



## Full wwPDB EM Validation Report ⓘ

May 2, 2026 – 01:31 PM EDT

PDB ID : 9DGV / pdb\_00009dgv  
EMDB ID : EMD-46849  
Title : structure of dynactin, dynein tail with TRAK2 from dynein-dynactin-TRAK2 on microtubules  
Authors : Rao, Q.; Chai, P.; Zhang, K.  
Deposited on : 2024-09-03  
Resolution : 8.80 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

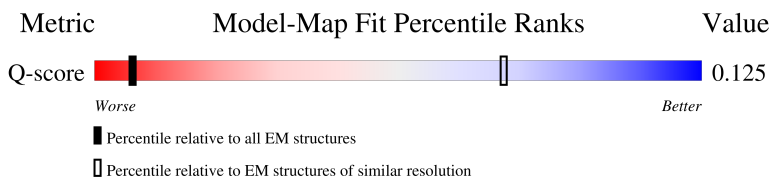
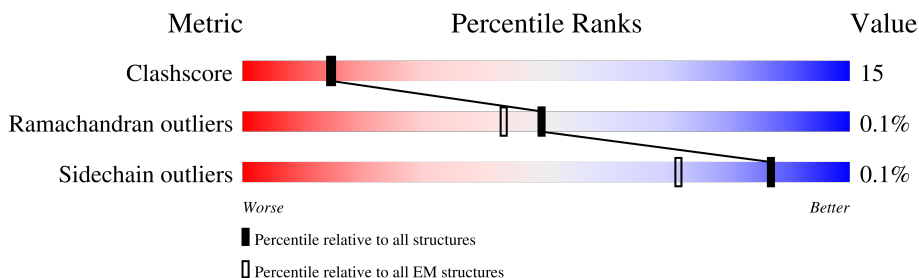
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 8.80 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	265 ( 8.30 - 9.30 )

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  $\geq 3$ , 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	376	
1	B	376	
1	C	376	
1	D	376	

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Mol	Chain	Length	Quality of chain
1	E	376	
1	F	376	
1	G	376	
1	I	376	
2	H	375	
3	J	417	
4	K	286	
5	L	272	
6	M	405	
6	N	405	
6	P	405	
6	Q	405	
7	O	186	
7	R	186	
8	U	190	
9	V	182	
10	W	1281	
10	Z	1281	
11	Y	467	
12	a	913	
12	b	913	
13	e	4646	
13	f	4646	
13	m	4646	
13	n	4646	

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Mol	Chain	Length	Quality of chain
14	g	612	<div><div></div><div>56%</div><div></div><div>42%</div></div>
14	h	612	<div><div></div><div>39%</div><div>20%</div><div>42%</div></div>
14	o	612	<div><div></div><div>41%</div><div>17%</div><div>42%</div></div>
14	p	612	<div><div>8%</div><div>42%</div><div>17%</div><div>42%</div></div>

## 2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 86528 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Alpha-centractin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	370	Total	C	N	O	S	0	0
			2944	1886	509	539	10		
1	B	370	Total	C	N	O	S	0	0
			2956	1892	509	545	10		
1	C	375	Total	C	N	O	S	0	0
			2998	1918	514	556	10		
1	D	370	Total	C	N	O	S	0	0
			2956	1892	509	545	10		
1	E	370	Total	C	N	O	S	0	0
			2956	1892	509	545	10		
1	F	370	Total	C	N	O	S	0	0
			2956	1892	509	545	10		
1	G	370	Total	C	N	O	S	0	0
			2956	1892	509	545	10		
1	I	370	Total	C	N	O	S	0	0
			2941	1885	509	537	10		

- Molecule 2 is a protein called Actin, cytoplasmic 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	370	Total	C	N	O	S	0	0
			2885	1827	486	550	22		

- Molecule 3 is a protein called Actin-related protein 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	379	Total	C	N	O	S	0	0
			2932	1888	496	532	16		

- Molecule 4 is a protein called F-actin-capping protein subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	278	Total	C	N	O	S	0	0
			2264	1428	396	434	6		

- Molecule 5 is a protein called F-actin-capping protein subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	269	Total	C	N	O	S	0	0
			2121	1323	370	417	11		

- Molecule 6 is a protein called Dynactin subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	M	340	Total	C	N	O	S	0	0
			2238	1382	408	443	5		
6	N	280	Total	C	N	O	S	0	0
			1767	1089	327	346	5		
6	P	325	Total	C	N	O	S	0	0
			2262	1413	397	446	6		
6	Q	343	Total	C	N	O	S	0	0
			2349	1471	423	451	4		

- Molecule 7 is a protein called Dynactin subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	O	179	Total	C	N	O	S	0	0
			1183	736	210	233	4		
7	R	170	Total	C	N	O	S	0	0
			1082	679	208	194	1		

- Molecule 8 is a protein called Dynactin subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	U	167	Total	C	N	O	S	0	0
			1224	771	212	231	10		

- Molecule 9 is a protein called Dynactin subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	V	179	Total	C	N	O	S	0	0
			1260	818	222	211	9		

- Molecule 10 is a protein called Dynactin subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	W	152	Total	C	N	O	S	0	0
			937	574	186	174	3		
10	Z	192	Total	C	N	O	S	0	0
			1444	904	262	275	3		

- Molecule 11 is a protein called Dynactin subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Y	410	Total	C	N	O	S	0	0
			2960	1868	543	529	20		

- Molecule 12 is a protein called Trafficking protein, kinesin binding 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	a	106	Total	C	N	O	S	0	0
			527	315	106	106			
12	b	105	Total	C	N	O	S	0	0
			522	312	105	105			

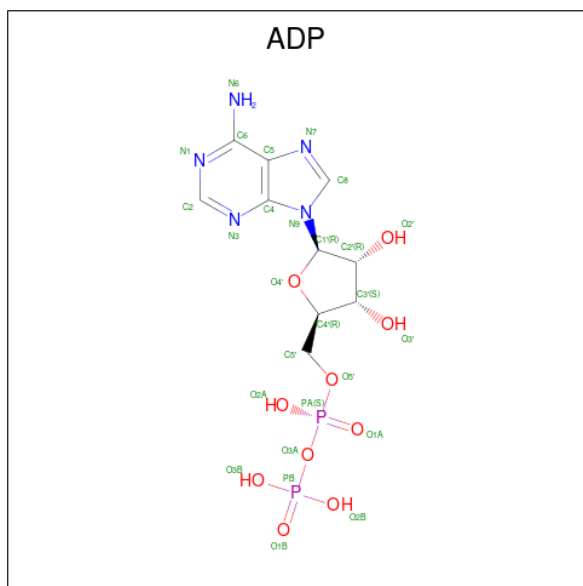
- Molecule 13 is a protein called Cytoplasmic dynein 1 heavy chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	e	798	Total	C	N	O	S	0	0
			4724	2897	879	944	4		
13	f	808	Total	C	N	O	S	0	0
			6570	4162	1175	1216	17		
13	m	792	Total	C	N	O	S	0	0
			5722	3529	1090	1089	14		
13	n	755	Total	C	N	O	S	0	0
			5424	3342	1034	1036	12		

- Molecule 14 is a protein called Cytoplasmic dynein 1 intermediate chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	g	358	Total	C	N	O	S	0	0
			1767	1051	358	358			
14	h	358	Total	C	N	O	S	0	0
			2808	1771	490	532	15		
14	o	358	Total	C	N	O	S	0	0
			2808	1771	490	532	15		
14	p	358	Total	C	N	O	S	0	0
			2808	1771	490	532	15		

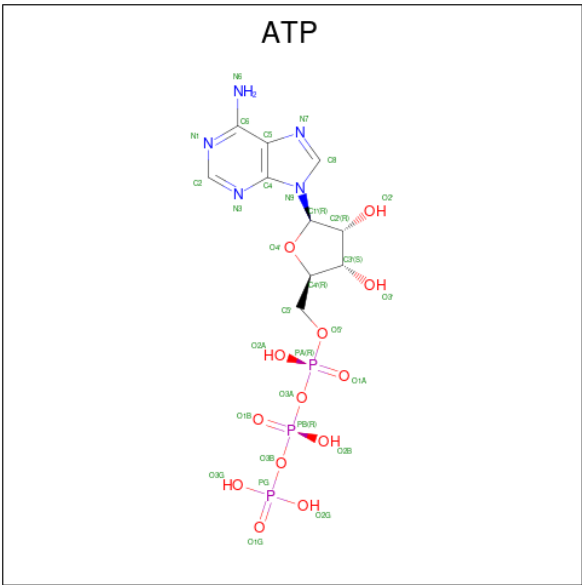
- Molecule 15 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms					AltConf
15	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
15	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
15	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
15	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
15	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
15	F	1	Total	C	N	O	P	0
			27	10	5	10	2	
15	G	1	Total	C	N	O	P	0
			27	10	5	10	2	
15	I	1	Total	C	N	O	P	0
			27	10	5	10	2	
15	J	1	Total	C	N	O	P	0
			27	10	5	10	2	

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





Mol	Chain	Residues	Atoms					AltConf
16	H	1	Total	C	N	O	P	0
			31	10	5	13	3	

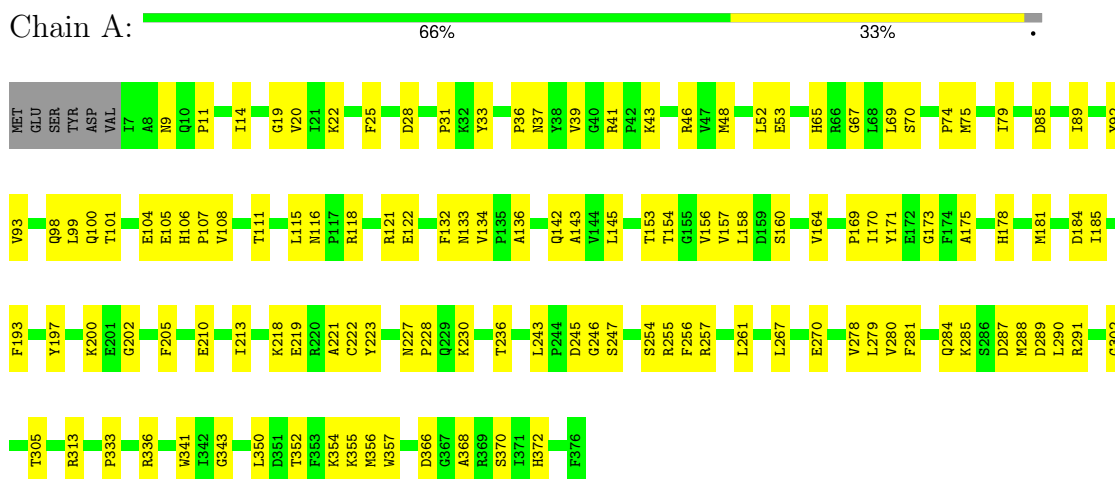
- Molecule 17 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
17	Y	3	Total	Zn	0
			3	3	

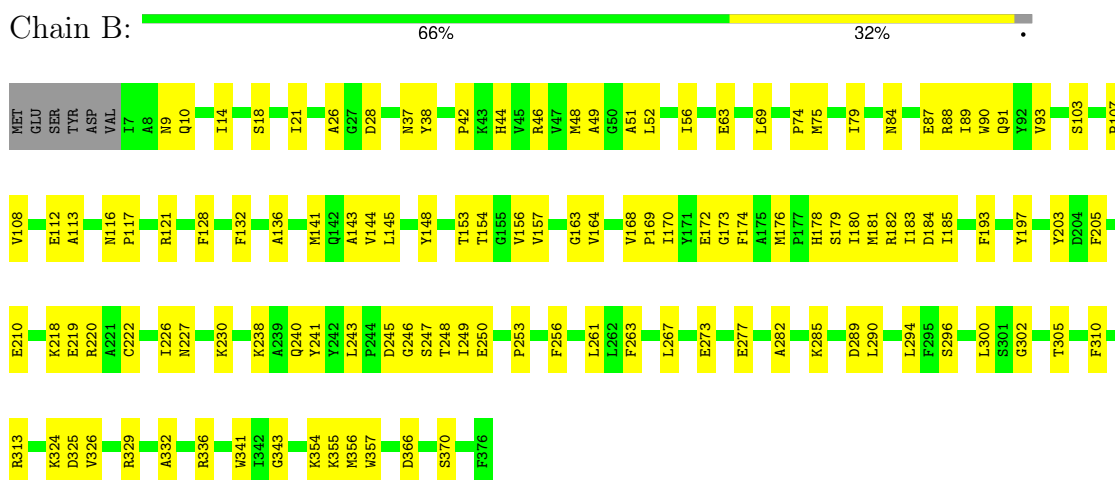
### 3 Residue-property plots

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: Alpha-centractin

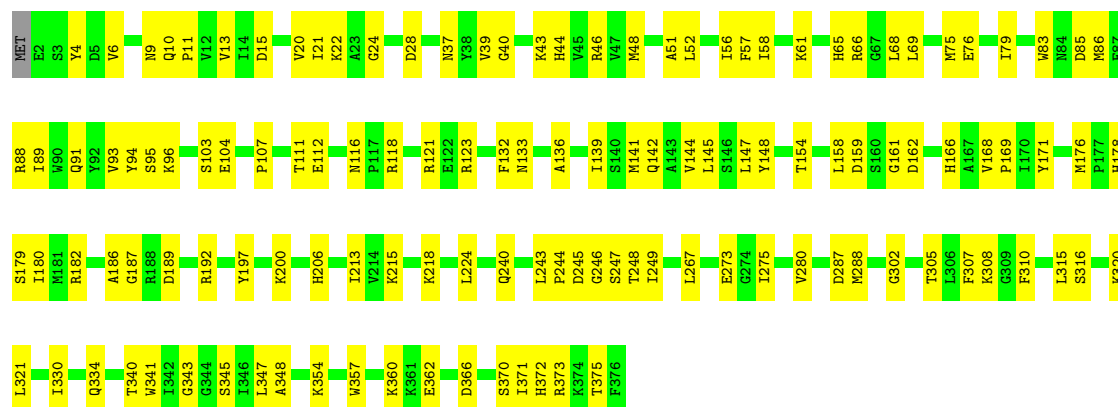


#### • Molecule 1: Alpha-centractin



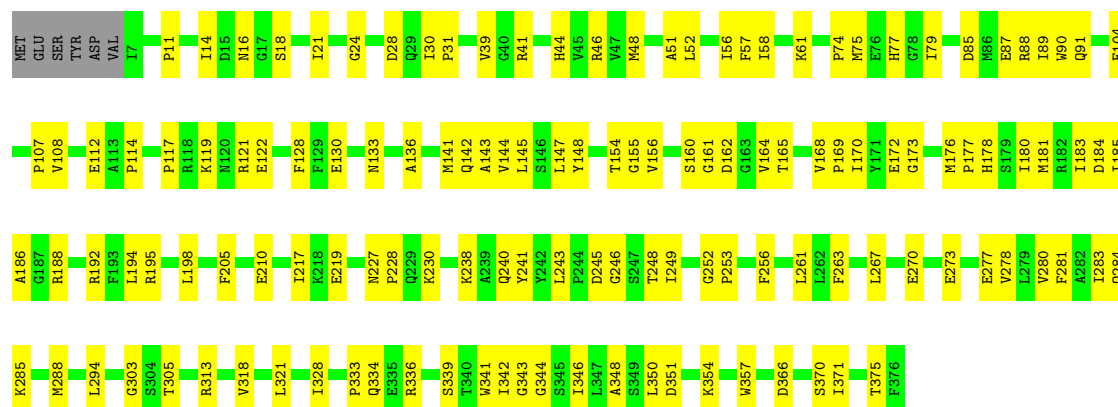
#### • Molecule 1: Alpha-centractin





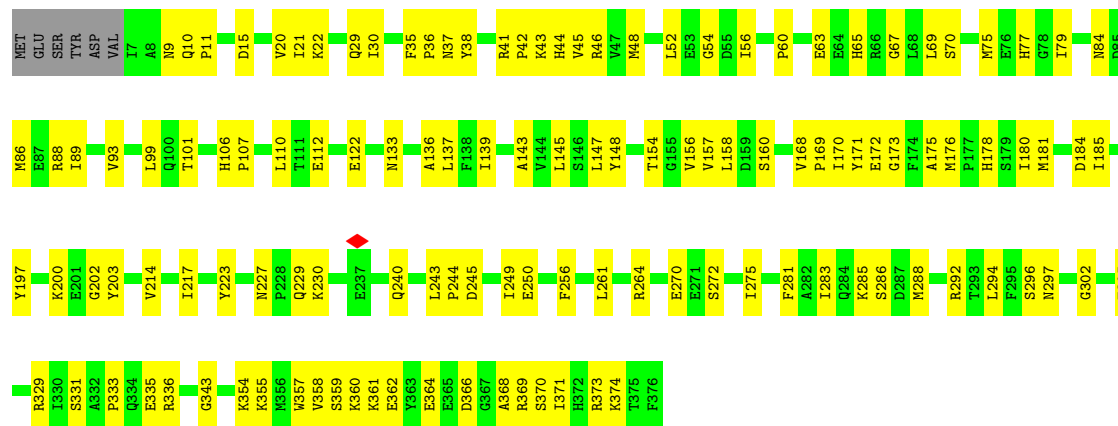
• Molecule 1: Alpha-centractin

Chain D: 63% 35%



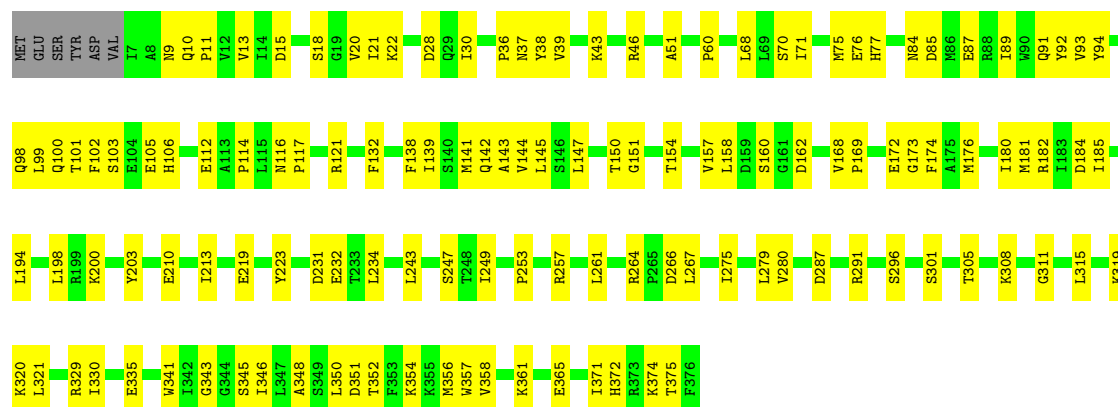
• Molecule 1: Alpha-centractin

Chain E: 65% 33%

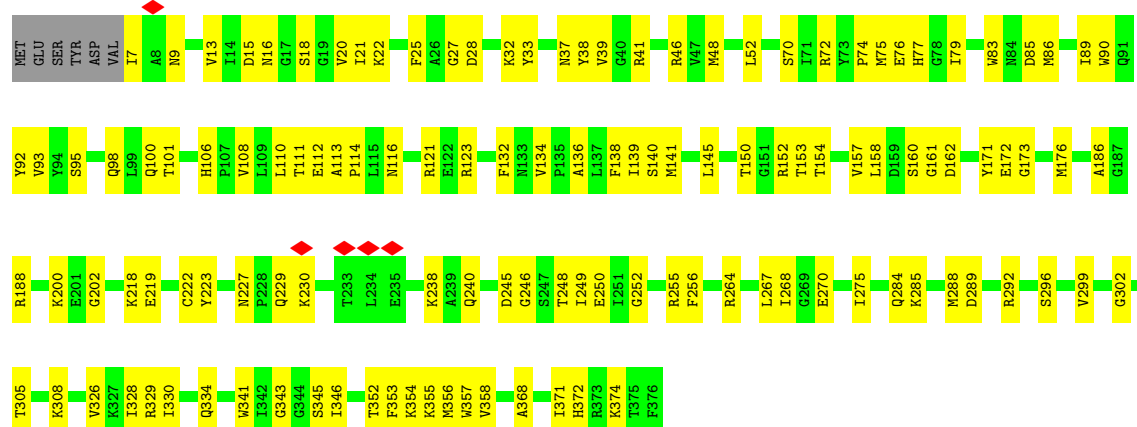


• Molecule 1: Alpha-centractin

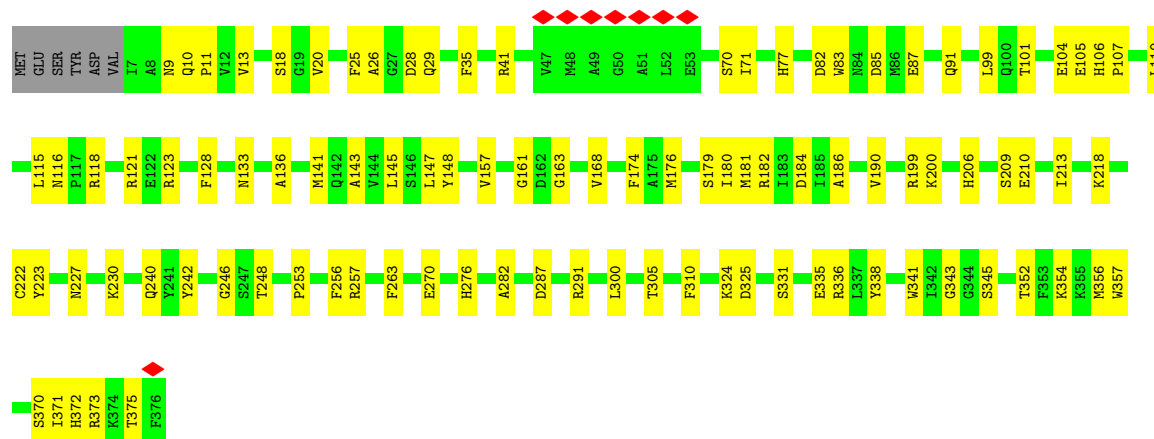
Chain F: 64% 34%



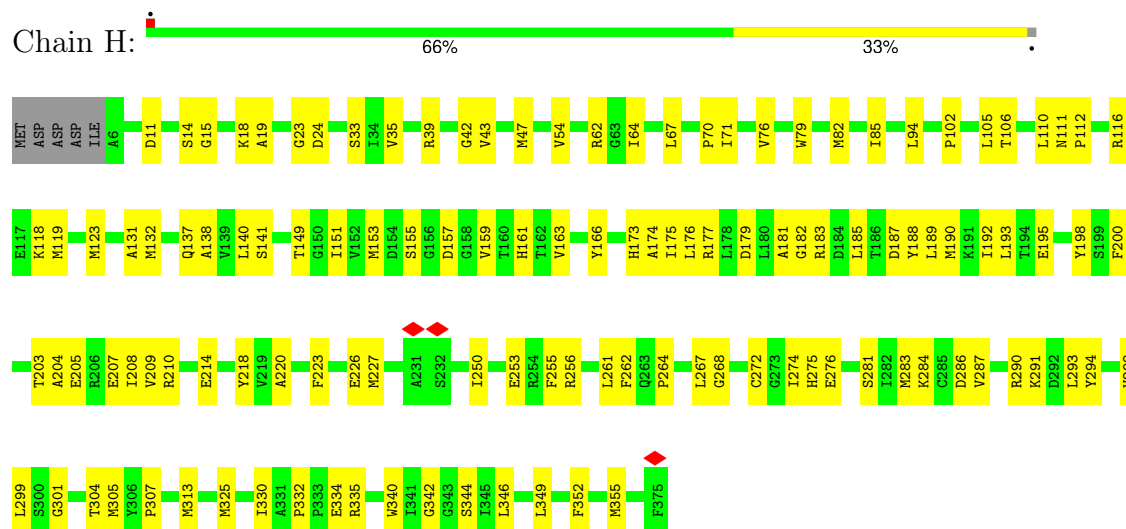
• Molecule 1: Alpha-centractin



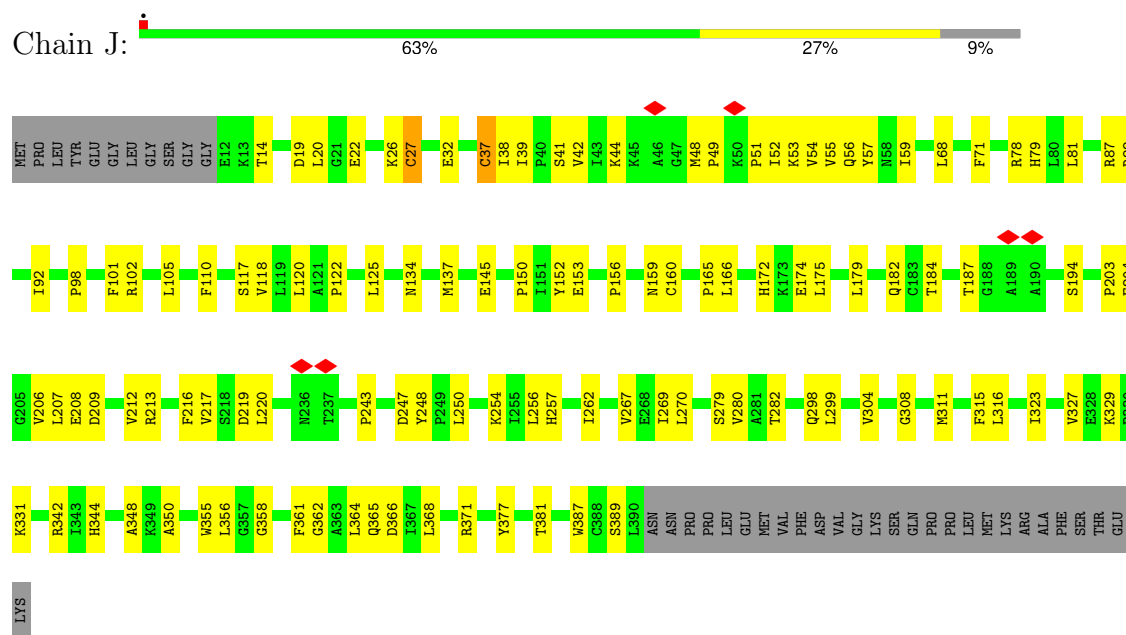
• Molecule 1: Alpha-centractin



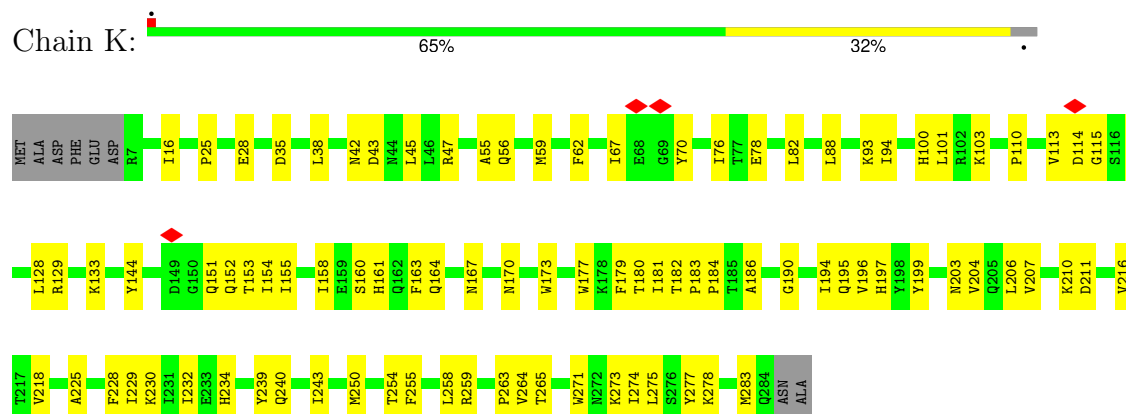
• Molecule 2: Actin, cytoplasmic 1



• Molecule 3: Actin-related protein 10

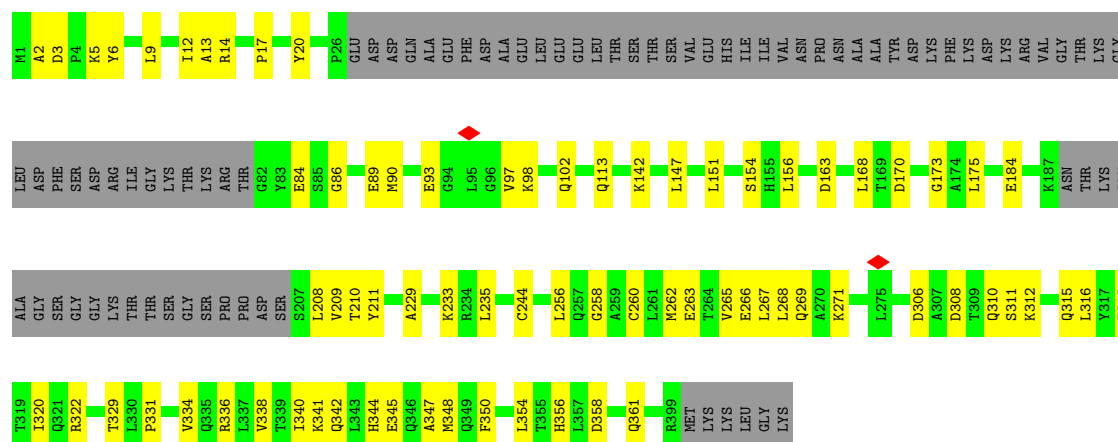


• Molecule 4: F-actin-capping protein subunit alpha-1



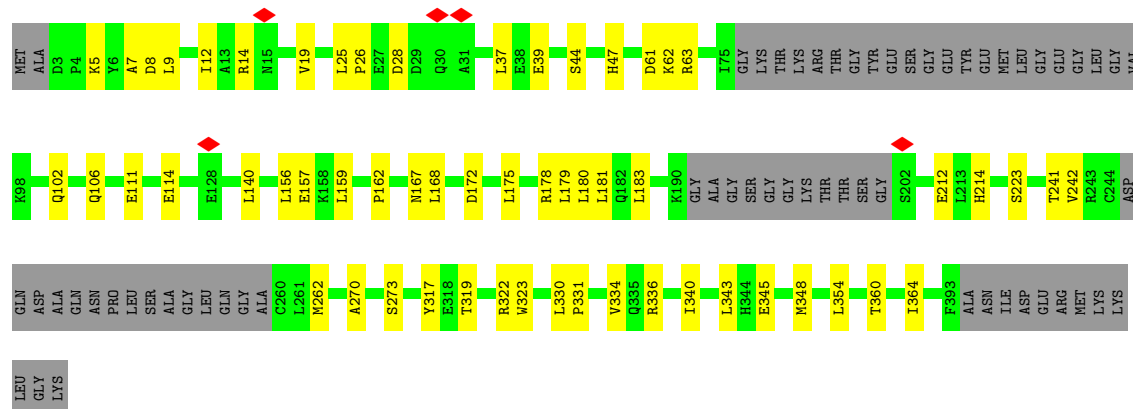


Chain P:  61% 19% 20%




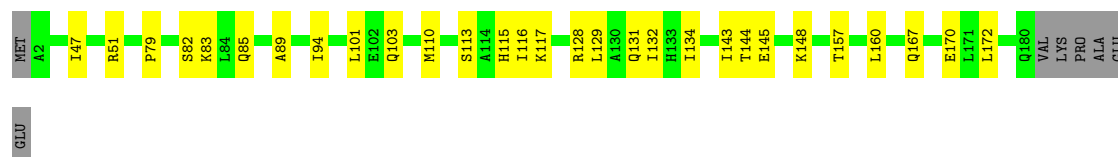
### • Molecule 6: Dynactin subunit 2

Chain Q:  70% 14% 15%




### • Molecule 7: Dynactin subunit 3

Chain O:  81% 16% 3%



### • Molecule 7: Dynactin subunit 3

Chain R:  76% 16% 9%

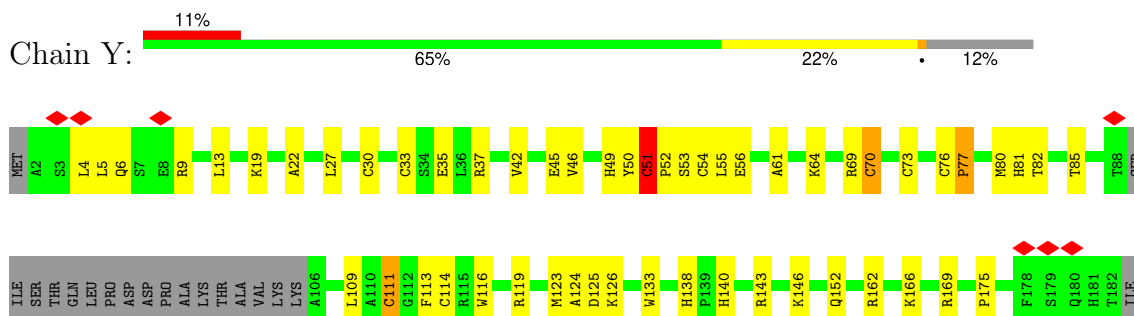








- Molecule 11: Dynactin subunit 4





- Molecule 12: Trafficking protein, kinesin binding 2

[illegible]

- Molecule 13: Cytoplasmic dynein 1 heavy chain 1

Chain e:



SER	VAL	VAL	GLY	ILE	SER	SER	ARG	GLY	GLY	GLY	GLY	GLY	ASP	PHE	ASP	LEU	LYS	LEU	GLU	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GL
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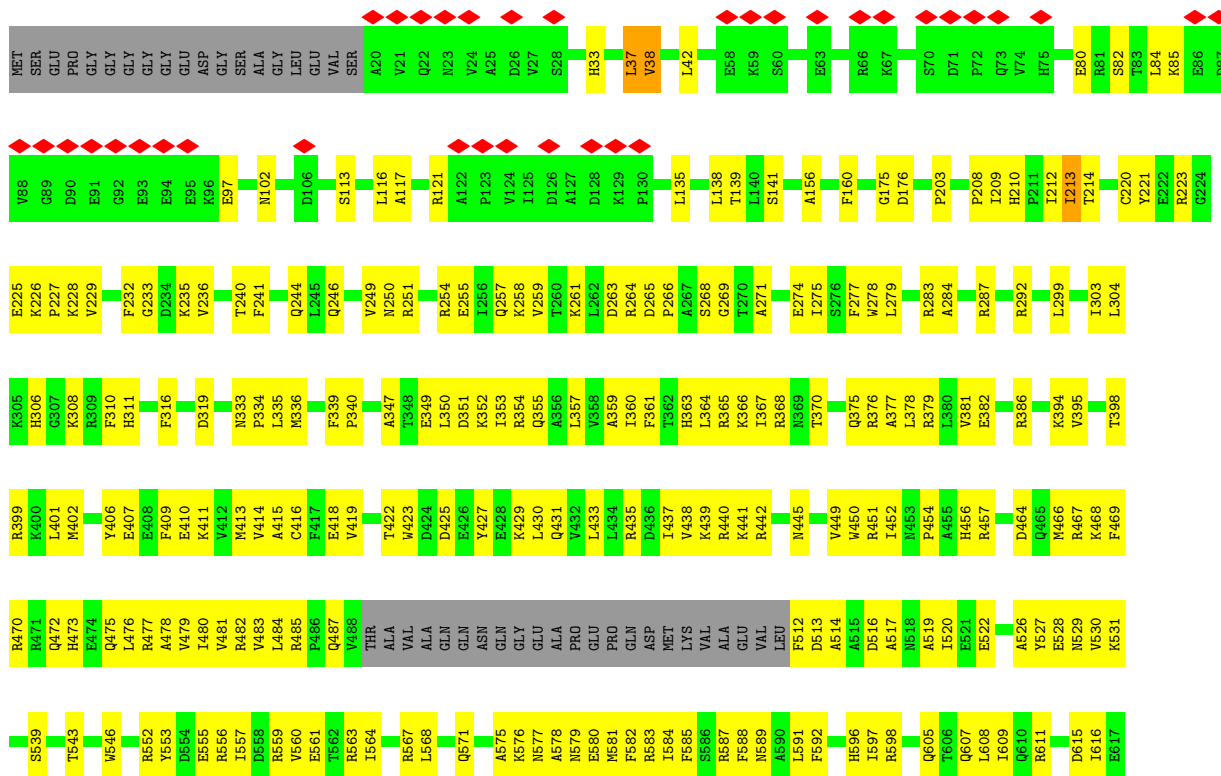




LEU	ASN	THR	ALA	SER	LEU	ASP	LEU	GLN	ASP	GLY	LEU	THR	GLN	THR	ASP	GLY	THR	ILE	GLN	ASN
ASN	THR	THR	THR	VAL	SER	ASP	ASP	ASP	ARG	ARG	PRO	ASP	PRO	GLY	ARG	GLY	THR	THR	THR	PRO
THR	THR	THR	ALA	GLN	ALA	VAL	VAL	GLN	ALA	ALA	THR	THR	GLN	VAL	VAL	VAL	THR	THR	THR	VAL
ALA	CYS	ALA	ALA	ALA	ALA	GLN	GLN	GLN	TRP	TRP	GLN	THR	THR	ASP	ASP	VAL	THR	THR	THR	ALA
ASP	SER	SER	SER	ALA	ALA	VAL	VAL	VAL	MET	MET	THR	THR	THR	THR	THR	THR	THR	THR	THR	ASN
LEU	THR	THR	PHE	SER	SER	CYS	CYS	PRO	ARG	ARG	PRO	PRO	PRO	ASN	ASN	ASN	ASN	ASN	ASN	LEU
LEU	THR	THR	VAL	GLY	GLY	GLY	GLY	GLY	THR	THR	SER	SER	GLY	THR	THR	THR	THR	THR	THR	LEU
PHE	THR	THR	VAL	GLY	GLY	GLY	GLY	GLY	LEU	LEU	HIS	THR	GLY	THR	ASP	PHE	THR	THR	THR	ARG
THR	THR	THR	THR	ALA	ALA	LYS	LYS	LYS	THR	THR	THR	THR	GLY	GLY	LYS	GLN	ARG	THR	THR	ALA
VAL	ASP	LEU	LEU	GLU	GLY	LYS	LYS	LYS	THR	THR	THR	THR	LEU	ARG	ARG	ARG	THR	THR	THR	GLY
ASP	PHE	LEU	LYS	LEU	LYS	GLN	GLN	GLN	ALA	ALA	PRO	PRO	PRO	VAL	VAL	ILE	THR	THR	THR	ARG
PHE	GLU	GLU	LEU	LYS	LYS	THR	THR	THR	SER	SER	ASN	ASN	ASN	ASN	ASN	ASN	THR	THR	THR	LYS
ILE	GLN	GLN	GLN	ILE	ILE	ILE	TYR	TYR	TRP	LEU	ALA	ALA	ALA	THR	THR	THR	THR	THR	THR	PHE
ALA	ALA	GLY	GLY	THR	THR	THR	HIS	VAL	THR	HIS	ARG	ARG	GLY	GLY	THR	THR	THR	THR	THR	GLY
THR	LYS	THR	THR	VAL	CYS	ARG	ARG	VAL	LEU	LEU	THR	THR	GLN	THR	THR	THR	THR	THR	THR	GLY
LYS	GLU	GLU	CYS	VAL	CYS	THR	THR	THR	LEU	LEU	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY
GLU	GLU	GLU	ASN	THR	THR	ILE	ILE	ILE	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY
ASP	ASP	ASP	SER	GLY	GLY	ILE	ILE	ILE	GLY	GLY	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	ASP
PRO	PRO	ASN	ASN	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ASN	ASN	ASN	THR	THR	THR	THR	THR	THR	PRO
ASN	ASN	ASN	ASN	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ASN	ASN	ASN	THR	THR	THR	THR	THR	THR	GLY
ARG	ARG	ASN	ASN	LEU	LEU	LEU	LEU	LEU	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	VAL
SER	SER	LYS	LYS	PHE	LEU	LEU	LEU	LEU	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	ASN
PHE	PHE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	ALA
TYR	TYR	SER	SER	VAL	VAL	VAL	VAL	VAL	SER	SER	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ASN
GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	ASN
ARG	ARG	ASN	ASN	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ASN
VAL	VAL	VAL	VAL	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
VAL	VAL	VAL	VAL	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
ASN	ASN	ASN	ASN	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
VAL	VAL	VAL	VAL	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
ALA	ALA	ALA	ALA	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
VAL	VAL	VAL	VAL	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
ASN	ASN	ASN	ASN	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU

