



Full wwPDB EM Validation Report ⓘ

Apr 29, 2024 – 12:11 am BST

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 : 2012-07-17
Resolution : 37.00 Å(reported)
Based on initial model : 2WPD

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev92
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

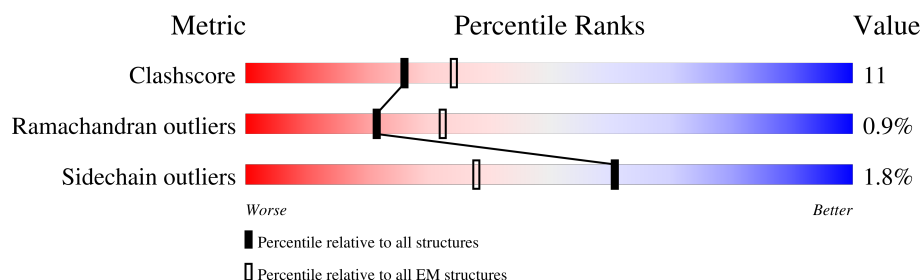
1 Overall quality at a glance

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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	485	<div> <div>8%</div> <div>61%</div> <div>38%</div> </div>
1	C	485	<div> <div>16%</div> <div>65%</div> <div>35%</div> </div>
1	a	485	<div> <div>9%</div> <div>99%</div> </div>
1	c	485	<div> <div>16%</div> <div>100%</div> </div>
2	B	486	<div> <div>16%</div> <div>63%</div> <div>37%</div> </div>
2	b	486	<div> <div>16%</div> <div>100%</div> </div>
3	D	470	<div> <div>15%</div> <div>63%</div> <div>37%</div> </div>
3	d	470	<div> <div>14%</div> <div>99%</div> </div>

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Mol	Chain	Length	Quality of chain
4	E	473	
4	F	473	
4	e	473	
4	f	473	
5	G	278	
5	g	278	
6	H	132	
6	h	132	
7	I	59	
7	i	59	
8	J	76	
8	K	76	
8	L	76	
8	M	76	
8	N	76	
8	O	76	
8	P	76	
8	Q	76	
8	R	76	
8	S	76	
8	j	76	
8	k	76	
8	l	76	
8	m	76	
8	n	76	

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Mol	Chain	Length	Quality of chain
8	o	76	
8	p	76	
8	q	76	
8	r	76	
8	s	76	
9	T	129	
9	t	129	
10	U	120	
10	u	120	
11	V	66	
11	v	66	
12	W	120	
12	w	120	

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

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

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

- 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		

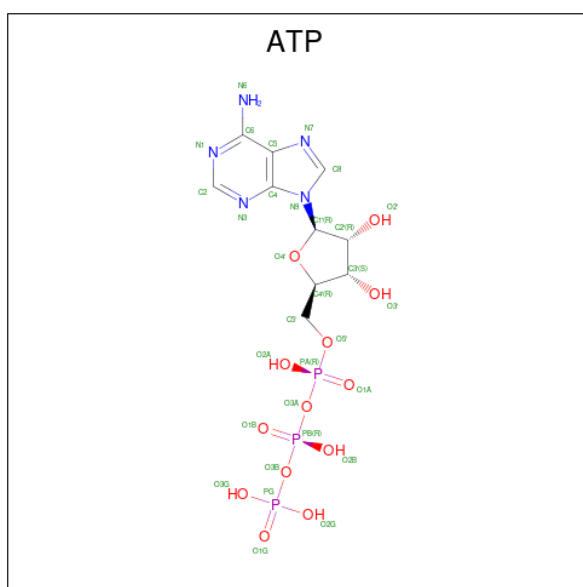
- Molecule 11 is a protein called ATP SYNTHASE-COUPPLING FACTOR 6, MITOCHONDRIAL.

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).

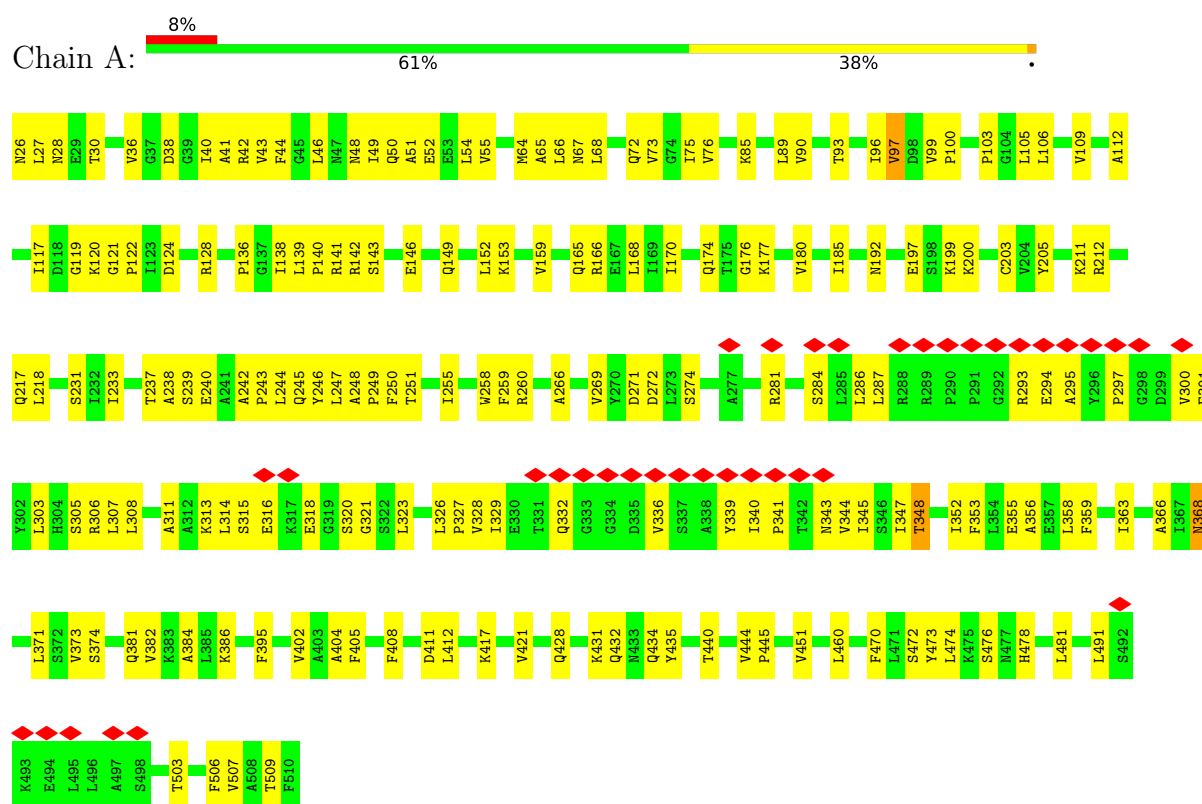
Mol	Chain	Residues	Atoms		AltConf
14	A	1	Total	Mg	0
			1	1	
14	B	1	Total	Mg	0
			1	1	
14	C	1	Total	Mg	0
			1	1	
14	D	1	Total	Mg	0
			1	1	
14	F	1	Total	Mg	0
			1	1	
14	a	1	Total	Mg	0
			1	1	
14	b	1	Total	Mg	0
			1	1	
14	c	1	Total	Mg	0
			1	1	
14	d	1	Total	Mg	0
			1	1	
14	f	1	Total	Mg	0
			1	1	

- Molecule 15 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

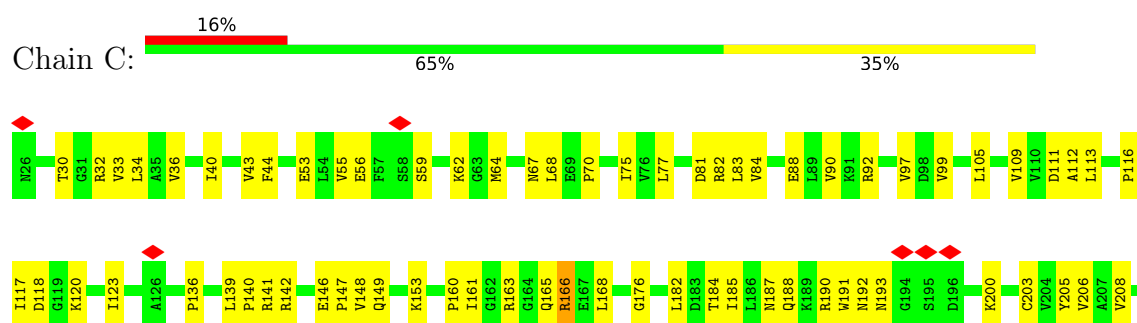
3 Residue-property plots

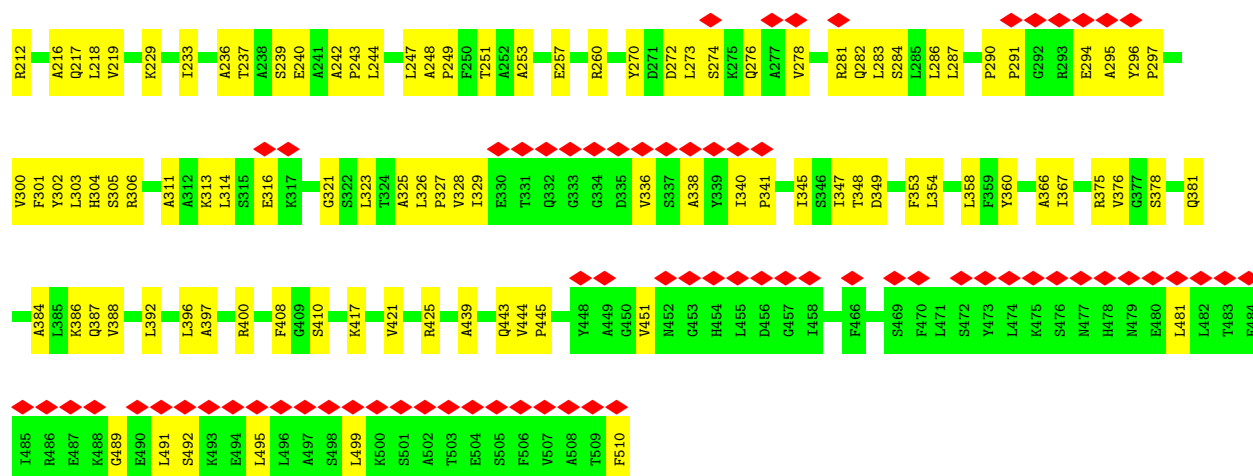
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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

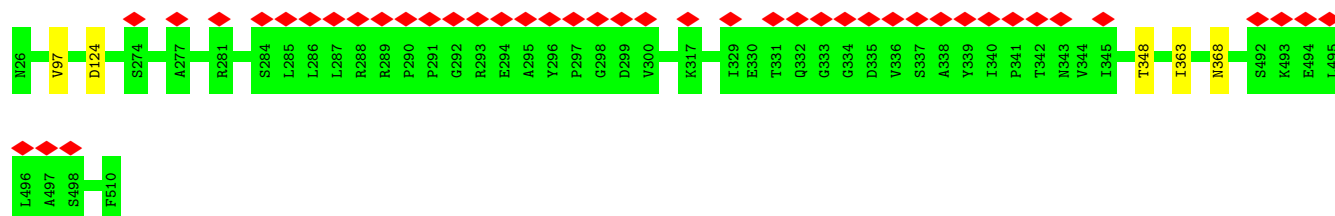


• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

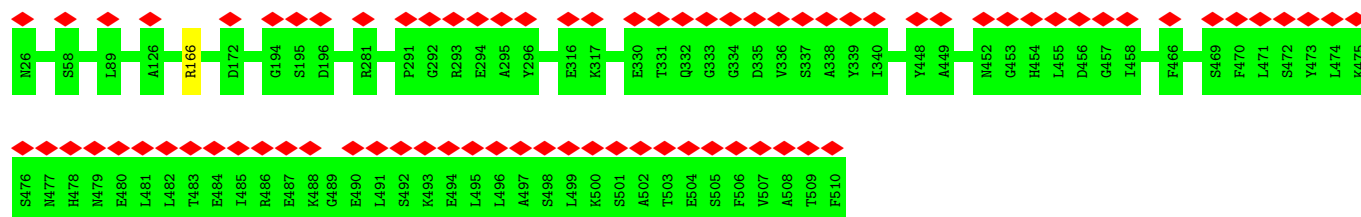




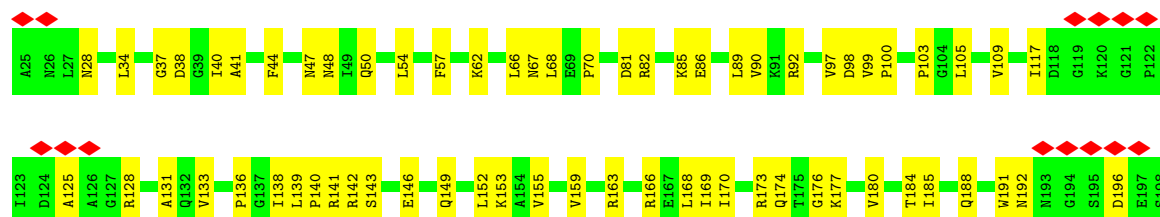
• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

