



## Full wwPDB EM Validation Report ⓘ

Oct 20, 2025 – 01:06 PM EDT

PDB ID : 9DGS / pdb\_00009dgs  
EMDB ID : EMD-46846  
Title : Dynactin and dynein tail region of dynein-dynactin complex on microtubules  
Authors : Rao, Q.; Chai, P.; Zhang, K.  
Deposited on : 2024-09-03  
Resolution : 3.90 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:

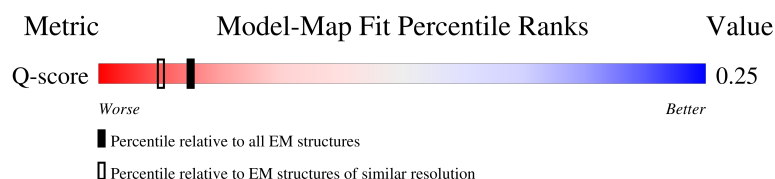
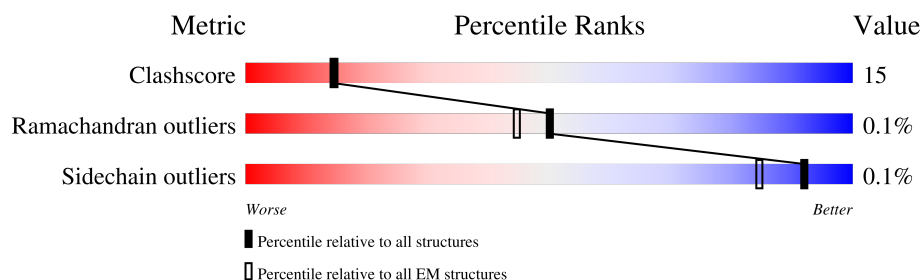
EMDB validation analysis : 0.0.1.dev129  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
EM percentile statistics : 202505.v01 (Using data in the EMDB 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) : 2.46

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.90 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	8855 ( 3.40 - 4.40 )

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	

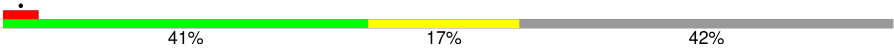
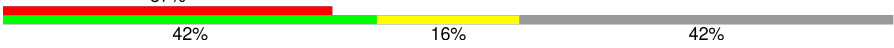
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Mol	Chain	Length	Quality of chain
1	E	376	
1	F	376	
1	G	376	
1	I	376	
2	H	375	
3	J	417	
4	K	286	
5	L	272	
6	M	405	
6	N	405	
6	P	405	
6	Q	405	
7	O	186	
7	R	186	
8	U	190	
9	V	182	
10	W	1281	
10	Z	1281	
11	Y	467	
12	e	4646	
12	f	4646	
12	m	4646	
12	n	4646	
13	g	612	
13	h	612	

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Mol	Chain	Length	Quality of chain
13	o	612	 41% 17% 42%
13	p	612	 37% 42% 16% 42%

## 2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 85480 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
			2122	1323	370	418	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		

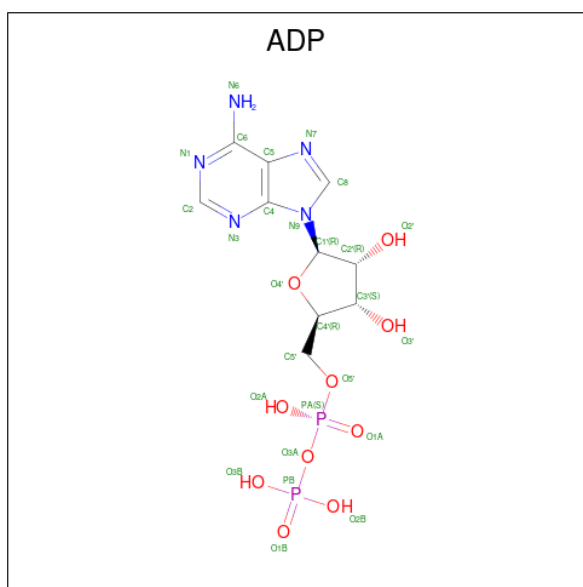
- Molecule 12 is a protein called Cytoplasmic dynein 1 heavy chain 1.

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

- Molecule 13 is a protein called Cytoplasmic dynein 1 intermediate chain 2.

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

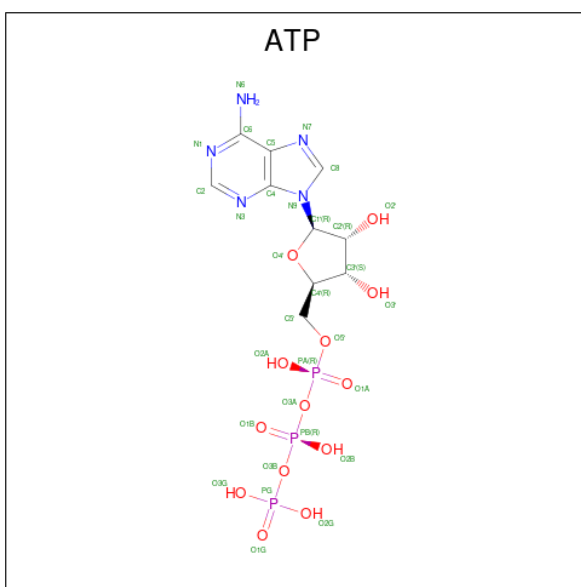
- Molecule 14 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



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

- Molecule 15 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).





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

- Molecule 16 is ZINC ION (CCD ID: ZN) (formula:  $\text{Zn}$ ).

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

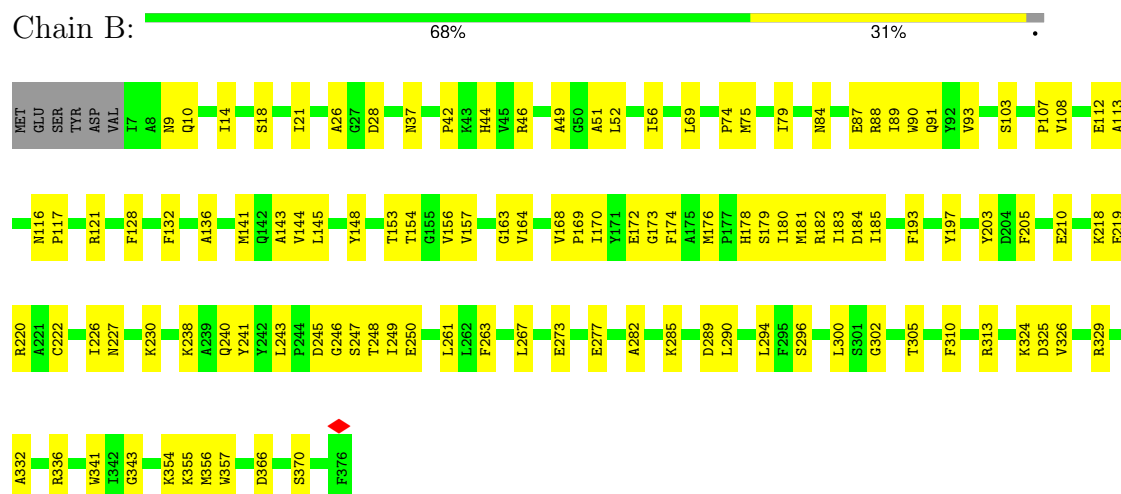
### 3 Residue-property plots

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.

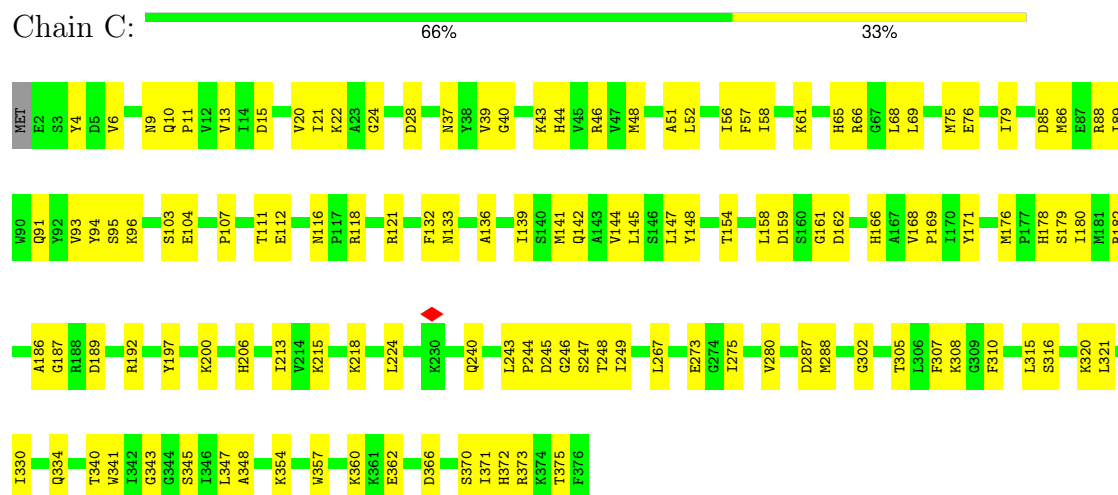
#### • Molecule 1: Alpha-centractin



#### • Molecule 1: Alpha-centractin



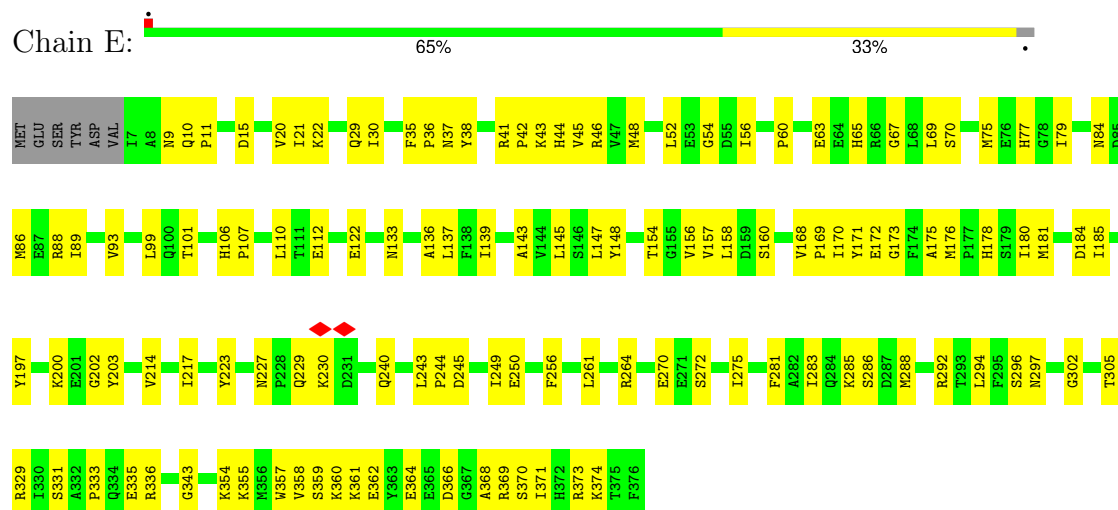
#### • Molecule 1: Alpha-centractin



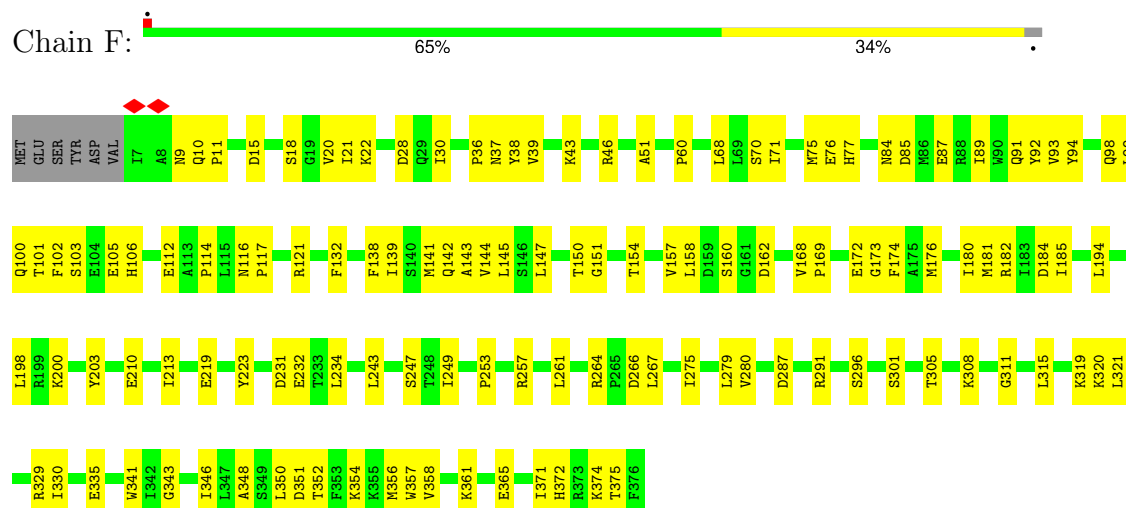
• Molecule 1: Alpha-centractin



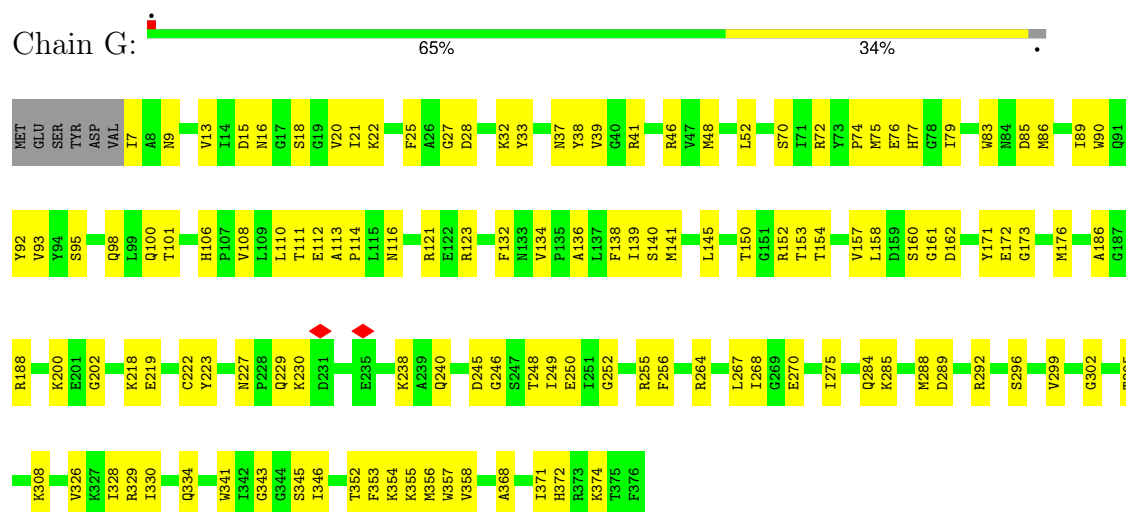
• Molecule 1: Alpha-centractin



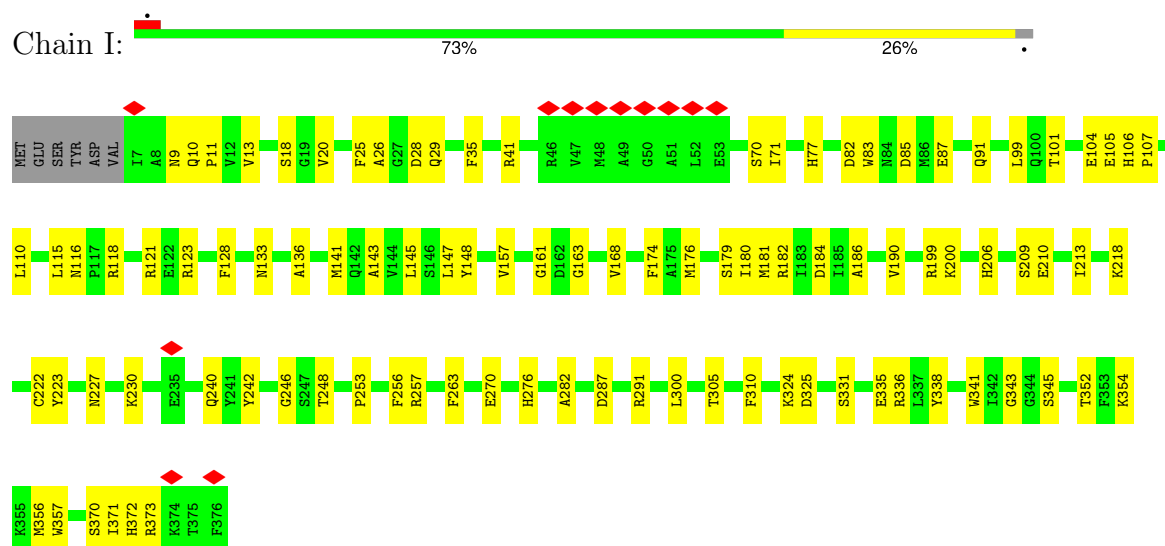
• Molecule 1: Alpha-centractin



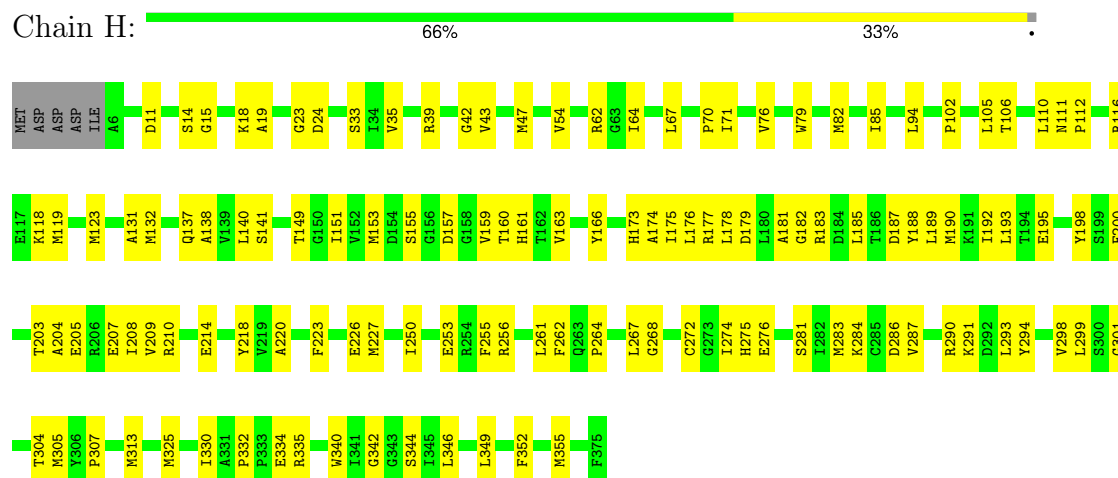
• Molecule 1: Alpha-centractin



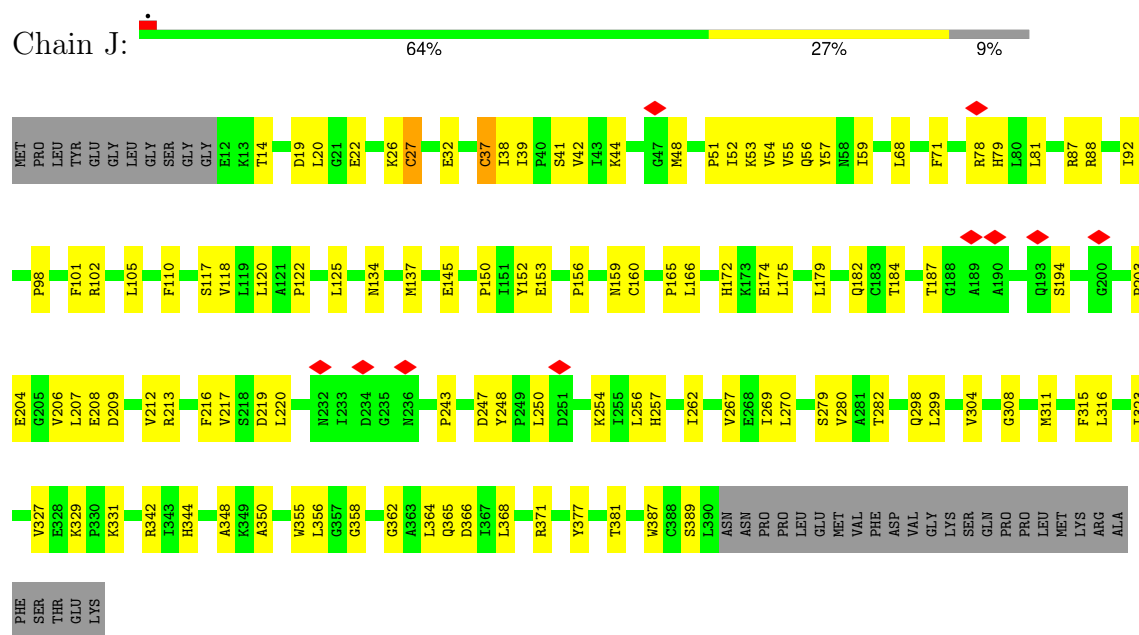
• Molecule 1: Alpha-centractin



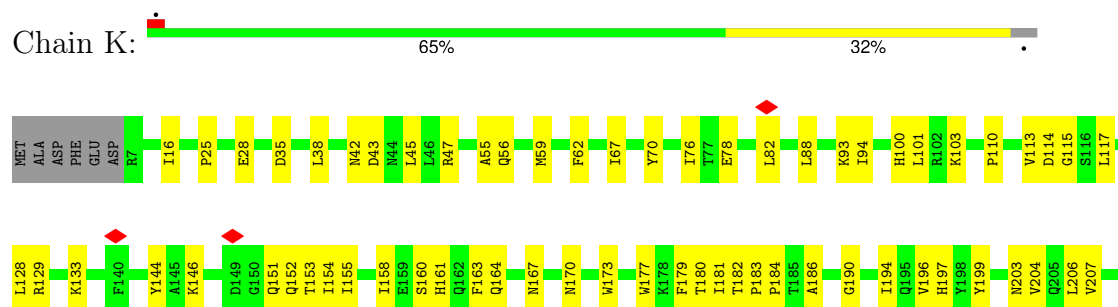
- Molecule 2: Actin, cytoplasmic 1



- Molecule 3: Actin-related protein 10

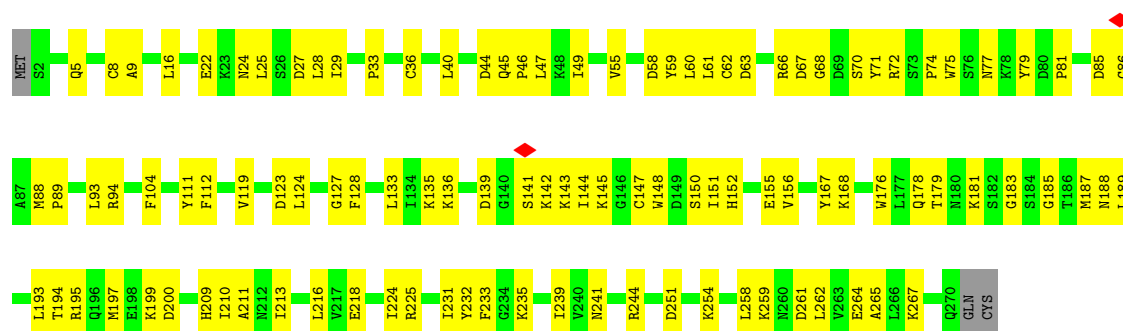


- Molecule 4: F-actin-capping protein subunit alpha-1

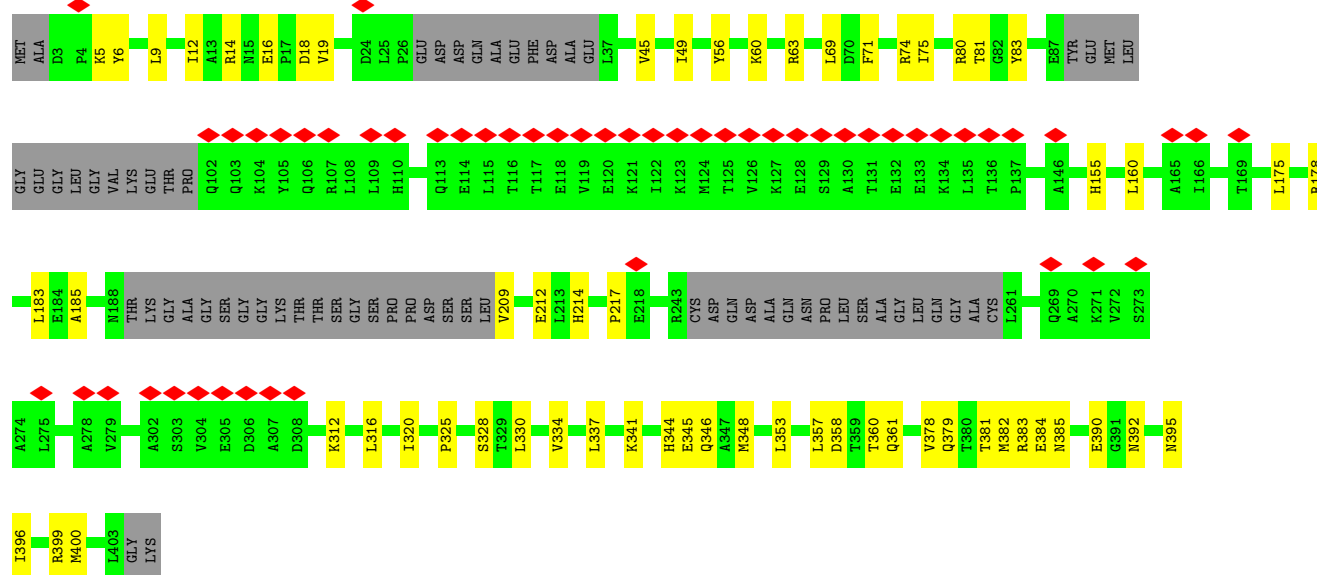




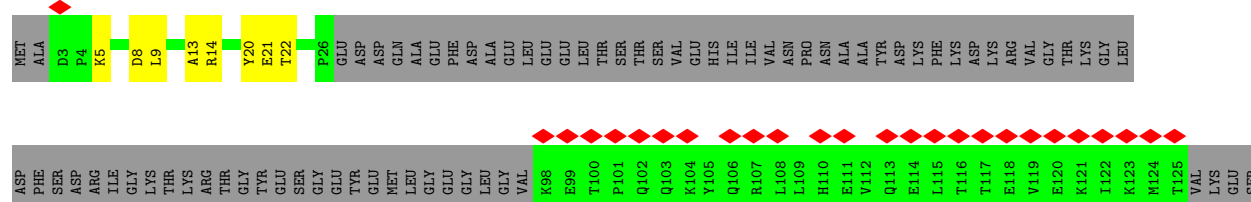
• Molecule 5: F-actin-capping protein subunit beta



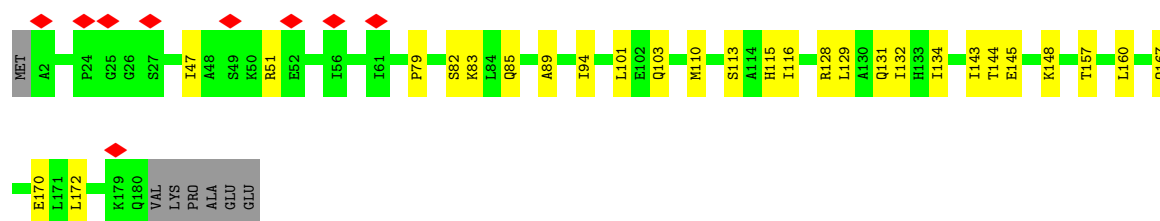
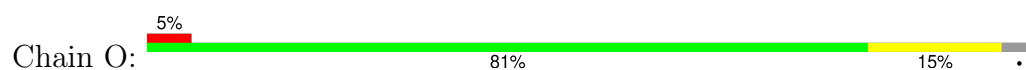
• Molecule 6: Dynactin subunit 2



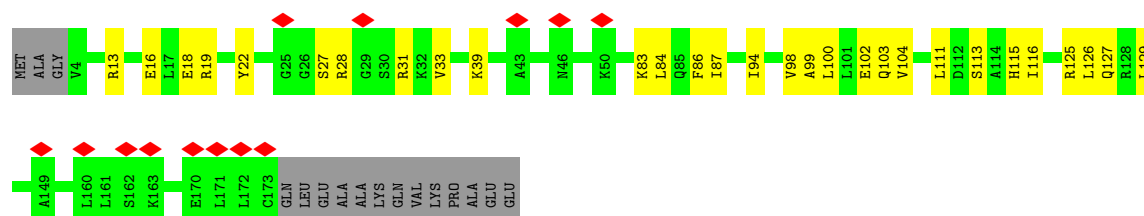
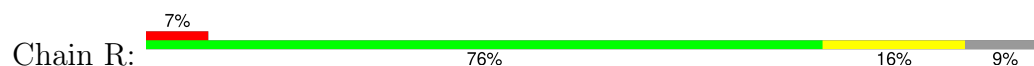
• Molecule 6: Dynactin subunit 2