- Molecule 13: Cytoplasmic dynein 1 heavy chain 1

Chain f:  10% 7% 83%



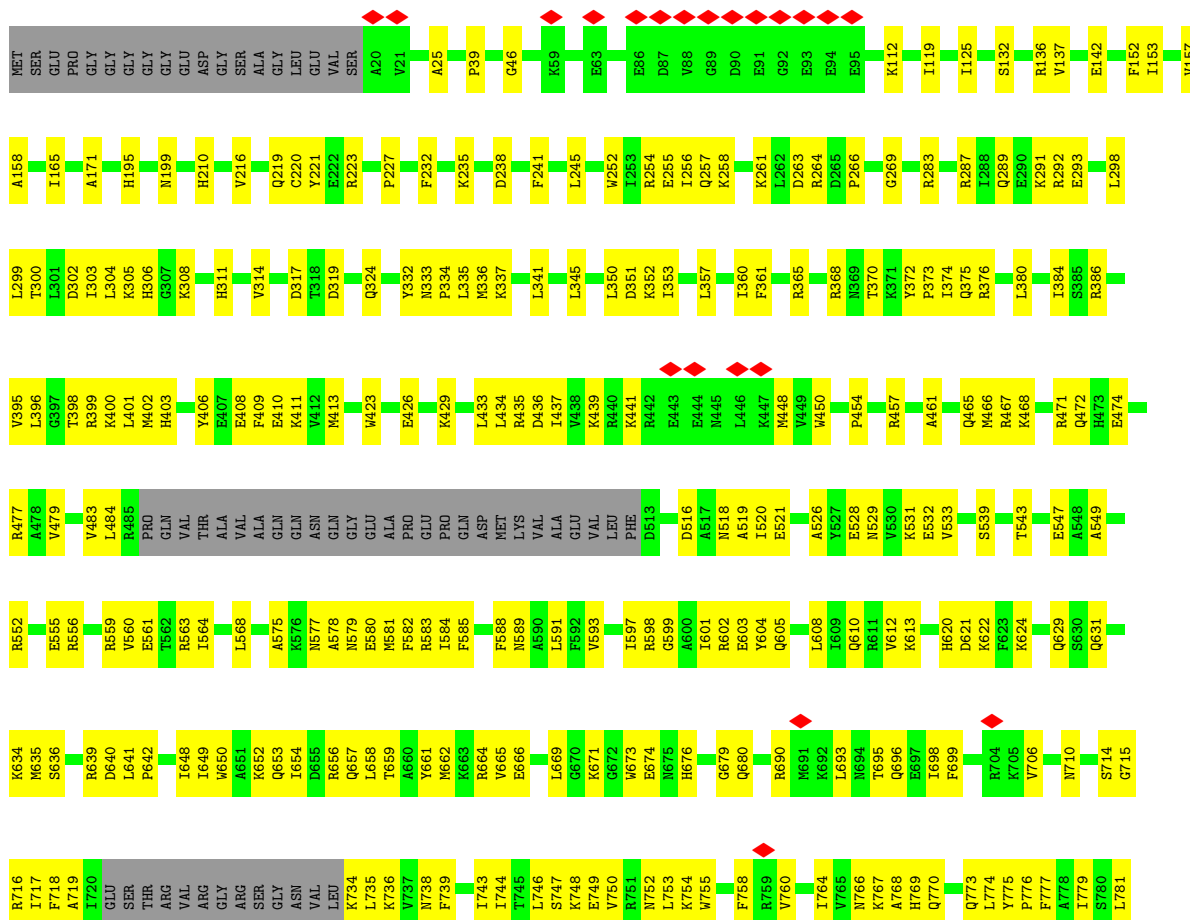


S618	L619	H620	D621	K622	F623	K624	V625	Q626	Y627	P628	Q629	A632	C633	K634	M635	S636	H637	V638	R639	D640	L641	P642	S647	I648	W650	A651	K652	Q653	I654	D655	R656	Q657	A660	Y661	R664	V665	L669	W673	V677	E678	K681	L682	K683	F689	T695	Q696	E697	I698																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
F699	D700	D701	R704	K705	V706	Q707	Q708	R709	N710	L711	G712	V713	R716	I717	F718	A719	I720	F721	S722	T723	S729	G730	N731	V732	L733	K734	L735	K736	N738	F739	L740	P741	E742	I743	I744	L746	S747	K748	E749	V750	R751	N752	L753	K754	W755	L756	G757	F758	R759	V760	I764	V765	N766																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
K767	A768	H769	Q770	Q773	F777	L781	L782	E783	S784	V785	T786	T787	R790	I794	V805	K810	I816	A817	I820	V823	W824	Y827	L829	P831	T832	V833	F843	Q844	V847	D848	L850	I851	I852	I853	I854	I855	I856	I857	I858	I859	I860	I861	I862	I863	I864	I865	I866	I867	I868	I869	I870	I871	I872	I873	I874	I875	I876	I877	I878	I879	I880	I881	I882	I883	I884	I885	I886	I887	I888	I889	I890	I891	I892	I893	I894	I895	I896	I897	I898	I899	I900	I901	I902	I903	I904	I905	I906	I907	I908	I909	I910	I911	I912	I913	I914	I915	I916	I917	I918	I919	I920	I921	I922	I923	I924	I925	I926	I927	I928	I929	I930	I931	I932	I933	I934	I935	I936	I937	I938	I939	I940	I941	I942	I943	I944	I945	I946	I947	I948	I949	I950	I951	I952	I953	I954	I955	I956	I957	I958	I959	I960	I961	I962	I963	I964	I965	I966	I967	I968	I969	I970	I971	I972	I973	I974	I975	I976	I977	I978	I979	I980	I981	I982	I983	I984	I985	I986	I987	I988	I989	I990	I991	I992	I993	I994	I995	I996	I997	I998	I999	I1000	I1001	I1002	I1003	I1004	I1005	I1006	I1007	I1008	I1009	I1010	I1011	I1012	I1013	I1014	I1015	I1016	I1017	I1018	I1019	I1020	I1021	I1022	I1023	I1024	I1025	I1026	I1027	I1028	I1029	I1030	I1031	I1032	I1033	I1034	I1035	I1036	I1037	I1038	I1039	I1040	I1041	I1042	I1043	I1044	I1045	I1046	I1047	I1048	I1049	I1050	I1051	I1052	I1053	I1054	I1055	I1056	I1057	I1058	I1059	I1060	I1061	I1062	I1063	I1064	I1065	I1066	I1067	I1068	I1069	I1070	I1071	I1072	I1073	I1074	I1075	I1076	I1077	I1078	I1079	I1080	I1081	I1082	I1083	I1084	I1085	I1086	I1087	I1088	I1089	I1090	I1091	I1092	I1093	I1094	I1095	I1096	I1097	I1098	I1099	I1100	I1101	I1102	I1103	I1104	I1105	I1106	I1107	I1108	I1109	I1110	I1111	I1112	I1113	I1114	I1115	I1116	I1117	I1118	I1119	I1120	I1121	I1122	I1123	I1124	I1125	I1126	I1127	I1128	I1129	I1130	I1131	I1132	I1133	I1134	I1135	I1136	I1137	I1138	I1139	I1140	I1141	I1142	I1143	I1144	I1145	I1146	I1147	I1148	I1149	I1150	I1151	I1152	I1153	I1154	I1155	I1156	I1157	I1158	I1159	I1160	I1161	I1162	I1163	I1164	I1165	I1166	I1167	I1168	I1169	I1170	I1171	I1172	I1173	I1174	I1175	I1176	I1177	I1178	I1179	I1180	I1181	I1182	I1183	I1184	I1185	I1186	I1187	I1188	I1189	I1190	I1191	I1192	I1193	I1194	I1195	I1196	I1197	I1198	I1199	I1200	I1201	I1202	I1203	I1204	I1205	I1206	I1207	I1208	I1209	I1210	I1211	I1212	I1213	I1214	I1215	I1216	I1217	I1218	I1219	I1220	I1221	I1222	I1223	I1224	I1225	I1226	I1227	I1228	I1229	I1230	I1231	I1232	I1233	I1234	I1235	I1236	I1237	I1238	I1239	I1240	I1241	I1242	I1243	I1244	I1245	I1246	I1247	I1248	I1249	I1250	I1251	I1252	I1253	I1254	I1255	I1256	I1257	I1258	I1259	I1260	I1261	I1262	I1263	I1264	I1265	I1266	I1267	I1268	I1269	I1270	I1271	I1272	I1273	I1274	I1275	I1276	I1277	I1278	I1279	I1280	I1281	I1282	I1283	I1284	I1285	I1286	I1287	I1288	I1289	I1290	I1291	I1292	I1293	I1294	I1295	I1296	I1297	I1298	I1299	I1300	I1301	I1302	I1303	I1304	I1305	I1306	I1307	I1308	I1309	I1310	I1311	I1312	I1313	I1314	I1315	I1316	I1317	I1318	I1319	I1320	I1321	I1322	I1323	I1324	I1325	I1326	I1327	I1328	I1329	I1330	I1331	I1332	I1333	I1334	I1335	I1336	I1337	I1338	I1339	I1340	I1341	I1342	I1343	I1344	I1345	I1346	I1347	I1348	I1349	I1350	I1351	I1352	I1353	I1354	I1355	I1356	I1357	I1358	I1359	I1360	I1361	I1362	I1363	I1364	I1365	I1366	I1367	I1368	I1369	I1370	I1371	I1372	I1373	I1374	I1375	I1376	I1377	I1378	I1379	I1380	I1381	I1382	I1383	I1384	I1385	I1386	I1387	I1388	I1389	I1390	I1391	I1392	I1393	I1394	I1395	I1396	I1397	I1398	I1399	I1400	I1401	I1402	I1403	I1404	I1405	I1406	I1407	I1408	I1409	I1410	I1411	I1412	I1413	I1414	I1415	I1416	I1417	I1418	I1419	I1420	I1421	I1422	I1423	I1424	I1425	I1426	I1427	I1428	I1429	I1430	I1431	I1432	I1433	I1434	I1435	I1436	I1437	I1438	I1439	I1440	I1441	I1442	I1443	I1444	I1445	I1446	I1447	I1448	I1449	I1450	I1451	I1452	I1453	I1454	I1455	I1456	I1457	I1458	I1459	I1460	I1461	I1462	I1463	I1464	I1465	I1466	I1467	I1468	I1469	I1470	I1471	I1472	I1473	I1474	I1475	I1476	I1477	I1478	I1479	I1480	I1481	I1482	I1483	I1484	I1485	I1486	I1487	I1488	I1489	I1490	I1491	I1492	I1493	I1494	I1495	I1496	I1497	I1498	I1499	I1500	I1501	I1502	I1503	I1504	I1505	I1506	I1507	I1508	I1509	I1510	I1511	I1512	I1513	I1514	I1515	I1516	I1517	I1518	I1519	I1520	I1521	I1522	I1523	I1524	I1525	I1526	I1527	I1528	I1529	I1530	I1531	I1532	I1533	I1534	I1535	I1536	I1537	I1538	I1539	I1540	I1541	I1542	I1543	I1544	I1545	I1546	I1547	I1548	I1549	I1550	I1551	I1552	I1553	I1554	I1555	I1556	I1557	I1558	I1559	I1560	I1561	I1562	I1563	I1564	I1565	I1566	I1567	I1568	I1569	I1570	I1571	I1572	I1573	I1574	I1575	I1576	I1577	I1578	I1579	I1580	I1581	I1582	I1583	I1584	I1585	I1586	I1587	I1588	I1589	I1590	I1591	I1592	I1593	I1594	I1595	I1596	I1597	I1598	I1599	I1600	I1601	I1602	I1603	I1604	I1605	I1606	I1607	I1608	I1609	I1610	I1611	I1612	I1613	I1614	I1615	I1616	I1617	I1618	I1619	I1620	I1621	I1622	I1623	I1624	I1625	I1626	I1627	I1628	I1629	I1630	I1631	I1632	I1633	I1634	I1635	I1636	I1637	I1638	I1639	I1640	I1641	I1642	I1643	I1644	I1645	I1646	I1647	I1648	I1649	I1650	I1651	I1652	I1653	I1654	I1655	I1656	I1657	I1658	I1659	I1660	I1661	I1662	I1663	I1664	I1665	I1666	I1667	I1668	I1669	I1670	I1671	I1672	I1673	I1674	I1675	I1676	I1677	I1678	I1679	I1680	I1681	I16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- Molecule 13: Cytoplasmic dynein 1 heavy chain 1

















- Molecule 14: Cytoplasmic dynein 1 intermediate chain 2

42%

E326	L359	V370	Q371	S409	Q419	T480	C484	F497	S500	L551	T562	E601	A619	E620	T621	ASN	ALA	ALA	ASN	ASN	ARG	ALA	ALA	ASP	ALA	GLU	GLU	GLU	ALA	ALA	THR	ARG	ILE	PRO	ALA
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- Molecule 14: Cytoplasmic dynein 1 intermediate chain 2

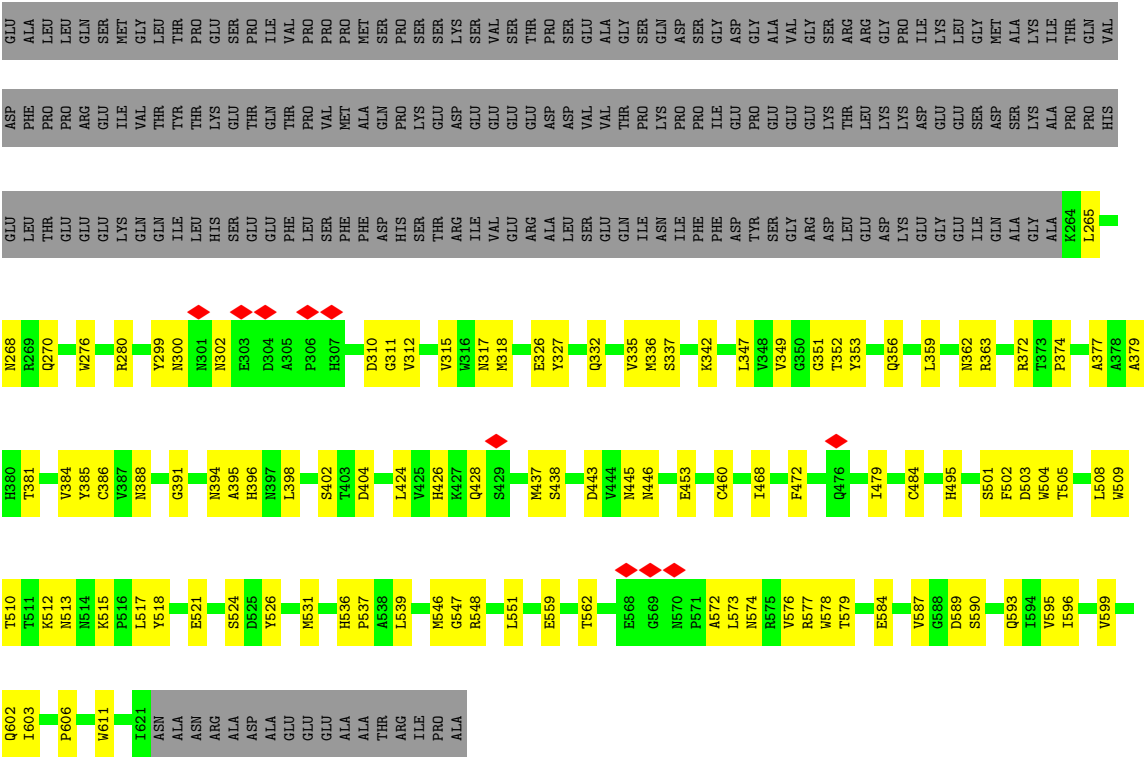
42%

I594	H483	C386	Q270
D598	H495	V390	F271
V599			
Q602	S500	Q393	V281
I603	S501	N394	V282
	F502		S283
E610	D503	S400	C284
	W504	I401	L285
	T505	S402	D286
R613	W509	T403	V287
F614	T510	D404	S288
		S405	
I621	N514	K406	Y291
ASN			P292
ALA		S409	E293
ASN	S524		L294
ARG	D525		L295
ALA	T526	K414	
ASP	Y527	L415	
ALA		S416	Y299
GLU			N300
GLU	W532	D420	
GLU			V312
ALA	H536	E423	
ALA			V316
ALA	L539	H426	N317
THR	F540	K427	N318
ARG	A541	Q428	
ILE			P325
PRO	D544	A433	
ALA	S545	V434	V328
	W546	T435	F329
	O547	S436	
	R548	K437	Q332
		S438	S333
	L551	F439	
	W552		N336
	N553	G450	
	L554	S451	L347
	N555	E452	V348
	N556	E453	
	D557	G454	T352
	T558	S455	
	E559	V456	G355
	W560	Y457	L359
	P561	T458	V360
	T562		
		K465	N365
	V567	L468	K366
	N570	S469	K367
		T470	T368
	L573	N471	P369
	N574	F472	
	R575	E473	R372
		G474	
	R583	H475	R380
	V587	T480	V384
			V289

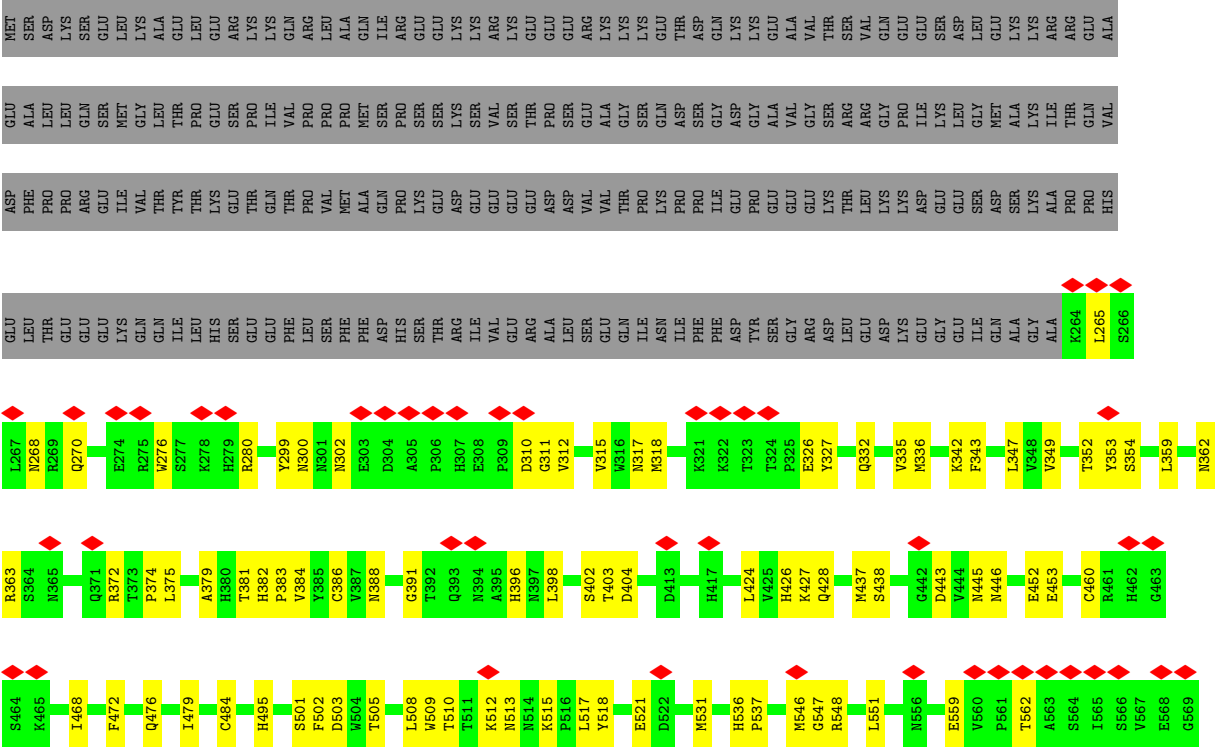
- Molecule 14: Cytoplasmic dynein 1 intermediate chain 2

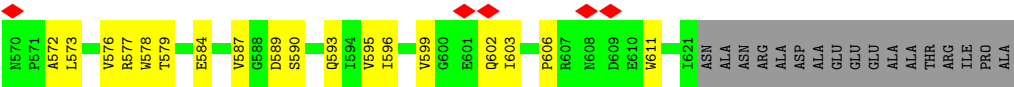
42%

MET	ASP	ASP	LYS	LYS	GLU	LEU	LYS	ALA	GLU	LEU	GLU	ARG	LYS	LYS	GLN	ARG	ARG	LEU	ALA	GLN	ILE	ARG	GLU	GLU	LYS	LYS	ARG	LYS	LYS	GLU	GLU	GLU	ARG	LYS	LYS	LYS	THR	GLU	GLU	ASP	GLN	LYS	LYS	LYS	VAL	THR	SER	VAL	GLN	GLU	GLU	SER	LEU	GLU	LYS	LYS	ARG	ARG	GLU	ALA
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● Molecule 14: Cytoplasmic dynein 1 intermediate chain 2





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	52920	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.187	Depositor
Minimum map value	-0.296	Depositor
Average map value	-0.008	Depositor
Map value standard deviation	0.051	Depositor
Recommended contour level	0.2	Depositor
Map size ( $\text{\AA}$ )	633.6, 633.6, 633.6	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	3.3, 3.3, 3.3	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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	0.14	0/3013	0.35	0/4070
1	B	0.17	0/3025	0.42	0/4085
1	C	0.17	0/3068	0.40	0/4144
1	D	0.16	0/3025	0.37	0/4085
1	E	0.17	0/3025	0.41	0/4085
1	F	0.17	0/3025	0.41	0/4085
1	G	0.17	0/3025	0.39	0/4085
1	I	0.14	0/3010	0.36	0/4066
2	H	0.16	0/2948	0.36	0/3991
3	J	0.23	0/2994	0.44	0/4066
4	K	0.14	0/2316	0.34	0/3135
5	L	0.18	0/2155	0.36	0/2905
6	M	0.17	0/2259	0.43	0/3090
6	N	0.16	0/1783	0.40	0/2451
6	P	0.16	0/2287	0.39	0/3119
6	Q	0.16	0/2375	0.38	0/3246
7	O	0.15	0/1194	0.42	0/1631
7	R	0.18	0/1093	0.49	0/1498
8	U	0.19	0/1241	0.48	0/1691
9	V	0.14	0/1286	0.38	0/1757
10	W	0.15	0/940	0.43	0/1281
10	Z	0.17	0/1467	0.44	0/1992
11	Y	0.36	0/3020	0.56	2/4119 (0.0%)
12	a	0.24	0/525	0.51	0/730
12	b	0.87	0/520	1.13	0/723
13	e	0.27	0/4754	0.47	0/6541
13	f	0.23	0/6683	0.46	2/9015 (0.0%)
13	m	0.18	0/5807	0.35	0/7751
13	n	0.27	0/5501	0.45	0/7337
14	g	0.11	0/1766	0.29	0/2457
14	h	0.13	0/2887	0.35	0/3938
14	o	0.12	0/2887	0.32	1/3938 (0.0%)



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
14	p	0.12	0/2887	0.32	1/3938 (0.0%)
All	All	0.20	0/87791	0.42	6/119045 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
11	Y	0	1
13	n	0	2
All	All	0	3

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	Y	294	PRO	N-CA-CB	-9.68	93.09	103.25
14	o	428	GLN	CB-CA-C	-5.20	110.56	116.54
14	p	428	GLN	CB-CA-C	-5.20	110.56	116.54
11	Y	51	CYS	CB-CA-C	5.05	116.40	108.63
13	f	37	LEU	CA-C-N	5.01	131.40	122.13
13	f	37	LEU	C-N-CA	5.01	131.40	122.13

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	Y	37	ARG	Sidechain
13	n	704	ARG	Sidechain
13	n	709	ARG	Sidechain

## 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	2944	0	2938	87	0
1	B	2956	0	2950	117	0
1	C	2998	0	2983	100	0
1	D	2956	0	2950	106	0
1	E	2956	0	2950	104	0
1	F	2956	0	2950	97	0
1	G	2956	0	2950	97	0
1	I	2941	0	2936	72	0
2	H	2885	0	2856	97	0
3	J	2932	0	3001	85	0
4	K	2264	0	2186	79	0
5	L	2121	0	2110	81	0
6	M	2238	0	1829	64	0
6	N	1767	0	1356	42	0
6	P	2262	0	2060	81	0
6	Q	2349	0	2069	59	0
7	O	1183	0	981	36	0
7	R	1082	0	881	33	0
8	U	1224	0	1215	39	0
9	V	1260	0	1213	37	0
10	W	937	0	707	33	0
10	Z	1444	0	1446	55	0
11	Y	2960	0	2711	83	0
12	a	527	0	234	7	0
12	b	522	0	232	9	0
13	e	4724	0	3273	57	0
13	f	6570	0	6693	307	0
13	m	5722	0	5269	219	0
13	n	5424	0	4963	260	0
14	g	1767	0	796	7	0
14	h	2808	0	2670	97	0
14	o	2808	0	2670	80	0
14	p	2808	0	2670	149	0
15	A	27	0	12	2	0
15	B	27	0	12	1	0
15	C	27	0	12	2	0
15	D	27	0	12	3	0
15	E	27	0	12	0	0
15	F	27	0	12	1	0
15	G	27	0	12	1	0
15	I	27	0	12	0	0
15	J	27	0	12	1	0
16	H	31	0	12	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	Y	3	0	0	0	0
All	All	86528	0	79818	2465	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 15.