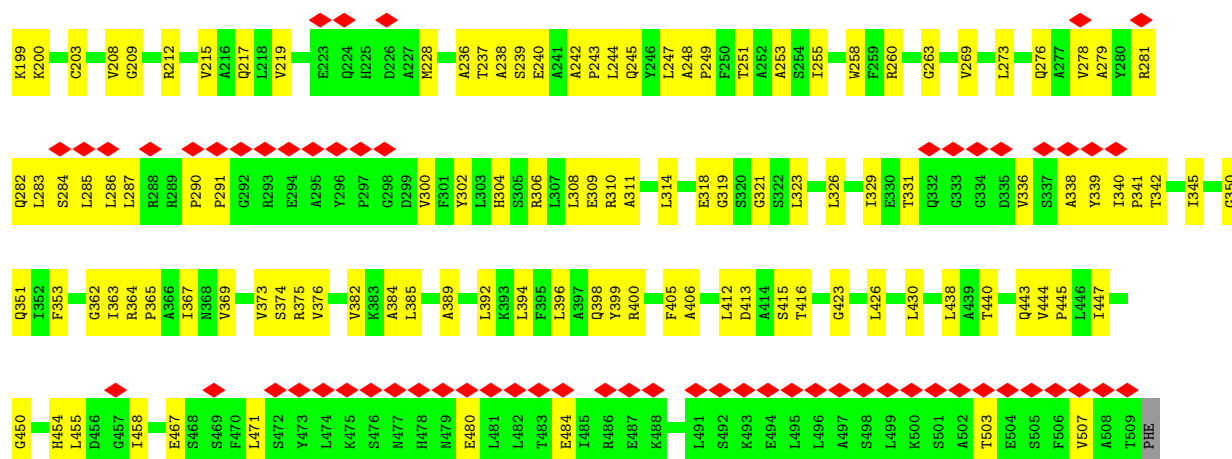


• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

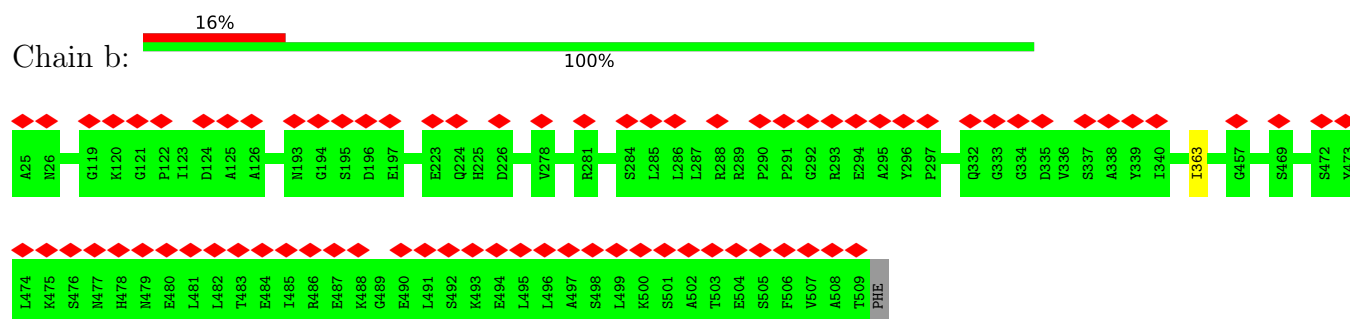


• Molecule 2: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

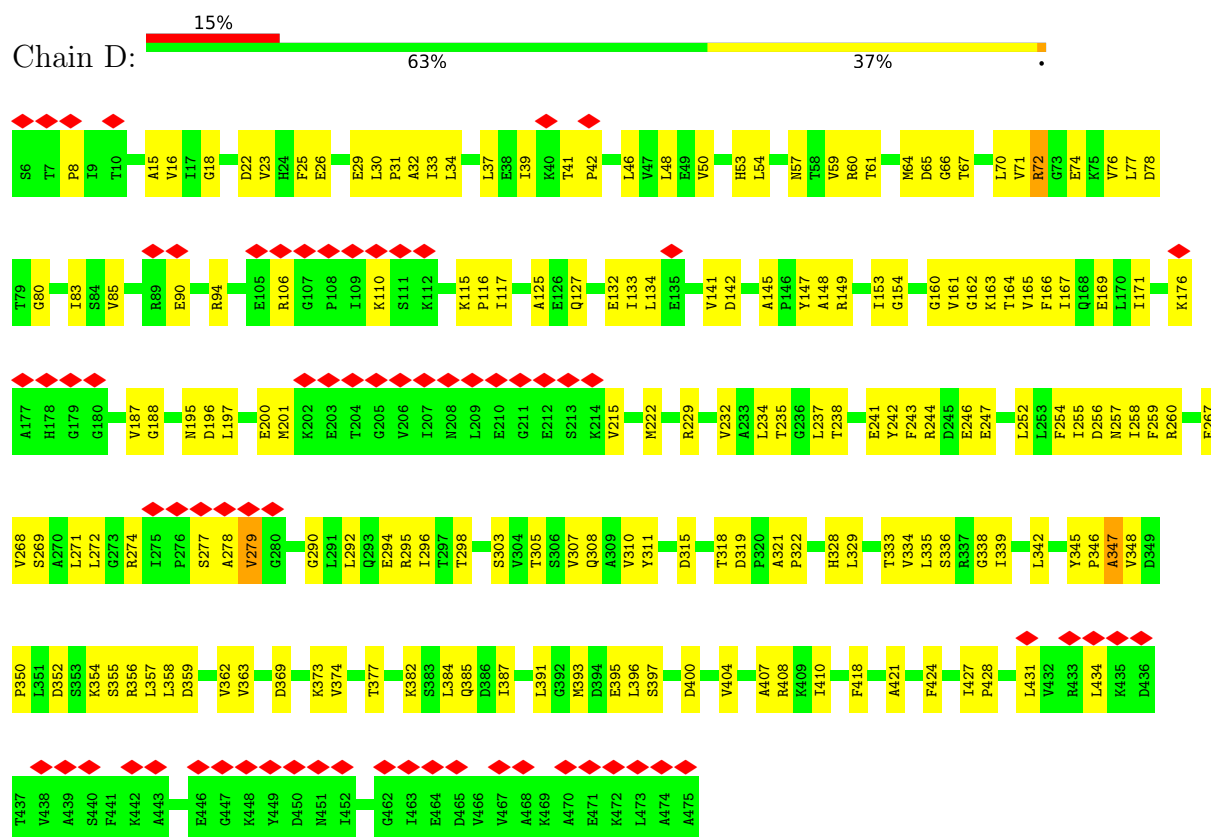




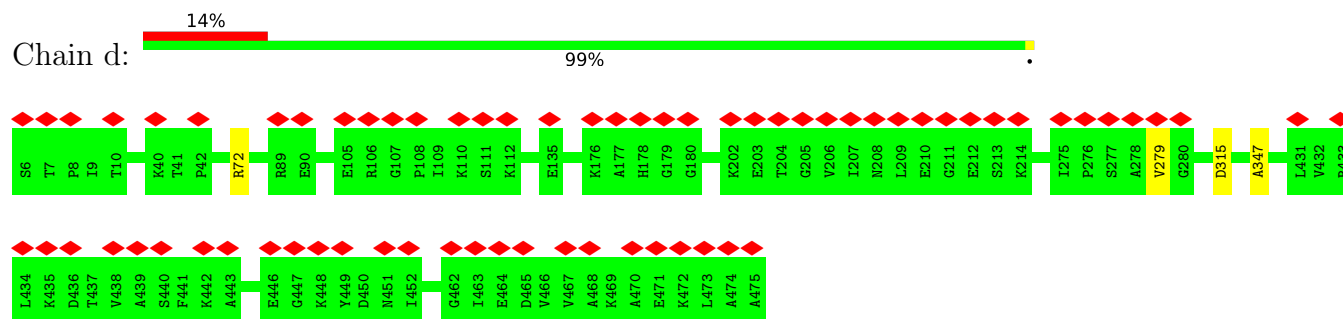
• Molecule 2: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL



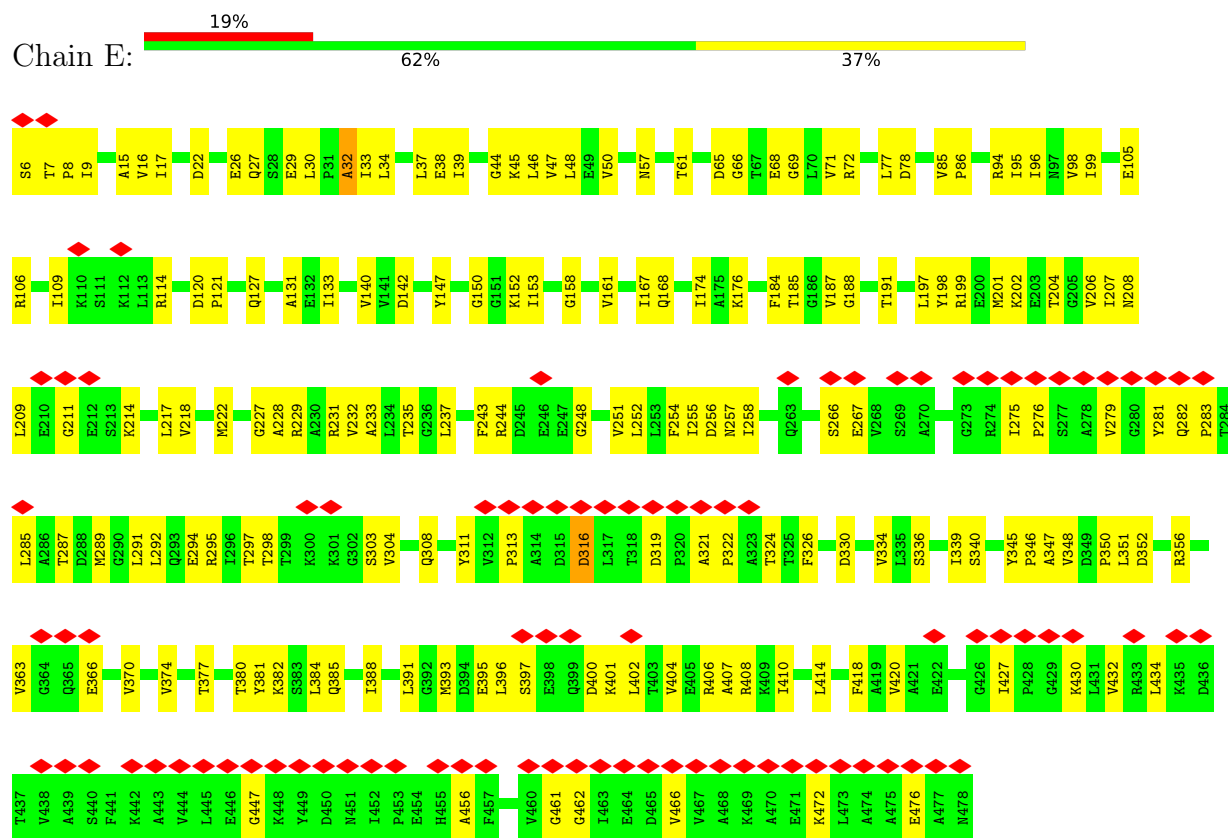
• Molecule 3: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL



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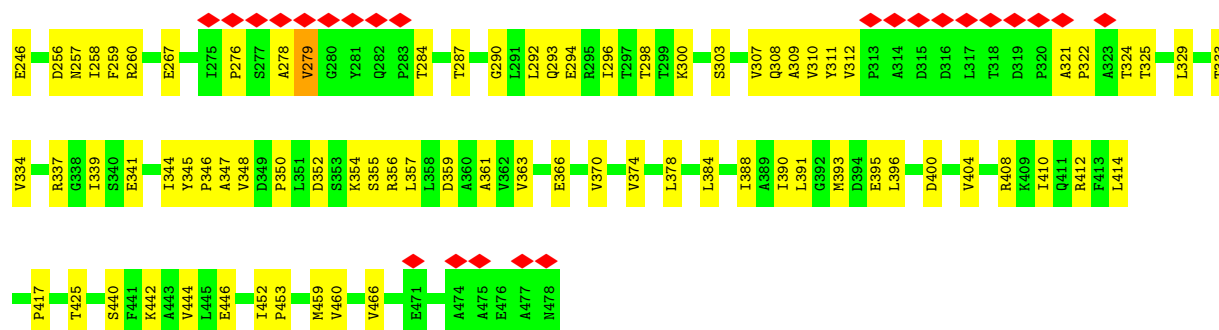


• Molecule 4: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

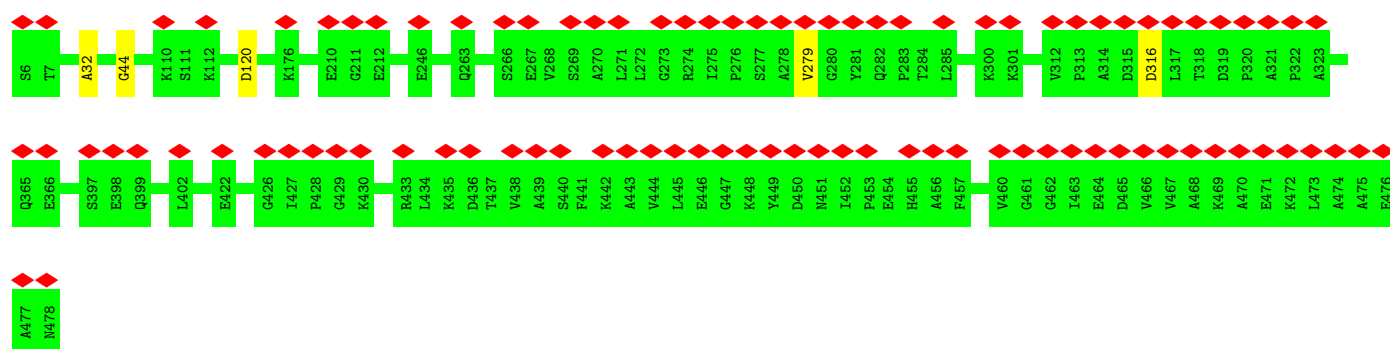


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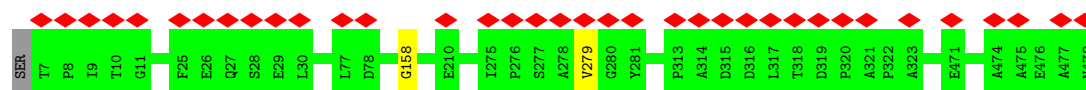




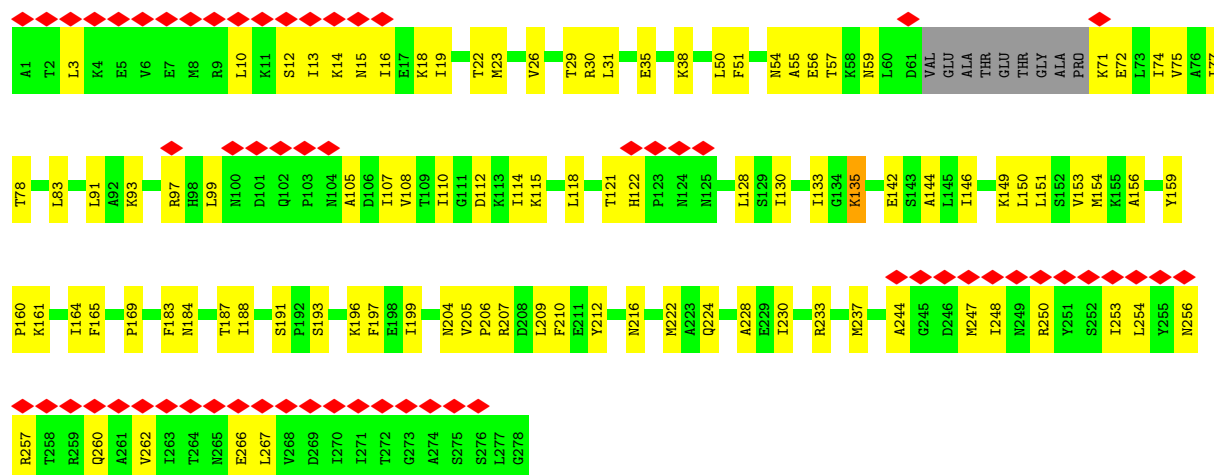
• Molecule 4: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL



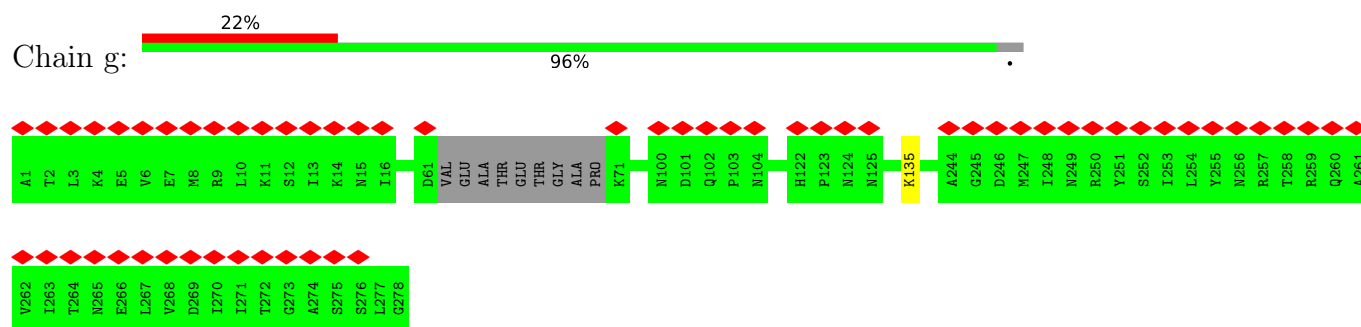
• Molecule 4: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL



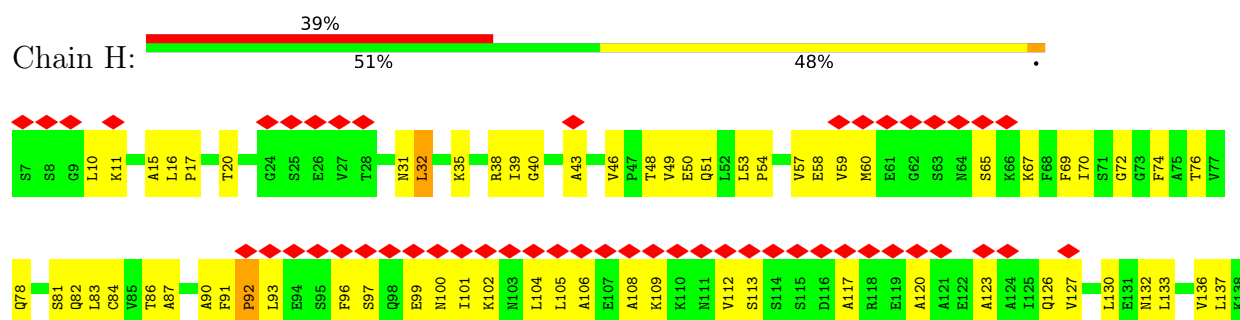
• Molecule 5: ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL



