:56:GLU:CD	12:W:53:ALA:CB	2.19	0.98
9:T:180:ARG:HH22	11:V:21:THR:HG21	1.26	0.98
9:T:116:ALA:HB1	9:T:120:LYS:HD2	1.46	0.97
8:L:4:VAL:CG2	8:M:5:LEU:HD23	1.95	0.97
1:A:119:GLY:C	11:V:51:TYR:OH	2.03	0.96
8:P:4:VAL:HG21	8:Q:5:LEU:CD2	1.95	0.96
9:T:134:MET:HG3	10:U:41:LEU:HD11	1.47	0.96
4:F:56:GLU:OE2	12:W:53:ALA:HB2	1.66	0.96
1:A:142:ARG:HG3	1:A:315:SER:HA	1.48	0.95
1:C:116:PRO:HD3	1:C:123:ILE:HG12	1.50	0.94
8:P:4:VAL:CG2	8:Q:5:LEU:HD23	1.96	0.94
2:B:174:GLN:HE21	4:E:356:ARG:HH11	1.16	0.94
4:F:56:GLU:OE2	12:W:53:ALA:N	2.01	0.94
1:C:239:SER:HB3	4:F:294:GLU:HG3	1.50	0.93
1:A:122:PRO:HD3	9:T:159:ILE:HG22	0.95	0.93
9:T:116:ALA:HB1	9:T:120:LYS:CD	1.98	0.93
9:T:116:ALA:HB1	9:T:120:LYS:HZ2	1.35	0.93
9:T:116:ALA:CB	9:T:120:LYS:NZ	2.32	0.92
1:A:404:ALA:HB2	5:G:18:LYS:HE2	1.51	0.92
1:A:473:TYR:CE1	10:U:13:VAL:HG11	2.05	0.92
12:W:23:TYR:CE1	12:W:32:LEU:HD11	2.05	0.91
2:B:217:GLN:HE22	4:E:131:ALA:HB2	1.35	0.91
2:B:398:GLN:HE22	4:F:412:ARG:HE	1.16	0.91
4:F:153:ILE:HD12	4:F:307:VAL:HG22	1.52	0.91
1:A:42:ARG:HD2	1:A:72:GLN:NE2	1.86	0.90
4:E:85:VAL:HG11	4:E:235:THR:HG23	1.53	0.90
1:A:472:SER:HB2	10:U:31:LYS:CE	2.02	0.90
1:A:476:SER:CB	10:U:12:TRP:N	2.32	0.89
1:A:28:ASN:HD21	11:V:8:VAL:HG21	1.38	0.89
5:G:247:MET:HG3	5:G:250:ARG:HH21	1.37	0.89
1:A:42:ARG:HD2	1:A:72:GLN:HE22	1.38	0.89
4:E:388:ILE:HG23	4:E:393:MET:HG2	1.55	0.89
3:D:125:ALA:HB1	11:V:50:MET:HG2	1.55	0.88
1:A:122:PRO:HB3	9:T:163:ASN:ND2	1.88	0.88
11:V:9:GLN:C	11:V:10:LYS:CA	2.42	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:T:116:ALA:CB	9:T:120:LYS:HZ2	2.02	0.88
9:T:201:LEU:HD12	11:V:7:PRO:CG	2.03	0.87
9:T:118:VAL:O	9:T:119:GLN:C	2.13	0.87
1:A:119:GLY:C	11:V:51:TYR:CZ	2.48	0.87
1:A:27:LEU:HD23	9:T:202:LYS:HE2	1.52	0.87
1:A:119:GLY:O	11:V:51:TYR:OH	1.93	0.86
8:R:4:VAL:HG21	8:S:5:LEU:HD23	1.56	0.86
2:B:217:GLN:NE2	4:E:131:ALA:HB2	1.90	0.86
1:A:28:ASN:HD22	11:V:8:VAL:CG1	1.88	0.86
1:A:473:TYR:CE1	10:U:13:VAL:CG1	2.59	0.86
9:T:134:MET:CG	10:U:41:LEU:HD11	2.06	0.85
2:B:389:ALA:HB2	2:B:447:ILE:HG21	1.59	0.85
4:F:37:LEU:HB2	4:F:48:LEU:HB2	1.59	0.85
2:B:174:GLN:HE21	4:E:356:ARG:NH1	1.75	0.85
9:T:201:LEU:HD13	11:V:7:PRO:CD	2.07	0.84
9:T:117:LEU:HD23	9:T:117:LEU:H	1.42	0.84
1:A:119:GLY:CA	11:V:50:MET:SD	2.66	0.84
4:F:56:GLU:OE2	12:W:53:ALA:CB	2.24	0.84
5:G:93:LYS:HE2	5:G:97:ARG:HH21	1.43	0.83
8:K:4:VAL:HG21	8:L:5:LEU:CD2	2.06	0.83
1:C:249:PRO:HG2	1:C:276:GLN:OE1	1.79	0.83
3:D:142:ASP:HB3	3:D:434:LEU:HD13	1.59	0.83
1:A:122:PRO:HG3	9:T:159:ILE:HG23	1.59	0.82
1:A:122:PRO:CB	9:T:163:ASN:HD21	1.93	0.82
12:W:26:ALA:HB2	12:W:81:LEU:HD12	1.62	0.82
8:J:5:LEU:HD23	8:S:4:VAL:HG21	1.62	0.82
1:C:273:LEU:HB3	1:C:304:HIS:CE1	2.15	0.81
9:T:173:MET:CG	11:V:22:LYS:HE2	2.10	0.81
9:T:201:LEU:CG	11:V:7:PRO:HG3	2.08	0.81
1:A:85:LYS:HE2	3:D:32:ALA:HB2	1.63	0.81
1:C:378:SER:HB2	1:C:386:LYS:HE2	1.63	0.81
1:A:122:PRO:HD2	9:T:159:ILE:HG21	1.33	0.81
8:K:4:VAL:CG2	8:L:5:LEU:HD23	2.07	0.81
1:A:122:PRO:HG2	9:T:159:ILE:HG21	1.63	0.81
12:W:45:ILE:HD11	12:W:76:GLU:OE1	1.81	0.81
10:U:60:VAL:HG22	10:U:61:ALA:H	1.46	0.80
5:G:110:ILE:HG23	5:G:130:ILE:HB	1.64	0.80
9:T:134:MET:HG3	10:U:41:LEU:CD1	2.11	0.80
1:A:239:SER:HB3	3:D:294:GLU:HG3	1.63	0.80
4:E:168:GLN:HE21	4:E:201:MET:HG2	1.46	0.80
9:T:116:ALA:O	9:T:120:LYS:CB	2.22	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:321:ALA:HB3	3:D:322:PRO:HD3	1.64	0.80
4:E:98:VAL:HG11	4:E:228:ALA:HB1	1.64	0.79
8:K:40:ASN:HD22	8:K:43:ILE:HG22	1.48	0.79
5:G:50:LEU:HG	6:H:78:GLN:HE21	1.47	0.79
4:F:298:THR:HG23	4:F:303:SER:HA	1.62	0.79
12:W:31:LYS:O	12:W:35:VAL:HG23	1.83	0.79
12:W:99:PRO:HA	12:W:102:ILE:HD12	1.63	0.78
6:H:38:ARG:HD2	8:M:41:PRO:HG3	1.66	0.78
1:A:472:SER:CB	10:U:31:LYS:CE	2.51	0.78
4:F:50:VAL:HA	4:F:61:THR:HG22	1.66	0.77
1:A:473:TYR:HE1	10:U:13:VAL:HG11	1.46	0.77
12:W:46:LEU:HD11	12:W:95:LEU:O	1.85	0.77
1:A:122:PRO:HD3	9:T:159:ILE:CG2	1.76	0.77
9:T:203:LEU:HD21	12:W:84:ASN:CG	2.04	0.76
2:B:398:GLN:HE22	4:F:412:ARG:NE	1.83	0.76
3:D:26:GLU:HB2	3:D:29:GLU:OE1	1.84	0.76
12:W:35:VAL:HG22	12:W:81:LEU:CB	2.15	0.76
2:B:240:GLU:HB3	2:B:244:LEU:HD12	1.67	0.76
4:E:174:ILE:HG21	4:E:252:LEU:HD11	1.68	0.76
3:D:85:VAL:HG11	3:D:235:THR:HG23	1.68	0.76
4:E:336:SER:HB3	4:E:339:ILE:HG12	1.68	0.76
12:W:69:LEU:HD23	12:W:86:ILE:HG23	1.67	0.76
1:A:103:PRO:HD3	1:A:258:TRP:CH2	2.21	0.76
2:B:239:SER:HB2	4:E:121:PRO:HG3	1.68	0.75
12:W:42:VAL:HA	12:W:45:ILE:HD12	1.68	0.75
1:A:28:ASN:ND2	11:V:8:VAL:HG21	2.01	0.75
12:W:55:LEU:HD22	12:W:95:LEU:HD13	1.69	0.75
4:E:15:ALA:HB3	4:E:22:ASP:HB2	1.69	0.75
8:Q:4:VAL:HG21	8:R:5:LEU:CD2	2.09	0.75
12:W:15:GLU:O	12:W:101:VAL:HG13	1.87	0.75
1:A:472:SER:OG	10:U:31:LYS:HE3	1.85	0.74
1:C:217:GLN:HE22	4:F:356:ARG:HD2	1.52	0.74
9:T:134:MET:CG	10:U:41:LEU:CD1	2.65	0.74
1:A:119:GLY:O	11:V:51:TYR:CE2	2.39	0.74
1:C:417:LYS:O	1:C:421:VAL:HG23	1.87	0.74
1:A:159:VAL:HG13	1:A:374:SER:HB2	1.70	0.74
8:O:4:VAL:HA	8:P:6:ALA:HB2	1.70	0.74
9:T:120:LYS:HD3	10:U:18:ILE:CG2	2.18	0.73
2:B:152:LEU:HD12	2:B:180:VAL:HG13	1.70	0.73
9:T:176:TRP:CE3	11:V:22:LYS:HD3	2.23	0.73
3:D:125:ALA:HB1	11:V:50:MET:CG	2.19	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:LEU:HD12	3:D:16:VAL:HB	1.70	0.73
1:A:27:LEU:HD22	9:T:202:LYS:NZ	2.02	0.73
10:U:13:VAL:O	10:U:17:GLU:HG2	1.89	0.73
9:T:176:TRP:HZ3	11:V:22:LYS:CA	2.01	0.73
1:A:143:SER:HB3	4:E:199:ARG:HH22	1.54	0.72
2:B:249:PRO:HG3	2:B:276:GLN:NE2	2.04	0.72
9:T:122:HIS:HD2	9:T:126:ASP:OD2	1.72	0.72
2:B:103:PRO:HD3	2:B:258:TRP:CH2	2.24	0.72
4:F:310:VAL:HG21	4:F:325:THR:HG21	1.71	0.72
1:C:56:GLU:HG2	1:C:62:LYS:HG2	1.72	0.72
4:E:206:VAL:HG23	4:E:207:ILE:HG13	1.72	0.72
6:H:49:VAL:HG22	6:H:76:THR:HG23	1.71	0.72
6:H:60:MET:HA	6:H:65:SER:CB	2.20	0.72
4:E:106:ARG:NH1	4:E:209:LEU:HD22	2.05	0.71
1:A:168:LEU:HB2	1:A:348:THR:HG21	1.72	0.71
4:F:257:ASN:HD21	4:F:311:TYR:N	1.88	0.71
9:T:117:LEU:HD23	9:T:117:LEU:N	2.05	0.71
4:E:298:THR:HG23	4:E:303:SER:HB3	1.72	0.71
9:T:176:TRP:CZ3	11:V:30:VAL:HG21	2.26	0.71
4:F:374:VAL:HG13	4:F:410:ILE:HG21	1.72	0.71
2:B:138:ILE:HD11	4:F:95:ILE:HG21	1.73	0.71
3:D:391:LEU:HB3	3:D:395:GLU:HG3	1.72	0.71
4:E:402:LEU:O	4:E:406:ARG:HG3	1.91	0.71
3:D:134:LEU:HD13	3:D:149:ARG:HE	1.55	0.71
1:A:240:GLU:HB3	1:A:244:LEU:HD12	1.73	0.70
2:B:219:VAL:HG13	2:B:228:MET:HE3	1.73	0.70
4:F:30:LEU:HD21	4:F:57:ASN:HA	1.73	0.70
12:W:78:PHE:CD1	12:W:82:THR:HG21	2.26	0.70
2:B:338:ALA:HB3	2:B:341:PRO:HG2	1.73	0.70
8:K:40:ASN:ND2	8:K:43:ILE:HG22	2.05	0.70
12:W:78:PHE:CD2	12:W:86:ILE:HD11	2.26	0.70
8:M:57:LEU:HD22	8:N:55:PHE:CZ	2.26	0.70
1:C:444:VAL:HB	1:C:445:PRO:HD3	1.74	0.70
4:F:106:ARG:NE	4:F:209:LEU:HD22	2.06	0.70
8:M:40:ASN:HD21	8:M:43:ILE:HG12	1.56	0.70
1:C:336:VAL:HG11	1:C:353:PHE:HE2	1.57	0.70
1:A:26:ASN:OD1	11:V:8:VAL:HG13	1.92	0.70
1:C:142:ARG:HH22	1:C:316:GLU:HB2	1.57	0.70
8:Q:4:VAL:CG2	8:R:5:LEU:HD23	2.09	0.70
2:B:243:PRO:HG3	2:B:283:LEU:HD11	1.73	0.70
1:A:50:GLN:HA	4:E:71:VAL:HG22	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:W:39:LEU:HB3	12:W:102:ILE:HG23	1.74	0.69
12:W:82:THR:O	12:W:86:ILE:HD13	1.92	0.69
12:W:35:VAL:HG22	12:W:81:LEU:HB2	1.75	0.69
12:W:12:TYR:N	12:W:12:TYR:CD1	2.61	0.69
1:A:119:GLY:CA	11:V:50:MET:HE2	2.09	0.69
4:E:430:LYS:HG3	4:E:461:GLY:HA3	1.74	0.69
9:T:176:TRP:CE3	11:V:22:LYS:HB2	2.27	0.69
9:T:176:TRP:HE3	11:V:22:LYS:HD3	1.56	0.69
3:D:397:SER:HB3	3:D:400:ASP:OD2	1.92	0.69
5:G:108:VAL:HG13	5:G:128:LEU:HB3	1.75	0.69
9:T:116:ALA:CB	9:T:120:LYS:HD2	2.23	0.69
1:A:314:LEU:HD22	1:A:318:GLU:HG2	1.75	0.69
1:C:240:GLU:HB3	1:C:244:LEU:HD12	1.75	0.69
4:F:417:PRO:HG3	4:F:459:MET:HG3	1.75	0.69
10:U:116:LYS:O	10:U:119:GLU:HB3	1.93	0.69
4:E:106:ARG:HH12	4:E:209:LEU:HD22	1.58	0.69
6:H:91:PHE:CE1	6:H:96:PHE:HB3	2.28	0.69
1:A:168:LEU:HD12	1:A:327:PRO:O	1.93	0.68
1:C:99:VAL:HG11	1:C:251:THR:HB	1.75	0.68
4:F:153:ILE:HB	4:F:307:VAL:HA	1.76	0.68
6:H:60:MET:HA	6:H:65:SER:HB3	1.75	0.68
1:A:120:LYS:N	11:V:51:TYR:OH	2.26	0.68
1:A:476:SER:HB3	10:U:11:ASP:HA	1.75	0.68
4:F:258:ILE:HG22	4:F:309:ALA:O	1.94	0.68
9:T:176:TRP:CZ3	11:V:22:LYS:CB	2.59	0.68
9:T:189:GLN:HA	9:T:192:GLU:CD	2.14	0.68
1:A:476:SER:HB2	10:U:12:TRP:H	1.54	0.68
8:N:57:LEU:HD22	8:O:55:PHE:CZ	2.29	0.68
1:A:473:TYR:CD1	10:U:13:VAL:HB	2.29	0.68
4:F:102:PRO:HG3	4:F:109:ILE:HG13	1.75	0.68
1:A:311:ALA:HB1	1:A:323:LEU:O	1.93	0.67
1:A:166:ARG:HD2	1:A:308:LEU:HB3	1.76	0.67
4:F:36:ALA:O	4:F:37:LEU:HD23	1.95	0.67
1:C:349:ASP:HA	1:C:375:ARG:HD2	1.77	0.67
12:W:38:GLU:HB3	12:W:82:THR:HG21	1.75	0.67
12:W:39:LEU:HD21	12:W:85:LEU:CD2	2.24	0.67
4:F:56:GLU:OE1	12:W:53:ALA:HB1	1.86	0.67
1:C:67:ASN:ND2	1:C:287:LEU:HB3	2.10	0.67
8:J:47:VAL:CG1	8:K:34:ILE:HG23	2.25	0.67
9:T:180:ARG:NH1	11:V:21:THR:HG23	2.10	0.67
12:W:26:ALA:HB2	12:W:81:LEU:CD1	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:SER:CB	10:U:12:TRP:HB2	2.25	0.67
2:B:454:HIS:HB3	2:B:507:VAL:HG21	1.77	0.67
4:F:134:LEU:HD13	4:F:149:ARG:HD2	1.77	0.67
5:G:55:ALA:HB2	5:G:197:PHE:HE2	1.59	0.67
9:T:144:LEU:O	9:T:147:VAL:HG22	1.95	0.67
9:T:180:ARG:CZ	11:V:21:THR:HG21	2.25	0.67
1:A:473:TYR:HE1	10:U:13:VAL:CG1	2.03	0.66
1:A:51:ALA:HB3	4:E:69:GLY:H	1.60	0.66
2:B:174:GLN:NE2	4:E:356:ARG:HH11	1.90	0.66
4:E:244:ARG:HD3	4:E:304:VAL:HG23	1.78	0.66
9:T:203:LEU:CD2	12:W:84:ASN:CB	2.41	0.66
5:G:204:ASN:HD22	5:G:207:ARG:HG3	1.60	0.66
1:A:211:LYS:HD3	3:D:328:HIS:HA	1.78	0.66
1:C:510:PHE:HD1	1:C:510:PHE:OXT	1.78	0.66
9:T:122:HIS:CD2	9:T:126:ASP:OD2	2.49	0.66
12:W:63:SER:O	12:W:66:VAL:HG12	1.95	0.66
1:A:138:ILE:HD13	4:E:191:THR:HG23	1.77	0.66
9:T:119:GLN:CG	9:T:120:LYS:H	2.09	0.66
1:A:217:GLN:HG2	3:D:356:ARG:HH12	1.60	0.66
3:D:187:VAL:HG22	3:D:232:VAL:HG13	1.78	0.66
6:H:69:PHE:HB3	6:H:91:PHE:HB3	1.78	0.66
1:C:510:PHE:CD1	1:C:510:PHE:OXT	2.49	0.66