All (2465) 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)
13:n:755:TRP:CZ2	14:p:453:GLU:CA	1.80	1.63
13:n:755:TRP:CZ2	14:p:453:GLU:HA	1.19	1.63
13:e:717:ILE:HA	13:e:824:TRP:CE2	1.39	1.55
13:n:779:ILE:CG2	14:p:375:LEU:HD22	1.33	1.54
13:n:779:ILE:HG21	14:p:375:LEU:CD2	1.33	1.52
13:n:755:TRP:CE2	14:p:453:GLU:HA	1.45	1.51
13:e:717:ILE:CB	13:e:824:TRP:CD2	1.97	1.48
13:n:755:TRP:CH2	14:p:453:GLU:HA	1.48	1.43
13:n:755:TRP:CE2	14:p:453:GLU:CA	1.89	1.43
13:e:717:ILE:N	13:e:824:TRP:CD1	1.87	1.41
13:n:748:LYS:NZ	14:p:383:PRO:HG2	1.07	1.39
13:n:748:LYS:NZ	14:p:383:PRO:CG	1.85	1.37
13:n:775:TYR:OH	14:p:354:SER:CA	1.73	1.36
13:e:717:ILE:CA	13:e:824:TRP:CE2	2.11	1.34
13:n:755:TRP:CZ2	14:p:453:GLU:C	2.05	1.32
13:n:755:TRP:CE2	14:p:453:GLU:CB	1.84	1.30
13:n:776:PRO:CB	14:p:375:LEU:O	1.81	1.28
13:n:779:ILE:CG2	14:p:375:LEU:CD2	1.97	1.28
13:n:779:ILE:CB	14:p:375:LEU:HD22	1.62	1.28
13:n:776:PRO:HB2	14:p:375:LEU:O	1.33	1.27
13:n:755:TRP:CE2	14:p:453:GLU:HB3	1.55	1.26
13:n:755:TRP:CZ3	14:p:452:GLU:O	1.89	1.25
13:n:748:LYS:CE	14:p:383:PRO:HG2	1.67	1.25
13:n:775:TYR:CE2	14:p:381:THR:O	1.90	1.24
13:n:755:TRP:NE1	14:p:453:GLU:CB	1.80	1.18
13:n:755:TRP:HB2	14:p:453:GLU:OE2	1.40	1.14
13:n:775:TYR:HE2	14:p:381:THR:O	1.26	1.12
13:e:717:ILE:CB	13:e:824:TRP:CE3	2.33	1.10
13:n:748:LYS:HZ3	14:p:383:PRO:CG	1.53	1.08
13:e:720:ILE:CB	13:e:820:ILE:HD12	1.84	1.07
13:n:751:ARG:NH2	14:p:403:THR:HB	1.72	1.05
13:e:717:ILE:HA	13:e:824:TRP:NE1	1.73	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:e:716:ARG:C	13:e:824:TRP:CD1	2.36	1.04
13:e:717:ILE:N	13:e:824:TRP:NE1	2.05	1.04
13:e:717:ILE:HA	13:e:824:TRP:CZ2	1.92	1.03
13:e:717:ILE:CA	13:e:824:TRP:NE1	2.22	1.02
13:n:779:ILE:HB	14:p:375:LEU:HD22	1.42	1.01
13:n:775:TYR:OH	14:p:354:SER:HA	0.84	1.00
13:n:755:TRP:CZ3	14:p:453:GLU:HA	1.96	1.00
13:n:779:ILE:HG21	14:p:375:LEU:HD21	1.02	1.00
13:n:755:TRP:CD2	14:p:453:GLU:HA	1.98	0.99
13:e:717:ILE:CB	13:e:824:TRP:CG	2.48	0.97
13:m:578:ALA:HA	13:m:581:MET:HE2	1.47	0.96
13:n:755:TRP:NE1	14:p:453:GLU:HB3	0.97	0.96
1:E:65:HIS:HD1	1:G:171:TYR:HH	1.13	0.96
13:e:716:ARG:C	13:e:824:TRP:NE1	2.26	0.94
13:n:748:LYS:HZ1	14:p:383:PRO:CG	1.67	0.94
13:n:755:TRP:CH2	14:p:452:GLU:O	2.21	0.93
13:n:755:TRP:CD2	14:p:453:GLU:CA	2.52	0.93
13:n:755:TRP:HE1	14:p:453:GLU:HB3	1.20	0.93
13:f:278:TRP:HB2	13:f:336:MET:HE3	1.49	0.92
7:R:28:ARG:NH1	7:R:28:ARG:O	2.03	0.90
6:N:348:MET:HE1	10:Z:1135:HIS:H	1.33	0.90
13:n:751:ARG:NH2	14:p:403:THR:CB	2.34	0.90
13:e:717:ILE:CA	13:e:824:TRP:CD2	2.47	0.90
13:e:717:ILE:H	13:e:824:TRP:CD1	1.83	0.89
13:n:755:TRP:HZ2	14:p:453:GLU:C	1.80	0.88
1:E:30:ILE:HG12	6:Q:5:LYS:HZ3	1.36	0.88
6:P:147:LEU:HD11	10:Z:1214:VAL:HG11	1.55	0.88
6:P:262:MET:HE3	7:R:33:VAL:HG22	1.55	0.88
13:m:402:MET:HB3	13:m:531:LYS:HG3	1.52	0.88
13:n:775:TYR:CD2	14:p:381:THR:O	2.26	0.88
6:Q:12:ILE:HB	6:Q:14:ARG:NH1	1.89	0.88
1:C:48:MET:HB3	1:E:173:GLY:HA2	1.52	0.88
13:e:717:ILE:CB	13:e:824:TRP:CE2	2.48	0.88
13:f:82:SER:HA	13:f:113:SER:HA	1.56	0.87
13:n:755:TRP:CB	14:p:453:GLU:OE2	2.09	0.87
1:B:107:PRO:HB3	1:B:136:ALA:HB3	1.57	0.86
1:A:288:MET:HE1	4:K:167:ASN:HA	1.58	0.86
13:f:402:MET:SD	13:f:470:ARG:NH2	2.48	0.86
13:m:526:ALA:HB2	13:m:556:ARG:HD2	1.58	0.86
13:n:755:TRP:CZ2	14:p:453:GLU:O	2.27	0.86
6:P:312:LYS:O	6:Q:317:TYR:OH	1.95	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:n:776:PRO:HB3	14:p:375:LEU:O	1.77	0.84
6:Q:63:ARG:HE	10:Z:1209:LYS:HZ1	1.26	0.84
6:M:341:LYS:HA	7:O:110:MET:HE1	1.58	0.84
13:n:748:LYS:HZ1	14:p:383:PRO:HG3	1.41	0.84
6:M:212:GLU:HB2	10:W:1255:LYS:HB3	1.59	0.83
11:Y:55:LEU:HB3	11:Y:298:PRO:HB3	1.61	0.83
13:f:378:LEU:HB3	13:f:452:ILE:HD11	1.58	0.83
13:n:751:ARG:HH22	14:p:403:THR:CB	1.93	0.82
13:f:275:ILE:HA	13:f:336:MET:HE1	1.62	0.82
13:n:779:ILE:HG22	14:p:375:LEU:HD22	1.57	0.82
1:F:30:ILE:HD13	6:N:5:LYS:HZ1	1.43	0.82
1:A:48:MET:HE3	1:C:147:LEU:HD11	1.60	0.81
6:N:379:GLN:HB3	6:N:383:ARG:HH12	1.44	0.81
13:f:529:ASN:HB3	13:f:552:ARG:HE	1.44	0.81
1:C:308:LYS:HD2	6:Q:39:GLU:HB2	1.61	0.80
5:L:88:MET:HE2	5:L:94:ARG:HB2	1.63	0.80
13:f:232:PHE:HB3	13:f:235:LYS:HB2	1.63	0.80
13:n:755:TRP:CH2	14:p:453:GLU:CA	2.31	0.80
1:G:110:LEU:HB3	1:G:139:ILE:HG22	1.63	0.80
13:n:748:LYS:NZ	14:p:383:PRO:HG3	1.95	0.79
13:f:399:ARG:NH1	13:f:416:CYS:SG	2.56	0.79
13:n:755:TRP:HZ2	14:p:453:GLU:O	1.61	0.79
13:f:85:LYS:HA	13:f:97:GLU:HA	1.65	0.79
14:h:465:LYS:NZ	14:h:469:SER:OG	2.16	0.79
10:W:1105:MET:HE2	10:Z:1105:MET:SD	2.23	0.79
1:B:164:VAL:HG21	1:B:182:ARG:HH11	1.47	0.79
13:e:717:ILE:N	13:e:824:TRP:CG	2.50	0.79
6:M:383:ARG:HA	6:Q:183:LEU:HD11	1.65	0.78
1:A:107:PRO:HB3	1:A:136:ALA:HB3	1.65	0.78
1:D:283:ILE:HD12	1:D:294:LEU:HB3	1.65	0.78
6:Q:241:THR:HG22	7:R:33:VAL:HG23	1.63	0.78
1:E:107:PRO:HB3	1:E:136:ALA:HB3	1.62	0.78
1:A:227:ASN:HB3	1:A:230:LYS:HG2	1.64	0.78
1:I:121:ARG:HH21	1:I:141:MET:HE1	1.49	0.78
13:e:717:ILE:CA	13:e:824:TRP:CD1	2.61	0.78
1:B:179:SER:HA	1:B:285:LYS:HD2	1.65	0.78
1:G:346:ILE:HD11	6:M:56:TYR:HB2	1.64	0.78
13:n:755:TRP:CE3	14:p:453:GLU:HA	2.19	0.78
1:B:87:GLU:HA	1:B:90:TRP:CE3	2.19	0.78
1:D:48:MET:HB3	1:F:173:GLY:HA2	1.66	0.77
1:B:145:LEU:HA	1:B:148:TYR:HD2	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:n:591:LEU:HB2	13:n:601:ILE:HD11	1.64	0.77
14:o:547:GLY:HA2	14:o:573:LEU:HD23	1.67	0.77
13:f:431:GLN:HB3	13:f:435:ARG:HH12	1.48	0.77
6:P:354:LEU:HD11	7:R:125:ARG:HH21	1.50	0.77
10:Z:1267:ARG:HG2	10:Z:1269:ARG:HH22	1.48	0.77
2:H:200:PHE:HB3	2:H:205:GLU:HB3	1.65	0.77
13:n:775:TYR:HH	14:p:354:SER:CA	1.74	0.77
1:G:227:ASN:HB3	1:G:230:LYS:HG2	1.65	0.76
6:M:399:ARG:NH2	6:N:397:ASP:OD1	2.14	0.76
14:p:424:LEU:HD12	14:p:468:ILE:HG13	1.68	0.76
7:R:28:ARG:HH12	7:R:31:ARG:HH12	1.34	0.76
6:N:379:GLN:HB3	6:N:383:ARG:NH1	2.00	0.75
1:D:107:PRO:HB3	1:D:136:ALA:HB3	1.68	0.75
14:p:547:GLY:HA2	14:p:573:LEU:HD23	1.67	0.75
13:n:456:HIS:O	13:n:460:GLN:N	2.19	0.75
13:e:718:PHE:CB	13:e:819:GLY:O	2.35	0.75
13:n:748:LYS:CE	14:p:383:PRO:CG	2.46	0.74
14:o:424:LEU:HD12	14:o:468:ILE:HG13	1.68	0.74
7:O:148:LYS:HD3	6:P:142:LYS:HD3	1.69	0.74
13:f:409:PHE:CZ	13:f:470:ARG:HD2	2.22	0.74
13:n:779:ILE:HG22	14:p:375:LEU:CD2	2.13	0.74
1:B:290:LEU:HB3	1:B:294:LEU:HD23	1.69	0.74
10:W:1105:MET:HE1	10:Z:1106:ARG:HG2	1.68	0.74
13:n:775:TYR:CZ	14:p:354:SER:HA	2.14	0.74
11:Y:111:CYS:SG	11:Y:114:CYS:N	2.57	0.73
13:f:269:GLY:O	13:f:386:ARG:NH2	2.20	0.73
13:f:616:ILE:HD12	13:f:682:LEU:HD11	1.68	0.73
6:Q:212:GLU:HB2	10:Z:1269:ARG:HE	1.53	0.73
9:V:53:ALA:HB2	9:V:71:PRO:HG3	1.69	0.73
6:N:392:ASN:HD21	10:Z:1179:ILE:HG12	1.53	0.73
1:G:354:LYS:HA	1:G:357:TRP:CZ3	2.23	0.73
13:n:232:PHE:HB3	13:n:235:LYS:HB2	1.71	0.73
9:V:73:PHE:HA	9:V:82:PHE:HA	1.70	0.73
11:Y:294:PRO:HB2	11:Y:302:LYS:HZ1	1.53	0.73
1:G:358:VAL:HG22	1:G:374:LYS:HD2	1.70	0.72
4:K:154:ILE:HB	4:K:179:PHE:HB3	1.69	0.72
5:L:47:LEU:HD21	5:L:151:ILE:HD11	1.71	0.72
8:U:43:ALA:HB2	8:U:48:ILE:HG12	1.71	0.72
9:V:58:GLY:HA3	9:V:89:ASP:HA	1.70	0.72
13:f:716:ARG:HG2	13:f:823:VAL:HG12	1.70	0.72
13:f:466:MET:HA	13:f:469:PHE:CE1	2.24	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:m:255:GLU:HA	13:m:258:LYS:HE2	1.71	0.72
13:f:361:PHE:HD2	13:f:430:LEU:HD23	1.55	0.72
13:f:395:VAL:HG12	13:f:399:ARG:HE	1.55	0.72
14:h:282:VAL:O	14:h:574:ASN:ND2	2.22	0.72
8:U:101:MET:HB2	8:U:119:LEU:HB2	1.70	0.72
13:f:406:TYR:HA	13:f:409:PHE:CE1	2.25	0.72
13:e:739:PHE:CB	13:e:824:TRP:CE2	2.73	0.72
13:f:117:ALA:N	13:f:138:LEU:O	2.17	0.72
1:F:158:LEU:HD11	1:F:275:ILE:HD11	1.72	0.71
11:Y:162:ARG:HG2	11:Y:166:LYS:NZ	2.05	0.71
11:Y:294:PRO:HB2	11:Y:302:LYS:NZ	2.05	0.71
13:e:344:LEU:HA	13:e:356:ALA:HB1	1.71	0.71
13:n:751:ARG:CZ	14:p:403:THR:HB	2.20	0.71
2:H:153:MET:HE3	2:H:299:LEU:HD22	1.71	0.71
7:R:22:TYR:O	7:R:27:SER:OG	2.08	0.71
13:f:466:MET:HA	13:f:469:PHE:CD1	2.26	0.71
1:C:107:PRO:HB3	1:C:136:ALA:HB3	1.70	0.70
1:A:46:ARG:NH2	1:A:52:LEU:O	2.24	0.70
2:H:190:MET:HE1	2:H:209:VAL:HG21	1.73	0.70
13:f:575:ALA:HB3	13:f:584:ILE:HD13	1.74	0.70
1:B:56:ILE:HD13	1:B:88:ARG:HD3	1.73	0.70
13:f:720:ILE:HD12	13:f:733:LEU:HD13	1.73	0.70
13:m:368:ARG:HD2	13:m:433:LEU:HD11	1.73	0.70
13:n:755:TRP:CZ3	14:p:452:GLU:C	2.69	0.70
1:G:229:GLN:HE22	1:G:264:ARG:HH22	1.37	0.70
10:W:1282:ASP:HA	10:W:1285:ILE:HG22	1.73	0.70
11:Y:70:CYS:SG	11:Y:73:CYS:N	2.61	0.70
13:f:817:ALA:HA	13:f:820:ILE:HD12	1.73	0.70
13:m:227:PRO:HB2	13:m:299:LEU:HD22	1.71	0.70
1:E:185:ILE:HD11	1:E:261:LEU:HG	1.73	0.69
13:f:626:GLN:HB2	13:f:629:GLN:HG2	1.73	0.69
9:V:13:TYR:HB2	9:V:24:ARG:HG3	1.73	0.69
1:G:28:ASP:HB2	1:G:341:TRP:HH2	1.58	0.69
7:O:160:LEU:HD22	6:Q:179:LEU:HD12	1.74	0.69
1:A:366:ASP:HB3	1:A:370:SER:HB3	1.75	0.69
1:C:116:ASN:OD1	1:C:182:ARG:NH1	2.26	0.69
5:L:179:THR:HB	5:L:187:MET:HB3	1.74	0.69
1:B:10:GLN:HG2	13:n:246:GLN:HE22	1.58	0.69
1:B:267:LEU:O	1:C:178:HIS:NE2	2.25	0.69
13:e:718:PHE:CB	13:e:822:LEU:O	2.41	0.69
13:n:748:LYS:HE2	14:p:383:PRO:HG2	1.71	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:e:486:PRO:HA	13:e:512:PHE:HA	1.76	0.68
6:Q:102:GLN:NE2	6:Q:106:GLN:OE1	2.26	0.68
14:h:471:MET:O	14:h:514:ASN:ND2	2.24	0.68
13:n:755:TRP:CD1	14:p:453:GLU:OE1	2.16	0.68
3:J:365:GLN:HA	3:J:368:LEU:HD12	1.75	0.68
14:h:369:PRO:O	14:h:372:ARG:NH2	2.26	0.68
4:K:128:LEU:HD11	4:K:158:ILE:HD11	1.74	0.68
1:D:57:PHE:HA	1:D:61:LYS:HE2	1.74	0.68
6:P:265:VAL:HA	6:P:268:LEU:HD12	1.74	0.68
13:m:750:VAL:HG22	13:m:760:VAL:HG11	1.76	0.68
13:n:779:ILE:HG22	14:p:375:LEU:HD13	1.76	0.68
8:U:165:ASP:HA	8:U:168:MET:HE1	1.76	0.68
10:W:1275:GLU:O	10:W:1279:GLN:NE2	2.27	0.68
12:a:133:GLY:HA2	12:b:133:GLY:HA2	1.73	0.68
13:f:431:GLN:HB3	13:f:435:ARG:NH1	2.09	0.68
1:C:154:THR:HG23	1:C:171:TYR:HA	1.75	0.67
13:f:365:ARG:HH21	13:f:433:LEU:HB2	1.60	0.67
14:h:414:MET:HE3	14:h:416:SER:HB2	1.76	0.67
1:A:154:THR:HG23	1:A:171:TYR:HA	1.77	0.67
14:o:505:THR:HG22	14:o:521:GLU:HG2	1.75	0.67
7:O:157:THR:HG22	6:Q:179:LEU:HB3	1.77	0.67
6:P:316:LEU:HG	6:Q:317:TYR:CE2	2.28	0.67
13:n:580:GLU:HG3	13:n:583:ARG:HH12	1.60	0.67
6:M:383:ARG:NH1	6:Q:183:LEU:O	2.26	0.67
1:B:143:ALA:HB1	1:B:157:VAL:HB	1.77	0.67
1:F:158:LEU:HD22	1:F:279:LEU:HD21	1.77	0.67
11:Y:42:VAL:HG13	11:Y:282:LEU:HD12	1.75	0.67
13:n:775:TYR:OH	14:p:354:SER:CB	2.43	0.67
1:C:267:LEU:O	1:D:178:HIS:NE2	2.27	0.67
13:f:529:ASN:OD1	13:f:556:ARG:NH1	2.28	0.67
13:n:779:ILE:CG2	14:p:375:LEU:HD21	1.92	0.67
1:I:26:ALA:O	1:I:345:SER:OG	2.13	0.67
13:f:751:ARG:HH21	14:h:433:ALA:HB1	1.60	0.67
11:Y:258:GLN:OE1	11:Y:272:ARG:NH1	2.28	0.67
11:Y:358:ASP:O	11:Y:423:THR:OG1	2.09	0.66
14:p:505:THR:HG22	14:p:521:GLU:HG2	1.75	0.66
1:G:354:LYS:HA	1:G:357:TRP:CE3	2.31	0.66
4:K:82:LEU:HD13	4:K:88:LEU:HD21	1.76	0.66
10:W:1130:ALA:O	10:W:1134:LEU:N	2.25	0.66
13:f:279:LEU:HB3	13:f:283:ARG:HH12	1.60	0.66
14:h:426:HIS:CD2	14:h:427:LYS:HG2	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:f:363:HIS:HA	13:f:366:LYS:HE3	1.77	0.66
13:m:829:LEU:HA	13:m:832:TYR:HB3	1.77	0.66
2:H:220:ALA:HB1	2:H:226:GLU:HG3	1.78	0.66
8:U:98:ALA:HB3	8:U:101:MET:HE3	1.76	0.66
13:n:280:ASN:OD1	13:n:283:ARG:NH2	2.28	0.66
1:A:111:THR:HG22	1:A:142:GLN:HG2	1.77	0.66
1:E:229:GLN:HE22	1:E:264:ARG:HH22	1.44	0.66
1:I:305:THR:O	1:I:336:ARG:NH1	2.29	0.66
13:f:526:ALA:HB1	13:f:553:TYR:HD1	1.61	0.66
1:E:21:ILE:HG23	1:E:37:ASN:HB2	1.77	0.65
4:K:152:GLN:HG3	4:K:181:ILE:HB	1.78	0.65
13:f:449:VAL:HG13	13:f:451:ARG:HD3	1.77	0.65
13:e:283:ARG:HA	13:f:175:GLY:HA3	1.78	0.65
14:h:602:GLN:HG2	14:h:603:ILE:HD12	1.77	0.65
13:m:648:ILE:HD13	13:m:753:LEU:HD11	1.78	0.65
6:P:147:LEU:HD11	10:Z:1214:VAL:CG1	2.26	0.65
13:f:413:MET:HE2	13:f:466:MET:HE1	1.76	0.65
1:B:46:ARG:NH2	1:B:52:LEU:O	2.29	0.65
13:n:255:GLU:HA	13:n:258:LYS:HD2	1.78	0.65
2:H:151:ILE:HB	2:H:293:LEU:HD12	1.79	0.65
5:L:161:SER:O	5:L:163:ARG:N	2.30	0.65
13:m:653:GLN:HG3	14:o:526:TYR:HE1	1.61	0.65
13:n:779:ILE:HG22	14:p:375:LEU:CD1	2.27	0.65
5:L:45:GLN:NE2	5:L:46:PRO:HD2	2.12	0.65
8:U:113:VAL:O	8:U:115:ARG:NH2	2.30	0.65
1:I:104:GLU:OE2	1:I:133:ASN:ND2	2.30	0.65
8:U:118:ILE:HB	8:U:136:VAL:HG23	1.78	0.65
13:f:829:LEU:O	13:f:833:VAL:N	2.30	0.65
13:m:776:PRO:HB3	14:o:377:ALA:HA	1.78	0.65
2:H:42:GLY:HA3	3:J:387:TRP:HA	1.79	0.65
4:K:204:VAL:HG21	5:L:232:TYR:HB3	1.78	0.65
13:n:591:LEU:HD13	13:n:597:ILE:HG21	1.79	0.65
1:D:46:ARG:NH2	1:D:52:LEU:O	2.30	0.64
6:N:210:THR:HA	10:W:1255:LYS:HZ1	1.60	0.64
13:m:436:ASP:HA	13:m:439:LYS:HD2	1.78	0.64
3:J:308:GLY:HA2	3:J:311:MET:HE3	1.77	0.64
13:m:695:THR:HG23	13:m:698:ILE:HD12	1.78	0.64
13:m:257:GLN:HB3	13:m:261:LYS:HE2	1.79	0.64
4:K:144:TYR:HB2	4:K:155:ILE:HB	1.79	0.64
14:o:386:CYS:HB3	14:o:437:MET:SD	2.37	0.64
1:C:94:TYR:HE2	1:C:103:SER:HA	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:62:CYS:HB2	5:L:133:LEU:HD21	1.80	0.64
13:e:777:PHE:HA	13:e:833:VAL:HG11	1.80	0.64
1:B:336:ARG:NH2	6:P:84:GLU:O	2.30	0.64
6:M:378:VAL:HG21	6:N:375:LEU:HD22	1.80	0.64
13:n:546:TRP:NE1	13:n:550:MET:HE3	2.13	0.64
1:C:144:VAL:HG13	1:C:145:LEU:HD12	1.79	0.64
13:f:716:ARG:HA	13:f:823:VAL:HA	1.79	0.64
13:f:844:GLN:NE2	13:f:848:ASP:OD2	2.30	0.64
13:n:775:TYR:HH	14:p:354:SER:HA	0.82	0.64
1:I:11:PRO:HB3	1:I:107:PRO:HG2	1.79	0.64
3:J:150:PRO:HG2	3:J:160:CYS:HB2	1.79	0.64
6:N:340:ILE:HD12	6:N:344:HIS:HE1	1.63	0.64
13:f:516:ASP:OD2	13:f:567:ARG:NH2	2.29	0.64
13:f:652:LYS:HE2	13:f:756:LEU:HD22	1.80	0.64
13:f:740:LEU:HB3	13:f:742:GLU:HG2	1.79	0.64
13:f:790:ARG:HG3	13:f:794:LYS:HE3	1.80	0.64
14:h:328:VAL:O	14:h:367:ARG:NE	2.29	0.64
1:C:366:ASP:HB2	1:C:370:SER:HB3	1.78	0.64
1:F:10:GLN:O	1:F:106:HIS:ND1	2.30	0.64
1:G:76:GLU:OE1	1:G:188:ARG:NH1	2.31	0.64
1:G:112:GLU:OE2	1:G:121:ARG:NE	2.31	0.64
13:n:569:ARG:HH12	13:n:600:ALA:HB1	1.63	0.64
1:D:346:ILE:HG23	13:m:311:HIS:HA	1.80	0.63
1:D:119:LYS:HA	1:D:122:GLU:HG2	1.81	0.63
13:f:661:TYR:HA	13:f:664:ARG:HD2	1.81	0.63
14:o:531:MET:HE2	14:o:578:TRP:HD1	1.63	0.63
14:p:386:CYS:HB3	14:p:437:MET:SD	2.37	0.63
1:F:330:ILE:HB	6:N:20:TYR:HB2	1.80	0.63
4:K:258:LEU:HD21	5:L:148:TRP:HB2	1.80	0.63
13:m:824:TRP:HA	13:m:829:LEU:HD11	1.80	0.63
14:p:336:MET:HE1	14:p:353:TYR:HA	1.80	0.63
4:K:186:ALA:N	4:K:216:VAL:O	2.30	0.63
8:U:25:GLY:HA3	8:U:43:ALA:HB3	1.81	0.63
13:n:716:ARG:NH1	13:n:820:ILE:O	2.31	0.63
1:A:267:LEU:O	1:B:178:HIS:NE2	2.32	0.63
1:I:110:LEU:HD21	1:I:128:PHE:HE2	1.62	0.63
13:f:746:LEU:HD22	13:f:768:ALA:HB2	1.80	0.63
14:o:402:SER:OG	14:o:404:ASP:OD1	2.15	0.63
14:p:531:MET:HE2	14:p:578:TRP:HD1	1.63	0.63
1:B:156:VAL:HG23	1:B:294:LEU:HD12	1.81	0.63
2:H:174:ALA:HA	2:H:284:LYS:HD2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:f:753:LEU:HB3	13:f:758:PHE:HB2	1.81	0.63
1:C:158:LEU:HD21	1:C:275:ILE:HD11	1.80	0.63
9:V:143:PHE:HA	9:V:157:LEU:HB2	1.81	0.63
1:C:141:MET:O	1:C:145:LEU:HD13	1.99	0.62
1:F:112:GLU:HG2	1:F:139:ILE:HD11	1.81	0.62
1:F:358:VAL:HG22	1:F:374:LYS:HD2	1.81	0.62
13:e:717:ILE:CA	13:e:824:TRP:CG	2.77	0.62
13:f:306:HIS:O	13:f:308:LYS:NZ	2.31	0.62
13:m:152:PHE:O	13:m:157:VAL:N	2.27	0.62
1:C:148:TYR:CE2	1:C:347:LEU:HD12	2.34	0.62
1:C:206:HIS:NE2	1:D:270:GLU:OE2	2.32	0.62
1:F:243:LEU:HD12	1:F:247:SER:HB2	1.81	0.62
6:N:13:ALA:O	6:N:14:ARG:NE	2.29	0.62
6:P:322:ARG:NH2	10:W:1114:HIS:HA	2.14	0.62
13:f:121:ARG:H	13:f:135:LEU:HA	1.64	0.62
13:f:401:LEU:HD12	13:f:409:PHE:HB2	1.80	0.62
13:f:619:LEU:HD12	13:f:622:LYS:HD2	1.81	0.62
14:o:336:MET:HE1	14:o:353:TYR:HA	1.80	0.62
1:B:164:VAL:HG23	1:B:184:ASP:HA	1.81	0.62
1:E:244:PRO:O	1:G:292:ARG:NH1	2.32	0.62
13:m:341:LEU:HA	13:m:360:ILE:HD11	1.80	0.62
4:K:151:GLN:NE2	4:K:181:ILE:O	2.32	0.62
13:f:653:GLN:HB3	13:f:656:ARG:HH21	1.65	0.62
13:n:279:LEU:HB3	13:n:283:ARG:HH12	1.65	0.62
1:E:245:ASP:H	1:G:288:MET:HE1	1.64	0.62
11:Y:54:CYS:O	11:Y:54:CYS:SG	2.57	0.62
13:n:748:LYS:CE	14:p:383:PRO:CD	2.77	0.62
1:A:39:VAL:HG21	1:A:85:ASP:HB3	1.82	0.62
1:C:51:ALA:HB2	1:E:173:GLY:HA3	1.80	0.62
14:h:402:SER:OG	14:h:404:ASP:OD1	2.14	0.62
13:n:437:ILE:HA	13:n:441:LYS:HZ1	1.65	0.62
1:D:303:GLY:HA3	15:D:800:ADP:H5'2	1.81	0.62
13:e:270:THR:O	13:e:274:GLU:N	2.25	0.62
13:m:591:LEU:HD23	13:m:597:ILE:HG21	1.80	0.62
13:n:673:TRP:HA	13:n:676:HIS:HD2	1.63	0.62
1:C:57:PHE:HA	1:C:61:LYS:HE2	1.82	0.62
2:H:106:THR:HB	2:H:137:GLN:HG2	1.82	0.62
12:a:305:LYS:HA	12:b:305:LYS:HA	1.80	0.62
13:f:351:ASP:OD2	13:f:355:GLN:NE2	2.32	0.62
13:n:227:PRO:HB2	13:n:299:LEU:HD22	1.82	0.62
1:E:154:THR:HG23	1:E:171:TYR:HA	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:207:GLU:OE2	2:H:210:ARG:NH2	2.33	0.62
1:I:199:ARG:NH1	3:J:145:GLU:OE1	2.33	0.62
9:V:38:GLY:HA3	9:V:59:ARG:HA	1.82	0.62
13:n:266:PRO:HB3	13:n:376:ARG:HG3	1.82	0.62
13:n:748:LYS:HZ3	14:p:383:PRO:HG2	0.80	0.62
1:G:154:THR:HG23	1:G:171:TYR:HA	1.81	0.61
5:L:49:ILE:HD11	5:L:58:ASP:HB3	1.81	0.61
13:m:738:ASN:HB3	13:m:824:TRP:HE1	1.65	0.61
13:n:699:PHE:HD1	13:n:753:LEU:HD23	1.65	0.61
14:p:551:LEU:O	14:p:562:THR:N	2.33	0.61
2:H:261:LEU:HB3	2:H:274:ILE:HD13	1.81	0.61
12:a:126:LEU:HA	12:b:126:LEU:HA	1.82	0.61
1:B:366:ASP:HB2	1:B:370:SER:HB3	1.82	0.61
1:E:202:GLY:HA2	1:F:117:PRO:HG3	1.83	0.61
13:f:656:ARG:NH1	13:f:657:GLN:OE1	2.28	0.61
13:n:598:ARG:O	13:n:602:ARG:HG3	2.00	0.61
11:Y:42:VAL:HG23	11:Y:284:CYS:HA	1.82	0.61
13:f:464:ASP:OD2	13:f:467:ARG:NH2	2.32	0.61
13:m:351:ASP:OD1	13:m:352:LYS:N	2.33	0.61
13:n:561:GLU:HB3	13:n:596:HIS:HD2	1.64	0.61
1:A:48:MET:HE2	1:A:48:MET:HA	1.81	0.61
5:L:147:CYS:HB3	5:L:176:TRP:HB3	1.83	0.61
6:Q:63:ARG:HH21	10:Z:1209:LYS:HZ3	1.47	0.61
14:h:555:ASN:ND2	14:h:610:GLU:OE1	2.32	0.61
13:m:283:ARG:HD3	13:n:175:GLY:HA3	1.82	0.61
13:n:334:PRO:HA	13:n:337:LYS:HZ2	1.65	0.61
5:L:136:LYS:HB3	5:L:148:TRP:HB3	1.82	0.61
7:O:129:LEU:HD12	7:O:132:ILE:HD11	1.83	0.61
1:G:268:ILE:HG23	1:G:270:GLU:OE1	2.01	0.61
5:L:161:SER:C	5:L:163:ARG:H	2.08	0.61
11:Y:295:GLU:O	11:Y:296:PHE:C	2.43	0.61
1:E:56:ILE:HD13	1:E:88:ARG:HD3	1.82	0.61
9:V:3:LEU:HD13	11:Y:5:LEU:HD13	1.83	0.61
13:f:718:PHE:HB3	13:f:735:LEU:HD11	1.82	0.61
3:J:329:LYS:HD3	3:J:331:LYS:H	1.66	0.60
6:M:345:GLU:HA	6:M:348:MET:HE2	1.83	0.60
1:I:87:GLU:O	1:I:91:GLN:HG2	2.02	0.60
6:Q:178:ARG:HA	6:Q:181:LEU:HG	1.82	0.60
1:E:46:ARG:NH2	1:E:54:GLY:O	2.34	0.60
13:f:454:PRO:HB2	13:f:457:ARG:HB2	1.82	0.60
14:o:508:LEU:O	14:o:517:LEU:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:357:TRP:HZ3	1:E:359:SER:HA	1.66	0.60
1:F:99:LEU:HD12	1:F:101:THR:H	1.66	0.60
1:I:270:GLU:OE2	3:J:159:ASN:ND2	2.32	0.60
14:p:508:LEU:O	14:p:517:LEU:N	2.35	0.60
9:V:98:VAL:HB	9:V:115:VAL:HG22	1.83	0.60
1:E:20:VAL:O	1:E:22:LYS:NZ	2.34	0.60
13:m:744:ILE:HG22	13:m:748:LYS:HE3	1.84	0.60
14:o:551:LEU:O	14:o:562:THR:N	2.33	0.60
14:p:335:VAL:HG22	14:p:352:THR:HG22	1.84	0.60
1:I:181:MET:HG2	1:I:282:ALA:HB2	1.83	0.60
13:n:779:ILE:CB	14:p:375:LEU:CD2	2.54	0.60
1:A:185:ILE:HD11	1:A:270:GLU:HG2	1.82	0.60
1:C:141:MET:HA	1:C:141:MET:HE3	1.83	0.60
1:E:331:SER:HA	6:Q:19:VAL:HG12	1.83	0.60
1:G:150:THR:HB	1:G:152:ARG:HD3	1.84	0.60
14:h:365:ASN:O	14:h:367:ARG:NH1	2.34	0.60
1:C:58:ILE:O	1:C:61:LYS:NZ	2.35	0.60
1:F:200:LYS:NZ	1:G:116:ASN:O	2.35	0.60
7:O:47:ILE:O	7:O:51:ARG:N	2.33	0.60
9:V:47:ILE:HB	9:V:68:VAL:HG23	1.84	0.60
10:W:1255:LYS:NZ	10:W:1256:VAL:O	2.35	0.60
13:m:454:PRO:HB2	13:m:457:ARG:HG2	1.84	0.60
13:n:751:ARG:NH2	14:p:403:THR:OG1	2.34	0.60
1:D:318:VAL:HG12	1:D:328:ILE:HD13	1.83	0.59
5:L:70:SER:HA	5:L:81:PRO:HD2	1.83	0.59
13:n:755:TRP:CH2	14:p:453:GLU:C	2.72	0.59
1:C:56:ILE:HD13	1:C:88:ARG:HD3	1.84	0.59
1:G:200:LYS:NZ	2:H:111:ASN:O	2.33	0.59
3:J:279:SER:N	3:J:282:THR:OG1	2.31	0.59
1:A:284:GLN:NE2	5:L:231:ILE:HG12	2.16	0.59
13:e:403:HIS:HA	13:e:532:GLU:HA	1.83	0.59
1:I:41:ARG:O	1:I:70:SER:N	2.34	0.59
1:I:253:PRO:O	1:I:257:ARG:HG2	2.03	0.59
13:e:716:ARG:C	13:e:824:TRP:HE1	2.08	0.59
13:f:480:ILE:HG23	13:f:484:LEU:HB2	1.85	0.59
8:U:20:GLU:HG3	8:U:37:PRO:HB3	1.83	0.59
13:f:480:ILE:HG21	13:f:520:ILE:HG12	1.84	0.59
14:h:457:TYR:HE1	14:h:471:MET:HG2	1.67	0.59
13:m:579:ASN:ND2	14:o:559:GLU:O	2.36	0.59
13:m:653:GLN:O	13:m:657:GLN:HG2	2.02	0.59
14:p:513:ASN:HD21	14:p:515:LYS:HE3	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:p:546:MET:HE1	14:p:548:ARG:HH21	1.67	0.59
8:U:55:LEU:HD11	8:U:89:VAL:HG13	1.84	0.59
9:V:28:LEU:HD13	9:V:34:ILE:HD11	1.83	0.59
13:m:153:ILE:O	13:m:158:ALA:N	2.34	0.59
1:C:189:ASP:OD1	1:C:192:ARG:NH2	2.35	0.59
3:J:92:ILE:HD11	3:J:358:GLY:HA3	1.84	0.59
4:K:228:PHE:O	4:K:232:ILE:HG12	2.02	0.59
5:L:181:LYS:O	5:L:185:GLY:N	2.32	0.59
13:n:396:LEU:HD11	13:n:463:LEU:HD11	1.84	0.59
1:D:121:ARG:NH1	1:D:375:THR:OG1	2.36	0.59
2:H:332:PRO:O	2:H:335:ARG:NH1	2.35	0.59
1:I:9:ASN:ND2	1:I:105:GLU:O	2.30	0.59
5:L:72:ARG:HE	5:L:79:TYR:HE2	1.49	0.59
13:m:822:LEU:HD21	13:m:828:LYS:HD3	1.85	0.59
14:p:438:SER:OG	14:p:484:CYS:N	2.36	0.59
1:B:176:MET:HE1	4:K:265:THR:HG22	1.85	0.59
1:B:325:ASP:HA	6:P:93:GLU:H	1.68	0.59
1:F:28:ASP:HB2	1:F:341:TRP:HH2	1.68	0.59
2:H:24:ASP:HB2	2:H:340:TRP:HH2	1.67	0.59
4:K:259:ARG:HH11	5:L:225:ARG:HD2	1.68	0.59
13:n:375:GLN:HG3	13:n:447:LYS:HD3	1.85	0.59
1:A:356:MET:HE1	5:L:258:LEU:HB3	1.85	0.59
1:D:141:MET:HE2	1:D:168:VAL:HG21	1.84	0.59
1:C:6:VAL:O	1:C:9:ASN:ND2	2.35	0.58
4:K:42:ASN:HB3	4:K:45:LEU:HB3	1.83	0.58
4:K:161:HIS:HE1	4:K:163:PHE:HB3	1.68	0.58
5:L:194:THR:O	5:L:195:ARG:NH1	2.35	0.58
7:O:82:SER:HB2	10:W:1108:HIS:HB2	1.85	0.58
11:Y:45:GLU:N	11:Y:281:SER:O	2.35	0.58
13:f:212:ILE:HG21	13:f:235:LYS:HE2	1.85	0.58
14:h:610:GLU:OE2	14:h:613:ARG:NH1	2.36	0.58
14:o:335:VAL:HG22	14:o:352:THR:HG22	1.84	0.58
1:B:49:ALA:N	1:D:148:TYR:OH	2.34	0.58
1:B:153:THR:HB	1:B:172:GLU:HA	1.85	0.58
13:f:605:GLN:HA	13:f:608:LEU:HB2	1.84	0.58
13:n:546:TRP:HE1	13:n:550:MET:HE3	1.68	0.58
14:o:438:SER:OG	14:o:484:CYS:N	2.36	0.58
13:n:215:ASN:O	13:n:218:LYS:HG3	2.03	0.58
1:C:46:ARG:NH2	1:C:52:LEU:O	2.36	0.58
1:D:185:ILE:HD11	1:D:261:LEU:HG	1.86	0.58
1:F:94:TYR:HE1	1:F:103:SER:HA	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:18:SER:HB2	1:G:162:ASP:HB3	1.84	0.58
3:J:311:MET:HE2	3:J:350:ALA:HB3	1.85	0.58
13:m:601:ILE:HG22	13:m:605:GLN:HG3	1.86	0.58
13:n:675:ASN:O	13:n:680:GLN:NE2	2.36	0.58
14:o:280:ARG:NH1	14:o:300:ASN:O	2.34	0.58
1:B:87:GLU:HA	1:B:90:TRP:HE3	1.66	0.58
1:G:108:VAL:HG12	1:G:134:VAL:HG11	1.85	0.58
3:J:122:PRO:HG2	3:J:125:LEU:HB3	1.84	0.58
13:n:573:GLY:HA3	14:o:394:ASN:HB3	1.85	0.58
14:o:513:ASN:HD21	14:o:515:LYS:HE3	1.67	0.58
1:E:354:LYS:HA	1:E:357:TRP:CD1	2.38	0.58
3:J:175:LEU:HD23	3:J:179:LEU:HD23	1.85	0.58
13:f:335:LEU:HD23	13:f:366:LYS:HB2	1.85	0.58
13:f:652:LYS:HG3	13:f:695:THR:HG21	1.84	0.58
13:m:710:ASN:HA	13:m:767:LYS:HZ1	1.69	0.58
1:C:354:LYS:HA	1:C:357:TRP:NE1	2.18	0.58
1:F:168:VAL:HG22	1:F:180:ILE:HG23	1.86	0.58
3:J:342:ARG:NH2	11:Y:228:ALA:O	2.37	0.58
5:L:161:SER:C	5:L:163:ARG:N	2.60	0.58
6:Q:214:HIS:HB3	10:Z:1250:THR:HB	1.86	0.58
13:m:578:ALA:HA	13:m:581:MET:CE	2.28	0.58
1:A:22:LYS:NZ	15:A:800:ADP:O1B	2.33	0.58
1:B:14:ILE:HD13	1:B:108:VAL:HG23	1.84	0.58
1:F:76:GLU:HG2	1:F:77:HIS:HD2	1.68	0.58
2:H:283:MET:O	2:H:290:ARG:NH2	2.36	0.58
6:N:399:ARG:HD3	7:O:172:LEU:HB3	1.86	0.58
13:f:264:ARG:HH21	13:f:274:GLU:HB2	1.69	0.58
13:n:465:GLN:HB3	13:n:546:TRP:HH2	1.69	0.58
1:A:43:LYS:NZ	1:A:69:LEU:O	2.32	0.58
1:E:48:MET:HE2	1:G:173:GLY:CA	2.33	0.58
1:E:243:LEU:HD11	1:E:249:ILE:HD12	1.86	0.58
1:F:154:THR:HG22	1:F:172:GLU:H	1.69	0.58
7:R:16:GLU:OE1	7:R:19:ARG:NH1	2.36	0.58
9:V:123:LYS:HZ1	11:Y:299:THR:N	2.02	0.58
13:f:519:ALA:HB1	13:f:560:VAL:HG23	1.84	0.58
1:A:14:ILE:HD13	1:A:108:VAL:HG13	1.86	0.58
13:f:638:VAL:HG22	14:h:300:ASN:HD21	1.69	0.58
14:o:546:MET:HE1	14:o:548:ARG:HH21	1.67	0.58
1:E:60:PRO:HA	1:E:63:GLU:HG2	1.85	0.57
13:m:332:TYR:HB3	13:m:336:MET:HE1	1.84	0.57
13:m:583:ARG:NH1	14:o:518:TYR:OH	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:328:SER:O	10:Z:1125:LYS:NZ	2.36	0.57
13:f:284:ALA:HA	13:f:287:ARG:HD2	1.87	0.57
13:f:375:GLN:HA	13:f:378:LEU:HD12	1.85	0.57
1:C:68:LEU:HD11	1:E:171:TYR:CD2	2.39	0.57
1:C:224:LEU:HD22	1:C:310:PHE:HA	1.86	0.57
6:P:262:MET:HE1	7:R:33:VAL:HA	1.86	0.57
13:e:80:GLU:HA	13:e:115:SER:HA	1.87	0.57
13:f:275:ILE:HA	13:f:336:MET:CE	2.33	0.57
13:f:482:ARG:NH1	13:f:587:ARG:O	2.37	0.57
13:n:266:PRO:HB2	13:n:379:ARG:HB2	1.85	0.57
1:D:141:MET:HB3	1:D:144:VAL:HG22	1.85	0.57
1:I:227:ASN:HB3	1:I:230:LYS:HE3	1.86	0.57
13:f:588:PHE:HB3	13:f:591:LEU:HD11	1.85	0.57
13:m:402:MET:HE3	13:m:466:MET:HE1	1.85	0.57
3:J:212:VAL:HG21	11:Y:252:LEU:HD12	1.85	0.57
6:M:56:TYR:O	6:M:60:LYS:HB2	2.05	0.57
6:N:374:LEU:HD21	10:Z:1168:ASN:HB3	1.85	0.57
11:Y:340:VAL:HA	11:Y:373:VAL:HG12	1.85	0.57
13:n:457:ARG:HA	13:n:460:GLN:HB3	1.86	0.57
14:o:391:GLY:HA3	14:o:396:HIS:HA	1.86	0.57
3:J:20:LEU:HD13	3:J:55:VAL:HG11	1.87	0.57
4:K:250:MET:HG2	4:K:254:THR:HB	1.86	0.57
14:h:525:ASP:OD2	14:h:546:MET:N	2.38	0.57
13:m:748:LYS:O	13:m:752:ASN:ND2	2.38	0.57
1:E:335:GLU:OE1	1:E:335:GLU:N	2.37	0.57
7:O:85:GLN:HG3	10:W:1105:MET:HB2	1.87	0.57
5:L:62:CYS:SG	5:L:63:ASP:N	2.78	0.57
14:h:409:SER:N	14:h:420:ASP:O	2.25	0.57
13:m:39:PRO:O	13:m:46:GLY:N	2.37	0.57
13:n:252:TRP:O	13:n:256:ILE:HG12	2.05	0.57
1:D:164:VAL:HG23	1:D:184:ASP:HA	1.87	0.57
1:G:141:MET:HE3	1:G:141:MET:HA	1.87	0.57
6:P:308:ASP:O	6:P:311:SER:OG	2.19	0.57
11:Y:6:GLN:HB3	11:Y:9:ARG:HG3	1.86	0.57
11:Y:279:LYS:HD3	11:Y:297:ASN:ND2	2.19	0.57
13:m:648:ILE:HA	13:m:695:THR:HG21	1.87	0.57
1:D:104:GLU:HG2	1:D:133:ASN:HB2	1.87	0.57
5:L:167:TYR:N	5:L:199:LYS:O	2.31	0.57
13:f:220:CYS:O	13:f:225:GLU:N	2.37	0.57
13:m:739:PHE:HE2	13:m:744:ILE:HD11	1.70	0.57
1:D:156:VAL:HG11	1:D:283:ILE:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:182:THR:HG22	4:K:184:PRO:HD2	1.86	0.56
4:K:240:GLN:NE2	5:L:244:ARG:O	2.31	0.56
5:L:74:PRO:O	5:L:94:ARG:NH1	2.38	0.56
11:Y:77:PRO:HD3	11:Y:271:PRO:HB3	1.87	0.56
1:F:354:LYS:HA	1:F:357:TRP:NE1	2.19	0.56
14:h:390:VAL:HG11	14:h:439:PHE:CE2	2.39	0.56
1:D:168:VAL:HG13	1:D:180:ILE:HG12	1.86	0.56
1:E:154:THR:HG22	1:E:297:ASN:HD21	1.70	0.56
2:H:204:ALA:O	2:H:208:ILE:HD12	2.04	0.56
6:M:185:ALA:HA	7:R:127:GLN:HG2	1.88	0.56
6:Q:270:ALA:O	6:Q:273:SER:OG	2.22	0.56
8:U:46:GLY:N	8:U:64:ASN:OD1	2.31	0.56
11:Y:52:PRO:HD3	11:Y:277:LEU:HD23	1.88	0.56
11:Y:374:LEU:HA	11:Y:405:ASN:HB3	1.86	0.56
13:n:751:ARG:NH1	14:p:382:HIS:CD2	2.73	0.56
13:n:751:ARG:NH1	14:p:403:THR:C	2.64	0.56
13:n:772:ASN:OD1	14:p:382:HIS:NE2	2.38	0.56
14:p:276:TRP:HB3	14:p:312:VAL:HG11	1.87	0.56
14:p:280:ARG:NH1	14:p:310:ASP:O	2.38	0.56
14:p:391:GLY:HA3	14:p:396:HIS:HA	1.86	0.56
2:H:187:ASP:HA	2:H:190:MET:HG2	1.88	0.56
12:a:119:LEU:HA	12:b:119:LEU:HA	1.87	0.56
14:h:284:CYS:HA	14:h:575:ARG:HG2	1.87	0.56
13:m:220:CYS:HA	13:m:223:ARG:HE	1.71	0.56
14:o:280:ARG:NH1	14:o:310:ASP:O	2.38	0.56
1:I:116:ASN:HB2	1:I:121:ARG:HH12	1.70	0.56
6:P:316:LEU:HG	6:Q:317:TYR:CZ	2.40	0.56
13:e:165:ILE:O	13:e:171:ALA:N	2.38	0.56
13:n:669:LEU:HD13	13:n:676:HIS:HB2	1.86	0.56
14:p:342:LYS:NZ	14:p:388:ASN:OD1	2.30	0.56
1:E:43:LYS:NZ	1:E:67:GLY:O	2.38	0.56
1:G:238:LYS:HB3	1:G:250:GLU:HB3	1.87	0.56
6:P:90:MET:HE2	6:P:90:MET:HA	1.87	0.56
10:Z:1204:SER:HA	10:Z:1207:ILE:HG12	1.88	0.56
13:n:226:LYS:HE3	13:n:227:PRO:HD2	1.87	0.56
1:C:244:PRO:O	1:E:292:ARG:NH1	2.39	0.56
1:E:283:ILE:O	1:E:286:SER:OG	2.23	0.56
1:G:16:ASN:HA	1:G:21:ILE:HG22	1.88	0.56
3:J:19:ASP:HB3	3:J:26:LYS:HB2	1.87	0.56
3:J:137:MET:HG2	3:J:299:LEU:HB3	1.87	0.56
5:L:145:LYS:O	5:L:178:GLN:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:124:ALA:O	11:Y:126:LYS:NZ	2.37	0.56
13:m:426:GLU:OE1	13:m:429:LYS:NZ	2.26	0.56
13:n:751:ARG:CZ	14:p:403:THR:CB	2.82	0.56
14:o:299:TYR:HB2	14:o:312:VAL:HB	1.86	0.56
1:D:108:VAL:HG11	1:D:128:PHE:CE2	2.40	0.56
14:h:271:PHE:HB2	14:h:594:ILE:HB	1.88	0.56
13:m:717:ILE:HD13	13:m:829:LEU:HD22	1.86	0.56
13:m:718:PHE:HB3	13:m:820:ILE:HD13	1.88	0.56
13:m:816:ILE:O	13:m:820:ILE:HG12	2.06	0.56
1:B:113:ALA:HB3	1:B:116:ASN:HD21	1.71	0.56
13:f:582:PHE:CG	13:f:664:ARG:HG2	2.41	0.56
13:n:480:ILE:HA	13:n:484:LEU:HD23	1.87	0.56
13:n:660:ALA:O	13:n:664:ARG:HG2	2.06	0.56
1:D:366:ASP:HB3	1:D:370:SER:HB3	1.87	0.56
6:Q:167:ASN:OD1	6:Q:168:LEU:N	2.38	0.56
13:e:283:ARG:HA	13:f:176:ASP:H	1.70	0.56
14:h:394:ASN:O	13:m:599:GLY:HA3	2.06	0.56
13:m:365:ARG:HD2	13:m:429:LYS:HE2	1.87	0.56
14:o:276:TRP:HB3	14:o:312:VAL:HG11	1.87	0.56
14:p:299:TYR:HB2	14:p:312:VAL:HB	1.86	0.56
1:G:13:VAL:HG21	1:G:345:SER:HA	1.87	0.55
1:G:355:LYS:HB2	6:M:63:ARG:HH22	1.71	0.55
2:H:182:GLY:HA2	2:H:185:LEU:HD12	1.87	0.55
1:I:107:PRO:HB3	1:I:136:ALA:HB3	1.87	0.55
3:J:39:ILE:HD13	3:J:79:HIS:CD2	2.40	0.55
4:K:183:PRO:HA	4:K:218:VAL:HB	1.88	0.55
5:L:9:ALA:HB1	5:L:28:LEU:HD21	1.88	0.55
6:M:396:ILE:O	6:M:400:MET:HG3	2.06	0.55
14:h:457:TYR:HB3	14:h:468:ILE:HG23	1.88	0.55
13:m:245:LEU:HB3	13:m:304:LEU:HD21	1.86	0.55
14:p:402:SER:OG	14:p:404:ASP:OD1	2.15	0.55
1:B:144:VAL:HG12	1:B:148:TYR:HE2	1.70	0.55
1:B:356:MET:HE1	4:K:277:TYR:CD1	2.40	0.55
1:D:267:LEU:O	1:E:178:HIS:NE2	2.39	0.55
1:D:354:LYS:HA	1:D:357:TRP:NE1	2.21	0.55
1:I:354:LYS:HA	1:I:357:TRP:NE1	2.20	0.55
6:P:320:ILE:HG22	7:R:94:ILE:HD11	1.88	0.55
13:n:278:TRP:HE1	13:n:376:ARG:HH21	1.54	0.55
14:p:573:LEU:HA	14:p:589:ASP:HA	1.88	0.55
1:A:25:PHE:HZ	1:A:101:THR:HG21	1.70	0.55
2:H:43:VAL:HG11	3:J:156:PRO:HG2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:f:439:LYS:HA	13:f:442:ARG:HG2	1.88	0.55
13:m:373:PRO:HB2	13:m:376:ARG:HB2	1.87	0.55
13:m:575:ALA:HB1	13:m:581:MET:SD	2.47	0.55
13:n:696:GLN:HA	13:n:758:PHE:CE1	2.41	0.55
1:B:144:VAL:HG12	1:B:148:TYR:CE2	2.42	0.55
1:B:354:LYS:HA	1:B:357:TRP:NE1	2.21	0.55
2:H:157:ASP:N	16:H:401:ATP:O2B	2.28	0.55
1:I:13:VAL:O	1:I:341:TRP:NE1	2.38	0.55
1:I:121:ARG:NH2	1:I:141:MET:HE1	2.19	0.55
6:P:211:TYR:HD1	10:Z:1256:VAL:HG22	1.71	0.55
6:P:354:LEU:HD22	7:R:126:LEU:HD11	1.87	0.55
13:e:152:PHE:O	13:e:157:VAL:N	2.35	0.55
13:f:274:GLU:OE2	13:f:278:TRP:NE1	2.35	0.55
13:f:350:LEU:HD13	13:f:353:ILE:HD12	1.87	0.55
14:h:409:SER:HB3	14:h:420:ASP:HB3	1.88	0.55
13:m:474:GLU:OE1	13:m:477:ARG:NH2	2.38	0.55
13:n:334:PRO:HA	13:n:337:LYS:NZ	2.21	0.55
1:A:243:LEU:HD12	1:A:247:SER:HB2	1.88	0.55
1:B:10:GLN:HG2	13:n:246:GLN:NE2	2.22	0.55
1:F:176:MET:HA	1:F:176:MET:HE3	1.88	0.55
1:G:330:ILE:HG22	6:M:45:VAL:HG23	1.87	0.55
1:G:334:GLN:HE22	6:M:49:ILE:HA	1.71	0.55
2:H:123:MET:HE2	2:H:123:MET:N	2.21	0.55
1:I:263:PHE:HD2	1:I:276:HIS:HD2	1.53	0.55
6:M:330:LEU:O	6:M:334:VAL:HG23	2.06	0.55
6:N:341:LYS:HE2	10:Z:1132:PRO:HD2	1.88	0.55
7:R:99:ALA:HA	7:R:102:GLU:OE1	2.07	0.55
10:W:1272:LEU:HB3	10:W:1276:GLN:HB3	1.87	0.55
13:f:413:MET:HE1	13:f:467:ARG:HA	1.88	0.55
13:f:711:LEU:HD12	13:f:746:LEU:HD12	1.89	0.55
13:m:269:GLY:O	13:m:386:ARG:NH2	2.38	0.55
13:m:333:ASN:O	13:m:337:LYS:HG2	2.06	0.55
13:m:649:ILE:O	13:m:653:GLN:HG2	2.05	0.55
13:n:438:VAL:HG13	13:n:444:GLU:HB2	1.88	0.55
1:D:14:ILE:HD13	1:D:108:VAL:HG13	1.89	0.55
1:E:48:MET:HE1	1:G:153:THR:HB	1.89	0.55
4:K:164:GLN:HG3	4:K:167:ASN:H	1.72	0.55
13:m:601:ILE:HD12	13:m:604:TYR:OH	2.07	0.55
1:C:52:LEU:HG	1:E:172:GLU:OE2	2.06	0.55
2:H:214:GLU:HG2	16:H:401:ATP:C4	2.42	0.55
3:J:216:PHE:HE1	3:J:243:PRO:HG3	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:h:291:TYR:HB3	14:h:294:LEU:HD23	1.89	0.55
13:n:751:ARG:NH1	14:p:403:THR:OG1	2.38	0.55
1:E:355:LYS:HD2	6:P:356:HIS:CE1	2.41	0.55
1:F:335:GLU:N	1:F:335:GLU:OE1	2.40	0.55
3:J:137:MET:O	3:J:304:VAL:N	2.39	0.55
6:M:14:ARG:O	6:M:16:GLU:HG3	2.06	0.55
7:O:134:ILE:HD11	6:P:168:LEU:HB3	1.89	0.55
8:U:63:ILE:HD12	8:U:65:ALA:HB3	1.88	0.55
13:m:119:ILE:O	13:m:136:ARG:N	2.40	0.55
13:m:479:VAL:O	13:m:483:VAL:HG22	2.07	0.55
13:n:467:ARG:HD3	13:n:471:ARG:HH22	1.70	0.55
3:J:209:ASP:OD2	3:J:248:TYR:OH	2.25	0.55
13:e:483:VAL:O	13:e:512:PHE:N	2.40	0.55
13:f:620:HIS:ND1	13:f:624:LYS:HE3	2.22	0.55
13:m:372:TYR:OH	13:m:376:ARG:NH1	2.33	0.55
13:m:568:LEU:HD21	13:m:597:ILE:HG23	1.89	0.55
14:p:510:THR:HG22	14:p:512:LYS:H	1.72	0.55
1:C:10:GLN:OE1	10:Z:1234:PHE:HB3	2.07	0.55
1:D:155:GLY:N	1:D:170:ILE:O	2.36	0.55
1:E:77:HIS:CE1	1:E:184:ASP:HB3	2.42	0.55
1:E:112:GLU:OE1	1:E:112:GLU:N	2.38	0.55
2:H:188:TYR:HB2	2:H:267:LEU:HD21	1.88	0.55
4:K:275:LEU:HD21	5:L:211:ALA:HB2	1.89	0.55
13:f:357:LEU:HD21	13:f:423:TRP:HB2	1.88	0.55
13:f:620:HIS:HD2	13:f:689:PHE:HB2	1.71	0.55
1:G:76:GLU:HG3	1:G:77:HIS:CD2	2.42	0.54
1:G:355:LYS:HB2	6:M:63:ARG:NH2	2.22	0.54
13:f:365:ARG:HH22	13:f:430:LEU:HD22	1.72	0.54
13:f:378:LEU:HD13	13:f:450:TRP:HA	1.88	0.54
13:f:723:THR:OG1	13:f:736:LYS:NZ	2.25	0.54
13:m:375:GLN:NE2	13:m:448:MET:SD	2.71	0.54
2:H:173:HIS:HB2	2:H:284:LYS:HZ1	1.70	0.54
6:P:336:ARG:O	6:P:340:ILE:HG12	2.08	0.54
13:f:575:ALA:HB1	13:f:580:GLU:HB3	1.89	0.54
14:h:270:GLN:NE2	14:h:594:ILE:O	2.40	0.54
13:n:608:LEU:HD13	13:n:668:VAL:HG22	1.88	0.54
14:o:573:LEU:HA	14:o:589:ASP:HA	1.88	0.54
1:A:193:PHE:CE2	1:A:197:TYR:HE2	2.25	0.54
1:F:11:PRO:HG2	1:F:348:ALA:HB1	1.90	0.54
6:Q:7:ALA:HA	6:Q:14:ARG:NH2	2.21	0.54
13:e:777:PHE:CB	13:e:824:TRP:HZ3	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:f:555:GLU:OE1	13:f:559:ARG:NH2	2.38	0.54
13:m:395:VAL:O	13:m:398:THR:OG1	2.19	0.54
13:m:484:LEU:HD12	13:m:516:ASP:HA	1.90	0.54
13:n:446:LEU:HD12	13:n:447:LYS:HB2	1.89	0.54
14:o:536:HIS:HA	14:o:606:PRO:HG3	1.89	0.54
14:o:602:GLN:HG2	14:o:603:ILE:HG13	1.89	0.54
1:B:74:PRO:HG3	1:B:89:ILE:HD12	1.88	0.54
5:L:22:GLU:HG2	5:L:45:GLN:NE2	2.23	0.54
8:U:112:TYR:OH	8:U:115:ARG:NH1	2.40	0.54
13:m:232:PHE:HB3	13:m:235:LYS:HB2	1.89	0.54
1:C:371:ILE:O	1:C:375:THR:OG1	2.21	0.54
2:H:149:THR:HG23	2:H:166:TYR:HA	1.90	0.54
3:J:26:LYS:HB3	3:J:355:TRP:CD1	2.43	0.54
3:J:68:LEU:HD13	3:J:105:LEU:HD23	1.90	0.54
14:g:409:SER:O	14:g:419:GLN:N	2.40	0.54
13:n:457:ARG:NH1	13:n:458:LYS:HB2	2.22	0.54
13:n:776:PRO:CA	14:p:375:LEU:O	2.53	0.54
1:B:42:PRO:HA	1:B:69:LEU:HA	1.89	0.54
1:D:108:VAL:HG11	1:D:128:PHE:HE2	1.72	0.54
1:F:143:ALA:HA	1:F:157:VAL:HG11	1.89	0.54
1:I:71:ILE:HD12	1:I:209:SER:HA	1.89	0.54
11:Y:162:ARG:HG2	11:Y:166:LYS:HZ2	1.72	0.54
13:f:529:ASN:O	13:f:552:ARG:NH2	2.38	0.54
14:h:551:LEU:O	14:h:562:THR:N	2.41	0.54
13:n:269:GLY:O	13:n:386:ARG:NH2	2.40	0.54
14:o:510:THR:HG22	14:o:512:LYS:H	1.72	0.54
1:E:52:LEU:HG	1:G:172:GLU:HB3	1.90	0.54
1:E:229:GLN:NE2	1:E:264:ARG:HH22	2.04	0.54
2:H:214:GLU:HG2	16:H:401:ATP:C5	2.42	0.54
2:H:352:PHE:HA	2:H:355:MET:HE2	1.89	0.54
3:J:247:ASP:OD1	3:J:257:HIS:ND1	2.28	0.54
3:J:362:GLY:HA2	3:J:368:LEU:HD21	1.90	0.54
5:L:16:LEU:HD13	5:L:24:ASN:HB3	1.88	0.54
11:Y:255:ARG:NH1	11:Y:264:ILE:HA	2.23	0.54
13:m:529:ASN:HB3	13:m:552:ARG:HH21	1.73	0.54
13:m:734:LYS:O	13:m:736:LYS:NZ	2.41	0.54
1:B:145:LEU:HA	1:B:148:TYR:CD2	2.38	0.54
1:F:346:ILE:HG12	13:f:311:HIS:HB3	1.89	0.54
5:L:187:MET:HA	5:L:187:MET:HE2	1.89	0.54
6:P:184:GLU:HG2	10:Z:1283:ARG:HH22	1.72	0.54
6:Q:63:ARG:HE	10:Z:1209:LYS:NZ	2.02	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:f:382:GLU:HG3	13:f:452:ILE:HD12	1.89	0.54
13:n:361:PHE:O	13:n:365:ARG:HG2	2.08	0.54
1:B:296:SER:O	1:B:329:ARG:NE	2.41	0.54
1:F:296:SER:O	1:F:329:ARG:HB3	2.07	0.54
4:K:94:ILE:HA	4:K:110:PRO:HA	1.90	0.54
6:P:163:ASP:OD1	6:Q:223:SER:HB3	2.08	0.54
6:Q:172:ASP:HA	6:Q:175:LEU:HB2	1.90	0.54
8:U:58:GLU:OE1	9:V:49:ARG:NH1	2.33	0.54
13:f:279:LEU:HB3	13:f:283:ARG:NH1	2.23	0.54
13:n:522:GLU:HB3	13:n:556:ARG:HG2	1.90	0.54
14:p:602:GLN:HG2	14:p:603:ILE:HG13	1.89	0.54
6:M:155:HIS:O	6:M:160:LEU:N	2.33	0.54
10:Z:1267:ARG:HG2	10:Z:1269:ARG:NH2	2.20	0.54
13:f:539:SER:O	13:f:543:THR:N	2.37	0.54
13:f:638:VAL:HG21	14:h:281:VAL:HG11	1.89	0.54
13:m:639:ARG:NH2	14:o:574:ASN:OD1	2.41	0.54
13:m:714:SER:O	13:m:738:ASN:ND2	2.41	0.54
14:p:536:HIS:HA	14:p:606:PRO:HG3	1.89	0.54
1:F:9:ASN:HB3	1:F:106:HIS:CE1	2.43	0.53
4:K:56:GLN:HA	4:K:59:MET:HE2	1.91	0.53
8:U:108:GLU:OE1	8:U:127:ALA:N	2.41	0.53
11:Y:255:ARG:HH12	11:Y:264:ILE:HA	1.72	0.53
14:h:380:HIS:NE2	14:h:400:SER:OG	2.40	0.53
14:p:384:VAL:HA	14:p:402:SER:HA	1.90	0.53
1:F:264:ARG:NH1	6:M:75:ILE:O	2.41	0.53
5:L:142:LYS:HG3	5:L:144:ILE:H	1.72	0.53
14:h:390:VAL:HG11	14:h:439:PHE:CD2	2.43	0.53
2:H:105:LEU:HG	2:H:132:MET:HE1	1.90	0.53
2:H:159:VAL:HG12	2:H:179:ASP:HA	1.90	0.53
4:K:101:LEU:O	4:K:103:LYS:NZ	2.38	0.53
6:P:151:LEU:O	6:P:154:SER:OG	2.23	0.53
13:m:374:ILE:HD12	13:m:434:LEU:HD22	1.91	0.53
1:E:203:TYR:CE2	1:E:249:ILE:HG23	2.44	0.53
2:H:110:LEU:O	2:H:177:ARG:NH1	2.40	0.53
11:Y:69:ARG:HH12	11:Y:272:ARG:NE	2.07	0.53
13:f:805:VAL:HG11	13:f:847:VAL:HG22	1.90	0.53
1:A:287:ASP:N	1:A:287:ASP:OD1	2.39	0.53
1:G:353:PHE:HA	1:G:356:MET:HB2	1.90	0.53
5:L:155:GLU:OE2	5:L:168:LYS:HG2	2.09	0.53
11:Y:51:CYS:SG	11:Y:54:CYS:N	2.78	0.53
13:f:349:GLU:HG3	13:f:352:LYS:H	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:f:744:ILE:O	13:f:748:LYS:HG3	2.09	0.53
13:m:254:ARG:O	13:m:258:LYS:HG3	2.08	0.53
14:p:280:ARG:NH1	14:p:300:ASN:O	2.34	0.53
1:C:75:MET:HE3	1:C:76:GLU:N	2.23	0.53
1:C:362:GLU:OE2	1:C:373:ARG:NH2	2.42	0.53
1:G:48:MET:HA	1:G:48:MET:HE2	1.90	0.53
3:J:38:ILE:HG21	11:Y:256:LEU:HD12	1.90	0.53
3:J:269:ILE:HG13	3:J:270:LEU:HD12	1.91	0.53
4:K:263:PRO:HD3	5:L:111:TYR:CZ	2.44	0.53
5:L:142:LYS:HE3	5:L:144:ILE:HG12	1.90	0.53
6:P:3:ASP:HA	6:P:6:TYR:CE1	2.43	0.53
14:o:384:VAL:HA	14:o:402:SER:HA	1.90	0.53
5:L:61:LEU:HB3	5:L:71:TYR:CE1	2.43	0.53
5:L:77:ASN:OD1	5:L:94:ARG:NH1	2.42	0.53
13:e:753:LEU:O	13:e:757:GLY:N	2.40	0.53
13:f:156:ALA:O	13:f:160:PHE:N	2.26	0.53
13:f:829:LEU:O	13:f:833:VAL:HG23	2.08	0.53
13:m:777:PHE:HB3	13:m:833:VAL:HG11	1.91	0.53
6:N:396:ILE:HG22	6:N:400:MET:HE3	1.90	0.53
1:D:130:GLU:HG2	13:f:440:ARG:HH21	1.74	0.53
3:J:204:GLU:HA	3:J:207:LEU:HD12	1.91	0.53
6:M:381:THR:HA	6:M:384:GLU:HG2	1.91	0.53
8:U:10:LYS:HB2	8:U:28:THR:HA	1.91	0.53
11:Y:55:LEU:CB	11:Y:298:PRO:HB3	2.37	0.53
13:f:619:LEU:HD23	13:f:689:PHE:HE2	1.74	0.53
13:m:776:PRO:HA	14:o:381:THR:HG21	1.89	0.53
14:o:342:LYS:NZ	14:o:388:ASN:OD1	2.30	0.53
1:A:236:THR:HG21	1:A:256:PHE:HE2	1.74	0.53
1:C:39:VAL:HG21	1:C:85:ASP:HB3	1.90	0.53
1:C:75:MET:HE1	1:C:79:ILE:N	2.24	0.53
4:K:271:TRP:CE3	4:K:274:ILE:HD11	2.43	0.53
5:L:193:LEU:HD22	5:L:224:ILE:HG13	1.90	0.53
11:Y:162:ARG:HG2	11:Y:166:LYS:HZ3	1.74	0.53
13:f:33:HIS:O	13:f:37:LEU:N	2.35	0.53
13:f:220:CYS:HB3	13:f:225:GLU:HB2	1.91	0.53
13:f:240:THR:O	13:f:244:GLN:HG3	2.09	0.53
13:f:335:LEU:HA	13:f:366:LYS:HD2	1.91	0.53
13:n:689:PHE:HA	13:n:692:LYS:HD2	1.90	0.53
1:C:118:ARG:HD2	1:C:372:HIS:CE1	2.43	0.52
1:F:346:ILE:HG23	13:f:311:HIS:HA	1.91	0.52
1:G:48:MET:HE3	1:I:147:LEU:HD11	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:47:MET:HE1	3:J:371:ARG:HE	1.75	0.52
2:H:64:ILE:HD11	3:J:152:TYR:HB3	1.91	0.52
1:I:354:LYS:HA	1:I:357:TRP:HE1	1.73	0.52
13:m:735:LEU:HB3	13:m:785:VAL:HG22	1.91	0.52
13:n:257:GLN:NE2	13:n:319:ASP:O	2.41	0.52
1:A:158:LEU:HD12	1:A:279:LEU:HB2	1.92	0.52
1:A:354:LYS:HA	1:A:357:TRP:NE1	2.25	0.52
1:D:343:GLY:HA2	1:D:346:ILE:HD12	1.90	0.52
1:G:158:LEU:HD12	1:G:275:ILE:HD11	1.92	0.52
1:I:145:LEU:HD12	1:I:343:GLY:C	2.35	0.52
11:Y:317:ARG:HE	11:Y:333:LEU:HD11	1.74	0.52
13:e:717:ILE:H	13:e:824:TRP:CG	2.17	0.52
13:f:576:LYS:O	13:f:611:ARG:NH1	2.42	0.52
13:f:738:ASN:HB3	13:f:824:TRP:HE1	1.74	0.52
14:h:293:GLU:HB2	14:h:318:MET:HB3	1.91	0.52
1:B:240:GLN:OE1	1:B:249:ILE:N	2.41	0.52
1:D:28:ASP:HB2	1:D:341:TRP:HH2	1.74	0.52
7:O:85:GLN:OE1	7:O:85:GLN:N	2.39	0.52
13:f:208:PRO:O	13:f:251:ARG:NH2	2.42	0.52
13:f:335:LEU:HG	13:f:370:THR:HG21	1.91	0.52
13:f:479:VAL:HG22	13:f:482:ARG:NH2	2.24	0.52
13:m:132:SER:H	13:n:41:LEU:C	2.17	0.52
13:n:293:GLU:HA	13:n:298:LEU:HD21	1.92	0.52
13:n:572:LEU:HD22	13:n:604:TYR:HE1	1.75	0.52
1:A:11:PRO:HB3	1:A:107:PRO:HB2	1.91	0.52
1:A:48:MET:HE1	1:C:148:TYR:CE2	2.44	0.52
1:D:160:SER:HA	1:D:165:THR:HG23	1.91	0.52
1:F:138:PHE:HB2	1:F:357:TRP:HB3	1.92	0.52
4:K:177:TRP:CE3	4:K:190:GLY:HA3	2.44	0.52
13:m:648:ILE:O	13:m:652:LYS:HG2	2.09	0.52
13:n:590:ALA:O	13:n:593:VAL:HG12	2.10	0.52
1:E:41:ARG:O	1:E:70:SER:N	2.34	0.52
1:G:27:GLY:N	1:G:345:SER:OG	2.42	0.52
4:K:25:PRO:HG2	4:K:28:GLU:HB2	1.91	0.52
13:e:435:ARG:HA	13:e:447:LYS:HA	1.90	0.52
13:e:739:PHE:CB	13:e:824:TRP:CZ2	2.92	0.52
13:f:221:TYR:HE1	13:f:227:PRO:HD3	1.74	0.52
1:C:40:GLY:HA3	1:C:69:LEU:HD13	1.91	0.52
1:D:141:MET:HG3	1:D:143:ALA:H	1.74	0.52
1:D:280:VAL:HG11	1:D:321:LEU:HB3	1.92	0.52
1:G:20:VAL:O	1:G:22:LYS:NZ	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:190:MET:HE3	2:H:190:MET:HA	1.90	0.52
6:N:21:GLU:OE2	6:N:22:THR:N	2.43	0.52
6:N:360:THR:O	6:N:364:ILE:HG12	2.10	0.52
1:C:215:LYS:NZ	15:C:800:ADP:H2'	2.24	0.52
1:C:240:GLN:OE1	1:C:249:ILE:N	2.41	0.52
1:E:168:VAL:HG13	1:E:180:ILE:HG22	1.91	0.52
1:E:358:VAL:HG22	1:E:374:LYS:HD2	1.91	0.52
6:Q:340:ILE:HD11	6:Q:343:LEU:HD22	1.90	0.52
13:f:80:GLU:N	13:f:102:ASN:O	2.27	0.52
13:m:719:ALA:O	13:m:736:LYS:NZ	2.34	0.52
13:n:528:GLU:O	13:n:532:GLU:HG2	2.10	0.52
1:B:141:MET:O	1:B:145:LEU:HD23	2.10	0.52
1:E:158:LEU:HD11	1:E:275:ILE:HD11	1.92	0.52
3:J:342:ARG:NH1	11:Y:228:ALA:O	2.43	0.52
6:P:312:LYS:O	6:P:315:GLN:N	2.42	0.52
13:e:716:ARG:CA	13:e:824:TRP:CD1	2.92	0.52
13:f:347:ALA:HB1	13:f:352:LYS:HB3	1.91	0.52
13:f:641:LEU:HG	14:h:502:PHE:HE2	1.74	0.52
1:C:89:ILE:O	1:C:93:VAL:HG23	2.10	0.52
1:E:86:MET:HA	1:E:86:MET:HE2	1.91	0.52
2:H:193:LEU:HD11	2:H:250:ILE:HG22	1.92	0.52
1:I:287:ASP:O	1:I:291:ARG:HG3	2.10	0.52
5:L:89:PRO:HG2	5:L:93:LEU:HD22	1.92	0.52
6:N:340:ILE:CD1	6:N:344:HIS:HE1	2.23	0.52
7:O:82:SER:HA	7:O:85:GLN:NE2	2.25	0.52
9:V:60:HIS:O	9:V:90:HIS:HA	2.10	0.52
11:Y:45:GLU:HB2	11:Y:281:SER:HB3	1.92	0.52
13:f:442:ARG:NH1	13:f:445:ASN:O	2.41	0.52
13:f:787:THR:OG1	14:h:332:GLN:NE2	2.24	0.52
13:m:659:THR:O	13:m:662:MET:HG2	2.10	0.52
13:n:459:LEU:HD22	13:n:538:VAL:HG11	1.90	0.52
13:n:755:TRP:HD1	14:p:453:GLU:OE1	1.77	0.52
14:p:576:VAL:HA	14:p:587:VAL:HG12	1.92	0.52
1:B:289:ASP:N	1:B:289:ASP:OD1	2.43	0.52
1:D:205:PHE:HB3	1:D:210:GLU:HB3	1.92	0.52
1:F:351:ASP:N	13:f:319:ASP:OD2	2.41	0.52
2:H:71:ILE:O	2:H:183:ARG:NH1	2.43	0.52
3:J:98:PRO:HB2	3:J:101:PHE:HB3	1.92	0.52
4:K:163:PHE:HA	4:K:170:ASN:HA	1.91	0.52
6:M:379:GLN:O	6:M:383:ARG:HG2	2.09	0.52
6:M:392:ASN:O	6:M:396:ILE:HG12	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:33:THR:OG1	8:U:54:ASN:O	2.26	0.52
11:Y:235:LEU:HD12	11:Y:236:PRO:HD2	1.92	0.52
13:n:569:ARG:NH1	13:n:604:TYR:OH	2.43	0.52
1:C:334:GLN:HE21	6:Q:47:HIS:HB3	1.75	0.51
1:D:351:ASP:N	13:m:319:ASP:OD1	2.39	0.51
2:H:11:ASP:HB3	2:H:18:LYS:HB2	1.91	0.51
2:H:272:CYS:HB2	2:H:276:GLU:HB3	1.92	0.51
6:N:210:THR:OG1	10:W:1266:GLN:O	2.22	0.51
6:P:269:GLN:HG2	7:R:39:LYS:NZ	2.24	0.51
10:W:1120:LYS:O	10:W:1124:MET:HG2	2.10	0.51
11:Y:230:ASP:OD1	11:Y:231:GLU:N	2.43	0.51
13:f:748:LYS:HA	13:f:751:ARG:HD3	1.90	0.51
13:f:777:PHE:HB3	13:f:829:LEU:HD21	1.92	0.51
13:m:659:THR:OG1	13:m:690:ARG:NH2	2.43	0.51
1:B:183:ILE:HG22	1:B:185:ILE:HG22	1.92	0.51
1:B:290:LEU:HB3	1:B:294:LEU:CD2	2.40	0.51
1:E:366:ASP:HB2	1:E:370:SER:HB3	1.92	0.51
2:H:189:LEU:HD12	2:H:192:ILE:HD11	1.92	0.51
2:H:334:GLU:N	2:H:334:GLU:OE1	2.42	0.51
3:J:172:HIS:NE2	3:J:208:GLU:HG2	2.25	0.51
13:f:367:ILE:HG23	13:f:437:ILE:HD11	1.91	0.51
13:n:485:ARG:HH12	13:n:487:GLN:HG2	1.75	0.51
1:B:325:ASP:HA	6:P:93:GLU:N	2.25	0.51
1:D:145:LEU:HD22	1:D:344:GLY:HA2	1.92	0.51
1:E:160:SER:HB3	1:E:305:THR:HG23	1.92	0.51
6:N:214:HIS:HB2	10:W:1271:VAL:HG22	1.92	0.51
13:f:350:LEU:HD12	13:f:419:VAL:HG21	1.92	0.51
13:f:783:GLU:OE1	13:f:786:ARG:NH2	2.43	0.51
13:n:335:LEU:O	13:n:363:HIS:NE2	2.41	0.51
1:B:9:ASN:OD1	13:n:250:ASN:ND2	2.43	0.51
6:P:102:GLN:HA	6:Q:140:LEU:HD21	1.92	0.51
13:m:350:LEU:HD23	13:m:353:ILE:HD12	1.92	0.51
13:m:555:GLU:HG3	13:m:559:ARG:HH12	1.75	0.51
13:n:229:VAL:HG13	13:n:236:VAL:HG11	1.92	0.51
1:D:351:ASP:H	13:m:319:ASP:CG	2.18	0.51
2:H:262:PHE:HD1	2:H:275:HIS:HD2	1.58	0.51
6:P:322:ARG:HE	10:W:1117:SER:HB2	1.75	0.51
13:f:519:ALA:HA	13:f:522:GLU:CD	2.35	0.51
14:h:426:HIS:O	14:h:427:LYS:HE2	2.10	0.51
1:E:110:LEU:HB3	1:E:139:ILE:HG22	1.93	0.51
1:F:68:LEU:HD12	2:H:166:TYR:HD2	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:7:ILE:HG22	1:G:9:ASN:H	1.76	0.51
2:H:253:GLU:HA	2:H:256:ARG:HB3	1.93	0.51
6:M:183:LEU:HD22	10:W:1283:ARG:NH1	2.25	0.51
6:M:320:ILE:HD11	7:O:94:ILE:HD11	1.91	0.51
11:Y:143:ARG:HH11	11:Y:146:LYS:HD2	1.74	0.51
13:f:357:LEU:O	13:f:361:PHE:HD1	1.93	0.51
13:f:365:ARG:NH2	13:f:430:LEU:HD22	2.26	0.51
13:f:653:GLN:HG3	14:h:503:ASP:HA	1.92	0.51
13:n:755:TRP:HZ3	14:p:452:GLU:O	1.80	0.51
2:H:111:ASN:OD1	2:H:177:ARG:NH1	2.43	0.51
4:K:55:ALA:O	4:K:59:MET:HG2	2.10	0.51
5:L:72:ARG:HH22	5:L:89:PRO:HD3	1.75	0.51
6:M:69:LEU:HD12	6:M:83:TYR:H	1.76	0.51
6:P:256:LEU:HA	6:P:267:LEU:HD23	1.91	0.51
10:Z:1112:LEU:O	10:Z:1116:ASN:ND2	2.43	0.51
12:a:130:ALA:N	12:b:129:ALA:HB1	2.26	0.51
13:m:706:VAL:HG12	13:m:764:ILE:HD12	1.93	0.51
1:B:18:SER:OG	1:B:163:GLY:N	2.42	0.51
1:E:359:SER:N	1:E:362:GLU:OE1	2.33	0.51
3:J:217:VAL:HG22	3:J:267:VAL:HG21	1.93	0.51
4:K:117:LEU:HD21	4:K:152:GLN:HB2	1.92	0.51
6:M:360:THR:HB	6:N:361:GLN:NE2	2.25	0.51
6:N:385:ASN:HD21	10:Z:1175:HIS:HA	1.74	0.51
9:V:123:LYS:HE3	11:Y:299:THR:HA	1.92	0.51
13:e:717:ILE:CB	13:e:824:TRP:HA	2.40	0.51
13:f:552:ARG:O	13:f:555:GLU:HG3	2.11	0.51
13:n:526:ALA:HB2	13:n:556:ARG:HD2	1.93	0.51
1:B:168:VAL:HG22	1:B:180:ILE:HG12	1.91	0.51
1:B:227:ASN:HB3	1:B:230:LYS:HB3	1.93	0.51
1:E:197:TYR:HD1	1:E:200:LYS:HD3	1.76	0.51
6:P:210:THR:HB	10:Z:1257:THR:HB	1.92	0.51
14:h:299:TYR:HB2	14:h:312:VAL:HB	1.92	0.51
14:h:386:CYS:HB3	14:h:437:MET:HG2	1.92	0.51
13:m:302:ASP:HA	13:m:305:LYS:HD2	1.92	0.51
14:o:576:VAL:HA	14:o:587:VAL:HG12	1.92	0.51
1:A:210:GLU:HA	1:A:213:ILE:HD12	1.93	0.51
1:D:165:THR:HB	1:D:183:ILE:HG13	1.93	0.51
1:D:281:PHE:HA	1:D:284:GLN:HE21	1.76	0.51
1:D:371:ILE:O	1:D:375:THR:OG1	2.21	0.51
4:K:271:TRP:HE1	5:L:218:GLU:CD	2.18	0.51
5:L:162:GLY:H	12:b:144:SER:CB	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:R:100:LEU:O	7:R:104:VAL:HG23	2.11	0.51
11:Y:253:GLN:O	11:Y:257:LEU:HG	2.10	0.51
14:h:426:HIS:HD2	14:h:471:MET:HE3	1.76	0.51
13:n:232:PHE:HE1	13:n:299:LEU:HD21	1.76	0.51
14:p:443:ASP:OD1	14:p:446:ASN:N	2.44	0.51
1:A:281:PHE:O	1:A:284:GLN:NE2	2.44	0.50
1:F:76:GLU:HG2	1:F:77:HIS:CD2	2.47	0.50
3:J:134:ASN:ND2	3:J:153:GLU:HG2	2.25	0.50
5:L:261:ASP:O	5:L:264:GLU:HG3	2.11	0.50
6:Q:8:ASP:OD1	6:Q:9:LEU:N	2.44	0.50
8:U:97:GLN:HB3	8:U:115:ARG:HH21	1.77	0.50
10:Z:1141:LEU:O	10:Z:1145:GLU:N	2.44	0.50
13:f:254:ARG:O	13:f:258:LYS:HG2	2.11	0.50
13:f:568:LEU:HA	13:f:571:GLN:HG2	1.92	0.50
14:h:456:VAL:HB	14:h:509:TRP:HZ3	1.75	0.50
13:m:696:GLN:HA	13:m:758:PHE:HE1	1.75	0.50
1:A:281:PHE:HA	1:A:284:GLN:HE21	1.77	0.50
1:F:39:VAL:HG21	1:F:85:ASP:HB3	1.93	0.50
4:K:250:MET:SD	4:K:255:PHE:HB2	2.51	0.50
7:O:128:ARG:HA	7:O:131:GLN:CD	2.36	0.50
9:V:5:GLU:O	9:V:175:LYS:NZ	2.44	0.50
1:G:352:THR:HA	6:M:63:ARG:CZ	2.42	0.50
11:Y:111:CYS:SG	11:Y:114:CYS:O	2.68	0.50
13:f:418:GLU:O	13:f:422:THR:OG1	2.23	0.50
13:f:530:VAL:HG13	13:f:546:TRP:HZ3	1.76	0.50
14:o:315:VAL:O	14:o:326:GLU:N	2.45	0.50
4:K:197:HIS:NE2	4:K:203:ASN:OD1	2.44	0.50
6:M:74:ARG:O	6:M:80:ARG:NH1	2.40	0.50
6:M:175:LEU:HA	6:M:178:ARG:HD3	1.93	0.50
6:M:316:LEU:HD11	6:N:317:TYR:HA	1.94	0.50
13:e:777:PHE:CB	13:e:833:VAL:HG11	2.41	0.50
13:f:581:MET:CE	13:f:608:LEU:HG	2.41	0.50
13:f:619:LEU:HG	13:f:654:ILE:HG23	1.93	0.50
1:C:21:ILE:HG12	1:C:37:ASN:HB2	1.94	0.50
1:D:87:GLU:O	1:D:91:GLN:HG2	2.12	0.50
1:D:245:ASP:OD1	1:D:246:GLY:N	2.44	0.50
1:F:315:LEU:HD11	6:N:22:THR:HG23	1.91	0.50
1:G:136:ALA:HB1	1:G:357:TRP:HB3	1.92	0.50
3:J:219:ASP:OD1	3:J:220:LEU:N	2.44	0.50
5:L:67:ASP:OD1	5:L:67:ASP:N	2.44	0.50
13:f:591:LEU:CD1	13:f:597:ILE:HG21	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:f:699:PHE:CE1	13:f:758:PHE:HB3	2.46	0.50
13:m:252:TRP:O	13:m:256:ILE:HG12	2.11	0.50
1:C:168:VAL:HG13	1:C:180:ILE:HG22	1.93	0.50
1:E:133:ASN:HA	1:E:360:LYS:HZ1	1.77	0.50
1:F:18:SER:HB2	1:F:162:ASP:HB3	1.93	0.50
1:G:141:MET:O	1:G:145:LEU:HD13	2.11	0.50
2:H:218:TYR:HB2	2:H:307:PRO:HB2	1.93	0.50
1:I:145:LEU:HD13	1:I:148:TYR:CD2	2.46	0.50
3:J:216:PHE:CE1	3:J:243:PRO:HG3	2.47	0.50
7:O:167:GLN:O	7:O:170:GLU:HG3	2.11	0.50
6:P:344:HIS:CE1	6:P:348:MET:HE3	2.46	0.50
13:f:274:GLU:OE2	13:f:376:ARG:NE	2.38	0.50
13:f:578:ALA:HA	13:f:581:MET:HG3	1.94	0.50
13:f:642:PRO:HG3	13:f:749:GLU:HG2	1.92	0.50
13:f:673:TRP:CZ3	13:f:683:LYS:HB2	2.46	0.50
13:f:711:LEU:HB3	13:f:743:ILE:HG12	1.94	0.50
13:f:748:LYS:O	13:f:752:ASN:ND2	2.45	0.50
13:n:776:PRO:HB3	14:p:375:LEU:C	2.37	0.50
14:p:332:GLN:HE22	14:p:372:ARG:HH12	1.60	0.50
1:B:227:ASN:HB2	6:P:113:GLN:CD	2.37	0.50
1:E:20:VAL:HA	1:E:36:PRO:HA	1.94	0.50
1:F:76:GLU:OE1	1:F:76:GLU:N	2.44	0.50
3:J:323:ILE:O	3:J:327:VAL:HG23	2.12	0.50
5:L:29:ILE:HG12	5:L:36:CYS:HB2	1.94	0.50
6:M:183:LEU:HD22	10:W:1283:ARG:CZ	2.42	0.50
10:W:1106:ARG:O	10:W:1109:ILE:HG22	2.11	0.50
1:A:143:ALA:HB1	1:A:157:VAL:HB	1.94	0.50
1:B:88:ARG:HA	1:B:91:GLN:CD	2.36	0.50
1:B:154:THR:HG22	1:B:172:GLU:H	1.76	0.50
1:B:290:LEU:HG	4:K:264:VAL:HG11	1.92	0.50
1:F:43:LYS:HB3	1:F:70:SER:HB3	1.94	0.50
1:G:160:SER:OG	1:G:305:THR:HG23	2.12	0.50
3:J:362:GLY:HA2	3:J:368:LEU:HD11	1.94	0.50
13:m:410:GLU:OE2	13:m:467:ARG:NE	2.32	0.50
13:m:561:GLU:HA	13:m:564:ILE:HD12	1.94	0.50
13:m:832:TYR:HA	13:m:835:ARG:HE	1.75	0.50
1:B:10:GLN:HG3	13:n:309:ARG:HD2	1.94	0.50
1:G:25:PHE:HZ	1:G:101:THR:HG21	1.76	0.50
1:G:240:GLN:CD	1:G:248:THR:HB	2.36	0.50
6:N:341:LYS:HE3	10:Z:1131:LEU:HD22	1.94	0.50
13:m:195:HIS:O	13:m:199:ASN:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:m:543:THR:O	13:m:547:GLU:HG2	2.11	0.50
13:n:274:GLU:OE1	13:n:376:ARG:NH2	2.44	0.50
13:n:607:GLN:NE2	13:n:608:LEU:HG	2.26	0.50
14:o:426:HIS:HB2	14:o:468:ILE:HD13	1.94	0.50
1:A:164:VAL:HG23	1:A:184:ASP:HA	1.94	0.49
1:D:238:LYS:HG2	1:D:252:GLY:HA3	1.93	0.49
1:F:223:TYR:HA	1:F:308:LYS:HG3	1.93	0.49
1:G:371:ILE:HG13	1:G:372:HIS:N	2.27	0.49
6:M:312:LYS:HB3	6:N:313:VAL:HG12	1.94	0.49
6:Q:360:THR:O	6:Q:364:ILE:HG12	2.12	0.49
13:f:661:TYR:O	13:f:665:VAL:HG23	2.12	0.49
14:h:435:THR:H	14:h:451:SER:HA	1.77	0.49
14:h:436:SER:O	14:h:450:GLY:N	2.40	0.49
1:B:302:GLY:O	1:B:305:THR:OG1	2.28	0.49
1:C:287:ASP:OD1	1:C:288:MET:N	2.44	0.49
1:G:93:VAL:HA	1:G:98:GLN:NE2	2.27	0.49
12:b:337:LEU:O	12:b:341:HIS:N	2.42	0.49
13:f:638:VAL:HG11	14:h:281:VAL:HG21	1.94	0.49
13:m:289:GLN:NE2	13:m:293:GLU:OE1	2.45	0.49
13:m:650:TRP:O	13:m:654:ILE:HG12	2.12	0.49
13:n:394:LYS:O	13:n:398:THR:HG23	2.12	0.49
13:n:435:ARG:NH1	13:n:448:MET:O	2.45	0.49
14:o:332:GLN:HE22	14:o:372:ARG:HH12	1.60	0.49
1:A:28:ASP:HB2	1:A:341:TRP:HH2	1.76	0.49
1:C:243:LEU:HD13	1:E:288:MET:HE2	1.94	0.49
1:D:18:SER:OG	1:D:188:ARG:NH2	2.45	0.49
1:G:113:ALA:HB3	1:G:116:ASN:HD21	1.77	0.49
3:J:41:SER:HB2	3:J:54:VAL:HG22	1.95	0.49
13:f:394:LYS:O	13:f:398:THR:HG23	2.11	0.49
13:f:748:LYS:O	13:f:751:ARG:HG2	2.11	0.49
13:m:621:ASP:HA	13:m:624:LYS:HD2	1.93	0.49
14:o:537:PRO:HB3	14:o:611:TRP:CZ3	2.48	0.49
14:o:572:ALA:HB3	14:o:590:SER:HB3	1.94	0.49
1:B:9:ASN:HB3	13:n:246:GLN:HE21	1.77	0.49
1:G:218:LYS:HA	1:G:222:CYS:SG	2.52	0.49
3:J:57:TYR:CD1	3:J:98:PRO:HG2	2.47	0.49
3:J:203:PRO:HG2	3:J:206:VAL:HG12	1.95	0.49
9:V:107:TYR:HE1	9:V:166:ILE:HD11	1.76	0.49
10:W:1101:GLN:O	10:W:1105:MET:HB3	2.12	0.49
13:f:249:VAL:HG21	13:f:304:LEU:HD11	1.94	0.49
13:f:292:ARG:HG2	13:f:316:PHE:HZ	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:m:335:LEU:HB2	13:m:370:THR:HG21	1.93	0.49
14:p:531:MET:HE2	14:p:578:TRP:CD1	2.45	0.49
1:E:44:HIS:CD2	1:G:176:MET:HB3	2.48	0.49
1:E:46:ARG:HD2	6:M:83:TYR:O	2.11	0.49
1:F:352:THR:O	1:F:356:MET:HG2	2.11	0.49
1:I:206:HIS:CE1	3:J:165:PRO:HG3	2.47	0.49
3:J:348:ALA:HB2	3:J:356:LEU:HD22	1.94	0.49
6:Q:322:ARG:HH11	6:Q:323:TRP:NE1	2.10	0.49
9:V:108:VAL:C	9:V:165:MET:HE1	2.38	0.49
13:f:639:ARG:NH2	14:h:574:ASN:OD1	2.45	0.49
13:m:533:VAL:HG21	13:m:549:ALA:HB2	1.95	0.49
13:m:631:GLN:HB3	14:o:572:ALA:HB2	1.94	0.49
13:n:86:GLU:O	13:n:96:LYS:N	2.42	0.49
13:n:361:PHE:CG	13:n:426:GLU:HB3	2.48	0.49
13:n:482:ARG:HH21	13:n:485:ARG:HH21	1.60	0.49
13:n:669:LEU:HD11	13:n:678:GLU:HB2	1.93	0.49
14:p:315:VAL:O	14:p:326:GLU:N	2.45	0.49
1:C:112:GLU:N	1:C:112:GLU:OE1	2.45	0.49
1:G:46:ARG:NH2	1:G:52:LEU:O	2.33	0.49
3:J:54:VAL:HG11	3:J:71:PHE:CD1	2.48	0.49
13:f:755:TRP:NE1	14:h:453:GLU:O	2.45	0.49
13:m:361:PHE:CG	13:m:426:GLU:HB3	2.48	0.49
13:n:315:SER:O	13:n:319:ASP:N	2.45	0.49
13:n:368:ARG:HB3	13:n:433:LEU:HD11	1.95	0.49
1:A:178:HIS:NE2	5:L:241:ASN:OD1	2.45	0.49
1:B:89:ILE:O	1:B:93:VAL:HG23	2.12	0.49
2:H:275:HIS:HA	2:H:313:MET:HE1	1.95	0.49
3:J:187:THR:HG23	3:J:254:LYS:HG2	1.94	0.49
6:P:2:ALA:HB1	6:P:5:LYS:HD2	1.95	0.49
6:P:266:GLU:HA	6:P:269:GLN:OE1	2.12	0.49
13:f:805:VAL:HB	13:f:843:PHE:HE1	1.77	0.49
13:m:715:GLY:O	13:m:824:TRP:N	2.46	0.49
13:m:747:SER:HA	13:m:768:ALA:HB1	1.95	0.49
13:n:483:VAL:HG13	13:n:484:LEU:HD22	1.94	0.49
1:E:169:PRO:HG2	1:E:176:MET:HB2	1.94	0.49
1:G:9:ASN:HB3	1:G:106:HIS:ND1	2.28	0.49
6:P:329:THR:HG22	10:W:1128:LEU:HD12	1.95	0.49
11:Y:166:LYS:HA	11:Y:169:ARG:HH11	1.78	0.49
13:f:769:HIS:CE1	13:f:773:GLN:HE21	2.31	0.49
13:m:552:ARG:O	13:m:555:GLU:HG2	2.13	0.49
13:m:597:ILE:O	13:m:601:ILE:HG12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:m:657:GLN:HG3	14:o:504:TRP:CE3	2.47	0.49
13:n:569:ARG:HD2	14:o:395:ALA:HB3	1.94	0.49
13:n:607:GLN:HE22	13:n:608:LEU:HG	1.78	0.49
13:n:776:PRO:C	14:p:375:LEU:O	2.56	0.49
14:p:426:HIS:HB2	14:p:468:ILE:HD13	1.94	0.49
2:H:181:ALA:O	2:H:185:LEU:HG	2.13	0.49
3:J:102:ARG:HD2	3:J:120:LEU:HD22	1.94	0.49
4:K:153:THR:HG22	4:K:180:THR:HG23	1.94	0.49
5:L:143:LYS:HZ3	5:L:181:LYS:HB2	1.77	0.49
9:V:129:LEU:HD12	9:V:147:SER:HB2	1.94	0.49
13:e:539:SER:O	13:e:543:THR:N	2.43	0.49
13:f:257:GLN:O	13:f:261:LYS:HG2	2.12	0.49
1:E:21:ILE:HD11	1:E:35:PHE:CZ	2.48	0.49
1:E:42:PRO:HA	1:E:69:LEU:HA	1.95	0.49
1:F:280:VAL:HG21	1:F:321:LEU:HB2	1.95	0.49
4:K:93:LYS:HE2	4:K:113:VAL:HB	1.95	0.49
6:M:325:PRO:HB3	10:Z:1120:LYS:HB3	1.95	0.49
6:M:390:GLU:HA	6:Q:180:LEU:HD13	1.95	0.49
13:f:699:PHE:HZ	13:f:759:ARG:HG3	1.77	0.49
13:m:306:HIS:O	13:m:308:LYS:NZ	2.45	0.49
13:n:250:ASN:HA	13:n:253:ILE:HG22	1.94	0.49
1:B:108:VAL:HG21	1:B:128:PHE:HE2	1.77	0.48
1:C:40:GLY:C	1:C:69:LEU:HD22	2.38	0.48
1:E:29:GLN:NE2	6:Q:5:LYS:HE3	2.26	0.48
1:F:84:ASN:O	1:F:87:GLU:HG3	2.12	0.48
1:G:98:GLN:O	1:G:100:GLN:N	2.45	0.48
6:M:346:GLN:HG2	10:Z:1139:LEU:HD13	1.95	0.48
13:m:608:LEU:O	13:m:612:VAL:HG23	2.12	0.48
14:o:443:ASP:OD1	14:o:446:ASN:N	2.44	0.48
1:D:133:ASN:HD21	13:f:368:ARG:HD2	1.78	0.48
2:H:189:LEU:HA	2:H:192:ILE:HG12	1.95	0.48
6:P:338:VAL:O	6:P:341:LYS:HB3	2.13	0.48
6:Q:63:ARG:HH21	10:Z:1209:LYS:NZ	2.12	0.48
13:f:209:ILE:O	13:f:210:HIS:C	2.57	0.48
13:f:583:ARG:NH1	14:h:559:GLU:O	2.46	0.48
13:f:777:PHE:HD1	13:f:833:VAL:HG21	1.78	0.48
14:h:536:HIS:HB3	14:h:539:LEU:HB3	1.94	0.48
14:p:572:ALA:HB3	14:p:590:SER:HB3	1.94	0.48
1:B:273:GLU:HB3	1:B:277:GLU:HB2	1.95	0.48
1:D:346:ILE:HG12	13:m:311:HIS:HB3	1.94	0.48
6:P:316:LEU:O	6:P:320:ILE:HG12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:f:709:ARG:HH21	13:f:711:LEU:HD11	1.78	0.48
13:n:755:TRP:CZ3	14:p:453:GLU:CA	2.83	0.48
14:p:388:ASN:HB2	14:p:437:MET:HE3	1.95	0.48
14:p:537:PRO:HB3	14:p:611:TRP:CZ3	2.48	0.48
1:B:136:ALA:HB1	1:B:357:TRP:CG	2.48	0.48
1:E:172:GLU:OE2	1:E:172:GLU:O	2.31	0.48
2:H:195:GLU:OE1	1:I:118:ARG:N	2.47	0.48
5:L:235:LYS:O	5:L:239:ILE:HG12	2.14	0.48
6:Q:175:LEU:O	6:Q:178:ARG:HG3	2.12	0.48
11:Y:4:LEU:H	11:Y:4:LEU:HD12	1.78	0.48
13:n:288:ILE:HA	13:n:291:LYS:HD2	1.95	0.48
14:o:388:ASN:HB2	14:o:437:MET:HE3	1.95	0.48
1:B:103:SER:HB2	1:B:132:PHE:HB3	1.95	0.48
1:C:44:HIS:CD2	1:E:176:MET:HE1	2.48	0.48
1:E:361:LYS:O	1:E:364:GLU:HG3	2.13	0.48
2:H:187:ASP:O	2:H:190:MET:HB2	2.14	0.48
8:U:58:GLU:HG2	8:U:92:VAL:HG13	1.94	0.48
13:f:246:GLN:NE2	13:f:250:ASN:OD1	2.46	0.48
13:f:266:PRO:HB3	13:f:376:ARG:HG3	1.95	0.48
13:f:333:ASN:HA	13:f:336:MET:HB3	1.96	0.48
13:m:483:VAL:HB	13:m:588:PHE:CD1	2.49	0.48
13:m:516:ASP:O	13:m:520:ILE:HG13	2.14	0.48
13:m:539:SER:O	13:m:543:THR:N	2.40	0.48
13:m:634:LYS:HE3	13:m:635:MET:HE3	1.96	0.48
13:n:395:VAL:O	13:n:398:THR:OG1	2.23	0.48
1:A:122:GLU:HG2	1:A:368:ALA:HB1	1.96	0.48