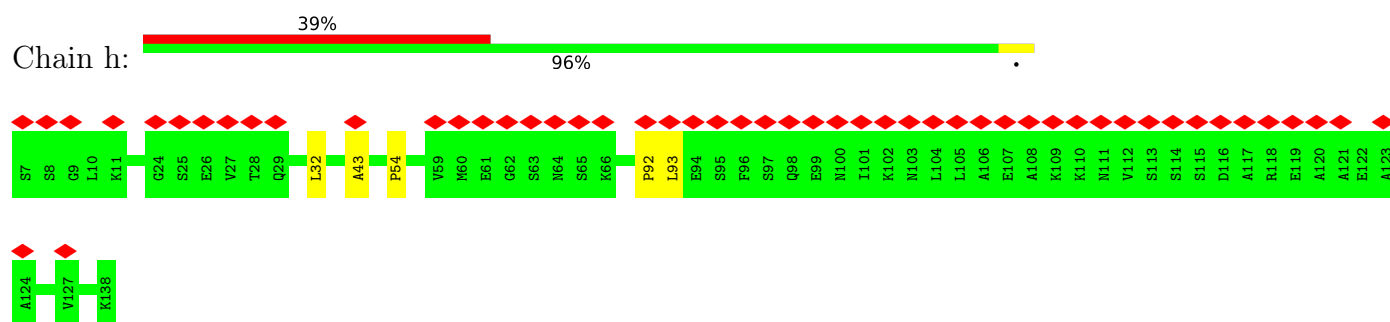
- Molecule 5: ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL



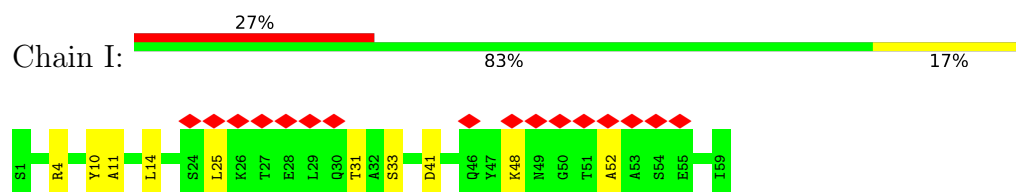
- Molecule 6: ATP SYNTHASE SUBUNIT DELTA, MITOCHONDRIAL



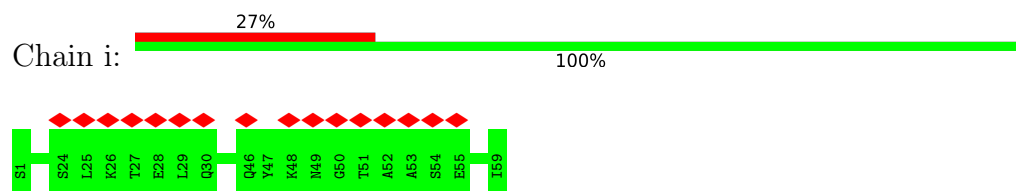
- Molecule 6: ATP SYNTHASE SUBUNIT DELTA, MITOCHONDRIAL



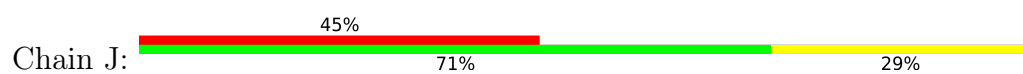
- Molecule 7: ATP SYNTHASE SUBUNIT EPSILON, MITOCHONDRIAL



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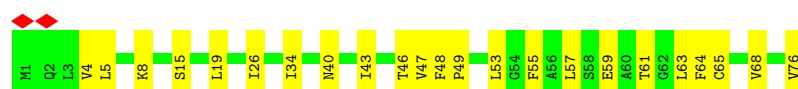
- Molecule 8: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL



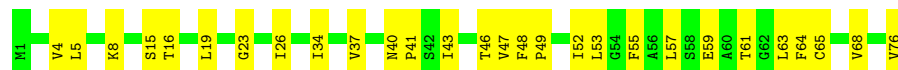
- Molecule 8: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL



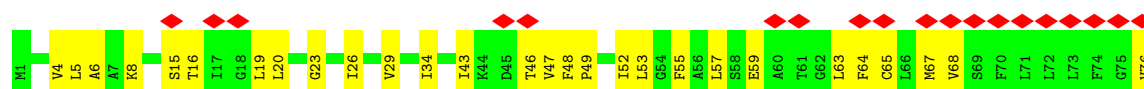
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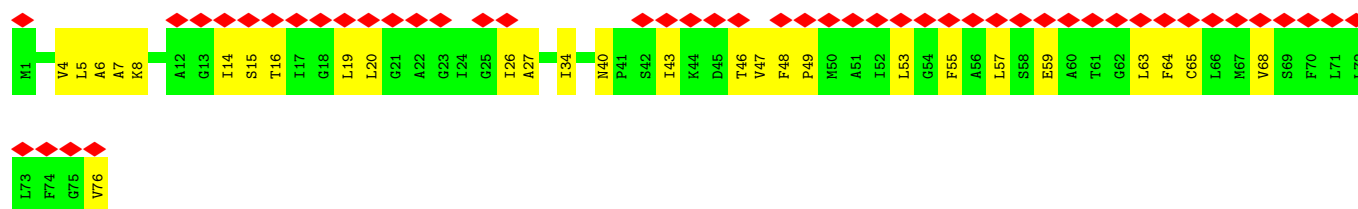
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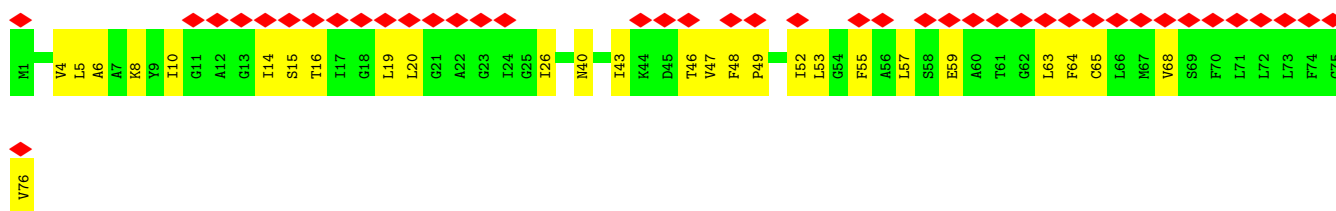


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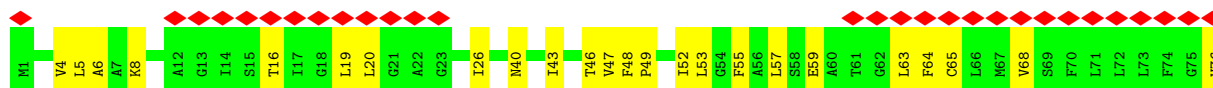
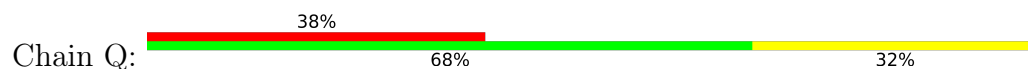


- Molecule 8: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

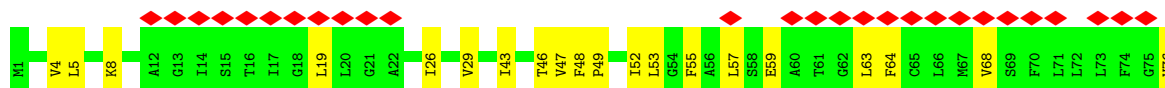
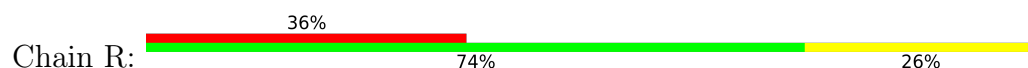




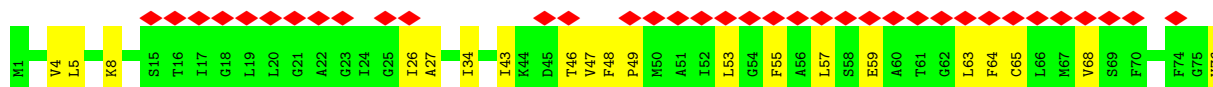
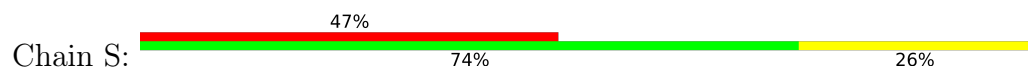
• Molecule 8: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL



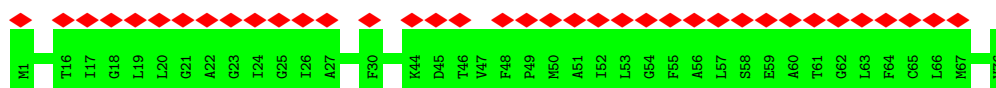
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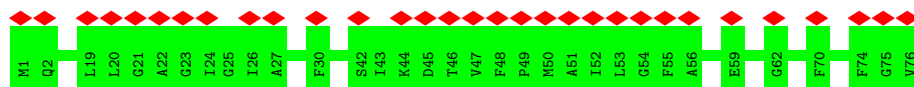
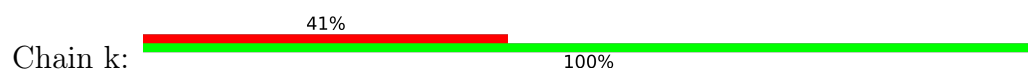
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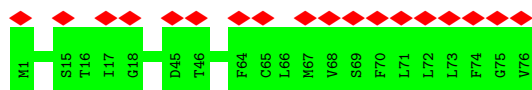
- Molecule 8: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

Chain m: 100%

There are no outlier residues recorded for this chain.

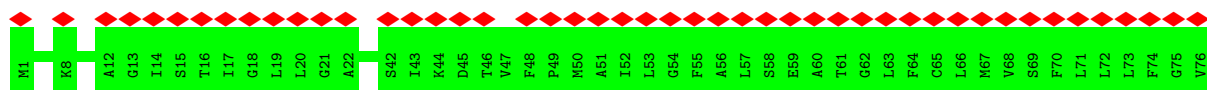
- Molecule 8: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

Chain n: 24% 100%



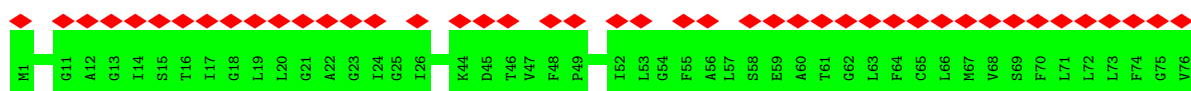
- Molecule 8: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

Chain o: 62% 100%



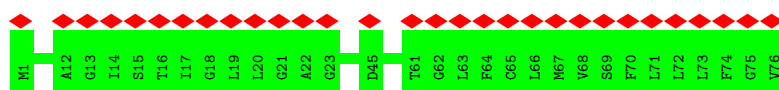
- Molecule 8: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

Chain p: 58% 100%



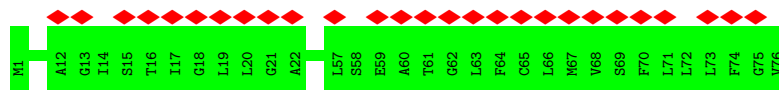
- Molecule 8: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

Chain q: 39% 100%



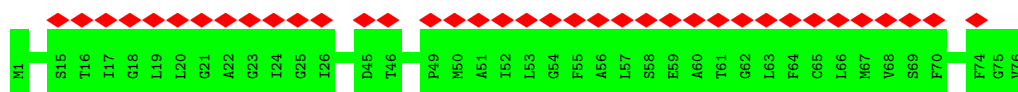
- Molecule 8: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

Chain r: 36% 100%



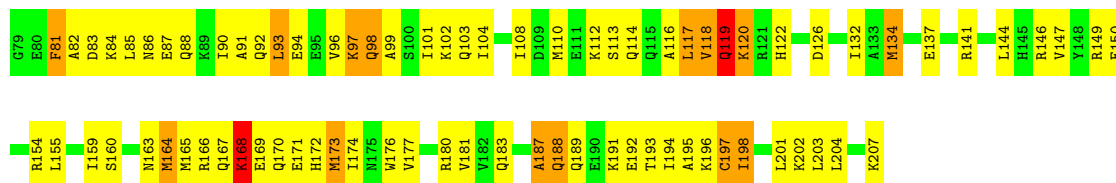
- Molecule 8: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

Chain s: 49% 100%



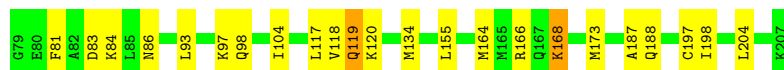
• Molecule 9: ATP SYNTHASE SUBUNIT B, MITOCHONDRIAL

Chain T: 39% 49% 11%



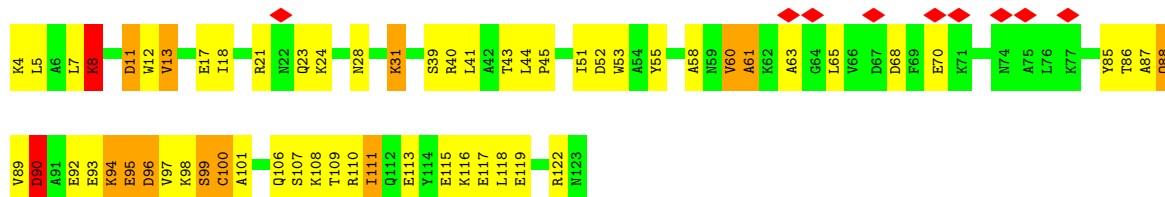
• Molecule 9: ATP SYNTHASE SUBUNIT B, MITOCHONDRIAL

Chain t: 82% 16%



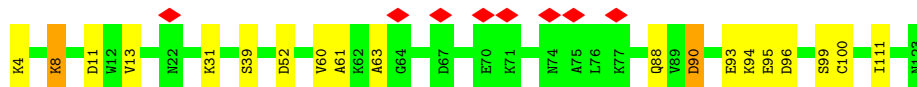
• Molecule 10: ATP SYNTHASE SUBUNIT D, MITOCHONDRIAL

Chain U: 8% 50% 38% 10%



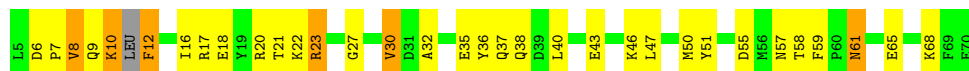
• Molecule 10: ATP SYNTHASE SUBUNIT D, MITOCHONDRIAL