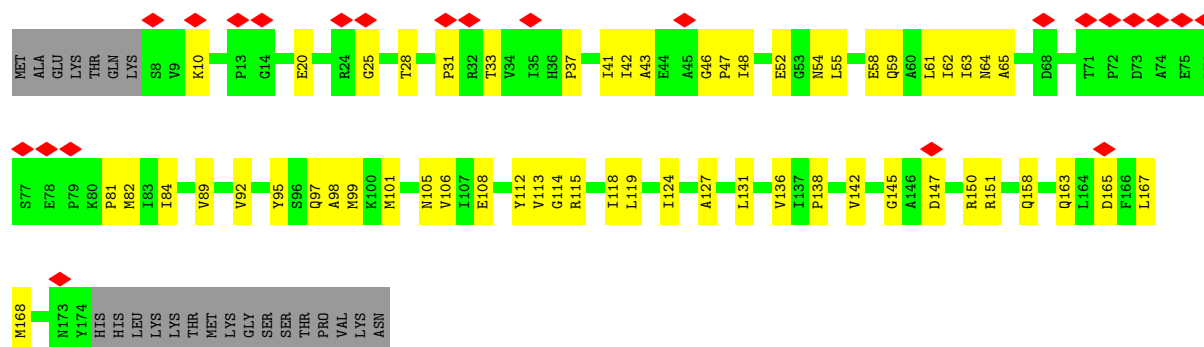




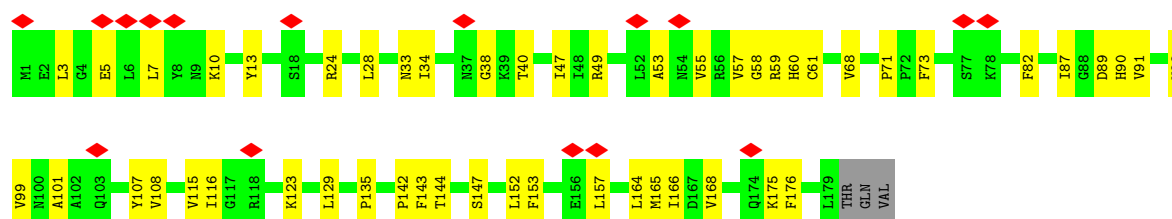
• Molecule 7: Dynactin subunit 3



• Molecule 8: Dynactin subunit 6



• Molecule 9: Dynactin subunit 5



• Molecule 10: Dynactin subunit 1



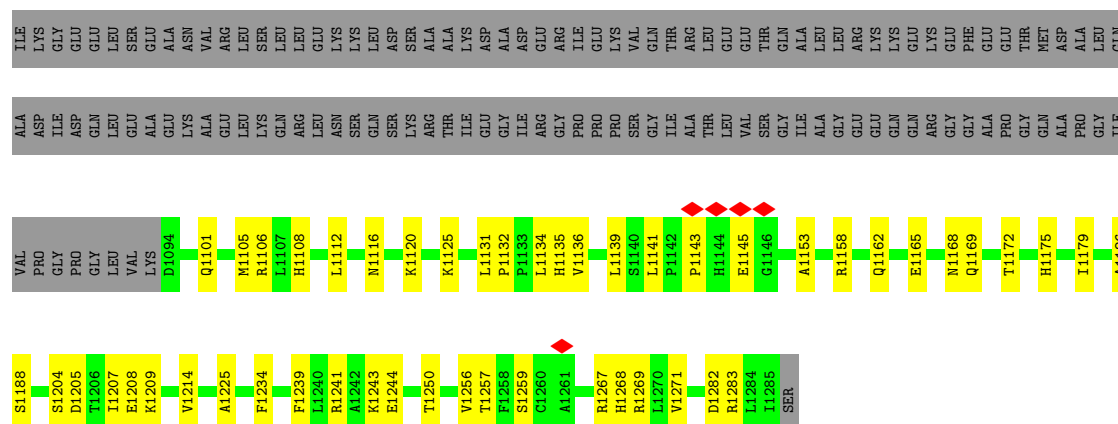




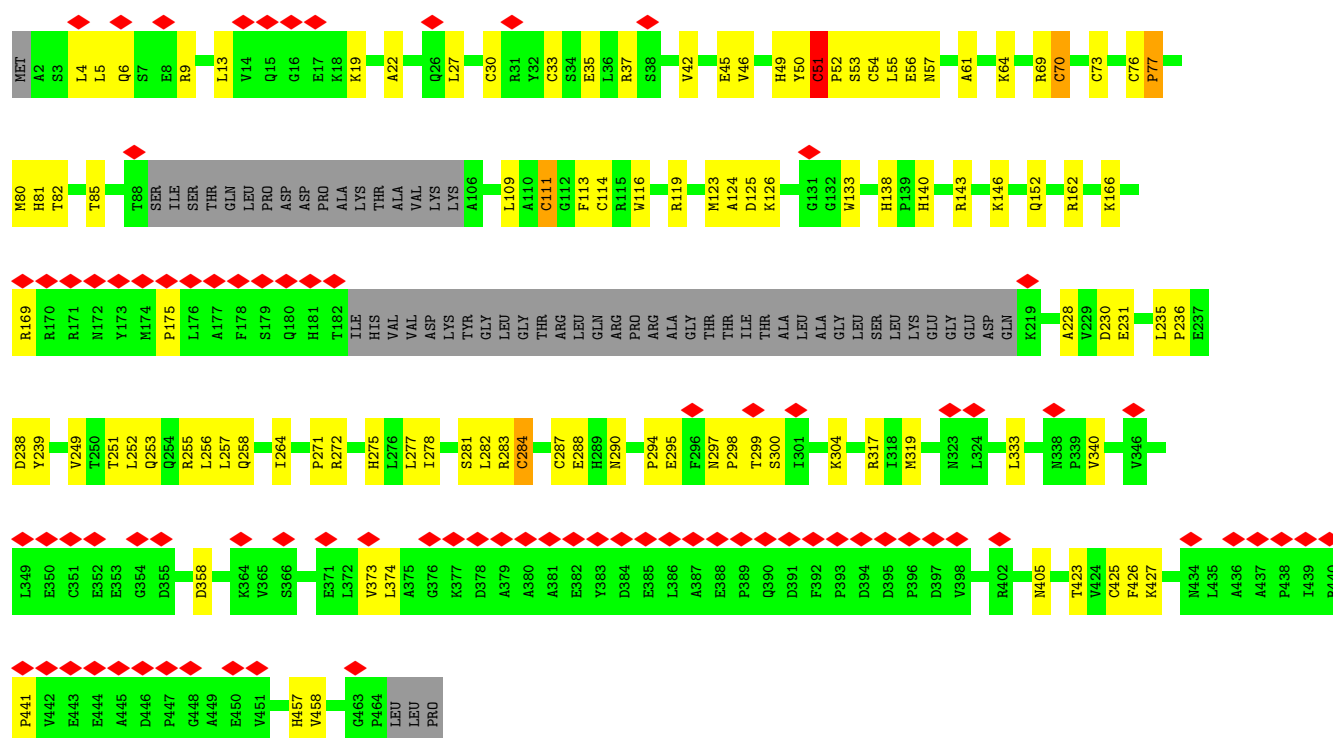


Chain Z:  11% 85%

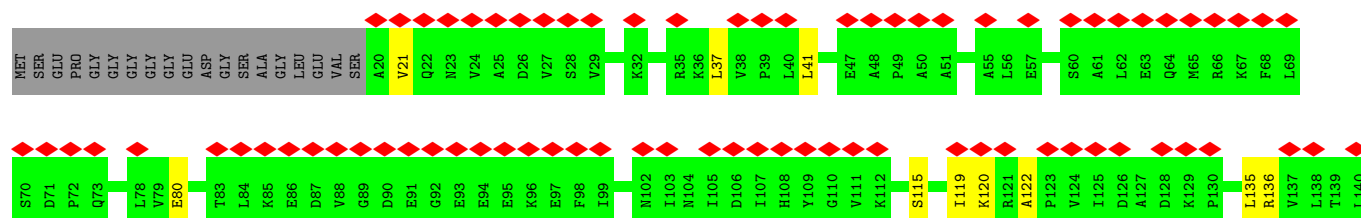




• Molecule 11: Dynactin subunit 4



• Molecule 12: Cytoplasmic dynein 1 heavy chain 1





























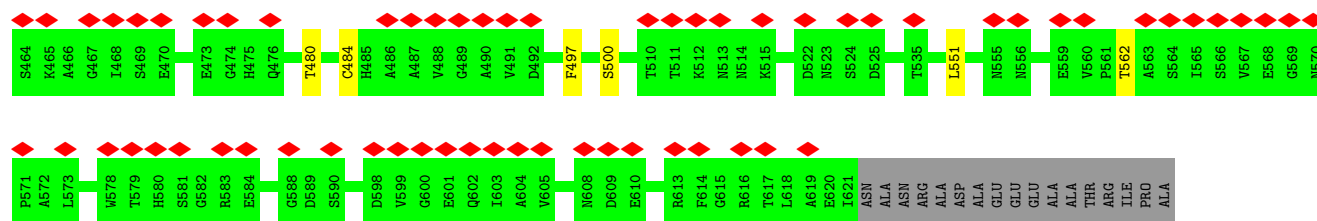






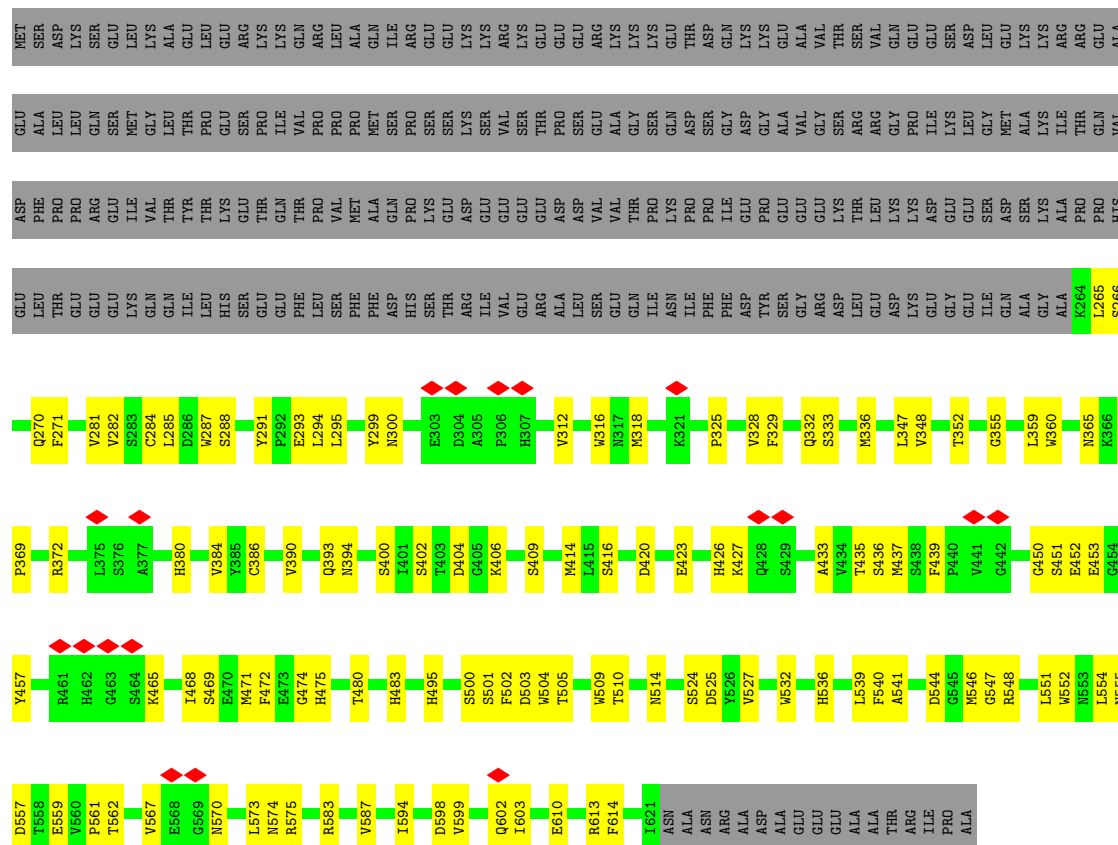
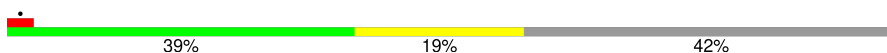






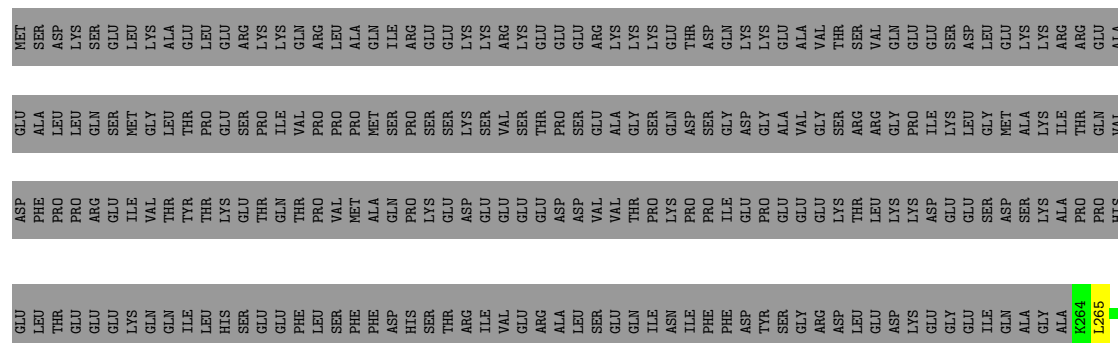
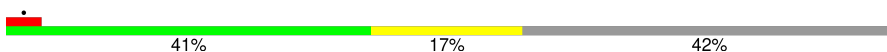
• Molecule 13: Cytoplasmic dynein 1 intermediate chain 2

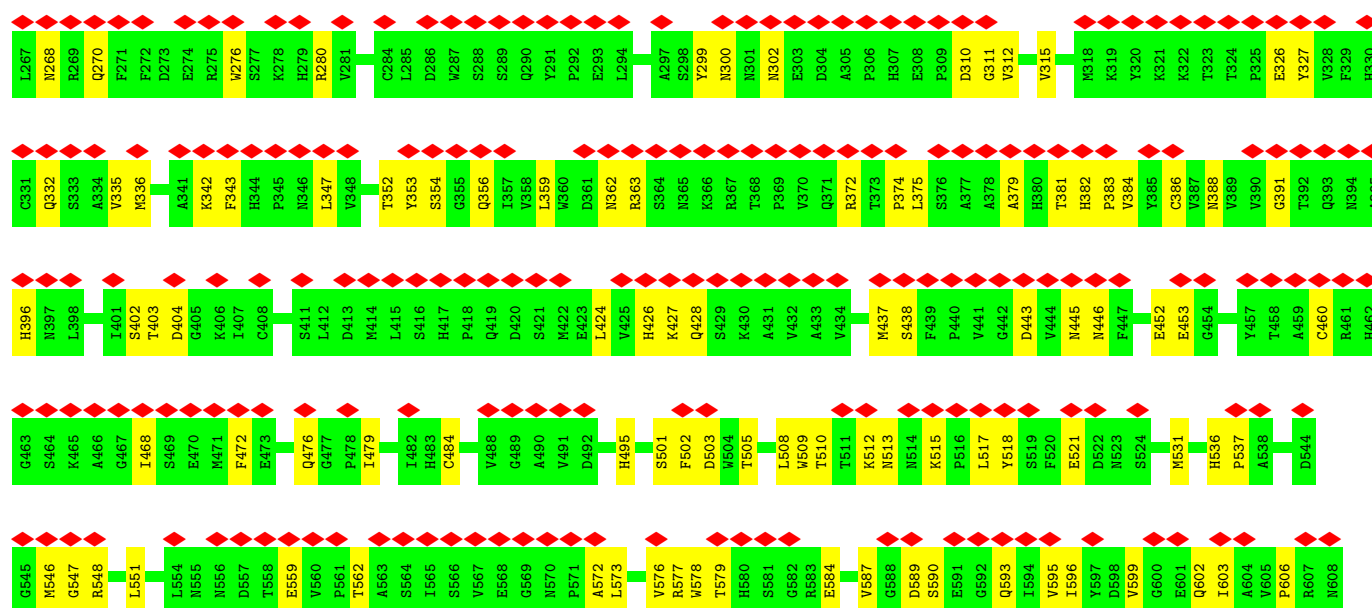
Chain h:



• Molecule 13: Cytoplasmic dynein 1 intermediate chain 2

Chain o:





D609	E610	W611	A612	F613	F614	G615	R616	T617	L618	A619	E620	F621	ASN	ALA	ASN	ARG	ALA	ALA	ASP	ALA	GLU	GLU	GLU	ALA	ALA	THR	ARG	ILE	PRO	ALA
------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	62404	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	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	0.582	Depositor
Minimum map value	-0.224	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.13	Depositor
Map size (Å)	633.6, 633.6, 633.6	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2375, 1.2375, 1.2375	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.14	0/3013	0.35	0/4070
1	B	0.16	0/3025	0.42	0/4085
1	C	0.17	0/3068	0.40	0/4144
1	D	0.15	0/3025	0.37	0/4085
1	E	0.16	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	0.13	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	0.14	0/2156	0.32	0/2906
6	M	0.16	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	0.14	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	0.16	0/1467	0.44	0/1992
11	Y	0.34	0/3020	0.51	1/4119 (0.0%)
12	e	0.27	0/4754	0.47	0/6541
12	f	0.23	0/6683	0.46	2/9015 (0.0%)
12	m	0.17	0/5807	0.35	0/7751
12	n	0.27	0/5501	0.45	0/7337
13	g	0.11	0/1766	0.28	0/2457
13	h	0.13	0/2887	0.35	0/3938
13	o	0.12	0/2887	0.32	1/3938 (0.0%)
13	p	0.12	0/2887	0.32	1/3938 (0.0%)
All	All	0.19	0/86747	0.40	5/117593 (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
12	n	0	2
All	All	0	3

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	o	428	GLN	CB-CA-C	-5.17	110.59	116.54
13	p	428	GLN	CB-CA-C	-5.17	110.59	116.54
11	Y	51	CYS	CB-CA-C	5.05	116.40	108.63
12	f	37	LEU	CA-C-N	5.03	131.44	122.13
12	f	37	LEU	C-N-CA	5.03	131.44	122.13