1:B:108:VAL:HG21	1:B:128:PHE:CE2	2.48	0.48
1:B:219:GLU:HG2	15:B:800:ADP:C4	2.48	0.48
6:N:209:VAL:HA	10:W:1266:GLN:HB2	1.96	0.48
10:W:1255:LYS:NZ	10:W:1257:THR:OG1	2.26	0.48
10:Z:1241:ARG:HA	10:Z:1244:GLU:OE1	2.14	0.48
13:f:265:ASP:HB3	13:f:268:SER:HB2	1.95	0.48
13:f:464:ASP:O	13:f:468:LYS:HG2	2.14	0.48
13:f:598:ARG:HH22	13:f:669:LEU:HA	1.78	0.48
14:h:368:THR:HG22	14:h:372:ARG:HH22	1.79	0.48
13:m:409:PHE:O	13:m:413:MET:HG2	2.12	0.48
14:o:531:MET:HE2	14:o:578:TRP:CD1	2.45	0.48
1:A:205:PHE:HB3	1:A:210:GLU:HB3	1.95	0.48
1:E:46:ARG:NH2	1:E:52:LEU:O	2.47	0.48
1:F:30:ILE:HD12	6:N:9:LEU:HD21	1.96	0.48
1:G:229:GLN:NE2	1:G:264:ARG:HH22	2.09	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:240:GLN:CD	1:I:248:THR:HB	2.39	0.48
13:f:553:TYR:O	13:f:557:ILE:HG12	2.14	0.48
14:g:551:LEU:O	14:g:562:THR:N	2.47	0.48
13:m:674:GLU:CD	13:m:674:GLU:H	2.22	0.48
13:n:748:LYS:HE3	14:p:383:PRO:CD	2.43	0.48
1:B:145:LEU:HD12	1:B:343:GLY:C	2.39	0.48
2:H:23:GLY:N	2:H:344:SER:OG	2.46	0.48
3:J:44:LYS:NZ	3:J:48:MET:O	2.36	0.48
5:L:189:LEU:HD13	5:L:233:PHE:HE1	1.79	0.48
6:P:12:ILE:HB	6:P:14:ARG:NH1	2.29	0.48
13:f:475:GLN:O	13:f:479:VAL:HG23	2.14	0.48
14:h:336:MET:SD	14:h:336:MET:N	2.77	0.48
13:n:401:LEU:O	13:n:470:ARG:NH1	2.43	0.48
1:C:176:MET:HB3	1:C:179:SER:HB2	1.96	0.48
1:C:243:LEU:HD12	1:C:247:SER:HB2	1.95	0.48
1:F:114:PRO:HB3	1:F:141:MET:SD	2.53	0.48
4:K:161:HIS:CE1	4:K:163:PHE:HB3	2.48	0.48
10:Z:1101:GLN:O	10:Z:1105:MET:HG3	2.14	0.48
13:f:435:ARG:HA	13:f:438:VAL:HG22	1.95	0.48
13:m:263:ASP:OD1	13:m:264:ARG:N	2.47	0.48
13:n:375:GLN:O	13:n:379:ARG:HG2	2.14	0.48
13:n:426:GLU:OE2	13:n:429:LYS:NZ	2.40	0.48
13:n:577:ASN:OD1	13:n:578:ALA:N	2.47	0.48
1:A:115:LEU:O	1:A:115:LEU:HD23	2.13	0.48
1:A:302:GLY:O	1:A:305:THR:OG1	2.30	0.48
1:C:197:TYR:HD1	1:C:200:LYS:HD3	1.79	0.48
1:G:41:ARG:O	1:G:70:SER:N	2.38	0.48
1:I:168:VAL:HG13	1:I:180:ILE:HG12	1.96	0.48
4:K:228:PHE:CE1	4:K:232:ILE:HD11	2.49	0.48
7:O:89:ALA:HB2	10:Z:1106:ARG:HD3	1.94	0.48
13:e:37:LEU:O	13:e:41:LEU:N	2.39	0.48
13:e:120:LYS:HA	13:e:135:LEU:HA	1.96	0.48
13:f:650:TRP:CE2	13:f:654:ILE:HD11	2.49	0.48
13:f:660:ALA:O	13:f:664:ARG:HG3	2.14	0.48
13:f:735:LEU:HD23	13:f:785:VAL:HG22	1.96	0.48
14:h:540:PHE:CE1	14:h:552:TRP:HB2	2.48	0.48
13:m:483:VAL:HG23	13:m:484:LEU:HD22	1.96	0.48
13:n:353:ILE:HD11	13:n:395:VAL:HG21	1.95	0.48
1:A:98:GLN:O	1:A:100:GLN:N	2.47	0.47
1:G:83:TRP:CE2	1:G:123:ARG:HG2	2.48	0.47
1:I:13:VAL:HG21	1:I:345:SER:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:R:113:SER:HB3	7:R:116:ILE:HD12	1.95	0.47
13:f:609:ILE:HG21	13:f:678:GLU:HB3	1.96	0.47
14:o:589:ASP:OD1	14:o:593:GLN:N	2.47	0.47
1:A:75:MET:HG2	1:A:79:ILE:C	2.39	0.47
1:B:74:PRO:HG3	1:B:89:ILE:CD1	2.45	0.47
1:B:84:ASN:O	1:B:87:GLU:HG3	2.14	0.47
1:C:112:GLU:CD	1:C:139:ILE:HG23	2.39	0.47
1:C:145:LEU:HD23	1:C:340:THR:O	2.14	0.47
1:I:223:TYR:CZ	1:I:256:PHE:HB3	2.50	0.47
4:K:255:PHE:CE2	5:L:225:ARG:HG3	2.50	0.47
5:L:124:LEU:HB3	5:L:127:GLY:O	2.14	0.47
6:P:263:GLU:OE1	6:P:263:GLU:N	2.35	0.47
13:m:266:PRO:HG3	13:m:376:ARG:HG3	1.95	0.47
13:n:616:ILE:HG12	13:n:661:TYR:HB3	1.96	0.47
13:n:661:TYR:O	13:n:665:VAL:HG23	2.14	0.47
13:n:755:TRP:CE3	14:p:453:GLU:CA	2.93	0.47
1:A:118:ARG:HB2	1:A:372:HIS:CE1	2.48	0.47
1:D:58:ILE:H	1:D:61:LYS:HZ3	1.61	0.47
1:E:43:LYS:HG3	1:E:44:HIS:CD2	2.50	0.47
1:F:219:GLU:HG2	15:F:800:ADP:C4	2.48	0.47
1:G:334:GLN:NE2	6:M:49:ILE:HD13	2.28	0.47
2:H:138:ALA:O	2:H:141:SER:OG	2.30	0.47
2:H:301:GLY:O	2:H:304:THR:OG1	2.32	0.47
4:K:160:SER:HB3	4:K:173:TRP:HB3	1.96	0.47
8:U:82:MET:HA	8:U:99:MET:O	2.14	0.47
10:W:1253:MET:HE2	10:W:1253:MET:HA	1.96	0.47
13:m:779:ILE:HA	13:m:782:ILE:HG22	1.96	0.47
13:n:705:LYS:HD3	13:n:709:ARG:HH21	1.79	0.47
1:A:288:MET:HE1	4:K:167:ASN:HD22	1.79	0.47
1:E:112:GLU:H	1:E:112:GLU:CD	2.23	0.47
1:F:203:TYR:CE1	1:F:249:ILE:HG22	2.49	0.47
1:G:46:ARG:HB2	1:I:174:PHE:CE1	2.49	0.47
1:I:145:LEU:HA	1:I:148:TYR:HD2	1.78	0.47
6:Q:336:ARG:HD3	7:R:111:LEU:HD22	1.96	0.47
9:V:57:VAL:HA	9:V:87:ILE:HB	1.96	0.47
10:Z:1205:ASP:O	10:Z:1208:GLU:HG3	2.14	0.47
13:f:476:LEU:O	13:f:479:VAL:HB	2.14	0.47
14:g:359:LEU:N	14:g:371:GLN:O	2.42	0.47
13:n:272:LEU:HB2	13:n:341:LEU:HD22	1.95	0.47
13:n:409:PHE:CD2	13:n:470:ARG:HD2	2.48	0.47
1:A:284:GLN:NE2	1:A:285:LYS:HG3	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:MET:HA	1:A:291:ARG:HG3	1.96	0.47
1:D:90:TRP:CD2	1:D:128:PHE:HE1	2.32	0.47
1:D:177:PRO:HA	1:D:180:ILE:HD12	1.97	0.47
4:K:211:ASP:OD1	4:K:211:ASP:N	2.47	0.47
6:P:170:ASP:OD2	6:P:173:GLY:N	2.47	0.47
6:P:306:ASP:O	6:P:310:GLN:HG2	2.14	0.47
6:Q:12:ILE:HB	6:Q:14:ARG:HH12	1.73	0.47
13:m:559:ARG:O	13:m:563:ARG:HG3	2.14	0.47
13:m:582:PHE:CE2	13:m:664:ARG:HB3	2.49	0.47
13:n:335:LEU:HB2	13:n:370:THR:HG21	1.96	0.47
13:n:675:ASN:OD1	13:n:676:HIS:N	2.47	0.47
1:A:352:THR:O	1:A:356:MET:HG2	2.15	0.47
1:B:296:SER:O	1:B:329:ARG:HB3	2.13	0.47
1:C:145:LEU:O	1:C:343:GLY:HA3	2.15	0.47
1:D:156:VAL:HA	1:D:169:PRO:HA	1.97	0.47
1:E:354:LYS:H	1:E:354:LYS:HD3	1.79	0.47
6:Q:61:ASP:OD1	6:Q:62:LYS:N	2.47	0.47
11:Y:30:CYS:SG	11:Y:33:CYS:N	2.81	0.47
12:a:312:LEU:HA	12:b:312:LEU:HA	1.97	0.47
13:f:579:ASN:HA	13:f:582:PHE:CD1	2.49	0.47
13:m:437:ILE:O	13:m:441:LYS:N	2.41	0.47
13:m:585:PHE:O	13:m:589:ASN:N	2.47	0.47
13:n:365:ARG:O	13:n:368:ARG:NH1	2.48	0.47
13:n:673:TRP:HA	13:n:676:HIS:CD2	2.48	0.47
13:n:748:LYS:CE	14:p:383:PRO:HD2	2.45	0.47
1:B:220:ARG:HD3	1:B:241:TYR:HE1	1.80	0.47
1:C:95:SER:OG	1:C:96:LYS:N	2.48	0.47
1:C:354:LYS:HA	1:C:357:TRP:HE1	1.80	0.47
1:G:302:GLY:O	1:G:305:THR:OG1	2.32	0.47
3:J:344:HIS:CD2	11:Y:228:ALA:HB2	2.50	0.47
6:N:397:ASP:O	6:N:401:LYS:HG2	2.14	0.47
6:P:208:LEU:HD12	10:Z:1259:SER:HA	1.97	0.47
6:P:354:LEU:HD11	7:R:125:ARG:NH2	2.24	0.47
7:R:28:ARG:NH1	7:R:31:ARG:HH12	2.08	0.47
8:U:37:PRO:HG2	9:V:49:ARG:HH21	1.80	0.47
11:Y:143:ARG:HD2	11:Y:146:LYS:HD2	1.97	0.47
11:Y:427:LYS:HA	11:Y:457:HIS:HA	1.96	0.47
13:f:578:ALA:HB3	13:f:615:ASP:OD2	2.15	0.47
13:f:638:VAL:HG22	14:h:300:ASN:ND2	2.29	0.47
13:m:221:TYR:HE1	13:m:227:PRO:HD3	1.80	0.47
13:m:357:LEU:HD11	13:m:423:TRP:HE3	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:m:461:ALA:O	13:m:465:GLN:HG3	2.15	0.47
13:m:471:ARG:NH1	13:m:472:GLN:OE1	2.43	0.47
13:m:622:LYS:NZ	14:o:524:SER:O	2.46	0.47
13:n:696:GLN:HA	13:n:758:PHE:HE1	1.79	0.47
1:E:46:ARG:HH22	1:E:54:GLY:N	2.13	0.47
1:F:15:ASP:HB3	1:F:22:LYS:HB2	1.96	0.47
1:G:202:GLY:HA2	2:H:112:PRO:HG3	1.97	0.47
1:I:335:GLU:OE1	1:I:335:GLU:N	2.47	0.47
3:J:184:THR:HG22	3:J:194:SER:HB2	1.97	0.47
13:n:530:VAL:HG22	13:n:549:ALA:HB1	1.97	0.47
1:A:20:VAL:HA	1:A:36:PRO:HA	1.96	0.47
1:I:242:TYR:CE2	1:I:246:GLY:HA2	2.50	0.47
3:J:270:LEU:HD23	3:J:280:VAL:HG11	1.97	0.47
4:K:55:ALA:HA	4:K:100:HIS:ND1	2.29	0.47
6:N:356:HIS:CD2	6:P:156:LEU:HD21	2.50	0.47
10:Z:1267:ARG:HG2	10:Z:1269:ARG:HH12	1.79	0.47
13:f:513:ASP:OD1	13:f:514:ALA:N	2.48	0.47
14:o:374:PRO:HG2	14:o:379:ALA:HB2	1.97	0.47
14:p:501:SER:OG	14:p:502:PHE:N	2.46	0.47
1:A:181:MET:HB3	1:A:278:VAL:HG13	1.97	0.47
1:B:261:LEU:HA	1:B:267:LEU:HD12	1.96	0.47
1:D:75:MET:HG2	1:D:79:ILE:C	2.40	0.47
1:D:227:ASN:HB3	1:D:230:LYS:HE3	1.96	0.47
1:E:11:PRO:HA	1:E:107:PRO:HD2	1.97	0.47
1:F:112:GLU:OE1	1:F:116:ASN:ND2	2.48	0.47
1:F:145:LEU:O	1:F:343:GLY:HA3	2.14	0.47
6:P:229:ALA:O	6:P:233:LYS:HG2	2.15	0.47
9:V:91:VAL:HG22	9:V:108:VAL:HG12	1.97	0.47
11:Y:251:THR:O	11:Y:255:ARG:HG3	2.15	0.47
13:e:435:ARG:O	13:e:447:LYS:N	2.48	0.47
13:f:513:ASP:O	13:f:517:ALA:N	2.37	0.47
14:h:266:SER:O	14:h:598:ASP:N	2.41	0.47
13:m:293:GLU:HA	13:m:298:LEU:HD21	1.97	0.47
13:n:253:ILE:HD11	13:n:319:ASP:HB3	1.97	0.47
1:A:200:LYS:O	1:B:117:PRO:HA	2.15	0.46
1:C:4:TYR:CG	10:Z:1243:LYS:HB3	2.50	0.46
1:C:43:LYS:HE3	1:C:44:HIS:CE1	2.51	0.46
11:Y:53:SER:HB2	11:Y:82:THR:HG21	1.97	0.46
13:f:407:GLU:O	13:f:411:LYS:HG2	2.14	0.46
14:g:315:VAL:O	14:g:326:GLU:N	2.48	0.46
14:h:552:TRP:CZ2	14:h:561:PRO:HG3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:n:772:ASN:OD1	14:p:382:HIS:CE1	2.68	0.46
1:A:41:ARG:O	1:A:70:SER:N	2.38	0.46
1:A:333:PRO:O	1:A:336:ARG:HG3	2.14	0.46
1:B:243:LEU:HD12	1:B:247:SER:HB2	1.97	0.46
2:H:67:LEU:HB2	2:H:203:THR:HB	1.96	0.46
1:I:161:GLY:O	1:I:186:ALA:HB1	2.15	0.46
7:O:131:GLN:HA	7:O:134:ILE:HD12	1.97	0.46
6:P:347:ALA:HA	6:P:350:PHE:CD2	2.50	0.46
13:m:357:LEU:HD21	13:m:423:TRP:HA	1.96	0.46
13:m:406:TYR:CD2	13:m:474:GLU:HG2	2.49	0.46
13:m:716:ARG:HA	13:m:823:VAL:HA	1.96	0.46
13:m:718:PHE:HE1	13:m:781:LEU:HD22	1.80	0.46
14:o:501:SER:OG	14:o:502:PHE:N	2.46	0.46
2:H:18:LYS:NZ	16:H:401:ATP:O3A	2.49	0.46
6:P:341:LYS:NZ	6:P:345:GLU:OE2	2.36	0.46
13:f:364:LEU:HB3	13:f:430:LEU:HD11	1.98	0.46
13:f:650:TRP:O	13:f:654:ILE:HG13	2.16	0.46
13:f:790:ARG:O	13:f:794:LYS:HG3	2.16	0.46
14:h:541:ALA:HB2	14:h:551:LEU:HG	1.98	0.46
13:n:706:VAL:HG12	13:n:764:ILE:HD12	1.97	0.46
1:D:240:GLN:CD	1:D:248:THR:HB	2.41	0.46
1:E:354:LYS:HA	1:E:357:TRP:NE1	2.29	0.46
1:G:223:TYR:HA	1:G:308:LYS:HB3	1.98	0.46
2:H:193:LEU:HD12	2:H:198:TYR:HD2	1.80	0.46
14:h:333:SER:HB2	14:h:352:THR:HB	1.97	0.46
13:m:408:GLU:HA	13:m:411:LYS:HE2	1.98	0.46
13:n:228:LYS:N	13:n:231:ASP:OD2	2.49	0.46
13:n:706:VAL:CG1	13:n:764:ILE:HD12	2.45	0.46
1:B:10:GLN:C	1:B:107:PRO:HD2	2.40	0.46
1:B:193:PHE:HZ	1:B:197:TYR:HH	1.62	0.46
1:B:226:ILE:HG22	6:P:113:GLN:HG2	1.98	0.46
1:B:227:ASN:HB3	1:B:230:LYS:HE3	1.98	0.46
1:C:15:ASP:HA	1:C:111:THR:HG22	1.97	0.46
1:C:176:MET:O	1:C:180:ILE:HG23	2.16	0.46
1:E:75:MET:HG2	1:E:79:ILE:C	2.40	0.46
1:F:18:SER:HA	1:F:75:MET:SD	2.56	0.46
1:F:36:PRO:HB2	1:F:38:TYR:CE2	2.51	0.46
2:H:14:SER:O	2:H:33:SER:OG	2.33	0.46
5:L:161:SER:O	5:L:163:ARG:HG2	2.15	0.46
13:e:119:ILE:O	13:e:136:ARG:N	2.49	0.46
14:h:480:THR:HG23	14:h:501:SER:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:n:462:ARG:O	13:n:466:MET:HG2	2.16	0.46
13:n:541:GLU:CD	13:n:541:GLU:H	2.23	0.46
14:p:374:PRO:HG2	14:p:379:ALA:HB2	1.97	0.46
1:D:114:PRO:HB3	1:D:141:MET:HE1	1.97	0.46
1:E:369:ARG:O	1:E:373:ARG:HG3	2.16	0.46
1:F:21:ILE:HG12	1:F:37:ASN:HB2	1.98	0.46
2:H:332:PRO:O	2:H:335:ARG:HG3	2.15	0.46
4:K:35:ASP:HB3	5:L:8:CYS:HB3	1.97	0.46
6:M:353:LEU:O	6:M:357:LEU:HB2	2.15	0.46
7:O:82:SER:O	7:O:83:LYS:NZ	2.46	0.46
8:U:124:ILE:HB	8:U:142:VAL:HG13	1.98	0.46
9:V:135:PRO:HB2	11:Y:81:HIS:CE1	2.50	0.46
13:e:783:GLU:HA	13:e:786:ARG:HH21	1.80	0.46
13:f:38:VAL:O	13:f:42:LEU:N	2.35	0.46
13:f:754:LYS:HE2	13:f:760:VAL:H	1.80	0.46
13:m:610:GLN:HA	13:m:613:LYS:HD3	1.97	0.46
13:n:560:VAL:O	13:n:564:ILE:HG13	2.16	0.46
1:A:43:LYS:HB3	1:A:70:SER:HB3	1.96	0.46
1:B:170:ILE:HG23	1:B:174:PHE:C	2.40	0.46
1:B:205:PHE:HB3	1:B:210:GLU:HB3	1.97	0.46
1:C:15:ASP:HB3	1:C:22:LYS:HB2	1.98	0.46
1:C:28:ASP:HB2	1:C:341:TRP:HH2	1.81	0.46
1:C:104:GLU:HG3	1:C:133:ASN:HB2	1.97	0.46
1:E:48:MET:HE2	1:G:173:GLY:N	2.31	0.46
1:F:89:ILE:O	1:F:93:VAL:HG23	2.16	0.46
1:G:219:GLU:HG2	15:G:800:ADP:C4	2.50	0.46
1:I:29:GLN:CD	6:M:5:LYS:HD2	2.41	0.46
3:J:298:GLN:OE1	3:J:298:GLN:N	2.27	0.46
4:K:128:LEU:HA	4:K:229:ILE:HG21	1.98	0.46
6:P:244:CYS:N	6:Q:262:MET:HE1	2.30	0.46
7:R:98:VAL:O	7:R:102:GLU:OE1	2.34	0.46
10:W:1109:ILE:HD12	10:Z:1105:MET:HE2	1.96	0.46
11:Y:282:LEU:O	11:Y:290:ASN:HB3	2.15	0.46
13:f:339:PHE:CZ	13:f:360:ILE:HG23	2.51	0.46
14:h:355:GLY:HA2	14:h:384:VAL:HG23	1.98	0.46
13:n:335:LEU:H	13:n:370:THR:HG21	1.81	0.46
1:A:170:ILE:HG12	1:A:175:ALA:HB2	1.97	0.46
1:C:273:GLU:OE1	1:C:273:GLU:N	2.49	0.46
1:D:77:HIS:ND1	1:D:184:ASP:HB2	2.30	0.46
1:D:334:GLN:HE22	6:P:14:ARG:HA	1.81	0.46
1:F:361:LYS:O	1:F:365:GLU:OE1	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:371:ILE:HG13	1:F:372:HIS:N	2.31	0.46
2:H:218:TYR:CE1	2:H:255:PHE:HB3	2.50	0.46
1:I:28:ASP:HB2	1:I:341:TRP:HH2	1.81	0.46
1:I:218:LYS:HA	1:I:222:CYS:SG	2.56	0.46
4:K:160:SER:O	4:K:173:TRP:N	2.35	0.46
6:M:209:VAL:HG22	10:W:1258:PHE:HD1	1.81	0.46
13:f:649:ILE:O	13:f:653:GLN:HG2	2.16	0.46
14:h:557:ASP:OD1	14:h:562:THR:OG1	2.33	0.46
13:m:750:VAL:HA	13:m:760:VAL:HG21	1.98	0.46
13:m:753:LEU:HD12	13:m:758:PHE:HB2	1.98	0.46
13:m:791:THR:O	13:m:795:VAL:HG23	2.14	0.46
13:n:408:GLU:O	13:n:411:LYS:HG2	2.15	0.46
13:n:484:LEU:HB3	13:n:516:ASP:CG	2.41	0.46
1:B:218:LYS:HA	1:B:222:CYS:SG	2.56	0.46
1:D:16:ASN:HA	1:D:21:ILE:HD12	1.97	0.46
1:E:45:VAL:HG22	6:M:81:THR:HG22	1.96	0.46
1:F:87:GLU:O	1:F:91:GLN:OE1	2.33	0.46
1:F:232:GLU:HG2	6:M:74:ARG:HG3	1.98	0.46
3:J:27:CYS:HB2	3:J:37:CYS:HB3	1.77	0.46
9:V:7:LEU:HG	9:V:175:LYS:HD2	1.98	0.46
10:Z:1141:LEU:HB3	10:Z:1143:PRO:HD2	1.98	0.46
10:Z:1162:GLN:O	10:Z:1165:GLU:HG3	2.16	0.46
13:f:246:GLN:OE1	13:f:311:HIS:NE2	2.49	0.46
14:h:495:HIS:ND1	14:h:510:THR:OG1	2.37	0.46
13:m:657:GLN:HG3	14:o:504:TRP:CZ3	2.50	0.46
13:m:666:GLU:HB2	13:m:673:TRP:CE2	2.51	0.46
13:m:832:TYR:HB2	13:m:835:ARG:HH21	1.81	0.46
13:n:395:VAL:O	13:n:399:ARG:HG2	2.15	0.46
1:B:145:LEU:HD13	1:B:148:TYR:CD2	2.51	0.46
1:D:31:PRO:HD2	6:P:9:LEU:HD21	1.97	0.46
1:G:21:ILE:HG23	1:G:37:ASN:HB2	1.98	0.46
1:G:161:GLY:O	1:G:186:ALA:HB1	2.16	0.46
1:G:368:ALA:HA	1:G:371:ILE:HG12	1.97	0.46
2:H:305:MET:SD	16:H:401:ATP:N6	2.89	0.46
1:I:116:ASN:HB2	1:I:121:ARG:NH1	2.31	0.46
3:J:22:GLU:N	15:J:800:ADP:O1B	2.49	0.46
4:K:93:LYS:NZ	4:K:113:VAL:O	2.48	0.46
5:L:25:LEU:HD21	5:L:40:LEU:HD23	1.97	0.46
13:f:340:PRO:HD3	13:f:363:HIS:ND1	2.31	0.46
13:f:577:ASN:OD1	13:f:578:ALA:N	2.49	0.46
13:m:528:GLU:O	13:m:532:GLU:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:m:629:GLN:OE1	13:m:629:GLN:N	2.49	0.46
13:n:253:ILE:HD12	13:n:316:PHE:HA	1.99	0.46
14:p:315:VAL:HB	14:p:327:TYR:HB2	1.98	0.46
1:B:18:SER:HA	1:B:75:MET:HE1	1.98	0.45
1:B:305:THR:O	1:B:336:ARG:NH1	2.49	0.45
1:F:141:MET:HB3	1:F:144:VAL:HG23	1.98	0.45
1:F:160:SER:HB3	1:F:305:THR:HG23	1.98	0.45
2:H:173:HIS:HB2	2:H:284:LYS:NZ	2.29	0.45
1:I:82:ASP:HB3	1:I:85:ASP:HB2	1.97	0.45
9:V:164:LEU:O	9:V:168:VAL:HG23	2.16	0.45
10:W:1105:MET:HE1	10:Z:1106:ARG:CG	2.43	0.45
13:e:535:GLY:HA2	13:e:546:TRP:HA	1.97	0.45
13:f:375:GLN:O	13:f:379:ARG:HG2	2.15	0.45
13:f:477:ARG:O	13:f:481:VAL:HG23	2.16	0.45
13:f:529:ASN:HB3	13:f:552:ARG:NE	2.23	0.45
13:f:759:ARG:HD2	13:f:759:ARG:O	2.15	0.45
13:m:690:ARG:HA	13:m:693:LEU:HB2	1.97	0.45
13:m:801:ILE:HG21	13:m:850:LEU:HB3	1.98	0.45
13:n:612:VAL:O	13:n:616:ILE:HG13	2.16	0.45
1:A:9:ASN:HB3	1:A:106:HIS:CE1	2.52	0.45
1:B:75:MET:HG2	1:B:79:ILE:C	2.40	0.45
1:E:145:LEU:O	1:E:343:GLY:HA3	2.15	0.45
6:M:346:GLN:OE1	10:Z:1136:VAL:HB	2.17	0.45
11:Y:119:ARG:NH1	11:Y:125:ASP:OD2	2.49	0.45
13:f:116:LEU:HA	13:f:139:THR:HA	1.98	0.45
13:f:582:PHE:CD2	13:f:664:ARG:HG2	2.51	0.45
13:f:620:HIS:HA	13:f:689:PHE:CE1	2.51	0.45
14:h:288:SER:HB3	14:h:291:TYR:HB2	1.96	0.45
13:n:475:GLN:O	13:n:479:VAL:HG12	2.16	0.45
14:p:268:ASN:N	14:p:596:ILE:O	2.49	0.45
1:A:289:ASP:OD2	1:A:290:LEU:N	2.48	0.45
1:C:112:GLU:C	1:C:142:GLN:HE22	2.24	0.45
1:G:200:LYS:O	2:H:112:PRO:HA	2.16	0.45
1:G:245:ASP:OD1	1:G:246:GLY:N	2.50	0.45
1:I:331:SER:HA	6:M:19:VAL:HG12	1.97	0.45
4:K:259:ARG:HG3	5:L:112:PHE:CE2	2.51	0.45
6:P:358:ASP:HB2	7:R:129:LEU:HD21	1.98	0.45
6:Q:212:GLU:HB2	10:Z:1269:ARG:NE	2.28	0.45
9:V:135:PRO:HG3	11:Y:113:PHE:HB2	1.97	0.45
13:f:395:VAL:HB	13:f:399:ARG:HH21	1.81	0.45
13:f:414:VAL:O	13:f:418:GLU:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:m:669:LEU:HB2	13:m:673:TRP:HB3	1.98	0.45
13:n:333:ASN:HA	13:n:336:MET:HB2	1.97	0.45
1:B:263:PHE:CZ	1:B:313:ARG:HG2	2.51	0.45
1:B:300:LEU:HD12	1:B:332:ALA:HB2	1.97	0.45
1:D:51:ALA:HB2	1:F:173:GLY:HA3	1.98	0.45
1:D:273:GLU:HB3	1:D:277:GLU:HB2	1.98	0.45
1:E:143:ALA:HA	1:E:157:VAL:HG11	1.97	0.45
1:E:178:HIS:O	1:E:285:LYS:NZ	2.38	0.45
1:E:181:MET:HE1	1:E:281:PHE:CB	2.47	0.45
1:G:267:LEU:O	2:H:173:HIS:NE2	2.49	0.45
1:G:343:GLY:O	1:G:346:ILE:HG22	2.16	0.45
13:f:113:SER:O	13:f:141:SER:HA	2.17	0.45
13:m:766:ASN:O	13:m:770:GLN:HG2	2.15	0.45
13:m:774:LEU:HA	13:m:777:PHE:CD2	2.51	0.45
13:n:233:GLY:O	13:n:236:VAL:HG22	2.17	0.45
13:n:278:TRP:NE1	13:n:376:ARG:HH21	2.14	0.45
1:B:203:TYR:CE1	1:B:249:ILE:HG12	2.52	0.45
1:C:162:ASP:HB2	15:C:800:ADP:H4'	1.97	0.45
1:C:169:PRO:HG2	1:C:176:MET:HB2	1.98	0.45
1:D:11:PRO:HG2	1:D:348:ALA:HB1	1.99	0.45
1:F:311:GLY:HA3	6:N:20:TYR:CZ	2.51	0.45
2:H:102:PRO:HB3	2:H:131:ALA:HB3	1.99	0.45
1:I:115:LEU:HB2	1:I:182:ARG:HD2	1.98	0.45
4:K:254:THR:HG23	5:L:144:ILE:HD12	1.99	0.45
6:M:348:MET:SD	7:O:115:HIS:ND1	2.90	0.45
7:O:144:THR:C	7:O:148:LYS:HZ2	2.25	0.45
6:P:258:GLY:O	6:P:260:CYS:N	2.48	0.45
9:V:3:LEU:HB3	11:Y:317:ARG:HG3	1.98	0.45
13:f:82:SER:O	13:f:84:LEU:N	2.50	0.45
13:f:377:ALA:O	13:f:381:VAL:HG23	2.17	0.45
13:f:480:ILE:HG12	13:f:484:LEU:HD12	1.98	0.45
13:f:581:MET:SD	13:f:582:PHE:N	2.89	0.45
14:h:483:HIS:ND1	14:h:532:TRP:HB2	2.31	0.45
13:n:572:LEU:HD22	13:n:604:TYR:CE1	2.51	0.45
1:A:53:GLU:N	1:A:53:GLU:OE2	2.50	0.45
1:A:116:ASN:O	1:A:121:ARG:NH1	2.48	0.45
1:B:240:GLN:CD	1:B:248:THR:HB	2.42	0.45
1:B:354:LYS:HA	1:B:357:TRP:HE1	1.81	0.45
1:C:48:MET:HE1	1:E:148:TYR:CE2	2.52	0.45
2:H:70:PRO:HG3	2:H:85:ILE:HD12	1.98	0.45
2:H:214:GLU:HA	16:H:401:ATP:C2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:168:VAL:HG22	1:I:180:ILE:HG23	1.98	0.45
3:J:364:LEU:HD22	11:Y:152:GLN:HA	1.97	0.45
3:J:366:ASP:N	3:J:366:ASP:OD1	2.48	0.45
5:L:251:ASP:HA	5:L:254:LYS:HD2	1.98	0.45
6:M:334:VAL:HG22	7:O:103:GLN:HE21	1.81	0.45
6:Q:25:LEU:HD12	6:Q:26:PRO:HD2	1.98	0.45
11:Y:50:TYR:HA	11:Y:56:GLU:O	2.16	0.45
13:f:357:LEU:HD11	13:f:423:TRP:HE3	1.82	0.45
13:m:805:VAL:HB	13:m:843:PHE:HE1	1.81	0.45
13:n:481:VAL:O	13:n:485:ARG:HD2	2.17	0.45
13:n:561:GLU:HG2	13:n:597:ILE:HD11	1.99	0.45
14:o:268:ASN:N	14:o:596:ILE:O	2.49	0.45
14:o:270:GLN:HE22	14:o:595:VAL:HG12	1.81	0.45
1:A:254:SER:HA	1:A:257:ARG:HB2	1.97	0.45
1:B:10:GLN:CG	13:n:246:GLN:HE22	2.26	0.45
1:B:156:VAL:CG2	1:B:294:LEU:HD12	2.46	0.45
1:C:91:GLN:OE1	1:C:91:GLN:HA	2.17	0.45
1:C:302:GLY:O	1:C:305:THR:OG1	2.30	0.45
1:F:94:TYR:CE1	1:F:103:SER:HA	2.51	0.45
3:J:32:GLU:HB2	3:J:355:TRP:HH2	1.82	0.45
4:K:55:ALA:HA	4:K:100:HIS:CE1	2.51	0.45
6:N:336:ARG:O	6:N:340:ILE:HG12	2.16	0.45
8:U:165:ASP:HA	8:U:168:MET:CE	2.46	0.45
13:f:479:VAL:O	13:f:483:VAL:N	2.42	0.45
13:m:402:MET:HE3	13:m:466:MET:CE	2.46	0.45
1:A:202:GLY:HA2	1:B:117:PRO:HG3	1.99	0.45
1:A:228:PRO:HD3	1:A:313:ARG:NH1	2.31	0.45
1:B:273:GLU:OE1	1:B:273:GLU:N	2.49	0.45
1:C:86:MET:HA	1:C:89:ILE:HG22	1.98	0.45
1:D:161:GLY:O	1:D:186:ALA:HB1	2.17	0.45
1:E:9:ASN:OD1	1:E:10:GLN:N	2.48	0.45
1:E:11:PRO:HB3	1:E:107:PRO:HB2	1.97	0.45
1:I:18:SER:OG	1:I:163:GLY:N	2.50	0.45
1:I:143:ALA:HA	1:I:157:VAL:HG11	1.99	0.45
6:M:395:ASN:O	6:M:399:ARG:HG2	2.17	0.45
7:R:28:ARG:HH12	7:R:31:ARG:NH1	2.10	0.45
11:Y:22:ALA:HB3	11:Y:27:LEU:HD21	1.99	0.45
11:Y:61:ALA:O	11:Y:64:LYS:HG2	2.17	0.45
13:f:271:ALA:O	13:f:275:ILE:HG12	2.17	0.45
13:f:354:ARG:HB2	13:f:422:THR:HG21	1.98	0.45
14:h:347:LEU:HD22	14:h:359:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:m:755:TRP:CD1	14:o:453:GLU:HB3	2.51	0.45
14:o:280:ARG:NH2	14:o:302:ASN:HB2	2.32	0.45
1:A:261:LEU:HA	1:A:267:LEU:HD12	1.98	0.45
1:D:58:ILE:H	1:D:61:LYS:NZ	2.15	0.45
1:F:147:LEU:HA	1:F:150:THR:HG22	1.98	0.45
3:J:78:ARG:NE	3:J:78:ARG:HA	2.32	0.45
4:K:62:PHE:HA	4:K:76:ILE:O	2.17	0.45
4:K:197:HIS:CE1	4:K:199:TYR:HB3	2.51	0.45
6:N:399:ARG:HD2	7:O:172:LEU:HD13	1.99	0.45
6:P:269:GLN:HG2	7:R:39:LYS:HZ1	1.81	0.45
9:V:40:THR:HG23	9:V:61:CYS:HB3	1.99	0.45
11:Y:69:ARG:HD3	11:Y:275:HIS:HA	1.99	0.45
13:f:250:ASN:O	13:f:254:ARG:HG2	2.17	0.45
13:f:299:LEU:O	13:f:303:ILE:HG12	2.16	0.45
13:f:368:ARG:HA	13:f:437:ILE:HG12	1.99	0.45
14:h:527:VAL:HA	14:h:544:ASP:HA	1.99	0.45
14:h:547:GLY:HA2	14:h:573:LEU:HG	1.99	0.45
13:n:613:LYS:HE2	13:n:613:LYS:HB3	1.76	0.45
1:A:145:LEU:O	1:A:343:GLY:HA3	2.17	0.45
1:F:185:ILE:H	1:F:185:ILE:HD12	1.82	0.45
5:L:156:VAL:HG11	5:L:209:HIS:CE1	2.52	0.45
13:f:229:VAL:HG22	13:f:303:ILE:HD13	1.99	0.45
13:n:334:PRO:HB2	13:n:370:THR:OG1	2.17	0.45
13:n:779:ILE:HB	14:p:375:LEU:CD2	2.28	0.45
1:B:28:ASP:HB2	1:B:341:TRP:HH2	1.81	0.44
1:I:20:VAL:HG23	1:I:35:PHE:C	2.42	0.44
3:J:182:GLN:HB2	3:J:262:ILE:HD11	1.99	0.44
4:K:129:ARG:O	4:K:133:LYS:HG2	2.17	0.44
10:Z:1153:ALA:O	10:Z:1158:ARG:NH1	2.48	0.44
13:f:364:LEU:O	13:f:367:ILE:HG22	2.17	0.44
13:f:368:ARG:HB3	13:f:433:LEU:HD11	1.98	0.44
13:f:483:VAL:O	13:f:567:ARG:NH1	2.50	0.44
14:h:360:TRP:CE2	14:h:369:PRO:HG3	2.52	0.44
13:m:802:SER:O	13:m:806:ALA:HB2	2.17	0.44
1:B:243:LEU:HD13	1:D:288:MET:HE2	1.99	0.44
1:F:210:GLU:HA	1:F:213:ILE:HD13	1.98	0.44
1:F:354:LYS:HA	1:F:357:TRP:CE2	2.52	0.44
1:G:75:MET:HG2	1:G:79:ILE:C	2.43	0.44
1:G:326:VAL:HG23	1:G:328:ILE:HG23	1.99	0.44
4:K:38:LEU:O	5:L:5:GLN:NE2	2.46	0.44
5:L:200:ASP:N	5:L:200:ASP:OD1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:R:84:LEU:HA	7:R:87:ILE:HG12	1.98	0.44
13:f:213:ILE:HG13	13:f:214:THR:N	2.32	0.44
13:f:368:ARG:HH21	13:f:433:LEU:HD13	1.82	0.44
13:f:751:ARG:NH2	14:h:433:ALA:HB1	2.31	0.44
13:m:300:THR:O	13:m:304:LEU:HD23	2.17	0.44
13:m:518:ASN:O	13:m:521:GLU:HG3	2.17	0.44
13:m:605:GLN:NE2	13:m:669:LEU:HA	2.32	0.44
1:B:355:LYS:C	1:B:356:MET:HE2	2.41	0.44
1:C:224:LEU:HD13	1:C:307:PHE:HB3	1.99	0.44
1:C:315:LEU:HD13	6:Q:44:SER:HB2	1.99	0.44
1:D:154:THR:HB	1:D:172:GLU:H	1.82	0.44
1:D:227:ASN:HB3	1:D:230:LYS:HG2	1.99	0.44
1:G:86:MET:SD	1:G:89:ILE:HD11	2.57	0.44
2:H:223:PHE:CE1	2:H:227:MET:HE3	2.53	0.44
2:H:286:ASP:OD1	2:H:287:VAL:N	2.51	0.44
6:M:379:GLN:O	6:M:382:MET:HB2	2.17	0.44
13:m:593:VAL:O	13:m:598:ARG:NH2	2.47	0.44
13:m:649:ILE:HG21	14:o:502:PHE:HD2	1.82	0.44
14:p:476:GLN:N	14:p:503:ASP:OD2	2.36	0.44
1:A:43:LYS:NZ	1:A:67:GLY:O	2.50	0.44
1:A:228:PRO:HD3	1:A:313:ARG:HH12	1.83	0.44
1:E:156:VAL:HG23	1:E:294:LEU:HD12	2.00	0.44
1:G:39:VAL:HG21	1:G:85:ASP:HB3	1.98	0.44
3:J:56:GLN:HB2	3:J:59:ILE:HD13	1.99	0.44
3:J:248:TYR:O	3:J:256:LEU:N	2.40	0.44
11:Y:143:ARG:HA	11:Y:146:LYS:HG2	1.99	0.44
13:f:339:PHE:HA	13:f:340:PRO:HD3	1.84	0.44
13:m:395:VAL:O	13:m:399:ARG:HG2	2.17	0.44
13:m:560:VAL:O	13:m:564:ILE:HG13	2.17	0.44
13:n:367:ILE:HD11	13:n:372:TYR:HB3	1.99	0.44
1:A:89:ILE:O	1:A:93:VAL:HG23	2.17	0.44
1:B:49:ALA:N	1:D:148:TYR:HH	2.15	0.44
1:D:112:GLU:C	1:D:142:GLN:HE21	2.26	0.44
2:H:190:MET:CE	2:H:200:PHE:HB2	2.47	0.44
4:K:114:ASP:OD1	4:K:115:GLY:N	2.51	0.44
5:L:139:ASP:OD2	5:L:141:SER:OG	2.30	0.44
7:O:85:GLN:HG3	10:W:1105:MET:SD	2.58	0.44
6:P:267:LEU:O	6:P:271:LYS:HG2	2.18	0.44
10:Z:1282:ASP:OD1	10:Z:1283:ARG:N	2.50	0.44
13:e:286:TYR:CB	13:f:175:GLY:HA2	2.48	0.44
13:f:375:GLN:HB3	13:f:379:ARG:HH12	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:f:473:HIS:CE1	13:f:527:TYR:HB2	2.52	0.44
13:f:649:ILE:HG12	13:f:756:LEU:HD11	2.00	0.44
13:f:713:VAL:HG23	13:f:743:ILE:HD12	1.98	0.44
13:m:292:ARG:NH2	13:m:317:ASP:OD1	2.46	0.44
13:n:669:LEU:HB2	13:n:673:TRP:HB2	2.00	0.44
1:A:245:ASP:OD1	1:A:246:GLY:N	2.51	0.44
1:B:88:ARG:HA	1:B:91:GLN:NE2	2.33	0.44
1:B:220:ARG:HD3	1:B:241:TYR:CE1	2.53	0.44
1:B:238:LYS:HB3	1:B:250:GLU:HB3	2.00	0.44
1:E:214:VAL:HA	1:E:217:ILE:HD12	2.00	0.44
1:G:15:ASP:HA	1:G:111:THR:OG1	2.18	0.44
2:H:305:MET:SD	16:H:401:ATP:C6	3.11	0.44
4:K:194:ILE:HD13	4:K:239:TYR:HE1	1.82	0.44
7:O:79:PRO:HG3	10:W:1107:LEU:HD22	2.00	0.44
8:U:42:ILE:HD12	8:U:63:ILE:HG22	1.99	0.44
8:U:147:ASP:HB2	8:U:150:ARG:HH22	1.81	0.44
13:f:410:GLU:O	13:f:414:VAL:HG23	2.17	0.44
14:o:315:VAL:HB	14:o:327:TYR:HB2	1.98	0.44
14:o:531:MET:HE2	14:o:578:TRP:H	1.82	0.44
1:C:308:LYS:HD3	6:Q:37:LEU:O	2.17	0.44
2:H:346:LEU:HA	2:H:349:LEU:HD12	1.99	0.44
3:J:110:PHE:CZ	3:J:118:VAL:HG12	2.52	0.44
4:K:43:ASP:O	4:K:47:ARG:HG2	2.18	0.44
6:M:6:TYR:HB3	6:M:12:ILE:HG21	2.00	0.44
6:M:185:ALA:O	7:R:127:GLN:NE2	2.45	0.44
6:N:8:ASP:OD1	6:N:9:LEU:N	2.51	0.44
6:Q:7:ALA:HA	6:Q:14:ARG:HH21	1.82	0.44
11:Y:138:HIS:HE1	11:Y:140:HIS:HB2	1.83	0.44
11:Y:238:ASP:OD1	11:Y:239:TYR:N	2.50	0.44
13:f:278:TRP:HB2	13:f:336:MET:CE	2.34	0.44
13:m:266:PRO:HG3	13:m:376:ARG:CG	2.48	0.44
13:m:710:ASN:HA	13:m:767:LYS:NZ	2.33	0.44
13:n:564:ILE:HG21	13:n:591:LEU:HD21	1.99	0.44
14:p:518:TYR:OH	14:p:559:GLU:OE2	2.34	0.44
14:p:531:MET:HE2	14:p:578:TRP:H	1.82	0.44
1:A:355:LYS:HZ1	5:L:258:LEU:HA	1.83	0.44
1:D:77:HIS:HD1	1:D:184:ASP:HB2	1.82	0.44
7:O:144:THR:O	7:O:148:LYS:HG2	2.18	0.44
8:U:42:ILE:HB	8:U:63:ILE:HG22	1.99	0.44
9:V:123:LYS:HD3	9:V:142:PRO:HD3	1.99	0.44
13:f:241:PHE:HA	13:f:244:GLN:HE21	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:f:333:ASN:O	13:f:336:MET:N	2.49	0.44
13:f:641:LEU:HG	14:h:502:PHE:CE2	2.52	0.44
14:h:457:TYR:CE1	14:h:471:MET:HG2	2.51	0.44
13:n:305:LYS:HE2	13:n:305:LYS:HB2	1.85	0.44
1:D:162:ASP:HB2	15:D:800:ADP:H4'	2.00	0.44
1:D:263:PHE:CZ	1:D:313:ARG:HG2	2.52	0.44
1:F:158:LEU:O	1:F:301:SER:N	2.51	0.44
1:F:264:ARG:HB3	1:F:266:ASP:OD1	2.18	0.44
2:H:298:VAL:HA	2:H:330:ILE:HB	2.00	0.44
1:I:210:GLU:O	1:I:213:ILE:HG22	2.18	0.44
4:K:38:LEU:HD23	5:L:8:CYS:SG	2.58	0.44
4:K:210:LYS:NZ	5:L:183:GLY:O	2.51	0.44
11:Y:426:PHE:CE1	11:Y:458:VAL:HB	2.53	0.44
13:e:716:ARG:CA	13:e:824:TRP:HD1	2.31	0.44
13:f:410:GLU:O	13:f:413:MET:HG2	2.18	0.44
13:f:584:ILE:HG13	13:f:585:PHE:HD1	1.83	0.44
13:m:580:GLU:O	13:m:584:ILE:HG13	2.18	0.44
14:o:495:HIS:ND1	14:o:510:THR:HG23	2.33	0.44
1:A:219:GLU:HG2	15:A:800:ADP:C4	2.53	0.43
1:B:263:PHE:CE2	1:B:313:ARG:HG2	2.53	0.43
1:F:46:ARG:HH11	1:F:51:ALA:HB3	1.83	0.43
1:G:90:TRP:HB3	1:G:132:PHE:CZ	2.54	0.43
2:H:138:ALA:HB2	2:H:161:HIS:CD2	2.53	0.43
4:K:16:ILE:HG23	5:L:27:ASP:HB3	2.00	0.43
4:K:239:TYR:O	4:K:243:ILE:HG12	2.17	0.43
11:Y:42:VAL:HG23	11:Y:284:CYS:CA	2.48	0.43
11:Y:425:CYS:HB3	11:Y:457:HIS:NE2	2.33	0.43
13:f:232:PHE:HE1	13:f:299:LEU:HD21	1.83	0.43
13:f:292:ARG:O	13:f:292:ARG:NH1	2.46	0.43
13:f:482:ARG:NH1	13:f:587:ARG:HG2	2.33	0.43
13:f:635:MET:HA	13:f:635:MET:HE3	2.00	0.43
14:h:554:LEU:HD12	14:h:614:PHE:HE1	1.84	0.43
13:n:365:ARG:HH22	13:n:429:LYS:HD2	1.83	0.43
13:n:487:GLN:NE2	13:n:587:ARG:HA	2.33	0.43
1:B:227:ASN:HB2	6:P:113:GLN:NE2	2.33	0.43
1:E:223:TYR:CZ	1:E:256:PHE:HB3	2.53	0.43
5:L:189:LEU:HD13	5:L:233:PHE:CE1	2.53	0.43
6:P:347:ALA:O	7:R:115:HIS:NE2	2.51	0.43
11:Y:76:CYS:SG	11:Y:80:MET:N	2.92	0.43
10:Z:1186:ALA:O	10:Z:1188:SER:N	2.51	0.43
13:f:233:GLY:O	13:f:236:VAL:HG12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:h:480:THR:H	14:h:501:SER:HA	1.82	0.43
14:h:503:ASP:O	14:h:505:THR:HG23	2.18	0.43
13:m:264:ARG:O	13:m:376:ARG:NH2	2.51	0.43
14:p:270:GLN:HE22	14:p:595:VAL:HG12	1.81	0.43
14:p:280:ARG:NH2	14:p:302:ASN:HB2	2.32	0.43
1:A:223:TYR:CE1	1:A:256:PHE:HB3	2.54	0.43
1:C:240:GLN:CD	1:C:248:THR:HB	2.43	0.43
1:D:39:VAL:HB	1:D:56:ILE:HD11	2.00	0.43
1:G:72:ARG:NH1	1:G:85:ASP:OD2	2.52	0.43
2:H:19:ALA:HB1	2:H:94:LEU:HD11	2.01	0.43
1:I:10:GLN:CD	1:I:25:PHE:HB3	2.44	0.43
1:I:11:PRO:HG2	1:I:26:ALA:HB2	2.01	0.43
6:P:361:GLN:NE2	7:R:129:LEU:HG	2.33	0.43
11:Y:319:MET:HE2	11:Y:333:LEU:HB3	1.99	0.43
13:e:283:ARG:CA	13:f:176:ASP:H	2.29	0.43
13:f:415:ALA:O	13:f:419:VAL:HG23	2.18	0.43
13:f:766:ASN:O	13:f:770:GLN:HG2	2.17	0.43
13:m:400:LYS:HB3	13:m:403:HIS:HD1	1.83	0.43
13:m:518:ASN:CG	13:m:563:ARG:HH12	2.26	0.43
13:m:769:HIS:O	13:m:773:GLN:HG2	2.17	0.43
13:n:235:LYS:NZ	13:n:238:ASP:OD2	2.48	0.43
13:n:425:ASP:OD1	13:n:426:GLU:N	2.51	0.43
13:n:569:ARG:HD3	13:n:569:ARG:HA	1.81	0.43
14:o:576:VAL:HG23	14:o:587:VAL:HG12	2.00	0.43
1:A:284:GLN:HE22	1:A:285:LYS:HG3	1.84	0.43
1:B:108:VAL:HG11	1:B:128:PHE:HD2	1.83	0.43
1:C:24:GLY:HA3	1:C:341:TRP:HZ2	1.83	0.43
1:F:77:HIS:ND1	1:F:184:ASP:HB3	2.33	0.43
1:G:252:GLY:H	1:G:255:ARG:HH12	1.66	0.43
2:H:140:LEU:HD12	2:H:342:GLY:C	2.43	0.43
1:I:300:LEU:HD13	1:I:310:PHE:HE2	1.84	0.43
8:U:58:GLU:HG3	8:U:59:GLN:H	1.83	0.43
8:U:158:GLN:OE1	8:U:158:GLN:N	2.51	0.43
13:f:485:ARG:HA	13:f:512:PHE:CE2	2.54	0.43
13:f:677:VAL:O	13:f:681:LYS:HG2	2.18	0.43
14:h:483:HIS:CE1	14:h:532:TRP:HB2	2.54	0.43
14:h:573:LEU:HD13	14:h:587:VAL:HG21	2.00	0.43
13:m:25:ALA:N	13:m:125:ILE:O	2.52	0.43
13:n:263:ASP:OD1	13:n:264:ARG:N	2.51	0.43
14:p:531:MET:SD	14:p:577:ARG:HD3	2.58	0.43
1:B:332:ALA:H	6:P:86:GLY:HA3	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:GLY:O	1:C:186:ALA:HB1	2.18	0.43
1:D:145:LEU:O	1:D:343:GLY:HA3	2.18	0.43
1:D:228:PRO:HD3	1:D:313:ARG:HH12	1.83	0.43
1:F:20:VAL:O	1:F:22:LYS:NZ	2.43	0.43
1:F:102:PHE:N	1:F:105:GLU:OE2	2.51	0.43
1:G:38:TYR:HA	1:G:74:PRO:HD3	2.01	0.43
2:H:123:MET:HG3	2:H:132:MET:SD	2.58	0.43
1:I:338:TYR:CD2	6:M:9:LEU:HD13	2.54	0.43
3:J:78:ARG:NH2	11:Y:278:ILE:HG22	2.33	0.43
3:J:174:GLU:HG2	3:J:269:ILE:HG21	2.00	0.43
4:K:207:VAL:HG23	5:L:188:ASN:HB3	2.00	0.43
6:M:385:ASN:HB3	6:N:386:LEU:HD13	2.00	0.43
7:O:148:LYS:CD	6:P:142:LYS:HD3	2.43	0.43
8:U:163:GLN:O	8:U:167:LEU:HG	2.18	0.43
13:e:777:PHE:CA	13:e:833:VAL:HG11	2.46	0.43
13:f:632:ALA:HA	13:f:635:MET:HB2	2.00	0.43
13:n:581:MET:HE1	13:n:607:GLN:OE1	2.17	0.43
13:n:685:ASP:OD1	13:n:685:ASP:N	2.51	0.43
14:o:531:MET:SD	14:o:577:ARG:HD3	2.58	0.43
1:B:9:ASN:HB3	13:n:246:GLN:NE2	2.33	0.43
1:B:51:ALA:HB2	1:D:173:GLY:HA3	2.01	0.43
1:D:181:MET:HG3	1:D:278:VAL:HG13	2.00	0.43
1:E:15:ASP:HB3	1:E:22:LYS:HE2	2.01	0.43
1:E:30:ILE:HG12	6:Q:5:LYS:NZ	2.20	0.43
1:E:147:LEU:HA	1:E:147:LEU:HD23	1.74	0.43
2:H:14:SER:HA	2:H:71:ILE:HD12	1.99	0.43
2:H:163:VAL:HG13	2:H:175:ILE:HG12	2.00	0.43
1:I:25:PHE:HZ	1:I:101:THR:HG21	1.82	0.43
3:J:53:LYS:C	3:J:56:GLN:HE22	2.25	0.43
4:K:59:MET:HG3	4:K:78:GLU:OE2	2.18	0.43
5:L:197:MET:HE1	5:L:216:LEU:HB3	2.01	0.43
6:P:312:LYS:C	6:Q:317:TYR:HH	2.14	0.43
6:Q:26:PRO:O	6:Q:28:ASP:N	2.51	0.43
13:f:441:LYS:O	13:f:445:ASN:N	2.33	0.43
13:f:619:LEU:HD22	13:f:661:TYR:HE2	1.84	0.43
13:f:746:LEU:CD2	13:f:768:ALA:HB2	2.46	0.43
13:m:620:HIS:O	13:m:624:LYS:HG3	2.18	0.43
13:n:476:LEU:HD21	13:n:594:ARG:NH1	2.34	0.43
14:p:576:VAL:HG23	14:p:587:VAL:HG12	2.00	0.43
1:C:20:VAL:O	1:C:22:LYS:NZ	2.44	0.43
1:D:219:GLU:HG2	15:D:800:ADP:C4	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:197:TYR:CD1	1:E:200:LYS:HD3	2.54	0.43
1:G:18:SER:HA	1:G:75:MET:HE1	2.01	0.43
2:H:262:PHE:HD1	2:H:275:HIS:CD2	2.36	0.43
3:J:81:LEU:HB3	11:Y:49:HIS:CE1	2.54	0.43
4:K:177:TRP:CD2	4:K:232:ILE:HD12	2.54	0.43
5:L:259:LYS:HD3	5:L:262:LEU:HD23	2.00	0.43
6:M:382:MET:HA	6:N:382:MET:HE1	2.01	0.43
9:V:144:THR:HG23	9:V:153:PHE:CE2	2.53	0.43
13:f:334:PRO:HB2	13:f:370:THR:HG22	2.00	0.43
13:f:427:TYR:OH	13:f:452:ILE:HB	2.19	0.43
13:f:479:VAL:HA	13:f:482:ARG:NH2	2.33	0.43
13:f:651:ALA:HB3	13:f:695:THR:HG22	2.00	0.43
13:n:365:ARG:HB3	13:n:368:ARG:HH12	1.84	0.43
13:n:369:ASN:OD1	13:n:369:ASN:N	2.52	0.43
1:A:132:PHE:HB2	1:A:134:VAL:HG23	2.01	0.43
1:B:305:THR:HG22	1:B:310:PHE:HE1	1.84	0.43
1:C:15:ASP:OD2	1:C:340:THR:OG1	2.32	0.43
1:I:242:TYR:HE2	1:I:246:GLY:HA2	1.84	0.43
6:M:358:ASP:O	6:M:361:GLN:HB3	2.19	0.43
8:U:138:PRO:HG2	8:U:151:ARG:HH22	1.84	0.43
13:f:722:SER:C	13:f:731:ASN:HB2	2.43	0.43
14:h:480:THR:HG22	14:h:502:PHE:CE1	2.54	0.43
1:B:245:ASP:OD1	1:B:246:GLY:N	2.52	0.43
1:E:67:GLY:HA3	1:G:289:ASP:HB3	2.00	0.43
1:F:371:ILE:O	1:F:375:THR:HG23	2.19	0.43
2:H:163:VAL:HG22	2:H:175:ILE:HG23	2.00	0.43
4:K:273:LYS:HB3	4:K:277:TYR:OH	2.19	0.43
6:P:3:ASP:HA	6:P:6:TYR:CZ	2.54	0.43
8:U:41:ILE:HD12	8:U:62:ILE:HD12	2.00	0.43
13:f:220:CYS:HA	13:f:223:ARG:HD2	2.00	0.43
13:f:478:ALA:O	13:f:482:ARG:HG3	2.19	0.43
14:h:316:TRP:CH2	14:h:325:PRO:HG3	2.54	0.43
13:m:324:GLN:OE1	13:m:324:GLN:N	2.42	0.43
13:m:717:ILE:HG22	13:m:824:TRP:CD2	2.54	0.43
13:n:357:LEU:HD21	13:n:423:TRP:HB2	2.00	0.43
14:o:472:PHE:HB3	14:o:509:TRP:CZ3	2.54	0.43
14:p:495:HIS:ND1	14:p:510:THR:HG23	2.33	0.43
1:A:280:VAL:O	1:A:284:GLN:HG3	2.18	0.43
1:C:245:ASP:OD1	1:C:246:GLY:N	2.51	0.43
1:D:24:GLY:HA3	1:D:341:TRP:HZ2	1.83	0.43
2:H:39:ARG:NH1	2:H:64:ILE:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:186:ALA:O	1:I:190:VAL:HG23	2.19	0.43
1:I:324:LYS:HG2	1:I:325:ASP:CG	2.44	0.43
3:J:42:VAL:HG12	3:J:53:LYS:HA	2.01	0.43
6:P:235:LEU:HD21	7:R:13:ARG:HB3	2.00	0.43
9:V:33:ASN:HB2	9:V:53:ALA:O	2.19	0.43
13:f:226:LYS:HB2	13:f:228:LYS:NZ	2.33	0.43
13:f:437:ILE:O	13:f:441:LYS:NZ	2.39	0.43
14:g:359:LEU:O	14:g:370:VAL:N	2.51	0.43
14:g:480:THR:N	14:g:500:SER:O	2.52	0.43
13:m:254:ARG:NH2	13:m:257:GLN:OE1	2.46	0.43
13:m:636:SER:HB2	13:m:641:LEU:HD23	2.01	0.43
13:m:783:GLU:HG2	13:m:786:ARG:HE	1.84	0.43
13:m:785:VAL:O	13:m:789:GLU:HG2	2.19	0.43
13:n:232:PHE:CE1	13:n:299:LEU:HD21	2.53	0.43
13:n:473:HIS:O	13:n:477:ARG:HD2	2.19	0.43
13:n:581:MET:CE	13:n:607:GLN:HE22	2.32	0.43
14:p:384:VAL:HG22	14:p:402:SER:HB3	2.01	0.43
1:A:92:TYR:HE2	1:A:98:GLN:HE21	1.67	0.42
1:B:21:ILE:HG12	1:B:37:ASN:HB2	2.01	0.42
1:C:68:LEU:H	1:C:68:LEU:HD12	1.84	0.42
1:G:92:TYR:C	1:G:98:GLN:HE21	2.25	0.42
2:H:116:ARG:HA	2:H:119:MET:HG2	2.00	0.42
13:f:378:LEU:HD11	13:f:450:TRP:CD1	2.54	0.42
14:h:329:PHE:HB3	14:h:360:TRP:CE2	2.53	0.42
14:h:475:HIS:ND1	14:h:501:SER:HB3	2.34	0.42
13:m:216:VAL:O	13:m:219:GLN:HG2	2.19	0.42
13:m:717:ILE:HG13	13:m:718:PHE:HD1	1.84	0.42
14:o:332:GLN:HE22	14:o:372:ARG:HH22	1.67	0.42
14:o:347:LEU:HB3	14:o:359:LEU:HD11	2.01	0.42
1:A:160:SER:OG	1:A:305:THR:HG23	2.19	0.42
1:D:74:PRO:HG3	1:D:89:ILE:HD12	2.00	0.42
1:G:240:GLN:OE1	1:G:249:ILE:N	2.53	0.42
1:I:200:LYS:O	3:J:98:PRO:HA	2.19	0.42
3:J:78:ARG:HA	3:J:78:ARG:HE	1.83	0.42
5:L:59:TYR:HB3	5:L:75:TRP:HZ3	1.84	0.42
6:N:212:GLU:OE1	10:W:1267:ARG:NH2	2.52	0.42
6:Q:157:GLU:HA	6:Q:162:PRO:HG2	2.01	0.42
8:U:89:VAL:HB	8:U:106:VAL:HG13	2.01	0.42
13:f:581:MET:O	13:f:584:ILE:HG12	2.19	0.42
13:f:628:PRO:HD3	13:f:647:SER:HB3	2.01	0.42
13:f:698:ILE:HA	13:f:701:ASP:OD2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:h:583:ARG:NH2	14:h:599:VAL:O	2.44	0.42
13:m:750:VAL:O	13:m:754:LYS:HG2	2.19	0.42
14:p:332:GLN:NE2	14:p:372:ARG:HH12	2.17	0.42
14:p:589:ASP:OD1	14:p:593:GLN:N	2.47	0.42
1:C:187:GLY:O	1:C:218:LYS:NZ	2.51	0.42
1:C:315:LEU:HD12	1:C:330:ILE:HD12	2.01	0.42
1:D:217:ILE:HG12	1:D:241:TYR:CE2	2.54	0.42
1:E:89:ILE:O	1:E:93:VAL:HG23	2.20	0.42
1:F:103:SER:HB2	1:F:132:PHE:HB3	2.01	0.42
2:H:291:LYS:HA	2:H:325:MET:SD	2.58	0.42
6:Q:319:THR:O	6:Q:323:TRP:HE3	2.01	0.42
9:V:99:VAL:HG22	9:V:116:ILE:HD12	2.01	0.42
10:W:1109:ILE:HD11	10:Z:1108:HIS:ND1	2.34	0.42
10:Z:1225:ALA:HB1	10:Z:1239:PHE:CD2	2.54	0.42
13:f:340:PRO:HG2	13:f:359:ALA:C	2.43	0.42
13:f:483:VAL:HG22	13:f:588:PHE:CE1	2.54	0.42
13:f:528:GLU:O	13:f:531:LYS:HB3	2.19	0.42
14:h:455:SER:HA	14:h:472:PHE:O	2.19	0.42
13:n:255:GLU:O	13:n:259:VAL:HG23	2.19	0.42
13:n:706:VAL:HA	13:n:709:ARG:HD2	2.02	0.42
14:p:311:GLY:HA3	14:p:335:VAL:HG23	2.01	0.42
1:B:156:VAL:HG22	1:B:169:PRO:HB3	2.01	0.42
1:C:316:SER:O	1:C:320:LYS:HG3	2.20	0.42
1:G:114:PRO:HA	1:G:141:MET:HE2	2.01	0.42
2:H:218:TYR:HA	2:H:307:PRO:HD2	2.01	0.42
4:K:67:ILE:HD11	4:K:70:TYR:HB2	2.01	0.42
4:K:230:LYS:O	4:K:234:HIS:ND1	2.47	0.42
6:Q:330:LEU:N	6:Q:331:PRO:HD2	2.34	0.42
9:V:3:LEU:HB3	11:Y:317:ARG:CG	2.48	0.42
11:Y:46:VAL:HG13	11:Y:278:ILE:HD11	2.01	0.42
13:f:753:LEU:HD22	13:f:758:PHE:HD2	1.84	0.42
13:f:827:TYR:O	13:f:831:PRO:HD2	2.19	0.42
13:n:221:TYR:HE1	13:n:227:PRO:HD3	1.84	0.42
13:n:373:PRO:HB2	13:n:376:ARG:HB3	2.02	0.42
14:o:332:GLN:NE2	14:o:372:ARG:HH12	2.17	0.42
14:o:503:ASP:O	14:o:505:THR:HG23	2.20	0.42
14:p:265:LEU:HD23	14:p:599:VAL:HG12	2.01	0.42
14:p:280:ARG:CZ	14:p:302:ASN:HB2	2.49	0.42
1:A:350:LEU:HD22	5:L:265:ALA:HB1	2.01	0.42
1:C:65:HIS:HB3	1:C:68:LEU:HD13	2.02	0.42
1:E:43:LYS:NZ	1:E:69:LEU:O	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:39:ILE:HG21	3:J:79:HIS:NE2	2.34	0.42
5:L:254:LYS:O	5:L:258:LEU:HG	2.19	0.42
6:N:392:ASN:ND2	10:Z:1179:ILE:HG12	2.30	0.42
6:P:331:PRO:HA	6:P:334:VAL:HG22	2.01	0.42
6:Q:111:GLU:O	6:Q:114:GLU:HG2	2.19	0.42
13:f:263:ASP:OD1	13:f:264:ARG:N	2.53	0.42
13:f:746:LEU:HD11	13:f:764:ILE:CG2	2.50	0.42
13:m:577:ASN:HB2	13:m:580:GLU:OE1	2.19	0.42
13:m:640:ASP:HB2	14:o:385:TYR:CE2	2.55	0.42
13:m:805:VAL:HG12	13:m:846:LYS:HB3	2.02	0.42
13:n:435:ARG:CZ	13:n:450:TRP:HB3	2.49	0.42
13:n:556:ARG:HG3	13:n:559:ARG:NH2	2.35	0.42
13:n:608:LEU:HD23	13:n:608:LEU:HA	1.83	0.42
14:o:518:TYR:OH	14:o:559:GLU:OE2	2.34	0.42
14:p:503:ASP:O	14:p:505:THR:HG23	2.20	0.42
1:B:108:VAL:HG11	1:B:128:PHE:CD2	2.55	0.42
1:D:238:LYS:HA	1:D:252:GLY:HA2	2.00	0.42
5:L:66:ARG:NE	5:L:68:GLY:O	2.53	0.42
6:Q:214:HIS:HB2	10:Z:1271:VAL:HG22	2.01	0.42
8:U:47:PRO:HD2	8:U:81:PRO:HB3	2.01	0.42
11:Y:123:MET:HB3	11:Y:133:TRP:HZ3	1.84	0.42
13:e:780:SER:CB	13:e:833:VAL:HB	2.50	0.42
13:f:468:LYS:O	13:f:472:GLN:HG2	2.20	0.42
13:f:618:SER:O	13:f:622:LYS:HG3	2.19	0.42
13:m:333:ASN:HB3	13:m:334:PRO:HD3	2.00	0.42
13:m:653:GLN:NE2	13:m:656:ARG:HH22	2.17	0.42
1:B:181:MET:HE1	1:B:282:ALA:HA	2.02	0.42
1:C:121:ARG:HE	1:C:139:ILE:HG21	1.85	0.42
1:D:253:PRO:HA	1:D:256:PHE:CE2	2.54	0.42
1:E:137:LEU:HD21	1:E:139:ILE:HG23	2.00	0.42
1:G:284:GLN:NE2	1:G:285:LYS:HG3	2.34	0.42
4:K:230:LYS:HG2	4:K:234:HIS:CE1	2.55	0.42
6:M:69:LEU:HD21	6:M:71:PHE:CD2	2.54	0.42
6:N:348:MET:SD	6:N:352:GLN:NE2	2.93	0.42
7:O:145:GLU:HA	7:O:148:LYS:HG2	2.01	0.42
6:P:211:TYR:CD1	10:Z:1256:VAL:HG22	2.53	0.42
6:Q:345:GLU:HA	6:Q:348:MET:HG2	2.02	0.42
7:R:99:ALA:O	7:R:103:GLN:OE1	2.38	0.42
11:Y:138:HIS:CE1	11:Y:140:HIS:HB2	2.55	0.42
13:f:482:ARG:HH11	13:f:587:ARG:HG2	1.84	0.42
14:h:474:GLY:HA3	14:h:509:TRP:CZ2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:m:241:PHE:O	13:m:245:LEU:HG	2.20	0.42
13:m:435:ARG:HG2	13:m:450:TRP:CH2	2.55	0.42
13:m:775:TYR:O	13:m:779:ILE:HG12	2.19	0.42
13:n:331:ASP:O	13:n:334:PRO:HD2	2.19	0.42
13:n:482:ARG:O	13:n:485:ARG:NE	2.52	0.42
13:n:604:TYR:O	13:n:607:GLN:NE2	2.53	0.42
14:o:352:THR:OG1	14:o:356:GLN:O	2.34	0.42
14:p:472:PHE:HB3	14:p:509:TRP:CZ3	2.54	0.42
14:p:579:THR:HG21	14:p:584:GLU:HB2	2.01	0.42
1:A:19:GLY:O	1:A:37:ASN:N	2.41	0.42
1:B:148:TYR:CD1	4:K:283:MET:HE1	2.55	0.42
1:B:305:THR:HG22	1:B:310:PHE:CE1	2.55	0.42
1:D:147:LEU:HD23	1:D:147:LEU:HA	1.84	0.42
1:E:9:ASN:HD21	1:E:106:HIS:CE1	2.38	0.42
1:E:270:GLU:HG3	1:E:272:SER:HB2	2.02	0.42
1:E:296:SER:O	1:E:329:ARG:HB3	2.20	0.42
1:F:98:GLN:O	1:F:100:GLN:N	2.53	0.42
4:K:196:VAL:HB	4:K:206:LEU:HB3	2.02	0.42
6:N:298:ALA:HB1	10:W:1100:GLN:HG2	2.02	0.42
6:Q:242:VAL:HG22	7:R:33:VAL:HG21	2.00	0.42
7:R:18:GLU:O	7:R:22:TYR:N	2.52	0.42
13:f:423:TRP:NE1	13:f:456:HIS:HE1	2.17	0.42
13:f:476:LEU:HD23	13:f:557:ILE:HD12	2.01	0.42
14:h:567:VAL:HG23	14:h:570:ASN:HA	2.02	0.42
13:m:400:LYS:HB3	13:m:403:HIS:ND1	2.34	0.42
13:m:738:ASN:O	13:m:824:TRP:NE1	2.53	0.42
13:n:409:PHE:O	13:n:413:MET:HG2	2.19	0.42
13:n:483:VAL:HG11	13:n:590:ALA:HB2	2.01	0.42
14:p:347:LEU:HB3	14:p:359:LEU:HD11	2.01	0.42
1:C:11:PRO:HG2	1:C:348:ALA:HB1	2.02	0.42
1:C:112:GLU:OE1	1:C:139:ILE:HG23	2.20	0.42
1:D:334:GLN:NE2	6:P:13:ALA:O	2.53	0.42
1:G:296:SER:O	1:G:329:ARG:HB3	2.20	0.42
2:H:283:MET:HE3	2:H:294:TYR:OH	2.20	0.42
1:I:77:HIS:CE1	1:I:184:ASP:HB3	2.54	0.42
1:I:352:THR:O	1:I:356:MET:HG2	2.20	0.42
5:L:85:ASP:OD1	5:L:86:GLY:N	2.53	0.42
6:P:147:LEU:HD12	6:P:147:LEU:HA	1.78	0.42
13:f:335:LEU:HD21	13:f:367:ILE:HB	2.02	0.42
13:f:357:LEU:HD11	13:f:423:TRP:CE3	2.55	0.42
13:f:425:ASP:O	13:f:429:LYS:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:f:653:GLN:HG3	14:h:502:PHE:O	2.20	0.42
13:m:518:ASN:HB3	13:m:563:ARG:HH22	1.85	0.42
13:m:653:GLN:OE1	13:m:656:ARG:NH1	2.30	0.42
13:n:580:GLU:HG3	13:n:583:ARG:NH1	2.29	0.42
14:o:280:ARG:CZ	14:o:302:ASN:HB2	2.49	0.42
14:o:336:MET:HE1	14:o:353:TYR:CA	2.47	0.42
14:p:270:GLN:NE2	14:p:595:VAL:HG12	2.35	0.42
1:E:305:THR:O	1:E:336:ARG:NH1	2.53	0.42
1:F:180:ILE:O	1:F:181:MET:HE2	2.20	0.42
1:F:350:LEU:HD13	13:f:319:ASP:HB2	2.01	0.42
1:G:32:LYS:HG3	1:G:33:TYR:CD2	2.55	0.42
2:H:35:VAL:HG12	2:H:54:VAL:HG22	2.02	0.42
1:I:10:GLN:O	1:I:106:HIS:ND1	2.34	0.42
1:I:176:MET:HB3	1:I:179:SER:HB2	2.01	0.42
11:Y:283:ARG:NE	11:Y:288:GLU:O	2.53	0.42
11:Y:296:PHE:O	11:Y:297:ASN:C	2.63	0.42
13:f:751:ARG:CZ	14:h:452:GLU:HG2	2.49	0.42
14:h:287:TRP:CZ3	14:h:295:LEU:HB2	2.54	0.42
13:m:468:LYS:O	13:m:472:GLN:HG2	2.20	0.42
13:m:774:LEU:HD13	13:m:824:TRP:CE3	2.55	0.42
14:o:265:LEU:HD23	14:o:599:VAL:HG12	2.01	0.42
14:p:479:ILE:HD13	14:p:501:SER:HB2	2.01	0.42
1:A:288:MET:HA	1:A:291:ARG:CG	2.50	0.41
1:E:36:PRO:HB2	1:E:38:TYR:CE2	2.54	0.41
1:E:60:PRO:O	1:E:63:GLU:HG2	2.20	0.41
1:F:77:HIS:O	1:F:182:ARG:NH2	2.53	0.41
2:H:79:TRP:CZ2	2:H:118:LYS:HB3	2.55	0.41
3:J:166:LEU:HB3	3:J:270:LEU:HG	2.02	0.41
4:K:230:LYS:CG	4:K:234:HIS:HE1	2.33	0.41
4:K:271:TRP:HA	4:K:274:ILE:HG12	2.00	0.41
5:L:210:ILE:HA	5:L:213:ILE:HG12	2.03	0.41
6:M:334:VAL:HG22	7:O:103:GLN:NE2	2.35	0.41
7:O:113:SER:HB2	7:O:116:ILE:HD12	2.02	0.41
6:Q:102:GLN:O	6:Q:106:GLN:HG2	2.19	0.41
8:U:105:ASN:OD1	8:U:105:ASN:N	2.52	0.41
13:f:255:GLU:O	13:f:259:VAL:HG23	2.20	0.41
13:f:413:MET:HG3	13:f:414:VAL:N	2.31	0.41
13:f:485:ARG:HH21	13:f:487:GLN:HG2	1.85	0.41
14:h:285:LEU:HD12	14:h:295:LEU:HD11	2.01	0.41
14:h:501:SER:OG	14:h:502:PHE:N	2.53	0.41
13:m:842:ASN:O	13:m:846:LYS:HG2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:n:485:ARG:HH12	13:n:487:GLN:CG	2.33	0.41
14:o:311:GLY:HA3	14:o:335:VAL:HG23	2.01	0.41
14:p:332:GLN:HE22	14:p:372:ARG:HH22	1.67	0.41
14:p:336:MET:HE1	14:p:353:TYR:CA	2.47	0.41
1:A:25:PHE:CE2	1:A:99:LEU:HD23	2.55	0.41
1:A:156:VAL:HA	1:A:169:PRO:HA	2.02	0.41
1:B:153:THR:O	1:B:173:GLY:N	2.45	0.41
1:D:192:ARG:HG2	1:D:195:ARG:HH21	1.84	0.41
1:D:339:SER:HA	1:D:342:ILE:HG22	2.01	0.41
1:F:20:VAL:HA	1:F:36:PRO:HA	2.03	0.41
2:H:71:ILE:CG1	2:H:82:MET:HE1	2.49	0.41
3:J:213:ARG:HD2	11:Y:249:VAL:HG23	2.02	0.41
5:L:55:VAL:HG21	5:L:75:TRP:HB2	2.01	0.41
6:M:344:HIS:HB2	7:O:116:ILE:HD11	2.02	0.41
7:O:113:SER:C	7:O:117:LYS:HZ3	2.27	0.41
6:P:17:PRO:HG2	6:P:20:TYR:CZ	2.55	0.41
8:U:31:PRO:HD2	8:U:52:GLU:HB3	2.01	0.41
9:V:34:ILE:HG22	9:V:55:VAL:HB	2.02	0.41
13:f:627:TYR:HB3	13:f:628:PRO:HD3	2.02	0.41
13:m:658:LEU:O	13:m:662:MET:HE3	2.20	0.41
13:m:699:PHE:CD2	13:m:758:PHE:HB3	2.54	0.41
13:n:305:LYS:HG3	13:n:310:PHE:CE1	2.56	0.41
13:n:448:MET:HE3	13:n:450:TRP:CZ3	2.55	0.41
14:o:384:VAL:HG22	14:o:402:SER:HB3	2.01	0.41
1:C:66:ARG:HH12	1:C:213:ILE:HG12	1.85	0.41
1:D:44:HIS:CG	1:F:176:MET:HE1	2.55	0.41
1:E:84:ASN:O	1:E:88:ARG:HG3	2.20	0.41
1:F:169:PRO:HG2	1:F:176:MET:HB2	2.02	0.41
1:F:287:ASP:O	1:F:291:ARG:HG3	2.20	0.41
1:F:372:HIS:HA	1:F:375:THR:HG23	2.01	0.41
3:J:250:LEU:HD11	3:J:256:LEU:HB2	2.01	0.41
6:M:214:HIS:ND1	6:P:209:VAL:O	2.49	0.41
7:O:143:ILE:HG13	7:O:144:THR:N	2.36	0.41
6:P:338:VAL:O	6:P:342:GLN:OE1	2.39	0.41
8:U:115:ARG:NE	8:U:115:ARG:HA	2.34	0.41
13:f:361:PHE:HA	13:f:364:LEU:HD12	2.01	0.41
13:f:661:TYR:O	13:f:664:ARG:HB2	2.20	0.41
14:h:524:SER:H	14:h:548:ARG:HH22	1.69	0.41
13:n:241:PHE:O	13:n:245:LEU:HG	2.19	0.41
1:B:324:LYS:O	1:B:326:VAL:HG23	2.20	0.41
1:D:243:LEU:HD11	1:D:249:ILE:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:305:THR:O	1:D:336:ARG:NH1	2.53	0.41
1:F:91:GLN:HG3	1:F:132:PHE:HE1	1.84	0.41
1:G:140:SER:OG	1:G:141:MET:N	2.53	0.41
5:L:60:LEU:HD21	5:L:135:LYS:HB2	2.02	0.41
6:M:212:GLU:OE1	6:M:212:GLU:N	2.53	0.41
13:f:579:ASN:HA	13:f:582:PHE:HD1	1.85	0.41
13:f:580:GLU:O	13:f:584:ILE:HG23	2.19	0.41
14:h:436:SER:N	14:h:450:GLY:O	2.39	0.41
13:m:137:VAL:O	13:n:139:THR:N	2.53	0.41
13:m:287:ARG:O	13:m:291:LYS:HG3	2.20	0.41
13:m:374:ILE:HG22	13:m:448:MET:HE1	2.01	0.41
13:m:603:GLU:HG3	13:m:604:TYR:H	1.85	0.41
13:n:413:MET:O	13:n:417:PHE:HD1	2.02	0.41
13:n:666:GLU:HA	13:n:673:TRP:CB	2.50	0.41
14:o:270:GLN:NE2	14:o:595:VAL:HG12	2.35	0.41
1:A:74:PRO:HG3	1:A:89:ILE:HD12	2.02	0.41
1:A:153:THR:HG21	5:L:267:LYS:HZ1	1.85	0.41
1:A:153:THR:O	1:A:173:GLY:N	2.53	0.41
1:A:218:LYS:HA	1:A:222:CYS:SG	2.61	0.41
1:C:103:SER:OG	1:C:132:PHE:HB3	2.21	0.41
1:C:197:TYR:CD1	1:C:200:LYS:HD3	2.55	0.41
1:D:30:ILE:HB	6:P:9:LEU:HD11	2.02	0.41
1:D:41:ARG:NH2	1:D:85:ASP:OD1	2.53	0.41
1:D:48:MET:HB3	1:F:173:GLY:CA	2.45	0.41
1:D:333:PRO:O	1:D:336:ARG:HG3	2.20	0.41
1:E:170:ILE:HD13	1:E:175:ALA:HA	2.01	0.41
1:F:60:PRO:HD2	1:F:92:TYR:OH	2.21	0.41
1:F:151:GLY:HA3	13:f:310:PHE:CD1	2.55	0.41
1:F:213:ILE:HD12	1:F:213:ILE:H	1.85	0.41
2:H:76:VAL:HG22	2:H:82:MET:HE3	2.00	0.41
2:H:155:SER:OG	2:H:304:THR:HG23	2.21	0.41
1:I:83:TRP:CE2	1:I:123:ARG:HG2	2.55	0.41
1:I:223:TYR:CE1	1:I:256:PHE:HB3	2.55	0.41
6:P:354:LEU:HB3	6:Q:354:LEU:HD11	2.03	0.41
6:Q:345:GLU:O	6:Q:348:MET:HG2	2.21	0.41
9:V:10:LYS:HB2	9:V:176:PHE:CE2	2.55	0.41
13:f:561:GLU:HG2	13:f:596:HIS:HB2	2.02	0.41
13:f:589:ASN:HA	13:f:592:PHE:CE2	2.56	0.41
13:f:628:PRO:HA	13:f:633:CYS:HB2	2.02	0.41
13:f:735:LEU:HD22	13:f:816:ILE:HG23	2.01	0.41
14:h:348:VAL:HB	14:h:360:TRP:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:h:546:MET:HB2	14:h:548:ARG:NE	2.36	0.41
13:m:396:LEU:HD22	13:m:401:LEU:HD11	2.01	0.41
13:m:743:ILE:HA	13:m:746:LEU:HB3	2.03	0.41
13:m:846:LYS:HD3	13:m:846:LYS:HA	1.82	0.41
13:n:365:ARG:NH2	13:n:429:LYS:HB2	2.35	0.41
1:A:221:ALA:O	1:A:255:ARG:HG3	2.20	0.41
1:E:99:LEU:O	1:E:101:THR:HG23	2.21	0.41
1:F:319:LYS:HB3	1:F:320:LYS:NZ	2.36	0.41
1:G:223:TYR:CZ	1:G:256:PHE:HB3	2.56	0.41
3:J:54:VAL:HG11	3:J:71:PHE:CG	2.56	0.41
6:P:97:VAL:HG22	6:P:98:LYS:H	1.86	0.41
6:P:175:LEU:HD13	10:Z:1268:HIS:HB3	2.01	0.41
11:Y:294:PRO:HG3	11:Y:302:LYS:HD2	2.03	0.41
10:Z:1268:HIS:O	10:Z:1269:ARG:NH2	2.54	0.41
13:f:578:ALA:HA	13:f:581:MET:CG	2.51	0.41
13:f:706:VAL:HA	13:f:709:ARG:HD3	2.02	0.41
13:m:112:LYS:H	13:m:142:GLU:C	2.29	0.41
13:n:462:ARG:NH1	13:n:538:VAL:HA	2.35	0.41
14:o:579:THR:HG21	14:o:584:GLU:HB2	2.01	0.41
1:B:9:ASN:ND2	13:n:247:SER:OG	2.50	0.41
1:C:141:MET:HB2	1:C:144:VAL:HG12	2.03	0.41
3:J:88:ARG:NH1	3:J:117:SER:OG	2.47	0.41
4:K:225:ALA:O	4:K:229:ILE:HG12	2.20	0.41
6:Q:354:LEU:HD13	7:R:126:LEU:HD21	2.01	0.41
11:Y:30:CYS:HB3	11:Y:35:GLU:O	2.19	0.41
13:f:264:ARG:HD3	13:f:277:PHE:CB	2.50	0.41
13:f:484:LEU:HB3	13:f:516:ASP:HB3	2.01	0.41
13:f:516:ASP:O	13:f:520:ILE:HG13	2.21	0.41
14:h:406:LYS:HA	14:h:423:GLU:HA	2.02	0.41
13:m:165:ILE:CA	13:m:171:ALA:H	2.34	0.41
13:m:775:TYR:HB3	13:m:776:PRO:HD3	2.03	0.41
13:n:563:ARG:HB3	13:n:567:ARG:HH21	1.85	0.41
1:C:200:LYS:O	1:D:117:PRO:HA	2.21	0.41
1:E:227:ASN:HB3	1:E:230:LYS:HG2	2.03	0.41
1:I:324:LYS:NZ	1:I:325:ASP:OD2	2.39	0.41
1:I:371:ILE:HG13	1:I:372:HIS:N	2.36	0.41
3:J:279:SER:HB2	3:J:282:THR:HG23	2.03	0.41
4:K:154:ILE:N	4:K:179:PHE:O	2.42	0.41
13:f:560:VAL:O	13:f:564:ILE:HG12	2.20	0.41
13:f:627:TYR:OH	13:f:636:SER:HB3	2.21	0.41
14:o:445:ASN:ND2	14:o:460:CYS:SG	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:PRO:HD3	1:A:341:TRP:CE3	2.56	0.41
1:E:240:GLN:HA	1:E:250:GLU:HA	2.02	0.41
1:E:302:GLY:O	1:E:305:THR:OG1	2.36	0.41
1:F:194:LEU:O	1:F:198:LEU:HD23	2.20	0.41
1:F:253:PRO:HB2	1:F:257:ARG:NE	2.36	0.41
1:G:270:GLU:OE1	1:G:270:GLU:N	2.54	0.41
2:H:262:PHE:CZ	2:H:274:ILE:HD11	2.56	0.41
1:I:118:ARG:HG2	1:I:372:HIS:CE1	2.56	0.41
3:J:14:THR:OG1	3:J:87:ARG:NH1	2.53	0.41
3:J:44:LYS:HE2	3:J:51:PRO:HB3	2.03	0.41
5:L:104:PHE:HD2	5:L:119:VAL:HG21	1.85	0.41
5:L:150:SER:HB2	5:L:152:HIS:NE2	2.36	0.41
6:N:348:MET:HE2	10:Z:1134:LEU:HD23	2.02	0.41
11:Y:13:LEU:HD21	11:Y:19:LYS:HG3	2.02	0.41
11:Y:114:CYS:O	11:Y:116:TRP:N	2.45	0.41
10:Z:1169:GLN:HA	10:Z:1172:THR:HG22	2.02	0.41
13:e:21:VAL:HA	13:e:122:ALA:HB1	2.03	0.41
13:f:264:ARG:HD3	13:f:277:PHE:HB2	2.02	0.41
13:f:375:GLN:NE2	13:f:449:VAL:O	2.44	0.41
13:f:571:GLN:OE1	13:f:584:ILE:HB	2.21	0.41
13:f:607:GLN:HG2	13:f:611:ARG:NE	2.36	0.41
13:m:519:ALA:HB1	13:m:560:VAL:HG13	2.03	0.41
13:m:642:PRO:HB2	13:m:749:GLU:OE2	2.21	0.41
13:m:661:TYR:O	13:m:665:VAL:HG23	2.21	0.41
13:m:666:GLU:OE2	13:m:671:LYS:NZ	2.37	0.41
13:m:676:HIS:O	13:m:680:GLN:HG3	2.20	0.41
13:m:770:GLN:O	13:m:774:LEU:HG	2.20	0.41
13:n:287:ARG:O	13:n:291:LYS:HG3	2.20	0.41
13:n:540:LYS:O	13:n:544:GLU:HG2	2.21	0.41
13:n:597:ILE:O	13:n:601:ILE:HG13	2.21	0.41
14:o:317:ASN:OD1	14:o:318:MET:N	2.54	0.41
14:o:362:ASN:OD1	14:o:363:ARG:N	2.54	0.41
14:p:362:ASN:OD1	14:p:363:ARG:N	2.54	0.41
1:A:105:GLU:HG3	1:A:106:HIS:CD2	2.56	0.41
1:B:44:HIS:CD2	1:D:176:MET:HG3	2.56	0.41
1:C:13:VAL:HG21	1:C:345:SER:HA	2.02	0.41
1:E:122:GLU:HG2	1:E:368:ALA:HB1	2.02	0.41
1:F:231:ASP:HA	1:F:234:LEU:HG	2.03	0.41
2:H:264:PRO:O	2:H:268:GLY:N	2.53	0.41
1:I:370:SER:HA	1:I:373:ARG:HG2	2.03	0.41
3:J:44:LYS:HZ1	3:J:49:PRO:C	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:123:ASP:HA	5:L:128:PHE:HA	2.03	0.41
6:M:344:HIS:CD2	7:O:113:SER:HB3	2.55	0.41
6:N:326:ILE:HB	7:O:101:LEU:HD21	2.02	0.41
6:P:322:ARG:NE	6:P:322:ARG:HA	2.36	0.41
9:V:123:LYS:NZ	11:Y:300:SER:H	2.19	0.41
13:f:335:LEU:HD11	13:f:367:ILE:HB	2.03	0.41
13:f:563:ARG:HD2	13:f:563:ARG:HA	1.94	0.41
13:f:621:ASP:HA	13:f:624:LYS:HD2	2.02	0.41
13:f:777:PHE:O	13:f:781:LEU:HG	2.20	0.41
14:h:500:SER:HB2	14:h:527:VAL:HG13	2.03	0.41
13:n:674:GLU:HA	13:n:679:GLY:HA3	2.03	0.41
13:n:755:TRP:CH2	14:p:452:GLU:C	2.95	0.41
1:B:112:GLU:OE1	1:B:121:ARG:HG2	2.20	0.40
1:B:329:ARG:HG3	6:P:89:GLU:OE2	2.21	0.40
1:C:280:VAL:HG11	1:C:321:LEU:HG	2.03	0.40
1:D:88:ARG:HA	1:D:91:GLN:HG2	2.04	0.40
1:F:261:LEU:HA	1:F:267:LEU:HD12	2.03	0.40
1:G:157:VAL:HG22	1:G:299:VAL:HB	2.03	0.40
2:H:176:LEU:HD12	2:H:281:SER:HB3	2.03	0.40
1:I:99:LEU:O	1:I:101:THR:HG23	2.20	0.40
7:O:128:ARG:HA	7:O:131:GLN:NE2	2.36	0.40
9:V:99:VAL:HG12	9:V:101:ALA:H	1.86	0.40
10:Z:1243:LYS:HA	10:Z:1243:LYS:HD3	1.83	0.40
13:m:238:ASP:OD2	13:m:241:PHE:N	2.52	0.40
13:n:247:SER:O	13:n:251:ARG:HG3	2.21	0.40
13:n:480:ILE:O	13:n:484:LEU:HB2	2.21	0.40
13:n:527:TYR:O	13:n:531:LYS:HG2	2.21	0.40
14:o:337:SER:O	14:o:351:GLY:N	2.46	0.40
14:o:479:ILE:HD13	14:o:501:SER:HB2	2.01	0.40
14:o:536:HIS:HB3	14:o:539:LEU:HB3	2.04	0.40
1:B:10:GLN:NE2	1:B:26:ALA:HB3	2.36	0.40
1:B:356:MET:HE2	1:B:356:MET:HA	2.01	0.40
1:C:360:LYS:HB2	1:C:360:LYS:HE2	1.96	0.40
1:E:357:TRP:HZ3	1:E:359:SER:CA	2.32	0.40
1:F:121:ARG:HG2	1:F:371:ILE:HD12	2.02	0.40
1:G:89:ILE:O	1:G:93:VAL:HG23	2.20	0.40
1:G:145:LEU:O	1:G:343:GLY:HA3	2.22	0.40
1:I:257:ARG:HH21	3:J:389:SER:H	1.68	0.40
3:J:48:MET:HE1	3:J:52:ILE:N	2.36	0.40
3:J:377:TYR:CZ	3:J:381:THR:HG21	2.57	0.40
6:P:318:GLU:O	6:P:322:ARG:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:114:GLY:H	8:U:131:LEU:HD12	1.86	0.40
11:Y:362:THR:H	11:Y:414:THR:HG1	1.67	0.40
14:g:484:CYS:HA	14:g:497:PHE:HA	2.03	0.40
14:h:265:LEU:HD11	14:h:551:LEU:HD13	2.04	0.40
13:m:232:PHE:CE1	13:m:303:ILE:HD11	2.56	0.40
13:m:292:ARG:HH21	13:m:317:ASP:HA	1.87	0.40
13:m:673:TRP:O	13:m:679:GLY:HA3	2.21	0.40
13:n:272:LEU:HB2	13:n:341:LEU:CD2	2.51	0.40
13:n:666:GLU:HA	13:n:673:TRP:CG	2.56	0.40
14:p:343:PHE:HD2	14:p:396:HIS:CG	2.39	0.40
1:A:33:TYR:HB3	1:A:98:GLN:OE1	2.22	0.40
1:B:48:MET:HE2	1:D:148:TYR:CE1	2.56	0.40
1:C:159:ASP:HB3	1:C:166:HIS:CE1	2.57	0.40
1:D:46:ARG:HB2	1:F:174:PHE:CE2	2.56	0.40
1:D:48:MET:CE	1:F:147:LEU:HB2	2.50	0.40
1:D:183:ILE:HB	1:D:185:ILE:HG22	2.03	0.40
1:D:240:GLN:OE1	1:D:248:THR:HB	2.21	0.40
1:D:346:ILE:O	1:D:350:LEU:HG	2.21	0.40
1:D:350:LEU:HD21	13:m:314:VAL:HG12	2.03	0.40
2:H:62:ARG:HG2	2:H:67:LEU:HD11	2.04	0.40
4:K:277:TYR:HD2	4:K:278:LYS:O	2.04	0.40
6:P:320:ILE:HD12	7:R:86:PHE:CE2	2.57	0.40
6:Q:334:VAL:HG21	10:W:1127:SER:HB3	2.03	0.40
13:f:350:LEU:O	13:f:353:ILE:HB	2.22	0.40
13:f:564:ILE:HG21	13:f:591:LEU:HD22	2.03	0.40
13:m:483:VAL:HB	13:m:588:PHE:HD1	1.86	0.40
13:m:602:ARG:HD2	13:m:602:ARG:HA	1.73	0.40
13:n:223:ARG:HE	13:n:223:ARG:HB2	1.73	0.40
13:n:513:ASP:OD1	13:n:514:ALA:N	2.54	0.40
14:p:445:ASN:ND2	14:p:460:CYS:SG	2.94	0.40
1:A:65:HIS:ND1	1:C:171:TYR:OH	2.30	0.40
1:B:84:ASN:O	1:B:88:ARG:HG3	2.22	0.40
1:C:83:TRP:CD2	1:C:123:ARG:HG2	2.56	0.40
1:E:48:MET:HE1	1:G:153:THR:CB	2.50	0.40
1:F:38:TYR:CG	1:F:71:ILE:HD11	2.57	0.40
1:G:92:TYR:HA	1:G:95:SER:HB2	2.03	0.40
2:H:15:GLY:N	16:H:401:ATP:O1B	2.55	0.40
2:H:261:LEU:HD23	2:H:274:ILE:HD13	2.03	0.40
1:I:371:ILE:O	1:I:375:THR:OG1	2.34	0.40
4:K:195:GLN:OE1	4:K:207:VAL:HG12	2.21	0.40
5:L:33:PRO:HA	5:L:36:CYS:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:18:ASP:OD1	6:M:18:ASP:N	2.54	0.40
6:P:310:GLN:HB3	7:R:83:LYS:HZ1	1.86	0.40
8:U:145:GLY:HA3	8:U:150:ARG:HH11	1.86	0.40
9:V:152:LEU:HG	9:V:153:PHE:H	1.85	0.40
13:e:435:ARG:HA	13:e:447:LYS:CA	2.51	0.40
13:f:583:ARG:HD2	14:h:559:GLU:HG2	2.04	0.40
13:f:657:GLN:HG3	14:h:504:TRP:CE3	2.57	0.40
14:h:474:GLY:HA3	14:h:509:TRP:CH2	2.55	0.40
14:h:556:ASN:OD1	14:h:613:ARG:NH2	2.44	0.40
13:m:380:LEU:O	13:m:384:ILE:HG13	2.21	0.40
13:m:797:GLU:HB2	13:m:798:ARG:HE	1.87	0.40
13:m:801:ILE:O	13:m:805:VAL:HG22	2.22	0.40
14:o:349:VAL:HG11	14:o:398:LEU:HD11	2.03	0.40
14:p:317:ASN:OD1	14:p:318:MET:N	2.54	0.40
14:p:426:HIS:CG	14:p:427:LYS:H	2.40	0.40
1:A:104:GLU:CD	1:A:133:ASN:HD21	2.29	0.40
1:B:38:TYR:OH	1:B:63:GLU:OE1	2.38	0.40
1:B:253:PRO:HA	1:B:256:PHE:CE2	2.56	0.40
1:C:371:ILE:HD12	1:C:371:ILE:HA	1.95	0.40
1:D:194:LEU:O	1:D:198:LEU:HD23	2.21	0.40
1:D:263:PHE:CE2	1:D:313:ARG:HG2	2.57	0.40
1:D:284:GLN:NE2	1:D:285:LYS:HG3	2.36	0.40
1:E:139:ILE:HG12	1:E:371:ILE:HD11	2.04	0.40
1:E:333:PRO:O	1:E:336:ARG:HG3	2.20	0.40
1:F:13:VAL:HG21	1:F:345:SER:HA	2.03	0.40
1:F:112:GLU:C	1:F:142:GLN:HE22	2.29	0.40
1:G:48:MET:HE1	1:I:148:TYR:CE2	2.57	0.40
1:G:138:PHE:CE2	1:G:140:SER:HB2	2.57	0.40
2:H:47:MET:HE3	3:J:361:PHE:HE1	1.86	0.40
2:H:62:ARG:HH12	2:H:208:ILE:HD11	1.87	0.40
3:J:315:PHE:HD1	3:J:316:LEU:HD22	1.87	0.40
4:K:258:LEU:HD23	4:K:259:ARG:HB2	2.03	0.40
6:M:337:LEU:HD12	7:O:103:GLN:HE22	1.86	0.40
6:M:378:VAL:O	6:M:382:MET:HG2	2.21	0.40
6:Q:156:LEU:HD12	6:Q:159:LEU:HD12	2.03	0.40
8:U:54:ASN:OD1	8:U:84:ILE:HG21	2.21	0.40
8:U:61:LEU:HB2	8:U:95:TYR:CD2	2.57	0.40
11:Y:85:THR:HG22	11:Y:109:LEU:HD11	2.04	0.40
10:Z:1115:GLU:HA	10:Z:1118:VAL:HG22	2.03	0.40
12:a:129:ALA:HB3	12:b:129:ALA:HB3	2.03	0.40
13:e:349:GLU:O	13:e:353:ILE:N	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:f:266:PRO:HB2	13:f:379:ARG:HG3	2.02	0.40
13:f:275:ILE:HG23	13:f:336:MET:SD	2.62	0.40
13:f:402:MET:HE2	13:f:531:LYS:N	2.37	0.40
13:f:810:LYS:HE3	13:f:810:LYS:HB2	1.87	0.40
14:h:336:MET:HE1	14:h:352:THR:C	2.46	0.40
14:h:458:THR:OG1	14:h:469:SER:HB2	2.22	0.40
13:m:341:LEU:O	13:m:345:LEU:HG	2.22	0.40
13:m:361:PHE:O	13:m:365:ARG:HG3	2.20	0.40
13:m:622:LYS:HE3	13:m:622:LYS:HB2	1.76	0.40
13:m:653:GLN:HE22	13:m:656:ARG:HH22	1.68	0.40
13:n:228:LYS:HG2	13:n:230:THR:H	1.87	0.40
13:n:477:ARG:NH1	13:n:478:ALA:HB2	2.35	0.40
13:n:748:LYS:NZ	14:p:353:TYR:CE1	2.90	0.40
14:p:349:VAL:HG11	14:p:398:LEU:HD11	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	368/376 (98%)	359 (98%)	9 (2%)	0	100	100
1	B	368/376 (98%)	355 (96%)	13 (4%)	0	100	100
1	C	373/376 (99%)	362 (97%)	11 (3%)	0	100	100
1	D	368/376 (98%)	356 (97%)	12 (3%)	0	100	100
1	E	368/376 (98%)	356 (97%)	12 (3%)	0	100	100
1	F	368/376 (98%)	357 (97%)	11 (3%)	0	100	100
1	G	368/376 (98%)	357 (97%)	11 (3%)	0	100	100
1	I	368/376 (98%)	354 (96%)	14 (4%)	0	100	100
2	H	368/375 (98%)	357 (97%)	11 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	J	377/417 (90%)	365 (97%)	12 (3%)	0	100	100
4	K	276/286 (96%)	268 (97%)	8 (3%)	0	100	100
5	L	267/272 (98%)	259 (97%)	6 (2%)	2 (1%)	18	56
6	M	330/405 (82%)	311 (94%)	18 (6%)	1 (0%)	36	72
6	N	270/405 (67%)	262 (97%)	7 (3%)	1 (0%)	30	67
6	P	319/405 (79%)	312 (98%)	7 (2%)	0	100	100
6	Q	335/405 (83%)	318 (95%)	17 (5%)	0	100	100
7	O	177/186 (95%)	165 (93%)	12 (7%)	0	100	100
7	R	168/186 (90%)	160 (95%)	8 (5%)	0	100	100
8	U	165/190 (87%)	157 (95%)	8 (5%)	0	100	100
9	V	177/182 (97%)	172 (97%)	5 (3%)	0	100	100
10	W	144/1281 (11%)	138 (96%)	5 (4%)	1 (1%)	18	56
10	Z	190/1281 (15%)	184 (97%)	6 (3%)	0	100	100
11	Y	404/467 (86%)	374 (93%)	25 (6%)	5 (1%)	10	44
12	a	102/913 (11%)	100 (98%)	2 (2%)	0	100	100
12	b	101/913 (11%)	101 (100%)	0	0	100	100
13	e	792/4646 (17%)	745 (94%)	45 (6%)	2 (0%)	36	72
13	f	804/4646 (17%)	763 (95%)	39 (5%)	2 (0%)	43	78
13	m	786/4646 (17%)	759 (97%)	26 (3%)	1 (0%)	48	83
13	n	747/4646 (16%)	721 (96%)	25 (3%)	1 (0%)	48	83
14	g	356/612 (58%)	353 (99%)	3 (1%)	0	100	100
14	h	356/612 (58%)	346 (97%)	10 (3%)	0	100	100
14	o	356/612 (58%)	349 (98%)	7 (2%)	0	100	100
14	p	356/612 (58%)	350 (98%)	6 (2%)	0	100	100
All	All	11672/32609 (36%)	11245 (96%)	411 (4%)	16 (0%)	49	83