Chain u: 7% 84% 14%



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

Chain V: 48% 41% 9%

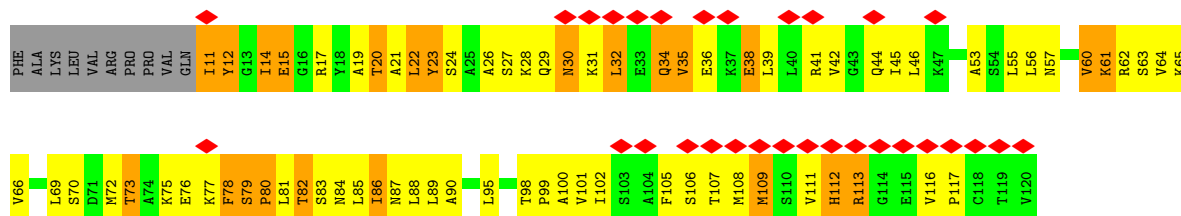


• Molecule 11: ATP SYNTHASE-COUPLING FACTOR 6, MITOCHONDRIAL

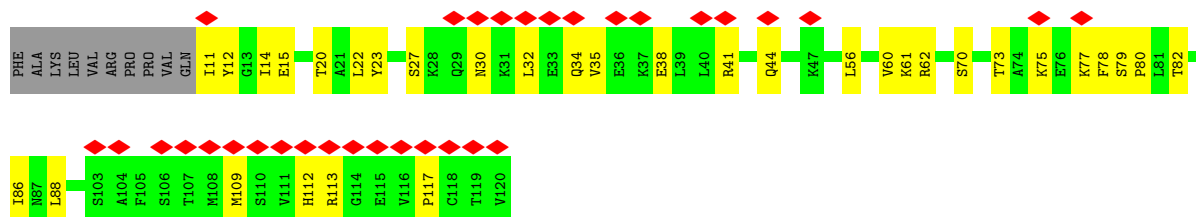
Chain v: 86% 12%



• Molecule 12: ATP SYNTHASE SUBUNIT O, MITOCHONDRIAL



• Molecule 12: ATP SYNTHASE SUBUNIT O, MITOCHONDRIAL



4 Experimental information

Property	Value	Source
EM reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of tilted images used	121	Depositor
Resolution determination method	Not provided	
CTF correction method	Not provided	
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
Maximum voxel value	11.211	Depositor
Minimum voxel value	0.610	Depositor
Average voxel value	5.106	Depositor
Voxel value standard deviation	1.447	Depositor
Recommended contour level	7.7	Depositor
Tomogram size (\AA)	518.4, 172.8, 345.6	wwPDB
Tomogram dimensions	90, 30, 60	wwPDB
Tomogram angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Grid spacing (\AA)	5.76, 5.76, 5.76	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.28	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
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
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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
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%)
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
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:472:SER:HB2	10:U:31:LYS:HE3	1.12	1.10
1:A:476:SER:HB3	10:U:12:TRP:H	0.94	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:176:TRP:HZ3	11:V:22:LYS:HB2	1.19	1.00
9:T:180:ARG:NH2	11:V:21:THR:HG21	1.75	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:HZ2	1.35	0.93
9:T:116:ALA:HB1	9:T:120:LYS:CD	1.98	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:H	9:T:117:LEU:HD23	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:A:122:PRO:HD2	9:T:159:ILE:HG21	1.33	0.81
1:C:378:SER:HB2	1:C:386:LYS:HE2	1.63	0.81
1:A:122:PRO:HG2	9:T:159:ILE:HG21	1.63	0.81
8:K:4:VAL:CG2	8:L:5:LEU:HD23	2.07	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
3:D:125:ALA:HB1	11:V:50:MET:CG	2.19	0.73
9:T:176:TRP:CE3	11:V:22:LYS:HD3	2.23	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
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
9:T:116:ALA:CB	9:T:120:LYS:HD2	2.23	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:A:120:LYS:N	11:V:51:TYR:OH	2.26	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: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
1:A:476:SER:HB2	10:U:12:TRP:H	1.54	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
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:51:ALA:HB3	4:E:69:GLY:H	1.60	0.66
1:A:473:TYR:HE1	10:U:13:VAL:CG1	2.03	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:OXT	1:C:510:PHE:HD1	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:OXT	1:C:510:PHE:CD1	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:39:LEU:HD21	12:W:85:LEU:HD21	1.78	0.65
12:W:65:LYS:O	12:W:69:LEU:HD13	1.96	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:404:ALA:HB3	5:G:22:THR:HG21	1.80	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:106:ARG:HE	4:F:209:LEU:HD22	1.62	0.64
4:F:201:MET:CE	4:F:215:VAL:HG11	2.28	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:H	1:C:166:ARG:HD2	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)
9:T:203:LEU:HG	12:W:84:ASN:ND2	2.14	0.63
12:W:39:LEU:HD12	12:W:105:PHE:CD2	2.34	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
2:B:50:GLN:HB3	4:F:69:GLY:HA2	1.81	0.61
3:D:336:SER:HB2	3:D:339:ILE:HG12	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:145:ALA:HB1	3:D:355:SER:HB2	1.83	0.61
3:D:154:GLY:HA3	3:D:329:LEU:HD13	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:H	4:E:282:GLN:CD	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
1:A:27:LEU:HD23	9:T:202:LYS:CE	2.19	0.60
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: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:120:LYS:CA	11:V:51:TYR:OH	2.49	0.60
1:A:476:SER:CB	10:U:12:TRP:CB	2.77	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
2:B:138:ILE:CD1	4:F:95:ILE:HG21	2.32	0.59
2:B:405:PHE:HZ	4:F:393:MET:SD	2.25	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
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:HB3	4:F:106:ARG:NH1	2.18	0.59
10:U:88:GLN:O	10:U:89:VAL:C	2.41	0.59
6:H:16:LEU:HD11	6:H:90:ALA:HB2	1.85	0.59
6:H:99:GLU:OE2	6:H:137:LEU:HD13	2.03	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:HB3	4:F:106:ARG:HH11	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
5:G:50:LEU:HG	6:H:78:GLN:NE2	2.17	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
4:F:102:PRO:HG2	4:F:108:PRO:HA	1.86	0.57
12:W:14:ILE:HD13	12:W:14:ILE:O	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
1:A:473:TYR:CE1	10:U:13:VAL:CB	2.87	0.57
2:B:248:ALA:N	2:B:249:PRO:HD2	2.19	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
5:G:212:TYR:OH	6:H:86:THR:HG22	2.04	0.57
6:H:59:VAL:O	6:H:65:SER:HB2	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:A:382:VAL:HG12	1:A:384:ALA:H	1.70	0.56
1:C:148:VAL:HB	1:C:161:ILE:HB	1.87	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:N	1:C:273:LEU:HD12	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:E:319:ASP:HA	5:G:260:GLN:HE22	1.71	0.56
4:F:293:GLN:HE22	4:F:308:GLN:HE22	1.54	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: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
9:T:198:ILE:HA	9:T:201:LEU:HD12	1.87	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:121:GLY:HA2	9:T:160:SER:OG	2.07	0.55
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
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:14:ILE:HD13	12:W:14:ILE:C	2.27	0.55
12:W:32:LEU:HD12	12:W:109:MET:CB	2.36	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:33:ILE:O	4:E:34:LEU:HB2	2.07	0.55
4:E:319:ASP:HA	5:G:260:GLN:NE2	2.22	0.55
1:A:301:PHE:HD2	4:E:229:ARG:HH12	1.54	0.55
3:D:94:ARG:NH2	3:D:106:ARG:HB2	2.22	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:68:LEU:HD23	4:F:72:ARG:HG3	1.89	0.55
2:B:283:LEU:O	2:B:287:LEU:HG	2.07	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:HG23	8:K:43:ILE:O	2.07	0.54
1:C:291:PRO:HB2	1:C:295:ALA:HA	1.89	0.54
4:E:316:ASP:OD2	5:G:256:ASN:HB3	2.08	0.54
5:G:193:SER:HB3	5:G:196:LYS:NZ	2.23	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:82:ARG:HD3	4:F:34:LEU:HD12	1.90	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
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:253:ALA:HB3	2:B:310:ARG:NH2	2.24	0.53
2:B:309:GLU:HG3	4:F:223:ASN:HB3	1.91	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
2:B:143:SER:HB2	4:F:196:ASP:OD1	2.10	0.52
1:C:34:LEU:HD11	1:C:44:PHE:HB2	1.92	0.52
1:C:260:ARG:O	1:C:321:GLY:HA3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:360:TYR:HE1	4:F:354:LYS:HZ1	1.61	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
9:T:201:LEU:HD12	11:V:7:PRO:CB	2.35	0.52
10:U:88:GLN:CD	10:U:88:GLN:H	2.13	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:67:ASN:ND2	1:C:287:LEU:HD13	2.25	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
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:160:PRO:HG3	1:C:381:GLN:HB2	1.91	0.52
1:C:274:SER:OG	1:C:329:ILE:HG23	2.10	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:E:276:PRO:HB2	5:G:267:LEU:HD21	1.92	0.51
4:F:370:VAL:O	4:F:374:VAL:HG23	2.11	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:30:THR:HB	1:A:89:LEU:HD11	1.94	0.51
1:A:205:TYR:CE2	1:A:218:LEU:HD13	2.46	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
9:T:201:LEU:HD11	11:V:7:PRO:HB3	1.93	0.50
10:U:86:THR:HG22	10:U:86:THR:O	2.11	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:54:LEU:HD21	4:F:60:ARG:HE	1.77	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
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:O	1:A:306:ARG:HG2	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:HD12	4:E:153:ILE:N	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:70:PRO:HD3	4:F:15:ALA:HB2	1.93	0.49
2:B:300:VAL:HG11	2:B:339:TYR:HE2	1.77	0.49
1:C:64:MET:HE2	1:C:97:VAL:HG21	1.93	0.49
1:C:282:GLN:CD	4:F:284:THR:HG22	2.33	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
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:43:VAL:HG11	1:A:90:VAL:CG1	2.42	0.49
1:A:105:LEU:HD12	1:A:255:ILE:HG23	1.95	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:N	10:U:96:ASP:OD1	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:A:217:GLN:HG2	3:D:356:ARG:NH1	2.27	0.49
1:C:191:TRP:O	1:C:200:LYS:HG2	2.13	0.49
4:E:72:ARG:HG3	4:E:72:ARG:HH11	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:96:ILE:HG21	4:E:68:GLU:OE2	2.13	0.49
1:A:395:PHE:HE2	1:A:451:VAL:HG13	1.78	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
1:A:408:PHE:HE2	5:G:22:THR:HG1	1.65	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
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:68:LEU:HB3	3:D:72:ARG:HD3	1.95	0.48
1:C:165:GLN:OE1	1:C:376:VAL:HG21	2.13	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:387:GLN:OE1	1:C:491:LEU:HB2	2.14	0.48
1:C:421:VAL:HG13	1:C:425:ARG:NH1	2.28	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:54:LEU:HD11	3:D:60:ARG:HH21	1.78	0.48
3:D:169:GLU:HG2	3:D:418:PHE:CD1	2.49	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:99:VAL:HG11	1:A:251:THR:HG23	1.96	0.48
1:A:473:TYR:CD1	10:U:13:VAL:CG1	2.97	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:HG2	10:U:122:ARG:O	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:CD1	12:W:23:TYR:O	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:122:PRO:HD2	9:T:159:ILE:CB	2.37	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
2:B:364:ARG:HA	2:B:365:PRO:C	2.35	0.47
1:C:141:ARG:HB2	3:D:195:ASN:CG	2.35	0.47
3:D:8:PRO:HB2	3:D:77:LEU:HD11	1.96	0.47
3:D:145:ALA:CB	3:D:355:SER:HB2	2.44	0.47
3:D:319:ASP:O	3:D:322:PRO:HD2	2.15	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
12:W:79:SER:O	12:W:83:SER:HB3	2.15	0.47
1:A:105:LEU:HD13	1:A:255:ILE:HD13	1.97	0.47
13:A:1511:ATP:O2B	13:A:1511:ATP:O2A	2.33	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:473:TYR:HD1	10:U:13:VAL:HB	1.77	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
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:37:LEU:O	4:F:47:VAL:HA	2.15	0.46
4:F:163:LYS:O	4:F:167:ILE:HG13	2.16	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:43:VAL:HG12	1:A:44:PHE:N	2.31	0.46
1:A:106:LEU:HD11	1:A:259:PHE:CZ	2.51	0.46
1:A:402:VAL:O	1:A:402:VAL:HG12	2.16	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:33:ILE:HA	4:F:50:VAL:HG11	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
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:50:VAL:HG13	3:D:59:VAL:CG1	2.46	0.46
3:D:255:ILE:HB	3:D:308:GLN:HG2	1.97	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:51:PHE:CE1	6:H:49:VAL:HG21	2.52	0.45
5:G:254:LEU:HG	5:G:257:ARG:HH22	1.81	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:48:LEU:HD23	4:F:63:ALA:HA	1.99	0.45
4:F:140:VAL:CG2	4:F:348:VAL:HG21	2.45	0.45
4:F:140:VAL:CG1	4:F:414:LEU:HB3	2.47	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:50:LEU:HD23	6:H:84:CYS:SG	2.57	0.45
5:G:75:VAL:HB	5:G:164:ILE:HD13	1.98	0.45
6:H:91:PHE:HE1	6:H:97:SER:N	2.14	0.45
8:O:7:ALA:HB1	8:P:10:ILE:HG13	1.98	0.45
8:O:40:ASN:HD21	8:O:43:ILE:HG12	1.81	0.45
9:T:119:GLN:CG	9:T:120:LYS:N	2.78	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:A:242:ALA:N	1:A:243:PRO:CD	2.80	0.45
1:C:136:PRO:HB2	1:C:141:ARG:HE	1.82	0.45
3:D:165:VAL:HG11	3:D:421:ALA:HB2	1.99	0.45
3:D:357:LEU:HD22	3:D:362:VAL:HG11	1.98	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:57:PHE:CD1	2:B:90:VAL:HG22	2.49	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
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
1:A:119:GLY:C	11:V:51:TYR:CE1	2.86	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