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	Y	37	ARG	Sidechain
12	n	704	ARG	Sidechain
12	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	114	0
1	C	2998	0	2983	98	0
1	D	2956	0	2950	105	0
1	E	2956	0	2950	103	0
1	F	2956	0	2950	96	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	2956	0	2950	96	0
1	I	2941	0	2936	70	0
2	H	2885	0	2856	98	0
3	J	2932	0	3001	83	0
4	K	2264	0	2186	78	0
5	L	2122	0	2113	77	0
6	M	2238	0	1829	65	0
6	N	1767	0	1356	42	0
6	P	2262	0	2060	82	0
6	Q	2349	0	2069	58	0
7	O	1183	0	981	35	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	34	0
10	Z	1444	0	1446	54	0
11	Y	2960	0	2711	79	0
12	e	4724	0	3273	56	0
12	f	6570	0	6693	307	0
12	m	5722	0	5269	216	0
12	n	5424	0	4963	264	0
13	g	1767	0	796	7	0
13	h	2808	0	2670	93	0
13	o	2808	0	2670	80	0
13	p	2808	0	2670	148	0
14	A	27	0	12	2	0
14	B	27	0	12	1	0
14	C	27	0	12	2	0
14	D	27	0	12	3	0
14	E	27	0	12	0	0
14	F	27	0	12	1	0
14	G	27	0	12	1	0
14	I	27	0	12	0	0
14	J	27	0	12	1	0
15	H	31	0	12	8	0
16	Y	3	0	0	0	0
All	All	85480	0	79355	2432	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 (2432) 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)
12:n:755:TRP:CZ2	13:p:453:GLU:HA	1.19	1.63
12:n:755:TRP:CZ2	13:p:453:GLU:CA	1.80	1.62
12:n:779:ILE:CG2	13:p:375:LEU:HD22	1.33	1.55
12:e:717:ILE:HA	12:e:824:TRP:CE2	1.39	1.54
12:n:779:ILE:HG21	13:p:375:LEU:CD2	1.33	1.52
12:n:755:TRP:CE2	13:p:453:GLU:HA	1.46	1.51
12:e:717:ILE:CB	12:e:824:TRP:CD2	1.97	1.48
12:n:755:TRP:CE2	13:p:453:GLU:CA	1.89	1.43
12:n:755:TRP:CH2	13:p:453:GLU:HA	1.48	1.43
12:e:717:ILE:N	12:e:824:TRP:CD1	1.87	1.41
12:n:748:LYS:NZ	13:p:383:PRO:HG2	1.07	1.39
12:n:748:LYS:NZ	13:p:383:PRO:CG	1.85	1.37
12:n:775:TYR:OH	13:p:354:SER:CA	1.73	1.36
12:e:717:ILE:CA	12:e:824:TRP:CE2	2.11	1.34
12:n:755:TRP:CZ2	13:p:453:GLU:C	2.05	1.31
12:n:755:TRP:CE2	13:p:453:GLU:CB	1.84	1.31
12:n:779:ILE:CB	13:p:375:LEU:HD22	1.62	1.28
12:n:776:PRO:CB	13:p:375:LEU:O	1.81	1.28
12:n:779:ILE:CG2	13:p:375:LEU:CD2	1.97	1.27
12:n:776:PRO:HB2	13:p:375:LEU:O	1.33	1.27
12:n:755:TRP:CE2	13:p:453:GLU:HB3	1.55	1.26
12:n:755:TRP:CZ3	13:p:452:GLU:O	1.89	1.25
12:n:748:LYS:CE	13:p:383:PRO:HG2	1.67	1.25
12:n:775:TYR:CE2	13:p:381:THR:O	1.90	1.24
12:n:755:TRP:NE1	13:p:453:GLU:CB	1.80	1.18
12:n:755:TRP:HB2	13:p:453:GLU:OE2	1.41	1.13
12:n:775:TYR:HE2	13:p:381:THR:O	1.26	1.12
12:e:717:ILE:CB	12:e:824:TRP:CE3	2.33	1.10
12:n:748:LYS:HZ3	13:p:383:PRO:CG	1.52	1.10
12:e:720:ILE:CB	12:e:820:ILE:HD12	1.84	1.07
12:n:751:ARG:NH2	13:p:403:THR:HB	1.72	1.05
12:e:716:ARG:C	12:e:824:TRP:CD1	2.36	1.04
12:e:717:ILE:HA	12:e:824:TRP:NE1	1.73	1.04
12:e:717:ILE:N	12:e:824:TRP:NE1	2.05	1.04
12:e:717:ILE:HA	12:e:824:TRP:CZ2	1.92	1.03
12:e:717:ILE:CA	12:e:824:TRP:NE1	2.22	1.02
12:n:779:ILE:HB	13:p:375:LEU:HD22	1.42	1.01
12:n:755:TRP:CZ3	13:p:453:GLU:HA	1.96	1.00
12:n:775:TYR:OH	13:p:354:SER:HA	0.84	1.00
12:n:779:ILE:HG21	13:p:375:LEU:HD21	1.02	1.00
12:n:755:TRP:CD2	13:p:453:GLU:HA	1.98	0.99
12:e:717:ILE:CB	12:e:824:TRP:CG	2.48	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:m:578:ALA:HA	12:m:581:MET:HE2	1.47	0.97
12:n:755:TRP:NE1	13:p:453:GLU:HB3	0.97	0.96
1:E:65:HIS:HD1	1:G:171:TYR:HH	1.13	0.95
12:e:716:ARG:C	12:e:824:TRP:NE1	2.26	0.94
12:n:755:TRP:CD2	13:p:453:GLU:CA	2.52	0.94
12:n:755:TRP:CH2	13:p:452:GLU:O	2.21	0.93
12:n:755:TRP:HE1	13:p:453:GLU:HB3	1.20	0.93
12:n:748:LYS:HZ1	13:p:383:PRO:CG	1.69	0.93
12:f:278:TRP:HB2	12:f:336:MET:HE3	1.49	0.92
7:R:28:ARG:NH1	7:R:28:ARG:O	2.03	0.91
12:e:717:ILE:H	12:e:824:TRP:CD1	1.83	0.90
12:e:717:ILE:CA	12:e:824:TRP:CD2	2.47	0.90
6:N:348:MET:HE1	10:Z:1135:HIS:H	1.33	0.90
12:n:751:ARG:NH2	13:p:403:THR:CB	2.34	0.90
12:m:402:MET:HB3	12:m:531:LYS:HG3	1.52	0.89
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
12:n:775:TYR:CD2	13:p:381:THR:O	2.26	0.88
6:Q:12:ILE:HB	6:Q:14:ARG:NH1	1.89	0.88
12:n:755:TRP:HZ2	13:p:453:GLU:C	1.80	0.88
12:n:755:TRP:CB	13:p:453:GLU:OE2	2.09	0.88
1:C:48:MET:HB3	1:E:173:GLY:HA2	1.52	0.88
12:e:717:ILE:CB	12:e:824:TRP:CE2	2.48	0.87
12:f:82:SER:HA	12:f:113:SER:HA	1.56	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
12:f:402:MET:SD	12:f:470:ARG:NH2	2.48	0.86
12:n:755:TRP:CZ2	13:p:453:GLU:O	2.27	0.86
12:m:526:ALA:HB2	12:m:556:ARG:HD2	1.58	0.85
6:P:312:LYS:O	6:Q:317:TYR:OH	1.95	0.85
12:n:776:PRO:HB3	13: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	0.83
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
12:f:378:LEU:HB3	12:f:452:ILE:HD11	1.59	0.83
12:n:748:LYS:HZ1	13:p:383:PRO:HG3	1.43	0.82
12:n:751:ARG:HH22	13:p:403:THR:CB	1.93	0.82
12:n:779:ILE:HG22	13:p:375:LEU:HD22	1.57	0.82
12:f:275:ILE:HA	12:f:336:MET:HE1	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
12:n:775:TYR:HH	13:p:354:SER:HA	1.00	0.81
6:N:379:GLN:HB3	6:N:383:ARG:HH12	1.44	0.81
12:f:529:ASN:HB3	12:f:552:ARG:HE	1.44	0.81
1:C:308:LYS:HD2	6:Q:39:GLU:HB2	1.61	0.81
5:L:88:MET:HE2	5:L:94:ARG:HB2	1.63	0.80
12:f:232:PHE:HB3	12:f:235:LYS:HB2	1.63	0.80
1:G:110:LEU:HB3	1:G:139:ILE:HG22	1.63	0.80
12:n:755:TRP:CH2	13:p:453:GLU:CA	2.31	0.80
12:n:748:LYS:NZ	13:p:383:PRO:HG3	1.95	0.79
13:h:465:LYS:NZ	13:h:469:SER:OG	2.15	0.79
12:f:85:LYS:HA	12:f:97:GLU:HA	1.65	0.79
12:f:399:ARG:NH1	12:f:416:CYS:SG	2.56	0.79
1:B:164:VAL:HG21	1:B:182:ARG:HH11	1.47	0.79
10:W:1105:MET:HE2	10:Z:1105:MET:SD	2.23	0.79
12:n:755:TRP:HZ2	13:p:453:GLU:O	1.61	0.79
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:M:383:ARG:HA	6:Q:183:LEU:HD11	1.65	0.78
12:e:717:ILE:N	12:e:824:TRP:CG	2.50	0.78
1:A:227:ASN:HB3	1:A:230:LYS:HG2	1.64	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:G:346:ILE:HD11	6:M:56:TYR:HB2	1.64	0.78
1:I:121:ARG:HH21	1:I:141:MET:HE1	1.49	0.78
12:e:717:ILE:CA	12:e:824:TRP:CD1	2.62	0.78
12:n:755:TRP:CE3	13: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	0.78
1:B:179:SER:HA	1:B:285:LYS:HD2	1.65	0.77
12:n:591:LEU:HB2	12:n:601:ILE:HD11	1.64	0.77
1:B:145:LEU:HA	1:B:148:TYR:HD2	1.49	0.77
13:o:547:GLY:HA2	13:o:573:LEU:HD23	1.67	0.77
12:f:431:GLN:HB3	12:f:435:ARG:HH12	1.48	0.77
2:H:200:PHE:HB3	2:H:205:GLU:HB3	1.65	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
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
13:p:424:LEU:HD12	13:p:468:ILE:HG13	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
13:p:547:GLY:HA2	13:p:573:LEU:HD23	1.67	0.75
12:e:718:PHE:CB	12:e:819:GLY:O	2.34	0.75
12:n:456:HIS:O	12:n:460:GLN:N	2.19	0.75
12:n:748:LYS:CE	13:p:383:PRO:CG	2.46	0.74
12:n:775:TYR:CZ	13:p:354:SER:HA	2.14	0.74
13:o:424:LEU:HD12	13:o:468:ILE:HG13	1.68	0.74
10:W:1105:MET:HE1	10:Z:1106:ARG:HG2	1.68	0.74
12:f:409:PHE:CZ	12:f:470:ARG:HD2	2.22	0.74
12:n:779:ILE:HG22	13:p:375:LEU:CD2	2.14	0.74
1:B:290:LEU:HB3	1:B:294:LEU:HD23	1.69	0.74
7:O:148:LYS:HD3	6:P:142:LYS:HD3	1.69	0.74
11:Y:70:CYS:SG	11:Y:73:CYS:N	2.61	0.74
11:Y:111:CYS:SG	11:Y:114:CYS:N	2.57	0.73
12:f:269:GLY:O	12:f:386:ARG:NH2	2.20	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	1.70	0.73
12:f:616:ILE:HD12	12:f:682:LEU:HD11	1.68	0.73
1:G:354:LYS:HA	1:G:357:TRP:CZ3	2.23	0.73
1:G:358:VAL:HG22	1:G:374:LYS:HD2	1.70	0.73
6:N:392:ASN:HD21	10:Z:1179:ILE:HG12	1.53	0.73
9:V:58:GLY:HA3	9:V:89:ASP:HA	1.70	0.73
5:L:47:LEU:HD21	5:L:151:ILE:HD11	1.71	0.73
9:V:73:PHE:HA	9:V:82:PHE:HA	1.70	0.73
12:n:232:PHE:HB3	12:n:235:LYS:HB2	1.71	0.73
4:K:154:ILE:HB	4:K:179:PHE:HB3	1.69	0.72
8:U:43:ALA:HB2	8:U:48:ILE:HG12	1.71	0.72
12:f:466:MET:HA	12:f:469:PHE:CE1	2.24	0.72
12:f:716:ARG:HG2	12:f:823:VAL:HG12	1.70	0.72
12:m:255:GLU:HA	12:m:258:LYS:HE2	1.71	0.72
13:h:282:VAL:O	13:h:574:ASN:ND2	2.22	0.72
12:f:361:PHE:HD2	12:f:430:LEU:HD23	1.55	0.72
12:f:395:VAL:HG12	12:f:399:ARG:HE	1.55	0.72
12:e:739:PHE:CB	12:e:824:TRP:CE2	2.73	0.72
8:U:101:MET:HB2	8:U:119:LEU:HB2	1.70	0.72
12:f:406:TYR:HA	12:f:409:PHE:CE1	2.25	0.72
12:n:779:ILE:CB	13:p:375:LEU:CD2	2.54	0.72
12:f:117:ALA:N	12:f:138:LEU:O	2.17	0.71
1:F:158:LEU:HD11	1:F:275:ILE:HD11	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:162:ARG:HG2	11:Y:166:LYS:NZ	2.06	0.71
12:n:751:ARG:CZ	13: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
1:C:107:PRO:HB3	1:C:136:ALA:HB3	1.70	0.71
12:e:344:LEU:HA	12:e:356:ALA:HB1	1.71	0.71
12:f:466:MET:HA	12:f:469:PHE:CD1	2.26	0.71
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
12:f:575:ALA:HB3	12:f:584:ILE:HD13	1.74	0.70
12:f:720:ILE:HD12	12:f:733:LEU:HD13	1.73	0.70
1:B:56:ILE:HD13	1:B:88:ARG:HD3	1.73	0.70
11:Y:358:ASP:O	11:Y:423:THR:OG1	2.09	0.70
12:m:368:ARG:HD2	12:m:433:LEU:HD11	1.73	0.70
12:f:817:ALA:HA	12:f:820:ILE:HD12	1.73	0.70
12:n:755:TRP:CZ3	13:p:452:GLU:C	2.70	0.70
10:W:1282:ASP:HA	10:W:1285:ILE:HG22	1.73	0.70
12:m:227:PRO:HB2	12:m:299:LEU:HD22	1.71	0.70
1:G:229:GLN:HE22	1:G:264:ARG:HH22	1.37	0.69
12:f:626:GLN:HB2	12:f:629:GLN:HG2	1.73	0.69
1:E:185:ILE:HD11	1:E:261:LEU:HG	1.73	0.69
7:O:160:LEU:HD22	6:Q:179:LEU:HD12	1.74	0.69
5:L:179:THR:HB	5:L:187:MET:HB3	1.74	0.69
1:A:366:ASP:HB3	1:A:370:SER:HB3	1.75	0.69
1:B:10:GLN:HG2	12:n:246:GLN:HE22	1.58	0.69
1:B:267:LEU:O	1:C:178:HIS:NE2	2.25	0.69
1:G:28:ASP:HB2	1:G:341:TRP:HH2	1.58	0.69
1:C:116:ASN:OD1	1:C:182:ARG:NH1	2.26	0.69
9:V:13:TYR:HB2	9:V:24:ARG:HG3	1.73	0.69
12:e:718:PHE:CB	12:e:822:LEU:O	2.41	0.69
12:n:748:LYS:HE2	13:p:383:PRO:HG2	1.71	0.69
12:e:486:PRO:HA	12:e:512:PHE:HA	1.75	0.68
13:h:471:MET:O	13:h:514:ASN:ND2	2.24	0.68
6:Q:102:GLN:NE2	6:Q:106:GLN:OE1	2.26	0.68
13:h:369:PRO:O	13:h:372:ARG:NH2	2.26	0.68
6:P:265:VAL:HA	6:P:268:LEU:HD12	1.74	0.68
4:K:128:LEU:HD11	4:K:158:ILE:HD11	1.74	0.68
3:J:365:GLN:HA	3:J:368:LEU:HD12	1.75	0.68
12:n:779:ILE:HG22	13:p:375:LEU:HD13	1.76	0.68
1:D:57:PHE:HA	1:D:61:LYS:HE2	1.74	0.68
12:n:755:TRP:CD1	13:p:453:GLU:OE1	2.16	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:m:750:VAL:HG22	12:m:760:VAL:HG11	1.76	0.68
12:f:365:ARG:HH21	12:f:433:LEU:HB2	1.59	0.67
12:f:431:GLN:HB3	12:f:435:ARG:NH1	2.09	0.67
1:A:154:THR:HG23	1:A:171:TYR:HA	1.77	0.67
1:C:154:THR:HG23	1:C:171:TYR:HA	1.75	0.67
6:M:383:ARG:NH1	6:Q:183:LEU:O	2.26	0.67
6:P:316:LEU:HG	6:Q:317:TYR:CE2	2.28	0.67
13:h:414:MET:HE3	13:h:416:SER:HB2	1.76	0.67
1:B:143:ALA:HB1	1:B:157:VAL:HB	1.76	0.67
12:n:580:GLU:HG3	12:n:583:ARG:HH12	1.60	0.67
1:F:158:LEU:HD22	1:F:279:LEU:HD21	1.77	0.67
7:O:157:THR:HG22	6:Q:179:LEU:HB3	1.77	0.67
10:W:1130:ALA:O	10:W:1134:LEU:N	2.25	0.67
12:n:775:TYR:OH	13:p:354:SER:CB	2.43	0.67
13:o:505:THR:HG22	13:o:521:GLU:HG2	1.75	0.67
11:Y:42:VAL:HG13	11:Y:282:LEU:HD12	1.75	0.67
12:f:529:ASN:OD1	12:f:556:ARG:NH1	2.28	0.67
12:f:751:ARG:HH21	13:h:433:ALA:HB1	1.60	0.67
13:p:505:THR:HG22	13:p:521:GLU:HG2	1.75	0.67
1:C:267:LEU:O	1:D:178:HIS:NE2	2.27	0.67
1:I:26:ALA:O	1:I:345:SER:OG	2.13	0.67
11:Y:258:GLN:OE1	11:Y:272:ARG:NH1	2.28	0.67
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
8:U:98:ALA:HB3	8:U:101:MET:HE3	1.76	0.66
12:f:279:LEU:HB3	12:f:283:ARG:HH12	1.60	0.66
12:m:829:LEU:HA	12:m:832:TYR:HB3	1.77	0.66
12:n:779:ILE:CG2	13:p:375:LEU:HD21	1.92	0.66
1:A:111:THR:HG22	1:A:142:GLN:HG2	1.77	0.66
2:H:220:ALA:HB1	2:H:226:GLU:HG3	1.78	0.66
13:h:426:HIS:CD2	13:h:427:LYS:HG2	2.29	0.66
1:E:229:GLN:HE22	1:E:264:ARG:HH22	1.44	0.66
12:f:363:HIS:HA	12:f:366:LYS:HE3	1.77	0.66
12:n:280:ASN:OD1	12:n:283:ARG:NH2	2.28	0.66
12:f:526:ALA:HB1	12:f:553:TYR:HD1	1.61	0.66
1:E:21:ILE:HG23	1:E:37:ASN:HB2	1.78	0.66
12:f:413:MET:HE2	12:f:466:MET:HE1	1.76	0.66
12:f:723:THR:OG1	12:f:736:LYS:NZ	2.25	0.65
12:m:648:ILE:HD13	12:m:753:LEU:HD11	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:305:THR:O	1:I:336:ARG:NH1	2.29	0.65
4:K:152:GLN:HG3	4:K:181:ILE:HB	1.78	0.65
12:e:283:ARG:HA	12:f:175:GLY:HA3	1.78	0.65
12:f:449:VAL:HG13	12:f:451:ARG:HD3	1.77	0.65
6:P:147:LEU:HD11	10:Z:1214:VAL:CG1	2.26	0.65
1:B:46:ARG:NH2	1:B:52:LEU:O	2.29	0.65
13:h:602:GLN:HG2	13:h:603:ILE:HD12	1.78	0.65
12:m:653:GLN:HG3	13:o:526:TYR:HE1	1.61	0.65
2:H:151:ILE:HB	2:H:293:LEU:HD12	1.79	0.65
5:L:45:GLN:NE2	5:L:46:PRO:HD2	2.12	0.65
12:n:255:GLU:HA	12:n:258:LYS:HD2	1.78	0.65
12:n:779:ILE:HG22	13:p:375:LEU:CD1	2.27	0.65
1:I:104:GLU:OE2	1:I:133:ASN:ND2	2.29	0.65
3:J:308:GLY:HA2	3:J:311:MET:HE3	1.77	0.65
8:U:113:VAL:O	8:U:115:ARG:NH2	2.30	0.65
8:U:118:ILE:HB	8:U:136:VAL:HG23	1.78	0.65
12:f:829:LEU:O	12:f:833:VAL:N	2.30	0.65
2:H:42:GLY:HA3	3:J:387:TRP:HA	1.79	0.65
12:m:695:THR:HG23	12:m:698:ILE:HD12	1.78	0.65
12:n:591:LEU:HD13	12:n:597:ILE:HG21	1.79	0.65
1:D:46:ARG:NH2	1:D:52:LEU:O	2.30	0.64
12:m:776:PRO:HB3	13:o:377:ALA:HA	1.78	0.64
6:N:210:THR:HA	10:W:1255:LYS:HZ1	1.60	0.64
13:o:386:CYS:HB3	13:o:437:MET:SD	2.37	0.64
4:K:204:VAL:HG21	5:L:232:TYR:HB3	1.78	0.64
12:m:436:ASP:HA	12:m:439:LYS:HD2	1.77	0.64
1:C:94:TYR:HE2	1:C:103:SER:HA	1.62	0.64
4:K:144:TYR:HB2	4:K:155:ILE:HB	1.79	0.64
5:L:62:CYS:HB2	5:L:133:LEU:HD21	1.80	0.64
6:M:378:VAL:HG21	6:N:375:LEU:HD22	1.80	0.64
12:m:257:GLN:HB3	12:m:261:LYS:HE2	1.79	0.64
1:B:336:ARG:NH2	6:P:84:GLU:O	2.30	0.64
12:e:777:PHE:HA	12:e:833:VAL:HG11	1.80	0.64
12:f:844:GLN:NE2	12:f:848:ASP:OD2	2.30	0.64
12:n:546:TRP:NE1	12:n:550:MET:HE3	2.13	0.64
1:C:144:VAL:HG13	1:C:145:LEU:HD12	1.79	0.64
6:N:340:ILE:HD12	6:N:344:HIS:HE1	1.63	0.64
12:f:716:ARG:HA	12:f:823:VAL:HA	1.79	0.64
1:F:10:GLN:O	1:F:106:HIS:ND1	2.30	0.64
1:G:112:GLU:OE2	1:G:121:ARG:NE	2.31	0.64
1:I:11:PRO:HB3	1:I:107:PRO:HG2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:652:LYS:HE2	12:f:756:LEU:HD22	1.80	0.64
12:f:740:LEU:HB3	12:f:742:GLU:HG2	1.79	0.64
12:n:569:ARG:HH12	12:n:600:ALA:HB1	1.62	0.64
1:G:76:GLU:OE1	1:G:188:ARG:NH1	2.31	0.64
12:f:790:ARG:HG3	12:f:794:LYS:HE3	1.80	0.64
13:p:386:CYS:HB3	13:p:437:MET:SD	2.37	0.64
1:C:366:ASP:HB2	1:C:370:SER:HB3	1.78	0.64
1:D:346:ILE:HG23	12:m:311:HIS:HA	1.80	0.63
3:J:150:PRO:HG2	3:J:160:CYS:HB2	1.79	0.63
12:f:516:ASP:OD2	12:f:567:ARG:NH2	2.29	0.63
13:h:328:VAL:O	13:h:367:ARG:NE	2.29	0.63
1:D:119:LYS:HA	1:D:122:GLU:HG2	1.81	0.63
4:K:186:ALA:N	4:K:216:VAL:O	2.30	0.63
13:o:531:MET:HE2	13:o:578:TRP:HD1	1.63	0.63
1:F:330:ILE:HB	6:N:20:TYR:HB2	1.80	0.63
12:f:661:TYR:HA	12:f:664:ARG:HD2	1.81	0.63
13:p:336:MET:HE1	13:p:353:TYR:HA	1.80	0.63
4:K:258:LEU:HD21	5:L:148:TRP:HB2	1.80	0.63
8:U:25:GLY:HA3	8:U:43:ALA:HB3	1.81	0.63
1:A:267:LEU:O	1:B:178:HIS:NE2	2.32	0.63
1:C:158:LEU:HD21	1:C:275:ILE:HD11	1.80	0.63
12:m:824:TRP:HA	12:m:829:LEU:HD11	1.80	0.63
12:n:716:ARG:NH1	12:n:820:ILE:O	2.31	0.63
2:H:174:ALA:HA	2:H:284:LYS:HD2	1.81	0.63
1:I:110:LEU:HD21	1:I:128:PHE:HE2	1.62	0.63
12:f:746:LEU:HD22	12:f:768:ALA:HB2	1.80	0.63
13:p:531:MET:HE2	13:p:578:TRP:HD1	1.63	0.63
12:f:753:LEU:HB3	12:f:758:PHE:HB2	1.81	0.63
12:e:717:ILE:CA	12:e:824:TRP:CG	2.77	0.63
12:m:152:PHE:O	12:m:157:VAL:N	2.27	0.63
13:o:336:MET:HE1	13:o:353:TYR:HA	1.80	0.63
1:B:156:VAL:HG23	1:B:294:LEU:HD12	1.81	0.62
9:V:143:PHE:HA	9:V:157:LEU:HB2	1.81	0.62
13:o:402:SER:OG	13:o:404:ASP:OD1	2.15	0.62
1:C:141:MET:O	1:C:145:LEU:HD13	1.99	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
1:F:358:VAL:HG22	1:F:374:LYS:HD2	1.81	0.62
6:P:322:ARG:NH2	10:W:1114:HIS:HA	2.14	0.62
12:m:341:LEU:HA	12:m:360:ILE:HD11	1.80	0.62
1:F:112:GLU:HG2	1:F:139:ILE:HD11	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:151:GLN:NE2	4:K:181:ILE:O	2.32	0.62
12:f:121:ARG:H	12:f:135:LEU:HA	1.65	0.62
12:f:306:HIS:O	12:f:308:LYS:NZ	2.31	0.62
12:f:401:LEU:HD12	12:f:409:PHE:HB2	1.80	0.62
12:f:619:LEU:HD12	12:f:622:LYS:HD2	1.81	0.62
1:B:164:VAL:HG23	1:B:184:ASP:HA	1.82	0.62
1:C:148:TYR:CE2	1:C:347:LEU:HD12	2.34	0.62
1:E:245:ASP:H	1:G:288:MET:HE1	1.64	0.62
12:n:748:LYS:CE	13:p:383:PRO:CD	2.77	0.62
12:n:279:LEU:HB3	12:n:283:ARG:HH12	1.65	0.62
1:A:39:VAL:HG21	1:A:85:ASP:HB3	1.82	0.62
1:E:244:PRO:O	1:G:292:ARG:NH1	2.32	0.62
6:N:13:ALA:O	6:N:14:ARG:NE	2.29	0.62
12:e:270:THR:O	12:e:274:GLU:N	2.25	0.62
12:f:653:GLN:HB3	12:f:656:ARG:HH21	1.65	0.62
11:Y:54:CYS:O	11:Y:54:CYS:SG	2.57	0.62
12:m:591:LEU:HD23	12:m:597:ILE:HG21	1.80	0.62
13:h:402:SER:OG	13:h:404:ASP:OD1	2.14	0.62
12:n:673:TRP:HA	12:n:676:HIS:HD2	1.63	0.62
1:C:57:PHE:HA	1:C:61:LYS:HE2	1.82	0.62
1:D:303:GLY:HA3	14:D:800:ADP:H5'2	1.81	0.62
1:G:154:THR:HG23	1:G:171:TYR:HA	1.81	0.62
12:n:266:PRO:HB3	12:n:376:ARG:HG3	1.82	0.62
1:E:154:THR:HG23	1:E:171:TYR:HA	1.82	0.62
2:H:207:GLU:OE2	2:H:210:ARG:NH2	2.33	0.62
9:V:38:GLY:HA3	9:V:59:ARG:HA	1.82	0.62
12:f:351:ASP:OD2	12:f:355:GLN:NE2	2.32	0.62
12:n:227:PRO:HB2	12:n:299:LEU:HD22	1.82	0.62
13:p:551:LEU:O	13:p:562:THR:N	2.33	0.62
1:C:51:ALA:HB2	1:E:173:GLY:HA3	1.80	0.61
2:H:106:THR:HB	2:H:137:GLN:HG2	1.82	0.61
1:I:199:ARG:NH1	3:J:145:GLU:OE1	2.33	0.61
5:L:49:ILE:HD11	5:L:58:ASP:HB3	1.81	0.61
11:Y:42:VAL:HG23	11:Y:284:CYS:HA	1.82	0.61
12:n:699:PHE:HD1	12:n:753:LEU:HD23	1.65	0.61
1:A:48:MET:HE2	1:A:48:MET:HA	1.81	0.61
12:n:598:ARG:O	12:n:602:ARG:HG3	2.00	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	1.82	0.61
2:H:261:LEU:HB3	2:H:274:ILE:HD13	1.81	0.61
6:Q:63:ARG:HH21	10:Z:1209:LYS:HZ3	1.47	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:464:ASP:OD2	12:f:467:ARG:NH2	2.32	0.61
13:h:555:ASN:ND2	13:h:610:GLU:OE1	2.32	0.61
12:m:738:ASN:HB3	12:m:824:TRP:HE1	1.65	0.61
12:n:437:ILE:HA	12:n:441:LYS:HZ1	1.65	0.61
12:f:656:ARG:NH1	12:f:657:GLN:OE1	2.28	0.61
12:m:283:ARG:HD3	12:n:175:GLY:HA3	1.82	0.61
12:m:351:ASP:OD1	12:m:352:LYS:N	2.33	0.61
12:n:561:GLU:HB3	12:n:596:HIS:HD2	1.64	0.61
5:L:147:CYS:HB3	5:L:176:TRP:HB3	1.83	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
7:O:47:ILE:O	7:O:51:ARG:N	2.33	0.61
1:G:268:ILE:HG23	1:G:270:GLU:OE1	2.01	0.61
1:E:56:ILE:HD13	1:E:88:ARG:HD3	1.82	0.61
3:J:329:LYS:HD3	3:J:331:LYS:H	1.66	0.61
12:f:718:PHE:HB3	12:f:735:LEU:HD11	1.82	0.61
6:M:345:GLU:HA	6:M:348:MET:HE2	1.83	0.60
6:Q:178:ARG:HA	6:Q:181:LEU:HG	1.82	0.60
9:V:3:LEU:HD13	11:Y:5:LEU:HD13	1.83	0.60
12:n:748:LYS:HZ3	13:p:383:PRO:HG2	0.79	0.60
1:F:99:LEU:HD12	1:F:101:THR:H	1.66	0.60
1:I:87:GLU:O	1:I:91:GLN:HG2	2.02	0.60
1:I:270:GLU:OE2	3:J:159:ASN:ND2	2.32	0.60
1:E:46:ARG:NH2	1:E:54:GLY:O	2.34	0.60
9:V:98:VAL:HB	9:V:115:VAL:HG22	1.83	0.60
12:f:454:PRO:HB2	12:f:457:ARG:HB2	1.82	0.60
12:m:744:ILE:HG22	12:m:748:LYS:HE3	1.84	0.60
13:o:508:LEU:O	13:o:517:LEU:N	2.35	0.60
13:p:508:LEU:O	13:p:517:LEU:N	2.35	0.60
1:A:22:LYS:NZ	14:A:800:ADP:O1B	2.33	0.60
1:E:20:VAL:O	1:E:22:LYS:NZ	2.34	0.60
1:E:357:TRP:HZ3	1:E:359:SER:HA	1.66	0.60
1:I:9:ASN:ND2	1:I:105:GLU:O	2.30	0.60
1:C:141:MET:HA	1:C:141:MET:HE3	1.83	0.60
1:C:58:ILE:O	1:C:61:LYS:NZ	2.34	0.60
1:F:200:LYS:NZ	1:G:116:ASN:O	2.35	0.60
1:G:150:THR:HB	1:G:152:ARG:HD3	1.84	0.60
10:W:1255:LYS:NZ	10:W:1256:VAL:O	2.35	0.60
12:m:454:PRO:HB2	12:m:457:ARG:HG2	1.84	0.60
13:o:551:LEU:O	13:o:562:THR:N	2.33	0.60
13:p:335:VAL:HG22	13:p:352:THR:HG22	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:331:SER:HA	6:Q:19:VAL:HG12	1.83	0.60
3:J:279:SER:N	3:J:282:THR:OG1	2.31	0.60
12:e:403:HIS:HA	12:e:532:GLU:HA	1.83	0.60
12:n:751:ARG:NH2	13:p:403:THR:OG1	2.34	0.60
1:A:185:ILE:HD11	1:A:270:GLU:HG2	1.82	0.59
9:V:47:ILE:HB	9:V:68:VAL:HG23	1.84	0.59
13:h:365:ASN:O	13:h:367:ARG:NH1	2.34	0.59
1:A:284:GLN:NE2	5:L:231:ILE:HG12	2.16	0.59
1:C:56:ILE:HD13	1:C:88:ARG:HD3	1.84	0.59
1:D:318:VAL:HG12	1:D:328:ILE:HD13	1.83	0.59
1:I:181:MET:HG2	1:I:282:ALA:HB2	1.83	0.59
12:e:716:ARG:C	12:e:824:TRP:HE1	2.08	0.59
5:L:70:SER:HA	5:L:81:PRO:HD2	1.83	0.59
1:I:41:ARG:O	1:I:70:SER:N	2.34	0.59
8:U:55:LEU:HD11	8:U:89:VAL:HG13	1.84	0.59
12:f:480:ILE:HG23	12:f:484:LEU:HB2	1.85	0.59
12:m:579:ASN:ND2	13:o:559:GLU:O	2.36	0.59
12:m:653:GLN:O	12:m:657:GLN:HG2	2.02	0.59
13:p:546:MET:HE1	13:p:548:ARG:HH21	1.67	0.59
1:G:200:LYS:NZ	2:H:111:ASN:O	2.33	0.59
1:I:253:PRO:O	1:I:257:ARG:HG2	2.03	0.59
1:F:28:ASP:HB2	1:F:341:TRP:HH2	1.67	0.59
5:L:181:LYS:O	5:L:185:GLY:N	2.32	0.59
9:V:28:LEU:HD13	9:V:34:ILE:HD11	1.83	0.59
12:f:480:ILE:HG21	12:f:520:ILE:HG12	1.84	0.59
13:h:457:TYR:HE1	13:h:471:MET:HG2	1.67	0.59
13:p:513:ASN:HD21	13:p:515:LYS:HE3	1.67	0.59
1:C:189:ASP:OD1	1:C:192:ARG:NH2	2.35	0.59
1:D:121:ARG:NH1	1:D:375:THR:OG1	2.36	0.59
4:K:228:PHE:O	4:K:232:ILE:HG12	2.02	0.59
8:U:20:GLU:HG3	8:U:37:PRO:HB3	1.83	0.59
1:B:325:ASP:HA	6:P:93:GLU:H	1.68	0.59
3:J:92:ILE:HD11	3:J:358:GLY:HA3	1.84	0.59
4:K:259:ARG:HH11	5:L:225:ARG:HD2	1.68	0.59
12:m:153:ILE:O	12:m:158:ALA:N	2.34	0.59
12:n:755:TRP:CH2	13:p:453:GLU:C	2.72	0.59
1:B:153:THR:HB	1:B:172:GLU:HA	1.85	0.59
1:B:176:MET:HE1	4:K:265:THR:HG22	1.85	0.59
1:D:141:MET:HE2	1:D:168:VAL:HG21	1.84	0.59
2:H:332:PRO:O	2:H:335:ARG:NH1	2.35	0.59
5:L:72:ARG:HE	5:L:79:TYR:HE2	1.49	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:194:THR:O	5:L:195:ARG:NH1	2.35	0.59
12:m:822:LEU:HD21	12:m:828:LYS:HD3	1.85	0.59
12:n:396:LEU:HD11	12:n:463:LEU:HD11	1.84	0.59
13:p:438:SER:OG	13:p:484:CYS:N	2.36	0.59
1:A:356:MET:HE1	5:L:258:LEU:HB3	1.85	0.59
1:C:6:VAL:O	1:C:9:ASN:ND2	2.35	0.59
2:H:24:ASP:HB2	2:H:340:TRP:HH2	1.67	0.59
1:B:49:ALA:N	1:D:148:TYR:OH	2.34	0.58
12:f:212:ILE:HG21	12:f:235:LYS:HE2	1.85	0.58
12:m:601:ILE:HG22	12:m:605:GLN:HG3	1.85	0.58
12:n:375:GLN:HG3	12:n:447:LYS:HD3	1.85	0.58
12:n:546:TRP:HE1	12:n:550:MET:HE3	1.68	0.58
13:o:438:SER:OG	13:o:484:CYS:N	2.36	0.58
1:B:87:GLU:HA	1:B:90:TRP:HE3	1.66	0.58
4:K:161:HIS:HE1	4:K:163:PHE:HB3	1.68	0.58
7:O:82:SER:HB2	10:W:1108:HIS:HB2	1.85	0.58
12:f:652:LYS:HG3	12:f:695:THR:HG21	1.84	0.58
13:h:610:GLU:OE2	13:h:613:ARG:NH1	2.36	0.58
12:n:215:ASN:O	12:n:218:LYS:HG3	2.03	0.58
13:o:335:VAL:HG22	13:o:352:THR:HG22	1.84	0.58
3:J:311:MET:HE2	3:J:350:ALA:HB3	1.85	0.58
4:K:42:ASN:HB3	4:K:45:LEU:HB3	1.83	0.58
11:Y:45:GLU:N	11:Y:281:SER:O	2.35	0.58
12:f:605:GLN:HA	12:f:608:LEU:HB2	1.84	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
1:G:18:SER:HB2	1:G:162:ASP:HB3	1.85	0.58
13:o:280:ARG:NH1	13:o:300:ASN:O	2.34	0.58
1:A:43:LYS:NZ	1:A:69:LEU:O	2.32	0.58
12:f:335:LEU:HD23	12:f:366:LYS:HB2	1.85	0.58
12:m:710:ASN:HA	12:m:767:LYS:HZ1	1.68	0.58
12:n:573:GLY:HA3	13:o:394:ASN:HB3	1.85	0.58
13:o:513:ASN:HD21	13:o:515:LYS:HE3	1.67	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:175:LEU:HD23	3:J:179:LEU:HD23	1.85	0.58
12:n:675:ASN:O	12:n:680:GLN:NE2	2.36	0.58
2:H:283:MET:O	2:H:290:ARG:NH2	2.36	0.58
1:B:14:ILE:HD13	1:B:108:VAL:HG23	1.84	0.58
1:E:60:PRO:HA	1:E:63:GLU:HG2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:243:LEU:HD11	1:E:249:ILE:HD12	1.86	0.58
1:E:354:LYS:HA	1:E:357:TRP:CD1	2.38	0.58
1:F:154:THR:HG22	1:F:172:GLU:H	1.69	0.58
1:G:108:VAL:HG12	1:G:134:VAL:HG11	1.85	0.58
3:J:342:ARG:NH2	11:Y:228:ALA:O	2.37	0.58
6:N:399:ARG:HD3	7:O:172:LEU:HB3	1.86	0.58
6:Q:214:HIS:HB3	10:Z:1250:THR:HB	1.86	0.58
12:n:465:GLN:HB3	12:n:546:TRP:HH2	1.69	0.58
1:F:76:GLU:HG2	1:F:77:HIS:HD2	1.68	0.58
3:J:122:PRO:HG2	3:J:125:LEU:HB3	1.84	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
12:f:519:ALA:HB1	12:f:560:VAL:HG23	1.84	0.58
12:m:332:TYR:HB3	12:m:336:MET:HE1	1.84	0.58
1:A:14:ILE:HD13	1:A:108:VAL:HG13	1.86	0.58
1:E:48:MET:HE2	1:G:173:GLY:CA	2.33	0.58
12:f:264:ARG:HH21	12:f:274:GLU:HB2	1.69	0.58
12:f:375:GLN:HA	12:f:378:LEU:HD12	1.85	0.58
12:f:638:VAL:HG22	13:h:300:ASN:HD21	1.69	0.58
12:m:578:ALA:HA	12:m:581:MET:CE	2.28	0.58
12:m:583:ARG:NH1	13:o:518:TYR:OH	2.37	0.58
13:o:546:MET:HE1	13:o:548:ARG:HH21	1.67	0.57
1:C:68:LEU:HD11	1:E:171:TYR:CD2	2.39	0.57
6:P:262:MET:HE1	7:R:33:VAL:HA	1.86	0.57
12:f:284:ALA:HA	12:f:287:ARG:HD2	1.87	0.57
13:h:409:SER:N	13:h:420:ASP:O	2.25	0.57
1:C:224:LEU:HD22	1:C:310:PHE:HA	1.86	0.57
12:e:80:GLU:HA	12:e:115:SER:HA	1.87	0.57
12:f:275:ILE:HA	12:f:336:MET:CE	2.33	0.57
12:f:482:ARG:NH1	12:f:587:ARG:O	2.37	0.57
13:o:391:GLY:HA3	13:o:396:HIS:HA	1.86	0.57
1:I:227:ASN:HB3	1:I:230:LYS:HE3	1.86	0.57
6:M:56:TYR:O	6:M:60:LYS:HB2	2.05	0.57
12:f:588:PHE:HB3	12:f:591:LEU:HD11	1.85	0.57
12:m:402:MET:HE3	12:m:466:MET:HE1	1.85	0.57
1:D:141:MET:HB3	1:D:144:VAL:HG22	1.85	0.57
6:M:328:SER:O	10:Z:1125:LYS:NZ	2.36	0.57
12:m:748:LYS:O	12:m:752:ASN:ND2	2.38	0.57
12:n:266:PRO:HB2	12:n:379:ARG:HB2	1.85	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	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:85:GLN:HG3	10:W:1105:MET:HB2	1.87	0.57
11:Y:340:VAL:HA	11:Y:373:VAL:HG12	1.85	0.57
12:n:334:PRO:HA	12:n:337:LYS:HZ2	1.70	0.57
1:G:141:MET:HE3	1:G:141:MET:HA	1.87	0.57
6:N:374:LEU:HD21	10:Z:1168:ASN:HB3	1.85	0.57
13:h:525:ASP:OD2	13:h:546:MET:N	2.38	0.57
12:n:457:ARG:HA	12:n:460:GLN:HB3	1.86	0.57
1:E:335:GLU:OE1	1:E:335:GLU:N	2.38	0.57
3:J:212:VAL:HG21	11:Y:252:LEU:HD12	1.85	0.57
5:L:62:CYS:SG	5:L:63:ASP:N	2.78	0.57
11:Y:6:GLN:HB3	11:Y:9:ARG:HG3	1.86	0.57
12:m:39:PRO:O	12:m:46:GLY:N	2.37	0.57
4:K:240:GLN:NE2	5:L:244:ARG:O	2.31	0.57
12:m:648:ILE:HA	12:m:695:THR:HG21	1.87	0.57
12:n:252:TRP:O	12:n:256:ILE:HG12	2.05	0.57
1:D:104:GLU:HG2	1:D:133:ASN:HB2	1.87	0.57
1:D:164:VAL:HG23	1:D:184:ASP:HA	1.87	0.57
2:H:204:ALA:O	2:H:208:ILE:HD12	2.04	0.57
4:K:182:THR:HG22	4:K:184:PRO:HD2	1.87	0.57
6:P:308:ASP:O	6:P:311:SER:OG	2.19	0.57
11:Y:77:PRO:HD3	11:Y:271:PRO:HB3	1.87	0.57
1:D:156:VAL:HG11	1:D:283:ILE:HD11	1.87	0.56
1:F:354:LYS:HA	1:F:357:TRP:NE1	2.19	0.56
5:L:167:TYR:N	5:L:199:LYS:O	2.31	0.56
12:f:220:CYS:O	12:f:225:GLU:N	2.37	0.56
13:h:390:VAL:HG11	13:h:439:PHE:CE2	2.39	0.56
12:m:739:PHE:HE2	12:m:744:ILE:HD11	1.70	0.56
5:L:74:PRO:O	5:L:94:ARG:NH1	2.38	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
6:M:185:ALA:HA	7:R:127:GLN:HG2	1.88	0.56
11:Y:52:PRO:HD3	11:Y:277:LEU:HD23	1.88	0.56
12:e:165:ILE:O	12:e:171:ALA:N	2.38	0.56
12:m:220:CYS:HA	12:m:223:ARG:HE	1.71	0.56
12:n:751:ARG:NH1	13:p:382:HIS:CD2	2.73	0.56
12:n:751:ARG:NH1	13:p:403:THR:C	2.64	0.56
12:n:772:ASN:OD1	13:p:382:HIS:NE2	2.39	0.56
13:o:280:ARG:NH1	13:o:310:ASP:O	2.38	0.56
13:p:280:ARG:NH1	13:p:310:ASP:O	2.38	0.56
13:p:391:GLY:HA3	13:p:396:HIS:HA	1.86	0.56
1:G:238:LYS:HB3	1:G:250:GLU:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:187:ASP:HA	2:H:190:MET:HG2	1.88	0.56
11:Y:374:LEU:HA	11:Y:405:ASN:HB3	1.86	0.56
12:n:669:LEU:HD13	12:n:676:HIS:HB2	1.86	0.56
13:p:276:TRP:HB3	13:p:312:VAL:HG11	1.87	0.56
1:I:116:ASN:HB2	1:I:121:ARG:HH12	1.70	0.56
3:J:19:ASP:HB3	3:J:26:LYS:HB2	1.87	0.56
6:P:316:LEU:HG	6:Q:317:TYR:CZ	2.40	0.56
6:Q:270:ALA:O	6:Q:273:SER:OG	2.22	0.56
12:n:226:LYS:HE3	12:n:227:PRO:HD2	1.87	0.56
1:D:108:VAL:HG11	1:D:128:PHE:CE2	2.40	0.56
6:P:90:MET:HE2	6:P:90:MET:HA	1.87	0.56
11:Y:124:ALA:O	11:Y:126:LYS:NZ	2.38	0.56
13:h:284:CYS:HA	13:h:575:ARG:HG2	1.87	0.56
12:n:751:ARG:CZ	13:p:403:THR:CB	2.82	0.56
1:C:244:PRO:O	1:E:292:ARG:NH1	2.39	0.56