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	L	161	SER
5	L	162	GLY
6	M	217	PRO
10	W	1142	PRO
11	Y	175	PRO

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Mol	Chain	Res	Type
11	Y	294	PRO
11	Y	441	PRO
13	f	38	VAL
13	f	203	PRO
11	Y	296	PHE
13	n	21	VAL
13	e	726	ARG
13	m	210	HIS
6	N	163	ASP
13	e	732	VAL
11	Y	77	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	315/324 (97%)	315 (100%)	0	100	100
1	B	318/324 (98%)	318 (100%)	0	100	100
1	C	323/324 (100%)	323 (100%)	0	100	100
1	D	318/324 (98%)	318 (100%)	0	100	100
1	E	318/324 (98%)	318 (100%)	0	100	100
1	F	318/324 (98%)	318 (100%)	0	100	100
1	G	318/324 (98%)	318 (100%)	0	100	100
1	I	314/324 (97%)	314 (100%)	0	100	100
2	H	313/318 (98%)	313 (100%)	0	100	100
3	J	323/363 (89%)	321 (99%)	2 (1%)	78	83
4	K	247/254 (97%)	247 (100%)	0	100	100
5	L	237/241 (98%)	237 (100%)	0	100	100
6	M	164/346 (47%)	164 (100%)	0	100	100
6	N	112/346 (32%)	112 (100%)	0	100	100
6	P	197/346 (57%)	197 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	Q	192/346 (56%)	192 (100%)	0	100	100
7	O	87/160 (54%)	87 (100%)	0	100	100
7	R	67/160 (42%)	67 (100%)	0	100	100
8	U	129/163 (79%)	129 (100%)	0	100	100
9	V	121/163 (74%)	121 (100%)	0	100	100
10	W	53/1078 (5%)	53 (100%)	0	100	100
10	Z	154/1078 (14%)	154 (100%)	0	100	100
11	Y	274/416 (66%)	268 (98%)	6 (2%)	45	64
13	e	230/4122 (6%)	230 (100%)	0	100	100
13	f	718/4122 (17%)	717 (100%)	1 (0%)	88	89
13	m	538/4122 (13%)	538 (100%)	0	100	100
13	n	504/4122 (12%)	502 (100%)	2 (0%)	84	84
14	h	309/535 (58%)	308 (100%)	1 (0%)	86	86
14	o	309/535 (58%)	309 (100%)	0	100	100
14	p	309/535 (58%)	309 (100%)	0	100	100
All	All	8129/26463 (31%)	8117 (100%)	12 (0%)	87	89