4:E:86:PRO:HD3	4:E:114:ARG:HH12	1.61	0.66
2:B:444:VAL:HB	2:B:445:PRO:HD3	1.79	0.65
9:T:180:ARG:NH2	11:V:18:GLU:OE1	2.29	0.65
3:D:298:THR:HG23	3:D:303:SER:HA	1.78	0.65
4:F:190:ARG:HD2	4:F:193:GLU:OE2	1.95	0.65
12:W:65:LYS:O	12:W:69:LEU:HD13	1.96	0.65
12:W:39:LEU:HD21	12:W:85:LEU:HD21	1.78	0.65
1:C:176:GLY:HA2	13:C:1511:ATP:O1A	1.96	0.65
9:T:180:ARG:NH1	11:V:21:THR:CG2	2.60	0.65
1:A:28:ASN:ND2	11:V:8:VAL:CG1	2.54	0.65
2:B:398:GLN:NE2	4:F:412:ARG:HE	1.93	0.65
12:W:19:ALA:HB1	12:W:105:PHE:HD2	1.62	0.65
6:H:10:LEU:HD21	6:H:83:LEU:N	2.08	0.64
8:J:55:PHE:CZ	8:S:57:LEU:HD22	2.33	0.64
12:W:46:LEU:HD22	12:W:98:THR:HG22	1.79	0.64
1:A:248:ALA:HB3	1:A:249:PRO:HD3	1.80	0.64
12:W:55:LEU:HD13	12:W:95:LEU:HD22	1.80	0.64
3:D:391:LEU:HD21	5:G:23:MET:HE3	1.79	0.64
9:T:176:TRP:HZ3	11:V:22:LYS:HA	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:V:6:ASP:N	11:V:7:PRO:HD2	2.13	0.64
2:B:89:LEU:HD23	2:B:90:VAL:N	2.12	0.64
4:E:346:PRO:HB3	4:E:418:PHE:HZ	1.62	0.64
4:F:140:VAL:HG21	4:F:348:VAL:HG21	1.80	0.64
6:H:46:VAL:HG21	8:K:38:SER:O	1.98	0.64
8:Q:57:LEU:HD22	8:R:55:PHE:CZ	2.33	0.64
4:E:142:ASP:HB3	4:E:434:LEU:HD13	1.80	0.64
9:T:116:ALA:CB	9:T:120:LYS:HZ1	2.09	0.64
1:A:358:LEU:HB2	1:A:366:ALA:HB1	1.78	0.64
4:F:9:ILE:HG23	4:F:27:GLN:OE1	1.98	0.64
8:M:4:VAL:HA	8:N:6:ALA:HB2	1.79	0.64
1:A:473:TYR:CE1	10:U:13:VAL:HB	2.32	0.64
2:B:340:ILE:HB	2:B:341:PRO:HD3	1.80	0.64
3:D:153:ILE:HD12	3:D:307:VAL:HG22	1.80	0.64
4:F:201:MET:CE	4:F:215:VAL:HG11	2.28	0.64
4:F:106:ARG:HE	4:F:209:LEU:HD22	1.62	0.64
1:A:404:ALA:HB3	5:G:22:THR:HG21	1.80	0.64
6:H:83:LEU:HD23	6:H:84:CYS:N	2.13	0.64
8:L:43:ILE:HG22	8:L:47:VAL:HG23	1.80	0.64
4:F:56:GLU:OE2	12:W:53:ALA:CA	2.45	0.64
8:P:40:ASN:HD21	8:P:43:ILE:HG12	1.63	0.64
12:W:90:ALA:HB2	12:W:95:LEU:HD11	1.80	0.64
9:T:98:GLN:O	9:T:101:ILE:HG13	1.97	0.64
9:T:176:TRP:CE3	11:V:22:LYS:CD	2.81	0.64
1:C:166:ARG:HD2	1:C:166:ARG:H	1.63	0.63
1:C:336:VAL:HG11	1:C:353:PHE:CE2	2.33	0.63
1:C:392:LEU:O	1:C:396:LEU:HD13	1.98	0.63
4:E:237:LEU:HD22	4:E:292:LEU:HD12	1.81	0.63
1:A:28:ASN:HB3	1:A:48:ASN:ND2	2.14	0.63
3:D:23:VAL:HG11	3:D:76:VAL:HG21	1.80	0.63
4:E:30:LEU:HD21	4:E:57:ASN:HA	1.80	0.63
12:W:78:PHE:CE2	12:W:86:ILE:HD11	2.34	0.63
12:W:98:THR:N	12:W:99:PRO:CD	2.62	0.63
1:A:371:LEU:O	1:A:373:VAL:HG13	1.99	0.63
8:K:40:ASN:HD22	8:K:43:ILE:CG2	2.12	0.63
12:W:73:THR:HG23	12:W:86:ILE:HG12	1.81	0.63
9:T:203:LEU:HD21	12:W:84:ASN:HB2	0.68	0.63
8:L:57:LEU:HD22	8:M:55:PHE:CZ	2.34	0.63
9:T:90:ILE:HG23	9:T:91:ALA:N	2.14	0.63
12:W:78:PHE:O	12:W:79:SER:CB	2.46	0.63
9:T:119:GLN:HG3	9:T:120:LYS:H	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:W:39:LEU:HD12	12:W:105:PHE:CD2	2.34	0.63
9:T:203:LEU:HG	12:W:84:ASN:ND2	2.14	0.63
1:A:43:VAL:HG11	1:A:90:VAL:HG11	1.81	0.62
2:B:131:ALA:HB1	2:B:247:LEU:HD11	1.81	0.62
4:F:185:THR:HA	4:F:218:VAL:O	1.99	0.62
1:A:153:LYS:HG3	1:A:432:GLN:OE1	1.99	0.62
5:G:93:LYS:HE2	5:G:97:ARG:NH2	2.13	0.62
9:T:180:ARG:HH12	11:V:21:THR:CG2	2.12	0.62
12:W:73:THR:HG22	12:W:78:PHE:CB	2.29	0.62
3:D:188:GLY:HA3	3:D:260:ARG:HG3	1.81	0.62
2:B:67:ASN:HB2	4:F:17:ILE:HG12	1.81	0.62
8:O:57:LEU:HD22	8:P:55:PHE:CZ	2.35	0.62
1:A:340:ILE:HB	1:A:341:PRO:HD3	1.81	0.62
4:F:229:ARG:NH2	4:F:267:GLU:OE2	2.33	0.62
5:G:54:ASN:HD22	6:H:78:GLN:NE2	1.97	0.62
5:G:78:THR:HG22	5:G:91:LEU:HD23	1.81	0.62
12:W:35:VAL:HG13	12:W:81:LEU:HB3	1.81	0.62
4:E:243:PHE:HB2	4:E:251:VAL:HG21	1.82	0.62
5:G:199:ILE:HD11	5:G:205:VAL:HB	1.82	0.62
6:H:112:VAL:HG12	6:H:120:ALA:HA	1.82	0.62
1:A:176:GLY:HA2	13:A:1511:ATP:O1A	2.00	0.62
1:C:248:ALA:HB3	1:C:249:PRO:HD3	1.81	0.62
8:R:43:ILE:HG23	8:R:46:THR:HB	1.81	0.62
1:A:476:SER:HB2	10:U:12:TRP:HB2	1.81	0.62
1:A:212:ARG:HB2	3:D:127:GLN:HE21	1.65	0.62
2:B:153:LYS:HG2	2:B:443:GLN:HG2	1.82	0.62
1:A:217:GLN:CD	3:D:356:ARG:HH22	2.03	0.61
1:C:338:ALA:HB3	1:C:341:PRO:HG2	1.82	0.61
9:T:132:ILE:HD12	10:U:85:TYR:HB2	1.81	0.61
10:U:96:ASP:O	10:U:100:CYS:HB3	1.99	0.61
1:A:212:ARG:CG	1:A:237:THR:HG21	2.30	0.61
3:D:336:SER:HB2	3:D:339:ILE:HG12	1.81	0.61
2:B:50:GLN:HB3	4:F:69:GLY:HA2	1.81	0.61
1:A:314:LEU:HD13	1:A:318:GLU:HG3	1.82	0.61
4:E:176:LYS:NZ	4:E:214:LYS:HE2	2.15	0.61
8:R:43:ILE:CG2	8:R:46:THR:HB	2.29	0.61
3:D:257:ASN:ND2	3:D:259:PHE:HB3	2.16	0.61
3:D:154:GLY:HA3	3:D:329:LEU:HD13	1.83	0.61
3:D:145:ALA:HB1	3:D:355:SER:HB2	1.83	0.61
8:M:43:ILE:HG23	8:M:46:THR:HB	1.83	0.61
4:E:127:GLN:HE22	4:E:297:THR:HG21	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:282:GLN:CD	4:E:282:GLN:H	2.04	0.61
12:W:32:LEU:HD13	12:W:105:PHE:CE1	2.35	0.61
2:B:57:PHE:HD1	2:B:90:VAL:HG22	1.66	0.61
3:D:125:ALA:CB	11:V:50:MET:HG2	2.29	0.61
10:U:86:THR:HA	10:U:88:GLN:NE2	2.16	0.61
1:A:300:VAL:HG11	1:A:339:TYR:HE2	1.66	0.61
2:B:503:THR:O	2:B:507:VAL:HG23	2.01	0.61
1:C:185:ILE:HG23	1:C:203:CYS:SG	2.41	0.61
4:E:402:LEU:HG	4:E:406:ARG:HE	1.65	0.61
9:T:173:MET:HG3	11:V:22:LYS:CE	2.20	0.61
2:B:242:ALA:HB3	2:B:243:PRO:HD3	1.83	0.60
1:C:302:TYR:HA	1:C:305:SER:OG	2.01	0.60
3:D:163:LYS:HB2	15:D:1476:ADP:O1B	2.01	0.60
1:A:27:LEU:HD23	9:T:202:LYS:CE	2.19	0.60
1:C:67:ASN:HD21	1:C:287:LEU:HB3	1.66	0.60
6:H:97:SER:HB2	6:H:102:LYS:HE3	1.83	0.60
3:D:255:ILE:HD12	3:D:308:GLN:HE21	1.65	0.60
4:F:197:LEU:O	4:F:201:MET:HG2	2.01	0.60
9:T:93:LEU:HA	9:T:96:VAL:HB	1.83	0.60
1:A:54:LEU:HD23	1:A:64:MET:HB3	1.83	0.60
1:A:476:SER:CB	10:U:12:TRP:CB	2.77	0.60
1:A:120:LYS:CA	11:V:51:TYR:OH	2.49	0.60
12:W:32:LEU:HD12	12:W:109:MET:HB2	1.83	0.60
1:A:239:SER:CB	3:D:294:GLU:HG3	2.31	0.60
8:M:43:ILE:HG22	8:M:47:VAL:HG23	1.83	0.60
9:T:170:GLN:O	9:T:174:ILE:HG12	2.02	0.60
1:A:99:VAL:HG21	1:A:251:THR:HG23	1.84	0.60
3:D:257:ASN:ND2	3:D:259:PHE:H	2.00	0.60
2:B:192:ASN:HA	2:B:200:LYS:HG2	1.83	0.60
1:C:205:TYR:HB3	1:C:233:ILE:HD12	1.84	0.60
4:E:388:ILE:HD11	4:E:396:LEU:HD11	1.84	0.60
4:F:374:VAL:O	4:F:378:LEU:HG	2.00	0.60
5:G:3:LEU:HD23	5:G:3:LEU:O	2.02	0.60
1:C:341:PRO:O	1:C:345:ILE:HG13	2.02	0.60
4:E:26:GLU:HB2	4:E:29:GLU:OE1	2.02	0.60
12:W:29:GLN:O	12:W:30:ASN:CB	2.50	0.60
4:F:157:GLY:H	4:F:312:VAL:HG23	1.67	0.60
1:C:381:GLN:HE21	1:C:386:LYS:HA	1.68	0.59
3:D:334:VAL:HG21	3:D:352:ASP:OD2	2.02	0.59
6:H:105:LEU:O	6:H:109:LYS:HG2	2.03	0.59
2:B:290:PRO:HB3	4:F:276:PRO:HG3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:388:ILE:HD11	4:F:396:LEU:HD11	1.83	0.59
4:E:319:ASP:O	4:E:322:PRO:HG2	2.03	0.59
4:E:366:GLU:O	4:E:370:VAL:HG23	2.03	0.59
2:B:405:PHE:HZ	4:F:393:MET:SD	2.25	0.59
2:B:138:ILE:CD1	4:F:95:ILE:HG21	2.32	0.59
5:G:184:ASN:HA	5:G:210:PHE:CD1	2.37	0.59
8:N:65:CYS:SG	8:O:19:LEU:HD12	2.42	0.59
8:R:47:VAL:CG1	8:S:34:ILE:HG23	2.32	0.59
12:W:73:THR:HG22	12:W:78:PHE:HB2	1.84	0.59
3:D:279:VAL:HG12	3:D:279:VAL:O	2.03	0.59
8:O:65:CYS:SG	8:P:19:LEU:HD12	2.42	0.59
8:R:43:ILE:HG22	8:R:47:VAL:HG23	1.84	0.59
2:B:48:ASN:O	2:B:92:ARG:NH1	2.36	0.59
4:E:340:SER:HB3	4:E:347:ALA:HB2	1.85	0.59
6:H:91:PHE:HE1	6:H:96:PHE:HB3	1.68	0.59
1:A:281:ARG:HG3	1:A:295:ALA:O	2.03	0.59
8:N:43:ILE:HG23	8:N:46:THR:HB	1.85	0.59
4:F:106:ARG:NH1	4:F:106:ARG:HB3	2.18	0.59
10:U:88:GLN:O	10:U:89:VAL:C	2.41	0.59
6:H:99:GLU:OE2	6:H:137:LEU:HD13	2.03	0.59
6:H:16:LEU:HD11	6:H:90:ALA:HB2	1.85	0.59
4:E:140:VAL:HG11	4:E:348:VAL:HB	1.85	0.58
6:H:35:LYS:HB2	6:H:51:GLN:HG3	1.85	0.58
9:T:177:VAL:O	9:T:181:VAL:HG23	2.03	0.58
5:G:144:ALA:HB1	7:I:11:ALA:HB1	1.85	0.58
9:T:176:TRP:CZ3	11:V:22:LYS:HA	2.39	0.58
2:B:153:LYS:HD3	2:B:438:LEU:HD12	1.85	0.58
6:H:72:GLY:HA3	7:I:14:LEU:HD22	1.86	0.58
8:L:43:ILE:HG23	8:L:46:THR:HB	1.86	0.58
2:B:38:ASP:O	2:B:286:LEU:HD13	2.03	0.58
10:U:12:TRP:CZ3	10:U:31:LYS:HG2	2.39	0.58
11:V:65:GLU:HG2	11:V:68:LYS:CE	2.34	0.58
12:W:98:THR:HG22	12:W:99:PRO:HD3	1.86	0.58
8:P:43:ILE:HG22	8:P:47:VAL:HG23	1.85	0.58
8:P:48:PHE:N	8:P:49:PRO:HD2	2.19	0.58
8:Q:48:PHE:N	8:Q:49:PRO:HD2	2.19	0.58
3:D:125:ALA:CB	11:V:50:MET:CG	2.82	0.58
4:F:106:ARG:HH11	4:F:106:ARG:HB3	1.68	0.58
5:G:23:MET:HG2	5:G:237:MET:HE2	1.86	0.58
8:J:48:PHE:N	8:J:49:PRO:HD2	2.19	0.58
1:A:146:GLU:OE1	1:A:313:LYS:HE2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:212:ARG:HG2	4:E:294:GLU:OE1	2.04	0.58
8:L:48:PHE:N	8:L:49:PRO:HD2	2.19	0.58
8:N:48:PHE:N	8:N:49:PRO:HD2	2.19	0.58
1:A:428:GLN:NE2	1:A:431:LYS:HD2	2.19	0.58
6:H:15:ALA:HB1	6:H:20:THR:HG22	1.86	0.58
6:H:60:MET:HA	6:H:65:SER:HB2	1.86	0.58
5:G:50:LEU:HG	6:H:78:GLN:NE2	2.17	0.58
4:F:102:PRO:HG2	4:F:108:PRO:HA	1.86	0.57
12:W:14:ILE:O	12:W:14:ILE:HD13	2.04	0.57
3:D:163:LYS:NZ	3:D:311:TYR:HA	2.19	0.57
8:O:48:PHE:N	8:O:49:PRO:HD2	2.19	0.57
8:R:48:PHE:N	8:R:49:PRO:HD2	2.19	0.57
1:A:444:VAL:HB	1:A:445:PRO:HD3	1.86	0.57
5:G:78:THR:CG2	5:G:91:LEU:HD23	2.34	0.57
6:H:106:ALA:HA	6:H:130:LEU:HD13	1.86	0.57
1:A:293:ARG:HD3	1:A:339:TYR:CD1	2.40	0.57
2:B:248:ALA:N	2:B:249:PRO:HD2	2.19	0.57
1:A:473:TYR:CE1	10:U:13:VAL:CB	2.87	0.57
3:D:348:VAL:O	3:D:350:PRO:HD3	2.04	0.57
8:K:48:PHE:N	8:K:49:PRO:HD2	2.19	0.57
8:Q:40:ASN:HD21	8:Q:43:ILE:HG12	1.69	0.57
1:A:27:LEU:HD21	9:T:202:LYS:CE	2.08	0.57
3:D:243:PHE:HA	3:D:247:GLU:HB3	1.86	0.57
4:F:162:GLY:O	4:F:166:PHE:HB2	2.05	0.57
6:H:59:VAL:O	6:H:65:SER:HB2	2.04	0.57
5:G:212:TYR:OH	6:H:86:THR:HG22	2.04	0.57
8:M:48:PHE:N	8:M:49:PRO:HD2	2.19	0.57
9:T:110:MET:HG3	10:U:107:SER:OG	2.05	0.57
9:T:118:VAL:HG12	9:T:119:GLN:H	1.69	0.57
9:T:164:MET:HE2	9:T:165:MET:N	2.20	0.57
9:T:191:LYS:HA	9:T:194:ILE:HG12	1.86	0.57
10:U:99:SER:O	10:U:100:CYS:O	2.23	0.57
1:A:68:LEU:HD23	1:A:73:VAL:HG13	1.87	0.57
1:C:481:LEU:HD21	1:C:499:LEU:HB2	1.86	0.57
4:F:178:HIS:CD2	4:F:180:GLY:H	2.23	0.57
6:H:32:LEU:HD12	6:H:32:LEU:O	2.05	0.57
8:S:48:PHE:N	8:S:49:PRO:HD2	2.19	0.57
10:U:108:LYS:HA	10:U:111:ILE:HG22	1.87	0.57
9:T:114:GLN:O	9:T:118:VAL:HG23	2.05	0.57
10:U:24:LYS:HE2	10:U:28:ASN:HD21	1.69	0.57