1:D:366:ASP:HB3	1:D:370:SER:HB3	1.87	0.56
1:G:16:ASN:HA	1:G:21:ILE:HG22	1.88	0.56
8:U:46:GLY:N	8:U:64:ASN:OD1	2.31	0.56
10:Z:1204:SER:HA	10:Z:1207:ILE:HG12	1.88	0.56
13:o:299:TYR:HB2	13:o:312:VAL:HB	1.86	0.56
1:G:13:VAL:HG21	1:G:345:SER:HA	1.86	0.56
5:L:145:LYS:O	5:L:178:GLN:N	2.38	0.56
13:h:271:PHE:HB2	13:h:594:ILE:HB	1.88	0.56
12:n:480:ILE:HA	12:n:484:LEU:HD23	1.87	0.56
1:B:113:ALA:HB3	1:B:116:ASN:HD21	1.71	0.56
1:E:43:LYS:NZ	1:E:67:GLY:O	2.38	0.56
1:E:283:ILE:O	1:E:286:SER:OG	2.23	0.56
1:G:355:LYS:HB2	6:M:63:ARG:HH22	1.71	0.56
2:H:157:ASP:N	15:H:401:ATP:O2B	2.28	0.56
3:J:137:MET:HG2	3:J:299:LEU:HB3	1.87	0.56
6:Q:167:ASN:OD1	6:Q:168:LEU:N	2.38	0.56
12:f:582:PHE:CG	12:f:664:ARG:HG2	2.41	0.56
12:m:816:ILE:O	12:m:820:ILE:HG12	2.06	0.56
13:o:276:TRP:HB3	13:o:312:VAL:HG11	1.87	0.56
13:p:299:TYR:HB2	13:p:312:VAL:HB	1.86	0.56
13:p:342:LYS:NZ	13:p:388:ASN:OD1	2.30	0.56
1:B:144:VAL:HG12	1:B:148:TYR:HE2	1.70	0.56
2:H:182:GLY:HA2	2:H:185:LEU:HD12	1.87	0.56
1:I:107:PRO:HB3	1:I:136:ALA:HB3	1.87	0.56
3:J:39:ILE:HD13	3:J:79:HIS:CD2	2.40	0.56
6:M:396:ILE:O	6:M:400:MET:HG3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:h:394:ASN:O	12:m:599:GLY:HA3	2.06	0.56
12:m:717:ILE:HD13	12:m:829:LEU:HD22	1.86	0.56
12:m:718:PHE:HB3	12:m:820:ILE:HD13	1.88	0.56
5:L:9:ALA:HB1	5:L:28:LEU:HD21	1.88	0.55
6:P:320:ILE:HG22	7:R:94:ILE:HD11	1.88	0.55
12:m:245:LEU:HB3	12:m:304:LEU:HD21	1.86	0.55
12:m:365:ARG:HD2	12:m:429:LYS:HE2	1.87	0.55
12:m:426:GLU:OE1	12:m:429:LYS:NZ	2.26	0.55
12:n:660:ALA:O	12:n:664:ARG:HG2	2.06	0.55
12:n:696:GLN:HA	12:n:758:PHE:CE1	2.41	0.55
1:B:356:MET:HE1	4:K:277:TYR:CD1	2.41	0.55
1:D:354:LYS:HA	1:D:357:TRP:NE1	2.21	0.55
1:I:13:VAL:O	1:I:341:TRP:NE1	2.38	0.55
4:K:183:PRO:HA	4:K:218:VAL:HB	1.88	0.55
12:e:283:ARG:HA	12:f:176:ASP:H	1.71	0.55
12:f:439:LYS:HA	12:f:442:ARG:HG2	1.88	0.55
13:h:457:TYR:HB3	13:h:468:ILE:HG23	1.88	0.55
12:n:334:PRO:HA	12:n:337:LYS:NZ	2.21	0.55
13:p:573:LEU:HA	13:p:589:ASP:HA	1.88	0.55
1:D:267:LEU:O	1:E:178:HIS:NE2	2.39	0.55
1:G:334:GLN:HE22	6:M:49:ILE:HA	1.71	0.55
1:I:354:LYS:HA	1:I:357:TRP:NE1	2.20	0.55
6:M:330:LEU:O	6:M:334:VAL:HG23	2.06	0.55
12:e:152:PHE:O	12:e:157:VAL:N	2.35	0.55
13:h:409:SER:HB3	13:h:420:ASP:HB3	1.88	0.55
12:m:269:GLY:O	12:m:386:ARG:NH2	2.38	0.55
12:n:278:TRP:HE1	12:n:376:ARG:HH21	1.54	0.55
1:A:25:PHE:HZ	1:A:101:THR:HG21	1.70	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
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
10:W:1272:LEU:HB3	10:W:1276:GLN:HB3	1.87	0.55
12:f:274:GLU:OE2	12:f:278:TRP:NE1	2.35	0.55
12:m:333:ASN:O	12:m:337:LYS:HG2	2.06	0.55
12:m:373:PRO:HB2	12:m:376:ARG:HB2	1.87	0.55
12:m:474:GLU:OE1	12:m:477:ARG:NH2	2.38	0.55
12:m:575:ALA:HB1	12:m:581:MET:SD	2.47	0.55
13:p:402:SER:OG	13:p:404:ASP:OD1	2.15	0.55
1:A:243:LEU:HD12	1:A:247:SER:HB2	1.88	0.55
1:B:10:GLN:HG2	12:n:246:GLN:NE2	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:LEU:HG	1:E:172:GLU:OE2	2.06	0.55
1:D:14:ILE:HD13	1:D:108:VAL:HG13	1.89	0.55
1:E:355:LYS:HD2	6:P:356:HIS:CE1	2.41	0.55
1:F:176:MET:HA	1:F:176:MET:HE3	1.88	0.55
2:H:43:VAL:HG11	3:J:156:PRO:HG2	1.88	0.55
2:H:123:MET:HE2	2:H:123:MET:N	2.21	0.55
4:K:164:GLN:HG3	4:K:167:ASN:H	1.72	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
12:f:711:LEU:HD12	12:f:746:LEU:HD12	1.89	0.55
12:m:649:ILE:O	12:m:653:GLN:HG2	2.05	0.55
12:n:751:ARG:NH1	13:p:403:THR:OG1	2.38	0.55
1:G:330:ILE:HG22	6:M:45:VAL:HG23	1.87	0.55
2:H:214:GLU:HG2	15:H:401:ATP:C4	2.42	0.55
1:I:263:PHE:HD2	1:I:276:HIS:HD2	1.53	0.55
6:P:354:LEU:HD22	7:R:126:LEU:HD11	1.87	0.55
12:f:350:LEU:HD13	12:f:353:ILE:HD12	1.87	0.55
12:f:413:MET:HE1	12:f:467:ARG:HA	1.88	0.55
12:m:601:ILE:HD12	12:m:604:TYR:OH	2.07	0.55
12:n:438:VAL:HG13	12:n:444:GLU:HB2	1.88	0.55
1:E:48:MET:HE1	1:G:153:THR:HB	1.89	0.55
1:E:112:GLU:OE1	1:E:112:GLU:N	2.38	0.55
1:F:335:GLU:N	1:F:335:GLU:OE1	2.40	0.55
12:f:620:HIS:HD2	12:f:689:PHE:HB2	1.71	0.55
3:J:216:PHE:HE1	3:J:243:PRO:HG3	1.72	0.55
12:f:378:LEU:HD13	12:f:450:TRP:HA	1.88	0.55
13:h:291:TYR:HB3	13:h:294:LEU:HD23	1.89	0.55
2:H:188:TYR:HB2	2:H:267:LEU:HD21	1.88	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	2.07	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
12:f:620:HIS:ND1	12:f:624:LYS:HE3	2.22	0.55
12:m:119:ILE:O	12:m:136:ARG:N	2.40	0.55
12:m:479:VAL:O	12:m:483:VAL:HG22	2.07	0.55
12:m:568:LEU:HD21	12:m:597:ILE:HG23	1.89	0.55
1:C:10:GLN:OE1	10:Z:1234:PHE:HB3	2.07	0.55
1:E:77:HIS:CE1	1:E:184:ASP:HB3	2.42	0.55
3:J:209:ASP:OD2	3:J:248:TYR:OH	2.25	0.55
12:e:483:VAL:O	12:e:512:PHE:N	2.40	0.55
13:h:270:GLN:NE2	13:h:594:ILE:O	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:n:467:ARG:HD3	12:n:471:ARG:HH22	1.70	0.55
13:o:573:LEU:HA	13:o:589:ASP:HA	1.88	0.55
13:p:510:THR:HG22	13:p:512:LYS:H	1.72	0.55
1:B:74:PRO:HG3	1:B:89:ILE:HD12	1.88	0.54
1:G:355:LYS:HB2	6:M:63:ARG:NH2	2.22	0.54
12:f:365:ARG:HH22	12:f:430:LEU:HD22	1.72	0.54
12:f:575:ALA:HB1	12:f:580:GLU:HB3	1.89	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
1:G:76:GLU:HG3	1:G:77:HIS:CD2	2.43	0.54
6:P:336:ARG:O	6:P:340:ILE:HG12	2.08	0.54
12:e:777:PHE:CB	12:e:824:TRP:HZ3	2.21	0.54
12:f:357:LEU:HD21	12:f:423:TRP:HB2	1.88	0.54
12:n:446:LEU:HD12	12:n:447:LYS:HB2	1.89	0.54
12:n:608:LEU:HD13	12:n:668:VAL:HG22	1.88	0.54
12:n:776:PRO:CA	13:p:375:LEU:O	2.53	0.54
13:o:602:GLN:HG2	13:o:603:ILE:HG13	1.89	0.54
4:K:275:LEU:HD21	5:L:211:ALA:HB2	1.90	0.54
5:L:22:GLU:HG2	5:L:45:GLN:NE2	2.23	0.54
12:m:372:TYR:OH	12:m:376:ARG:NH1	2.33	0.54
12:n:457:ARG:NH1	12:n:458:LYS:HB2	2.22	0.54
1:C:371:ILE:O	1:C:375:THR:OG1	2.21	0.54
1:I:71:ILE:HD12	1:I:209:SER:HA	1.89	0.54
8:U:112:TYR:OH	8:U:115:ARG:NH1	2.40	0.54
12:f:555:GLU:OE1	12:f:559:ARG:NH2	2.38	0.54
13:g:409:SER:O	13:g:419:GLN:N	2.40	0.54
12:m:232:PHE:HB3	12:m:235:LYS:HB2	1.90	0.54
12:m:484:LEU:HD12	12:m:516:ASP:HA	1.90	0.54
13:o:536:HIS:HA	13:o:606:PRO:HG3	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
2:H:149:THR:HG23	2:H:166:TYR:HA	1.90	0.54
2:H:352:PHE:HA	2:H:355:MET:HE2	1.89	0.54
3:J:68:LEU:HD13	3:J:105:LEU:HD23	1.90	0.54
5:L:16:LEU:HD13	5:L:24:ASN:HB3	1.88	0.54
6:Q:7:ALA:HA	6:Q:14:ARG:NH2	2.22	0.54
13:o:510:THR:HG22	13:o:512:LYS:H	1.72	0.54
1:B:42:PRO:HA	1:B:69:LEU:HA	1.89	0.54
1:B:145:LEU:HA	1:B:148:TYR:CD2	2.38	0.54
3:J:26:LYS:HB3	3:J:355:TRP:CD1	2.43	0.54
13:h:551:LEU:O	13:h:562:THR:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:n:269:GLY:O	12:n:386:ARG:NH2	2.40	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
4:K:94:ILE:HA	4:K:110:PRO:HA	1.90	0.54
6:Q:63:ARG:HE	10:Z:1209:LYS:NZ	2.02	0.54
11:Y:255:ARG:NH1	11:Y:264:ILE:HA	2.23	0.54
12:m:375:GLN:NE2	12:m:448:MET:SD	2.71	0.54
12:m:529:ASN:HB3	12:m:552:ARG:HH21	1.73	0.54
12:m:734:LYS:O	12:m:736:LYS:NZ	2.41	0.54
12:n:361:PHE:O	12: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
3:J:362:GLY:HA2	3:J:368:LEU:HD21	1.90	0.54
6:P:163:ASP:OD1	6:Q:223:SER:HB3	2.08	0.54
12:m:395:VAL:O	12:m:398:THR:OG1	2.19	0.54
12:n:522:GLU:HB3	12:n:556:ARG:HG2	1.90	0.54
13:p:602:GLN:HG2	13:p:603:ILE:HG13	1.89	0.54
1:F:346:ILE:HG12	12:f:311:HIS:HB3	1.89	0.54
2:H:214:GLU:HG2	15:H:401:ATP:C5	2.42	0.54
6:Q:172:ASP:HA	6:Q:175:LEU:HB2	1.90	0.54
11:Y:162:ARG:HG2	11:Y:166:LYS:HZ2	1.72	0.54
10:Z:1267:ARG:HG2	10:Z:1269:ARG:NH2	2.20	0.54
12:f:279:LEU:HB3	12:f:283:ARG:NH1	2.23	0.54
12:f:382:GLU:HG3	12:f:452:ILE:HD12	1.89	0.54
12:f:529:ASN:O	12:f:552:ARG:NH2	2.38	0.54
12:f:539:SER:O	12:f:543:THR:N	2.37	0.54
12:f:638:VAL:HG21	13:h:281:VAL:HG11	1.89	0.54
12:m:714:SER:O	12:m:738:ASN:ND2	2.41	0.54
1:F:9:ASN:HB3	1:F:106:HIS:CE1	2.43	0.54
5:L:142:LYS:HG3	5:L:144:ILE:H	1.72	0.54
5:L:187:MET:HA	5:L:187:MET:HE2	1.88	0.54
6:P:184:GLU:HG2	10:Z:1283:ARG:HH22	1.72	0.54
12:m:639:ARG:NH2	13:o:574:ASN:OD1	2.41	0.54
1:F:264:ARG:NH1	6:M:75:ILE:O	2.41	0.53
4:K:56:GLN:HA	4:K:59:MET:HE2	1.91	0.53
6:M:155:HIS:O	6:M:160:LEU:N	2.33	0.53
8:U:108:GLU:OE1	8:U:127:ALA:N	2.41	0.53
12:f:805:VAL:HG11	12:f:847:VAL:HG22	1.90	0.53
1:A:287:ASP:N	1:A:287:ASP:OD1	2.39	0.53
8:U:58:GLU:OE1	9:V:49:ARG:NH1	2.33	0.53
12:m:374:ILE:HD12	12:m:434:LEU:HD22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:p:536:HIS:HA	13:p:606:PRO:HG3	1.90	0.53
2:H:105:LEU:HG	2:H:132:MET:HE1	1.90	0.53
2:H:110:LEU:O	2:H:177:ARG:NH1	2.40	0.53
2:H:159:VAL:HG12	2:H:179:ASP:HA	1.90	0.53
3:J:247:ASP:OD1	3:J:257:HIS:ND1	2.28	0.53
11:Y:69:ARG:HH12	11:Y:272:ARG:NE	2.07	0.53
11:Y:255:ARG:HH12	11:Y:264:ILE:HA	1.72	0.53
13:h:380:HIS:NE2	13:h:400:SER:OG	2.40	0.53
13:h:390:VAL:HG11	13:h:439:PHE:CD2	2.43	0.53
13:p:280:ARG:NH1	13:p:300:ASN:O	2.34	0.53
13:p:384:VAL:HA	13:p:402:SER: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
12:f:349:GLU:HG3	12:f:352:LYS:H	1.74	0.53
12:m:254:ARG:O	12:m:258:LYS:HG3	2.08	0.53
1:C:75:MET:HE3	1:C:76:GLU:N	2.23	0.53
1:E:203:TYR:CE2	1:E:249:ILE:HG23	2.44	0.53
1:G:48:MET:HA	1:G:48:MET:HE2	1.90	0.53
6:P:3:ASP:HA	6:P:6:TYR:CE1	2.43	0.53
11:Y:51:CYS:SG	11:Y:54:CYS:N	2.78	0.53
12:e:753:LEU:O	12:e:757:GLY:N	2.40	0.53
13:o:384:VAL:HA	13:o:402:SER:HA	1.90	0.53
1:C:362:GLU:OE2	1:C:373:ARG:NH2	2.42	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
5:L:155:GLU:OE2	5:L:168:LYS:HG2	2.09	0.53
1:C:39:VAL:HG21	1:C:85:ASP:HB3	1.90	0.53
4:K:263:PRO:HD3	5:L:111:TYR:CZ	2.44	0.53
5:L:77:ASN:OD1	5:L:94:ARG:NH1	2.42	0.53
5:L:142:LYS:HE3	5:L:144:ILE:HG12	1.90	0.53
6:N:396:ILE:HG22	6:N:400:MET:HE3	1.90	0.53
12:f:156:ALA:O	12:f:160:PHE:N	2.26	0.53
12:f:744:ILE:O	12:f:748:LYS:HG3	2.09	0.53
1:D:130:GLU:HG2	12:f:440:ARG:HH21	1.73	0.53
1:D:155:GLY:N	1:D:170:ILE:O	2.36	0.53
1:G:353:PHE:HA	1:G:356:MET:HB2	1.90	0.53
5:L:61:LEU:HB3	5:L:71:TYR:CE1	2.43	0.53
6:M:381:THR:HA	6:M:384:GLU:HG2	1.91	0.53
12:m:777:PHE:HB3	12:m:833:VAL:HG11	1.91	0.53
8:U:10:LYS:HB2	8:U:28:THR:HA	1.91	0.53
12:f:335:LEU:HA	12:f:366:LYS:HD2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:829:LEU:O	12:f:833:VAL:HG23	2.08	0.53
1:C:118:ARG:HD2	1:C:372:HIS:CE1	2.43	0.53
1:D:28:ASP:HB2	1:D:341:TRP:HH2	1.74	0.53
1:D:343:GLY:HA2	1:D:346:ILE:HD12	1.90	0.53
4:K:271:TRP:CE3	4:K:274:ILE:HD11	2.43	0.53
12:m:776:PRO:HA	13:o:381:THR:HG21	1.90	0.53
12:n:257:GLN:NE2	12:n:319:ASP:O	2.41	0.53
1:A:158:LEU:HD12	1:A:279:LEU:HB2	1.92	0.52
1:A:236:THR:HG21	1:A:256:PHE:HE2	1.74	0.52
1:B:240:GLN:OE1	1:B:249:ILE:N	2.41	0.52
1:C:75:MET:HE1	1:C:79:ILE:N	2.24	0.52
1:G:48:MET:HE3	1:I:147:LEU:HD11	1.90	0.52
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:145:LEU:HD12	1:I:343:GLY:C	2.35	0.52
3:J:204:GLU:HA	3:J:207:LEU:HD12	1.91	0.52
5:L:193:LEU:HD22	5:L:224:ILE:HG13	1.90	0.52
7:O:85:GLN:OE1	7:O:85:GLN:N	2.39	0.52
11:Y:55:LEU:CB	11:Y:298:PRO:HB3	2.37	0.52
11:Y:317:ARG:HE	11:Y:333:LEU:HD11	1.74	0.52
12:f:33:HIS:O	12:f:37:LEU:N	2.36	0.52
12:f:220:CYS:HB3	12:f:225:GLU:HB2	1.91	0.52
12:f:240:THR:O	12:f:244:GLN:HG3	2.09	0.52
12:m:735:LEU:HB3	12:m:785:VAL:HG22	1.91	0.52
12:n:689:PHE:HA	12:n:692:LYS:HD2	1.89	0.52
11:Y:162:ARG:HG2	11:Y:166:LYS:HZ3	1.74	0.52
12:e:717:ILE:H	12:e:824:TRP:CG	2.17	0.52
12:f:479:VAL:HG22	12:f:482:ARG:NH2	2.24	0.52
12:f:576:LYS:O	12:f:611:ARG:NH1	2.42	0.52
12:f:619:LEU:HD23	12:f:689:PHE:HE2	1.74	0.52
13:h:293:GLU:HB2	13:h:318:MET:HB3	1.91	0.52
12:m:132:SER:H	12:n:41:LEU:C	2.17	0.52
1:F:346:ILE:HG23	12:f:311:HIS:HA	1.91	0.52
1:G:158:LEU:HD12	1:G:275:ILE:HD11	1.92	0.52
4:K:177:TRP:CE3	4:K:190:GLY:HA3	2.44	0.52
12:e:435:ARG:HA	12:e:447:LYS:HA	1.90	0.52
12:f:208:PRO:O	12:f:251:ARG:NH2	2.42	0.52
12:f:335:LEU:HG	12:f:370:THR:HG21	1.91	0.52
12:f:738:ASN:HB3	12:f:824:TRP:HE1	1.74	0.52
12:n:293:GLU:HA	12:n:298:LEU:HD21	1.92	0.52
1:A:11:PRO:HB3	1:A:107:PRO:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:LYS:HA	1:A:357:TRP:NE1	2.25	0.52
2:H:190:MET:HE3	2:H:190:MET:HA	1.90	0.52
1:I:354:LYS:HA	1:I:357:TRP:HE1	1.73	0.52
12:m:719:ALA:O	12:m:736:LYS:NZ	2.34	0.52
12:n:572:LEU:HD22	12:n:604:TYR:HE1	1.75	0.52
12:n:590:ALA:O	12:n:593:VAL:HG12	2.10	0.52
1:A:48:MET:HE1	1:C:148:TYR:CE2	2.44	0.52
1:C:40:GLY:HA3	1:C:69:LEU:HD13	1.91	0.52
1:D:160:SER:HA	1:D:165:THR:HG23	1.91	0.52
1:E:168:VAL:HG13	1:E:180:ILE:HG22	1.91	0.52
1:F:138:PHE:HB2	1:F:357:TRP:HB3	1.92	0.52
1:G:20:VAL:O	1:G:22:LYS:NZ	2.42	0.52
6:N:21:GLU:OE2	6:N:22:THR:N	2.43	0.52
6:Q:340:ILE:HD11	6:Q:343:LEU:HD22	1.90	0.52
12:f:80:GLU:N	12:f:102:ASN:O	2.27	0.52
12:f:641:LEU:HG	13:h:502:PHE:HE2	1.74	0.52
1:C:215:LYS:NZ	14:C:800:ADP:H2'	2.24	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: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
6:P:312:LYS:O	6:P:315:GLN:N	2.42	0.52
12:f:221:TYR:HE1	12:f:227:PRO:HD3	1.74	0.52
12:m:648:ILE:O	12:m:652:LYS:HG2	2.09	0.52
1:B:141:MET:O	1:B:145:LEU:HD23	2.10	0.52
1:C:240:GLN:OE1	1:C:249:ILE:N	2.41	0.52
1:D:351:ASP:N	12:m:319:ASP:OD1	2.39	0.52
3:J:342:ARG:NH1	11:Y:228:ALA:O	2.43	0.52
6:N:210:THR:OG1	10:W:1266:GLN:O	2.23	0.52
6:N:360:THR:O	6:N:364:ILE:HG12	2.10	0.52
12:e:739:PHE:CB	12:e:824:TRP:CZ2	2.92	0.52
12:n:528:GLU:O	12:n:532:GLU:HG2	2.10	0.52
1:E:41:ARG:O	1:E:70:SER:N	2.34	0.52
1:E:86:MET:HA	1:E:86:MET:HE2	1.91	0.52
1:E:358:VAL:HG22	1:E:374:LYS:HD2	1.91	0.52
1:I:287:ASP:O	1:I:291:ARG:HG3	2.10	0.52
9:V:60:HIS:O	9:V:90:HIS:HA	2.10	0.52
11:Y:235:LEU:HD12	11:Y:236:PRO:HD2	1.92	0.52
12:n:459:LEU:HD22	12:n:538:VAL:HG11	1.90	0.52
12:n:755:TRP:HD1	13:p:453:GLU:OE1	1.77	0.52
1:C:89:ILE:O	1:C:93:VAL:HG23	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:71:ILE:O	2:H:183:ARG:NH1	2.43	0.52
2:H:193:LEU:HD11	2:H:250:ILE:HG22	1.92	0.52
2:H:272:CYS:HB2	2:H:276:GLU:HB3	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
8:U:33:THR:OG1	8:U:54:ASN:O	2.26	0.52
11:Y:45:GLU:HB2	11:Y:281:SER:HB3	1.92	0.52
12:f:367:ILE:HG23	12:f:437:ILE:HD11	1.91	0.52
12:f:748:LYS:HA	12:f:751:ARG:HD3	1.90	0.52
13:p:576:VAL:HA	13: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:E:158:LEU:HD11	1:E:275:ILE:HD11	1.92	0.52
3:J:172:HIS:NE2	3:J:208:GLU:HG2	2.25	0.52
5:L:89:PRO:HG2	5:L:93:LEU:HD22	1.92	0.52
6:M:392:ASN:O	6:M:396:ILE:HG12	2.10	0.52
12:f:347:ALA:HB1	12:f:352:LYS:HB3	1.91	0.52
12:f:442:ARG:NH1	12:f:445:ASN:O	2.41	0.52
12:m:659:THR:O	12:m:662:MET:HG2	2.10	0.52
1:C:334:GLN:HE21	6:Q:47:HIS:HB3	1.75	0.51
1:D:145:LEU:HD22	1:D:344:GLY:HA2	1.92	0.51
11:Y:230:ASP:OD1	11:Y:231:GLU:N	2.43	0.51
12:e:716:ARG:CA	12:e:824:TRP:CD1	2.92	0.51
12:f:777:PHE:HB3	12:f:829:LEU:HD21	1.92	0.51
12:n:335:LEU:O	12:n:363:HIS:NE2	2.41	0.51
12:n:569:ARG:NH1	12:n:604:TYR:OH	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:B:325:ASP:HA	6:P:93:GLU:N	2.25	0.51
1:E:160:SER:HB3	1:E:305:THR:HG23	1.92	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	1.93	0.51
2:H:334:GLU:N	2:H:334:GLU:OE1	2.42	0.51
3:J:98:PRO:HB2	3:J:101:PHE:HB3	1.92	0.51
4:K:163:PHE:HA	4:K:170:ASN:HA	1.91	0.51
6:M:379:GLN:O	6:M:383:ARG:HG2	2.09	0.51
6:P:269:GLN:HG2	7:R:39:LYS:NZ	2.25	0.51
10:W:1120:LYS:O	10:W:1124:MET:HG2	2.10	0.51
12:f:350:LEU:HD12	12:f:419:VAL:HG21	1.92	0.51
12:f:783:GLU:OE1	12:f:786:ARG:NH2	2.43	0.51
1:B:9:ASN:OD1	12:n:250:ASN:ND2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:359:SER:N	1:E:362:GLU:OE1	2.33	0.51
1:F:351:ASP:N	12:f:319:ASP:OD2	2.41	0.51
2:H:11:ASP:HB3	2:H:18:LYS:HB2	1.91	0.51
6:N:214:HIS:HB2	10:W:1271:VAL:HG22	1.92	0.51
12:m:659:THR:OG1	12:m:690:ARG:NH2	2.43	0.51
12:n:229:VAL:HG13	12:n:236:VAL:HG11	1.92	0.51
12:n:485:ARG:HH12	12:n:487:GLN:HG2	1.75	0.51
6:P:102:GLN:HA	6:Q:140:LEU:HD21	1.92	0.51
6:P:322:ARG:HE	10:W:1117:SER:HB2	1.75	0.51
13:h:426:HIS:O	13:h:427:LYS:HE2	2.10	0.51
1:F:68:LEU:HD12	2:H:166:TYR:HD2	1.76	0.51
6:M:320:ILE:HD11	7:O:94:ILE:HD11	1.91	0.51
12:f:357:LEU:O	12:f:361:PHE:HD1	1.94	0.51
12:f:519:ALA:HA	12:f:522:GLU:CD	2.35	0.51
12:f:653:GLN:HG3	13:h:503:ASP:HA	1.92	0.51
12:f:787:THR:OG1	13:h:332:GLN:NE2	2.24	0.51
12:m:350:LEU:HD23	12:m:353:ILE:HD12	1.92	0.51
12:m:555:GLU:HG3	12:m:559:ARG:HH12	1.75	0.51
1:D:351:ASP:H	12:m:319:ASP:CG	2.18	0.51
1:E:110:LEU:HB3	1:E:139:ILE:HG22	1.93	0.51
2:H:253:GLU:HA	2:H:256:ARG:HB3	1.93	0.51
4:K:271:TRP:HE1	5:L:218:GLU:CD	2.18	0.51
6:N:385:ASN:HD21	10:Z:1175:HIS:HA	1.74	0.51
11:Y:143:ARG:HH11	11:Y:146:LYS:HD2	1.74	0.51
12:f:365:ARG:NH2	12:f:430:LEU:HD22	2.26	0.51
1:G:7:ILE:HG22	1:G:9:ASN:H	1.76	0.51
2:H:111:ASN:OD1	2:H:177:ARG:NH1	2.43	0.51
2:H:262:PHE:HD1	2:H:275:HIS:HD2	1.58	0.51
6:M:183:LEU:HD22	10:W:1283:ARG:NH1	2.25	0.51
6:M:360:THR:HB	6:N:361:GLN:NE2	2.25	0.51
6:P:256:LEU:HA	6:P:267:LEU:HD23	1.91	0.51
9:V:123:LYS:HE3	11:Y:299:THR:HA	1.92	0.51
13:h:386:CYS:HB3	13:h:437:MET:HG2	1.92	0.51
12:m:706:VAL:HG12	12:m:764:ILE:HD12	1.93	0.51
13:o:576:VAL:HA	13:o:587:VAL:HG12	1.92	0.51
1:B:168:VAL:HG22	1:B:180:ILE:HG12	1.91	0.51
1:D:165:THR:HB	1:D:183:ILE:HG13	1.93	0.51
5:L:72:ARG:HH22	5:L:89:PRO:HD3	1.75	0.51
6:M:212:GLU:N	10:W:1255:LYS:O	2.35	0.51
10:Z:1112:LEU:O	10:Z:1116:ASN:ND2	2.43	0.51
12:e:717:ILE:CB	12:e:824:TRP:HA	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:552:ARG:O	12:f:555:GLU:HG3	2.11	0.51
12:n:526:ALA:HB2	12:n:556:ARG:HD2	1.93	0.51
1:D:281:PHE:HA	1:D:284:GLN:HE21	1.76	0.51
1:E:197:TYR:HD1	1:E:200:LYS:HD3	1.76	0.51
3:J:217:VAL:HG22	3:J:267:VAL:HG21	1.93	0.51
4:K:55:ALA:O	4:K:59:MET:HG2	2.10	0.51
4:K:117:LEU:HD21	4:K:152:GLN:HB2	1.92	0.51
6:M:69:LEU:HD12	6:M:83:TYR:H	1.76	0.51
1:A:210:GLU:HA	1:A:213:ILE:HD12	1.93	0.51
1:B:227:ASN:HB3	1:B:230:LYS:HB3	1.93	0.51
3:J:134:ASN:ND2	3:J:153:GLU:HG2	2.25	0.51
6:Q:8:ASP:OD1	6:Q:9:LEU:N	2.44	0.51
7:R:100:LEU:O	7:R:104:VAL:HG23	2.11	0.51
12:f:254:ARG:O	12:f:258:LYS:HG2	2.11	0.51
12:m:302:ASP:HA	12:m:305:LYS:HD2	1.92	0.51
12:n:232:PHE:HE1	12:n:299:LEU:HD21	1.76	0.51
13:p:443:ASP:OD1	13:p:446:ASN:N	2.44	0.51
1:A:281:PHE:O	1:A:284:GLN:NE2	2.44	0.50
1:B:18:SER:OG	1:B:163:GLY:N	2.42	0.50
1:F:76:GLU:HG2	1:F:77:HIS:CD2	2.47	0.50
5:L:261:ASP:O	5:L:264:GLU:HG3	2.11	0.50
7:O:128:ARG:HA	7:O:131:GLN:CD	2.36	0.50
8:U:97:GLN:HB3	8:U:115:ARG:HH21	1.77	0.50
11:Y:253:GLN:O	11:Y:257:LEU:HG	2.11	0.50
11:Y:294:PRO:HA	11:Y:304:LYS:HE2	1.92	0.50
13:h:299:TYR:HB2	13:h:312:VAL:HB	1.92	0.50
13:h:426:HIS:HD2	13:h:471:MET:HE3	1.76	0.50
1:D:371:ILE:O	1:D:375:THR:OG1	2.21	0.50
1:F:315:LEU:HD11	6:N:22:THR:HG23	1.91	0.50
6:P:210:THR:HB	10:Z:1257:THR:HB	1.92	0.50
11:Y:111:CYS:SG	11:Y:114:CYS:O	2.68	0.50
10:Z:1141:LEU:O	10:Z:1145:GLU:N	2.45	0.50
12:f:530:VAL:HG13	12:f:546:TRP:HZ3	1.76	0.50
12:f:568:LEU:HA	12:f:571:GLN:HG2	1.92	0.50
12:f:619:LEU:HG	12:f:654:ILE:HG23	1.93	0.50
12:n:755:TRP:HZ3	13:p:452:GLU:O	1.80	0.50
1:A:281:PHE:HA	1:A:284:GLN:HE21	1.77	0.50
1:G:136:ALA:HB1	1:G:357:TRP:HB3	1.92	0.50
4:K:197:HIS:NE2	4:K:203:ASN:OD1	2.44	0.50
4:K:250:MET:SD	4:K:255:PHE:HB2	2.51	0.50
6:M:316:LEU:HD11	6:N:317:TYR:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:581:MET:CE	12:f:608:LEU:HG	2.41	0.50
13:h:456:VAL:HB	13:h:509:TRP:HZ3	1.75	0.50
12:m:696:GLN:HA	12:m:758:PHE:HE1	1.75	0.50
13:o:315:VAL:O	13:o:326:GLU:N	2.45	0.50
1:G:352:THR:HA	6:M:63:ARG:CZ	2.42	0.50
3:J:219:ASP:OD1	3:J:220:LEU:N	2.44	0.50
6:M:74:ARG:O	6:M:80:ARG:NH1	2.40	0.50
7:O:167:GLN:O	7:O:170:GLU:HG3	2.11	0.50
12:e:777:PHE:CB	12:e:833:VAL:HG11	2.41	0.50
12:f:699:PHE:CE1	12:f:758:PHE:HB3	2.46	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:F:39:VAL:HG21	1:F:85:ASP:HB3	1.93	0.50
1:F:76:GLU:OE1	1:F:76:GLU:N	2.44	0.50
1:G:141:MET:O	1:G:145:LEU:HD13	2.11	0.50
5:L:67:ASP:OD1	5:L:67:ASP:N	2.44	0.50
9:V:5:GLU:O	9:V:175:LYS:NZ	2.44	0.50
12:f:591:LEU:CD1	12:f:597:ILE:HG21	2.41	0.50
12:f:642:PRO:HG3	12:f:749:GLU:HG2	1.92	0.50
12:f:711:LEU:HB3	12:f:743:ILE:HG12	1.94	0.50
12:m:410:GLU:OE2	12:m:467:ARG:NE	2.32	0.50
1:C:168:VAL:HG13	1:C:180:ILE:HG22	1.93	0.50
1:E:20:VAL:HA	1:E:36:PRO:HA	1.94	0.50
1:E:133:ASN:HA	1:E:360:LYS:HZ1	1.77	0.50
3:J:216:PHE:CE1	3:J:243:PRO:HG3	2.47	0.50
6:M:175:LEU:HA	6:M:178:ARG:HD3	1.93	0.50
6:M:183:LEU:HD22	10:W:1283:ARG:CZ	2.42	0.50
6:P:344:HIS:CE1	6:P:348:MET:HE3	2.46	0.50
12:f:578:ALA:HA	12:f:581:MET:HG3	1.94	0.50
12:f:748:LYS:O	12:f:752:ASN:ND2	2.45	0.50
1:B:154:THR:HG22	1:B:172:GLU:H	1.76	0.50
1:B:227:ASN:HB2	6:P:113:GLN:CD	2.37	0.50
1:B:302:GLY:O	1:B:305:THR:OG1	2.28	0.50
1:D:245:ASP:OD1	1:D:246:GLY:N	2.45	0.50
1:F:18:SER:HB2	1:F:162:ASP:HB3	1.94	0.50
1:I:145:LEU:HD13	1:I:148:TYR:CD2	2.46	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
10:W:1106:ARG:O	10:W:1109:ILE:HG22	2.11	0.50
12:f:418:GLU:O	12:f:422:THR:OG1	2.24	0.50
12:m:252:TRP:O	12:m:256:ILE:HG12	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:n:776:PRO:HB3	13:p:375:LEU:C	2.37	0.50
13:p:332:GLN:HE22	13:p:372:ARG:HH12	1.60	0.50
1:A:143:ALA:HB1	1:A:157:VAL:HB	1.94	0.50
1:A:164:VAL:HG23	1:A:184:ASP:HA	1.94	0.50
1:B:10:GLN:HG3	12:n:309:ARG:HD2	1.94	0.50
1:F:43:LYS:HB3	1:F:70:SER:HB3	1.94	0.50
1:G:25:PHE:HZ	1:G:101:THR:HG21	1.76	0.50
1:G:160:SER:OG	1:G:305:THR:HG23	2.12	0.50
2:H:218:TYR:HB2	2:H:307:PRO:HB2	1.93	0.50
5:L:143:LYS:HZ3	5:L:181:LYS:HB2	1.76	0.50
6:N:341:LYS:HE3	10:Z:1131:LEU:HD22	1.94	0.50
12:f:673:TRP:CZ3	12:f:683:LYS:HB2	2.46	0.50
12:m:561:GLU:HA	12:m:564:ILE:HD12	1.94	0.50
12:n:274:GLU:OE1	12:n:376:ARG:NH2	2.44	0.50
1:B:290:LEU:HG	4:K:264:VAL:HG11	1.92	0.50
3:J:362:GLY:HA2	3:J:368:LEU:HD11	1.94	0.50
12:f:274:GLU:OE2	12:f:376:ARG:NE	2.38	0.50
12:f:748:LYS:O	12:f:751:ARG:HG2	2.11	0.50
12:m:543:THR:O	12:m:547:GLU:HG2	2.11	0.50
12:m:832:TYR:HA	12:m:835:ARG:HE	1.75	0.50
1:A:28:ASP:HB2	1:A:341:TRP:HH2	1.76	0.49
1:B:88:ARG:HA	1:B:91:GLN:CD	2.36	0.49
1:D:238:LYS:HG2	1:D:252:GLY:HA3	1.93	0.49
1:G:46:ARG:NH2	1:G:52:LEU:O	2.33	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:h:435:THR:H	13:h:451:SER:HA	1.77	0.49
12:m:195:HIS:O	12:m:199:ASN:N	2.45	0.49
12:m:335:LEU:HB2	12:m:370:THR:HG21	1.93	0.49
12:m:650:TRP:O	12:m:654:ILE:HG12	2.12	0.49
12:n:435:ARG:NH1	12:n:448:MET:O	2.45	0.49
12:n:607:GLN:NE2	12:n:608:LEU:HG	2.26	0.49
13:o:332:GLN:HE22	13:o:372:ARG:HH12	1.60	0.49
13:o:426:HIS:HB2	13:o:468:ILE:HD13	1.94	0.49
1:C:287:ASP:OD1	1:C:288:MET:N	2.44	0.49
1:F:223:TYR:HA	1:F:308:LYS:HG3	1.93	0.49
1:G:113:ALA:HB3	1:G:116:ASN:HD21	1.77	0.49
1:G:240:GLN:CD	1:G:248:THR:HB	2.36	0.49
1:G:371:ILE:HG13	1:G:372:HIS:N	2.27	0.49
3:J:57:TYR:CD1	3:J:98:PRO:HG2	2.47	0.49
12:f:661:TYR:O	12:f:665:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:m:289:GLN:NE2	12:m:293:GLU:OE1	2.45	0.49
13:o:572:ALA:HB3	13:o:590:SER:HB3	1.94	0.49
1:B:9:ASN:HB3	12:n:246:GLN:HE21	1.77	0.49
1:D:18:SER:OG	1:D:188:ARG:NH2	2.45	0.49
1:E:46:ARG:HD2	6:M:83:TYR:O	2.12	0.49
1:G:93:VAL:HA	1:G:98:GLN:NE2	2.27	0.49
12:f:394:LYS:O	12:f:398:THR:HG23	2.11	0.49
13:h:436:SER:O	13:h:450:GLY:N	2.40	0.49
12:m:621:ASP:HA	12:m:624:LYS:HD2	1.93	0.49
13:o:537:PRO:HB3	13:o:611:TRP:CZ3	2.48	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: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
12:f:249:VAL:HG21	12:f:304:LEU:HD11	1.94	0.49
12:f:292:ARG:HG2	12:f:316:PHE:HZ	1.76	0.49
12:f:638:VAL:HG11	13:h:281:VAL:HG21	1.94	0.49
12:n:394:LYS:O	12:n:398:THR:HG23	2.12	0.49
12:n:482:ARG:HH21	12:n:485:ARG:HH21	1.60	0.49
12:n:669:LEU:HD11	12:n:678:GLU:HB2	1.93	0.49
1:C:243:LEU:HD13	1:E:288:MET:HE2	1.94	0.49
1:E:44:HIS:CD2	1:G:176:MET:HB3	2.48	0.49
6:P:2:ALA:HB1	6:P:5:LYS:HD2	1.94	0.49
9:V:108:VAL:C	9:V:165:MET:HE1	2.38	0.49
12:m:533:VAL:HG21	12:m:549:ALA:HB2	1.95	0.49
12:n:86:GLU:O	12:n:96:LYS:N	2.42	0.49
12:n:361:PHE:CG	12:n:426:GLU:HB3	2.48	0.49
12:n:483:VAL:HG13	12:n:484:LEU:HD22	1.94	0.49
13:p:315:VAL:O	13:p:326:GLU:N	2.45	0.49
1:E:169:PRO:HG2	1:E:176:MET:HB2	1.94	0.49
1:G:218:LYS:HA	1:G:222:CYS:SG	2.52	0.49
2:H:275:HIS:HA	2:H:313:MET:HE1	1.95	0.49
3:J:41:SER:HB2	3:J:54:VAL:HG22	1.95	0.49
3:J:54:VAL:HG11	3:J:71:PHE:CD1	2.48	0.49
3:J:348:ALA:HB2	3:J:356:LEU:HD22	1.94	0.49
12:f:639:ARG:NH2	13:h:574:ASN:OD1	2.45	0.49
12:f:805:VAL:HB	12:f:843:PHE:HE1	1.77	0.49
12:m:361:PHE:CG	12:m:426:GLU:HB3	2.48	0.49
12:m:631:GLN:HB3	13:o:572:ALA:HB2	1.94	0.49
12:m:715:GLY:O	12:m:824:TRP:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:n:315:SER:O	12:n:319:ASP:N	2.45	0.49
12:n:368:ARG:HB3	12:n:433:LEU:HD11	1.95	0.49
13:p:531:MET:HE2	13:p:578:TRP:CD1	2.45	0.49
6:P:266:GLU:HA	6:P:269:GLN:OE1	2.12	0.49
6:P:329:THR:HG22	10:W:1128:LEU:HD12	1.95	0.49
6:Q:322:ARG:HH11	6:Q:323:TRP:NE1	2.10	0.49
12:e:539:SER:O	12:e:543:THR:N	2.43	0.49
12:m:657:GLN:HG3	13:o:504:TRP:CE3	2.47	0.49
1:C:112:GLU:N	1:C:112:GLU:OE1	2.45	0.49
1:G:98:GLN:O	1:G:100:GLN:N	2.45	0.49
3:J:102:ARG:HD2	3:J:120:LEU:HD22	1.94	0.49
11:Y:166:LYS:HA	11:Y:169:ARG:HH11	1.78	0.49
12:f:699:PHE:HZ	12:f:759:ARG:HG3	1.77	0.49
12:f:755:TRP:NE1	13:h:453:GLU:O	2.45	0.49
12:m:306:HIS:O	12:m:308:LYS:NZ	2.45	0.49
12:m:597:ILE:O	12:m:601:ILE:HG12	2.12	0.49
12:m:747:SER:HA	12:m:768:ALA:HB1	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
1:F:280:VAL:HG21	1:F:321:LEU:HB2	1.95	0.49
2:H:181:ALA:O	2:H:185:LEU:HG	2.13	0.49
3:J:187:THR:HG23	3:J:254:LYS:HG2	1.94	0.49
4:K:93:LYS:HE2	4:K:113:VAL:HB	1.95	0.49
4:K:153:THR:HG22	4:K:180:THR:HG23	1.94	0.49
6:M:346:GLN:HG2	10:Z:1139:LEU:HD13	1.95	0.49
9:V:129:LEU:HD12	9:V:147:SER:HB2	1.94	0.49
12:f:769:HIS:CE1	12:f:773:GLN:HE21	2.31	0.49
12:n:776:PRO:C	13:p:375:LEU:O	2.56	0.49
1:B:108:VAL:HG21	1:B:128:PHE:HE2	1.77	0.49
1:C:40:GLY:C	1:C:69:LEU:HD22	2.38	0.49
1:E:21:ILE:HD11	1:E:35:PHE:CZ	2.48	0.49
1:F:84:ASN:O	1:F:87:GLU:HG3	2.12	0.49
1:G:9:ASN:HB3	1:G:106:HIS:ND1	2.28	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
12:m:552:ARG:O	12:m:555:GLU:HG2	2.13	0.49
12:n:569:ARG:HD2	13:o:395:ALA:HB3	1.94	0.49
12:n:607:GLN:HE22	12:n:608:LEU:HG	1.78	0.49
13:p:426:HIS:HB2	13:p:468:ILE:HD13	1.94	0.49
1:E:29:GLN:NE2	6:Q:5:LYS:HE3	2.26	0.48
1:E:42:PRO:HA	1:E:69:LEU:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Q:63:ARG:HH21	10:Z:1209:LYS:NZ	2.12	0.48
12:f:257:GLN:O	12:f:261:LYS:HG2	2.12	0.48
1:D:346:ILE:HG12	12:m:311:HIS:HB3	1.94	0.48
2:H:189:LEU:HA	2:H:192:ILE:HG12	1.95	0.48
6:P:316:LEU:O	6:P:320:ILE:HG12	2.13	0.48
12:f:209:ILE:O	12:f:210:HIS:C	2.56	0.48
12:f:709:ARG:HH21	12:f:711:LEU:HD11	1.78	0.48
12:f:777:PHE:HD1	12:f:833:VAL:HG21	1.78	0.48
12:m:608:LEU:O	12:m:612:VAL:HG23	2.12	0.48
11:Y:4:LEU:H	11:Y:4:LEU:HD12	1.78	0.48
12:f:583:ARG:NH1	13:h:559:GLU:O	2.46	0.48
13:h:336:MET:SD	13:h:336:MET:N	2.77	0.48
12:n:250:ASN:HA	12:n:253:ILE:HG22	1.94	0.48
12:n:288:ILE:HA	12:n:291:LYS:HD2	1.95	0.48
13:o:443:ASP:OD1	13:o:446:ASN:N	2.44	0.48
13:p:537:PRO:HB3	13:p:611:TRP:CZ3	2.48	0.48
13:p:572:ALA:HB3	13:p:590:SER:HB3	1.94	0.48
1:B:103:SER:HB2	1:B:132:PHE:HB3	1.95	0.48