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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
4:F:156:PHE:HB2	4:F:334:VAL:HG22	1.98	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:67:ASN:OD1	4:E:17:ILE:HG23	2.17	0.45
1:A:197:GLU:C	1:A:199:LYS:H	2.20	0.45
2:B:28:ASN:HB3	2:B:48:ASN:HD22	1.82	0.45
2:B:394:LEU:HD11	4:F:425:THR:HG22	1.99	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:54:LEU:HD13	2:B:97:VAL:HG22	1.99	0.45
2:B:196:ASP:OD2	2:B:199:LYS:HG2	2.17	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:HG2	1:C:166:ARG:O	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:60:VAL:HG11	12:W:65:LYS:HB2	1.98	0.44
12:W:63:SER:C	12:W:66:VAL:HG12	2.38	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:C	3:D:431:LEU:HD23	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:77:LEU:HD12	4:E:78:ASP:H	1.83	0.44
4:E:462:GLY:O	4:E:466:VAL:HG23	2.18	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:168:LEU:HD11	2:B:329:ILE:HG12	2.00	0.44
2:B:247:LEU:HG	2:B:251:THR:HG23	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:HA	10:U:94:LYS:HD2	1.71	0.44
12:W:23:TYR:CD1	12:W:23:TYR:C	2.91	0.44
12:W:31:LYS:HG3	12:W:81:LEU:HD21	2.00	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:109:MET:O	12:W:112:HIS:CE1	2.71	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:109:LYS:HD2	6:H:126:GLN:OE1	2.18	0.44
6:H:112:VAL:HB	6:H:123:ALA:HB2	1.99	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:6:ASP:N	11:V:7:PRO:CD	2.81	0.44
11:V:55:ASP:OD1	11:V:57:ASN:HB2	2.18	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:91:PHE:HZ	6:H:97:SER:HG	1.65	0.44
6:H:113:SER:HA	6:H:120:ALA:HB1	2.00	0.44
8:O:53:LEU:O	8:O:57:LEU:HG	2.18	0.44
9:T:176:TRP:CZ3	11:V:22:LYS:CA	2.91	0.44
10:U:55:TYR:O	10:U:58:ALA:HB3	2.18	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:55:VAL:HG21	1:A:75:ILE:HD13	2.00	0.44
1:A:67:ASN:HD21	1:A:287:LEU:HB3	1.83	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: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
5:G:149:LYS:O	5:G:153:VAL:HG12	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
2:B:82:ARG:HA	4:E:33:ILE:HB	1.99	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
4:E:377:THR:HG22	4:E:407:ALA:HB2	2.00	0.43
4:F:65:ASP:CG	4:F:66:GLY:H	2.21	0.43
4:F:145:ALA:HB1	4:F:355:SER:HB3	2.00	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:141:ARG:CZ	10:U:41:LEU:HD23	2.49	0.43
9:T:176:TRP:CZ3	11:V:22:LYS:CD	3.01	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)
1:A:119:GLY:C	11:V:50:MET:HE2	2.39	0.43
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:30:ARG:HB3	5:G:230:ILE:HD13	2.01	0.43
5:G:72:GLU:HG3	5:G:161:LYS:O	2.19	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
12:W:113:ARG:O	12:W:116:VAL:HG12	2.18	0.43
1:A:26:ASN:O	11:V:8:VAL:HG22	2.19	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: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:77:ILE:HD12	5:G:222:MET:HG2	2.01	0.43
5:G:209:LEU:HA	6:H:74:PHE:CE2	2.54	0.43
6:H:10:LEU:HG	6:H:81:SER:O	2.19	0.43
6:H:69:PHE:CE2	6:H:133:LEU:HD23	2.54	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:167:ILE:HD11	4:F:309:ALA:HB2	2.00	0.43
4:F:293:GLN:HE22	4:F:308:GLN:NE2	2.16	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:40:ILE:HG13	1:C:286:LEU:HB3	2.01	0.43
1:C:392:LEU:O	1:C:396:LEU:CD1	2.67	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:81:ASP:O	4:E:33:ILE:HD12	2.19	0.42
2:B:336:VAL:HG23	4:F:337:ARG:HH11	1.84	0.42
4:E:30:LEU:HD12	4:E:30:LEU:N	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:38:GLU:HB3	12:W:78:PHE:CD1	2.53	0.42
12:W:69:LEU:O	12:W:73:THR:OG1	2.35	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:64:MET:CE	3:D:83:ILE:HD11	2.49	0.42
3:D:404:VAL:O	3:D:408:ARG:HG3	2.19	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:30:THR:HA	1:C:90:VAL:O	2.19	0.42
1:C:118:ASP:OD1	1:C:120:LYS:HG3	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:46:LEU:O	1:A:49:ILE:HG22	2.19	0.42
1:A:212:ARG:CB	3:D:127:GLN:HE21	2.29	0.42
1:A:405:PHE:O	1:A:412:LEU:HD11	2.19	0.42
2:B:105:LEU:HD12	2:B:105:LEU:N	2.35	0.42
2:B:141:ARG:NH1	4:F:191:THR:HB	2.34	0.42
2:B:208:VAL:HG23	2:B:208:VAL:O	2.20	0.42
3:D:117:ILE:HA	3:D:238:THR:OG1	2.19	0.42
4:E:6:SER:C	4:E:8:PRO:CD	2.88	0.42
4:E:345:TYR:HA	4:E:346:PRO:C	2.40	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
9:T:176:TRP:CH2	11:V:30:VAL:HG21	2.55	0.42
10:U:92:GLU:O	10:U:95:GLU:N	2.53	0.42
10:U:99:SER:OG	10:U:100:CYS:N	2.52	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:HD12	1:C:105:LEU:N	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:46:LEU:HB3	1:A:49:ILE:HB	2.02	0.42
1:A:271:ASP:HA	1:A:272:ASP:HA	1.75	0.42
2:B:98:ASP:OD2	2:B:128:ARG:HB3	2.20	0.42
2:B:142:ARG:HA	4:F:195:ASN:HD21	1.85	0.42
2:B:375:ARG:HG2	15:F:1479:ADP:H5'1	2.02	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
4:E:30:LEU:HD12	4:E:30:LEU:H	1.84	0.42
4:E:150:GLY:HA2	4:E:304:VAL:O	2.20	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:47:VAL:CG1	8:O:34:ILE:HG23	2.50	0.42
8:N:64:PHE:HA	8:N:67:MET:HE3	2.00	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:375:ARG:NH1	4:F:190:ARG:CZ	2.83	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
4:F:220:GLY:HA3	4:F:232:VAL:HG21	2.02	0.42
8:J:6:ALA:HB2	8:S:4:VAL:HA	2.01	0.42
8:J:19:LEU:HD12	8:S:65:CYS:SG	2.60	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:9:ILE:HB	4:E:78:ASP:HB3	2.02	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
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:HD3	10:U:98:LYS:HA	1.79	0.41
12:W:78:PHE:CB	12:W:82:THR:HB	2.50	0.41
1:A:68:LEU:HD12	4:E:16:VAL:HB	2.03	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
2:B:159:VAL:HG12	2:B:374:SER:HB2	2.02	0.41
1:C:70:PRO:HA	3:D:72:ARG:NH2	2.36	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:33:ILE:HG22	3:D:34:LEU:N	2.35	0.41
3:D:176:LYS:HE2	3:D:176:LYS:HB3	1.87	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
1:A:332:GLN:HB3	3:D:318:THR:HB	2.03	0.41
2:B:47:ASN:HA	4:F:72:ARG:NH2	2.35	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
4:E:393:MET:HE1	4:E:408:ARG:HH21	1.86	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:HG22	1:A:352:ILE:O	2.20	0.41
1:C:68:LEU:HB2	3:D:16:VAL:HB	2.03	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
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:53:HIS:CD2	3:D:59:VAL:HG22	2.56	0.41
3:D:171:ILE:HG12	3:D:254:PHE:CZ	2.56	0.41
3:D:201:MET:CE	3:D:215:VAL:HG11	2.51	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:93:LEU:HD23	9:T:97:LYS:HE3	2.03	0.41
9:T:97:LYS:HD3	9:T:97:LYS:HA	1.82	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:HG13	4:E:258:ILE:O	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:HD23	12:W:55:LEU:HA	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:E:276:PRO:CB	5:G:267:LEU:HD21	2.51	0.41
4:F:97:ASN:HB2	4:F:103:ILE:CG2	2.51	0.41
4:F:300:LYS:HB2	4:F:300:LYS:HE3	1.90	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
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
3:D:37:LEU:HB2	3:D:48:LEU:HB2	2.03	0.41
3:D:384:LEU:HD22	3:D:387:ILE:HD12	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
5:G:22:THR:O	5:G:26:VAL:HG23	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:W:38:GLU:HG2	12:W:82:THR:OG1	2.21	0.41
12:W:57:ASN:ND2	12:W:60:VAL:CG2	2.84	0.41
12:W:112:HIS:ND1	12:W:113:ARG:N	2.69	0.41
2:B:82:ARG:HG3	4:E:33:ILE:O	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
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:145:ALA:CA	3:D:355:SER:HB2	2.51	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
4:F:95:ILE:HA	4:F:217:LEU:O	2.21	0.41
4:F:95:ILE:O	4:F:103:ILE:HG12	2.21	0.41
4:F:101:GLU:HA	4:F:102:PRO:HD3	1.95	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
9:T:203:LEU:CG	12:W:84:ASN:ND2	2.84	0.40
10:U:113:GLU:O	10:U:117:GLU:N	2.45	0.40
1:A:26:ASN:O	1:A:27:LEU:HB3	2.21	0.40
1:A:50:GLN:HG2	4:E:71:VAL:CG2	2.51	0.40
1:A:192:ASN:OD1	1:A:200:LYS:HB3	2.22	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
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:HE21	9:T:88:GLN:HB2	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:7:THR:HA	4:F:8:PRO:HD2	1.95	0.40
4:F:440:SER:O	4:F:444:VAL:HG23	2.21	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:52:GLU:OE1	4:E:68:GLU:HB2	2.21	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
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: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
9:T:146:ARG:O	9:T:150:GLU:HG3	2.21	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:HD23	12:W:39:LEU:HA	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%)	19	60
1	C	483/485 (100%)	450 (93%)	33 (7%)	0	100	100
1	a	483/485 (100%)	444 (92%)	35 (7%)	4 (1%)	19	60
1	c	483/485 (100%)	450 (93%)	33 (7%)	0	100	100
2	B	483/486 (99%)	447 (92%)	35 (7%)	1 (0%)	47	81
2	b	483/486 (99%)	447 (92%)	35 (7%)	1 (0%)	47	81
3	D	468/470 (100%)	443 (95%)	22 (5%)	3 (1%)	25	66
3	d	468/470 (100%)	443 (95%)	22 (5%)	3 (1%)	25	66
4	E	471/473 (100%)	436 (93%)	32 (7%)	3 (1%)	25	66
4	F	470/473 (99%)	438 (93%)	30 (6%)	2 (0%)	34	72
4	e	471/473 (100%)	436 (93%)	32 (7%)	3 (1%)	25	66
4	f	470/473 (99%)	438 (93%)	30 (6%)	2 (0%)	34	72
5	G	265/278 (95%)	247 (93%)	17 (6%)	1 (0%)	34	72
5	g	265/278 (95%)	247 (93%)	17 (6%)	1 (0%)	34	72
6	H	130/132 (98%)	115 (88%)	11 (8%)	4 (3%)	4	27
6	h	130/132 (98%)	115 (88%)	11 (8%)	4 (3%)	4	27
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	17
9	t	127/129 (98%)	100 (79%)	19 (15%)	8 (6%)	1	17
10	U	118/120 (98%)	88 (75%)	24 (20%)	6 (5%)	2	19
10	u	118/120 (98%)	88 (75%)	24 (20%)	6 (5%)	2	19
11	V	60/66 (91%)	52 (87%)	6 (10%)	2 (3%)	4	26
11	v	61/66 (92%)	52 (85%)	7 (12%)	2 (3%)	4	26
12	W	108/120 (90%)	92 (85%)	8 (7%)	8 (7%)	1	14
12	w	108/120 (90%)	92 (85%)	8 (7%)	8 (7%)	1	14
All	All	8927/9072 (98%)	8182 (92%)	661 (7%)	84 (1%)	21	57

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 [i](#)

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%)	92	95
1	C	391/391 (100%)	390 (100%)	1 (0%)	92	95
1	a	391/391 (100%)	390 (100%)	1 (0%)	92	95
1	c	391/391 (100%)	390 (100%)	1 (0%)	92	95
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%)	92	95
3	d	380/380 (100%)	379 (100%)	1 (0%)	92	95
4	E	382/382 (100%)	380 (100%)	2 (0%)	88	93
4	F	381/382 (100%)	381 (100%)	0	100	100
4	e	382/382 (100%)	380 (100%)	2 (0%)	88	93
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%)	78	87
6	h	111/111 (100%)	110 (99%)	1 (1%)	78	87
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%)	4	18
9	t	118/118 (100%)	103 (87%)	15 (13%)	4	18
10	U	104/104 (100%)	90 (86%)	14 (14%)	4	17
10	u	104/104 (100%)	90 (86%)	14 (14%)	4	17
11	V	58/60 (97%)	52 (90%)	6 (10%)	7	25
11	v	58/60 (97%)	52 (90%)	6 (10%)	7	25
12	W	95/104 (91%)	70 (74%)	25 (26%)	0	3
12	w	95/104 (91%)	70 (74%)	25 (26%)	0	3
All	All	7232/7312 (99%)	7100 (98%)	132 (2%)	61	77

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

Sometimes 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 monosaccharides 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$
15	ADP	d	1476	14	24,29,29	1.02	1 (4%)	29,45,45	1.42	4 (13%)
15	ADP	f	1479	14	24,29,29	0.93	1 (4%)	29,45,45	1.49	5 (17%)
13	ATP	b	1510	14	26,33,33	0.95	1 (3%)	31,52,52	1.50	5 (16%)
15	ADP	F	1479	14	24,29,29	0.93	1 (4%)	29,45,45	1.49	5 (17%)
13	ATP	C	1511	14	26,33,33	0.96	1 (3%)	31,52,52	1.61	5 (16%)
13	ATP	c	1511	14	26,33,33	0.95	1 (3%)	31,52,52	1.61	5 (16%)
13	ATP	B	1510	14	26,33,33	0.95	1 (3%)	31,52,52	1.50	5 (16%)
13	ATP	A	1511	14	26,33,33	0.92	1 (3%)	31,52,52	1.54	5 (16%)
15	ADP	D	1476	14	24,29,29	1.01	1 (4%)	29,45,45	1.41	4 (13%)
13	ATP	a	1511	14	26,33,33	0.90	1 (3%)	31,52,52	1.53	5 (16%)

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
15	ADP	d	1476	14	-	0/12/32/32	0/3/3/3
15	ADP	f	1479	14	-	1/12/32/32	0/3/3/3
13	ATP	b	1510	14	-	6/18/38/38	0/3/3/3
15	ADP	F	1479	14	-	1/12/32/32	0/3/3/3
13	ATP	C	1511	14	-	6/18/38/38	0/3/3/3
13	ATP	c	1511	14	-	6/18/38/38	0/3/3/3
13	ATP	B	1510	14	-	6/18/38/38	0/3/3/3
13	ATP	A	1511	14	-	6/18/38/38	0/3/3/3
15	ADP	D	1476	14	-	0/12/32/32	0/3/3/3
13	ATP	a	1511	14	-	6/18/38/38	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	D	1476	ADP	C5-C4	2.60	1.47	1.40
15	d	1476	ADP	C5-C4	2.60	1.47	1.40
13	c	1511	ATP	C5-C4	2.48	1.47	1.40
13	C	1511	ATP	C5-C4	2.48	1.47	1.40
13	B	1510	ATP	C5-C4	2.46	1.47	1.40
13	a	1511	ATP	C5-C4	2.46	1.47	1.40
13	b	1510	ATP	C5-C4	2.45	1.47	1.40
13	A	1511	ATP	C5-C4	2.45	1.47	1.40
15	f	1479	ADP	C5-C4	2.37	1.47	1.40
15	F	1479	ADP	C5-C4	2.35	1.47	1.40

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	c	1511	ATP	PB-O3B-PG	-4.51	117.35	132.83
13	C	1511	ATP	PB-O3B-PG	-4.49	117.42	132.83
13	A	1511	ATP	PA-O3A-PB	-3.85	119.61	132.83
13	a	1511	ATP	PA-O3A-PB	-3.82	119.71	132.83
15	F	1479	ADP	C3'-C2'-C1'	3.71	106.57	100.98
15	f	1479	ADP	C3'-C2'-C1'	3.71	106.56	100.98
13	B	1510	ATP	PA-O3A-PB	-3.65	120.31	132.83
13	b	1510	ATP	PA-O3A-PB	-3.64	120.34	132.83
13	A	1511	ATP	PB-O3B-PG	-3.54	120.67	132.83
13	a	1511	ATP	PB-O3B-PG	-3.53	120.72	132.83
15	f	1479	ADP	N3-C2-N1	-3.32	123.49	128.68
15	F	1479	ADP	N3-C2-N1	-3.29	123.53	128.68
15	d	1476	ADP	C3'-C2'-C1'	3.27	105.90	100.98
15	D	1476	ADP	C3'-C2'-C1'	3.24	105.86	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	c	1511	ATP	N3-C2-N1	-3.21	123.67	128.68
15	d	1476	ADP	N3-C2-N1	-3.20	123.67	128.68
13	B	1510	ATP	N3-C2-N1	-3.19	123.69	128.68
13	b	1510	ATP	N3-C2-N1	-3.19	123.70	128.68
13	C	1511	ATP	N3-C2-N1	-3.18	123.70	128.68
13	c	1511	ATP	PA-O3A-PB	-3.18	121.92	132.83
13	C	1511	ATP	PA-O3A-PB	-3.18	121.92	132.83
15	D	1476	ADP	N3-C2-N1	-3.16	123.74	128.68
13	b	1510	ATP	PB-O3B-PG	-3.12	122.13	132.83
13	B	1510	ATP	PB-O3B-PG	-3.12	122.13	132.83
15	d	1476	ADP	C4-C5-N7	-2.97	106.30	109.40
13	a	1511	ATP	N3-C2-N1	-2.96	124.06	128.68
13	A	1511	ATP	N3-C2-N1	-2.95	124.07	128.68
15	D	1476	ADP	C4-C5-N7	-2.95	106.33	109.40
13	b	1510	ATP	C3'-C2'-C1'	2.90	105.35	100.98
13	B	1510	ATP	C3'-C2'-C1'	2.85	105.27	100.98
15	F	1479	ADP	C4-C5-N7	-2.72	106.57	109.40
15	f	1479	ADP	C4-C5-N7	-2.71	106.57	109.40
15	D	1476	ADP	PA-O3A-PB	-2.68	123.64	132.83
15	d	1476	ADP	PA-O3A-PB	-2.67	123.66	132.83
13	a	1511	ATP	C3'-C2'-C1'	2.64	104.96	100.98
13	b	1510	ATP	C4-C5-N7	-2.64	106.65	109.40
13	B	1510	ATP	C4-C5-N7	-2.62	106.67	109.40
13	C	1511	ATP	C3'-C2'-C1'	2.61	104.91	100.98
13	c	1511	ATP	C3'-C2'-C1'	2.60	104.89	100.98
13	A	1511	ATP	C3'-C2'-C1'	2.60	104.89	100.98
15	F	1479	ADP	PA-O3A-PB	-2.57	124.00	132.83
15	f	1479	ADP	PA-O3A-PB	-2.56	124.04	132.83
13	C	1511	ATP	C4-C5-N7	-2.53	106.76	109.40
13	c	1511	ATP	C4-C5-N7	-2.51	106.78	109.40
13	A	1511	ATP	N6-C6-N1	2.08	122.89	118.57
15	F	1479	ADP	C1'-N9-C4	-2.08	122.99	126.64
13	a	1511	ATP	N6-C6-N1	2.07	122.86	118.57
15	f	1479	ADP	C1'-N9-C4	-2.06	123.03	126.64

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	1511	ATP	C5'-O5'-PA-O1A
13	A	1511	ATP	C5'-O5'-PA-O2A
13	A	1511	ATP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
13	A	1511	ATP	C3'-C4'-C5'-O5'
13	B	1510	ATP	C5'-O5'-PA-O1A
13	a	1511	ATP	C5'-O5'-PA-O1A
13	a	1511	ATP	C5'-O5'-PA-O2A
13	a	1511	ATP	O4'-C4'-C5'-O5'
13	a	1511	ATP	C3'-C4'-C5'-O5'
13	b	1510	ATP	C5'-O5'-PA-O1A
13	B	1510	ATP	C3'-C4'-C5'-O5'
13	b	1510	ATP	C3'-C4'-C5'-O5'
13	B	1510	ATP	O4'-C4'-C5'-O5'
13	b	1510	ATP	O4'-C4'-C5'-O5'
13	c	1511	ATP	O4'-C4'-C5'-O5'
13	B	1510	ATP	C5'-O5'-PA-O3A
13	b	1510	ATP	C5'-O5'-PA-O3A
13	C	1511	ATP	O4'-C4'-C5'-O5'
13	B	1510	ATP	PA-O3A-PB-O1B
13	b	1510	ATP	PA-O3A-PB-O1B
13	A	1511	ATP	PA-O3A-PB-O2B
13	C	1511	ATP	PG-O3B-PB-O2B
13	C	1511	ATP	PA-O3A-PB-O2B
13	a	1511	ATP	PA-O3A-PB-O2B
13	c	1511	ATP	PG-O3B-PB-O2B
13	c	1511	ATP	PA-O3A-PB-O2B
13	A	1511	ATP	C5'-O5'-PA-O3A
13	a	1511	ATP	C5'-O5'-PA-O3A
13	C	1511	ATP	C3'-C4'-C5'-O5'
13	c	1511	ATP	C3'-C4'-C5'-O5'
13	B	1510	ATP	PA-O3A-PB-O2B
13	C	1511	ATP	PG-O3B-PB-O1B
13	C	1511	ATP	PA-O3A-PB-O1B
13	b	1510	ATP	PA-O3A-PB-O2B
13	c	1511	ATP	PG-O3B-PB-O1B
13	c	1511	ATP	PA-O3A-PB-O1B
15	F	1479	ADP	C5'-O5'-PA-O1A
15	f	1479	ADP	C5'-O5'-PA-O1A

There are no ring outliers.