4:E:199:ARG:HA	4:E:202:LYS:HE2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:ARG:HB3	3:D:127:GLN:HG3	1.87	0.56
8:K:57:LEU:HD22	8:L:55:PHE:CZ	2.40	0.56
1:C:148:VAL:HB	1:C:161:ILE:HB	1.87	0.56
1:A:382:VAL:HG12	1:A:384:ALA:H	1.70	0.56
8:N:4:VAL:HG21	8:O:5:LEU:CD2	2.13	0.56
4:F:187:VAL:HG12	4:F:260:ARG:HB2	1.87	0.56
9:T:203:LEU:CD2	12:W:84:ASN:CG	2.71	0.56
10:U:43:THR:O	10:U:45:PRO:HD3	2.06	0.56
8:P:65:CYS:SG	8:Q:19:LEU:HD12	2.46	0.56
10:U:60:VAL:HG22	10:U:61:ALA:N	2.19	0.56
1:C:273:LEU:HD12	1:C:273:LEU:N	2.20	0.56
1:C:358:LEU:HB2	1:C:366:ALA:HB1	1.88	0.56
1:A:36:VAL:HG23	1:A:41:ALA:HB2	1.88	0.56
2:B:351:GLN:H	2:B:373:VAL:HG13	1.71	0.56
4:F:293:GLN:HE22	4:F:308:GLN:HE22	1.54	0.56
4:E:319:ASP:HA	5:G:260:GLN:HE22	1.71	0.56
6:H:69:PHE:CB	6:H:91:PHE:HD2	2.18	0.56
2:B:184:THR:O	2:B:188:GLN:HG2	2.05	0.56
9:T:198:ILE:HA	9:T:201:LEU:HD12	1.87	0.56
9:T:134:MET:HG2	10:U:41:LEU:CD1	2.36	0.56
9:T:169:GLU:HA	11:V:36:TYR:OH	2.06	0.56
1:A:142:ARG:HG3	1:A:315:SER:CA	2.30	0.56
1:A:177:LYS:HB2	13:A:1511:ATP:O1B	2.05	0.56
1:C:270:TYR:HB2	1:C:273:LEU:HD11	1.88	0.56
4:E:330:ASP:HA	4:E:356:ARG:HD3	1.87	0.56
8:R:57:LEU:HD22	8:S:55:PHE:CZ	2.41	0.56
9:T:187:ALA:O	9:T:188:GLN:C	2.45	0.56
1:A:473:TYR:HE1	10:U:13:VAL:CB	2.20	0.55
2:B:212:ARG:HD3	2:B:237:THR:HG21	1.88	0.55
4:E:27:GLN:O	4:E:29:GLU:HG3	2.06	0.55
5:G:212:TYR:HB2	7:I:10:TYR:HD2	1.71	0.55
1:A:121:GLY:HA2	9:T:160:SER:OG	2.07	0.55
11:V:20:ARG:O	11:V:23:ARG:HG3	2.06	0.55
1:A:212:ARG:HG3	1:A:237:THR:HG21	1.88	0.55
2:B:139:LEU:N	2:B:140:PRO:HD2	2.21	0.55
4:E:86:PRO:HD3	4:E:114:ARG:NH1	2.21	0.55
4:F:85:VAL:HG13	4:F:86:PRO:HD2	1.89	0.55
12:W:109:MET:O	12:W:112:HIS:ND1	2.39	0.55
1:A:301:PHE:HB3	4:E:267:GLU:OE2	2.06	0.55
4:F:220:GLY:N	4:F:232:VAL:HG21	2.22	0.55
4:F:345:TYR:HA	4:F:346:PRO:C	2.26	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:W:32:LEU:HD12	12:W:109:MET:CB	2.36	0.55
12:W:14:ILE:C	12:W:14:ILE:HD13	2.27	0.55
3:D:133:ILE:HA	3:D:357:LEU:CD1	2.36	0.55
8:O:15:SER:HA	8:P:16:THR:OG1	2.07	0.55
10:U:111:ILE:O	10:U:115:GLU:HG3	2.06	0.55
8:L:47:VAL:CG1	8:M:34:ILE:HG23	2.37	0.55
1:C:149:GLN:HG3	1:C:191:TRP:CH2	2.41	0.55
3:D:37:LEU:HD12	3:D:61:THR:HG21	1.89	0.55
4:E:319:ASP:HA	5:G:260:GLN:NE2	2.22	0.55
4:E:33:ILE:O	4:E:34:LEU:HB2	2.07	0.55
3:D:94:ARG:NH2	3:D:106:ARG:HB2	2.22	0.55
1:A:301:PHE:HD2	4:E:229:ARG:HH12	1.54	0.55
4:F:201:MET:HE1	4:F:215:VAL:HG11	1.91	0.55
4:F:257:ASN:HD21	4:F:311:TYR:H	1.54	0.55
8:R:47:VAL:HG11	8:S:34:ILE:HG23	1.88	0.55
11:V:65:GLU:HG2	11:V:68:LYS:HE3	1.89	0.55
4:E:197:LEU:O	4:E:201:MET:HG3	2.07	0.55
4:F:201:MET:HE3	4:F:215:VAL:HG11	1.89	0.55
12:W:12:TYR:HE1	12:W:100:ALA:HB1	1.72	0.55
2:B:283:LEU:O	2:B:287:LEU:HG	2.07	0.55
2:B:68:LEU:HD23	4:F:72:ARG:HG3	1.89	0.55
3:D:90:GLU:HG3	3:D:110:LYS:O	2.06	0.55
4:E:37:LEU:HB2	4:E:48:LEU:HB2	1.89	0.55
5:G:169:PRO:HD3	5:G:228:ALA:HB2	1.89	0.55
1:A:99:VAL:HG21	1:A:251:THR:CG2	2.38	0.54
4:F:90:GLU:HG3	4:F:109:ILE:HG23	1.89	0.54
5:G:244:ALA:O	5:G:248:ILE:HG13	2.07	0.54
8:K:43:ILE:O	8:K:43:ILE:HG23	2.07	0.54
1:C:291:PRO:HB2	1:C:295:ALA:HA	1.89	0.54
5:G:193:SER:HB3	5:G:196:LYS:NZ	2.23	0.54
4:E:316:ASP:OD2	5:G:256:ASN:HB3	2.08	0.54
8:L:65:CYS:SG	8:M:19:LEU:HD12	2.48	0.54
9:T:98:GLN:HG3	9:T:99:ALA:N	2.23	0.54
9:T:201:LEU:HD11	11:V:7:PRO:CB	2.36	0.54
1:C:149:GLN:HG3	1:C:191:TRP:HH2	1.72	0.54
4:F:344:ILE:HD11	4:F:412:ARG:HD3	1.89	0.54
4:F:98:VAL:HG22	4:F:232:VAL:HB	1.90	0.54
11:V:46:LYS:HG3	11:V:47:LEU:N	2.22	0.54
2:B:269:VAL:HG22	2:B:326:LEU:HB2	1.89	0.54
1:C:142:ARG:HB3	1:C:313:LYS:HG3	1.90	0.54
4:E:147:TYR:CD2	4:E:153:ILE:HG12	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:242:TYR:CE1	3:D:246:GLU:HG3	2.43	0.54
6:H:102:LYS:NZ	6:H:133:LEU:HB3	2.22	0.54
9:T:180:ARG:HH12	11:V:21:THR:HG23	1.72	0.54
3:D:421:ALA:HB1	3:D:424:PHE:HD2	1.72	0.54
6:H:11:LYS:HD2	6:H:82:GLN:HE21	1.73	0.54
9:T:116:ALA:CB	9:T:120:LYS:CE	2.78	0.54
1:A:192:ASN:HA	1:A:200:LYS:HG2	1.88	0.54
1:C:109:VAL:O	1:C:117:ILE:HG12	2.07	0.54
1:C:205:TYR:HB3	1:C:233:ILE:CD1	2.38	0.54
1:C:82:ARG:HD3	4:F:34:LEU:HD12	1.90	0.54
9:T:85:LEU:O	9:T:88:GLN:HB3	2.08	0.54
2:B:109:VAL:HG12	2:B:117:ILE:HD11	1.90	0.54
3:D:252:LEU:HD23	3:D:305:THR:HB	1.90	0.54
3:D:382:LYS:HA	3:D:385:GLN:HG2	1.89	0.54
4:E:27:GLN:HA	4:E:57:ASN:OD1	2.08	0.54
5:G:142:GLU:O	5:G:146:ILE:HG13	2.08	0.54
10:U:106:GLN:O	10:U:109:THR:HG22	2.08	0.54
11:V:35:GLU:HA	11:V:38:GLN:OE1	2.08	0.54
1:A:36:VAL:HG12	3:D:53:HIS:HB2	1.90	0.54
2:B:406:ALA:HB2	2:B:412:LEU:HD11	1.90	0.54
4:E:370:VAL:O	4:E:374:VAL:HG23	2.08	0.54
4:E:406:ARG:HH12	4:E:447:GLY:HA2	1.73	0.54
4:F:134:LEU:HD13	4:F:149:ARG:CD	2.38	0.54
4:F:400:ASP:O	4:F:404:VAL:HG23	2.08	0.54
9:T:201:LEU:CD1	11:V:7:PRO:HB3	2.36	0.54
10:U:90:ASP:OD1	10:U:90:ASP:N	2.35	0.54
12:W:23:TYR:CD1	12:W:32:LEU:HD21	2.44	0.53
1:A:106:LEU:HD11	1:A:259:PHE:HZ	1.73	0.53
2:B:278:VAL:O	2:B:281:ARG:HG2	2.08	0.53
2:B:302:TYR:HE2	2:B:306:ARG:HH21	1.55	0.53
4:E:152:LYS:HD2	4:E:152:LYS:N	2.23	0.53
4:E:400:ASP:O	4:E:404:VAL:HG23	2.09	0.53
2:B:152:LEU:CD1	2:B:180:VAL:HG13	2.38	0.53
2:B:450:GLY:HA2	2:B:455:LEU:HD12	1.90	0.53
3:D:162:GLY:O	3:D:166:PHE:HB2	2.08	0.53
5:G:204:ASN:HB3	5:G:207:ARG:HB2	1.90	0.53
10:U:87:ALA:HA	10:U:90:ASP:OD1	2.08	0.53
2:B:426:LEU:O	2:B:430:LEU:HG	2.09	0.53
3:D:71:VAL:O	3:D:74:GLU:HG3	2.09	0.53
5:G:83:LEU:O	5:G:233:ARG:HG3	2.09	0.53
8:N:43:ILE:HG22	8:N:47:VAL:HG23	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:GLY:N	11:V:51:TYR:OH	2.42	0.53
1:C:242:ALA:HB3	1:C:243:PRO:HD3	1.91	0.53
4:E:96:ILE:HB	4:E:218:VAL:HG22	1.90	0.53
8:N:4:VAL:CG2	8:O:5:LEU:HD23	2.13	0.53
12:W:31:LYS:O	12:W:34:GLN:N	2.41	0.53
1:C:272:ASP:HB2	1:C:328:VAL:O	2.08	0.53
3:D:400:ASP:O	3:D:404:VAL:HG23	2.09	0.53
8:N:15:SER:HA	8:O:16:THR:OG1	2.09	0.53
9:T:90:ILE:CG2	9:T:91:ALA:N	2.71	0.53
1:A:368:ASN:ND2	1:A:371:LEU:HG	2.24	0.53
1:C:182:LEU:HD13	1:C:218:LEU:HD11	1.91	0.53
3:D:46:LEU:HD23	3:D:70:LEU:HD21	1.91	0.53
4:F:85:VAL:HG21	4:F:235:THR:HG23	1.89	0.53
9:T:134:MET:HG2	10:U:41:LEU:HD11	1.90	0.53
12:W:60:VAL:HG11	12:W:65:LYS:CA	2.39	0.53
1:A:67:ASN:ND2	1:A:287:LEU:HD13	2.24	0.53
1:C:302:TYR:O	1:C:306:ARG:HG2	2.09	0.53
4:F:258:ILE:HD11	4:F:292:LEU:CD2	2.39	0.53
8:L:47:VAL:HG22	8:M:37:VAL:HG21	1.90	0.53
8:M:65:CYS:SG	8:N:19:LEU:HD12	2.49	0.53
12:W:78:PHE:CD1	12:W:82:THR:CG2	2.92	0.53
1:C:64:MET:CE	1:C:97:VAL:HG21	2.39	0.53
3:D:234:LEU:HD23	3:D:292:LEU:HD13	1.91	0.53
2:B:309:GLU:HG3	4:F:223:ASN:HB3	1.91	0.53
2:B:253:ALA:HB3	2:B:310:ARG:NH2	2.24	0.53
1:C:168:LEU:HA	1:C:327:PRO:HG2	1.91	0.53
1:C:296:TYR:CD2	1:C:340:ILE:HD11	2.44	0.53
9:T:81:PHE:CG	9:T:82:ALA:N	2.78	0.53
4:E:95:ILE:HD11	4:E:198:TYR:CD1	2.44	0.52
1:A:159:VAL:CG1	1:A:374:SER:HB2	2.39	0.52
1:C:217:GLN:NE2	4:F:356:ARG:HD2	2.23	0.52
3:D:339:ILE:HB	3:D:347:ALA:HB1	1.91	0.52
2:B:40:ILE:HG12	2:B:41:ALA:N	2.25	0.52
4:E:37:LEU:N	4:E:37:LEU:HD12	2.25	0.52
4:F:148:ALA:HB2	4:F:357:LEU:HD11	1.92	0.52
5:G:12:SER:O	5:G:16:ILE:HG13	2.10	0.52
9:T:110:MET:SD	10:U:110:ARG:NH1	2.82	0.52
12:W:23:TYR:CE1	12:W:32:LEU:HD21	2.44	0.52
1:C:260:ARG:O	1:C:321:GLY:HA3	2.09	0.52
1:C:34:LEU:HD11	1:C:44:PHE:HB2	1.92	0.52
1:C:360:TYR:HE1	4:F:354:LYS:HZ1	1.61	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:143:SER:HB2	4:F:196:ASP:OD1	2.10	0.52
4:F:19:ALA:O	4:F:20:ILE:HD13	2.10	0.52
9:T:118:VAL:O	9:T:119:GLN:O	2.27	0.52
10:U:88:GLN:CD	10:U:88:GLN:H	2.13	0.52
9:T:201:LEU:HD12	11:V:7:PRO:CB	2.35	0.52
12:W:35:VAL:CG1	12:W:81:LEU:HB3	2.40	0.52
1:A:239:SER:HB3	3:D:294:GLU:CG	2.38	0.52
1:A:272:ASP:OD2	1:A:274:SER:HB2	2.10	0.52
2:B:455:LEU:HA	2:B:458:ILE:HD12	1.92	0.52
1:C:273:LEU:HD23	1:C:304:HIS:ND1	2.25	0.52
1:C:381:GLN:NE2	1:C:386:LYS:HA	2.25	0.52
1:C:67:ASN:ND2	1:C:287:LEU:HD13	2.25	0.52
4:E:140:VAL:HG22	4:E:414:LEU:HB3	1.91	0.52
2:B:209:GLY:HA2	2:B:245:GLN:NE2	2.25	0.52
4:E:208:ASN:ND2	4:E:211:GLY:H	2.08	0.52
4:E:404:VAL:O	4:E:408:ARG:HG3	2.10	0.52
4:F:321:ALA:HB3	4:F:322:PRO:CD	2.40	0.52
8:P:4:VAL:HA	8:Q:6:ALA:HB2	1.92	0.52
9:T:172:HIS:O	9:T:176:TRP:HB2	2.09	0.52
12:W:78:PHE:HB3	12:W:82:THR:HB	1.92	0.52
1:A:99:VAL:HG23	1:A:100:PRO:HD2	1.92	0.52
1:A:470:PHE:O	1:A:474:LEU:HD13	2.10	0.52
4:F:53:HIS:ND1	4:F:59:VAL:HG12	2.25	0.52
6:H:100:ASN:O	6:H:104:LEU:HG	2.10	0.52
1:A:472:SER:OG	10:U:31:LYS:CE	2.57	0.52
1:C:253:ALA:O	1:C:257:GLU:HG3	2.10	0.52
1:C:272:ASP:OD2	1:C:274:SER:HB2	2.09	0.52
4:F:348:VAL:O	4:F:350:PRO:HD3	2.10	0.52
11:V:22:LYS:HD2	11:V:30:VAL:HG21	1.92	0.52
12:W:107:THR:O	12:W:111:VAL:HG23	2.09	0.52
1:C:274:SER:OG	1:C:329:ILE:HG23	2.10	0.52
1:C:160:PRO:HG3	1:C:381:GLN:HB2	1.91	0.52
1:C:439:ALA:O	1:C:443:GLN:HG3	2.10	0.52
12:W:19:ALA:HB1	12:W:105:PHE:CD2	2.44	0.52
1:A:27:LEU:HD22	9:T:202:LYS:HZ1	2.11	0.52
3:D:290:GLY:O	3:D:294:GLU:HG2	2.10	0.52
4:F:388:ILE:CD1	4:F:396:LEU:HD11	2.40	0.52
12:W:20:THR:HG23	12:W:108:MET:HB3	1.92	0.51
1:A:65:ALA:HB2	1:A:75:ILE:HG12	1.91	0.51
4:F:140:VAL:HG12	4:F:414:LEU:HB3	1.93	0.51
5:G:253:ILE:HG22	5:G:257:ARG:NH1	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:T:137:GLU:HG3	10:U:5:LEU:HD11	1.92	0.51
3:D:169:GLU:OE1	3:D:418:PHE:HB3	2.11	0.51
4:F:370:VAL:O	4:F:374:VAL:HG23	2.11	0.51
4:E:276:PRO:HB2	5:G:267:LEU:HD21	1.92	0.51
8:J:61:THR:HG21	8:K:23:GLY:N	2.25	0.51
8:K:47:VAL:CG1	8:L:34:ILE:HG23	2.41	0.51
9:T:108:ILE:HG23	9:T:112:LYS:HE3	1.92	0.51
2:B:236:ALA:HA	2:B:240:GLU:OE1	2.11	0.51
1:C:166:ARG:HG2	1:C:348:THR:HA	1.92	0.51
8:P:15:SER:HA	8:Q:16:THR:OG1	2.11	0.51
11:V:65:GLU:HG2	11:V:68:LYS:NZ	2.26	0.51
1:A:139:LEU:HB3	1:A:140:PRO:HD3	1.92	0.51
1:A:212:ARG:HG2	1:A:237:THR:HG21	1.91	0.51
1:A:250:PHE:CD1	1:A:307:LEU:HD13	2.46	0.51
4:F:187:VAL:HG22	4:F:232:VAL:HG13	1.91	0.51
5:G:91:LEU:HD11	5:G:165:PHE:HB3	1.93	0.51