1:B:273:GLU:HB3	1:B:277:GLU:HB2	1.95	0.48
1:D:133:ASN:HD21	12:f:368:ARG:HD2	1.78	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:P:338:VAL:O	6:P:341:LYS:HB3	2.13	0.48
6:Q:175:LEU:O	6:Q:178:ARG:HG3	2.12	0.48
13:h:536:HIS:HB3	13:h:539:LEU:HB3	1.94	0.48
13:p:388:ASN:HB2	13:p:437:MET:HE3	1.95	0.48
1:B:136:ALA:HB1	1:B:357:TRP:CG	2.48	0.48
1:C:44:HIS:CD2	1:E:176:MET:HE1	2.49	0.48
1:E:172:GLU:OE2	1:E:172:GLU:O	2.31	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
10:Z:1241:ARG:HA	10:Z:1244:GLU:OE1	2.14	0.48
12:f:266:PRO:HB3	12:f:376:ARG:HG3	1.95	0.48
12:f:333:ASN:HA	12:f:336:MET:HB3	1.96	0.48
12:m:483:VAL:HB	12:m:588:PHE:CD1	2.49	0.48
12:m:516:ASP:O	12:m:520:ILE:HG13	2.14	0.48
12:m:539:SER:O	12:m:543:THR:N	2.40	0.48
12:m:634:LYS:HE3	12:m:635:MET:HE3	1.96	0.48
12:n:748:LYS:HE3	13:p:383:PRO:CD	2.43	0.48
1:B:108:VAL:HG21	1:B:128:PHE:CE2	2.48	0.48
1:B:219:GLU:HG2	14:B:800:ADP:C4	2.48	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
6:N:209:VAL:HA	10:W:1266:GLN:HB2	1.96	0.48
8:U:58:GLU:HG2	8:U:92:VAL:HG13	1.94	0.48
12:f:246:GLN:NE2	12:f:250:ASN:OD1	2.46	0.48
12:f:265:ASP:HB3	12:f:268:SER:HB2	1.95	0.48
12:f:464:ASP:O	12:f:468:LYS:HG2	2.14	0.48
12:f:598:ARG:HH22	12:f:669:LEU:HA	1.78	0.48
12:n:401:LEU:O	12:n:470:ARG:NH1	2.43	0.48
12:n:426:GLU:OE2	12:n:429:LYS:NZ	2.40	0.48
12:n:755:TRP:CZ3	13:p:453:GLU:CA	2.83	0.48
13:o:388:ASN:HB2	13:o:437:MET:HE3	1.95	0.48
1:A:122:GLU:HG2	1:A:368:ALA:HB1	1.96	0.48
1:A:205:PHE:HB3	1:A:210:GLU:HB3	1.95	0.48
1:B:145:LEU:HD12	1:B:343:GLY:C	2.39	0.48
1:E:46:ARG:NH2	1:E:52:LEU:O	2.46	0.48
2:H:23:GLY:N	2:H:344:SER:OG	2.46	0.48
5:L:189:LEU:HD13	5:L:233:PHE:HE1	1.79	0.48
10:W:1255:LYS:NZ	10:W:1257:THR:OG1	2.26	0.48
12:f:553:TYR:O	12:f:557:ILE:HG12	2.14	0.48
13:g:551:LEU:O	13:g:562:THR:N	2.47	0.48
12:m:674:GLU:CD	12:m:674:GLU:H	2.22	0.48
1:C:176:MET:HB3	1:C:179:SER:HB2	1.96	0.48
1:F:114:PRO:HB3	1:F:141:MET:SD	2.53	0.48
1:G:229:GLN:NE2	1:G:264:ARG:HH22	2.09	0.48
13:h:368:THR:HG22	13:h:372:ARG:HH22	1.79	0.48
13:h:540:PHE:CE1	13:h:552:TRP:HB2	2.48	0.48
13:o:531:MET:HE2	13:o:578:TRP:CD1	2.45	0.48
1:A:302:GLY:O	1:A:305:THR:OG1	2.30	0.48
1:C:243:LEU:HD12	1:C:247:SER:HB2	1.95	0.48
1:F:30:ILE:HD12	6:N:9:LEU:HD21	1.96	0.48
4:K:228:PHE:CE1	4:K:232:ILE:HD11	2.49	0.48
6:P:12:ILE:HB	6:P:14:ARG:NH1	2.29	0.48
10:Z:1101:GLN:O	10:Z:1105:MET:HG3	2.14	0.48
12:f:475:GLN:O	12:f:479:VAL:HG23	2.14	0.48
12:f:660:ALA:O	12:f:664:ARG:HG3	2.14	0.48
12:m:409:PHE:O	12:m:413:MET:HG2	2.12	0.48
12:n:353:ILE:HD11	12:n:395:VAL:HG21	1.95	0.48
12:n:375:GLN:O	12:n:379:ARG:HG2	2.14	0.48
1:A:118:ARG:HB2	1:A:372:HIS:CE1	2.48	0.48
1:C:145:LEU:HD23	1:C:340:THR:O	2.14	0.48
1:C:197:TYR:HD1	1:C:200:LYS:HD3	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:89:ALA:HB2	10:Z:1106:ARG:HD3	1.94	0.48
6:P:263:GLU:OE1	6:P:263:GLU:N	2.35	0.48
11:Y:30:CYS:SG	11:Y:33:CYS:N	2.80	0.48
12:f:435:ARG:HA	12:f:438:VAL:HG22	1.95	0.48
12:f:650:TRP:CE2	12:f:654:ILE:HD11	2.49	0.48
12:m:263:ASP:OD1	12:m:264:ARG:N	2.47	0.48
12:m:483:VAL:HG23	12:m:484:LEU:HD22	1.96	0.48
12:n:755:TRP:CE3	13:p:453:GLU:CA	2.93	0.48
1:A:75:MET:HG2	1:A:79:ILE:C	2.39	0.47
1:A:115:LEU:O	1:A:115:LEU:HD23	2.13	0.47
1:B:74:PRO:HG3	1:B:89:ILE:CD1	2.44	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
1:I:13:VAL:HG21	1:I:345:SER:HA	1.96	0.47
1:I:168:VAL:HG13	1:I:180:ILE:HG12	1.96	0.47
1:I:223:TYR:CZ	1:I:256:PHE:HB3	2.49	0.47
3:J:44:LYS:NZ	3:J:48:MET:O	2.36	0.47
4:K:161:HIS:CE1	4:K:163:PHE:HB3	2.48	0.47
7:R:113:SER:HB3	7:R:116:ILE:HD12	1.95	0.47
10:W:1253:MET:HE2	10:W:1253:MET:HA	1.96	0.47
12:f:735:LEU:HD23	12:f:785:VAL:HG22	1.96	0.47
12:m:266:PRO:HG3	12:m:376:ARG:HG3	1.95	0.47
12:n:577:ASN:OD1	12:n:578:ALA:N	2.47	0.47
12:n:616:ILE:HG12	12:n:661:TYR:HB3	1.96	0.47
13:o:589:ASP:OD1	13:o:593:GLN:N	2.47	0.47
1:A:98:GLN:O	1:A:100:GLN:N	2.47	0.47
1:C:112:GLU:CD	1:C:139:ILE:HG23	2.39	0.47
1:G:46:ARG:HB2	1:I:174:PHE:CE1	2.49	0.47
4:K:160:SER:HB3	4:K:173:TRP:HB3	1.96	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:Q:12:ILE:HB	6:Q:14:ARG:HH12	1.73	0.47
12:e:37:LEU:O	12:e:41:LEU:N	2.39	0.47
12:e:120:LYS:HA	12:e:135:LEU:HA	1.96	0.47
12:n:661:TYR:O	12:n:665:VAL:HG23	2.14	0.47
1:B:84:ASN:O	1:B:87:GLU:HG3	2.14	0.47
1:F:219:GLU:HG2	14:F:800:ADP:C4	2.48	0.47
2:H:301:GLY:O	2:H:304:THR:OG1	2.32	0.47
8:U:82:MET:HA	8:U:99:MET:O	2.14	0.47
9:V:57:VAL:HA	9:V:87:ILE:HB	1.96	0.47
12:m:779:ILE:HA	12:m:782:ILE:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:177:PRO:HA	1:D:180:ILE:HD12	1.97	0.47
1:E:43:LYS:HG3	1:E:44:HIS:CD2	2.50	0.47
1:G:41:ARG:O	1:G:70:SER:N	2.38	0.47
1:I:145:LEU:HA	1:I:148:TYR:HD2	1.78	0.47
12:f:609:ILE:HG21	12:f:678:GLU:HB3	1.96	0.47
12:m:437:ILE:O	12:m:441:LYS:N	2.41	0.47
12:n:272:LEU:HB2	12:n:341:LEU:HD22	1.95	0.47
12:n:335:LEU:HB2	12:n:370:THR:HG21	1.96	0.47
12:n:705:LYS:HD3	12:n:709:ARG:HH21	1.79	0.47
1:A:288:MET:HE1	4:K:167:ASN:HD22	1.79	0.47
1:D:58:ILE:H	1:D:61:LYS:HZ3	1.61	0.47
1:D:90:TRP:CD2	1:D:128:PHE:HE1	2.32	0.47
1:D:156:VAL:HA	1:D:169:PRO:HA	1.97	0.47
1:F:203:TYR:CE1	1:F:249:ILE:HG22	2.50	0.47
1:G:83:TRP:CE2	1:G:123:ARG:HG2	2.48	0.47
4:K:211:ASP:OD1	4:K:211:ASP:N	2.47	0.47
10:Z:1205:ASP:O	10:Z:1208:GLU:HG3	2.14	0.47
12:f:476:LEU:O	12:f:479:VAL:HB	2.14	0.47
12:m:559:ARG:O	12:m:563:ARG:HG3	2.14	0.47
12:m:582:PHE:CE2	12:m:664:ARG:HB3	2.49	0.47
1:A:284:GLN:NE2	1:A:285:LYS:HG3	2.30	0.47
1:A:288:MET:HA	1:A:291:ARG:HG3	1.96	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:E:112:GLU:H	1:E:112:GLU:CD	2.23	0.47
1:E:354:LYS:H	1:E:354:LYS:HD3	1.79	0.47
1:G:302:GLY:O	1:G:305:THR:OG1	2.31	0.47
2:H:173:HIS:HB2	2:H:284:LYS:NZ	2.29	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:306:ASP:O	6:P:310:GLN:HG2	2.14	0.47
6:Q:61:ASP:OD1	6:Q:62:LYS:N	2.47	0.47
6:Q:336:ARG:HD3	7:R:111:LEU:HD22	1.96	0.47
7:R:28:ARG:NH1	7:R:31:ARG:HH12	2.08	0.47
12:m:585:PHE:O	12:m:589:ASN:N	2.47	0.47
12:n:365:ARG:O	12:n:368:ARG:NH1	2.48	0.47
12:n:409:PHE:CD2	12:n:470:ARG:HD2	2.48	0.47
12:n:675:ASN:OD1	12:n:676:HIS:N	2.47	0.47
12:n:748:LYS:CE	13:p:383:PRO:HD2	2.45	0.47
1:B:220:ARG:HD3	1:B:241:TYR:HE1	1.80	0.47
1:C:145:LEU:O	1:C:343:GLY:HA3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:354:LYS:HA	1:C:357:TRP:HE1	1.80	0.47
1:F:15:ASP:HB3	1:F:22:LYS:HB2	1.97	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	2.48	0.47
3:J:344:HIS:CD2	11:Y:228:ALA:HB2	2.50	0.47
6:P:170:ASP:OD2	6:P:173:GLY:N	2.47	0.47
11:Y:143:ARG:HD2	11:Y:146:LYS:HD2	1.97	0.47
12:f:578:ALA:HB3	12:f:615:ASP:OD2	2.15	0.47
12:f:579:ASN:HA	12:f:582:PHE:CD1	2.49	0.47
12:f:638:VAL:HG22	13:h:300:ASN:ND2	2.29	0.47
13:h:266:SER:O	13:h:598:ASP:N	2.41	0.47
12:m:221:TYR:HE1	12:m:227:PRO:HD3	1.80	0.47
12:m:461:ALA:O	12:m:465:GLN:HG3	2.15	0.47
12:n:673:TRP:HA	12:n:676:HIS:CD2	2.48	0.47
12:n:696:GLN:HA	12:n:758:PHE:HE1	1.79	0.47
13:p:501:SER:OG	13:p:502:PHE:N	2.46	0.47
1:B:261:LEU:HA	1:B:267:LEU:HD12	1.96	0.47
1:C:95:SER:OG	1:C:96:LYS:N	2.48	0.47
3:J:366:ASP:N	3:J:366:ASP:OD1	2.47	0.47
6:P:354:LEU:HD11	7:R:125:ARG:NH2	2.24	0.47
8:U:37:PRO:HG2	9:V:49:ARG:HH21	1.80	0.47
13:g:359:LEU:N	13:g:371:GLN:O	2.42	0.47
12:m:293:GLU:HA	12:m:298:LEU:HD21	1.96	0.47
12:m:357:LEU:HD11	12:m:423:TRP:HE3	1.80	0.47
12:m:622:LYS:NZ	13:o:524:SER:O	2.46	0.47
12:n:253:ILE:HD11	12:n:319:ASP:HB3	1.97	0.47
1:A:20:VAL:HA	1:A:36:PRO:HA	1.96	0.47
1:E:11:PRO:HA	1:E:107:PRO:HD2	1.97	0.47
1:E:46:ARG:HH22	1:E:54:GLY:N	2.12	0.47
3:J:184:THR:HG22	3:J:194:SER:HB2	1.97	0.47
3:J:270:LEU:HD23	3:J:280:VAL:HG11	1.97	0.47
11:Y:427:LYS:HA	11:Y:457:HIS:HA	1.96	0.47
10:Z:1267:ARG:HG2	10:Z:1269:ARG:HH12	1.79	0.47
12:e:435:ARG:O	12:e:447:LYS:N	2.48	0.47
12:m:471:ARG:NH1	12:m:472:GLN:OE1	2.43	0.47
13:o:374:PRO:HG2	13:o:379:ALA:HB2	1.97	0.47
1:A:333:PRO:O	1:A:336:ARG:HG3	2.14	0.47
1:D:75:MET:HG2	1:D:79:ILE:C	2.40	0.47
1:F:112:GLU:OE1	1:F:116:ASN:ND2	2.48	0.47
2:H:67:LEU:HB2	2:H:203:THR:HB	1.96	0.47
1:I:161:GLY:O	1:I:186:ALA:HB1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:242:TYR:CE2	1:I:246:GLY:HA2	2.50	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
9:V:91:VAL:HG22	9:V:108:VAL:HG12	1.97	0.47
12:n:530:VAL:HG22	12:n:549:ALA:HB1	1.97	0.47
12:n:772:ASN:OD1	13:p:382:HIS:CE1	2.68	0.47
13:o:501:SER:OG	13:o:502:PHE:N	2.46	0.47
1:A:181:MET:HB3	1:A:278:VAL:HG13	1.97	0.46
1:B:243:LEU:HD12	1:B:247:SER:HB2	1.97	0.46
1:C:4:TYR:CG	10:Z:1243:LYS:HB3	2.50	0.46
6:P:229:ALA:O	6:P:233:LYS:HG2	2.15	0.46
11:Y:53:SER:HB2	11:Y:82:THR:HG21	1.97	0.46
11:Y:251:THR:O	11:Y:255:ARG:HG3	2.15	0.46
12:f:513:ASP:OD1	12:f:514:ALA:N	2.48	0.46
13:g:315:VAL:O	13:g:326:GLU:N	2.48	0.46
12:m:406:TYR:CD2	12:m:474:GLU:HG2	2.49	0.46
12:m:718:PHE:HE1	12:m:781:LEU:HD22	1.80	0.46
1:A:200:LYS:O	1:B:117:PRO:HA	2.15	0.46
1:D:227:ASN:HB3	1:D:230:LYS:HE3	1.96	0.46
1:F:145:LEU:O	1:F:343:GLY:HA3	2.14	0.46
2:H:18:LYS:NZ	15:H:401:ATP:O3A	2.49	0.46
3:J:298:GLN:OE1	3:J:298:GLN:N	2.27	0.46
6:P:347:ALA:HA	6:P:350:PHE:CD2	2.50	0.46
12:f:407:GLU:O	12:f:411:LYS:HG2	2.14	0.46
12:f:790:ARG:O	12:f:794:LYS:HG3	2.16	0.46
13:h:541:ALA:HB2	13:h:551:LEU:HG	1.97	0.46
13:h:552:TRP:CZ2	13:h:561:PRO:HG3	2.50	0.46
1:A:41:ARG:O	1:A:70:SER:N	2.38	0.46
1:C:43:LYS:HE3	1:C:44:HIS:CE1	2.51	0.46
1:D:240:GLN:CD	1:D:248:THR:HB	2.41	0.46
1:E:75:MET:HG2	1:E:79:ILE:C	2.40	0.46
2:H:193:LEU:HD12	2:H:198:TYR:HD2	1.80	0.46
7:O:131:GLN:HA	7:O:134:ILE:HD12	1.97	0.46
12:f:513:ASP:O	12:f:517:ALA:N	2.37	0.46
12:f:650:TRP:O	12:f:654:ILE:HG13	2.15	0.46
12:m:716:ARG:HA	12:m:823:VAL:HA	1.97	0.46
1:B:10:GLN:C	1:B:107:PRO:HD2	2.40	0.46
1:B:226:ILE:HG22	6:P:113:GLN:HG2	1.98	0.46
1:C:15:ASP:HA	1:C:111:THR:HG22	1.97	0.46
1:G:223:TYR:HA	1:G:308:LYS:HB3	1.98	0.46
13:h:333:SER:HB2	13:h:352:THR:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:m:357:LEU:HD21	12:m:423:TRP:HA	1.96	0.46
12:m:408:GLU:HA	12:m:411:LYS:HE2	1.98	0.46
12:n:228:LYS:N	12:n:231:ASP:OD2	2.49	0.46
13:p:374:PRO:HG2	13:p:379:ALA:HB2	1.97	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	1.96	0.46
1:C:176:MET:O	1:C:180:ILE:HG23	2.16	0.46
1:D:330:ILE:N	6:P:20:TYR:O	2.43	0.46
1:E:369:ARG:O	1:E:373:ARG:HG3	2.16	0.46
1:F:18:SER:HA	1:F:75:MET:SD	2.56	0.46
1:F:21:ILE:HG12	1:F:37:ASN:HB2	1.97	0.46
1:F:36:PRO:HB2	1:F:38:TYR:CE2	2.51	0.46
2:H:218:TYR:CE1	2:H:255:PHE:HB3	2.50	0.46
3:J:27:CYS:HB2	3:J:37:CYS:HB3	1.77	0.46
7:O:82:SER:O	7:O:83:LYS:NZ	2.46	0.46
12:e:119:ILE:O	12:e:136:ARG:N	2.49	0.46
12:f:364:LEU:HB3	12:f:430:LEU:HD11	1.98	0.46
12:f:754:LYS:HE2	12:f:760:VAL:H	1.80	0.46
12:n:462:ARG:O	12:n:466:MET:HG2	2.16	0.46
12:n:541:GLU:CD	12:n:541:GLU:H	2.23	0.46
12:n:706:VAL:CG1	12:n:764:ILE:HD12	2.45	0.46
12:n:706:VAL:HG12	12:n:764:ILE:HD12	1.98	0.46
1:C:104:GLU:HG3	1:C:133:ASN:HB2	1.97	0.46
1:D:114:PRO:HB3	1:D:141:MET:HE1	1.97	0.46
1:F:20:VAL:O	1:F:22:LYS:NZ	2.43	0.46
1:F:87:GLU:O	1:F:91:GLN:OE1	2.33	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
6:P:244:CYS:N	6:Q:262:MET:HE1	2.30	0.46
11:Y:282:LEU:O	11:Y:290:ASN:HB3	2.15	0.46
12:e:783:GLU:HA	12:e:786:ARG:HH21	1.80	0.46
12:m:791:THR:O	12:m:795:VAL:HG23	2.14	0.46
12:n:335:LEU:H	12:n:370:THR:HG21	1.81	0.46
1:A:43:LYS:HB3	1:A:70:SER:HB3	1.96	0.46
1:B:227:ASN:HB3	1:B:230:LYS:HE3	1.98	0.46
1:C:15:ASP:HB3	1:C:22:LYS:HB2	1.98	0.46
1:C:273:GLU:OE1	1:C:273:GLU:N	2.49	0.46
1:E:354:LYS:HA	1:E:357:TRP:NE1	2.29	0.46
2:H:332:PRO:O	2:H:335:ARG:HG3	2.15	0.46
1:I:29:GLN:CD	6:M:5:LYS:HD2	2.41	0.46
4:K:128:LEU:HA	4:K:229:ILE:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:R:98:VAL:O	7:R:102:GLU:OE1	2.34	0.46
9:V:135:PRO:HB2	11:Y:81:HIS:CE1	2.50	0.46
10:W:1109:ILE:HD12	10:Z:1105:MET:HE2	1.96	0.46
12:f:339:PHE:CZ	12:f:360:ILE:HG23	2.51	0.46
13:h:480:THR:HG23	13:h:501:SER:HA	1.97	0.46
13:h:557:ASP:OD1	13:h:562:THR:OG1	2.33	0.46
12:m:657:GLN:HG3	13:o:504:TRP:CZ3	2.50	0.46
12:m:753:LEU:HD12	12:m:758:PHE:HB2	1.98	0.46
12:n:395:VAL:O	12:n:399:ARG:HG2	2.15	0.46
12:n:408:GLU:O	12:n:411:LYS:HG2	2.15	0.46
12:n:484:LEU:HB3	12:n:516:ASP:CG	2.41	0.46
12:n:560:VAL:O	12:n:564:ILE:HG13	2.16	0.46
1:A:170:ILE:HG12	1:A:175:ALA:HB2	1.97	0.46
1:C:28:ASP:HB2	1:C:341:TRP:HH2	1.81	0.46
1:D:16:ASN:HA	1:D:21:ILE:HD12	1.97	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: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:F:361:LYS:O	1:F:365:GLU:OE1	2.34	0.46
1:G:219:GLU:HG2	14:G:800:ADP:C4	2.50	0.46
1:G:368:ALA:HA	1:G:371:ILE:HG12	1.97	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:146:LYS:O	4:K:153:THR:OG1	2.30	0.46
5:L:25:LEU:HD21	5:L:40:LEU:HD23	1.97	0.46
8:U:124:ILE:HB	8:U:142:VAL:HG13	1.98	0.46
12:f:649:ILE:O	12:f:653:GLN:HG2	2.16	0.46
13:h:355:GLY:HA2	13:h:384:VAL:HG23	1.98	0.46
12:m:610:GLN:HA	12:m:613:LYS:HD3	1.97	0.46
12:m:690:ARG:HA	12:m:693:LEU:HB2	1.97	0.46
1:B:218:LYS:HA	1:B:222:CYS:SG	2.56	0.46
1:F:371:ILE:HG13	1:F:372:HIS:N	2.31	0.46
1:G:21:ILE:HG23	1:G:37:ASN:HB2	1.98	0.46
1:I:116:ASN:HB2	1:I:121:ARG:NH1	2.31	0.46
3:J:22:GLU:N	14:J:800:ADP:O1B	2.49	0.46
6:M:209:VAL:HG22	10:W:1258:PHE:HD1	1.81	0.46
6:P:341:LYS:NZ	6:P:345:GLU:OE2	2.36	0.46
9:V:7:LEU:HG	9:V:175:LYS:HD2	1.98	0.46
12:f:246:GLN:OE1	12:f:311:HIS:NE2	2.49	0.46
12:f:340:PRO:HD3	12:f:363:HIS:ND1	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:m:666:GLU:HB2	12:m:673:TRP:CE2	2.51	0.46
12:m:750:VAL:HA	12:m:760:VAL:HG21	1.98	0.46
12:m:832:TYR:HB2	12:m:835:ARG:HH21	1.81	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:F:141:MET:HB3	1:F:144:VAL:HG23	1.98	0.46
1:F:232:GLU:HG2	6:M:74:ARG:HG3	1.98	0.46
1:G:161:GLY:O	1:G:186:ALA:HB1	2.16	0.46
2:H:305:MET:SD	15:H:401:ATP:N6	2.89	0.46
4:K:93:LYS:NZ	4:K:113:VAL:O	2.48	0.46
6:Q:212:GLU:HB2	10:Z:1269:ARG:NE	2.28	0.46
10:W:1105:MET:HE1	10:Z:1106:ARG:CG	2.43	0.46
10:Z:1162:GLN:O	10:Z:1165:GLU:HG3	2.16	0.46
12:f:375:GLN:O	12:f:379:ARG:HG2	2.15	0.46
12:f:477:ARG:O	12:f:481:VAL:HG23	2.16	0.46
12:f:577:ASN:OD1	12:f:578:ALA:N	2.49	0.46
12:m:528:GLU:O	12:m:532:GLU:HG2	2.16	0.46
12:m:629:GLN:OE1	12:m:629:GLN:N	2.49	0.46
13:p:315:VAL:HB	13:p:327:TYR:HB2	1.98	0.46
1:B:18:SER:HA	1:B:75:MET:HE1	1.99	0.45
2:H:14:SER:O	2:H:33:SER:OG	2.32	0.45
1:I:331:SER:HA	6:M:19:VAL:HG12	1.97	0.45
9:V:164:LEU:O	9:V:168:VAL:HG23	2.16	0.45
10:Z:1141:LEU:HB3	10:Z:1143:PRO:HD2	1.98	0.45
12:f:759:ARG:HD2	12:f:759:ARG:O	2.15	0.45
12:m:801:ILE:HG21	12:m:850:LEU:HB3	1.98	0.45
12:n:253:ILE:HD12	12:n:316:PHE:HA	1.99	0.45
12:n:612:VAL:O	12: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:45:VAL:HG22	6:M:81:THR:HG22	1.96	0.45
1:E:178:HIS:O	1:E:285:LYS:NZ	2.38	0.45
1:F:160:SER:HB3	1:F:305:THR:HG23	1.98	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:82:ASP:HB3	1:I:85:ASP:HB2	1.97	0.45
1:I:115:LEU:HB2	1:I:182:ARG:HD2	1.98	0.45
4:K:160:SER:O	4:K:173:TRP:N	2.35	0.45
4:K:259:ARG:HG3	5:L:112:PHE:CE2	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:e:535:GLY:HA2	12:e:546:TRP:HA	1.97	0.45
12:f:38:VAL:O	12:f:42:LEU:N	2.35	0.45
12:f:116:LEU:HA	12:f:139:THR:HA	1.98	0.45
12:f:582:PHE:CD2	12:f:664:ARG:HG2	2.51	0.45
13:p:268:ASN:N	13:p:596:ILE:O	2.49	0.45
1:B:193:PHE:HZ	1:B:197:TYR:HH	1.62	0.45
1:B:263:PHE:CZ	1:B:313:ARG:HG2	2.51	0.45
1:B:305:THR:O	1:B:336:ARG:NH1	2.49	0.45
1:D:273:GLU:HB3	1:D:277:GLU:HB2	1.98	0.45
1:E:145:LEU:O	1:E:343:GLY:HA3	2.15	0.45
1:G:343:GLY:O	1:G:346:ILE:HG22	2.16	0.45
6:P:358:ASP:HB2	7:R:129:LEU:HD21	1.98	0.45
12:f:414:VAL:O	12:f:418:GLU:HG2	2.16	0.45
12:f:529:ASN:HB3	12:f:552:ARG:NE	2.23	0.45
13:h:288:SER:HB3	13:h:291:TYR:HB2	1.97	0.45
12:m:774:LEU:HA	12:m:777:PHE:CD2	2.51	0.45
12:n:475:GLN:O	12:n:479:VAL:HG12	2.16	0.45
12:n:613:LYS:HE2	12:n:613:LYS:HB3	1.76	0.45
1:A:289:ASP:OD2	1:A:290:LEU:N	2.48	0.45
1:B:354:LYS:HA	1:B:357:TRP:HE1	1.81	0.45
1:C:112:GLU:C	1:C:142:GLN:HE22	2.24	0.45
1:D:11:PRO:HG2	1:D:348:ALA:HB1	1.99	0.45
1:D:51:ALA:HB2	1:F:173:GLY:HA3	1.98	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
2:H:102:PRO:HB3	2:H:131:ALA:HB3	1.99	0.45
4:K:55:ALA:HA	4:K:100:HIS:CE1	2.51	0.45
5:L:251:ASP:HA	5:L:254:LYS:HD2	1.98	0.45
12:f:82:SER:O	12:f:84:LEU:N	2.50	0.45
12:f:113:SER:O	12:f:141:SER:HA	2.17	0.45
12:f:377:ALA:O	12:f:381:VAL:HG23	2.17	0.45
12:f:620:HIS:HA	12:f:689:PHE:CE1	2.51	0.45
13:h:483:HIS:ND1	13:h:532:TRP:HB2	2.31	0.45
13:h:495:HIS:ND1	13:h:510:THR:OG1	2.37	0.45
12:m:766:ASN:O	12:m:770:GLN:HG2	2.15	0.45
12:n:233:GLY:O	12:n:236:VAL:HG22	2.17	0.45
12:n:278:TRP:NE1	12:n:376:ARG:HH21	2.14	0.45
13:o:342:LYS:NZ	13:o:389:VAL:O	2.38	0.45
1:A:228:PRO:HD3	1:A:313:ARG:NH1	2.31	0.45
1:B:203:TYR:CE1	1:B:249:ILE:HG12	2.52	0.45
1:C:48:MET:HE1	1:E:148:TYR:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:PRO:HG2	1:C:176:MET:HB2	1.98	0.45
1:C:302:GLY:O	1:C:305:THR:OG1	2.30	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
6:N:336:ARG:O	6:N:340:ILE:HG12	2.16	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
8:U:165:ASP:HA	8:U:168:MET:CE	2.46	0.45
9:V:135:PRO:HG3	11:Y:113:PHE:HB2	1.97	0.45
12:f:395:VAL:HB	12:f:399:ARG:HH21	1.81	0.45
12:f:479:VAL:O	12:f:483:VAL:N	2.42	0.45
12:m:669:LEU:HB2	12:m:673:TRP:HB3	1.98	0.45
12:n:333:ASN:HA	12:n:336:MET:HB2	1.97	0.45
12:n:481:VAL:O	12:n:485:ARG:HD2	2.17	0.45
12:n:572:LEU:HD22	12:n:604:TYR:CE1	2.51	0.45
13:o:268:ASN:N	13:o:596:ILE:O	2.49	0.45
1:B:240:GLN:CD	1:B:248:THR:HB	2.42	0.45
1:C:162:ASP:HB2	14:C:800:ADP:H4'	1.97	0.45
1:F:311:GLY:HA3	6:N:20:TYR:CZ	2.51	0.45
2:H:70:PRO:HG3	2:H:85:ILE:HD12	1.98	0.45
2:H:214:GLU:HA	15:H:401:ATP:C2	2.52	0.45
6:M:334:VAL:HG22	7:O:103:GLN:HE21	1.81	0.45
9:V:3:LEU:HB3	11:Y:317:ARG:HG3	1.98	0.45
11:Y:50:TYR:HA	11:Y:56:GLU:O	2.16	0.45
12:f:357:LEU:HD11	12:f:423:TRP:HE3	1.82	0.45
12:m:755:TRP:CD1	13:o:453:GLU:HB3	2.51	0.45
12:n:561:GLU:HG2	12:n:597:ILE:HD11	1.99	0.45
1:A:53:GLU:N	1:A:53:GLU:OE2	2.50	0.45
1:B:49:ALA:N	1:D:148:TYR:HH	2.15	0.45
1:B:300:LEU:HD12	1:B:332:ALA:HB2	1.98	0.45
1:C:86:MET:HA	1:C:89:ILE:HG22	1.98	0.45
1:C:91:GLN:OE1	1:C:91:GLN:HA	2.17	0.45
1:D:161:GLY:O	1:D:186:ALA:HB1	2.17	0.45
1:E:11:PRO:HB3	1:E:107:PRO:HB2	1.97	0.45
1:E:143:ALA:HA	1:E:157:VAL:HG11	1.97	0.45
1:I:143:ALA:HA	1:I:157:VAL:HG11	1.99	0.45
3:J:32:GLU:HB2	3:J:355:TRP:HH2	1.82	0.45
3:J:364:LEU:HD22	11:Y:152:GLN:HA	1.97	0.45
6:Q:25:LEU:HD12	6:Q:26:PRO:HD2	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:271:ALA:O	12:f:275:ILE:HG12	2.17	0.45
12:f:480:ILE:HG12	12:f:484:LEU:HD12	1.98	0.45
12:m:805:VAL:HB	12:m:843:PHE:HE1	1.81	0.45
13:o:270:GLN:HE22	13:o:595:VAL:HG12	1.81	0.45
1:A:116:ASN:O	1:A:121:ARG:NH1	2.48	0.45
1:A:202:GLY:HA2	1:B:117:PRO:HG3	1.99	0.45
1:A:254:SER:HA	1:A:257:ARG:HB2	1.97	0.45
1:B:273:GLU:OE1	1:B:273:GLU:N	2.49	0.45
1:E:9:ASN:OD1	1:E:10:GLN:N	2.48	0.45
1:I:168:VAL:HG22	1:I:180:ILE:HG23	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
12:f:581:MET:SD	12:f:582:PHE:N	2.89	0.45
12:m:402:MET:HE3	12:m:466:MET:CE	2.46	0.45
1:A:355:LYS:HZ1	5:L:258:LEU:HA	1.82	0.45
1:B:10:GLN:CG	12:n:246:GLN:HE22	2.26	0.45
1:B:156:VAL:CG2	1:B:294:LEU:HD12	2.46	0.45
1:B:355:LYS:C	1:B:356:MET:HE2	2.41	0.45
1:D:58:ILE:H	1:D:61:LYS:NZ	2.15	0.45
1:F:94:TYR:CE1	1:F:103:SER:HA	2.51	0.45
1:F:210:GLU:HA	1:F:213:ILE:HD13	1.98	0.45
1:I:18:SER:OG	1:I:163:GLY:N	2.50	0.45
3:J:78:ARG:NE	3:J:78:ARG:HA	2.32	0.45
3:J:182:GLN:HB2	3:J:262:ILE:HD11	1.98	0.45
4:K:62:PHE:HA	4:K:76:ILE:O	2.17	0.45
6:N:399:ARG:HD2	7:O:172:LEU:HD13	1.99	0.45
12:f:229:VAL:HG22	12:f:303:ILE:HD13	1.99	0.45
12:f:250:ASN:O	12:f:254:ARG:HG2	2.17	0.45
12:f:299:LEU:O	12:f:303:ILE:HG12	2.16	0.45
12:f:368:ARG:HB3	12:f:433:LEU:HD11	1.98	0.45
12:f:368:ARG:HA	12:f:437:ILE:HG12	1.99	0.45
13:h:547:GLY:HA2	13:h:573:LEU:HG	1.99	0.45
12:n:334:PRO:HB2	12:n:370:THR:OG1	2.17	0.45
13:o:280:ARG:NH2	13:o:302:ASN:HB2	2.32	0.45
1:A:261:LEU:HA	1:A:267:LEU:HD12	1.98	0.45
1:F:147:LEU:HA	1:F:150:THR:HG22	1.98	0.45
4:K:129:ARG:O	4:K:133:LYS:HG2	2.17	0.45
4:K:197:HIS:CE1	4:K:199:TYR:HB3	2.51	0.45
5:L:156:VAL:HG11	5:L:209:HIS:CE1	2.52	0.45
9:V:40:THR:HG23	9:V:61:CYS:HB3	1.99	0.45
12:f:354:ARG:HB2	12:f:422:THR:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:364:LEU:O	12:f:367:ILE:HG22	2.17	0.45
13:h:347:LEU:HD22	13:h:359:LEU:HD21	1.98	0.45
13:h:527:VAL:HA	13:h:544:ASP:HA	1.99	0.45
1:A:145:LEU:O	1:A:343:GLY:HA3	2.17	0.44
1:B:28:ASP:HB2	1:B:341:TRP:HH2	1.81	0.44
1:B:243:LEU:HD13	1:D:288:MET:HE2	1.99	0.44
1:F:185:ILE:H	1:F:185:ILE:HD12	1.82	0.44
1:G:326:VAL:HG23	1:G:328:ILE:HG23	1.99	0.44
3:J:248:TYR:O	3:J:256:LEU:N	2.40	0.44
7:R:84:LEU:HA	7:R:87:ILE:HG12	1.98	0.44
11:Y:69:ARG:HD3	11:Y:275:HIS:HA	1.99	0.44
12:f:368:ARG:HH21	12:f:433:LEU:HD13	1.82	0.44
12:f:483:VAL:O	12:f:567:ARG:NH1	2.50	0.44
13:h:360:TRP:CE2	13:h:369:PRO:HG3	2.52	0.44
12:m:300:THR:O	12:m:304:LEU:HD23	2.17	0.44
12:m:802:SER:O	12:m:806:ALA:HB2	2.17	0.44
13:o:342:LYS:NZ	13:o:388:ASN:OD1	2.30	0.44
13:p:476:GLN:N	13:p:503:ASP:OD2	2.36	0.44
1:C:224:LEU:HD13	1:C:307:PHE:HB3	1.99	0.44
1:D:154:THR:HB	1:D:172:GLU:H	1.82	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: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
1:I:20:VAL:HG23	1:I:35:PHE:C	2.42	0.44
10:Z:1153:ALA:O	10:Z:1158:ARG:NH1	2.48	0.44
12:f:559:ARG:O	12:f:562:THR:OG1	2.35	0.44
12:m:518:ASN:O	12:m:521:GLU:HG3	2.18	0.44
12:m:649:ILE:HG21	13:o:502:PHE:HD2	1.82	0.44
12:m:666:GLU:OE2	12:m:671:LYS:NZ	2.37	0.44
1:A:228:PRO:HD3	1:A:313:ARG:HH12	1.83	0.44
1:C:315:LEU:HD13	6:Q:44:SER:HB2	1.99	0.44
1:D:227:ASN:HB3	1:D:230:LYS:HG2	1.99	0.44
5:L:200:ASP:N	5:L:200:ASP:OD1	2.50	0.44
6:M:379:GLN:O	6:M:382:MET:HB2	2.17	0.44
11:Y:143:ARG:HA	11:Y:146:LYS:HG2	1.99	0.44
12:f:649:ILE:HG12	12:f:756:LEU:HD11	2.00	0.44
12:f:713:VAL:HG23	12:f:743:ILE:HD12	1.98	0.44
12:m:593:VAL:O	12:m:598:ARG:NH2	2.47	0.44
12:n:779:ILE:HB	13:p:375:LEU:CD2	2.27	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:112:GLU:C	1:D:142:GLN:HE21	2.26	0.44
2:H:173:HIS:HB2	2:H:284:LYS:HZ1	1.81	0.44
4:K:38:LEU:O	5:L:5:GLN:NE2	2.46	0.44
5:L:139:ASP:OD2	5:L:141:SER:OG	2.30	0.44
8:U:147:ASP:HB2	8:U:150:ARG:HH22	1.81	0.44
12:e:286:TYR:CB	12:f:175:GLY:HA2	2.48	0.44
12:f:375:GLN:HB3	12:f:379:ARG:HH12	1.82	0.44
12:f:751:ARG:NH2	13:h:433:ALA:HB1	2.31	0.44
12:m:395:VAL:O	12:m:399:ARG:HG2	2.17	0.44
12:m:560:VAL:O	12:m:564:ILE:HG13	2.17	0.44
12:m:605:GLN:NE2	12:m:669:LEU:HA	2.32	0.44
12:n:367:ILE:HD11	12:n:372:TYR:HB3	1.99	0.44
13:o:315:VAL:HB	13:o:327:TYR:HB2	1.98	0.44
1:A:89:ILE:O	1:A:93:VAL:HG23	2.17	0.44
1:E:156:VAL:HG23	1:E:294:LEU:HD12	2.00	0.44
1:G:15:ASP:HA	1:G:111:THR:OG1	2.18	0.44
1:G:39:VAL:HG21	1:G:85:ASP:HB3	1.98	0.44
3:J:110:PHE:CZ	3:J:118:VAL:HG12	2.52	0.44
11:Y:57:ASN:ND2	11:Y:295:GLU:O	2.51	0.44
10:Z:1282:ASP:OD1	10:Z:1283:ARG:N	2.50	0.44
12:m:292:ARG:NH2	12:m:317:ASP:OD1	2.46	0.44
12:n:539:SER:O	12:n:543:THR:N	2.44	0.44
13:o:531:MET:HE2	13:o:578:TRP:H	1.82	0.44
1:A:43:LYS:NZ	1:A:67:GLY:O	2.50	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:D:77:HIS:HD1	1:D:184:ASP:HB2	1.82	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
4:K:194:ILE:HD13	4:K:239:TYR:HE1	1.82	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
8:U:42:ILE:HD12	8:U:63:ILE:HG22	1.99	0.44
12:n:564:ILE:HG21	12:n:591:LEU:HD21	1.99	0.44
12:n:669:LEU:HB2	12:n:673:TRP:HB2	2.00	0.44
1:A:245:ASP:OD1	1:A:246:GLY:N	2.51	0.44
1:B:238:LYS:HB3	1:B:250:GLU:HB3	2.00	0.44
1:C:308:LYS:HD3	6:Q:37:LEU:O	2.17	0.44
1:D:162:ASP:HB2	14:D:800:ADP:H4'	2.00	0.44
1:E:214:VAL:HA	1:E:217:ILE:HD12	2.00	0.44
1:F:264:ARG:HB3	1:F:266:ASP:OD1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:305:MET:SD	15:H:401:ATP:C6	3.11	0.44
2:H:346:LEU:HA	2:H:349:LEU:HD12	1.99	0.44
3:J:56:GLN:HB2	3:J:59:ILE:HD13	2.00	0.44
4:K:43:ASP:O	4:K:47:ARG:HG2	2.18	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
7:O:79:PRO:HG3	10:W:1107:LEU:HD22	2.00	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
12:f:241:PHE:HA	12:f:244:GLN:HE21	1.83	0.44
12:f:339:PHE:HA	12:f:340:PRO:HD3	1.84	0.44
12:f:410:GLU:O	12:f:414:VAL:HG23	2.17	0.44
12:f:473:HIS:CE1	12:f:527:TYR:HB2	2.52	0.44
12:m:710:ASN:HA	12:m:767:LYS:NZ	2.33	0.44
12:n:235:LYS:NZ	12:n:238:ASP:OD2	2.48	0.44
13:p:531:MET:HE2	13:p:578:TRP:H	1.82	0.44
4:K:16:ILE:HG23	5:L:27:ASP:HB3	2.00	0.44
6:M:6:TYR:HB3	6:M:12:ILE:HG21	2.00	0.44
6:Q:7:ALA:HA	6:Q:14:ARG:HH21	1.83	0.44
12:e:716:ARG:CA	12:e:824:TRP:HD1	2.31	0.44
12:f:635:MET:HA	12:f:635:MET:HE3	2.00	0.44
12:m:266:PRO:HG3	12:m:376:ARG:CG	2.48	0.44
1:A:219:GLU:HG2	14:A:800:ADP:C4	2.53	0.44
1:B:263:PHE:CE2	1:B:313:ARG:HG2	2.53	0.44
1:E:223:TYR:CZ	1:E:256:PHE:HB3	2.53	0.44
2:H:298:VAL:HA	2:H:330:ILE:HB	2.00	0.44
4:K:38:LEU:HD23	5:L:8:CYS:SG	2.58	0.44
4:K:239:TYR:O	4:K:243:ILE:HG12	2.17	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
11:Y:425:CYS:HB3	11:Y:457:HIS:NE2	2.33	0.44
11:Y:426:PHE:CE1	11:Y:458:VAL:HB	2.53	0.44
12:f:482:ARG:NH1	12:f:587:ARG:HG2	2.33	0.44
12:f:641:LEU:HG	13:h:502:PHE:CE2	2.52	0.44
13:h:457:TYR:CE1	13:h:471:MET:HG2	2.51	0.44
12:m:580:GLU:O	12:m:584:ILE:HG13	2.18	0.44
1:I:210:GLU:O	1:I:213:ILE:HG22	2.18	0.43
4:K:210:LYS:NZ	5:L:183:GLY:O	2.51	0.43
6:P:347:ALA:O	7:R:115:HIS:NE2	2.51	0.43
11:Y:42:VAL:HG23	11:Y:284:CYS:CA	2.48	0.43
10:Z:1186:ALA:O	10:Z:1188:SER:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:278:TRP:HB2	12:f:336:MET:CE	2.34	0.43
12:f:292:ARG:O	12:f:292:ARG:NH1	2.46	0.43
12:f:410:GLU:O	12:f:413:MET:HG2	2.18	0.43
12:f:584:ILE:HG13	12:f:585:PHE:HD1	1.83	0.43
13:h:503:ASP:O	13:h:505:THR:HG23	2.18	0.43
13:h:573:LEU:HD13	13:h:587:VAL:HG21	1.99	0.43
12:m:518:ASN:CG	12:m:563:ARG:HH12	2.26	0.43
12:n:305:LYS:HE2	12:n:305:LYS:HB2	1.85	0.43
12:n:487:GLN:NE2	12:n:587:ARG:HA	2.33	0.43
13:o:495:HIS:ND1	13:o:510:THR:HG23	2.33	0.43
13:p:518:TYR:OH	13:p:559:GLU:OE2	2.34	0.43
1:D:263:PHE:CZ	1:D:313:ARG:HG2	2.52	0.43
1:E:30:ILE:HG12	6:Q:5:LYS:NZ	2.20	0.43
1:F:158:LEU:O	1:F:301:SER:N	2.51	0.43
1:G:90:TRP:HB3	1:G:132:PHE:CZ	2.54	0.43
2:H:19:ALA:HB1	2:H:94:LEU:HD11	2.01	0.43
2:H:138:ALA:HB2	2:H:161:HIS:CD2	2.53	0.43
1:I:10:GLN:CD	1:I:25:PHE:HB3	2.44	0.43
5:L:189:LEU:HD13	5:L:233:PHE:CE1	2.53	0.43
8:U:158:GLN:OE1	8:U:158:GLN:N	2.51	0.43
12:e:777:PHE:CA	12:e:833:VAL:HG11	2.46	0.43
12:f:232:PHE:HE1	12:f:299:LEU:HD21	1.83	0.43
12:f:233:GLY:O	12:f:236:VAL:HG12	2.19	0.43
12:f:333:ASN:O	12:f:336:MET:N	2.49	0.43
12:f:415:ALA:O	12:f:419:VAL:HG23	2.18	0.43
13:h:480:THR:H	13:h:501:SER:HA	1.82	0.43
13:h:554:LEU:HD12	13:h:614:PHE:HE1	1.84	0.43
12:m:400:LYS:HB3	12:m:403:HIS:HD1	1.83	0.43
12:n:365:ARG:HH22	12:n:429:LYS:HD2	1.83	0.43