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	J	27	CYS
3	J	37	CYS
11	Y	51	CYS
11	Y	70	CYS
11	Y	111	CYS
11	Y	284	CYS
11	Y	287	CYS
11	Y	294	PRO
13	f	213	ILE
14	h	393	GLN
13	n	685	ASP
13	n	704	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	284	GLN
1	B	10	GLN
1	B	116	ASN
1	B	120	ASN
1	C	166	HIS
1	C	276	HIS
1	C	284	GLN
1	D	9	ASN
1	D	120	ASN
1	D	133	ASN
1	D	284	GLN
1	D	334	GLN
1	E	77	HIS
1	E	142	GLN
1	E	276	HIS
1	F	9	ASN
1	F	77	HIS
1	G	29	GLN
1	G	284	GLN
2	H	49	GLN
2	H	87	HIS
2	H	137	GLN
1	I	116	ASN
1	I	142	GLN
1	I	276	HIS
3	J	182	GLN
4	K	92	ASN
4	K	161	HIS
4	K	167	ASN
4	K	205	GLN
5	L	45	GLN
5	L	178	GLN
6	M	379	GLN
6	N	344	HIS
6	N	352	GLN
6	N	356	HIS
6	N	392	ASN
6	N	395	ASN
7	O	103	GLN
7	O	155	ASN
6	P	361	GLN
6	Q	150	GLN