5:G:188:ILE:HD13	5:G:209:LEU:HD23	1.93	0.51
9:T:119:GLN:O	9:T:120:LYS:C	2.48	0.51
3:D:132:GLU:OE1	3:D:149:ARG:HG2	2.11	0.51
3:D:229:ARG:NH2	3:D:267:GLU:OE1	2.43	0.51
3:D:358:LEU:O	3:D:358:LEU:HG	2.11	0.51
4:E:204:THR:HG23	4:E:206:VAL:H	1.76	0.51
4:E:406:ARG:HH12	4:E:447:GLY:CA	2.24	0.51
4:F:141:VAL:HG11	4:F:147:TYR:CE2	2.45	0.51
6:H:97:SER:HA	7:I:25:LEU:HA	1.93	0.51
8:O:43:ILE:HG23	8:O:46:THR:HB	1.94	0.51
8:P:57:LEU:HD22	8:Q:55:PHE:CZ	2.45	0.51
9:T:189:GLN:HA	9:T:192:GLU:OE2	2.11	0.51
13:A:1511:ATP:O2B	13:A:1511:ATP:O2G	2.29	0.51
4:F:393:MET:HA	4:F:396:LEU:HG	1.93	0.51
8:Q:65:CYS:SG	8:R:19:LEU:HD12	2.51	0.51
8:S:43:ILE:CG2	8:S:46:THR:HB	2.41	0.51
10:U:99:SER:O	10:U:100:CYS:C	2.50	0.51
11:V:61:ASN:OD1	11:V:61:ASN:N	2.44	0.51
1:A:205:TYR:CE2	1:A:218:LEU:HD13	2.46	0.51
1:A:30:THR:HB	1:A:89:LEU:HD11	1.94	0.51
1:C:294:GLU:O	1:C:295:ALA:HB3	2.11	0.51
3:D:39:ILE:HG23	3:D:46:LEU:HB3	1.93	0.51
4:E:167:ILE:HG23	4:E:254:PHE:CE2	2.46	0.51
5:G:112:ASP:OD1	5:G:115:LYS:HE3	2.11	0.51
8:N:4:VAL:HA	8:O:6:ALA:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:S:43:ILE:HG23	8:S:46:THR:HB	1.93	0.51
11:V:22:LYS:HZ2	11:V:30:VAL:HG22	1.76	0.51
1:A:381:GLN:NE2	1:A:386:LYS:HA	2.26	0.50
4:F:324:THR:O	4:F:324:THR:HG22	2.11	0.50
2:B:382:VAL:HG12	2:B:384:ALA:H	1.77	0.50
1:C:397:ALA:HA	1:C:400:ARG:NH2	2.26	0.50
4:F:46:LEU:C	4:F:46:LEU:HD23	2.32	0.50
6:H:39:ILE:HG13	6:H:50:GLU:OE1	2.12	0.50
10:U:86:THR:O	10:U:86:THR:HG22	2.11	0.50
9:T:201:LEU:HD11	11:V:7:PRO:HB3	1.93	0.50
12:W:20:THR:HG23	12:W:108:MET:CB	2.42	0.50
4:E:133:ILE:HG13	4:E:363:VAL:HG12	1.94	0.50
4:F:33:ILE:HA	4:F:50:VAL:CG1	2.41	0.50
5:G:59:ASN:HD22	5:G:183:PHE:HE1	1.59	0.50
7:I:48:LYS:CB	7:I:52:ALA:HB3	2.41	0.50
9:T:197:CYS:SG	12:W:28:LYS:NZ	2.85	0.50
1:A:40:ILE:HD13	1:A:287:LEU:CD2	2.41	0.50
1:A:68:LEU:O	4:E:15:ALA:HA	2.11	0.50
3:D:65:ASP:CG	3:D:66:GLY:H	2.15	0.50
4:E:208:ASN:HD22	4:E:211:GLY:HA3	1.76	0.50
4:F:67:THR:HB	4:F:70:LEU:HD12	1.93	0.50
8:N:43:ILE:CG2	8:N:46:THR:HB	2.41	0.50
3:D:237:LEU:HD21	3:D:295:ARG:HB2	1.94	0.50
4:E:237:LEU:HD21	4:E:295:ARG:HB2	1.94	0.50
4:F:225:PRO:HB3	4:F:226:PRO:HD2	1.94	0.50
4:F:442:LYS:O	4:F:446:GLU:HG3	2.11	0.50
4:F:54:LEU:HD21	4:F:60:ARG:HE	1.77	0.50
8:L:15:SER:HA	8:M:16:THR:OG1	2.12	0.50
12:W:73:THR:HA	12:W:78:PHE:HD2	1.77	0.50
1:A:67:ASN:HD22	1:A:287:LEU:HD22	1.77	0.50
3:D:18:GLY:O	3:D:67:THR:HG21	2.12	0.50
3:D:258:ILE:HG13	3:D:258:ILE:O	2.12	0.50
4:E:96:ILE:O	4:E:218:VAL:HA	2.12	0.50
1:A:306:ARG:HG2	1:A:306:ARG:O	2.12	0.50
2:B:480:GLU:O	2:B:484:GLU:HG2	2.12	0.50
4:E:168:GLN:NE2	4:E:201:MET:HG2	2.22	0.50
8:P:43:ILE:HG23	8:P:46:THR:HB	1.93	0.50
1:A:444:VAL:HG11	1:A:491:LEU:HD11	1.94	0.50
1:C:77:LEU:HD12	1:C:81:ASP:HB3	1.94	0.50
4:E:153:ILE:N	4:E:153:ILE:HD12	2.27	0.50
4:F:278:ALA:O	4:F:279:VAL:HB	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:T:117:LEU:N	9:T:117:LEU:CD2	2.72	0.50
9:T:193:THR:C	9:T:195:ALA:H	2.15	0.50
12:W:14:ILE:HG23	12:W:15:GLU:N	2.27	0.50
2:B:300:VAL:HG11	2:B:339:TYR:HE2	1.77	0.49
2:B:70:PRO:HD3	4:F:15:ALA:HB2	1.93	0.49
1:C:64:MET:HE2	1:C:97:VAL:HG21	1.93	0.49
4:E:334:VAL:HG21	4:E:352:ASP:HB3	1.94	0.49
4:F:188:GLY:HA2	4:F:222:MET:N	2.27	0.49
1:C:282:GLN:CD	4:F:284:THR:HG22	2.33	0.49
8:Q:43:ILE:HG22	8:Q:47:VAL:HG23	1.93	0.49
9:T:87:GLU:O	9:T:90:ILE:HG22	2.12	0.49
9:T:180:ARG:CZ	11:V:21:THR:CG2	2.90	0.49
2:B:217:GLN:NE2	4:E:131:ALA:CB	2.70	0.49
3:D:50:VAL:HA	3:D:61:THR:HG22	1.94	0.49
1:C:408:PHE:CD2	1:C:410:SER:HB2	2.47	0.49
3:D:393:MET:SD	3:D:396:LEU:HD12	2.53	0.49
4:F:279:VAL:HG12	4:F:279:VAL:O	2.12	0.49
1:A:105:LEU:HD12	1:A:255:ILE:HG23	1.95	0.49
1:A:43:VAL:HG11	1:A:90:VAL:CG1	2.42	0.49
2:B:146:GLU:HB2	2:B:163:ARG:HB2	1.94	0.49
4:F:287:THR:O	4:F:290:GLY:N	2.46	0.49
9:T:174:ILE:O	9:T:177:VAL:HB	2.13	0.49
10:U:96:ASP:OD1	10:U:96:ASP:N	2.44	0.49
2:B:170:ILE:HD11	2:B:331:THR:HG21	1.94	0.49
1:C:53:GLU:OE2	1:C:92:ARG:HD2	2.12	0.49
3:D:237:LEU:HD13	3:D:296:ILE:HG12	1.94	0.49
4:E:168:GLN:HB3	4:E:206:VAL:HG11	1.95	0.49
5:G:56:GLU:O	5:G:191:SER:HB3	2.12	0.49
11:V:58:THR:HG22	11:V:59:PHE:O	2.13	0.49
1:A:100:PRO:HD3	1:A:128:ARG:NH1	2.27	0.49
1:A:170:ILE:HD12	1:A:345:ILE:HD11	1.94	0.49
1:C:191:TRP:O	1:C:200:LYS:HG2	2.13	0.49
1:A:217:GLN:HG2	3:D:356:ARG:NH1	2.27	0.49
4:E:72:ARG:HH11	4:E:72:ARG:HG3	1.77	0.49
5:G:135:LYS:NZ	7:I:41:ASP:HB2	2.28	0.49
5:G:207:ARG:HB3	7:I:4:ARG:HH21	1.78	0.49
9:T:141:ARG:NH1	10:U:41:LEU:HD23	2.27	0.49
1:A:395:PHE:HE2	1:A:451:VAL:HG13	1.78	0.49
1:A:96:ILE:HG21	4:E:68:GLU:OE2	2.13	0.49
2:B:405:PHE:CZ	4:F:393:MET:SD	3.06	0.49
4:F:258:ILE:HD11	4:F:292:LEU:HD21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:T:191:LYS:HD3	9:T:194:ILE:HD11	1.94	0.49
3:D:197:LEU:O	3:D:201:MET:HG2	2.12	0.49
3:D:222:MET:HA	3:D:229:ARG:HD3	1.94	0.49
3:D:359:ASP:O	3:D:363:VAL:HG22	2.13	0.49
4:F:334:VAL:HG21	4:F:352:ASP:OD2	2.13	0.49
8:J:47:VAL:HG11	8:K:34:ILE:HG23	1.94	0.49
12:W:73:THR:HG22	12:W:78:PHE:HB3	1.94	0.49
3:D:78:ASP:OD1	3:D:80:GLY:N	2.46	0.49
4:E:158:GLY:O	4:E:161:VAL:HG22	2.13	0.49
4:E:256:ASP:HA	4:E:257:ASN:HA	1.57	0.49
4:F:24:HIS:ND1	4:F:57:ASN:O	2.46	0.49
1:A:408:PHE:HE2	5:G:22:THR:HG1	1.65	0.49
5:G:78:THR:HG21	5:G:114:ILE:HB	1.95	0.49
6:H:69:PHE:HB2	6:H:91:PHE:HD2	1.78	0.49
12:W:11:ILE:C	12:W:12:TYR:CD1	2.86	0.49
12:W:45:ILE:HG21	12:W:72:MET:HE1	1.96	0.49
1:A:109:VAL:O	1:A:117:ILE:HG12	2.13	0.49
4:E:311:TYR:O	4:E:313:PRO:HD3	2.13	0.49
4:F:157:GLY:HA3	4:F:161:VAL:HG21	1.95	0.49
8:M:47:VAL:CG1	8:N:34:ILE:HG23	2.43	0.49
1:C:165:GLN:OE1	1:C:376:VAL:HG21	2.13	0.48
1:C:68:LEU:HB3	3:D:72:ARG:HD3	1.95	0.48
4:E:266:SER:HA	4:E:282:GLN:OE1	2.13	0.48
2:B:169:ILE:HG21	2:B:177:LYS:O	2.13	0.48
1:C:236:ALA:HA	1:C:240:GLU:OE1	2.14	0.48
1:C:421:VAL:HG13	1:C:425:ARG:NH1	2.28	0.48
1:C:387:GLN:OE1	1:C:491:LEU:HB2	2.14	0.48
3:D:71:VAL:H	3:D:74:GLU:CD	2.16	0.48
8:L:40:ASN:HD21	8:L:43:ILE:HG12	1.78	0.48
1:A:46:LEU:HD13	1:A:49:ILE:HD12	1.95	0.48
2:B:345:ILE:HG23	2:B:351:GLN:CD	2.34	0.48
2:B:350:GLY:HA2	2:B:373:VAL:HG13	1.94	0.48
3:D:374:VAL:HG13	3:D:410:ILE:HG21	1.95	0.48
4:E:402:LEU:HG	4:E:406:ARG:NE	2.29	0.48
4:E:410:ILE:O	4:E:414:LEU:HG	2.13	0.48
5:G:247:MET:HA	5:G:250:ARG:HE	1.78	0.48
5:G:262:VAL:O	5:G:266:GLU:HG2	2.13	0.48
8:Q:43:ILE:CG2	8:Q:46:THR:HB	2.43	0.48
1:A:411:ASP:O	5:G:29:THR:HG21	2.13	0.48
3:D:169:GLU:HG2	3:D:418:PHE:CD1	2.49	0.48
3:D:54:LEU:HD11	3:D:60:ARG:HH21	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:427:ILE:HD12	4:E:427:ILE:N	2.29	0.48
11:V:22:LYS:HD2	11:V:30:VAL:CG2	2.43	0.48
2:B:273:LEU:HB3	2:B:304:HIS:CD2	2.49	0.48
1:C:270:TYR:CB	1:C:273:LEU:HD11	2.43	0.48
4:E:174:ILE:HG13	4:E:252:LEU:HD21	1.96	0.48
1:A:476:SER:HB3	10:U:11:ASP:CA	2.43	0.48
4:F:242:TYR:CZ	4:F:246:GLU:HG2	2.49	0.48
5:G:31:LEU:O	5:G:35:GLU:HG2	2.14	0.48
8:S:43:ILE:HG22	8:S:47:VAL:HG23	1.95	0.48
10:U:7:LEU:O	10:U:8:LYS:C	2.52	0.48
1:A:473:TYR:CD1	10:U:13:VAL:CG1	2.97	0.48
1:A:99:VAL:HG11	1:A:251:THR:HG23	1.96	0.48
2:B:400:ARG:HH22	4:F:341:GLU:CD	2.17	0.48
4:F:408:ARG:O	4:F:412:ARG:HG2	2.14	0.48
6:H:108:ALA:O	6:H:112:VAL:HG23	2.13	0.48
8:L:61:THR:HG21	8:M:23:GLY:N	2.29	0.48
4:E:176:LYS:HZ1	4:E:214:LYS:HE2	1.84	0.48
4:E:374:VAL:HG13	4:E:410:ILE:HG21	1.95	0.48
5:G:118:LEU:HA	5:G:121:THR:HG22	1.95	0.48
12:W:106:SER:O	12:W:109:MET:HE3	2.17	0.48
1:A:329:ILE:HD11	1:A:344:VAL:HG21	1.96	0.48
1:C:97:VAL:HG11	1:C:247:LEU:HD21	1.95	0.48
3:D:258:ILE:HG21	3:D:310:VAL:HG22	1.96	0.48
10:U:122:ARG:O	10:U:122:ARG:HG2	2.14	0.48
11:V:6:ASP:H	11:V:7:PRO:HD2	1.78	0.48
1:C:278:VAL:HG13	1:C:281:ARG:NH2	2.30	0.47
4:E:185:THR:HG21	4:E:233:ALA:HA	1.96	0.47
4:E:432:VAL:HG22	4:E:461:GLY:O	2.14	0.47
6:H:105:LEU:HB3	6:H:109:LYS:HE3	1.96	0.47
8:K:8:LYS:HD3	8:K:76:VAL:HG21	1.96	0.47
8:Q:43:ILE:HG23	8:Q:46:THR:HB	1.96	0.47
9:T:99:ALA:HB1	9:T:103:GLN:NE2	2.28	0.47
12:W:23:TYR:O	12:W:23:TYR:CD1	2.67	0.47
2:B:37:GLY:O	2:B:40:ILE:HG22	2.14	0.47
3:D:234:LEU:CD2	3:D:292:LEU:HD13	2.44	0.47
4:F:366:GLU:O	4:F:370:VAL:HG23	2.14	0.47
5:G:10:LEU:HG	5:G:14:LYS:HE3	1.96	0.47
8:J:8:LYS:HD3	8:J:76:VAL:HG21	1.96	0.47
1:A:149:GLN:NE2	1:A:440:THR:OG1	2.42	0.47
1:A:478:HIS:HB3	1:A:481:LEU:HD12	1.96	0.47
2:B:238:ALA:HA	2:B:245:GLN:NE2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:VAL:HG22	1:C:43:VAL:HG22	1.96	0.47
4:E:33:ILE:HG22	4:E:34:LEU:HG	1.97	0.47
8:Q:8:LYS:HD3	8:Q:76:VAL:HG21	1.97	0.47
8:R:8:LYS:HD3	8:R:76:VAL:HG21	1.97	0.47
10:U:96:ASP:O	10:U:97:VAL:C	2.52	0.47
2:B:173:ARG:HH12	4:E:326:PHE:HD2	1.62	0.47
3:D:257:ASN:HD22	3:D:259:PHE:HB3	1.79	0.47
4:E:39:ILE:HB	4:E:46:LEU:HB3	1.96	0.47
6:H:69:PHE:HB3	6:H:91:PHE:HD2	1.80	0.47
8:J:15:SER:HA	8:K:16:THR:OG1	2.15	0.47
8:L:8:LYS:HD3	8:L:76:VAL:HG21	1.96	0.47
8:S:8:LYS:HD3	8:S:76:VAL:HG21	1.97	0.47
10:U:21:ARG:C	10:U:23:GLN:H	2.17	0.47
3:D:196:ASP:O	3:D:200:GLU:HG2	2.15	0.47
3:D:346:PRO:O	3:D:348:VAL:N	2.48	0.47
4:E:38:GLU:OE1	4:E:45:LYS:HD2	2.14	0.47
4:F:182:SER:HB2	4:F:215:VAL:HB	1.96	0.47
12:W:32:LEU:O	12:W:36:GLU:CB	2.63	0.47
12:W:73:THR:HA	12:W:78:PHE:HB2	1.96	0.47
1:A:336:VAL:HG11	1:A:353:PHE:HE2	1.80	0.47
2:B:212:ARG:HB3	4:E:127:GLN:HG3	1.96	0.47
4:E:456:ALA:O	4:E:466:VAL:HG13	2.15	0.47
6:H:101:ILE:HG21	7:I:25:LEU:O	2.15	0.47
8:P:8:LYS:HD3	8:P:76:VAL:HG21	1.97	0.47
9:T:168:LYS:O	9:T:169:GLU:C	2.48	0.47
1:A:341:PRO:O	1:A:345:ILE:HG13	2.15	0.47
2:B:149:GLN:HB2	2:B:191:TRP:HH2	1.79	0.47
1:C:141:ARG:HB2	3:D:195:ASN:CG	2.35	0.47
3:D:145:ALA:CB	3:D:355:SER:HB2	2.44	0.47
3:D:8:PRO:HB2	3:D:77:LEU:HD11	1.96	0.47
5:G:205:VAL:HB	5:G:206:PRO:HD3	1.97	0.47
8:O:8:LYS:HD3	8:O:76:VAL:HG21	1.96	0.47
1:A:122:PRO:HD2	9:T:159:ILE:CB	2.37	0.47
2:B:364:ARG:HA	2:B:365:PRO:C	2.35	0.47
3:D:319:ASP:O	3:D:322:PRO:HD2	2.15	0.47