13:p:280:ARG:NH2	13:p:302:ASN:HB2	2.32	0.43
1:C:240:GLN:CD	1:C:248:THR:HB	2.43	0.43
1:D:145:LEU:O	1:D:343:GLY:HA3	2.18	0.43
1:F:46:ARG:HH11	1:F:51:ALA:HB3	1.83	0.43
1:G:72:ARG:NH1	1:G:85:ASP:OD2	2.52	0.43
8:U:58:GLU:HG3	8:U:59:GLN:H	1.83	0.43
9:V:123:LYS:HD3	9:V:142:PRO:HD3	2.00	0.43
11:Y:76:CYS:SG	11:Y:80:MET:N	2.92	0.43
11:Y:319:MET:HE2	11:Y:333:LEU:HB3	1.99	0.43
12:f:485:ARG:HA	12:f:512:PHE:CE2	2.54	0.43
12:f:632:ALA:HA	12:f:635:MET:HB2	2.00	0.43
12:f:766:ASN:O	12:f:770:GLN:HG2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:h:483:HIS:CE1	13:h:532:TRP:HB2	2.54	0.43
12:m:264:ARG:O	12:m:376:ARG:NH2	2.51	0.43
12:n:263:ASP:OD1	12:n:264:ARG:N	2.51	0.43
12:n:425:ASP:OD1	12:n:426:GLU:N	2.51	0.43
12:n:581:MET:HE1	12:n:607:GLN:OE1	2.17	0.43
1:A:223:TYR:CE1	1:A:256:PHE:HB3	2.54	0.43
1:A:284:GLN:HE22	1:A:285:LYS:HG3	1.84	0.43
1:B:227:ASN:HB2	6:P:113:GLN:NE2	2.33	0.43
1:B:332:ALA:H	6:P:86:GLY:HA3	1.82	0.43
1:C:24:GLY:HA3	1:C:341:TRP:HZ2	1.83	0.43
1:D:39:VAL:HB	1:D:56:ILE:HD11	2.00	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	2.00	0.43
1:G:252:GLY:H	1:G:255:ARG:HH12	1.66	0.43
4:K:207:VAL:HG23	5:L:188:ASN:HB3	2.00	0.43
7:O:148:LYS:CD	6:P:142:LYS:HD3	2.44	0.43
12:f:213:ILE:HG13	12:f:214:THR:N	2.32	0.43
12:f:746:LEU:CD2	12:f:768:ALA:HB2	2.46	0.43
12:m:25:ALA:N	12:m:125:ILE:O	2.52	0.43
12:n:685:ASP:OD1	12:n:685:ASP:N	2.51	0.43
13:p:531:MET:SD	13:p:577:ARG:HD3	2.58	0.43
1:B:305:THR:HG22	1:B:310:PHE:HE1	1.83	0.43
1:C:161:GLY:O	1:C:186:ALA:HB1	2.18	0.43
1:F:77:HIS:ND1	1:F:184:ASP:HB3	2.33	0.43
2:H:140:LEU:HD12	2:H:342:GLY:C	2.43	0.43
2:H:163:VAL:HG13	2:H:175:ILE:HG12	2.00	0.43
1:I:11:PRO:HG2	1:I:26:ALA:HB2	2.01	0.43
1:I:300:LEU:HD13	1:I:310:PHE:HE2	1.84	0.43
3:J:78:ARG:NH2	11:Y:278:ILE:HG22	2.33	0.43
4:K:59:MET:HG3	4:K:78:GLU:OE2	2.18	0.43
6:M:385:ASN:HB3	6:N:386:LEU:HD13	2.00	0.43
6:P:361:GLN:NE2	7:R:129:LEU:HG	2.33	0.43
12:e:283:ARG:CA	12:f:176:ASP:H	2.29	0.43
12:m:769:HIS:O	12:m:773:GLN:HG2	2.17	0.43
13:o:531:MET:SD	13:o:577:ARG:HD3	2.58	0.43
13:o:576:VAL:HG23	13:o:587:VAL:HG12	2.00	0.43
13:p:270:GLN:HE22	13:p:595:VAL:HG12	1.81	0.43
1:D:181:MET:HG3	1:D:278:VAL:HG13	2.01	0.43
1:D:228:PRO:HD3	1:D:313:ARG:HH12	1.83	0.43
1:G:18:SER:HA	1:G:75:MET:HE1	2.01	0.43
2:H:123:MET:HG3	2:H:132:MET:SD	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:338:TYR:CD2	6:M:9:LEU:HD13	2.54	0.43
6:M:382:MET:HA	6:N:382:MET:HE1	2.00	0.43
6:Q:26:PRO:O	6:Q:28:ASP:N	2.51	0.43
8:U:163:GLN:O	8:U:167:LEU:HG	2.18	0.43
9:V:144:THR:HG23	9:V:153:PHE:CE2	2.53	0.43
12:f:334:PRO:HB2	12:f:370:THR:HG22	2.00	0.43
12:f:479:VAL:HA	12:f:482:ARG:NH2	2.33	0.43
12:f:619:LEU:HD22	12:f:661:TYR:HE2	1.83	0.43
12:f:677:VAL:O	12:f:681:LYS:HG2	2.18	0.43
12:n:395:VAL:O	12:n:398:THR:OG1	2.23	0.43
12:n:476:LEU:HD21	12:n:594:ARG:NH1	2.34	0.43
12:n:569:ARG:HD3	12:n:569:ARG:HA	1.81	0.43
13:p:576:VAL:HG23	13:p:587:VAL:HG12	2.00	0.43
1:B:108:VAL:HG11	1:B:128:PHE:HD2	1.83	0.43
1:D:219:GLU:HG2	14:D:800:ADP:C4	2.54	0.43
1:E:15:ASP:HB3	1:E:22:LYS:HE2	2.01	0.43
1:F:371:ILE:O	1:F:375:THR:HG23	2.19	0.43
2:H:14:SER:HA	2:H:71:ILE:HD12	1.99	0.43
1:I:242:TYR:HE2	1:I:246:GLY:HA2	1.84	0.43
3:J:81:LEU:HB3	11:Y:49:HIS:CE1	2.54	0.43
3:J:174:GLU:HG2	3:J:269:ILE:HG21	2.00	0.43
4:K:273:LYS:HB3	4:K:277:TYR:OH	2.18	0.43
5:L:197:MET:HE1	5:L:216:LEU:HB3	2.01	0.43
12:f:427:TYR:OH	12:f:452:ILE:HB	2.19	0.43
12:f:651:ALA:HB3	12:f:695:THR:HG22	2.00	0.43
12:f:722:SER:C	12:f:731:ASN:HB2	2.43	0.43
13:h:480:THR:HG22	13:h:502:PHE:CE1	2.54	0.43
12:m:620:HIS:O	12:m:624:LYS:HG3	2.18	0.43
12:n:365:ARG:HB3	12:n:368:ARG:HH12	1.84	0.43
12:n:369:ASN:OD1	12:n:369:ASN:N	2.52	0.43
1:B:9:ASN:HB3	12:n:246:GLN:NE2	2.33	0.43
1:B:51:ALA:HB2	1:D:173:GLY:HA3	2.01	0.43
1:C:245:ASP:OD1	1:C:246:GLY:N	2.51	0.43
1:E:147:LEU:HA	1:E:147:LEU:HD23	1.74	0.43
2:H:39:ARG:NH1	2:H:64:ILE:O	2.51	0.43
3:J:53:LYS:C	3:J:56:GLN:HE22	2.25	0.43
4:K:177:TRP:CD2	4:K:232:ILE:HD12	2.54	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:h:316:TRP:CH2	13:h:325:PRO:HG3	2.54	0.43
13:o:472:PHE:HB3	13:o:509:TRP:CZ3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:PHE:HB2	1:A:134:VAL:HG23	2.01	0.43
1:C:20:VAL:O	1:C:22:LYS:NZ	2.44	0.43
1:E:67:GLY:HA3	1:G:289:ASP:HB3	2.00	0.43
1:E:197:TYR:CD1	1:E:200:LYS:HD3	2.54	0.43
2:H:163:VAL:HG22	2:H:175:ILE:HG23	2.00	0.43
1:I:25:PHE:HZ	1:I:101:THR:HG21	1.82	0.43
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
5:L:259:LYS:HD3	5:L:262:LEU:HD23	2.00	0.43
8:U:41:ILE:HD12	8:U:62:ILE:HD12	2.00	0.43
12:f:478:ALA:O	12:f:482:ARG:HG3	2.19	0.43
13:g:359:LEU:O	13:g:370:VAL:N	2.51	0.43
12:m:717:ILE:HG22	12:m:824:TRP:CD2	2.54	0.43
12:m:783:GLU:HG2	12:m:786:ARG:HE	1.84	0.43
12:n:357:LEU:HD21	12:n:423:TRP:HB2	2.00	0.43
12:n:581:MET:CE	12:n:607:GLN:HE22	2.32	0.43
1:A:280:VAL:O	1:A:284:GLN:HG3	2.18	0.43
1:B:245:ASP:OD1	1:B:246:GLY:N	2.52	0.43
1:C:15:ASP:OD2	1:C:340:THR:OG1	2.32	0.43
1:D:24:GLY:HA3	1:D:341:TRP:HZ2	1.83	0.43
2:H:116:ARG:HA	2:H:119:MET:HG2	2.00	0.43
3:J:42:VAL:HG12	3:J:53:LYS:HA	2.01	0.43
6:P:3:ASP:HA	6:P:6:TYR:CZ	2.54	0.43
12:f:220:CYS:HA	12:f:223:ARG:HD2	2.00	0.43
13:g:480:THR:N	13:g:500:SER:O	2.52	0.43
12:m:717:ILE:HG13	12:m:718:PHE:HD1	1.84	0.43
12:m:785:VAL:O	12:m:789:GLU:HG2	2.19	0.43
12:n:232:PHE:CE1	12:n:299:LEU:HD21	2.53	0.43
12:n:473:HIS:O	12:n:477:ARG:HD2	2.19	0.43
13:o:347:LEU:HB3	13:o:359:LEU:HD11	2.01	0.43
13:p:495:HIS:ND1	13:p:510:THR:HG23	2.33	0.43
1:B:21:ILE:HG12	1:B:37:ASN:HB2	2.01	0.42
2:H:262:PHE:HD1	2:H:275:HIS:CD2	2.36	0.42
2:H:291:LYS:HA	2:H:325:MET:SD	2.58	0.42
1:I:200:LYS:O	3:J:98:PRO:HA	2.19	0.42
6:P:269:GLN:HG2	7:R:39:LYS:HZ1	1.83	0.42
8:U:89:VAL:HB	8:U:106:VAL:HG13	2.01	0.42
9:V:33:ASN:HB2	9:V:53:ALA:O	2.19	0.42
12:f:581:MET:O	12:f:584:ILE:HG12	2.19	0.42
13:h:329:PHE:HB3	13:h:360:TRP:CE2	2.53	0.42
13:h:475:HIS:ND1	13:h:501:SER:HB3	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:m:636:SER:HB2	12:m:641:LEU:HD23	2.01	0.42
13:o:332:GLN:HE22	13:o:372:ARG:HH22	1.67	0.42
13:p:332:GLN:NE2	13:p:372:ARG:HH12	2.17	0.42
13:p:384:VAL:HG22	13:p:402:SER:HB3	2.01	0.42
13:p:589:ASP:OD1	13:p:593:GLN:N	2.47	0.42
1:A:160:SER:OG	1:A:305:THR:HG23	2.19	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
1:G:240:GLN:OE1	1:G:249:ILE:N	2.53	0.42
2:H:218:TYR:HA	2:H:307:PRO:HD2	2.01	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
10:Z:1225:ALA:HB1	10:Z:1239:PHE:CD2	2.54	0.42
12:f:226:LYS:HB2	12:f:228:LYS:NZ	2.34	0.42
12:f:378:LEU:HD11	12:f:450:TRP:CD1	2.54	0.42
12:f:483:VAL:HG22	12:f:588:PHE:CE1	2.54	0.42
12:f:528:GLU:O	12:f:531:LYS:HB3	2.19	0.42
12:f:628:PRO:HD3	12:f:647:SER:HB3	2.01	0.42
12:m:216:VAL:O	12:m:219:GLN:HG2	2.20	0.42
12:m:254:ARG:NH2	12:m:257:GLN:OE1	2.46	0.42
12:m:324:GLN:OE1	12:m:324:GLN:N	2.42	0.42
12:m:750:VAL:O	12:m:754:LYS:HG2	2.19	0.42
13:p:311:GLY:HA3	13:p:335:VAL:HG23	2.01	0.42
1:D:217:ILE:HG12	1:D:241:TYR:CE2	2.54	0.42
1:F:103:SER:HB2	1:F:132:PHE:HB3	2.01	0.42
3:J:78:ARG:HA	3:J:78:ARG:HE	1.83	0.42
6:P:235:LEU:HD21	7:R:13:ARG:HB3	2.00	0.42
10:W:1109:ILE:HD11	10:Z:1108:HIS:ND1	2.34	0.42
12:f:340:PRO:HG2	12:f:359:ALA:C	2.43	0.42
12:f:698:ILE:HA	12:f:701:ASP:OD2	2.19	0.42
12:f:753:LEU:HD22	12:f:758:PHE:HD2	1.84	0.42
13:h:455:SER:HA	13:h:472:PHE:O	2.19	0.42
12:n:706:VAL:HA	12:n:709:ARG:HD2	2.02	0.42
12:n:775:TYR:HH	13:p:354:SER:CA	1.94	0.42
1:B:156:VAL:HG22	1:B:169:PRO:HB3	2.00	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:E:89:ILE:O	1:E:93:VAL:HG23	2.20	0.42
4:K:230:LYS:O	4:K:234:HIS:ND1	2.47	0.42
6:P:331:PRO:HA	6:P:334:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Q:319:THR:O	6:Q:323:TRP:HE3	2.01	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
9:V:99:VAL:HG22	9:V:116:ILE:HD12	2.01	0.42
12:f:441:LYS:O	12:f:445:ASN:N	2.33	0.42
12:m:577:ASN:HB2	12:m:580:GLU:OE1	2.19	0.42
12:m:775:TYR:O	12:m:779:ILE:HG12	2.19	0.42
12:n:255:GLU:O	12:n:259:VAL:HG23	2.19	0.42
12:n:373:PRO:HB2	12:n:376:ARG:HB3	2.02	0.42
12:n:435:ARG:CZ	12:n:450:TRP:HB3	2.49	0.42
12:n:482:ARG:O	12:n:485:ARG:NE	2.52	0.42
13:o:332:GLN:NE2	13:o:372:ARG:HH12	2.17	0.42
13:p:265:LEU:HD23	13:p:599:VAL:HG12	2.01	0.42
13:p:280:ARG:CZ	13:p:302:ASN:HB2	2.49	0.42
1:A:153:THR:HG21	5:L:267:LYS:HZ1	1.84	0.42
1:C:65:HIS:HB3	1:C:68:LEU:HD13	2.02	0.42
1:G:114:PRO:HA	1:G:141:MET:HE2	2.01	0.42
4:K:67:ILE:HD11	4:K:70:TYR:HB2	2.01	0.42
4:K:230:LYS:HG2	4:K:234:HIS:CE1	2.55	0.42
5:L:66:ARG:NE	5:L:68:GLY:O	2.53	0.42
6:N:392:ASN:ND2	10:Z:1179:ILE:HG12	2.30	0.42
8:U:47:PRO:HD2	8:U:81:PRO:HB3	2.01	0.42
11:Y:46:VAL:HG13	11:Y:278:ILE:HD11	2.01	0.42
12:e:780:SER:CB	12:e:833:VAL:HB	2.49	0.42
12:f:618:SER:O	12:f:622:LYS:HG3	2.19	0.42
12:f:827:TYR:O	12:f:831:PRO:HD2	2.19	0.42
13:h:583:ARG:NH2	13:h:599:VAL:O	2.44	0.42
12:m:333:ASN:HB3	12:m:334:PRO:HD3	2.00	0.42
12:n:221:TYR:HE1	12:n:227:PRO:HD3	1.84	0.42
12:n:608:LEU:HD23	12:n:608:LEU:HA	1.83	0.42
13:p:347:LEU:HB3	13:p:359:LEU:HD11	2.01	0.42
13:p:352:THR:OG1	13:p:356:GLN:O	2.34	0.42
13:p:472:PHE:HB3	13:p:509:TRP:CZ3	2.54	0.42
1:B:108:VAL:HG11	1:B:128:PHE:CD2	2.55	0.42
1:B:148:TYR:CD1	4:K:283:MET:HE1	2.55	0.42
1:B:181:MET:HE1	1:B:282:ALA:HA	2.02	0.42
1:C:316:SER:O	1:C:320:LYS:HG3	2.20	0.42
1:D:238:LYS:HA	1:D:252:GLY:HA2	2.00	0.42
1:I:10:GLN:O	1:I:106:HIS:ND1	2.34	0.42
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:145:GLU:HA	7:O:148:LYS:HG2	2.01	0.42
6:Q:111:GLU:O	6:Q:114:GLU:HG2	2.19	0.42
6:Q:214:HIS:HB2	10:Z:1271:VAL:HG22	2.00	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	2.37	0.42
11:Y:123:MET:HB3	11:Y:133:TRP:HZ3	1.84	0.42
12:f:263:ASP:OD1	12:f:264:ARG:N	2.53	0.42
12:f:423:TRP:NE1	12:f:456:HIS:HE1	2.17	0.42
12:f:746:LEU:HD11	12:f:764:ILE:CG2	2.50	0.42
12:m:640:ASP:HB2	13:o:385:TYR:CE2	2.55	0.42
12:m:653:GLN:NE2	12:m:656:ARG:HH22	2.17	0.42
12:m:805:VAL:HG12	12:m:846:LYS:HB3	2.02	0.42
12:n:409:PHE:O	12:n:413:MET:HG2	2.19	0.42
12:n:556:ARG:HG3	12:n:559:ARG:NH2	2.35	0.42
13:o:503:ASP:O	13:o:505:THR:HG23	2.20	0.42
13:p:503:ASP:O	13:p:505:THR:HG23	2.20	0.42
1:A:350:LEU:HD22	5:L:265:ALA:HB1	2.01	0.42
1:B:305:THR:HG22	1:B:310:PHE:CE1	2.55	0.42
1:C:121:ARG:HE	1:C:139:ILE:HG21	1.85	0.42
1:D:74:PRO:HG3	1:D:89:ILE:HD12	2.00	0.42
1:D:253:PRO:HA	1:D:256:PHE:CE2	2.54	0.42
6:P:211:TYR:CD1	10:Z:1256:VAL:HG22	2.53	0.42
11:Y:138:HIS:CE1	11:Y:140:HIS:HB2	2.54	0.42
12:f:468:LYS:O	12:f:472:GLN:HG2	2.20	0.42
12:f:476:LEU:HD23	12:f:557:ILE:HD12	2.01	0.42
13:h:474:GLY:HA3	13:h:509:TRP:CZ2	2.55	0.42
13:h:567:VAL:HG23	13:h:570:ASN:HA	2.02	0.42
12:m:241:PHE:O	12:m:245:LEU:HG	2.20	0.42
12:m:738:ASN:O	12:m:824:TRP:NE1	2.53	0.42
12:n:331:ASP:O	12:n:334:PRO:HD2	2.19	0.42
1:C:112:GLU:OE1	1:C:139:ILE:HG23	2.20	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
1:F:350:LEU:HD13	12:f:319:ASP:HB2	2.01	0.42
1:G:284:GLN:NE2	1:G:285:LYS:HG3	2.34	0.42
1:I:77:HIS:CE1	1:I:184:ASP:HB3	2.54	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:N:348:MET:SD	6:N:352:GLN:NE2	2.93	0.42
6:P:312:LYS:C	6:Q:317:TYR:HH	2.15	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:357:LEU:HD11	12:f:423:TRP:CE3	2.55	0.42
12:m:435:ARG:HG2	12:m:450:TRP:CH2	2.55	0.42
12:m:518:ASN:HB3	12:m:563:ARG:HH22	1.85	0.42
12:m:846:LYS:HD3	12:m:846:LYS:HA	1.82	0.42
13:o:280:ARG:CZ	13:o:302:ASN:HB2	2.49	0.42
13:o:336:MET:HE1	13:o:353:TYR:CA	2.47	0.42
13:o:518:TYR:OH	13:o:559:GLU:OE2	2.34	0.42
13:p:579:THR:HG21	13:p:584:GLU:HB2	2.01	0.42
1:A:19:GLY:O	1:A:37:ASN:N	2.41	0.42
1:C:11:PRO:HG2	1:C:348:ALA:HB1	2.02	0.42
1:E:9:ASN:HD21	1:E:106:HIS:CE1	2.38	0.42
1:E:36:PRO:HB2	1:E:38:TYR:CE2	2.54	0.42
1:E:137:LEU:HD21	1:E:139:ILE:HG23	2.00	0.42
4:K:230:LYS:CG	4:K:234:HIS:HE1	2.33	0.42
4:K:271:TRP:HA	4:K:274:ILE:HG12	2.00	0.42
6:M:69:LEU:HD21	6:M:71:PHE:CD2	2.54	0.42
6:P:147:LEU:HD12	6:P:147:LEU:HA	1.78	0.42
6:Q:242:VAL:HG22	7:R:33:VAL:HG21	2.00	0.42
12:f:425:ASP:O	12:f:429:LYS:HG3	2.20	0.42
12:f:482:ARG:HH11	12:f:587:ARG:HG2	1.84	0.42
12:f:653:GLN:HG3	13:h:502:PHE:O	2.20	0.42
12:f:751:ARG:CZ	13:h:452:GLU:HG2	2.49	0.42
13:h:287:TRP:CZ3	13:h:295:LEU:HB2	2.54	0.42
12:m:400:LYS:HB3	12:m:403:HIS:ND1	2.34	0.42
12:m:653:GLN:OE1	12:m:656:ARG:NH1	2.30	0.42
12:n:604:TYR:O	12:n:607:GLN:NE2	2.53	0.42
13:p:270:GLN:NE2	13:p:595:VAL:HG12	2.35	0.42
1:D:334:GLN:NE2	6:P:13:ALA:O	2.53	0.42
1:E:60:PRO:O	1:E:63:GLU:HG2	2.20	0.42
1:G:32:LYS:HG3	1:G:33:TYR:CD2	2.55	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:176:MET:HB3	1:I:179:SER:HB2	2.01	0.42
1:I:352:THR:O	1:I:356:MET:HG2	2.20	0.42
5:L:60:LEU:HD21	5:L:135:LYS:HB2	2.02	0.42
5:L:85:ASP:OD1	5:L:86:GLY:N	2.53	0.42
5:L:210:ILE:HA	5:L:213:ILE:HG12	2.02	0.42
7:R:18:GLU:O	7:R:22:TYR:N	2.52	0.42
9:V:34:ILE:HG22	9:V:55:VAL:HB	2.02	0.42
11:Y:283:ARG:NE	11:Y:288:GLU:O	2.52	0.42
12:f:413:MET:HG3	12:f:414:VAL:N	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:m:468:LYS:O	12:m:472:GLN:HG2	2.20	0.42
12:m:699:PHE:CD2	12:m:758:PHE:HB3	2.54	0.42
12:n:441:LYS:HE2	12:n:441:LYS:HB2	1.93	0.42
13:o:265:LEU:HD23	13:o:599:VAL:HG12	2.01	0.42
1:A:25:PHE:CE2	1:A:99:LEU:HD23	2.55	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:E:305:THR:O	1:E:336:ARG:NH1	2.53	0.41
1:F:20:VAL:HA	1:F:36:PRO:HA	2.02	0.41
1:F:77:HIS:O	1:F:182:ARG:NH2	2.53	0.41
1:F:180:ILE:O	1:F:181:MET:HE2	2.20	0.41
1:F:372:HIS:HA	1:F:375:THR:HG23	2.01	0.41
2:H:71:ILE:CG1	2:H:82:MET:HE1	2.50	0.41
2:H:79:TRP:CZ2	2:H:118:LYS:HB3	2.55	0.41
6:M:334:VAL:HG22	7:O:103:GLN:NE2	2.35	0.41
6:M:344:HIS:HB2	7:O:116:ILE:HD11	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
12:f:255:GLU:O	12:f:259:VAL:HG23	2.20	0.41
12:f:335:LEU:HD21	12:f:367:ILE:HB	2.02	0.41
12:f:485:ARG:HH21	12:f:487:GLN:HG2	1.85	0.41
12:f:580:GLU:O	12:f:584:ILE:HG23	2.19	0.41
13:h:501:SER:OG	13:h:502:PHE:N	2.53	0.41
12:m:658:LEU:O	12:m:662:MET:HE3	2.20	0.41
12:m:842:ASN:O	12:m:846:LYS:HG2	2.19	0.41
12:n:483:VAL:HG11	12:n:590:ALA:HB2	2.01	0.41
12:n:485:ARG:HH12	12:n:487:GLN:CG	2.33	0.41
12:n:580:GLU:HG3	12:n:583:ARG:NH1	2.29	0.41
1:A:156:VAL:HA	1:A:169:PRO:HA	2.02	0.41
1:A:288:MET:HA	1:A:291:ARG:CG	2.50	0.41
1:D:147:LEU:HD23	1:D:147:LEU:HA	1.84	0.41
1:D:305:THR:O	1:D:336:ARG:NH1	2.53	0.41
1:F:151:GLY:HA3	12:f:310:PHE:CD1	2.55	0.41
1:F:169:PRO:HG2	1:F:176:MET:HB2	2.02	0.41
3:J:166:LEU:HB3	3:J:270:LEU:HG	2.02	0.41
3:J:213:ARG:HD2	11:Y:249:VAL:HG23	2.02	0.41
6:M:214:HIS:ND1	6:P:209:VAL:O	2.49	0.41
8:U:31:PRO:HD2	8:U:52:GLU:HB3	2.01	0.41
13:h:285:LEU:HD12	13:h:295:LEU:HD11	2.01	0.41
13:h:524:SER:H	13:h:548:ARG:HH22	1.69	0.41
12:m:774:LEU:HD13	12:m:824:TRP:CE3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:n:241:PHE:O	12:n:245:LEU:HG	2.19	0.41
12:n:305:LYS:HG3	12:n:310:PHE:CE1	2.56	0.41
12:n:349:GLU:OE1	12:n:399:ARG:NH2	2.47	0.41
13:o:270:GLN:NE2	13:o:595:VAL:HG12	2.35	0.41
13:o:311:GLY:HA3	13:o:335:VAL:HG23	2.01	0.41
13:p:336:MET:HE1	13:p:353:TYR:CA	2.47	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:287:ASP:O	1:F:291:ARG:HG3	2.20	0.41
1:G:140:SER:OG	1:G:141:MET:N	2.53	0.41
2:H:35:VAL:HG12	2:H:54:VAL:HG22	2.02	0.41
2:H:76:VAL:HG22	2:H:82:MET:HE3	2.00	0.41
1:I:223:TYR:CE1	1:I:256:PHE:HB3	2.55	0.41
7:O:113:SER:HB2	7:O:116:ILE:HD12	2.02	0.41
6:P:17:PRO:HG2	6:P:20:TYR:CZ	2.55	0.41
6:P:338:VAL:O	6:P:342:GLN:OE1	2.39	0.41
12:f:361:PHE:HA	12:f:364:LEU:HD12	2.01	0.41
12:f:484:LEU:HB3	12:f:516:ASP:HB3	2.01	0.41
12:f:661:TYR:O	12:f:664:ARG:HB2	2.20	0.41
12:m:603:GLU:HG3	12:m:604:TYR:H	1.85	0.41
12:m:743:ILE:HA	12:m:746:LEU:HB3	2.03	0.41
12:n:413:MET:O	12:n:417:PHE:HD1	2.02	0.41
12:n:448:MET:HE3	12:n:450:TRP:CZ3	2.55	0.41
13:p:479:ILE:HD13	13:p:501:SER:HB2	2.01	0.41
1:A:74:PRO:HG3	1:A:89:ILE:HD12	2.02	0.41
1:A:218:LYS:HA	1:A:222:CYS:SG	2.61	0.41
1:B:324:LYS:O	1:B:326:VAL:HG23	2.20	0.41
3:J:250:LEU:HD11	3:J:256:LEU:HB2	2.01	0.41
5:L:55:VAL:HG21	5:L:75:TRP:HB2	2.01	0.41
7:O:143:ILE:HG13	7:O:144:THR:N	2.35	0.41
6:Q:345:GLU:O	6:Q:348:MET:HG2	2.20	0.41
8:U:115:ARG:NE	8:U:115:ARG:HA	2.34	0.41
12:f:579:ASN:HA	12:f:582:PHE:HD1	1.85	0.41
12:f:628:PRO:HA	12:f:633:CYS:HB2	2.02	0.41
13:h:348:VAL:HB	13:h:360:TRP:HB2	2.02	0.41
13:h:546:MET:HB2	13:h:548:ARG:NE	2.36	0.41
12:m:137:VAL:O	12:n:139:THR:N	2.53	0.41
12:m:287:ARG:O	12:m:291:LYS:HG3	2.20	0.41
12:m:396:LEU:HD22	12:m:401:LEU:HD11	2.01	0.41
12:n:365:ARG:NH2	12:n:429:LYS:HB2	2.35	0.41
12:n:666:GLU:HA	12:n:673:TRP:CB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:p:332:GLN:HE22	13:p:372:ARG:HH22	1.67	0.41
1:B:9:ASN:ND2	12:n:247:SER:OG	2.51	0.41
1:B:153:THR:O	1:B:173:GLY:N	2.45	0.41
1:C:66:ARG:HH12	1:C:213:ILE:HG12	1.86	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:F:91:GLN:HG3	1:F:132:PHE:HE1	1.84	0.41
1:F:213:ILE:HD12	1:F:213:ILE:H	1.85	0.41
1:F:319:LYS:HB3	1:F:320:LYS:NZ	2.36	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
3:J:88:ARG:NH1	3:J:117:SER:OG	2.47	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
10:Z:1268:HIS:O	10:Z:1269:ARG:NH2	2.54	0.41
12:f:627:TYR:HB3	12:f:628:PRO:HD3	2.02	0.41
13:h:436:SER:N	13:h:450:GLY:O	2.39	0.41
12:n:462:ARG:NH1	12:n:538:VAL:HA	2.35	0.41
13:o:384:VAL:HG22	13:o:402:SER:HB3	2.01	0.41
1:C:197:TYR:CD1	1:C:200:LYS:HD3	2.55	0.41
1:C:200:LYS:O	1:D:117:PRO:HA	2.21	0.41
1:D:243:LEU:HD11	1:D:249:ILE:HG12	2.02	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: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:M:212:GLU:N	6:M:212:GLU:OE1	2.53	0.41
6:P:310:GLN:HB3	7:R:83:LYS:HZ1	1.85	0.41
9:V:10:LYS:HB2	9:V:176:PHE:CE2	2.55	0.41
12:f:264:ARG:HD3	12:f:277:PHE:CB	2.50	0.41
12:f:578:ALA:HA	12:f:581:MET:CG	2.51	0.41
12:f:589:ASN:HA	12:f:592:PHE:CE2	2.56	0.41
12:f:735:LEU:HD22	12:f:816:ILE:HG23	2.01	0.41
13:h:406:LYS:HA	13:h:423:GLU:HA	2.02	0.41
12:m:165:ILE:CA	12:m:171:ALA:H	2.34	0.41
12:m:374:ILE:HG22	12:m:448:MET:HE1	2.01	0.41
12:m:676:HIS:O	12:m:680:GLN:HG3	2.20	0.41
12:n:563:ARG:HB3	12:n:567:ARG:HH21	1.85	0.41
1:A:65:HIS:ND1	1:C:171:TYR:OH	2.30	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:THR:O	1:A:173:GLY:N	2.53	0.41
1:C:103:SER:OG	1:C:132:PHE:HB3	2.21	0.41
1:C:141:MET:HB2	1:C:144:VAL:HG12	2.03	0.41
1:E:99:LEU:O	1:E:101:THR:HG23	2.21	0.41
1:E:122:GLU:HG2	1:E:368:ALA:HB1	2.02	0.41
4:K:225:ALA:O	4:K:229:ILE:HG12	2.20	0.41
6:P:97:VAL:HG22	6:P:98:LYS:H	1.86	0.41
6:P:354:LEU:HB3	6:Q:354:LEU:HD11	2.03	0.41
12:m:112:LYS:H	12:m:142:GLU:C	2.29	0.41
12:m:775:TYR:HB3	12:m:776:PRO:HD3	2.03	0.41
13:o:579:THR:HG21	13:o:584:GLU:HB2	2.01	0.41
1:A:221:ALA:O	1:A:255:ARG:HG3	2.20	0.41
1:E:227:ASN:HB3	1:E:230:LYS:HG2	2.03	0.41
1:I:370:SER:HA	1:I:373:ARG:HG2	2.02	0.41
4:K:154:ILE:N	4:K:179:PHE:O	2.42	0.41
5:L:104:PHE:HD2	5:L:119:VAL:HG21	1.85	0.41
12:f:516:ASP:O	12:f:520:ILE:HG13	2.21	0.41
12:f:706:VAL:HA	12:f:709:ARG:HD3	2.02	0.41
12:m:642:PRO:HB2	12:m:749:GLU:OE2	2.21	0.41
13:o:445:ASN:ND2	13:o:460:CYS:SG	2.94	0.41
1:B:44:HIS:CD2	1:D:176:MET:HG3	2.56	0.41
1:E:302:GLY:O	1:E:305:THR:OG1	2.36	0.41
2:H:220:ALA:CB	2:H:226:GLU:HG3	2.50	0.41
2:H:264:PRO:O	2:H:268:GLY:N	2.53	0.41
1:I:118:ARG:HG2	1:I:372:HIS:CE1	2.56	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: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
3:J:279:SER:HB2	3:J:282:THR:HG23	2.03	0.41
6:N:326:ILE:HB	7:O:101:LEU:HD21	2.02	0.41
6:N:348:MET:HE2	10:Z:1134:LEU:HD23	2.02	0.41
6:P:175:LEU:HD13	10:Z:1268:HIS:HB3	2.01	0.41
9:V:123:LYS:NZ	11:Y:300:SER:H	2.19	0.41
11:Y:13:LEU:HD21	11:Y:19:LYS:HG3	2.01	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
12:e:21:VAL:HA	12:e:122:ALA:HB1	2.03	0.41
12:f:264:ARG:HD3	12:f:277:PHE:HB2	2.02	0.41
12:f:560:VAL:O	12:f:564:ILE:HG12	2.21	0.41
12:f:561:GLU:HG2	12:f:596:HIS:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:607:GLN:HG2	12:f:611:ARG:NE	2.36	0.41
12:f:627:TYR:OH	12:f:636:SER:HB3	2.20	0.41
12:f:777:PHE:O	12:f:781:LEU:HG	2.20	0.41
13:h:500:SER:HB2	13:h:527:VAL:HG13	2.03	0.41
12:m:519:ALA:HB1	12:m:560:VAL:HG13	2.03	0.41
12:m:770:GLN:O	12:m:774:LEU:HG	2.20	0.41
12:n:247:SER:O	12:n:251:ARG:HG3	2.21	0.41
12:n:287:ARG:O	12:n:291:LYS:HG3	2.20	0.41
12:n:540:LYS:O	12:n:544:GLU:HG2	2.21	0.41
13:o:317:ASN:OD1	13:o:318:MET:N	2.54	0.41
13:p:362:ASN:OD1	13:p:363:ARG:N	2.54	0.41
1:A:105:GLU:HG3	1:A:106:HIS:CD2	2.56	0.41
1:B:112:GLU:OE1	1:B:121:ARG:HG2	2.20	0.41
1:C:13:VAL:HG21	1:C:345:SER:HA	2.02	0.41
1:F:194:LEU:O	1:F:198:LEU:HD23	2.20	0.41
1:F:231:ASP:HA	1:F:234:LEU:HG	2.03	0.41
1:G:270:GLU:OE1	1:G:270:GLU:N	2.54	0.41
1:I:257:ARG:HH21	3:J:389:SER:H	1.68	0.41
5:L:123:ASP:HA	5:L:128:PHE:HA	2.03	0.41
5:L:150:SER:HB2	5:L:152:HIS:NE2	2.36	0.41
6:M:344:HIS:CD2	7:O:113:SER:HB3	2.55	0.41
7:O:128:ARG:HA	7:O:131:GLN:NE2	2.36	0.41
9:V:99:VAL:HG12	9:V:101:ALA:H	1.86	0.41
12:f:571:GLN:OE1	12:f:584:ILE:HB	2.21	0.41
12:f:621:ASP:HA	12:f:624:LYS:HD2	2.02	0.41
12:f:810:LYS:HE3	12:f:810:LYS:HB2	1.87	0.41
12:m:661:TYR:O	12:m:665:VAL:HG23	2.21	0.41
12:n:597:ILE:O	12:n:601:ILE:HG13	2.21	0.41
12:n:755:TRP:CH2	13:p:452:GLU:C	2.95	0.41
13:o:362:ASN:OD1	13:o:363:ARG:N	2.54	0.41
1:A:31:PRO:HD3	1:A:341:TRP:CE3	2.56	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:E:240:GLN:HA	1:E:250:GLU:HA	2.02	0.40
1:F:121:ARG:HG2	1:F:371:ILE:HD12	2.02	0.40
1:F:253:PRO:HB2	1:F:257:ARG:NE	2.36	0.40
2:H:262:PHE:CZ	2:H:274:ILE:HD11	2.56	0.40
1:I:99:LEU:O	1:I:101:THR:HG23	2.20	0.40
6:P:322:ARG:NE	6:P:322:ARG:HA	2.36	0.40
12:f:335:LEU:HD11	12:f:367:ILE:HB	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:375:GLN:NE2	12:f:449:VAL:O	2.44	0.40
13:g:484:CYS:HA	13:g:497:PHE:HA	2.03	0.40
13:h:265:LEU:HD11	13:h:551:LEU:HD13	2.04	0.40
12:m:483:VAL:HB	12:m:588:PHE:HD1	1.86	0.40
12:n:272:LEU:HB2	12:n:341:LEU:CD2	2.51	0.40
12:n:674:GLU:HA	12:n:679:GLY:HA3	2.03	0.40
13:o:536:HIS:HB3	13:o:539:LEU:HB3	2.03	0.40
1:B:356:MET:HE2	1:B:356:MET:HA	2.01	0.40
1:C:159:ASP:HB3	1:C:166:HIS:CE1	2.57	0.40
1:C:360:LYS:HB2	1:C:360:LYS:HE2	1.95	0.40
1:D:240:GLN:OE1	1:D:248:THR:HB	2.21	0.40
1:E:48:MET:HE1	1:G:153:THR:CB	2.50	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
3:J:48:MET:HE1	3:J:52:ILE:N	2.36	0.40
8:U:54:ASN:OD1	8:U:84:ILE:HG21	2.21	0.40
8:U:114:GLY:H	8:U:131:LEU:HD12	1.86	0.40
10:Z:1243:LYS:HA	10:Z:1243:LYS:HD3	1.83	0.40
12:f:350:LEU:O	12:f:353:ILE:HB	2.22	0.40
12:m:238:ASP:OD2	12:m:241:PHE:N	2.52	0.40
12:m:292:ARG:HH21	12:m:317:ASP:HA	1.87	0.40
12:n:480:ILE:O	12:n:484:LEU:HB2	2.21	0.40
13:o:479:ILE:HD13	13:o:501:SER:HB2	2.01	0.40
13:p:343:PHE:HD2	13:p:396:HIS:CG	2.39	0.40
13:p:445:ASN:ND2	13:p:460:CYS:SG	2.94	0.40
1:A:33:TYR:HB3	1:A:98:GLN:OE1	2.22	0.40
1:B:10:GLN:NE2	1:B:26:ALA:HB3	2.36	0.40
1:D:346:ILE:O	1:D:350:LEU:HG	2.21	0.40
1:D:350:LEU:HD21	12:m:314:VAL:HG12	2.03	0.40
1:E:333:PRO:O	1:E:336:ARG:HG3	2.20	0.40
1:F:38:TYR:CG	1:F:71:ILE:HD11	2.56	0.40
1:G:145:LEU:O	1:G:343:GLY:HA3	2.22	0.40
2:H:62:ARG:HG2	2:H:67:LEU:HD11	2.04	0.40
2:H:160:THR:HG23	2:H:178:LEU:HB3	2.03	0.40
2:H:261:LEU:HD23	2:H:274:ILE:HD13	2.03	0.40
3:J:377:TYR:CZ	3:J:381:THR:HG21	2.57	0.40
4:K:277:TYR:HD2	4:K:278:LYS:O	2.04	0.40
5:L:44:ASP:N	5:L:44:ASP:OD1	2.53	0.40
6:M:18:ASP:OD1	6:M:18:ASP:N	2.54	0.40
6:M:378:VAL:O	6:M:382:MET:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:P:318:GLU:O	6:P:322:ARG:HG2	2.21	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
9:V:152:LEU:HG	9:V:153:PHE:H	1.85	0.40
11:Y:294:PRO:O	11:Y:297:ASN:ND2	2.54	0.40
12:e:435:ARG:HA	12:e:447:LYS:CA	2.51	0.40
12:f:657:GLN:HG3	13:h:504:TRP:CE3	2.57	0.40
12:m:232:PHE:CE1	12:m:303:ILE:HD11	2.56	0.40
12:m:361:PHE:O	12:m:365:ARG:HG3	2.20	0.40
12:n:513:ASP:OD1	12:n:514:ALA:N	2.54	0.40
12:n:527:TYR:O	12:n:531:LYS:HG2	2.21	0.40
1:A:104:GLU:CD	1:A:133:ASN:HD21	2.29	0.40
1:A:134:VAL:HG12	1:A:136:ALA:H	1.87	0.40
1:D:48:MET:CE	1:F:147:LEU:HB2	2.51	0.40
1:D:89:ILE:O	1:D:93:VAL:HG23	2.21	0.40
1:D:183:ILE:HB	1:D:185:ILE:HG22	2.03	0.40
1:F:112:GLU:C	1:F:142:GLN:HE22	2.29	0.40
1:G:138:PHE:CE2	1:G:140:SER:HB2	2.57	0.40
2:H:15:GLY:N	15:H:401:ATP:O1B	2.55	0.40
5:L:33:PRO:HA	5:L:36:CYS:HB3	2.03	0.40
6:M:337:LEU:HD12	7:O:103:GLN:HE22	1.86	0.40
12:f:275:ILE:HG23	12:f:336:MET:SD	2.62	0.40
12:f:563:ARG:HD2	12:f:563:ARG:HA	1.94	0.40
12:f:564:ILE:HG21	12:f:591:LEU:HD22	2.03	0.40
12:m:341:LEU:O	12:m:345:LEU:HG	2.22	0.40
12:m:797:GLU:HB2	12:m:798:ARG:HE	1.87	0.40
12:m:801:ILE:O	12:m:805:VAL:HG22	2.22	0.40
12:n:228:LYS:HG2	12:n:230:THR:H	1.87	0.40
12:n:408:GLU:HA	12:n:411:LYS:HG2	2.04	0.40
12:n:477:ARG:NH1	12:n:478:ALA:HB2	2.35	0.40
12:n:748:LYS:NZ	13:p:353:TYR:CE1	2.90	0.40
13:o:349:VAL:HG11	13:o:398:LEU:HD11	2.03	0.40
13:p:426:HIS:CG	13:p:427:LYS:H	2.40	0.40
1:B:84:ASN:O	1:B:88:ARG:HG3	2.22	0.40
1:D:46:ARG:HB2	1:F:174:PHE:CE2	2.56	0.40
1:D:194:LEU:O	1:D:198:LEU:HD23	2.21	0.40
1:E:139:ILE:HG12	1:E:371:ILE:HD11	2.04	0.40
1:E:357:TRP:HZ3	1:E:359:SER:CA	2.32	0.40
1:G:89:ILE:O	1:G:93:VAL:HG23	2.20	0.40
1:G:92:TYR:HA	1:G:95:SER:HB2	2.03	0.40
2:H:62:ARG:HH12	2:H:208:ILE:HD11	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:315:PHE:HD1	3:J:316:LEU:HD22	1.87	0.40
8:U:61:LEU:HB2	8:U:95:TYR:CD2	2.56	0.40
8:U:145:GLY:HA3	8:U:150:ARG:HH11	1.86	0.40
11:Y:85:THR:HG22	11:Y:109:LEU:HD11	2.04	0.40
12:f:402:MET:HE2	12:f:531:LYS:N	2.37	0.40
12:f:583:ARG:HD2	13:h:559:GLU:HG2	2.04	0.40
12:f:735:LEU:HD12	12:f:735:LEU:HA	1.86	0.40
12:m:380:LEU:O	12:m:384:ILE:HG13	2.21	0.40
12:m:673:TRP:O	12:m:679:GLY:HA3	2.21	0.40
12:n:426:GLU:HA	12:n:429:LYS:HD2	2.03	0.40
12:n:666:GLU:HA	12:n:673:TRP:CG	2.56	0.40
13:o:337:SER:O	13:o:351:GLY:N	2.46	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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%)	361 (97%)	12 (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
3	J	377/417 (90%)	365 (97%)	12 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	K	276/286 (96%)	268 (97%)	8 (3%)	0	100	100
5	L	267/272 (98%)	261 (98%)	6 (2%)	0	100	100
6	M	330/405 (82%)	311 (94%)	18 (6%)	1 (0%)	37	70
6	N	270/405 (67%)	262 (97%)	7 (3%)	1 (0%)	30	65
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%)	19	54
10	Z	190/1281 (15%)	184 (97%)	6 (3%)	0	100	100
11	Y	404/467 (86%)	377 (93%)	24 (6%)	3 (1%)	19	54
12	e	792/4646 (17%)	745 (94%)	45 (6%)	2 (0%)	37	70
12	f	804/4646 (17%)	763 (95%)	39 (5%)	2 (0%)	44	75
12	m	786/4646 (17%)	758 (96%)	27 (3%)	1 (0%)	48	80
12	n	747/4646 (16%)	720 (96%)	26 (4%)	1 (0%)	48	80
13	g	356/612 (58%)	353 (99%)	3 (1%)	0	100	100
13	h	356/612 (58%)	346 (97%)	10 (3%)	0	100	100
13	o	356/612 (58%)	350 (98%)	6 (2%)	0	100	100
13	p	356/612 (58%)	350 (98%)	6 (2%)	0	100	100
All	All	11469/30783 (37%)	11047 (96%)	410 (4%)	12 (0%)	50	80