5 monomers are involved in 11 short contacts:

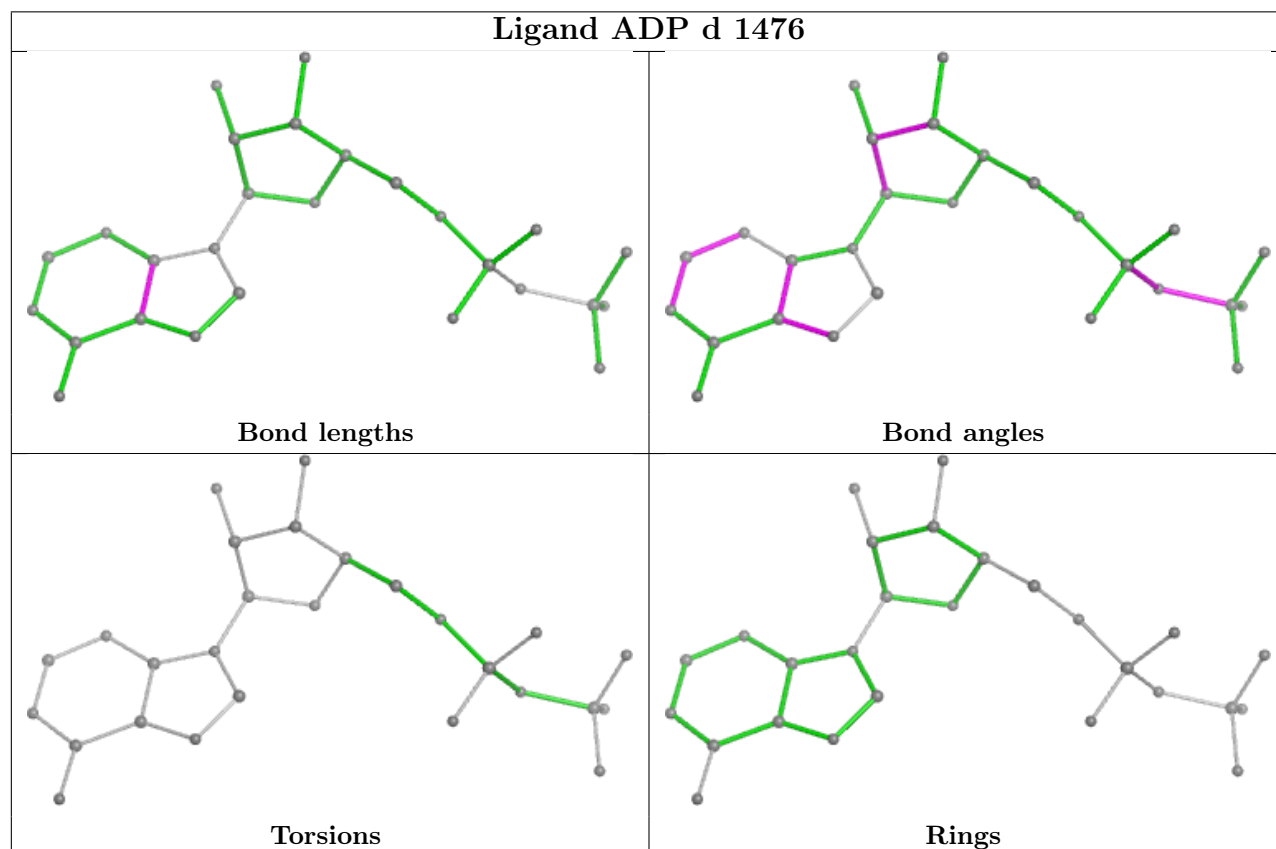
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	F	1479	ADP	2	0
13	C	1511	ATP	1	0

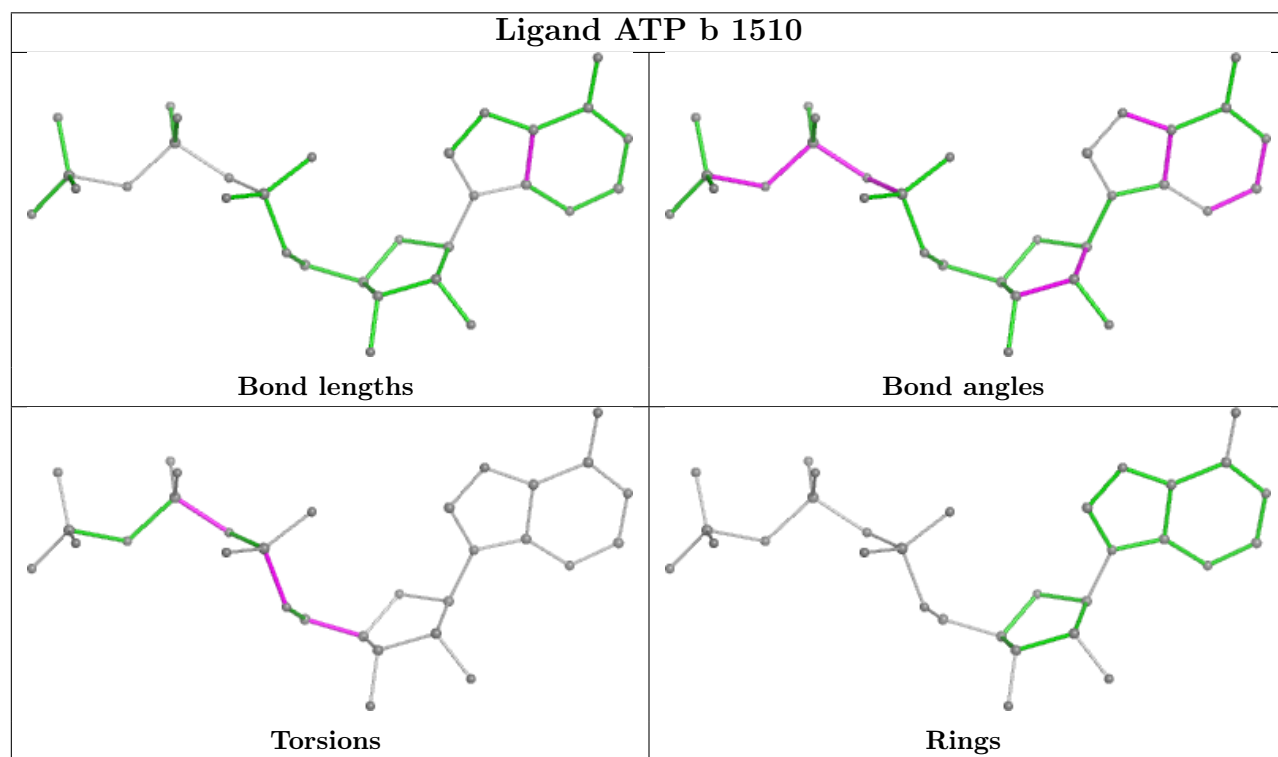
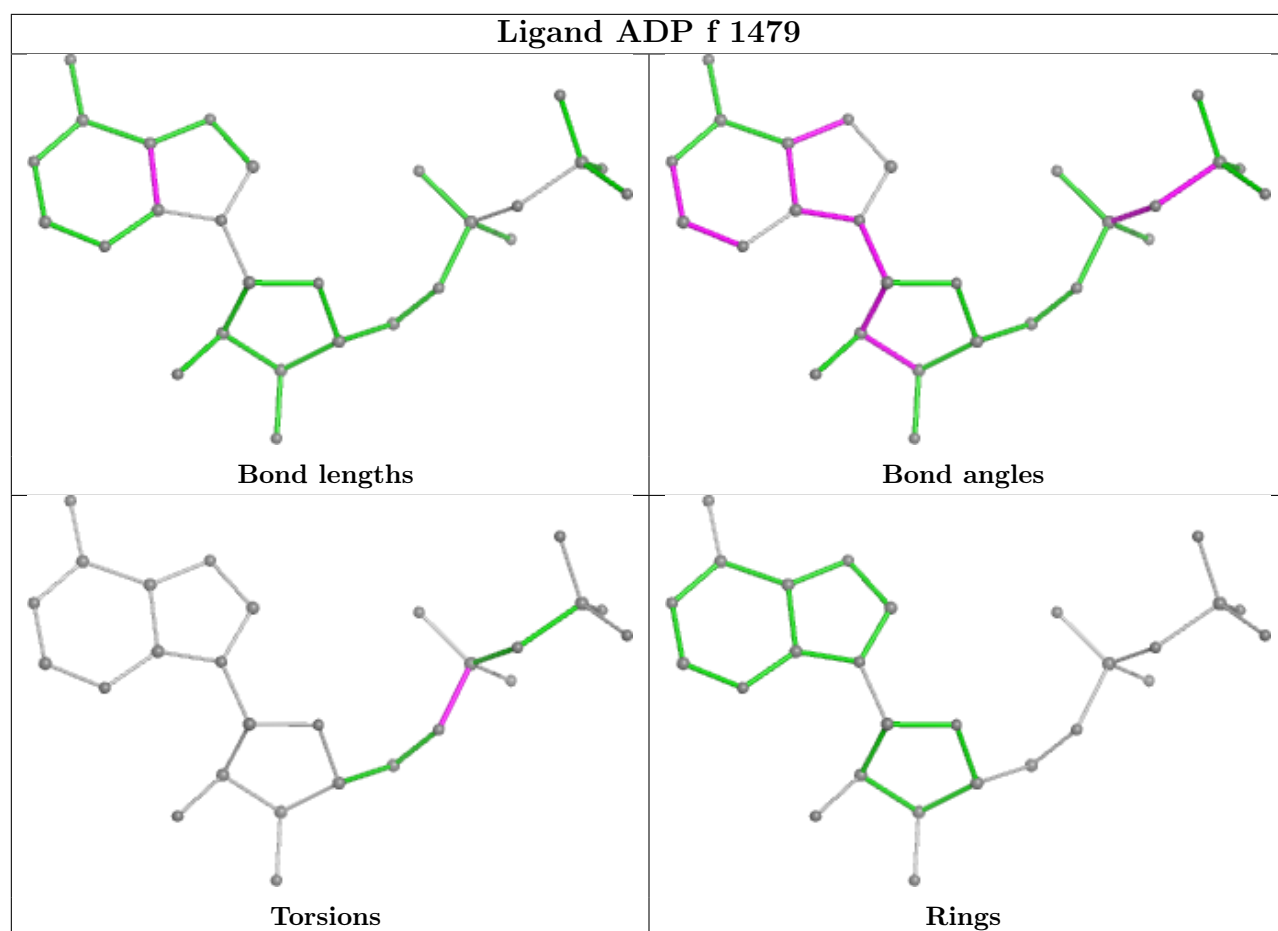
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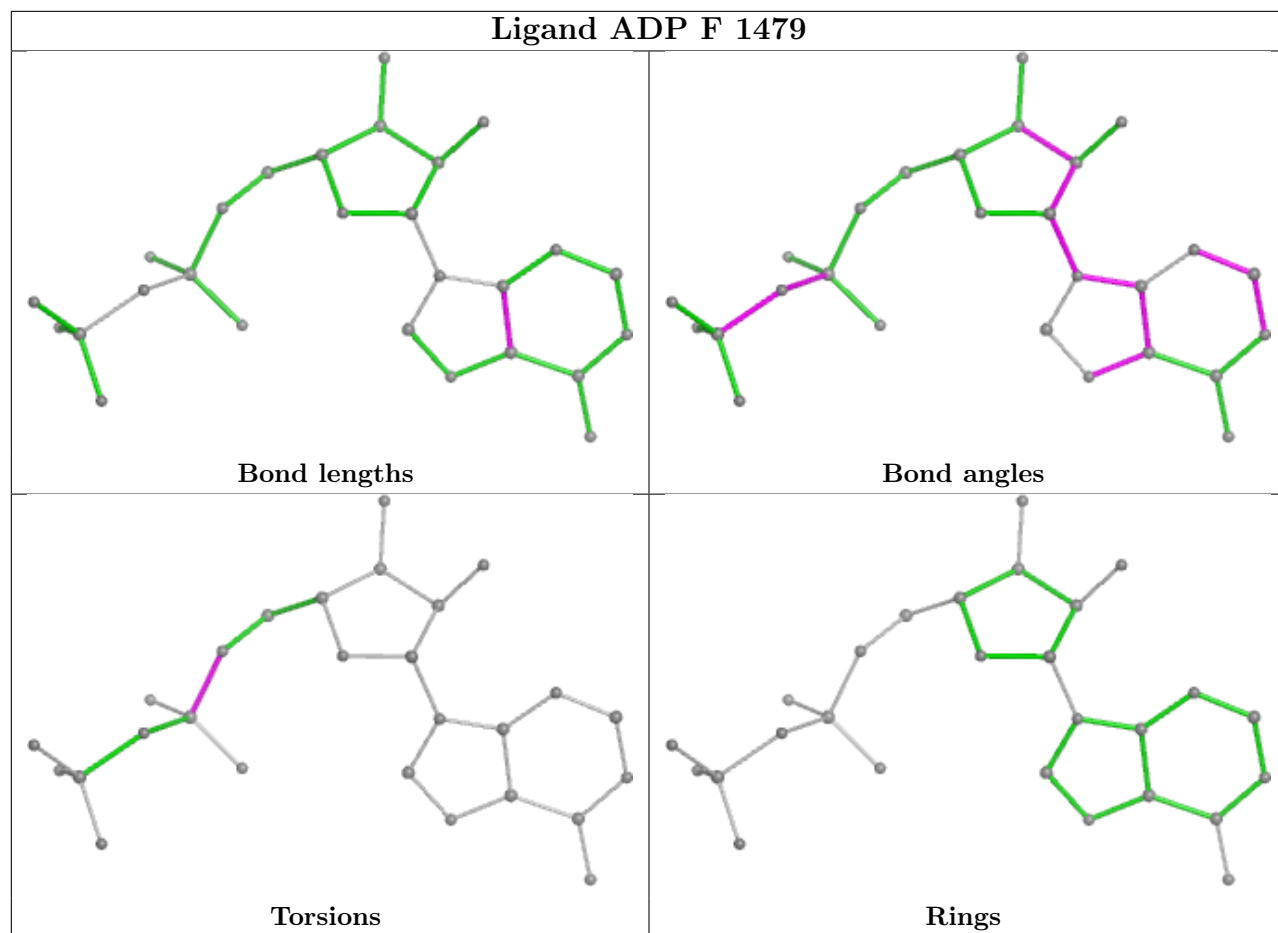
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	1510	ATP	1	0
13	A	1511	ATP	5	0
15	D	1476	ADP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