12:W:79:SER:O	12:W:83:SER:HB3	2.15	0.47
13:A:1511:ATP:O2B	13:A:1511:ATP:O2A	2.33	0.47
1:A:105:LEU:HD13	1:A:255:ILE:HD13	1.97	0.47
2:B:97:VAL:HG11	2:B:247:LEU:HD21	1.97	0.47
1:C:59:SER:OG	1:C:83:LEU:HB3	2.15	0.47
4:E:402:LEU:HD21	4:E:406:ARG:HH21	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:LYS:NZ	1:C:113:LEU:HD13	2.30	0.47
1:C:274:SER:O	1:C:278:VAL:HG23	2.15	0.47
3:D:133:ILE:HA	3:D:357:LEU:HD13	1.97	0.47
4:E:381:TYR:O	4:E:385:GLN:HG2	2.15	0.47
4:F:190:ARG:HB2	4:F:193:GLU:HG3	1.97	0.47
8:M:47:VAL:HG11	8:N:34:ILE:HG23	1.97	0.47
1:A:506:PHE:HA	1:A:509:THR:HG22	1.97	0.47
4:E:255:ILE:HB	4:E:308:GLN:HB3	1.96	0.47
8:N:8:LYS:HD3	8:N:76:VAL:HG21	1.97	0.47
8:O:43:ILE:CG2	8:O:46:THR:HB	2.45	0.47
8:O:43:ILE:HG22	8:O:47:VAL:HG23	1.97	0.47
9:T:90:ILE:CG2	9:T:91:ALA:H	2.28	0.47
1:A:473:TYR:HD1	10:U:13:VAL:HB	1.77	0.47
2:B:133:VAL:O	2:B:310:ARG:HD3	2.16	0.46
4:E:6:SER:C	4:E:8:PRO:HD3	2.35	0.46
8:M:8:LYS:HD3	8:M:76:VAL:HG21	1.97	0.46
1:A:212:ARG:HH12	1:A:239:SER:HG	1.63	0.46
1:A:242:ALA:HB3	1:A:243:PRO:HD3	1.97	0.46
1:A:356:ALA:O	1:A:359:PHE:HB3	2.15	0.46
4:E:397:SER:O	4:E:401:LYS:HG2	2.15	0.46
4:F:257:ASN:HD22	4:F:259:PHE:HB3	1.79	0.46
6:H:91:PHE:CE1	6:H:97:SER:HB3	2.51	0.46
12:W:23:TYR:HB2	12:W:105:PHE:CZ	2.51	0.46
2:B:66:LEU:HD11	2:B:67:ASN:HD22	1.81	0.46
4:E:252:LEU:N	4:E:252:LEU:HD12	2.30	0.46
4:F:163:LYS:O	4:F:167:ILE:HG13	2.16	0.46
4:F:37:LEU:O	4:F:47:VAL:HA	2.15	0.46
12:W:23:TYR:CB	12:W:105:PHE:CE2	2.98	0.46
12:W:73:THR:CG2	12:W:78:PHE:HB2	2.44	0.46
1:A:106:LEU:HD11	1:A:259:PHE:CZ	2.51	0.46
1:A:402:VAL:HG12	1:A:402:VAL:O	2.16	0.46
1:A:43:VAL:HG12	1:A:44:PHE:N	2.31	0.46
2:B:105:LEU:HD22	2:B:255:ILE:HG23	1.98	0.46
3:D:25:PHE:HB2	3:D:30:LEU:HD23	1.98	0.46
4:F:85:VAL:HG22	4:F:100:GLY:HA3	1.98	0.46
4:F:90:GLU:HG2	4:F:110:LYS:O	2.16	0.46
4:F:33:ILE:HA	4:F:50:VAL:HG11	1.98	0.46
8:M:15:SER:HA	8:N:16:THR:OG1	2.16	0.46
9:T:203:LEU:O	9:T:207:LYS:HG3	2.15	0.46
12:W:26:ALA:CB	12:W:35:VAL:HG21	2.46	0.46
12:W:31:LYS:C	12:W:35:VAL:HG23	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:ASN:ND2	11:V:8:VAL:CG2	2.77	0.46
2:B:99:VAL:HG11	2:B:251:THR:HB	1.97	0.46
1:C:283:LEU:O	1:C:287:LEU:HG	2.16	0.46
1:C:392:LEU:HD13	1:C:451:VAL:HG12	1.97	0.46
4:F:93:GLY:O	4:F:94:ARG:HD2	2.16	0.46
5:G:55:ALA:O	5:G:57:THR:HG23	2.15	0.46
10:U:40:ARG:CZ	10:U:44:LEU:HG	2.45	0.46
1:A:142:ARG:CG	1:A:315:SER:HA	2.34	0.46
1:C:116:PRO:HB3	1:C:123:ILE:HD11	1.97	0.46
1:C:492:SER:H	1:C:495:LEU:HD12	1.81	0.46
4:E:287:THR:O	4:E:291:LEU:HG	2.16	0.46
4:F:188:GLY:HA3	4:F:260:ARG:HG3	1.98	0.46
4:F:191:THR:HA	4:F:221:GLN:HE21	1.81	0.46
5:G:108:VAL:CG1	5:G:128:LEU:HB3	2.45	0.46
8:O:14:ILE:HG21	8:P:14:ILE:HG12	1.98	0.46
12:W:98:THR:CG2	12:W:99:PRO:HD3	2.45	0.46
2:B:185:ILE:HG12	2:B:203:CYS:SG	2.56	0.46
4:F:237:LEU:HD13	4:F:296:ILE:HG12	1.98	0.46
2:B:54:LEU:HD11	2:B:62:LYS:HB3	1.98	0.46
3:D:41:THR:HB	3:D:42:PRO:HD2	1.98	0.46
4:E:281:TYR:CE2	4:E:321:ALA:HB2	2.51	0.46
4:F:204:THR:OG1	4:F:206:VAL:HG23	2.16	0.46
4:F:238:THR:HA	4:F:241:GLU:OE2	2.15	0.46
8:N:20:LEU:HB2	8:O:20:LEU:HD22	1.98	0.46
12:W:86:ILE:HG22	12:W:87:ASN:N	2.31	0.46
3:D:255:ILE:HB	3:D:308:GLN:HG2	1.97	0.46
3:D:50:VAL:HG13	3:D:59:VAL:CG1	2.46	0.46
4:F:154:GLY:HA3	4:F:329:LEU:HD13	1.98	0.46
1:A:503:THR:O	1:A:507:VAL:HG23	2.16	0.46
4:F:162:GLY:HA2	15:F:1479:ADP:O1A	2.16	0.46
1:A:55:VAL:HA	1:A:93:THR:HG23	1.98	0.45
2:B:311:ALA:HB1	2:B:323:LEU:O	2.16	0.45
4:E:47:VAL:HG21	4:E:99:ILE:HD12	1.98	0.45
4:F:98:VAL:HG21	4:F:228:ALA:HB1	1.98	0.45
5:G:254:LEU:HG	5:G:257:ARG:HH22	1.81	0.45
5:G:51:PHE:CE1	6:H:49:VAL:HG21	2.52	0.45
11:V:17:ARG:O	11:V:20:ARG:HB2	2.16	0.45
12:W:45:ILE:CG2	12:W:55:LEU:HD11	2.46	0.45
1:A:112:ALA:O	1:A:251:THR:HG21	2.16	0.45
1:A:417:LYS:O	1:A:421:VAL:HG23	2.17	0.45
2:B:28:ASN:HB3	2:B:48:ASN:ND2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:ILE:HD12	1:C:287:LEU:CD2	2.46	0.45
4:F:140:VAL:CG1	4:F:414:LEU:HB3	2.47	0.45
4:F:140:VAL:CG2	4:F:348:VAL:HG21	2.45	0.45
4:F:48:LEU:HD23	4:F:63:ALA:HA	1.99	0.45
8:K:65:CYS:SG	8:L:19:LEU:HD12	2.57	0.45
8:O:20:LEU:HB2	8:P:20:LEU:HD22	1.99	0.45
12:W:20:THR:CG2	12:W:108:MET:HB3	2.46	0.45
2:B:412:LEU:HB3	2:B:416:THR:OG1	2.16	0.45
4:E:94:ARG:NH1	4:E:109:ILE:HG12	2.31	0.45
5:G:13:ILE:HD13	5:G:247:MET:HE3	1.97	0.45
5:G:75:VAL:HB	5:G:164:ILE:HD13	1.98	0.45
5:G:50:LEU:HD23	6:H:84:CYS:SG	2.57	0.45
6:H:91:PHE:HE1	6:H:97:SER:N	2.14	0.45
8:O:40:ASN:HD21	8:O:43:ILE:HG12	1.81	0.45
8:O:7:ALA:HB1	8:P:10:ILE:HG13	1.98	0.45
9:T:119:GLN:CG	9:T:120:LYS:N	2.78	0.45
1:A:242:ALA:N	1:A:243:PRO:CD	2.80	0.45
1:A:27:LEU:CD2	9:T:202:LYS:HE3	2.30	0.45
1:A:96:ILE:HG22	1:A:97:VAL:N	2.31	0.45
1:C:136:PRO:HB2	1:C:141:ARG:HE	1.82	0.45
3:D:357:LEU:HD22	3:D:362:VAL:HG11	1.98	0.45
3:D:165:VAL:HG11	3:D:421:ALA:HB2	1.99	0.45
4:E:228:ALA:O	4:E:232:VAL:HG23	2.17	0.45
8:M:43:ILE:CG2	8:M:47:VAL:HG23	2.45	0.45
12:W:26:ALA:HB1	12:W:35:VAL:HG21	1.99	0.45
12:W:79:SER:N	12:W:80:PRO:CD	2.79	0.45
1:A:52:GLU:HG2	1:A:66:LEU:HD23	1.98	0.45
2:B:279:ALA:O	2:B:282:GLN:HB3	2.17	0.45
2:B:351:GLN:H	2:B:373:VAL:CG1	2.30	0.45
2:B:57:PHE:CD1	2:B:90:VAL:HG22	2.49	0.45
3:D:164:THR:O	3:D:167:ILE:HG22	2.17	0.45
4:E:32:ALA:O	4:E:50:VAL:HG11	2.17	0.45
4:F:123:SER:HB2	4:F:126:GLU:HG3	1.99	0.45
8:Q:40:ASN:ND2	8:Q:43:ILE:HG12	2.32	0.45
9:T:196:LYS:HZ2	12:W:24:SER:HA	1.09	0.45
2:B:215:VAL:O	2:B:219:VAL:HG23	2.17	0.45
2:B:314:LEU:HB3	2:B:318:GLU:HB2	1.99	0.45
2:B:455:LEU:HD23	2:B:458:ILE:HD12	1.98	0.45
1:C:111:ASP:O	1:C:112:ALA:C	2.55	0.45
1:C:168:LEU:HD11	1:C:329:ILE:HG13	1.99	0.45
4:F:156:PHE:HB2	4:F:334:VAL:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:94:ARG:NH2	4:F:102:PRO:HB3	2.32	0.45
1:A:119:GLY:C	11:V:51:TYR:CE1	2.86	0.45
1:A:97:VAL:HG11	1:A:247:LEU:HD13	1.98	0.45
2:B:285:LEU:HD12	4:E:283:PRO:HB3	1.99	0.45
2:B:362:GLY:O	2:B:364:ARG:HG3	2.17	0.45
1:C:240:GLU:HB3	1:C:244:LEU:CD1	2.46	0.45
5:G:75:VAL:HB	5:G:164:ILE:CD1	2.47	0.45
1:A:197:GLU:C	1:A:199:LYS:H	2.20	0.45
1:A:67:ASN:OD1	4:E:17:ILE:HG23	2.17	0.45
2:B:394:LEU:HD11	4:F:425:THR:HG22	1.99	0.45
2:B:28:ASN:HB3	2:B:48:ASN:HD22	1.82	0.45
1:C:216:ALA:O	1:C:219:VAL:HG22	2.17	0.45
3:D:141:VAL:HG11	3:D:147:TYR:CE2	2.52	0.45
9:T:146:ARG:HA	9:T:149:ARG:NH1	2.31	0.45
1:A:139:LEU:HD23	4:E:105:GLU:OE2	2.17	0.45
1:A:284:SER:CB	1:A:297:PRO:HG2	2.47	0.45
2:B:196:ASP:OD2	2:B:199:LYS:HG2	2.17	0.45
2:B:54:LEU:HD13	2:B:97:VAL:HG22	1.99	0.45
4:F:46:LEU:HD23	4:F:47:VAL:N	2.32	0.45
8:S:26:ILE:HD13	8:S:55:PHE:CE1	2.52	0.45
12:W:61:LYS:CB	12:W:64:VAL:HG23	2.46	0.45
1:A:272:ASP:HB2	1:A:328:VAL:O	2.17	0.45
4:E:384:LEU:O	4:E:388:ILE:HG12	2.16	0.45
4:F:384:LEU:O	4:F:388:ILE:HG12	2.17	0.45
8:K:26:ILE:HD13	8:K:55:PHE:CE1	2.52	0.45
12:W:12:TYR:CE1	12:W:100:ALA:HB1	2.52	0.45
12:W:61:LYS:HB3	12:W:64:VAL:HG23	1.99	0.45
2:B:176:GLY:HA2	13:B:1510:ATP:O1A	2.17	0.44
1:C:166:ARG:O	1:C:166:ARG:HG2	2.18	0.44
4:E:244:ARG:O	4:E:248:GLY:HA2	2.17	0.44
8:P:26:ILE:HD13	8:P:55:PHE:CE1	2.53	0.44
11:V:37:GLN:OE1	11:V:40:LEU:HD23	2.18	0.44
12:W:63:SER:C	12:W:66:VAL:HG12	2.38	0.44
12:W:60:VAL:HG11	12:W:65:LYS:HB2	1.98	0.44
1:C:187:ASN:O	1:C:190:ARG:HG3	2.17	0.44
1:C:311:ALA:HB1	1:C:323:LEU:O	2.18	0.44
1:C:408:PHE:HD2	1:C:410:SER:HB2	1.83	0.44
3:D:431:LEU:HD23	3:D:431:LEU:C	2.38	0.44
5:G:38:LYS:HE2	5:G:224:GLN:HG3	1.98	0.44
8:J:26:ILE:HD13	8:J:55:PHE:CE1	2.53	0.44
8:O:26:ILE:HD13	8:O:55:PHE:CE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:TYR:CE2	1:A:218:LEU:CD1	3.01	0.44
1:A:434:GLN:HB2	13:A:1511:ATP:C6	2.52	0.44
3:D:377:THR:HG22	3:D:407:ALA:HB2	2.00	0.44
4:E:282:GLN:NE2	4:E:285:LEU:HD13	2.33	0.44
4:F:256:ASP:HA	4:F:257:ASN:HA	1.59	0.44
8:L:26:ILE:HD13	8:L:55:PHE:CE1	2.53	0.44
8:Q:26:ILE:HD13	8:Q:55:PHE:CE1	2.53	0.44
9:T:116:ALA:C	9:T:120:LYS:HD2	2.38	0.44
9:T:192:GLU:O	9:T:195:ALA:HB3	2.17	0.44
11:V:12:PHE:O	11:V:16:ILE:HG13	2.17	0.44
12:W:39:LEU:CD1	12:W:105:PHE:CD2	3.00	0.44
3:D:256:ASP:HA	3:D:257:ASN:HA	1.62	0.44
4:E:462:GLY:O	4:E:466:VAL:HG23	2.18	0.44
4:E:77:LEU:HD12	4:E:78:ASP:H	1.83	0.44
5:G:99:LEU:HD21	5:G:122:HIS:CG	2.53	0.44
6:H:58:GLU:HB2	6:H:67:LYS:HG3	2.00	0.44
8:J:43:ILE:CG2	8:J:46:THR:HB	2.47	0.44
8:L:47:VAL:HG11	8:M:34:ILE:HG23	2.00	0.44
8:M:26:ILE:HD13	8:M:55:PHE:CE1	2.53	0.44
8:R:26:ILE:HD13	8:R:55:PHE:CE1	2.53	0.44
9:T:88:GLN:O	9:T:92:GLN:HG2	2.18	0.44
10:U:7:LEU:HD23	10:U:7:LEU:HA	1.76	0.44
12:W:45:ILE:HG22	12:W:55:LEU:HD11	2.00	0.44
2:B:260:ARG:O	2:B:321:GLY:HA3	2.18	0.44
2:B:440:THR:O	2:B:444:VAL:HG23	2.18	0.44
8:M:57:LEU:HD22	8:N:55:PHE:CE1	2.53	0.44
8:R:53:LEU:O	8:R:57:LEU:HG	2.18	0.44
1:A:305:SER:HA	1:A:347:ILE:HD13	1.99	0.44
2:B:247:LEU:HG	2:B:251:THR:HG23	2.00	0.44
2:B:168:LEU:HD11	2:B:329:ILE:HG12	2.00	0.44
2:B:392:LEU:O	2:B:396:LEU:HG	2.18	0.44
4:E:65:ASP:CG	4:E:66:GLY:H	2.21	0.44
5:G:212:TYR:CE2	5:G:216:ASN:ND2	2.86	0.44
10:U:86:THR:HG21	10:U:89:VAL:HG23	2.00	0.44
10:U:94:LYS:HD2	10:U:94:LYS:HA	1.71	0.44
12:W:109:MET:O	12:W:112:HIS:CE1	2.71	0.44
12:W:23:TYR:CD1	12:W:23:TYR:C	2.91	0.44
12:W:42:VAL:HG11	12:W:89:LEU:HD13	2.00	0.44
12:W:45:ILE:HG22	12:W:55:LEU:CD1	2.48	0.44
12:W:73:THR:CG2	12:W:78:PHE:CB	2.96	0.44
12:W:31:LYS:HG3	12:W:81:LEU:HD21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:VAL:CG2	1:A:100:PRO:HD2	2.48	0.44
3:D:241:GLU:OE2	3:D:295:ARG:HB3	2.18	0.44
4:E:188:GLY:O	4:E:222:MET:HG2	2.18	0.44
4:E:275:ILE:HA	4:E:276:PRO:HD3	1.82	0.44
4:E:388:ILE:HD12	4:E:393:MET:HA	2.00	0.44
4:F:391:LEU:HD13	4:F:395:GLU:HG3	2.00	0.44
6:H:10:LEU:C	6:H:10:LEU:HD23	2.39	0.44
6:H:112:VAL:HB	6:H:123:ALA:HB2	1.99	0.44
6:H:109:LYS:HD2	6:H:126:GLN:OE1	2.18	0.44
8:M:43:ILE:CG2	8:M:46:THR:HB	2.48	0.44
9:T:167:GLN:O	9:T:171:GLU:HG3	2.18	0.44
11:V:55:ASP:OD1	11:V:57:ASN:HB2	2.18	0.44