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	M	217	PRO
10	W	1142	PRO
11	Y	175	PRO
11	Y	441	PRO
12	f	38	VAL
12	f	203	PRO
12	n	21	VAL
12	e	726	ARG
12	m	210	HIS

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Mol	Chain	Res	Type
6	N	163	ASP
12	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%)	84	88
4	K	247/254 (97%)	247 (100%)	0	100	100
5	L	238/241 (99%)	238 (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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	Z	154/1078 (14%)	154 (100%)	0	100	100
11	Y	274/416 (66%)	269 (98%)	5 (2%)	54	71
12	e	230/4122 (6%)	230 (100%)	0	100	100
12	f	718/4122 (17%)	717 (100%)	1 (0%)	92	95
12	m	538/4122 (13%)	538 (100%)	0	100	100
12	n	504/4122 (12%)	502 (100%)	2 (0%)	89	91
13	h	309/535 (58%)	308 (100%)	1 (0%)	91	92
13	o	309/535 (58%)	309 (100%)	0	100	100
13	p	309/535 (58%)	309 (100%)	0	100	100
All	All	8130/26463 (31%)	8119 (100%)	11 (0%)	92	95

All (11) 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
12	f	213	ILE
13	h	393	GLN
12	n	685	ASP
12	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	77	HIS
1	B	116	ASN
1	C	166	HIS
1	C	276	HIS
1	C	284	GLN
1	D	9	ASN