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Mol	Chain	Res	Type
6	Q	346	GLN
8	U	153	GLN
10	W	1114	HIS
10	W	1276	GLN
11	Y	81	HIS
10	Z	1199	GLN
13	e	799	ASN
13	e	842	ASN
13	f	215	ASN
13	f	257	GLN
13	f	752	ASN
13	f	770	GLN
13	f	773	GLN
13	f	799	ASN
14	h	356	GLN
14	h	397	ASN
14	h	426	HIS
14	h	446	ASN
13	m	210	HIS
13	m	250	ASN
13	m	475	GLN
13	m	589	ASN
13	m	605	GLN
13	m	657	GLN
13	n	246	GLN
13	n	250	ASN
13	n	431	GLN
13	n	475	GLN
13	n	487	GLN
13	n	607	GLN
13	n	676	HIS
13	n	769	HIS
13	n	799	ASN
13	n	842	ASN
14	o	330	HIS
14	o	419	GLN
14	o	462	HIS
14	o	593	GLN
14	p	268	ASN
14	p	330	HIS
14	p	419	GLN
14	p	462	HIS

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Mol	Chain	Res	Type
14	p	593	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 3 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	G	800	-	28,29,29	1.39	4 (14%)	43,45,45	1.84	8 (18%)
15	ADP	I	800	-	28,29,29	1.40	4 (14%)	43,45,45	1.88	10 (23%)
15	ADP	B	800	-	28,29,29	1.39	4 (14%)	43,45,45	1.83	9 (20%)
15	ADP	C	800	-	28,29,29	1.38	4 (14%)	43,45,45	1.79	8 (18%)
15	ADP	F	800	-	28,29,29	1.39	4 (14%)	43,45,45	1.82	9 (20%)
15	ADP	D	800	-	28,29,29	1.42	4 (14%)	43,45,45	1.84	9 (20%)
16	ATP	H	401	-	32,33,33	0.36	0	48,52,52	0.31	0
15	ADP	A	800	-	28,29,29	1.40	4 (14%)	43,45,45	1.83	8 (18%)
15	ADP	J	800	-	28,29,29	1.43	5 (17%)	43,45,45	1.85	9 (20%)
15	ADP	E	800	-	28,29,29	1.39	4 (14%)	43,45,45	1.83	9 (20%)

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	G	800	-	-	0/16/32/32	0/3/3/3
15	ADP	I	800	-	-	3/16/32/32	0/3/3/3
15	ADP	B	800	-	-	0/16/32/32	0/3/3/3
15	ADP	C	800	-	-	3/16/32/32	0/3/3/3
15	ADP	F	800	-	-	8/16/32/32	0/3/3/3
15	ADP	D	800	-	-	5/16/32/32	0/3/3/3
16	ATP	H	401	-	-	10/22/38/38	0/3/3/3
15	ADP	A	800	-	-	1/16/32/32	0/3/3/3
15	ADP	J	800	-	-	7/16/32/32	0/3/3/3
15	ADP	E	800	-	-	2/16/32/32	0/3/3/3

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	I	800	ADP	C5-C4	4.69	1.47	1.39
15	A	800	ADP	C5-C4	4.69	1.47	1.39
15	J	800	ADP	C5-C4	4.66	1.47	1.39
15	C	800	ADP	C5-C4	4.63	1.47	1.39
15	B	800	ADP	C5-C4	4.63	1.47	1.39
15	E	800	ADP	C5-C4	4.62	1.47	1.39
15	G	800	ADP	C5-C4	4.62	1.47	1.39
15	D	800	ADP	C5-C4	4.61	1.47	1.39
15	F	800	ADP	C5-C4	4.59	1.47	1.39
15	D	800	ADP	C5-C6	2.68	1.48	1.41
15	J	800	ADP	C5-C6	2.66	1.48	1.41
15	C	800	ADP	C5-C6	2.66	1.48	1.41
15	G	800	ADP	C5-C6	2.65	1.48	1.41
15	B	800	ADP	C5-C6	2.65	1.48	1.41
15	I	800	ADP	C5-C6	2.65	1.48	1.41
15	E	800	ADP	C5-C6	2.64	1.48	1.41
15	F	800	ADP	C5-C6	2.64	1.48	1.41
15	A	800	ADP	C5-C6	2.63	1.48	1.41
15	D	800	ADP	C5-N7	-2.38	1.34	1.39
15	B	800	ADP	C5-N7	-2.37	1.34	1.39
15	E	800	ADP	C5-N7	-2.37	1.34	1.39
15	G	800	ADP	C5-N7	-2.36	1.34	1.39
15	F	800	ADP	C5-N7	-2.35	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	C	800	ADP	C5-N7	-2.33	1.34	1.39
15	I	800	ADP	C5-N7	-2.31	1.34	1.39
15	J	800	ADP	C5-N7	-2.31	1.34	1.39
15	J	800	ADP	C8-N7	2.30	1.36	1.31
15	A	800	ADP	C5-N7	-2.29	1.34	1.39
15	D	800	ADP	C8-N7	2.28	1.36	1.31
15	I	800	ADP	C8-N7	2.25	1.36	1.31
15	A	800	ADP	C8-N7	2.24	1.36	1.31
15	G	800	ADP	C8-N7	2.23	1.36	1.31
15	B	800	ADP	C8-N7	2.23	1.36	1.31
15	E	800	ADP	C8-N7	2.22	1.36	1.31
15	C	800	ADP	C8-N7	2.22	1.35	1.31
15	F	800	ADP	C8-N7	2.19	1.35	1.31
15	J	800	ADP	PA-O3A	2.18	1.61	1.59

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	800	ADP	C5-C4-N3	-5.96	118.51	126.72
15	D	800	ADP	C5-C4-N3	-5.95	118.52	126.72
15	I	800	ADP	C5-C4-N3	-5.93	118.55	126.72
15	B	800	ADP	C5-C4-N3	-5.89	118.60	126.72
15	E	800	ADP	C5-C4-N3	-5.88	118.62	126.72
15	J	800	ADP	C5-C4-N3	-5.88	118.63	126.72
15	G	800	ADP	C5-C4-N3	-5.86	118.64	126.72
15	C	800	ADP	C5-C4-N3	-5.86	118.65	126.72
15	F	800	ADP	C5-C4-N3	-5.83	118.69	126.72
15	I	800	ADP	N3-C4-N9	4.82	135.37	127.17
15	A	800	ADP	N3-C4-N9	4.79	135.32	127.17
15	F	800	ADP	N3-C4-N9	4.74	135.23	127.17
15	D	800	ADP	N3-C4-N9	4.73	135.22	127.17
15	B	800	ADP	N3-C4-N9	4.71	135.18	127.17
15	E	800	ADP	N3-C4-N9	4.70	135.16	127.17
15	G	800	ADP	N3-C4-N9	4.69	135.15	127.17
15	J	800	ADP	N3-C4-N9	4.68	135.12	127.17
15	C	800	ADP	N3-C4-N9	4.67	135.11	127.17
15	A	800	ADP	C2-N3-C4	3.70	120.88	111.83
15	J	800	ADP	C2-N3-C4	3.67	120.78	111.83
15	G	800	ADP	C2-N3-C4	3.66	120.78	111.83
15	I	800	ADP	C2-N3-C4	3.66	120.77	111.83
15	E	800	ADP	C2-N3-C4	3.65	120.73	111.83
15	F	800	ADP	C2-N3-C4	3.62	120.68	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	C	800	ADP	C2-N3-C4	3.62	120.66	111.83
15	D	800	ADP	C2-N3-C4	3.61	120.66	111.83
15	B	800	ADP	C2-N3-C4	3.60	120.63	111.83
15	B	800	ADP	C4-C5-N7	-3.42	106.68	110.58
15	G	800	ADP	C4-C5-N7	-3.40	106.70	110.58
15	I	800	ADP	C4-C5-N7	-3.40	106.70	110.58
15	E	800	ADP	C4-C5-N7	-3.39	106.70	110.58
15	D	800	ADP	C4-C5-N7	-3.36	106.74	110.58
15	J	800	ADP	C4-C5-N7	-3.36	106.74	110.58
15	A	800	ADP	C4-C5-N7	-3.35	106.75	110.58
15	C	800	ADP	C4-C5-N7	-3.34	106.76	110.58
15	F	800	ADP	C4-C5-N7	-3.33	106.77	110.58
15	J	800	ADP	N3-C2-N1	-3.18	123.78	128.58
15	G	800	ADP	N3-C2-N1	-3.13	123.85	128.58
15	I	800	ADP	N3-C2-N1	-3.10	123.89	128.58
15	A	800	ADP	N3-C2-N1	-3.09	123.90	128.58
15	E	800	ADP	N3-C2-N1	-3.07	123.94	128.58
15	C	800	ADP	N3-C2-N1	-3.03	123.99	128.58
15	F	800	ADP	N3-C2-N1	-3.03	124.00	128.58
15	D	800	ADP	N3-C2-N1	-2.94	124.13	128.58
15	B	800	ADP	N3-C2-N1	-2.92	124.16	128.58
15	I	800	ADP	C4-N9-C8	2.83	108.71	105.74
15	F	800	ADP	C4-N9-C8	2.79	108.67	105.74
15	B	800	ADP	C4-N9-C8	2.68	108.56	105.74
15	G	800	ADP	C4-N9-C8	2.67	108.55	105.74
15	A	800	ADP	C4-N9-C8	2.65	108.52	105.74
15	E	800	ADP	C4-N9-C8	2.63	108.50	105.74
15	D	800	ADP	C4-N9-C8	2.61	108.48	105.74
15	A	800	ADP	C2'-C1'-N9	-2.59	106.87	113.30
15	J	800	ADP	C4-N9-C8	2.56	108.43	105.74
15	C	800	ADP	C4-N9-C8	2.55	108.41	105.74
15	I	800	ADP	C5-N7-C8	2.54	107.44	103.45
15	G	800	ADP	C5-N7-C8	2.52	107.42	103.45
15	B	800	ADP	C5-N7-C8	2.51	107.40	103.45
15	E	800	ADP	C5-N7-C8	2.49	107.37	103.45
15	B	800	ADP	C2'-C1'-N9	-2.49	107.11	113.30
15	F	800	ADP	C5-N7-C8	2.45	107.30	103.45
15	J	800	ADP	C5-N7-C8	2.44	107.29	103.45
15	D	800	ADP	C2'-C1'-N9	-2.43	107.25	113.30
15	C	800	ADP	C5-N7-C8	2.43	107.27	103.45
15	D	800	ADP	C5-N7-C8	2.42	107.26	103.45
15	A	800	ADP	C5-N7-C8	2.42	107.25	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	E	800	ADP	C2'-C1'-N9	-2.37	107.42	113.30
15	I	800	ADP	C3'-C2'-C1'	2.32	105.86	101.46
15	G	800	ADP	C3'-C2'-C1'	2.26	105.75	101.46
15	F	800	ADP	C2'-C1'-N9	-2.26	107.69	113.30
15	C	800	ADP	C2'-C1'-N9	-2.19	107.85	113.30
15	B	800	ADP	C3'-C2'-C1'	2.18	105.59	101.46
15	F	800	ADP	C3'-C2'-C1'	2.18	105.58	101.46
15	I	800	ADP	C2'-C1'-N9	-2.16	107.94	113.30
15	E	800	ADP	C3'-C2'-C1'	2.10	105.43	101.46
15	J	800	ADP	C2'-C3'-C4'	2.08	106.63	102.61
15	J	800	ADP	C3'-C2'-C1'	2.06	105.36	101.46
15	D	800	ADP	C3'-C2'-C1'	2.03	105.31	101.46
15	I	800	ADP	N9-C8-N7	-2.02	111.08	113.94

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	C	800	ADP	C5'-O5'-PA-O3A
15	D	800	ADP	C5'-O5'-PA-O2A
15	D	800	ADP	C5'-O5'-PA-O3A
15	D	800	ADP	C3'-C4'-C5'-O5'
15	F	800	ADP	C5'-O5'-PA-O1A
15	F	800	ADP	C5'-O5'-PA-O2A
15	F	800	ADP	C5'-O5'-PA-O3A
15	I	800	ADP	C5'-O5'-PA-O1A
15	I	800	ADP	C5'-O5'-PA-O3A
15	J	800	ADP	PA-O3A-PB-O3B
15	J	800	ADP	C5'-O5'-PA-O1A
15	J	800	ADP	C5'-O5'-PA-O2A
15	J	800	ADP	C5'-O5'-PA-O3A
16	H	401	ATP	C5'-O5'-PA-O1A
16	H	401	ATP	C5'-O5'-PA-O2A
16	H	401	ATP	C5'-O5'-PA-O3A
15	J	800	ADP	C3'-C4'-C5'-O5'
16	H	401	ATP	O4'-C4'-C5'-O5'
15	D	800	ADP	O4'-C4'-C5'-O5'
15	J	800	ADP	O4'-C4'-C5'-O5'
16	H	401	ATP	C3'-C4'-C5'-O5'
15	F	800	ADP	O4'-C4'-C5'-O5'
15	F	800	ADP	C3'-C4'-C5'-O5'
15	D	800	ADP	PA-O3A-PB-O1B

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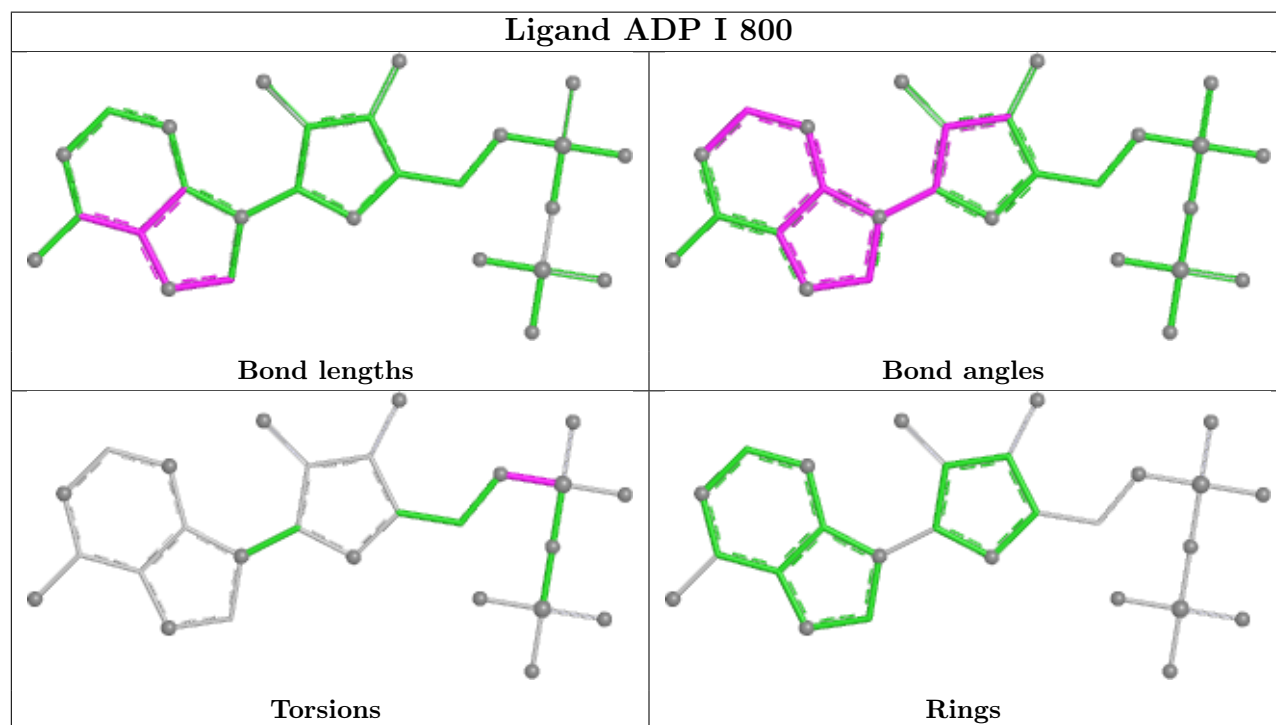
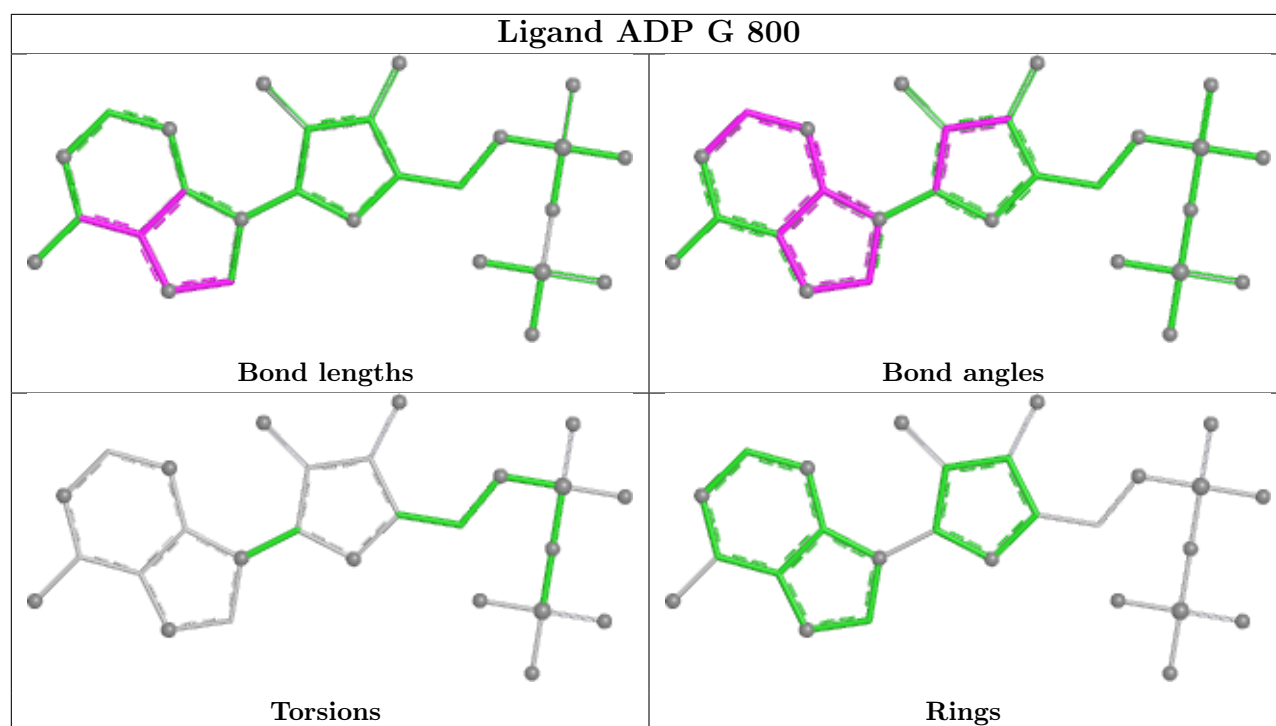
Mol	Chain	Res	Type	Atoms
16	H	401	ATP	PB-O3A-PA-O1A
16	H	401	ATP	PB-O3A-PA-O5'
15	C	800	ADP	C3'-C4'-C5'-O5'
15	C	800	ADP	C5'-O5'-PA-O1A
15	I	800	ADP	C5'-O5'-PA-O2A
15	J	800	ADP	PA-O3A-PB-O1B
16	H	401	ATP	PB-O3B-PG-O1G
15	F	800	ADP	PA-O3A-PB-O1B
15	E	800	ADP	PA-O3A-PB-O2B
15	F	800	ADP	PA-O3A-PB-O2B
15	F	800	ADP	PA-O3A-PB-O3B
16	H	401	ATP	PA-O3A-PB-O1B
15	A	800	ADP	O4'-C4'-C5'-O5'
15	E	800	ADP	O4'-C4'-C5'-O5'
16	H	401	ATP	PA-O3A-PB-O2B

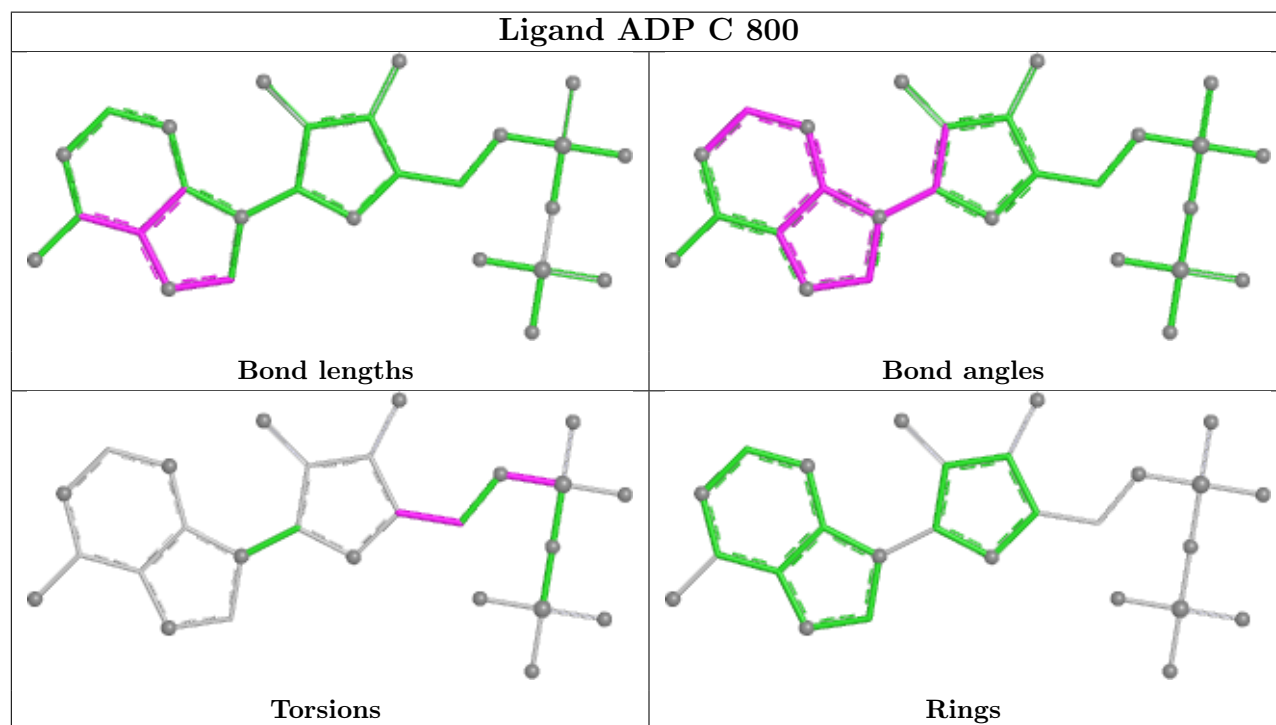
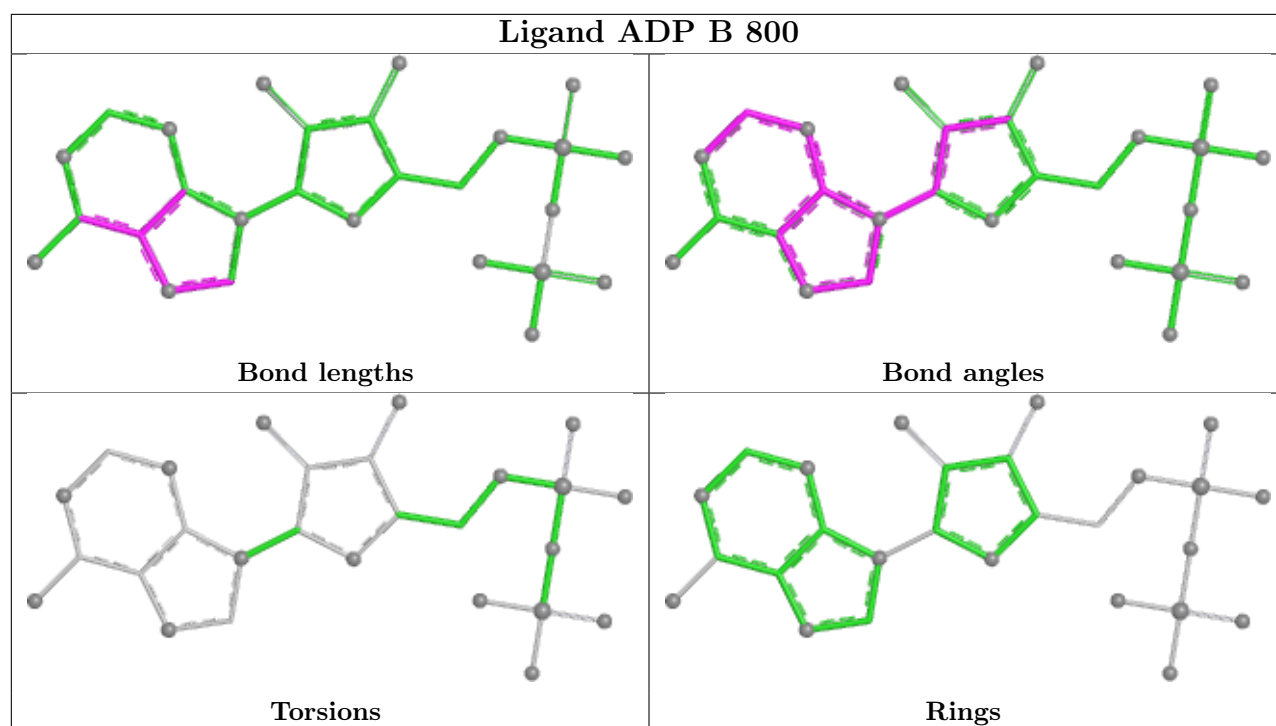
There are no ring outliers.

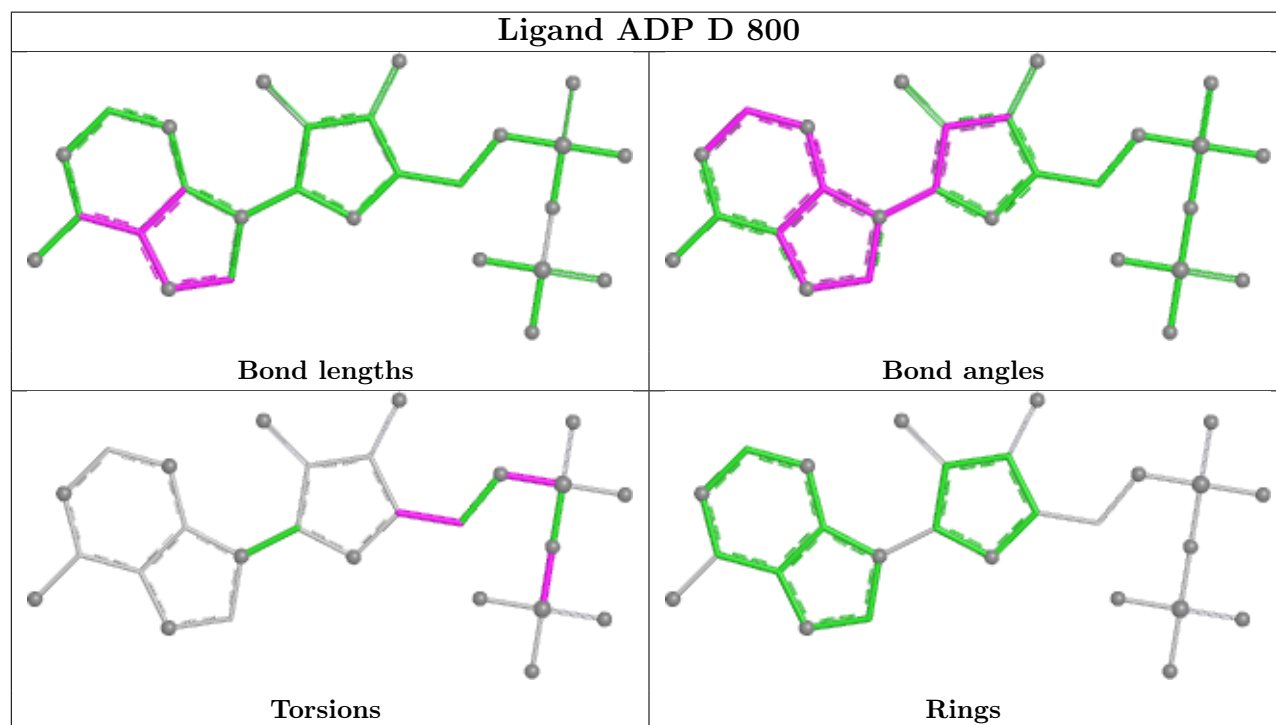
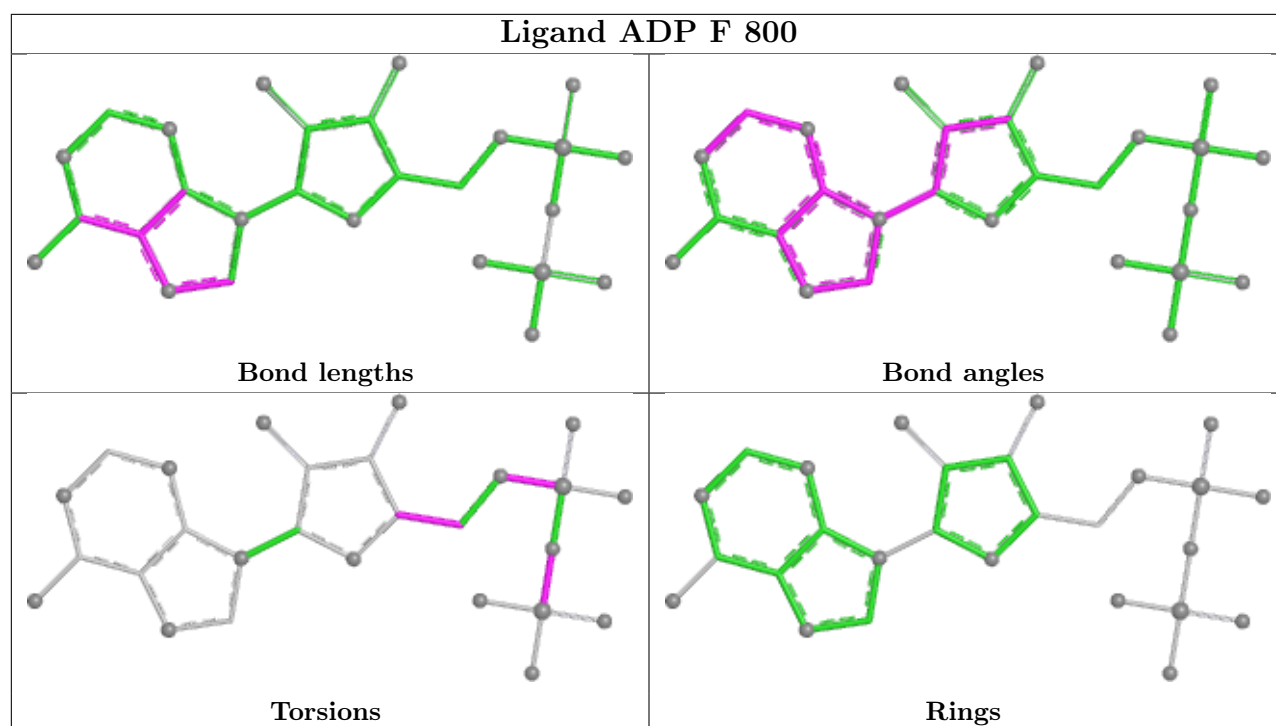
8 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	G	800	ADP	1	0
15	B	800	ADP	1	0
15	C	800	ADP	2	0
15	F	800	ADP	1	0
15	D	800	ADP	3	0
16	H	401	ATP	8	0
15	A	800	ADP	2	0
15	J	800	ADP	1	0

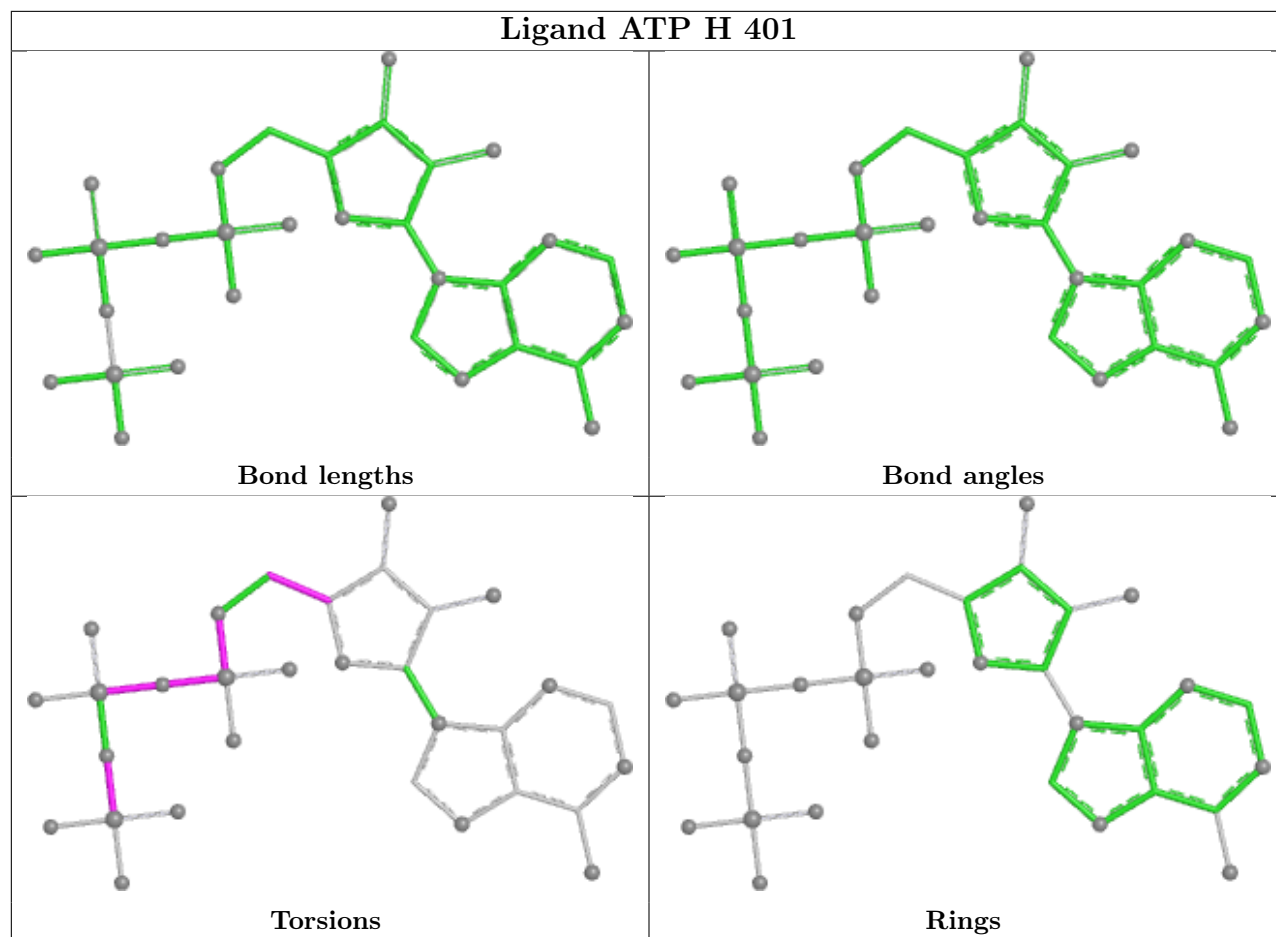
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



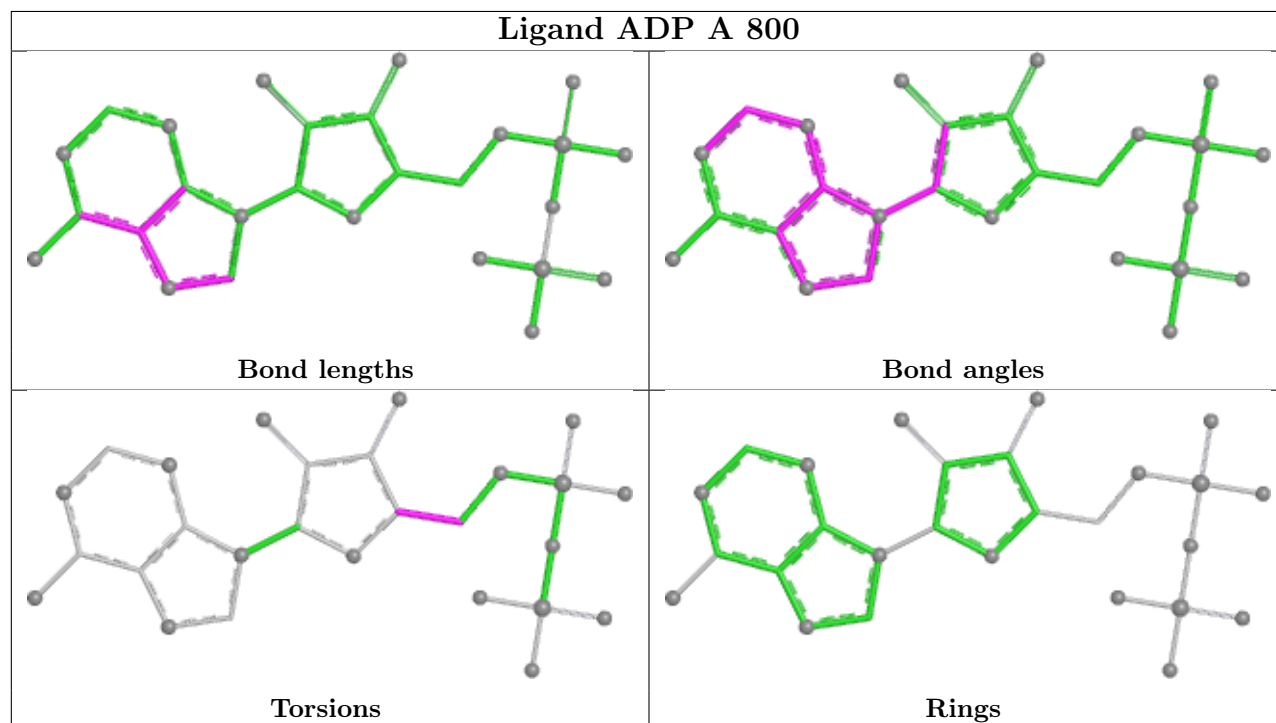


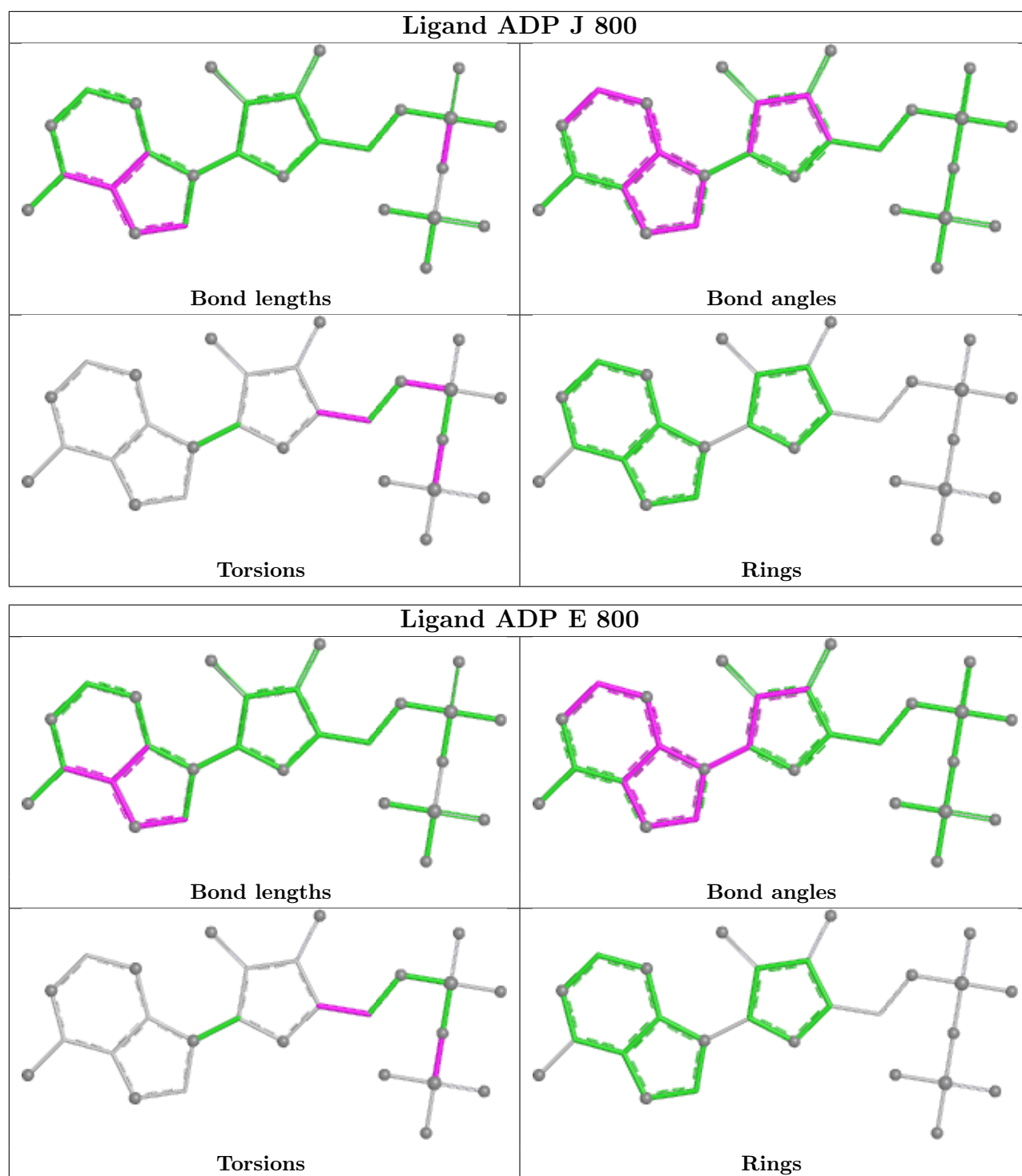


## Ligand ATP H 401



## Ligand ADP A 800





## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.