11:V:6:ASP:N	11:V:7:PRO:CD	2.81	0.44
1:A:260:ARG:O	1:A:321:GLY:HA3	2.18	0.44
2:B:133:VAL:HB	2:B:310:ARG:HH11	1.83	0.44
1:C:166:ARG:HD2	1:C:166:ARG:N	2.30	0.44
4:F:33:ILE:HG22	4:F:34:LEU:N	2.33	0.44
5:G:59:ASN:ND2	5:G:183:PHE:HE1	2.16	0.44
5:G:187:THR:O	5:G:187:THR:HG22	2.18	0.44
6:H:113:SER:HA	6:H:120:ALA:HB1	2.00	0.44
6:H:91:PHE:HZ	6:H:97:SER:HG	1.65	0.44
8:O:53:LEU:O	8:O:57:LEU:HG	2.18	0.44
10:U:55:TYR:O	10:U:58:ALA:HB3	2.18	0.44
9:T:176:TRP:CZ3	11:V:22:LYS:CA	2.91	0.44
12:W:22:LEU:HD21	12:W:81:LEU:O	2.18	0.44
12:W:78:PHE:CD2	12:W:86:ILE:CD1	2.98	0.44
1:A:67:ASN:HD21	1:A:287:LEU:HB3	1.83	0.44
1:A:55:VAL:HG21	1:A:75:ILE:HD13	2.00	0.44
3:D:163:LYS:HZ3	3:D:311:TYR:HA	1.83	0.44
3:D:369:ASP:O	3:D:373:LYS:HG3	2.18	0.44
4:E:380:THR:O	4:E:384:LEU:HG	2.18	0.44
4:E:396:LEU:HD13	4:E:404:VAL:HG21	1.99	0.44
5:G:149:LYS:O	5:G:153:VAL:HG12	2.18	0.44
5:G:13:ILE:CD1	5:G:247:MET:HE3	2.48	0.44
5:G:57:THR:HG22	5:G:191:SER:OG	2.18	0.44
6:H:16:LEU:HB3	6:H:17:PRO:HD2	2.00	0.44
8:J:53:LEU:O	8:J:57:LEU:HG	2.18	0.44
8:L:57:LEU:HD22	8:M:55:PHE:CE1	2.53	0.44
8:S:53:LEU:O	8:S:57:LEU:HG	2.18	0.44
8:S:64:PHE:O	8:S:68:VAL:HG23	2.18	0.44
12:W:78:PHE:O	12:W:79:SER:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:34:LEU:HD11	2:B:44:PHE:HB2	2.00	0.43
2:B:399:TYR:CE1	2:B:423:GLY:HA3	2.53	0.43
4:F:117:ILE:HA	4:F:238:THR:OG1	2.18	0.43
8:J:64:PHE:O	8:J:68:VAL:HG23	2.18	0.43
8:K:64:PHE:O	8:K:68:VAL:HG23	2.18	0.43
8:L:53:LEU:O	8:L:57:LEU:HG	2.18	0.43
8:M:53:LEU:O	8:M:57:LEU:HG	2.18	0.43
8:M:64:PHE:O	8:M:68:VAL:HG23	2.18	0.43
8:N:26:ILE:HD13	8:N:55:PHE:CE1	2.52	0.43
8:N:64:PHE:O	8:N:68:VAL:HG23	2.18	0.43
8:O:59:GLU:O	8:O:63:LEU:HG	2.19	0.43
8:Q:53:LEU:O	8:Q:57:LEU:HG	2.18	0.43
8:R:29:VAL:CG2	8:S:27:ALA:HA	2.48	0.43
8:R:64:PHE:O	8:R:68:VAL:HG23	2.18	0.43
12:W:89:LEU:HD21	12:W:98:THR:OG1	2.19	0.43
1:A:67:ASN:HD21	1:A:287:LEU:HD13	1.82	0.43
1:C:354:LEU:HD23	1:C:367:ILE:HA	2.01	0.43
1:C:384:ALA:HB2	1:C:489:GLY:O	2.18	0.43
2:B:82:ARG:HA	4:E:33:ILE:HB	1.99	0.43
4:E:377:THR:HG22	4:E:407:ALA:HB2	2.00	0.43
4:F:145:ALA:HB1	4:F:355:SER:HB3	2.00	0.43
4:F:65:ASP:CG	4:F:66:GLY:H	2.21	0.43
5:G:71:LYS:HE3	5:G:159:TYR:HA	2.01	0.43
6:H:132:ASN:O	6:H:136:VAL:HG23	2.18	0.43
8:K:59:GLU:O	8:K:63:LEU:HG	2.19	0.43
8:P:53:LEU:O	8:P:57:LEU:HG	2.18	0.43
9:T:176:TRP:CZ3	11:V:22:LYS:CD	3.01	0.43
9:T:141:ARG:CZ	10:U:41:LEU:HD23	2.49	0.43
10:U:51:ILE:O	10:U:53:TRP:N	2.51	0.43
12:W:20:THR:HA	12:W:23:TYR:CD2	2.53	0.43
1:A:260:ARG:HH11	1:A:314:LEU:HD11	1.84	0.43
1:C:284:SER:OG	1:C:297:PRO:HG3	2.18	0.43
1:C:388:VAL:O	1:C:451:VAL:HG21	2.19	0.43
3:D:115:LYS:HA	3:D:116:PRO:HD3	1.91	0.43
4:E:94:ARG:CZ	4:E:109:ILE:HG12	2.48	0.43
6:H:123:ALA:O	6:H:127:VAL:HG23	2.19	0.43
8:K:53:LEU:O	8:K:57:LEU:HG	2.18	0.43
8:L:64:PHE:O	8:L:68:VAL:HG23	2.18	0.43
8:M:59:GLU:O	8:M:63:LEU:HG	2.19	0.43
8:N:53:LEU:O	8:N:57:LEU:HG	2.18	0.43
8:N:59:GLU:O	8:N:63:LEU:HG	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:290:PRO:HA	2:B:291:PRO:HD2	1.93	0.43
4:F:121:PRO:HA	4:F:122:PRO:HD3	1.88	0.43
5:G:72:GLU:HG3	5:G:161:LYS:O	2.19	0.43
5:G:30:ARG:HB3	5:G:230:ILE:HD13	2.01	0.43
8:J:59:GLU:O	8:J:63:LEU:HG	2.19	0.43
8:O:64:PHE:O	8:O:68:VAL:HG23	2.18	0.43
8:P:64:PHE:O	8:P:68:VAL:HG23	2.18	0.43
8:Q:59:GLU:O	8:Q:63:LEU:HG	2.19	0.43
8:R:59:GLU:O	8:R:63:LEU:HG	2.19	0.43
1:A:119:GLY:C	11:V:50:MET:HE2	2.39	0.43
12:W:113:ARG:O	12:W:116:VAL:HG12	2.18	0.43
1:A:28:ASN:HB3	1:A:48:ASN:HD22	1.81	0.43
2:B:369:VAL:HG21	2:B:396:LEU:HD13	2.01	0.43
2:B:467:GLU:O	2:B:471:LEU:HG	2.18	0.43
1:C:273:LEU:N	1:C:273:LEU:CD1	2.82	0.43
1:C:305:SER:HA	1:C:347:ILE:HD13	2.01	0.43
9:T:176:TRP:CZ3	11:V:22:LYS:HD2	2.53	0.43
1:A:26:ASN:O	11:V:8:VAL:HG22	2.19	0.43
1:A:103:PRO:HA	1:A:106:LEU:HD13	2.01	0.43
1:A:316:GLU:HA	1:A:320:SER:OG	2.19	0.43
1:C:55:VAL:HG21	1:C:75:ILE:HD13	2.01	0.43
3:D:427:ILE:HG23	3:D:428:PRO:HD2	2.01	0.43
4:F:84:SER:HA	4:F:116:PRO:HA	2.00	0.43
5:G:209:LEU:HA	6:H:74:PHE:CE2	2.54	0.43
5:G:77:ILE:HD12	5:G:222:MET:HG2	2.01	0.43
6:H:69:PHE:CE2	6:H:133:LEU:HD23	2.54	0.43
6:H:10:LEU:HG	6:H:81:SER:O	2.19	0.43
10:U:100:CYS:SG	10:U:101:ALA:N	2.92	0.43
12:W:23:TYR:CD1	12:W:32:LEU:CD2	3.02	0.43
12:W:79:SER:HA	12:W:83:SER:HB2	2.01	0.43
12:W:90:ALA:HB2	12:W:95:LEU:CD1	2.48	0.43
4:E:204:THR:OG1	4:E:420:VAL:HB	2.19	0.43
4:F:293:GLN:HE22	4:F:308:GLN:NE2	2.16	0.43
4:F:167:ILE:HD11	4:F:309:ALA:HB2	2.00	0.43
4:F:452:ILE:HA	4:F:453:PRO:HD3	1.89	0.43
6:H:31:ASN:O	6:H:57:VAL:HA	2.19	0.43
6:H:35:LYS:HD2	6:H:53:LEU:HD11	2.01	0.43
8:P:59:GLU:O	8:P:63:LEU:HG	2.18	0.43
8:Q:64:PHE:O	8:Q:68:VAL:HG23	2.18	0.43
9:T:164:MET:HE1	11:V:40:LEU:HD12	2.04	0.43
9:T:180:ARG:NH1	11:V:21:THR:HG21	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:W:38:GLU:HB3	12:W:78:PHE:HD1	1.84	0.43
12:W:73:THR:HA	12:W:78:PHE:CD2	2.53	0.43
1:A:205:TYR:HB3	1:A:233:ILE:HD13	2.01	0.43
1:A:381:GLN:HE21	1:A:386:LYS:HA	1.84	0.43
1:C:242:ALA:N	1:C:243:PRO:CD	2.81	0.43
4:F:155:LEU:HD23	4:F:333:THR:HB	2.01	0.43
6:H:39:ILE:HG22	6:H:40:GLY:N	2.34	0.43
12:W:79:SER:O	12:W:83:SER:CB	2.66	0.43
1:C:392:LEU:O	1:C:396:LEU:CD1	2.67	0.43
1:C:40:ILE:HG13	1:C:286:LEU:HB3	2.01	0.43
3:D:64:MET:HE2	3:D:83:ILE:HD11	2.00	0.43
5:G:23:MET:HG2	5:G:237:MET:CE	2.49	0.43
5:G:74:ILE:HB	5:G:107:ILE:HG12	2.01	0.43
11:V:17:ARG:HH11	11:V:20:ARG:NH1	2.17	0.43
1:A:368:ASN:HD22	1:A:371:LEU:HB2	1.84	0.43
4:E:201:MET:HA	4:E:204:THR:HG22	2.00	0.43
4:F:339:ILE:HB	4:F:347:ALA:HB1	2.01	0.43
4:F:390:ILE:HD11	5:G:247:MET:HE1	2.09	0.43
6:H:112:VAL:O	6:H:120:ALA:HB2	2.19	0.43
12:W:17:ARG:O	12:W:21:ALA:N	2.50	0.43
2:B:336:VAL:HG23	4:F:337:ARG:HH11	1.84	0.42
2:B:81:ASP:O	4:E:33:ILE:HD12	2.19	0.42
4:E:30:LEU:N	4:E:30:LEU:HD12	2.34	0.42
4:F:30:LEU:N	4:F:30:LEU:HD12	2.34	0.42
8:K:47:VAL:HG11	8:L:34:ILE:HG23	2.01	0.42
8:M:61:THR:HG21	8:N:23:GLY:N	2.34	0.42
9:T:183:GLN:O	9:T:187:ALA:HB3	2.19	0.42
12:W:69:LEU:O	12:W:73:THR:OG1	2.35	0.42
12:W:38:GLU:HB3	12:W:78:PHE:CD1	2.53	0.42
1:A:136:PRO:HB2	1:A:141:ARG:HE	1.84	0.42
1:A:152:LEU:HD11	1:A:180:VAL:HA	2.01	0.42
3:D:404:VAL:O	3:D:408:ARG:HG3	2.19	0.42
3:D:64:MET:CE	3:D:83:ILE:HD11	2.49	0.42
5:G:150:LEU:O	5:G:154:MET:HB2	2.19	0.42
8:S:59:GLU:O	8:S:63:LEU:HG	2.19	0.42
12:W:98:THR:N	12:W:99:PRO:HD2	2.34	0.42
1:A:238:ALA:HA	1:A:245:GLN:NE2	2.33	0.42
2:B:136:PRO:HG2	2:B:141:ARG:HH21	1.84	0.42
1:C:118:ASP:OD1	1:C:120:LYS:HG3	2.19	0.42
1:C:30:THR:HA	1:C:90:VAL:O	2.19	0.42
9:T:113:SER:O	9:T:116:ALA:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:U:87:ALA:HA	10:U:90:ASP:CG	2.39	0.42
12:W:23:TYR:OH	12:W:112:HIS:HB3	2.20	0.42
1:A:405:PHE:O	1:A:412:LEU:HD11	2.19	0.42
1:A:46:LEU:O	1:A:49:ILE:HG22	2.19	0.42
2:B:105:LEU:N	2:B:105:LEU:HD12	2.35	0.42
2:B:208:VAL:HG23	2:B:208:VAL:O	2.20	0.42
1:A:212:ARG:CB	3:D:127:GLN:HE21	2.29	0.42
3:D:117:ILE:HA	3:D:238:THR:OG1	2.19	0.42
4:E:345:TYR:HA	4:E:346:PRO:C	2.40	0.42
4:E:6:SER:C	4:E:8:PRO:CD	2.88	0.42
2:B:141:ARG:NH1	4:F:191:THR:HB	2.34	0.42
4:F:359:ASP:OD2	4:F:361:ALA:HB3	2.20	0.42
5:G:159:TYR:HA	5:G:160:PRO:HD3	1.85	0.42
8:L:43:ILE:CG2	8:L:46:THR:HB	2.49	0.42
9:T:150:GLU:O	9:T:154:ARG:HG2	2.19	0.42
10:U:99:SER:OG	10:U:100:CYS:N	2.52	0.42
10:U:92:GLU:O	10:U:95:GLU:N	2.53	0.42
9:T:176:TRP:CH2	11:V:30:VAL:HG21	2.55	0.42
12:W:23:TYR:HA	12:W:26:ALA:HB3	2.02	0.42
12:W:60:VAL:HG21	12:W:65:LYS:HD2	2.01	0.42
2:B:365:PRO:HB2	2:B:367:ILE:HG13	2.00	0.42
2:B:376:VAL:HG11	4:F:192:ARG:NH1	2.35	0.42
1:C:146:GLU:HB2	1:C:163:ARG:HB2	2.01	0.42
1:C:283:LEU:N	1:C:283:LEU:HD12	2.35	0.42
4:E:244:ARG:HG3	4:E:303:SER:N	2.35	0.42
5:G:254:LEU:HG	5:G:257:ARG:NH2	2.35	0.42
1:A:38:ASP:HB3	1:A:286:LEU:HD22	2.01	0.42
1:A:64:MET:O	1:A:76:VAL:HG22	2.19	0.42
1:C:105:LEU:N	1:C:105:LEU:HD12	2.35	0.42
1:C:116:PRO:HD3	1:C:123:ILE:CG1	2.35	0.42
1:C:153:LYS:HG2	1:C:443:GLN:HG2	2.01	0.42
4:E:472:LYS:O	4:E:476:GLU:HG3	2.19	0.42
4:F:174:ILE:O	4:F:178:HIS:HB2	2.20	0.42
5:G:118:LEU:HD12	5:G:118:LEU:N	2.34	0.42
6:H:70:ILE:HD11	6:H:87:ALA:HB2	2.02	0.42
12:W:78:PHE:O	12:W:79:SER:HB2	2.18	0.42
1:A:271:ASP:HA	1:A:272:ASP:HA	1.75	0.42
1:A:46:LEU:HB3	1:A:49:ILE:HB	2.02	0.42
2:B:98:ASP:OD2	2:B:128:ARG:HB3	2.20	0.42
4:E:150:GLY:HA2	4:E:304:VAL:O	2.20	0.42
4:E:30:LEU:HD12	4:E:30:LEU:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:7:THR:N	4:E:8:PRO:CD	2.83	0.42
2:B:375:ARG:HG2	15:F:1479:ADP:H5'1	2.02	0.42
2:B:142:ARG:HA	4:F:195:ASN:HD21	1.85	0.42
6:H:109:LYS:NZ	6:H:130:LEU:HD11	2.35	0.42
8:L:59:GLU:O	8:L:63:LEU:HG	2.19	0.42
8:N:64:PHE:HA	8:N:67:MET:HE3	2.00	0.42
8:N:47:VAL:CG1	8:O:34:ILE:HG23	2.50	0.42
9:T:119:GLN:HG3	9:T:120:LYS:N	2.34	0.42
9:T:188:GLN:OE1	9:T:191:LYS:HG3	2.19	0.42
12:W:22:LEU:HD13	12:W:85:LEU:CD1	2.50	0.42
2:B:338:ALA:O	2:B:342:THR:HG23	2.20	0.42
2:B:385:LEU:HD22	2:B:447:ILE:HD12	2.02	0.42
1:C:166:ARG:HA	1:C:325:ALA:O	2.20	0.42
1:C:193:ASN:ND2	1:C:229:LYS:NZ	2.68	0.42
3:D:271:LEU:HD12	3:D:271:LEU:N	2.34	0.42
4:E:282:GLN:NE2	4:E:285:LEU:HB2	2.35	0.42
4:F:140:VAL:HG21	4:F:348:VAL:CG2	2.48	0.42
2:B:375:ARG:NH1	4:F:190:ARG:CZ	2.83	0.42
4:F:220:GLY:HA3	4:F:232:VAL:HG21	2.02	0.42
8:J:19:LEU:HD12	8:S:65:CYS:SG	2.60	0.42
8:J:6:ALA:HB2	8:S:4:VAL:HA	2.01	0.42
9:T:193:THR:HG23	9:T:194:ILE:N	2.35	0.42
12:W:60:VAL:HG11	12:W:65:LYS:HA	2.01	0.42
2:B:100:PRO:HB3	2:B:125:ALA:HB2	2.02	0.42
3:D:333:THR:O	3:D:333:THR:HG22	2.19	0.42
4:E:176:LYS:HZ2	4:E:214:LYS:HE2	1.82	0.42
4:E:351:LEU:CD1	4:E:382:LYS:HD2	2.50	0.42
4:E:9:ILE:HB	4:E:78:ASP:HB3	2.02	0.42
1:A:343:ASN:O	1:A:347:ILE:HG13	2.20	0.42
1:C:184:THR:O	1:C:188:GLN:HG2	2.20	0.42
1:C:270:TYR:O	1:C:328:VAL:HG23	2.20	0.42
3:D:33:ILE:HG22	3:D:34:LEU:HG	2.02	0.42
4:E:289:MET:HG2	4:E:324:THR:HG22	2.02	0.42
11:V:6:ASP:OD1	11:V:9:GLN:NE2	2.52	0.42