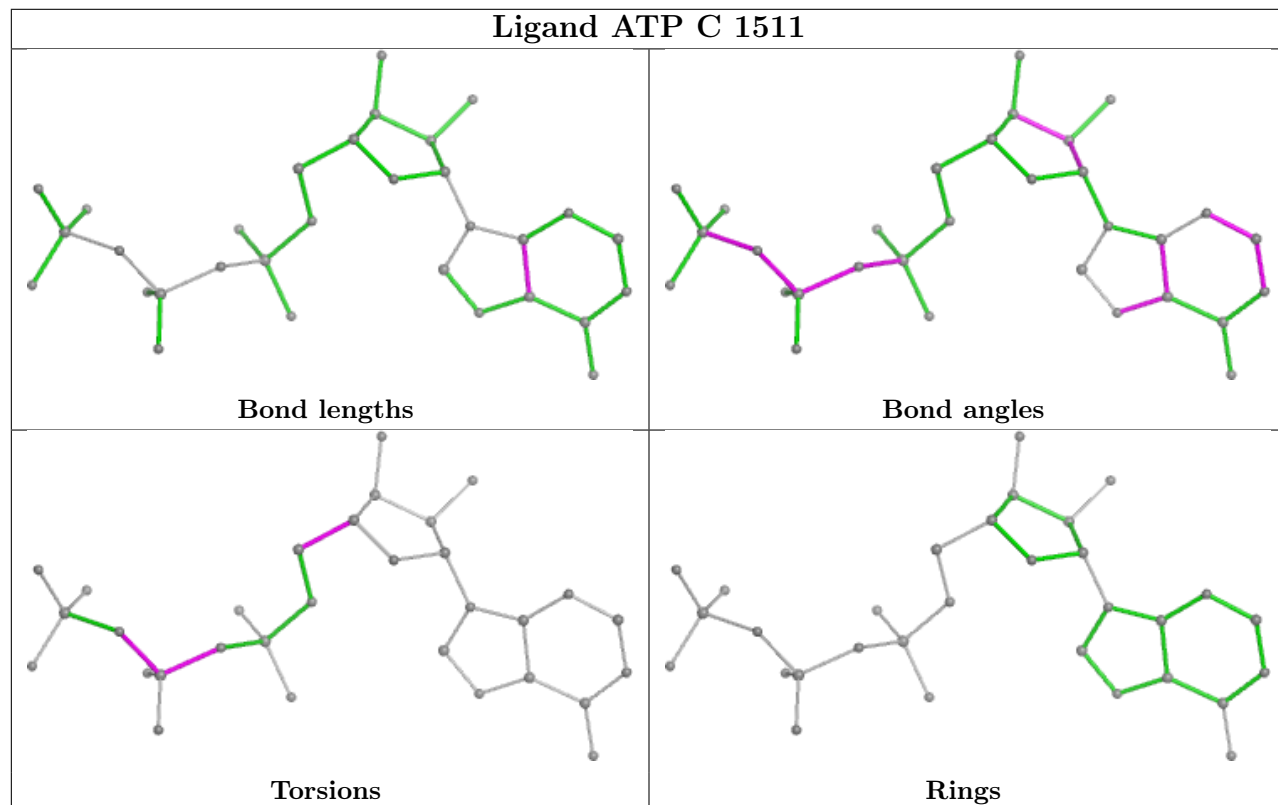


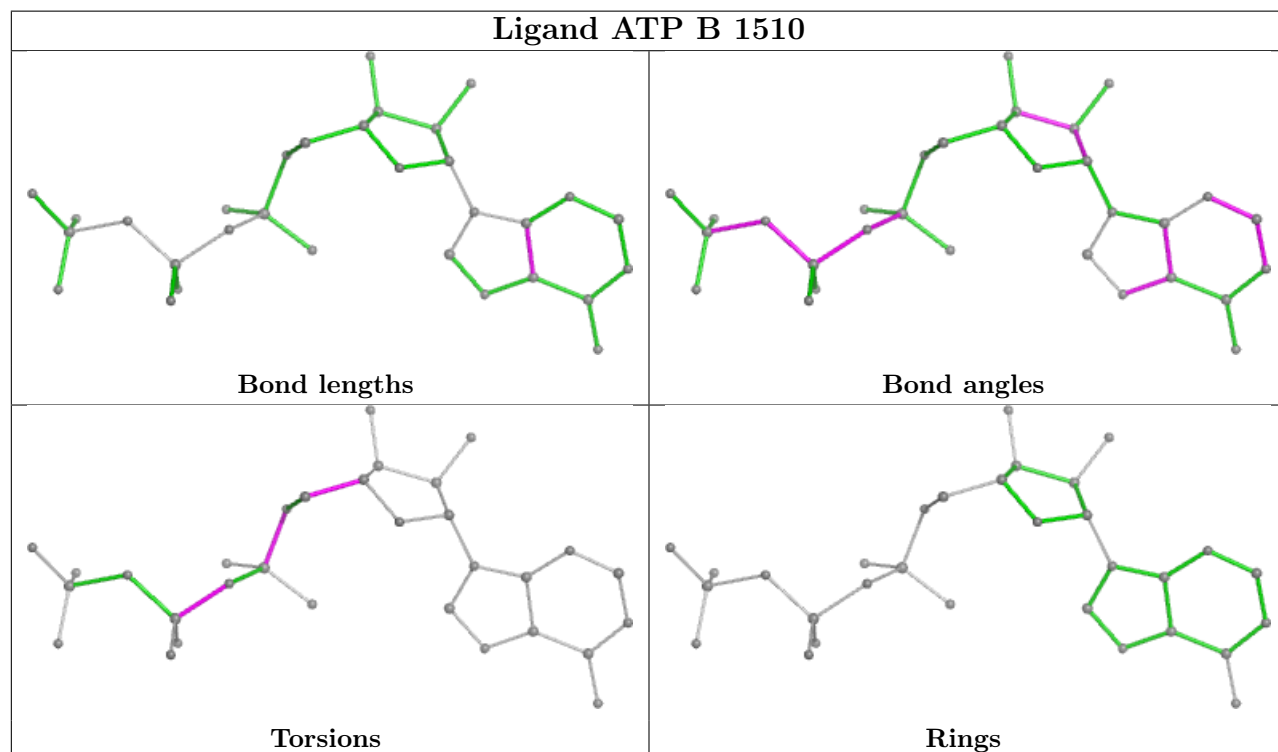
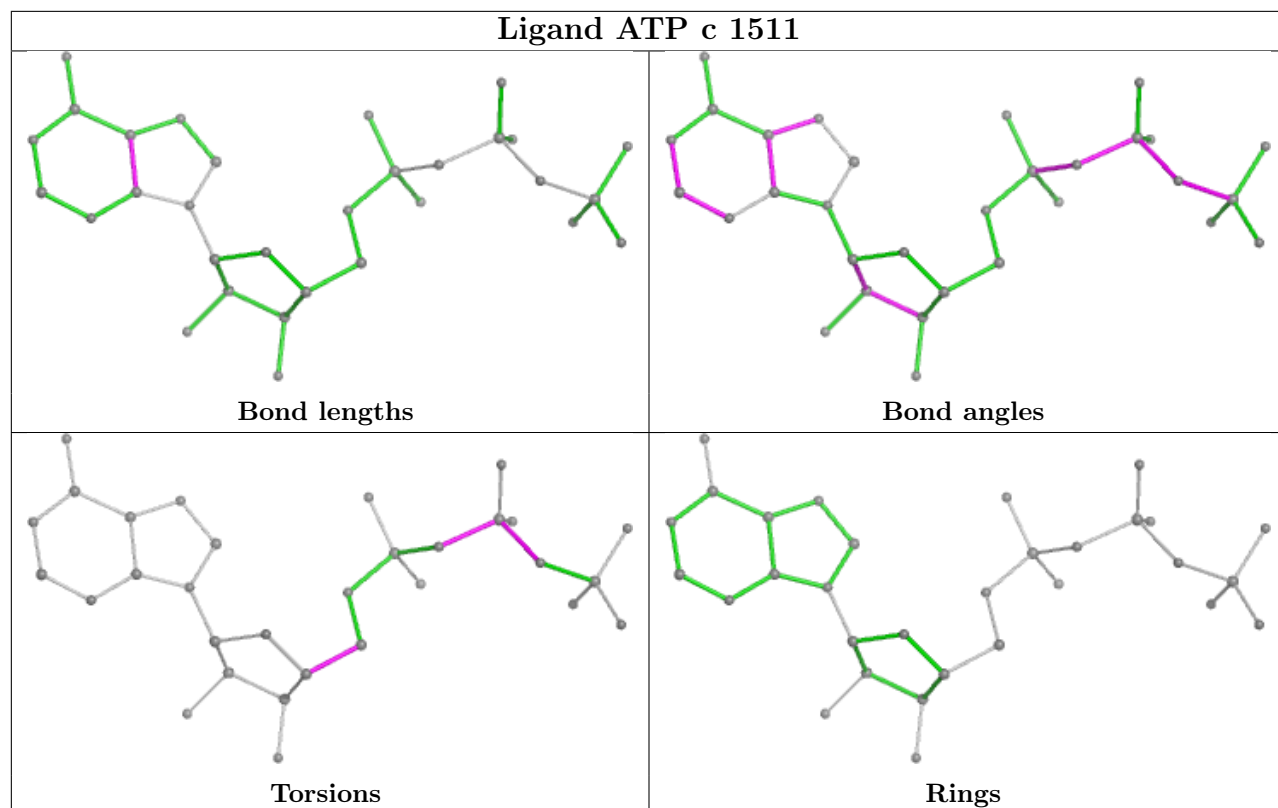


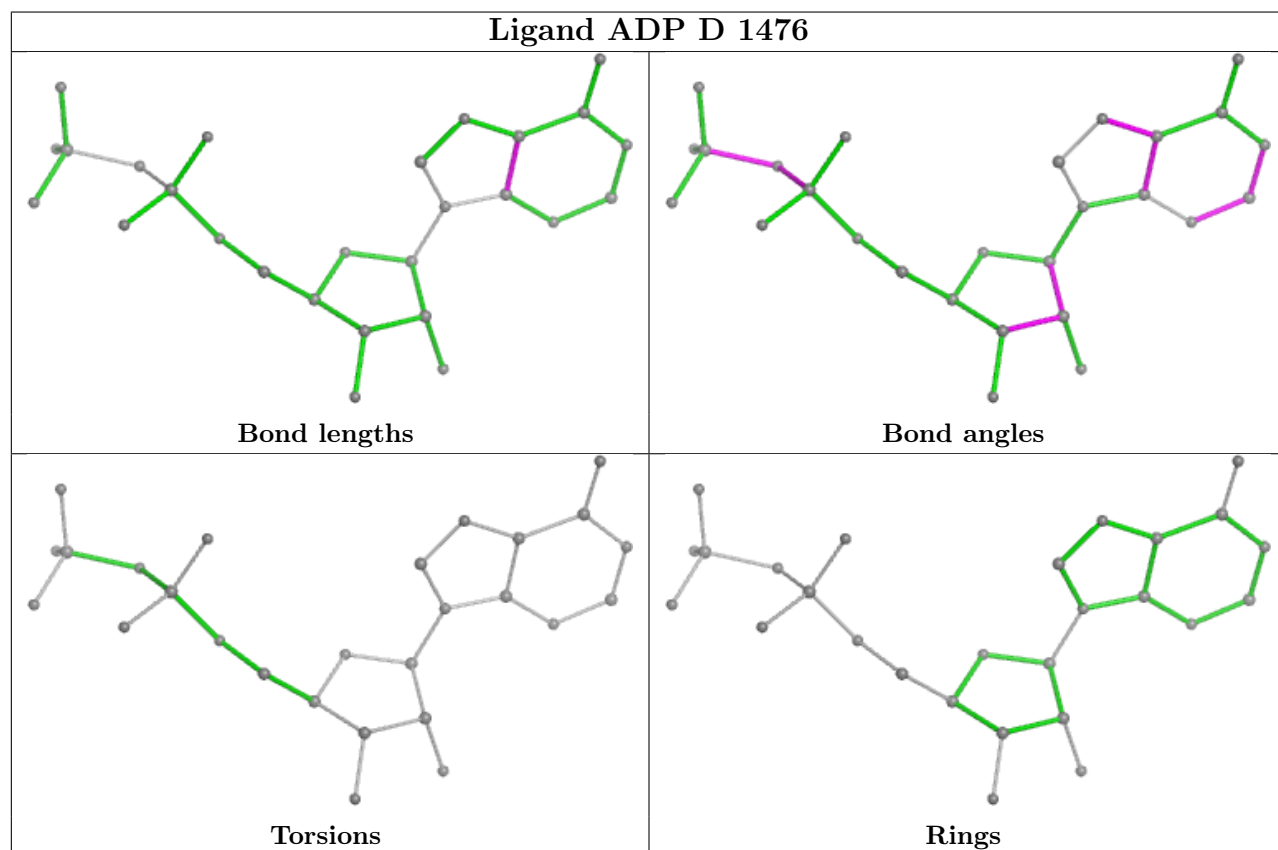
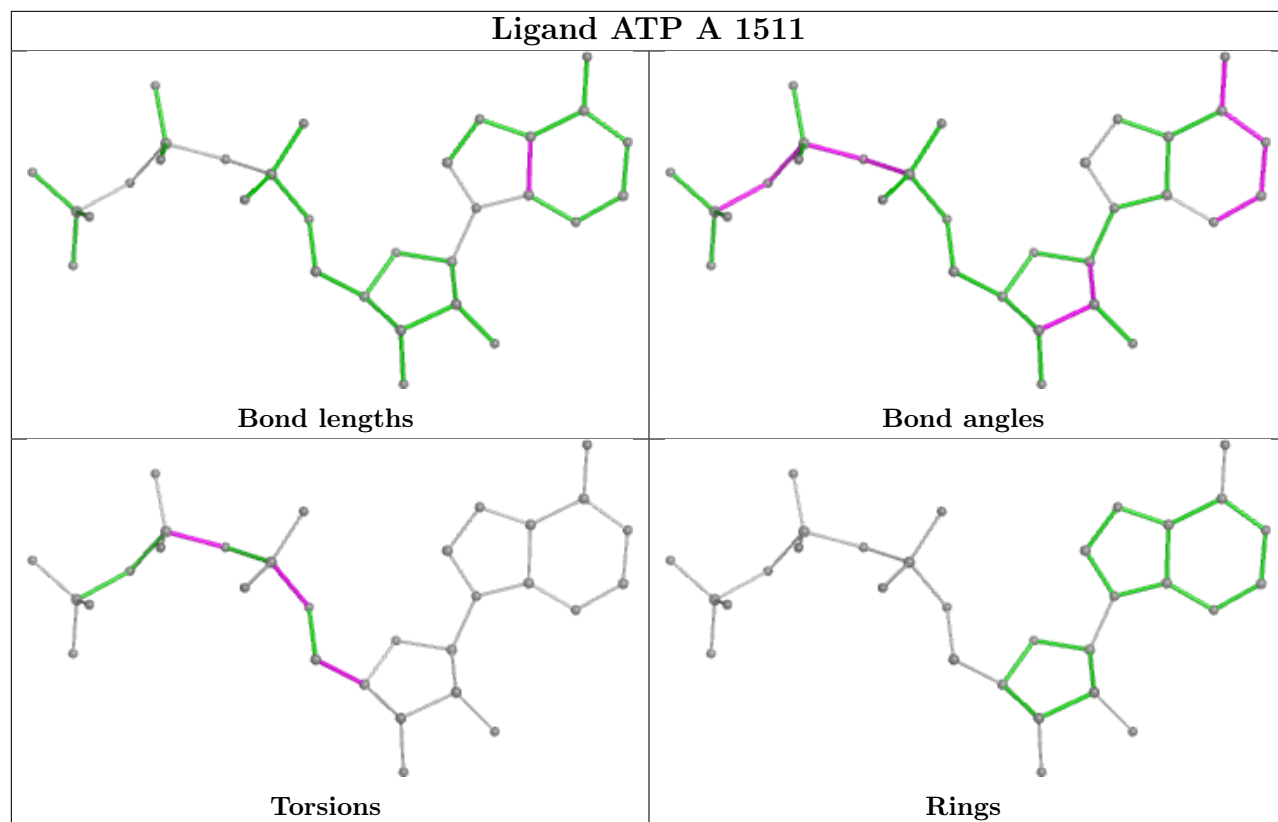
Ligand ADP F 1479