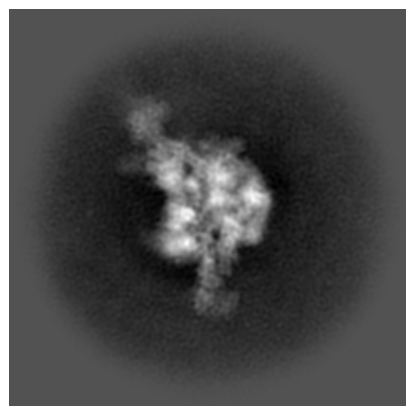
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46849. These allow visual inspection of the internal detail of the map and identification of artifacts.

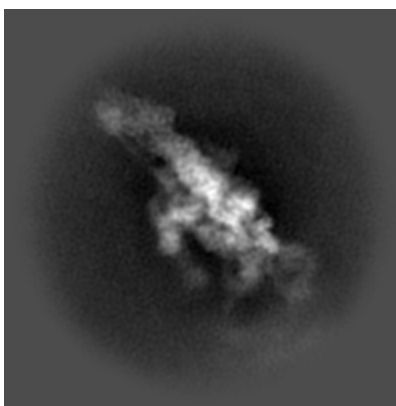
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

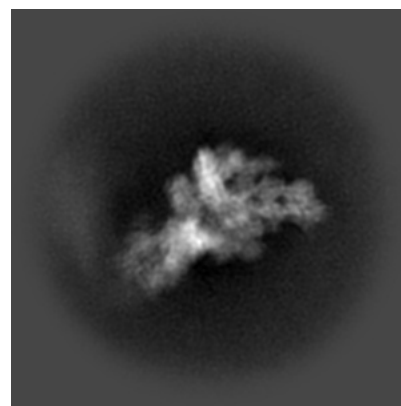
#### 6.1.1 Primary map



X

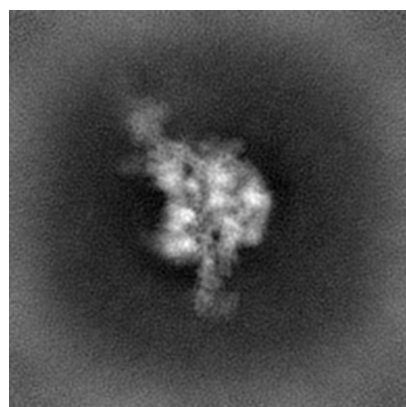


Y

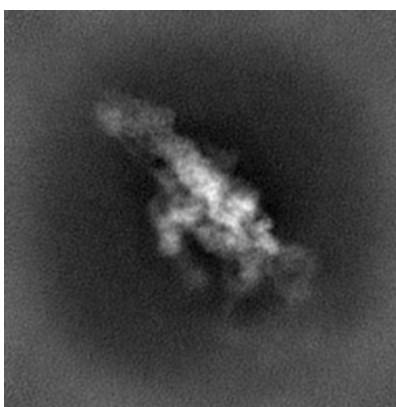


Z

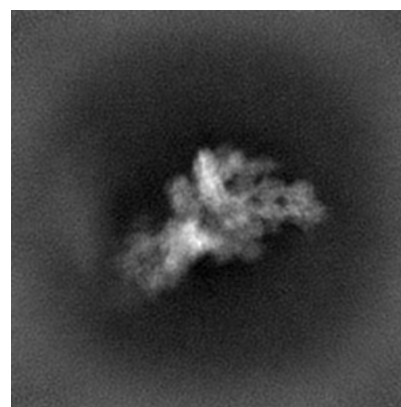
#### 6.1.2 Raw map



X



Y

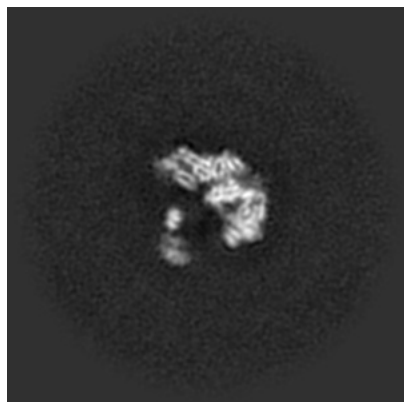


Z

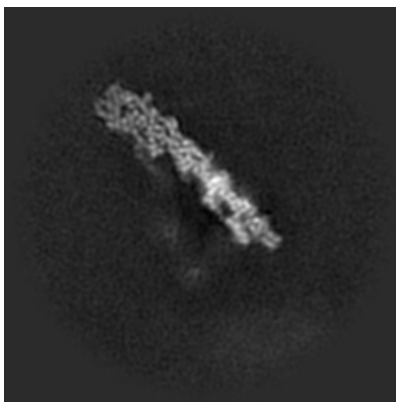
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

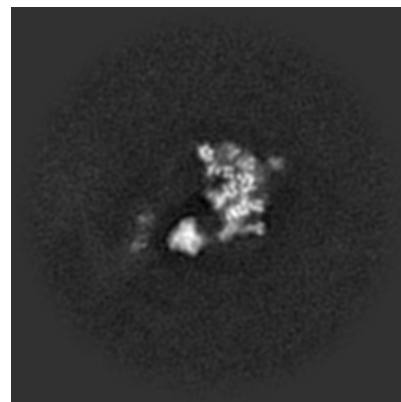
### 6.2.1 Primary map



X Index: 96

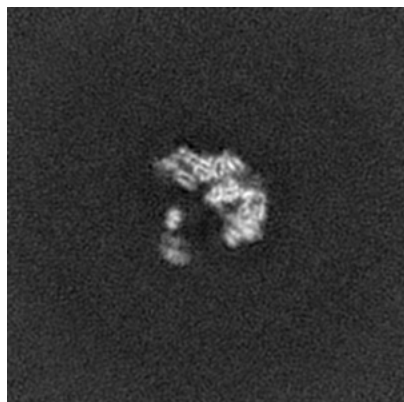


Y Index: 96

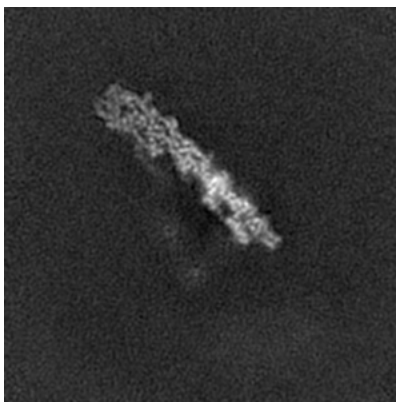


Z Index: 96

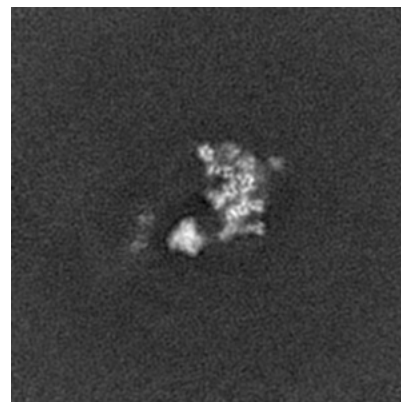
### 6.2.2 Raw map



X Index: 96



Y Index: 96

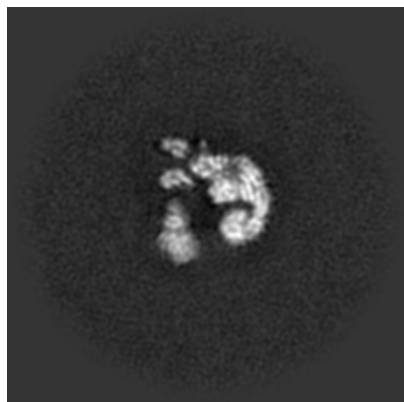


Z Index: 96

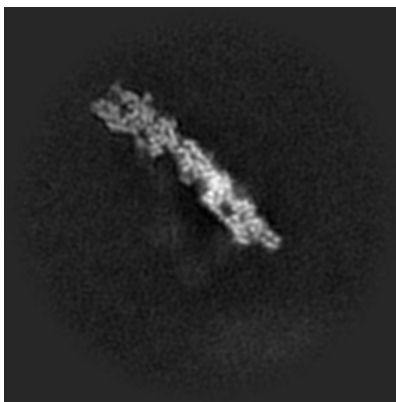
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

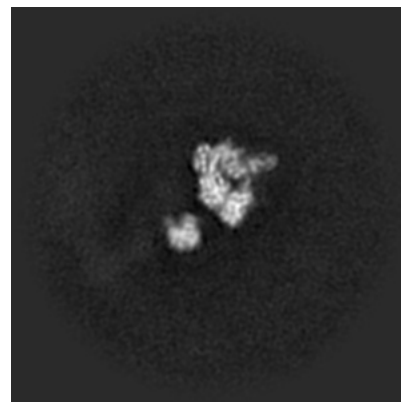
### 6.3.1 Primary map



X Index: 92

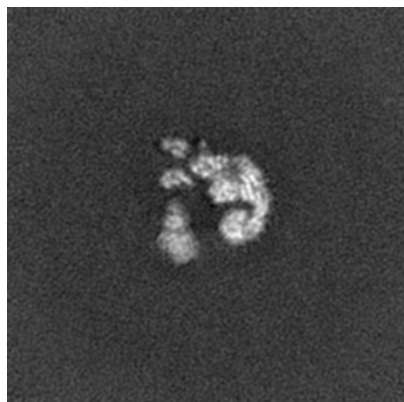


Y Index: 97

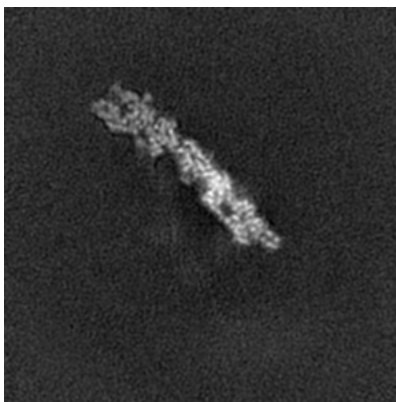


Z Index: 101

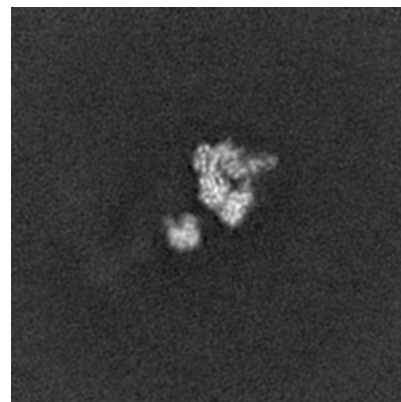
### 6.3.2 Raw map



X Index: 92



Y Index: 97

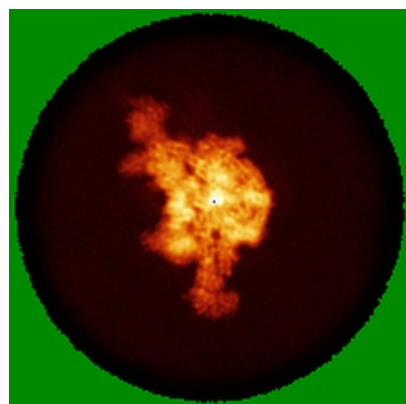


Z Index: 101

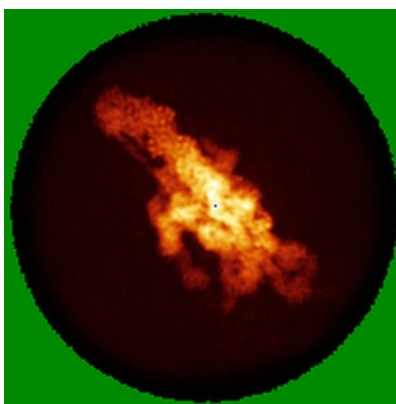
The images above show the largest variance slices of the map in three orthogonal directions.

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

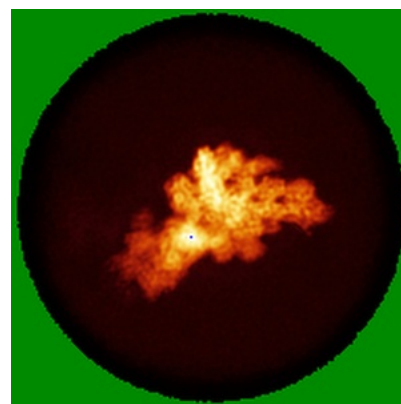
### 6.4.1 Primary map



X

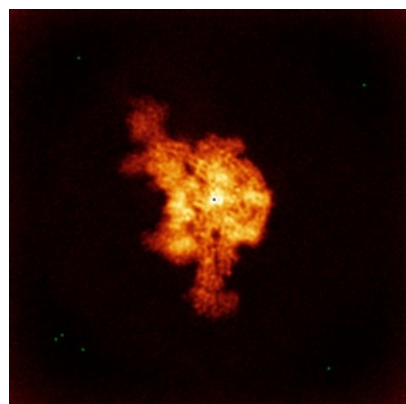


Y

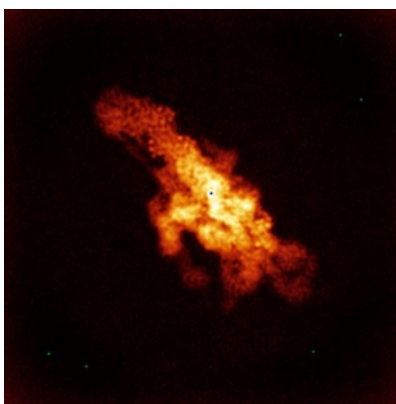


Z

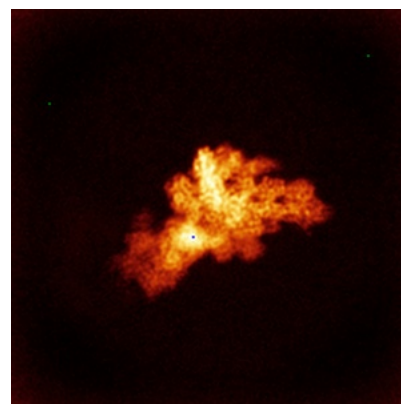
### 6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

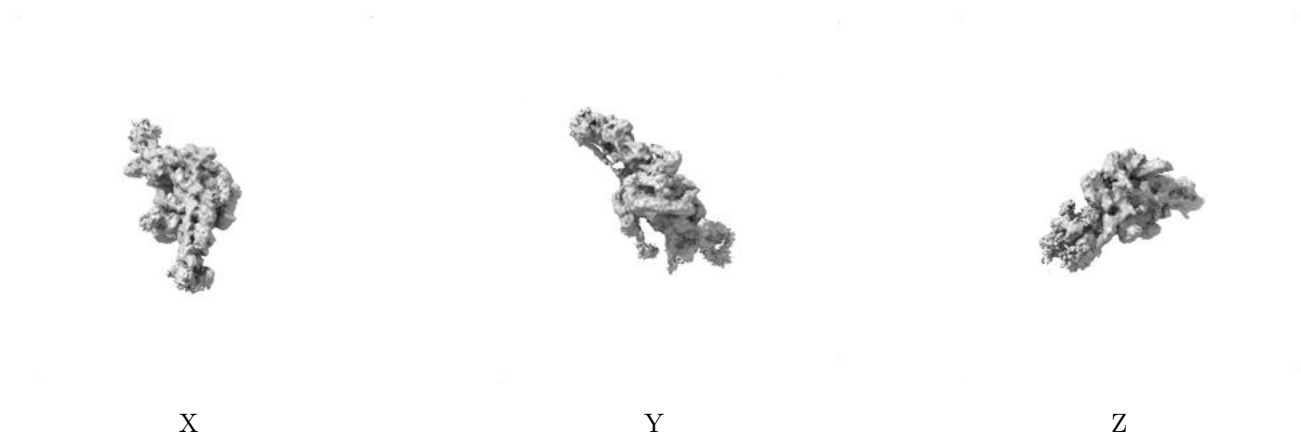
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

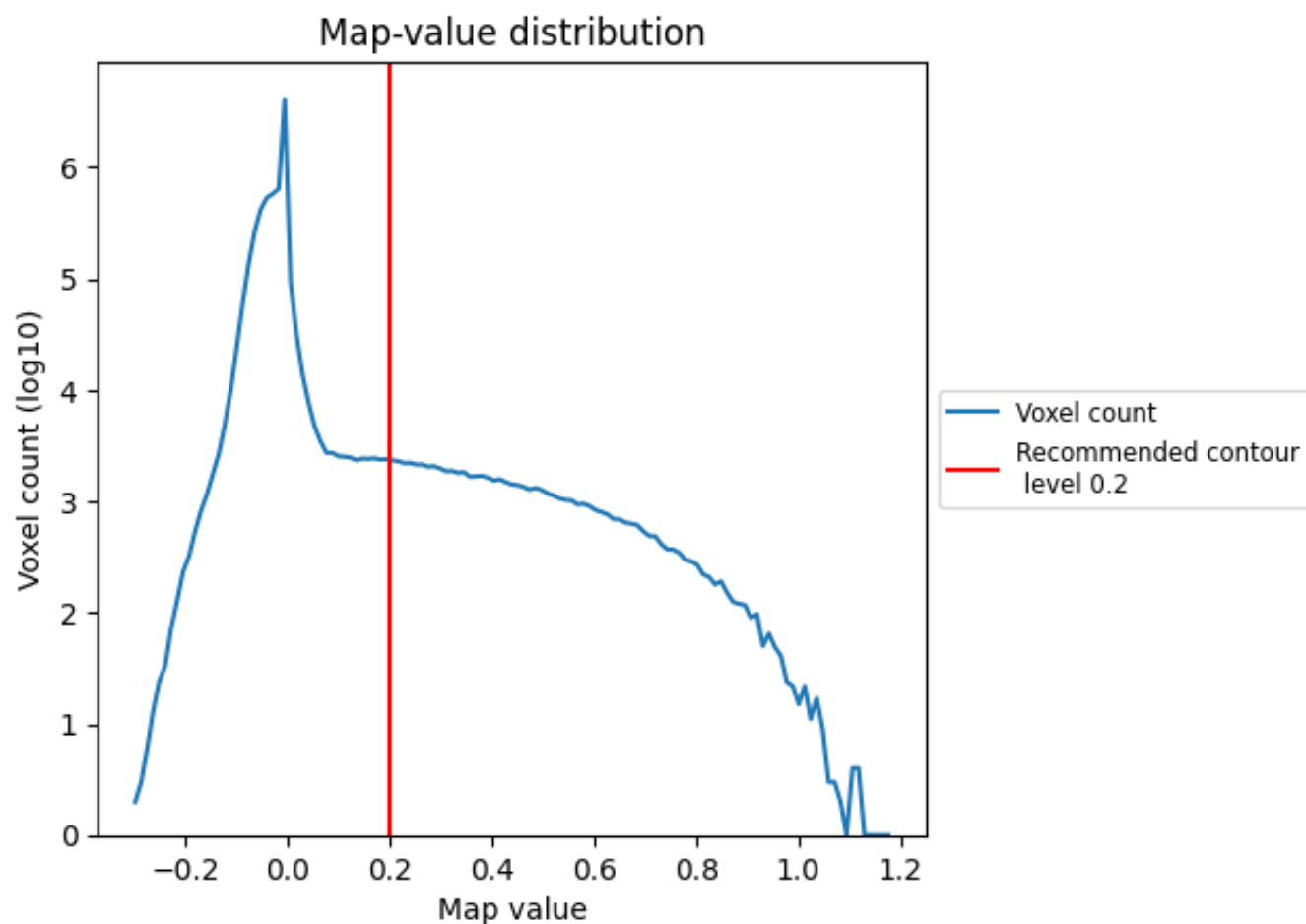
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

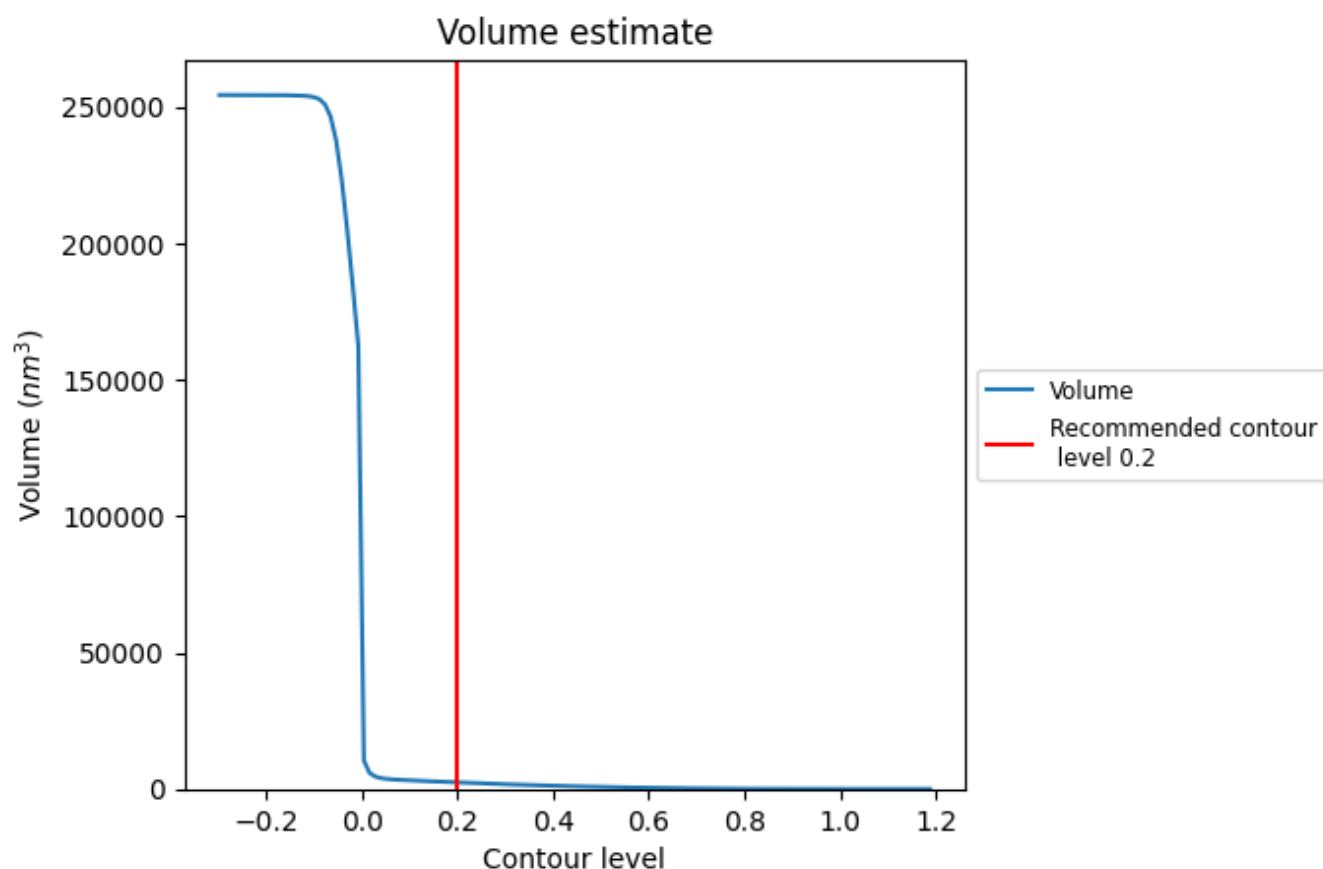
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

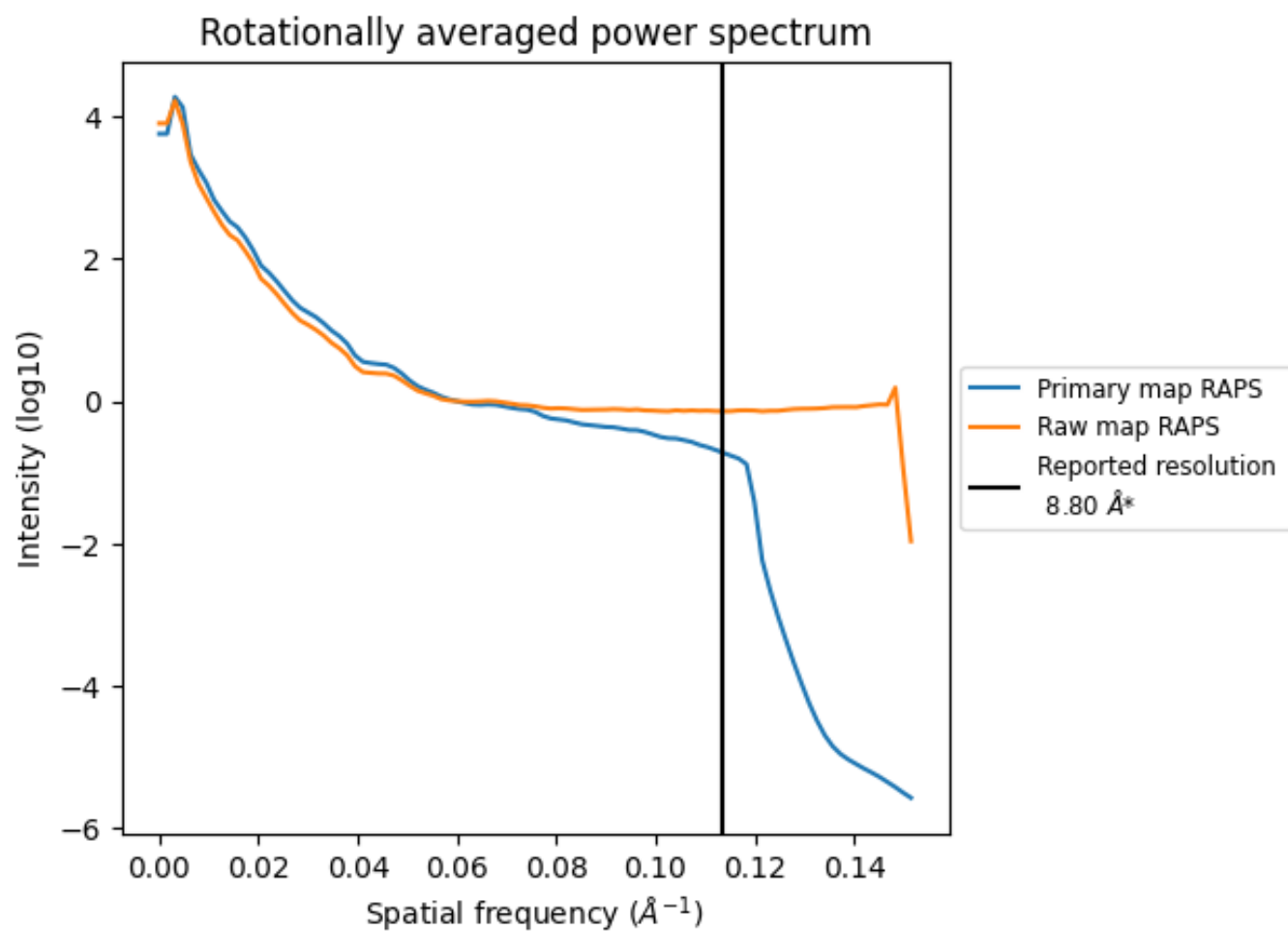
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2406  $\text{nm}^3$ ; this corresponds to an approximate mass of 2173 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ



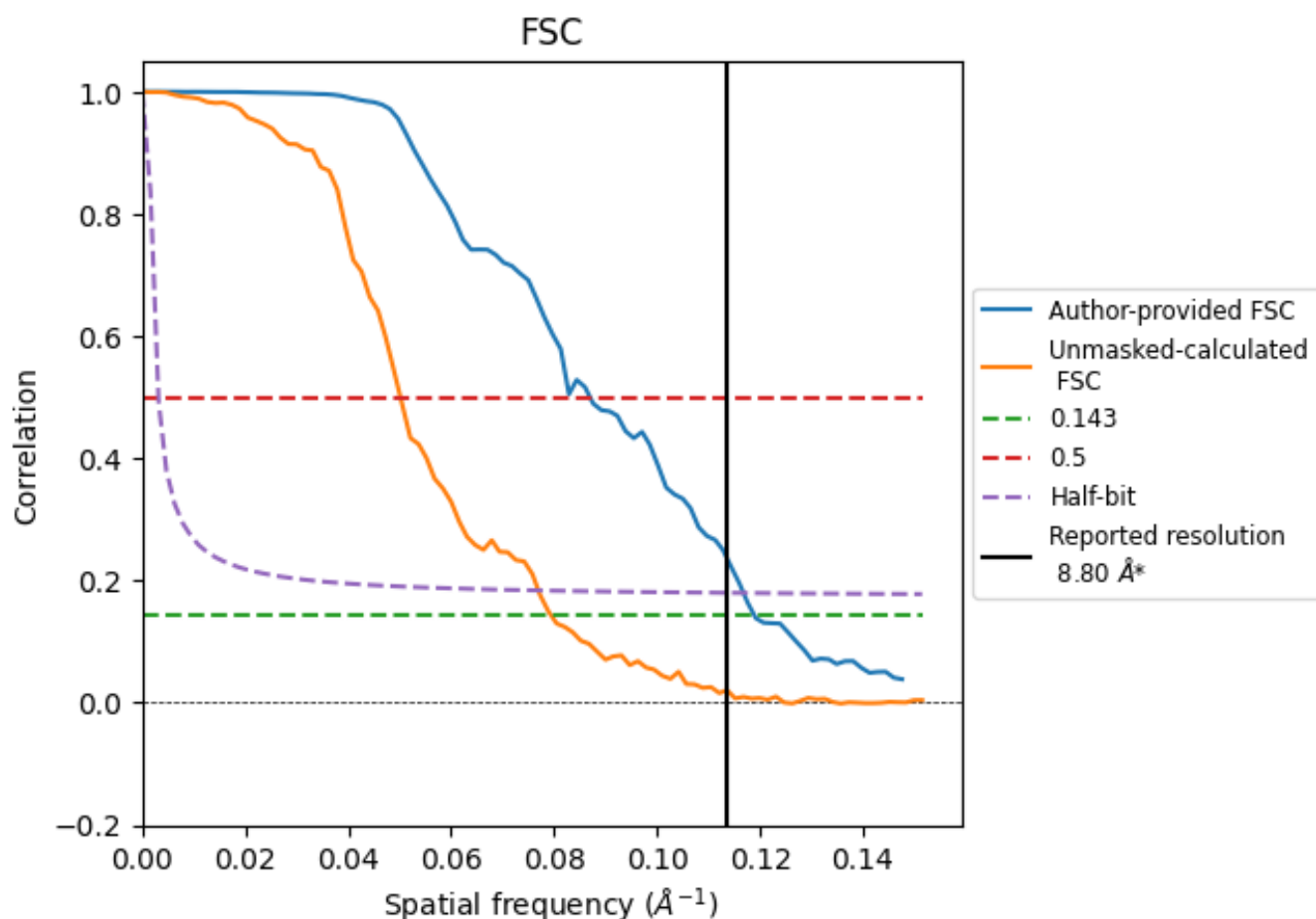
\*Reported resolution corresponds to spatial frequency of 0.114 Å<sup>-1</sup>



## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.114  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

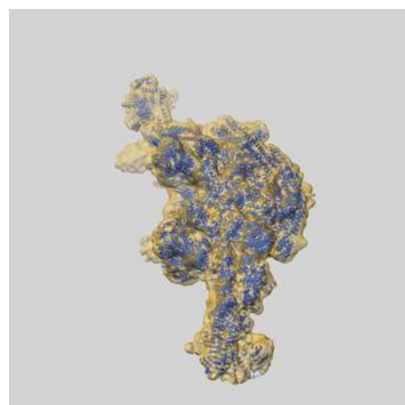
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	8.80	-	-
Author-provided FSC curve	8.41	11.49	8.56
Unmasked-calculated*	12.59	19.92	12.99

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 12.59 differs from the reported value 8.8 by more than 10 %

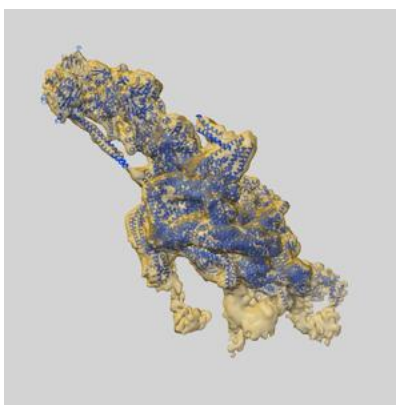
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-46849 and PDB model 9DGV. Per-residue inclusion information can be found in section [3](#) on page [10](#).

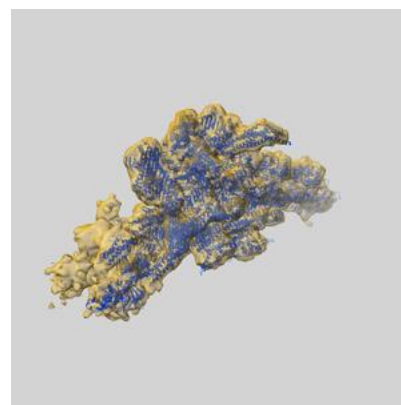
### 9.1 Map-model overlay [i](#)



X



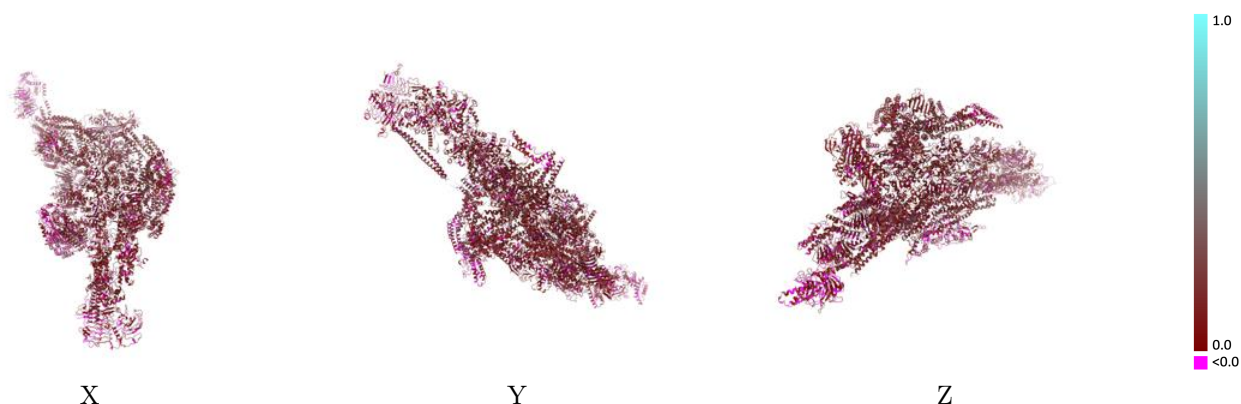
Y



Z

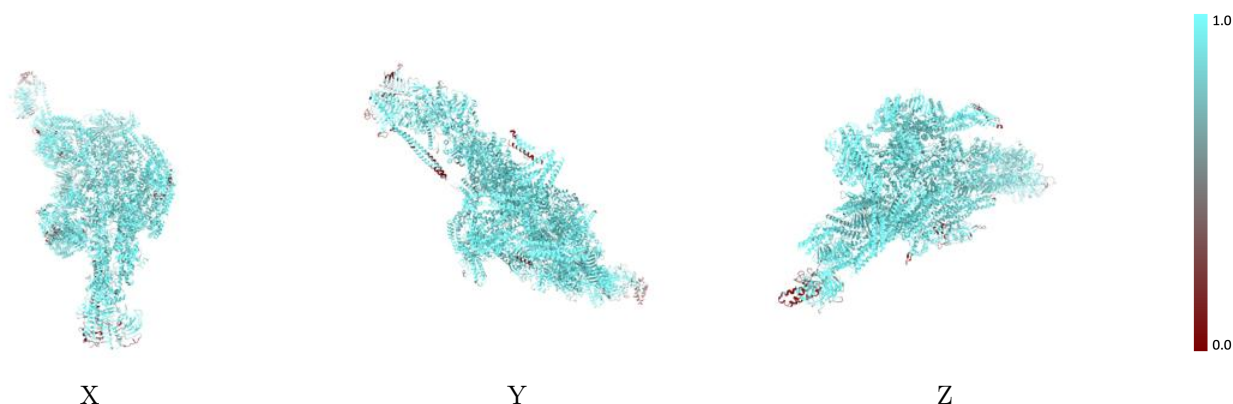
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



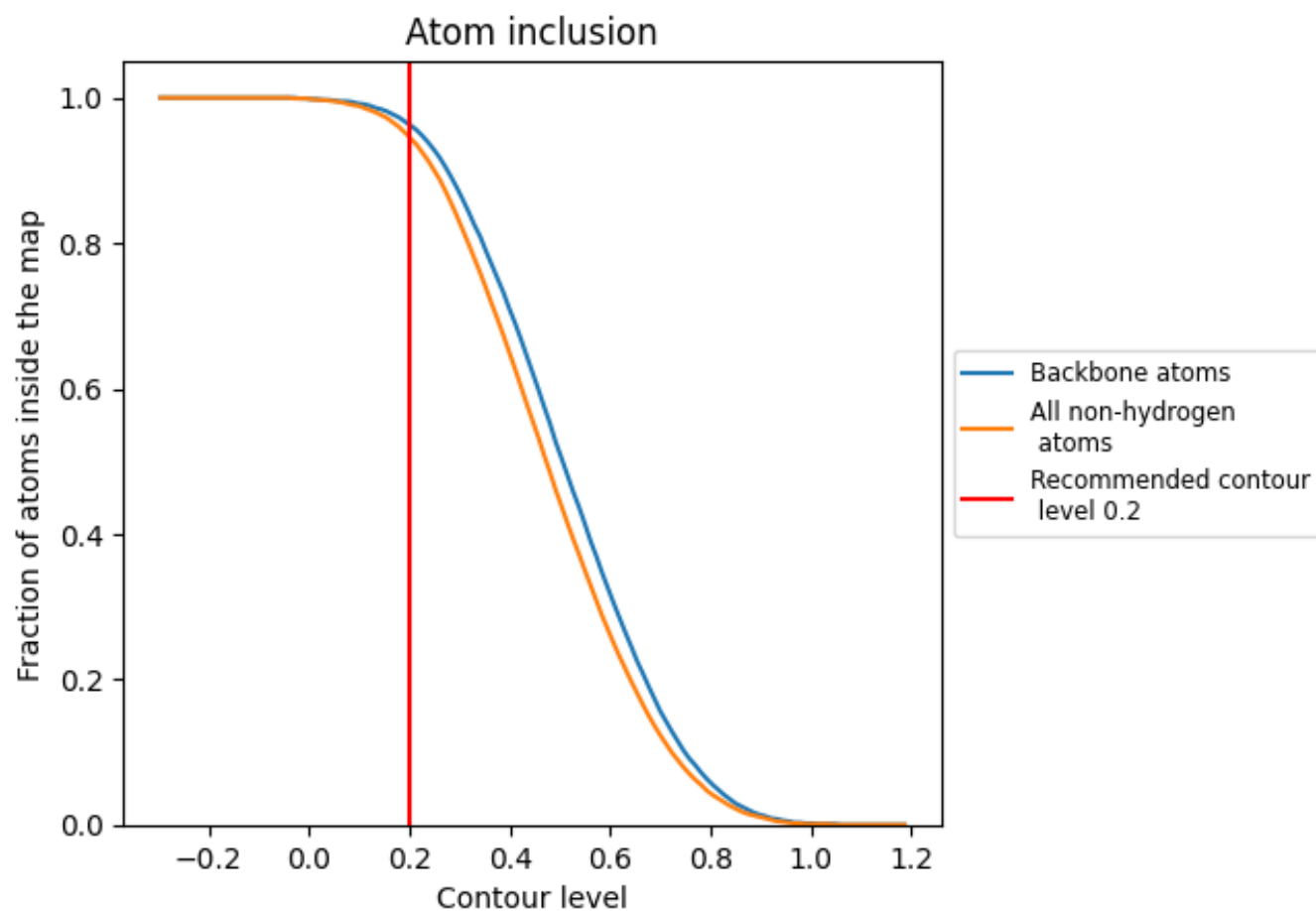
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.2).





































































## 9.4 Atom inclusion ⓘ



At the recommended contour level, 96% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9460	 0.1250
A	 0.9950	 0.1330
B	 0.9980	 0.1350
C	 0.9950	 0.1280
D	 0.9970	 0.1280
E	 0.9900	 0.1290
F	 0.9910	 0.1350
G	 0.9600	 0.1330
H	 0.9600	 0.1330
I	 0.9240	 0.1280
J	 0.9450	 0.1260
K	 0.9630	 0.1330
L	 0.9810	 0.1390
M	 0.9430	 0.1600
N	 0.9610	 0.1520
O	 1.0000	 0.1660
P	 0.9910	 0.1510
Q	 0.9780	 0.1610
R	 0.9940	 0.1620
U	 0.6620	 0.0840
V	 0.8690	 0.0880
W	 0.9800	 0.1510
Y	 0.8570	 0.1090
Z	 0.9970	 0.1410
a	 0.8220	 0.2020
b	 0.7760	 0.1550
e	 0.9350	 0.1040
f	 0.9300	 0.1130
g	 0.9920	 0.0820
h	 0.9870	 0.0990
m	 0.9630	 0.1370
n	 0.8700	 0.1360
o	 0.9550	 0.0910
p	 0.8260	 0.0530