12:W:78:PHE:CE1	12:W:82:THR:HG21	2.55	0.42
1:A:100:PRO:HD3	1:A:128:ARG:HH12	1.85	0.41
1:A:243:PRO:O	1:A:246:TYR:HB3	2.20	0.41
1:A:294:GLU:O	1:A:295:ALA:HB3	2.20	0.41
3:D:241:GLU:O	3:D:244:ARG:HB3	2.20	0.41
5:G:184:ASN:O	5:G:188:ILE:HG13	2.20	0.41
7:I:31:THR:HG23	7:I:33:SER:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:U:98:LYS:HA	10:U:98:LYS:HD3	1.79	0.41
12:W:78:PHE:CB	12:W:82:THR:HB	2.50	0.41
1:A:185:ILE:HG12	1:A:203:CYS:SG	2.60	0.41
1:A:250:PHE:HZ	1:A:303:LEU:HD12	1.86	0.41
1:A:266:ALA:O	1:A:323:LEU:HD12	2.20	0.41
1:A:68:LEU:HD12	4:E:16:VAL:HB	2.03	0.41
2:B:159:VAL:HG12	2:B:374:SER:HB2	2.02	0.41
1:C:206:VAL:HG12	1:C:208:VAL:HG23	2.02	0.41
1:C:300:VAL:O	1:C:303:LEU:HB3	2.21	0.41
3:D:15:ALA:HB3	3:D:22:ASP:HB2	2.03	0.41
3:D:176:LYS:HE2	3:D:176:LYS:HB3	1.87	0.41
3:D:33:ILE:HG22	3:D:34:LEU:N	2.35	0.41
1:C:70:PRO:HA	3:D:72:ARG:NH2	2.36	0.41
5:G:135:LYS:HZ3	7:I:41:ASP:HB2	1.94	0.41
10:U:53:TRP:CH2	10:U:70:GLU:HA	2.55	0.41
10:U:86:THR:CG2	10:U:89:VAL:HG23	2.50	0.41
12:W:23:TYR:HB3	12:W:105:PHE:CE2	2.55	0.41
12:W:35:VAL:CG2	12:W:81:LEU:CB	2.95	0.41
2:B:85:LYS:HG2	2:B:86:GLU:N	2.35	0.41
1:C:192:ASN:HA	1:C:200:LYS:HG2	2.03	0.41
1:A:332:GLN:HB3	3:D:318:THR:HB	2.03	0.41
4:E:393:MET:HE1	4:E:408:ARG:HH21	1.86	0.41
2:B:47:ASN:HA	4:F:72:ARG:NH2	2.35	0.41
6:H:102:LYS:HZ2	6:H:133:LEU:HB3	1.85	0.41
8:P:43:ILE:CG2	8:P:46:THR:HB	2.49	0.41
12:W:36:GLU:HB2	12:W:105:PHE:CE1	2.56	0.41
1:A:143:SER:HB3	4:E:199:ARG:NH2	2.30	0.41
1:A:174:GLN:HB3	3:D:354:LYS:HD2	2.02	0.41
1:A:352:ILE:O	1:A:352:ILE:HG22	2.20	0.41
3:D:94:ARG:HH21	3:D:106:ARG:HB2	1.85	0.41
3:D:161:VAL:CG1	3:D:335:LEU:HB3	2.51	0.41
1:C:68:LEU:HB2	3:D:16:VAL:HB	2.03	0.41
3:D:268:VAL:O	3:D:272:LEU:HD13	2.20	0.41
3:D:345:TYR:HA	3:D:346:PRO:C	2.40	0.41
4:E:227:GLY:O	4:E:231:ARG:HG2	2.20	0.41
4:F:133:ILE:HD13	4:F:363:VAL:HG12	2.03	0.41
4:F:412:ARG:HG2	4:F:412:ARG:HH11	1.85	0.41
5:G:72:GLU:HB3	5:G:105:ALA:CB	2.50	0.41
6:H:117:ALA:HA	6:H:120:ALA:HB3	2.02	0.41
1:A:434:GLN:O	1:A:435:TYR:HB2	2.20	0.41
2:B:166:ARG:HD2	2:B:308:LEU:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:201:MET:CE	3:D:215:VAL:HG11	2.51	0.41
3:D:171:ILE:HG12	3:D:254:PHE:CZ	2.56	0.41
3:D:53:HIS:CD2	3:D:59:VAL:HG22	2.56	0.41
4:E:391:LEU:HB2	4:E:395:GLU:HG3	2.02	0.41
4:F:106:ARG:HH21	4:F:209:LEU:HB3	1.85	0.41
4:F:207:ILE:HD11	4:F:215:VAL:HG13	2.03	0.41
6:H:91:PHE:HA	6:H:92:PRO:HD3	1.91	0.41
9:T:97:LYS:HD3	9:T:97:LYS:HA	1.82	0.41
9:T:93:LEU:HD23	9:T:97:LYS:HE3	2.03	0.41
12:W:32:LEU:HD13	12:W:105:PHE:HE1	1.85	0.41
1:A:460:LEU:O	1:A:460:LEU:HG	2.21	0.41
3:D:148:ALA:HA	3:D:357:LEU:HD11	2.03	0.41
4:F:35:ASN:O	4:F:49:GLU:HA	2.21	0.41
4:F:460:VAL:HG21	4:F:466:VAL:HG22	2.02	0.41
5:G:77:ILE:HD13	5:G:110:ILE:HD12	2.03	0.41
12:W:60:VAL:HG21	12:W:65:LYS:CD	2.51	0.41
3:D:160:GLY:N	15:D:1476:ADP:O3B	2.54	0.41
4:E:258:ILE:O	4:E:258:ILE:HG13	2.20	0.41
4:E:348:VAL:O	4:E:350:PRO:HD3	2.21	0.41
6:H:48:THR:HG22	6:H:50:GLU:HG3	2.03	0.41
8:N:29:VAL:CG2	8:O:27:ALA:HA	2.51	0.41
8:P:20:LEU:HB2	8:Q:20:LEU:HD22	2.03	0.41
12:W:55:LEU:HA	12:W:55:LEU:HD23	1.94	0.41
1:A:67:ASN:ND2	1:A:287:LEU:HB3	2.35	0.41
1:C:301:PHE:CE1	1:C:305:SER:HB3	2.56	0.41
4:F:300:LYS:HE3	4:F:300:LYS:HB2	1.90	0.41
4:F:97:ASN:HB2	4:F:103:ILE:CG2	2.51	0.41
4:E:276:PRO:CB	5:G:267:LEU:HD21	2.51	0.41
8:K:33:LEU:O	8:K:37:VAL:HG22	2.21	0.41
9:T:117:LEU:O	9:T:118:VAL:O	2.39	0.41
3:D:384:LEU:HD22	3:D:387:ILE:HD12	2.03	0.41
3:D:37:LEU:HB2	3:D:48:LEU:HB2	2.03	0.41
4:E:187:VAL:HG22	4:E:232:VAL:HB	2.02	0.41
4:F:220:GLY:CA	4:F:232:VAL:HG21	2.51	0.41
8:K:52:ILE:O	8:K:55:PHE:HB3	2.21	0.41
9:T:103:GLN:HB2	10:U:118:LEU:HD21	2.03	0.41
10:U:44:LEU:HD23	10:U:44:LEU:HA	1.91	0.41
12:W:112:HIS:ND1	12:W:113:ARG:N	2.69	0.41
2:B:170:ILE:HG23	2:B:353:PHE:HA	2.03	0.41
1:C:32:ARG:HA	1:C:88:GLU:O	2.21	0.41
1:C:82:ARG:HA	4:F:33:ILE:HB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:22:THR:O	5:G:26:VAL:HG23	2.21	0.41
12:W:57:ASN:ND2	12:W:60:VAL:CG2	2.84	0.41
12:W:38:GLU:HG2	12:W:82:THR:OG1	2.21	0.41
2:B:152:LEU:HD12	2:B:155:VAL:HG21	2.03	0.41
2:B:413:ASP:OD2	2:B:415:SER:HB3	2.21	0.41
2:B:82:ARG:HG3	4:E:33:ILE:O	2.21	0.41
1:C:260:ARG:HH11	1:C:314:LEU:HD11	1.86	0.41
1:C:326:LEU:HA	1:C:327:PRO:HD2	1.92	0.41
3:D:187:VAL:HG12	3:D:260:ARG:HB2	2.03	0.41
3:D:269:SER:HB2	3:D:274:ARG:HD2	2.02	0.41
3:D:145:ALA:CA	3:D:355:SER:HB2	2.51	0.41
4:F:101:GLU:HA	4:F:102:PRO:HD3	1.95	0.41
4:F:95:ILE:O	4:F:103:ILE:HG12	2.21	0.41
4:F:95:ILE:HA	4:F:217:LEU:O	2.21	0.41
8:J:52:ILE:O	8:J:55:PHE:HB3	2.21	0.41
8:M:52:ILE:O	8:M:55:PHE:HB3	2.21	0.41
9:T:116:ALA:HB2	9:T:120:LYS:HZ1	1.83	0.41
1:A:165:GLN:HG2	1:A:166:ARG:N	2.36	0.40
1:A:269:VAL:HG22	1:A:326:LEU:HB2	2.03	0.40
1:C:146:GLU:HA	1:C:147:PRO:HD2	1.94	0.40
3:D:338:GLY:O	3:D:342:LEU:HD13	2.21	0.40
4:E:167:ILE:HG23	4:E:254:PHE:CD2	2.56	0.40
8:N:52:ILE:O	8:N:55:PHE:HB3	2.21	0.40
8:P:52:ILE:O	8:P:55:PHE:HB3	2.21	0.40
8:R:52:ILE:O	8:R:55:PHE:HB3	2.21	0.40
9:T:91:ALA:O	9:T:94:GLU:HB3	2.21	0.40
10:U:113:GLU:O	10:U:117:GLU:N	2.45	0.40
9:T:203:LEU:CG	12:W:84:ASN:ND2	2.84	0.40
1:A:192:ASN:OD1	1:A:200:LYS:HB3	2.22	0.40
1:A:26:ASN:O	1:A:27:LEU:HB3	2.21	0.40
2:B:191:TRP:O	2:B:200:LYS:HG2	2.22	0.40
2:B:281:ARG:HA	2:B:284:SER:HB3	2.04	0.40
3:D:30:LEU:HA	3:D:31:PRO:HD2	1.93	0.40
3:D:30:LEU:HD11	3:D:57:ASN:HA	2.03	0.40
4:E:184:PHE:HB3	4:E:217:LEU:HD23	2.03	0.40
1:A:50:GLN:HG2	4:E:71:VAL:CG2	2.51	0.40
4:F:24:HIS:HE1	4:F:57:ASN:HB2	1.87	0.40
4:F:85:VAL:CG1	4:F:86:PRO:HD2	2.51	0.40
5:G:151:LEU:HD23	5:G:156:ALA:HB3	2.02	0.40
8:O:4:VAL:HG23	8:P:6:ALA:HA	2.03	0.40
9:T:88:GLN:HB2	9:T:88:GLN:HE21	1.77	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:U:12:TRP:HZ3	10:U:31:LYS:HG2	1.85	0.40
11:V:20:ARG:HA	11:V:23:ARG:HG2	2.04	0.40
12:W:61:LYS:CB	12:W:64:VAL:CG2	2.99	0.40
1:A:203:CYS:O	1:A:231:SER:HA	2.21	0.40
1:A:474:LEU:HD12	1:A:474:LEU:N	2.37	0.40
1:C:36:VAL:HG21	1:C:84:VAL:HB	2.02	0.40
4:E:168:GLN:NE2	4:E:201:MET:HA	2.36	0.40
4:F:440:SER:O	4:F:444:VAL:HG23	2.21	0.40
4:F:7:THR:HA	4:F:8:PRO:HD2	1.95	0.40
5:G:133:ILE:HG21	5:G:222:MET:CE	2.52	0.40
8:Q:52:ILE:O	8:Q:55:PHE:HB3	2.22	0.40
1:A:353:PHE:HE1	1:A:355:GLU:HG2	1.86	0.40
1:C:139:LEU:N	1:C:140:PRO:HD2	2.37	0.40
1:C:290:PRO:HA	1:C:291:PRO:HD2	1.86	0.40
3:D:277:SER:OG	3:D:278:ALA:N	2.55	0.40
1:A:52:GLU:OE1	4:E:68:GLU:HB2	2.21	0.40
4:F:120:ASP:HA	4:F:121:PRO:HD3	1.85	0.40
5:G:15:ASN:O	5:G:19:ILE:HG12	2.22	0.40
9:T:146:ARG:O	9:T:150:GLU:HG3	2.21	0.40
9:T:96:VAL:HG12	9:T:97:LYS:HE2	2.04	0.40
9:T:98:GLN:HE22	9:T:102:LYS:HD2	1.86	0.40
10:U:65:LEU:O	10:U:68:ASP:HB3	2.22	0.40
12:W:11:ILE:HG13	12:W:12:TYR:N	2.36	0.40
12:W:39:LEU:HA	12:W:39:LEU:HD23	1.92	0.40
12:W:69:LEU:O	12:W:72:MET:N	2.50	0.40
2:B:263:GLY:HA2	2:B:319:GLY:O	2.22	0.40
3:D:54:LEU:HD11	3:D:60:ARG:NH2	2.36	0.40
4:F:96:ILE:HD12	4:F:239:ILE:CD1	2.52	0.40
9:T:196:LYS:NZ	12:W:20:THR:O	2.54	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	A	483/485 (100%)	444 (92%)	35 (7%)	4 (1%)	22	67
1	C	483/485 (100%)	450 (93%)	33 (7%)	0	100	100
1	a	483/485 (100%)	444 (92%)	35 (7%)	4 (1%)	22	67
1	c	483/485 (100%)	450 (93%)	33 (7%)	0	100	100
2	B	483/486 (99%)	447 (92%)	35 (7%)	1 (0%)	51	84
2	b	483/486 (99%)	447 (92%)	35 (7%)	1 (0%)	51	84
3	D	468/470 (100%)	443 (95%)	22 (5%)	3 (1%)	28	71
3	d	468/470 (100%)	443 (95%)	22 (5%)	3 (1%)	28	71
4	E	471/473 (100%)	436 (93%)	32 (7%)	3 (1%)	28	71
4	F	470/473 (99%)	438 (93%)	30 (6%)	2 (0%)	38	77
4	e	471/473 (100%)	436 (93%)	32 (7%)	3 (1%)	28	71
4	f	470/473 (99%)	438 (93%)	30 (6%)	2 (0%)	38	77
5	G	265/278 (95%)	247 (93%)	17 (6%)	1 (0%)	38	77
5	g	265/278 (95%)	247 (93%)	17 (6%)	1 (0%)	38	77
6	H	130/132 (98%)	115 (88%)	11 (8%)	4 (3%)	5	37
6	h	130/132 (98%)	115 (88%)	11 (8%)	4 (3%)	5	37
7	I	57/59 (97%)	48 (84%)	9 (16%)	0	100	100
7	i	57/59 (97%)	48 (84%)	9 (16%)	0	100	100
8	J	74/76 (97%)	69 (93%)	5 (7%)	0	100	100
8	K	74/76 (97%)	68 (92%)	6 (8%)	0	100	100
8	L	74/76 (97%)	70 (95%)	4 (5%)	0	100	100
8	M	74/76 (97%)	68 (92%)	6 (8%)	0	100	100
8	N	74/76 (97%)	69 (93%)	5 (7%)	0	100	100
8	O	74/76 (97%)	70 (95%)	4 (5%)	0	100	100
8	P	74/76 (97%)	68 (92%)	6 (8%)	0	100	100
8	Q	74/76 (97%)	70 (95%)	4 (5%)	0	100	100
8	R	74/76 (97%)	70 (95%)	4 (5%)	0	100	100
8	S	74/76 (97%)	69 (93%)	5 (7%)	0	100	100
8	j	74/76 (97%)	69 (93%)	5 (7%)	0	100	100
8	k	74/76 (97%)	68 (92%)	6 (8%)	0	100	100
8	l	74/76 (97%)	70 (95%)	4 (5%)	0	100	100
8	m	74/76 (97%)	68 (92%)	6 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	n	74/76 (97%)	69 (93%)	5 (7%)	0	100	100
8	o	74/76 (97%)	70 (95%)	4 (5%)	0	100	100
8	p	74/76 (97%)	68 (92%)	6 (8%)	0	100	100
8	q	74/76 (97%)	70 (95%)	4 (5%)	0	100	100
8	r	74/76 (97%)	70 (95%)	4 (5%)	0	100	100
8	s	74/76 (97%)	69 (93%)	5 (7%)	0	100	100
9	T	127/129 (98%)	100 (79%)	19 (15%)	8 (6%)	1	22
9	t	127/129 (98%)	100 (79%)	19 (15%)	8 (6%)	1	22
10	U	118/120 (98%)	88 (75%)	24 (20%)	6 (5%)	2	26
10	u	118/120 (98%)	88 (75%)	24 (20%)	6 (5%)	2	26
11	V	60/66 (91%)	52 (87%)	6 (10%)	2 (3%)	4	35
11	v	61/66 (92%)	52 (85%)	7 (12%)	2 (3%)	4	35
12	W	108/120 (90%)	92 (85%)	8 (7%)	8 (7%)	1	18
12	w	108/120 (90%)	92 (85%)	8 (7%)	8 (7%)	1	18
All	All	8927/9072 (98%)	8182 (92%)	661 (7%)	84 (1%)	25	63

All (84) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	72	ARG
3	D	279	VAL
4	E	32	ALA
4	E	279	VAL
4	F	279	VAL
6	H	93	LEU
9	T	118	VAL
9	T	119	GLN
9	T	120	LYS
9	T	197	CYS
10	U	63	ALA
10	U	100	CYS
11	V	32	ALA
12	W	30	ASN
12	W	77	LYS
12	W	78	PHE
12	W	79	SER
12	W	80	PRO

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Mol	Chain	Res	Type
3	d	72	ARG
3	d	279	VAL
4	e	32	ALA
4	e	279	VAL
4	f	279	VAL
6	h	93	LEU
9	t	118	VAL
9	t	119	GLN
9	t	120	LYS
9	t	197	CYS
10	u	63	ALA