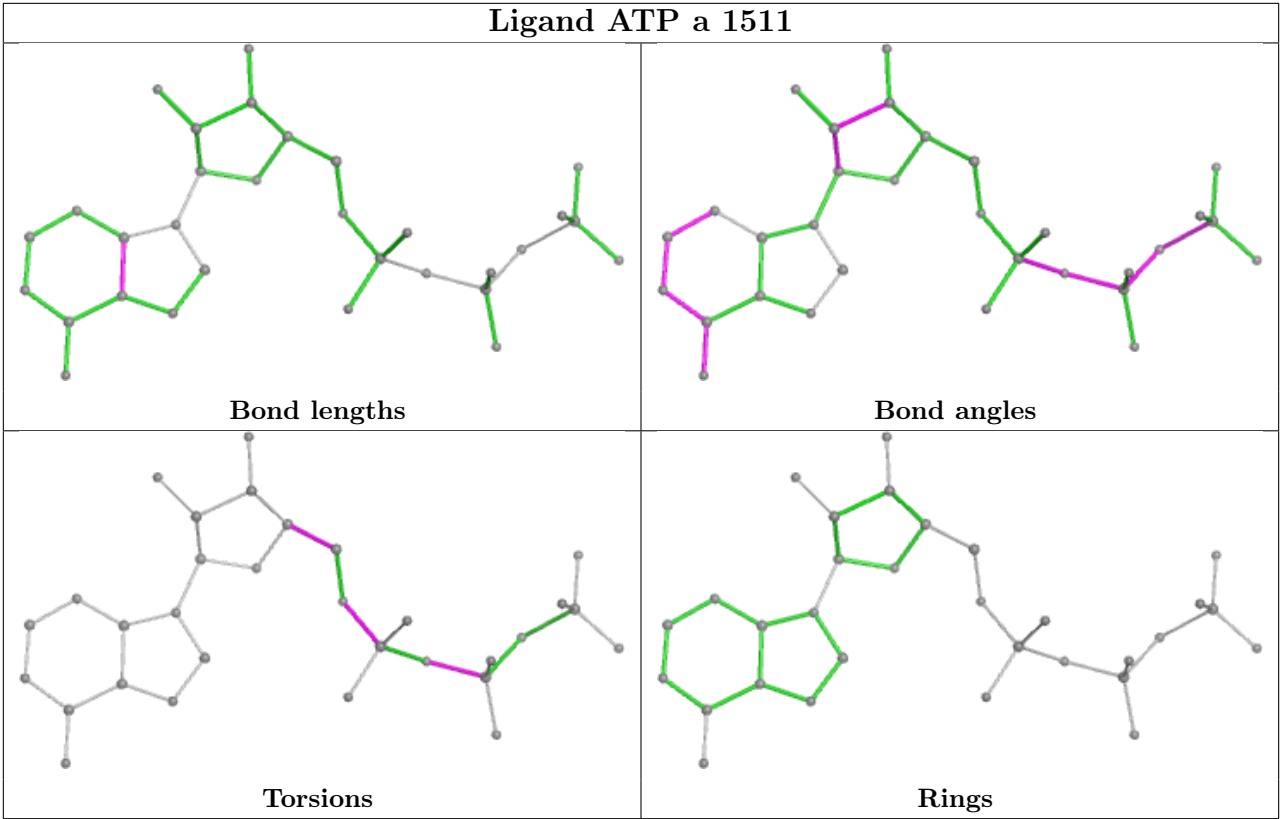


Ligand ATP C 1511









5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

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

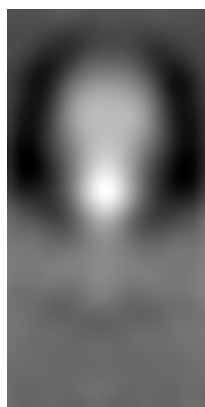
All chain breaks are listed below:

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

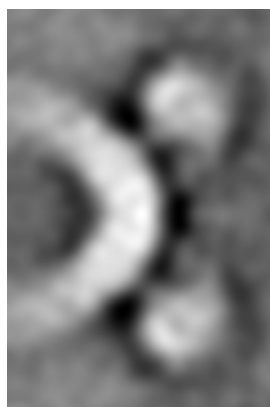
6 Tomogram visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2161. These allow visual inspection of the internal detail of the tomogram and identification of artifacts.

6.1 Orthogonal projections [i](#)



X



Y



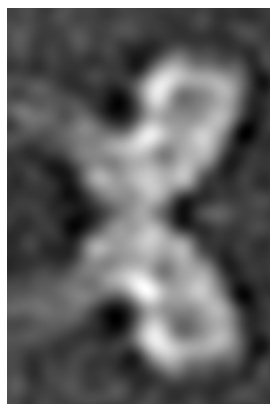
Z

The images above show the tomogram projected in three orthogonal directions.

6.2 Central slices [i](#)



X Index: 45



Y Index: 15



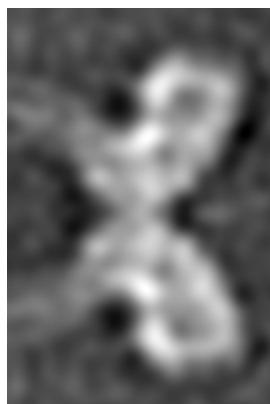
Z Index: 30

The images above show central slices of the tomogram in three orthogonal directions.

6.3 Largest variance slices [i](#)



X Index: 62



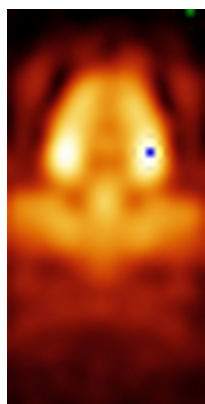
Y Index: 14



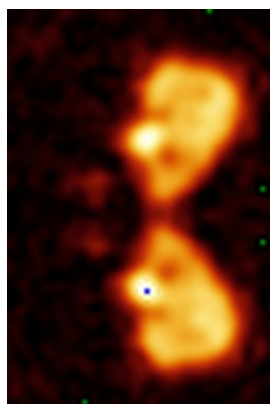
Z Index: 36

The images above show the largest variance slices of the tomogram in three orthogonal directions.

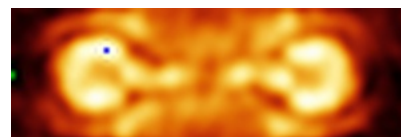
6.4 Orthogonal standard-deviation projections (False-color) [i](#)



X



Y



Z

The images above show the tomogram projected in three orthogonal directions.

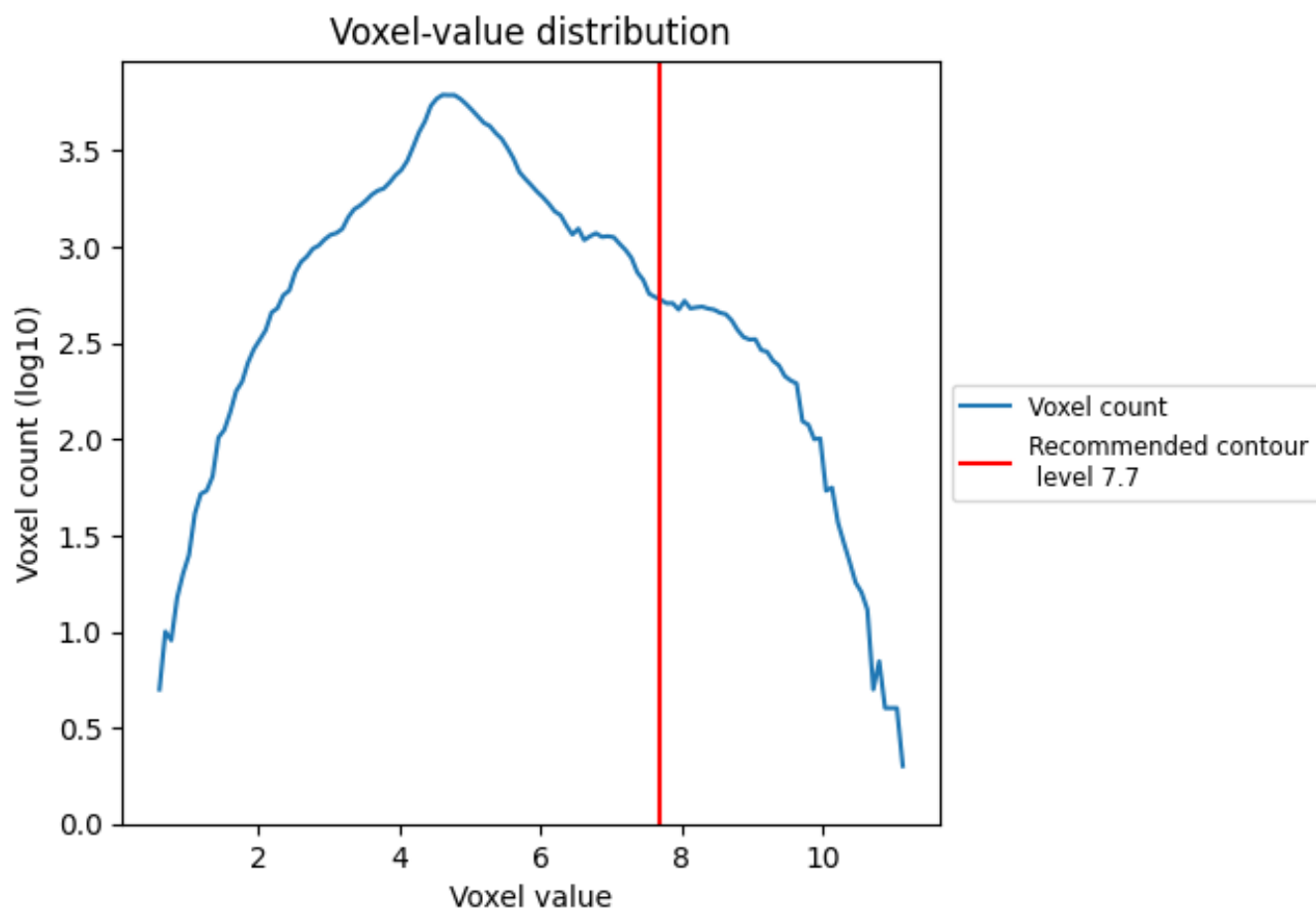
6.5 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Tomogram analysis [i](#)

This section contains the results of statistical analysis of the tomogram.

7.1 Voxel-value distribution [i](#)



The voxel-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic.

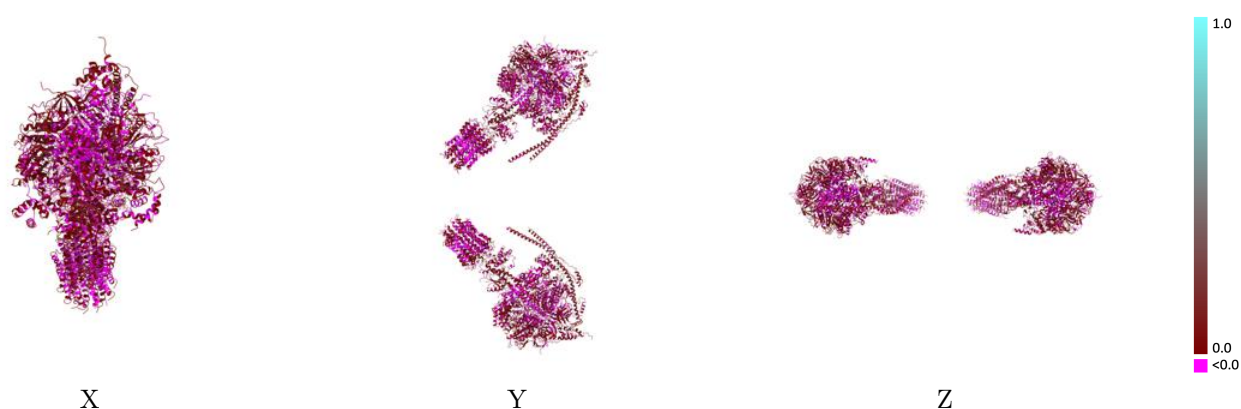
8 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-2161 and PDB model 4B2Q. Per-residue inclusion information can be found in section 3 on page 11.

8.1 Map-model overlay [i](#)

This section was not generated.

8.2 Q-score mapped to coordinate model [i](#)

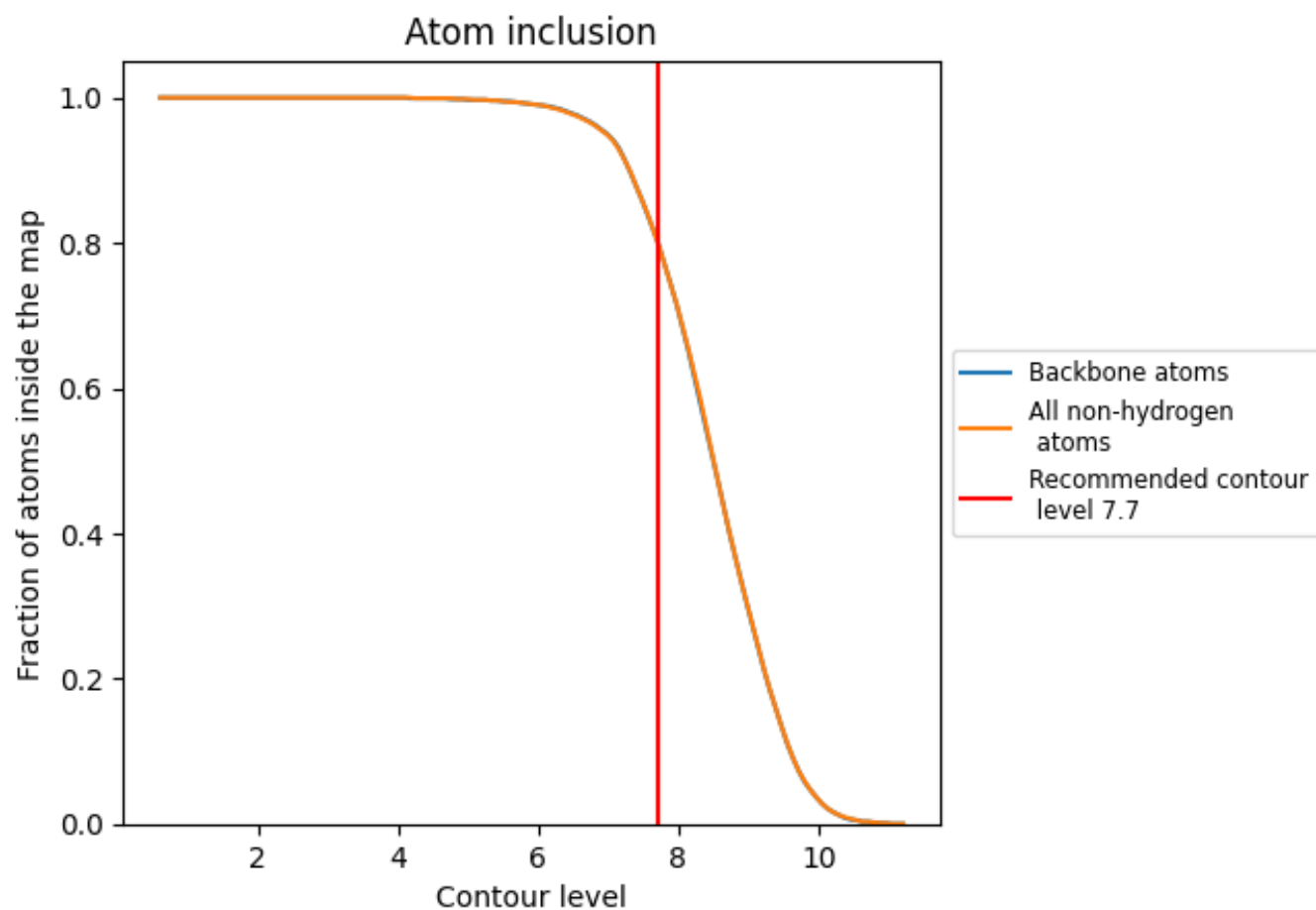


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

8.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.







































































8.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary ⓘ

























The table lists the average atom inclusion at the recommended contour level (7.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8030	 0.0310
A	 0.9100	 0.0020
B	 0.8240	 0.0350
C	 0.8190	 0.0260
D	 0.8450	 0.0330
E	 0.7930	 0.0410
F	 0.9100	 0.0440
G	 0.7630	 0.0290
H	 0.5930	 0.0280
I	 0.7420	 0.0370
J	 0.5350	 0.0280
K	 0.6750	 0.0070
L	 0.9410	 -0.0020
M	 0.9830	 0.0260
N	 0.6750	 0.0080
O	 0.3400	 0.0070
P	 0.4350	 0.0080
Q	 0.5830	 0.0280
R	 0.6330	 0.0320
S	 0.5170	 -0.0020
T	 0.9940	 0.1120
U	 0.9040	 0.0670
V	 0.9620	 0.0570
W	 0.7100	 0.0510
a	 0.9020	 0.0010
b	 0.8240	 0.0320
c	 0.8200	 0.0270
d	 0.8480	 0.0330
e	 0.7900	 0.0440
f	 0.9150	 0.0400
g	 0.7690	 0.0230
h	 0.5760	 0.0290
i	 0.7340	 0.0280
j	 0.5040	 0.0230
k	 0.5500	 0.0090



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Chain	Atom inclusion	Q-score
l	 0.9430	 0.0110
m	 0.9890	 0.0270
n	 0.7160	 0.0010
o	 0.3430	 -0.0060
p	 0.3970	 -0.0040
q	 0.5720	 0.0130
r	 0.6350	 0.0240
s	 0.5310	 0.0040
t	 0.9950	 0.1110
u	 0.9120	 0.0700
v	 0.9700	 0.0610
w	 0.6890	 0.0370