10	u	100	CYS
11	v	32	ALA
12	w	30	ASN
12	w	77	LYS
12	w	78	PHE
12	w	79	SER
12	w	80	PRO
1	A	348	THR
1	A	363	ILE
2	B	363	ILE
9	T	81	PHE
9	T	188	GLN
9	T	204	LEU
10	U	61	ALA
12	W	60	VAL
1	a	348	THR
1	a	363	ILE
2	b	363	ILE
9	t	81	PHE
9	t	188	GLN
9	t	204	LEU
10	u	61	ALA
12	w	60	VAL
1	A	368	ASN
6	H	43	ALA
9	T	187	ALA
12	W	61	LYS
1	a	368	ASN
6	h	43	ALA
9	t	187	ALA
12	w	61	LYS

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Mol	Chain	Res	Type
3	D	347	ALA
6	H	54	PRO
12	W	117	PRO
3	d	347	ALA
6	h	54	PRO
12	w	117	PRO
10	U	52	ASP
10	u	52	ASP
5	G	135	LYS
10	U	8	LYS
5	g	135	LYS
10	u	8	LYS
4	F	158	GLY
4	f	158	GLY
4	E	44	GLY
4	e	44	GLY
1	A	97	VAL
6	H	92	PRO
10	U	60	VAL
11	V	27	GLY
1	a	97	VAL
6	h	92	PRO
10	u	60	VAL
11	v	27	GLY

### 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	A	391/391 (100%)	390 (100%)	1 (0%)	94	96
1	C	391/391 (100%)	390 (100%)	1 (0%)	94	96
1	a	391/391 (100%)	390 (100%)	1 (0%)	94	96
1	c	391/391 (100%)	390 (100%)	1 (0%)	94	96
2	B	390/391 (100%)	390 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	b	390/391 (100%)	390 (100%)	0	100	100
3	D	380/380 (100%)	379 (100%)	1 (0%)	94	96
3	d	380/380 (100%)	379 (100%)	1 (0%)	94	96
4	E	382/382 (100%)	380 (100%)	2 (0%)	91	95
4	F	381/382 (100%)	381 (100%)	0	100	100
4	e	382/382 (100%)	380 (100%)	2 (0%)	91	95
4	f	381/382 (100%)	381 (100%)	0	100	100
5	G	230/236 (98%)	230 (100%)	0	100	100
5	g	230/236 (98%)	230 (100%)	0	100	100
6	H	111/111 (100%)	110 (99%)	1 (1%)	82	91
6	h	111/111 (100%)	110 (99%)	1 (1%)	82	91
7	I	25/46 (54%)	25 (100%)	0	100	100
7	i	25/46 (54%)	25 (100%)	0	100	100
8	J	56/56 (100%)	56 (100%)	0	100	100
8	K	56/56 (100%)	56 (100%)	0	100	100
8	L	56/56 (100%)	56 (100%)	0	100	100
8	M	56/56 (100%)	56 (100%)	0	100	100
8	N	56/56 (100%)	56 (100%)	0	100	100
8	O	56/56 (100%)	56 (100%)	0	100	100
8	P	56/56 (100%)	56 (100%)	0	100	100
8	Q	56/56 (100%)	56 (100%)	0	100	100
8	R	56/56 (100%)	56 (100%)	0	100	100
8	S	56/56 (100%)	56 (100%)	0	100	100
8	j	56/56 (100%)	56 (100%)	0	100	100
8	k	56/56 (100%)	56 (100%)	0	100	100
8	l	56/56 (100%)	56 (100%)	0	100	100
8	m	56/56 (100%)	56 (100%)	0	100	100
8	n	56/56 (100%)	56 (100%)	0	100	100
8	o	56/56 (100%)	56 (100%)	0	100	100
8	p	56/56 (100%)	56 (100%)	0	100	100
8	q	56/56 (100%)	56 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	r	56/56 (100%)	56 (100%)	0	100	100
8	s	56/56 (100%)	56 (100%)	0	100	100
9	T	118/118 (100%)	103 (87%)	15 (13%)	5	25
9	t	118/118 (100%)	103 (87%)	15 (13%)	5	25
10	U	104/104 (100%)	90 (86%)	14 (14%)	4	24
10	u	104/104 (100%)	90 (86%)	14 (14%)	4	24
11	V	58/60 (97%)	52 (90%)	6 (10%)	8	32
11	v	58/60 (97%)	52 (90%)	6 (10%)	8	32
12	W	95/104 (91%)	70 (74%)	25 (26%)	0	4
12	w	95/104 (91%)	70 (74%)	25 (26%)	0	4
All	All	7232/7312 (99%)	7100 (98%)	132 (2%)	67	84

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	124	ASP
1	C	166	ARG
3	D	315	ASP
4	E	120	ASP
4	E	316	ASP
6	H	32	LEU
9	T	83	ASP
9	T	84	LYS
9	T	86	ASN
9	T	93	LEU
9	T	97	LYS
9	T	98	GLN
9	T	104	ILE
9	T	117	LEU
9	T	119	GLN
9	T	134	MET
9	T	155	LEU
9	T	164	MET
9	T	166	ARG
9	T	168	LYS
9	T	198	ILE
10	U	4	LYS
10	U	8	LYS

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Mol	Chain	Res	Type
10	U	11	ASP
10	U	13	VAL
10	U	31	LYS
10	U	39	SER
10	U	88	GLN
10	U	90	ASP
10	U	93	GLU
10	U	94	LYS
10	U	95	GLU
10	U	96	ASP
10	U	99	SER
10	U	111	ILE
11	V	8	VAL
11	V	12	PHE
11	V	23	ARG
11	V	30	VAL
11	V	43	GLU
11	V	61	ASN
12	W	11	ILE
12	W	12	TYR
12	W	14	ILE
12	W	15	GLU
12	W	20	THR
12	W	22	LEU
12	W	23	TYR
12	W	27	SER
12	W	32	LEU
12	W	34	GLN
12	W	35	VAL
12	W	38	GLU
12	W	41	ARG
12	W	44	GLN
12	W	56	LEU
12	W	62	ARG
12	W	70	SER
12	W	73	THR
12	W	75	LYS
12	W	82	THR
12	W	86	ILE
12	W	88	LEU
12	W	109	MET
12	W	112	HIS

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Mol	Chain	Res	Type
12	W	113	ARG
1	a	124	ASP
1	c	166	ARG
3	d	315	ASP
4	e	120	ASP
4	e	316	ASP
6	h	32	LEU
9	t	83	ASP
9	t	84	LYS
9	t	86	ASN
9	t	93	LEU
9	t	97	LYS
9	t	98	GLN
9	t	104	ILE
9	t	117	LEU
9	t	119	GLN
9	t	134	MET
9	t	155	LEU
9	t	164	MET
9	t	166	ARG
9	t	168	LYS
9	t	198	ILE
10	u	4	LYS
10	u	8	LYS
10	u	11	ASP
10	u	13	VAL
10	u	31	LYS
10	u	39	SER
10	u	88	GLN
10	u	90	ASP
10	u	93	GLU
10	u	94	LYS
10	u	95	GLU
10	u	96	ASP
10	u	99	SER
10	u	111	ILE
11	v	8	VAL
11	v	12	PHE
11	v	23	ARG
11	v	30	VAL
11	v	43	GLU
11	v	61	ASN

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Mol	Chain	Res	Type
12	w	11	ILE
12	w	12	TYR
12	w	14	ILE
12	w	15	GLU
12	w	20	THR
12	w	22	LEU
12	w	23	TYR
12	w	27	SER
12	w	32	LEU
12	w	34	GLN
12	w	35	VAL
12	w	38	GLU
12	w	41	ARG
12	w	44	GLN
12	w	56	LEU
12	w	62	ARG
12	w	70	SER
12	w	73	THR
12	w	75	LYS
12	w	82	THR
12	w	86	ILE
12	w	88	LEU
12	w	109	MET
12	w	112	HIS
12	w	113	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (139) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	48	ASN
1	A	72	GLN
1	A	149	GLN
1	A	245	GLN
1	A	262	ASN
1	A	351	GLN
1	A	368	ASN
1	A	381	GLN
2	B	26	ASN
2	B	28	ASN
2	B	48	ASN
2	B	174	GLN

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Mol	Chain	Res	Type
2	B	217	GLN
2	B	245	GLN
2	B	276	GLN
2	B	343	ASN
2	B	398	GLN
2	B	477	ASN
2	B	478	HIS
1	C	193	ASN
1	C	225	HIS
1	C	245	GLN
1	C	262	ASN
1	C	343	ASN
1	C	368	ASN
1	C	381	GLN
3	D	52	GLN
3	D	249	GLN
3	D	257	ASN
3	D	308	GLN
4	E	52	GLN
4	E	118	HIS
4	E	127	GLN
4	E	168	GLN
4	E	208	ASN
4	E	308	GLN
4	F	35	ASN
4	F	52	GLN
4	F	118	HIS
4	F	178	HIS
4	F	195	ASN
4	F	257	ASN
4	F	293	GLN
5	G	49	GLN
5	G	59	ASN
5	G	117	GLN
5	G	125	ASN
5	G	204	ASN
5	G	243	ASN
5	G	260	GLN
6	H	78	GLN
6	H	82	GLN
6	H	111	ASN
8	K	40	ASN

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Mol	Chain	Res	Type
8	L	40	ASN
8	M	40	ASN
8	N	40	ASN
8	O	40	ASN
8	P	40	ASN
8	Q	40	ASN
8	R	40	ASN
8	S	40	ASN
9	T	88	GLN
9	T	98	GLN
9	T	103	GLN
9	T	163	ASN
10	U	28	ASN
12	W	97	ASN
1	a	28	ASN
1	a	48	ASN
1	a	72	GLN
1	a	149	GLN
1	a	245	GLN
1	a	262	ASN
1	a	351	GLN
1	a	368	ASN
1	a	381	GLN
2	b	26	ASN
2	b	28	ASN
2	b	48	ASN
2	b	174	GLN
2	b	192	ASN
2	b	217	GLN
2	b	245	GLN
2	b	276	GLN
2	b	343	ASN
2	b	398	GLN
2	b	477	ASN
2	b	478	HIS
1	c	193	ASN
1	c	225	HIS
1	c	245	GLN
1	c	262	ASN
1	c	343	ASN
1	c	368	ASN
1	c	381	GLN

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Mol	Chain	Res	Type
3	d	52	GLN
3	d	249	GLN
3	d	257	ASN
3	d	308	GLN
4	e	52	GLN
4	e	118	HIS
4	e	127	GLN
4	e	168	GLN
4	e	208	ASN
4	e	308	GLN
4	f	35	ASN
4	f	52	GLN
4	f	118	HIS
4	f	178	HIS
4	f	195	ASN
4	f	257	ASN
4	f	293	GLN
5	g	49	GLN
5	g	59	ASN
5	g	117	GLN
5	g	125	ASN
5	g	204	ASN
5	g	224	GLN
5	g	243	ASN
5	g	260	GLN
6	h	78	GLN
6	h	82	GLN
6	h	111	ASN
8	k	40	ASN
8	l	40	ASN
8	m	40	ASN
8	n	40	ASN
8	o	40	ASN
8	p	40	ASN
8	q	40	ASN
8	s	40	ASN
9	t	88	GLN
9	t	98	GLN
9	t	103	GLN
9	t	163	ASN
10	u	28	ASN
12	w	97	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 10 are monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
13	ATP	A	1511	14	27,33,33	0.94	1 (3%)	25,52,52	1.57	2 (8%)
13	ATP	B	1510	14	27,33,33	0.98	1 (3%)	25,52,52	1.60	2 (8%)
13	ATP	C	1511	14	27,33,33	0.98	1 (3%)	25,52,52	1.64	2 (8%)
15	ADP	D	1476	14	25,29,29	1.03	1 (4%)	24,45,45	1.66	2 (8%)
15	ADP	F	1479	14	25,29,29	0.94	1 (4%)	24,45,45	1.71	3 (12%)
13	ATP	a	1511	14	27,33,33	0.93	1 (3%)	25,52,52	1.56	2 (8%)
13	ATP	b	1510	14	27,33,33	0.98	1 (3%)	25,52,52	1.60	2 (8%)
13	ATP	c	1511	14	27,33,33	0.97	1 (3%)	25,52,52	1.64	2 (8%)
15	ADP	d	1476	14	25,29,29	1.04	1 (4%)	24,45,45	1.68	2 (8%)
15	ADP	f	1479	14	25,29,29	0.95	1 (4%)	24,45,45	1.72	3 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	ATP	A	1511	14	-	0/18/38/38	0/3/3/3
13	ATP	B	1510	14	-	0/18/38/38	0/3/3/3
13	ATP	C	1511	14	-	0/18/38/38	0/3/3/3
15	ADP	D	1476	14	-	0/12/32/32	0/3/3/3
15	ADP	F	1479	14	-	0/12/32/32	0/3/3/3
13	ATP	a	1511	14	-	0/18/38/38	0/3/3/3
13	ATP	b	1510	14	-	0/18/38/38	0/3/3/3
13	ATP	c	1511	14	-	0/18/38/38	0/3/3/3
15	ADP	d	1476	14	-	0/12/32/32	0/3/3/3
15	ADP	f	1479	14	-	0/12/32/32	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	F	1479	ADP	C5-C4	2.95	1.47	1.40
15	f	1479	ADP	C5-C4	2.97	1.47	1.40
13	A	1511	ATP	C5-C4	3.06	1.47	1.40
13	b	1510	ATP	C5-C4	3.06	1.47	1.40
13	a	1511	ATP	C5-C4	3.07	1.47	1.40
13	B	1510	ATP	C5-C4	3.08	1.47	1.40
13	C	1511	ATP	C5-C4	3.10	1.47	1.40
13	c	1511	ATP	C5-C4	3.10	1.47	1.40
15	d	1476	ADP	C5-C4	3.24	1.47	1.40
15	D	1476	ADP	C5-C4	3.25	1.47	1.40

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	f	1479	ADP	N3-C2-N1	-6.17	123.49	128.86
15	F	1479	ADP	N3-C2-N1	-6.11	123.53	128.86
13	c	1511	ATP	N3-C2-N1	-5.96	123.67	128.86
15	d	1476	ADP	N3-C2-N1	-5.96	123.67	128.86
13	B	1510	ATP	N3-C2-N1	-5.93	123.69	128.86
13	b	1510	ATP	N3-C2-N1	-5.92	123.70	128.86
13	C	1511	ATP	N3-C2-N1	-5.92	123.70	128.86
15	D	1476	ADP	N3-C2-N1	-5.88	123.74	128.86
13	a	1511	ATP	N3-C2-N1	-5.51	124.06	128.86
13	A	1511	ATP	N3-C2-N1	-5.50	124.07	128.86
15	d	1476	ADP	C4-C5-N7	-3.22	106.30	109.41
15	D	1476	ADP	C4-C5-N7	-3.19	106.33	109.41
15	F	1479	ADP	C4-C5-N7	-2.94	106.57	109.41
15	f	1479	ADP	C4-C5-N7	-2.94	106.57	109.41
13	b	1510	ATP	C4-C5-N7	-2.86	106.65	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	1510	ATP	C4-C5-N7	-2.84	106.67	109.41
13	C	1511	ATP	C4-C5-N7	-2.74	106.76	109.41
13	c	1511	ATP	C4-C5-N7	-2.72	106.78	109.41
15	F	1479	ADP	C1'-N9-C4	-2.11	122.99	126.64
15	f	1479	ADP	C1'-N9-C4	-2.09	123.03	126.64
13	a	1511	ATP	N6-C6-N1	2.07	122.86	118.77
13	A	1511	ATP	N6-C6-N1	2.08	122.89	118.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	A	1511	ATP	5	0
13	B	1510	ATP	1	0
13	C	1511	ATP	1	0
15	D	1476	ADP	2	0
15	F	1479	ADP	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
9	t	1
9	T	1
11	V	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	V	9:GLN	C	10:LYS	N	9.37
1	T	168:LYS	C	169:GLU	N	0.99
1	t	168:LYS	C	169:GLU	N	0.99