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Mol	Chain	Res	Type
1	D	120	ASN
1	D	133	ASN
1	D	284	GLN
1	D	334	GLN
1	E	77	HIS
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
6	Q	346	GLN
8	U	153	GLN
10	W	1114	HIS
10	W	1276	GLN
11	Y	81	HIS
11	Y	142	GLN
10	Z	1199	GLN
12	e	799	ASN
12	e	842	ASN

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Mol	Chain	Res	Type
12	f	215	ASN
12	f	257	GLN
12	f	610	GLN
12	f	752	ASN
12	f	770	GLN
12	f	773	GLN
12	f	799	ASN
13	h	356	GLN
13	h	397	ASN
13	h	426	HIS
13	h	446	ASN
12	m	210	HIS
12	m	250	ASN
12	m	475	GLN
12	m	589	ASN
12	m	605	GLN
12	m	657	GLN
12	n	246	GLN
12	n	250	ASN
12	n	431	GLN
12	n	473	HIS
12	n	475	GLN
12	n	487	GLN
12	n	607	GLN
12	n	676	HIS
12	n	769	HIS
12	n	799	ASN
12	n	842	ASN
13	o	419	GLN
13	o	462	HIS
13	o	593	GLN
13	p	268	ASN
13	p	419	GLN
13	p	462	HIS
13	p	593	GLN

### 5.3.3 RNA ⓘ

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	$\# Z  > 2$
14	ADP	G	800	-	24,29,29	0.88	0	29,45,45	1.18	2 (6%)
14	ADP	C	800	-	24,29,29	0.85	0	29,45,45	1.09	2 (6%)
15	ATP	H	401	-	28,33,33	0.70	0	34,52,52	0.61	1 (2%)
14	ADP	E	800	-	24,29,29	0.88	0	29,45,45	1.13	2 (6%)
14	ADP	D	800	-	24,29,29	0.90	0	29,45,45	1.19	2 (6%)
14	ADP	J	800	-	24,29,29	0.95	1 (4%)	29,45,45	1.24	3 (10%)
14	ADP	B	800	-	24,29,29	0.87	0	29,45,45	1.13	2 (6%)
14	ADP	I	800	-	24,29,29	0.88	0	29,45,45	1.19	2 (6%)
14	ADP	F	800	-	24,29,29	0.86	0	29,45,45	1.12	2 (6%)
14	ADP	A	800	-	24,29,29	0.89	0	29,45,45	1.11	2 (6%)

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
14	ADP	G	800	-	-	0/12/32/32	0/3/3/3
14	ADP	C	800	-	-	3/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	ATP	H	401	-	-	10/18/38/38	0/3/3/3
14	ADP	E	800	-	-	2/12/32/32	0/3/3/3
14	ADP	D	800	-	-	5/12/32/32	0/3/3/3
14	ADP	J	800	-	-	7/12/32/32	0/3/3/3
14	ADP	B	800	-	-	0/12/32/32	0/3/3/3
14	ADP	I	800	-	-	3/12/32/32	0/3/3/3
14	ADP	F	800	-	-	8/12/32/32	0/3/3/3
14	ADP	A	800	-	-	1/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	J	800	ADP	PA-O3A	2.18	1.61	1.59

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	J	800	ADP	N3-C2-N1	-3.62	123.76	128.67
14	G	800	ADP	N3-C2-N1	-3.58	123.81	128.67
14	I	800	ADP	N3-C2-N1	-3.53	123.88	128.67
14	A	800	ADP	N3-C2-N1	-3.50	123.92	128.67
14	E	800	ADP	N3-C2-N1	-3.46	123.97	128.67
14	F	800	ADP	N3-C2-N1	-3.46	123.97	128.67
14	C	800	ADP	N3-C2-N1	-3.43	124.02	128.67
14	B	800	ADP	N3-C2-N1	-3.37	124.10	128.67
14	D	800	ADP	N3-C2-N1	-3.34	124.14	128.67
14	B	800	ADP	C4-C5-N7	-2.52	106.68	109.34
14	D	800	ADP	C4-C5-N7	-2.49	106.70	109.34
14	E	800	ADP	C4-C5-N7	-2.48	106.71	109.34
14	G	800	ADP	C4-C5-N7	-2.47	106.72	109.34
14	I	800	ADP	C4-C5-N7	-2.46	106.74	109.34
14	C	800	ADP	C4-C5-N7	-2.44	106.76	109.34
14	F	800	ADP	C4-C5-N7	-2.44	106.76	109.34
14	A	800	ADP	C4-C5-N7	-2.43	106.77	109.34
14	J	800	ADP	C4-C5-N7	-2.41	106.79	109.34
15	H	401	ATP	C5-C6-N6	2.28	123.78	120.31
14	J	800	ADP	C2'-C3'-C4'	2.08	106.62	102.61

There are no chirality outliers.

All (39) torsion outliers are listed below:

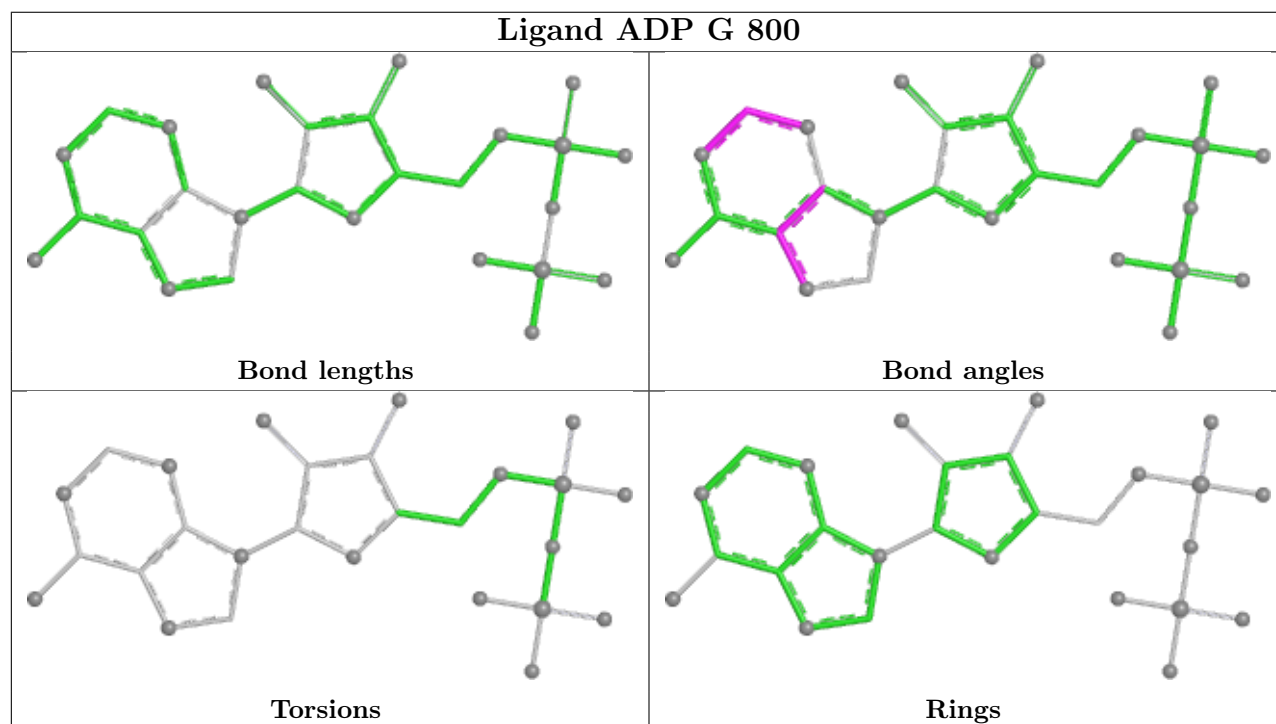
Mol	Chain	Res	Type	Atoms
14	C	800	ADP	C5'-O5'-PA-O3A
14	D	800	ADP	C5'-O5'-PA-O2A
14	D	800	ADP	C5'-O5'-PA-O3A
14	D	800	ADP	C3'-C4'-C5'-O5'
14	F	800	ADP	C5'-O5'-PA-O1A
14	F	800	ADP	C5'-O5'-PA-O2A
14	F	800	ADP	C5'-O5'-PA-O3A
14	I	800	ADP	C5'-O5'-PA-O1A
14	I	800	ADP	C5'-O5'-PA-O3A
14	J	800	ADP	PA-O3A-PB-O3B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

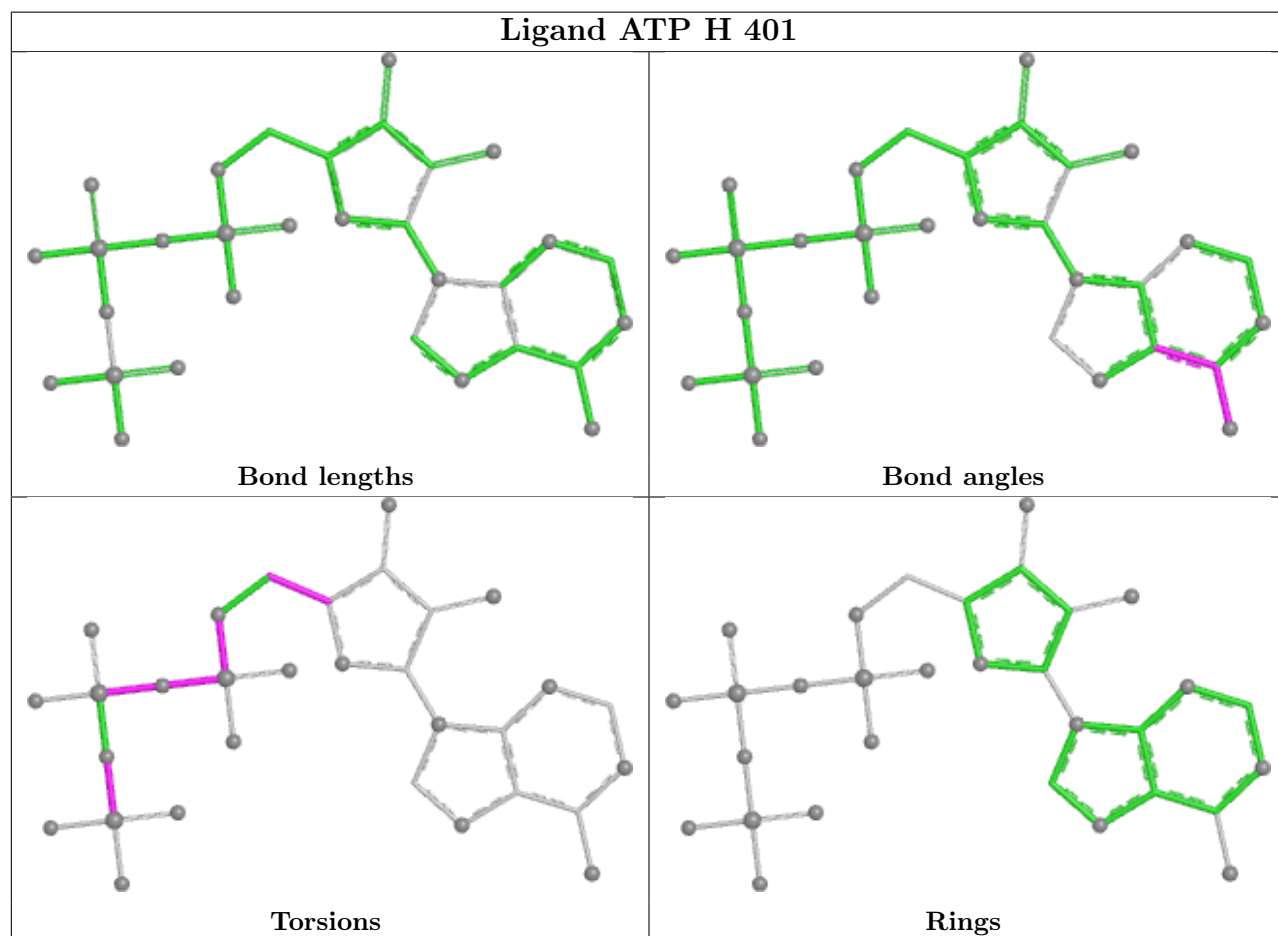
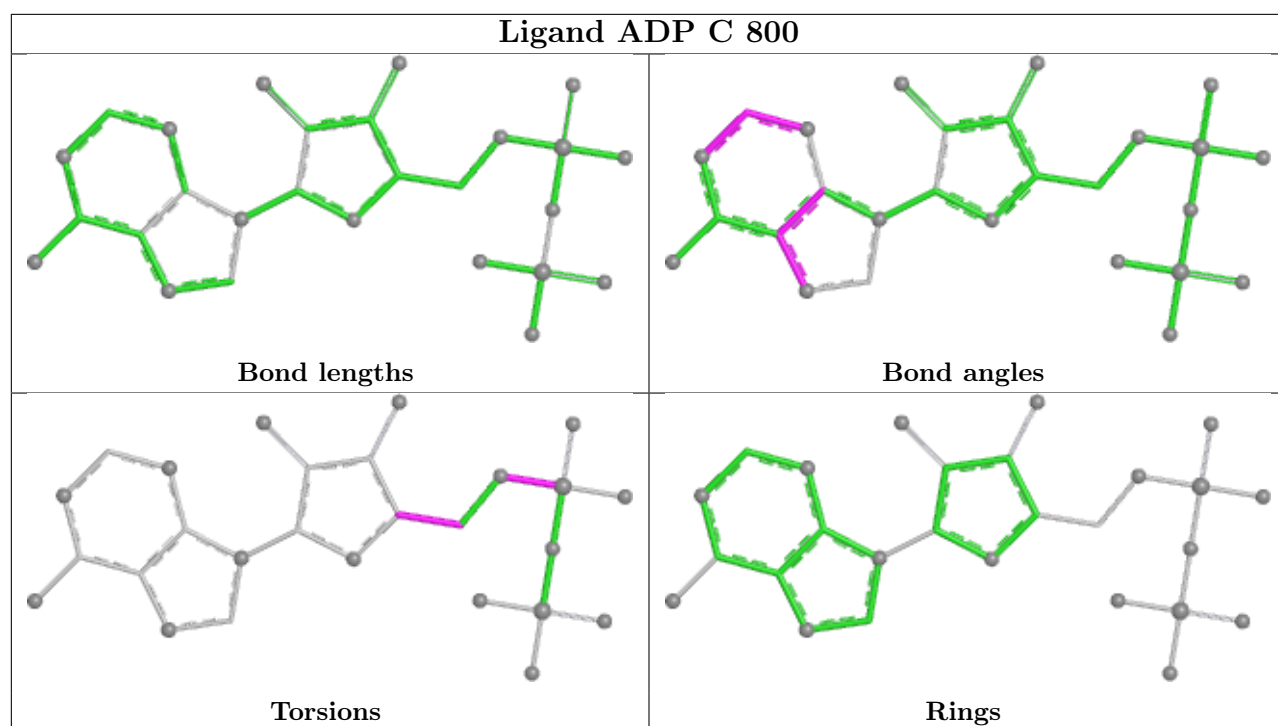
There are no ring outliers.

8 monomers are involved in 19 short contacts:

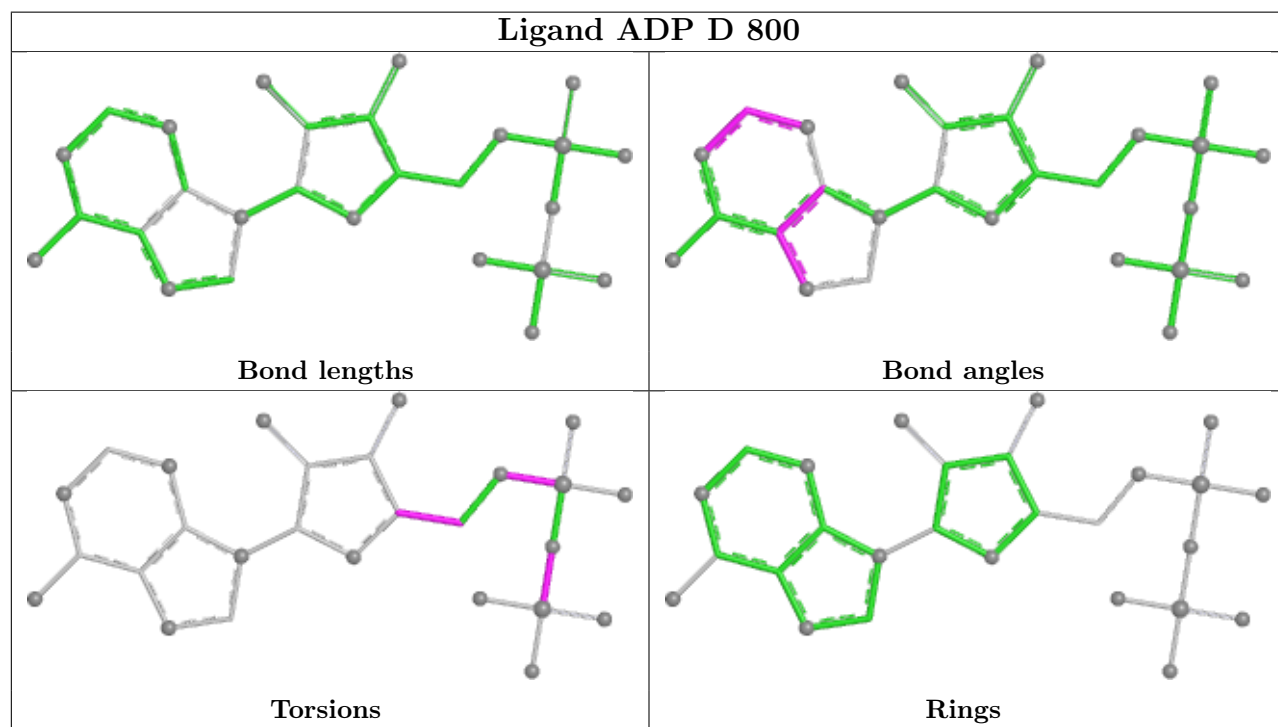
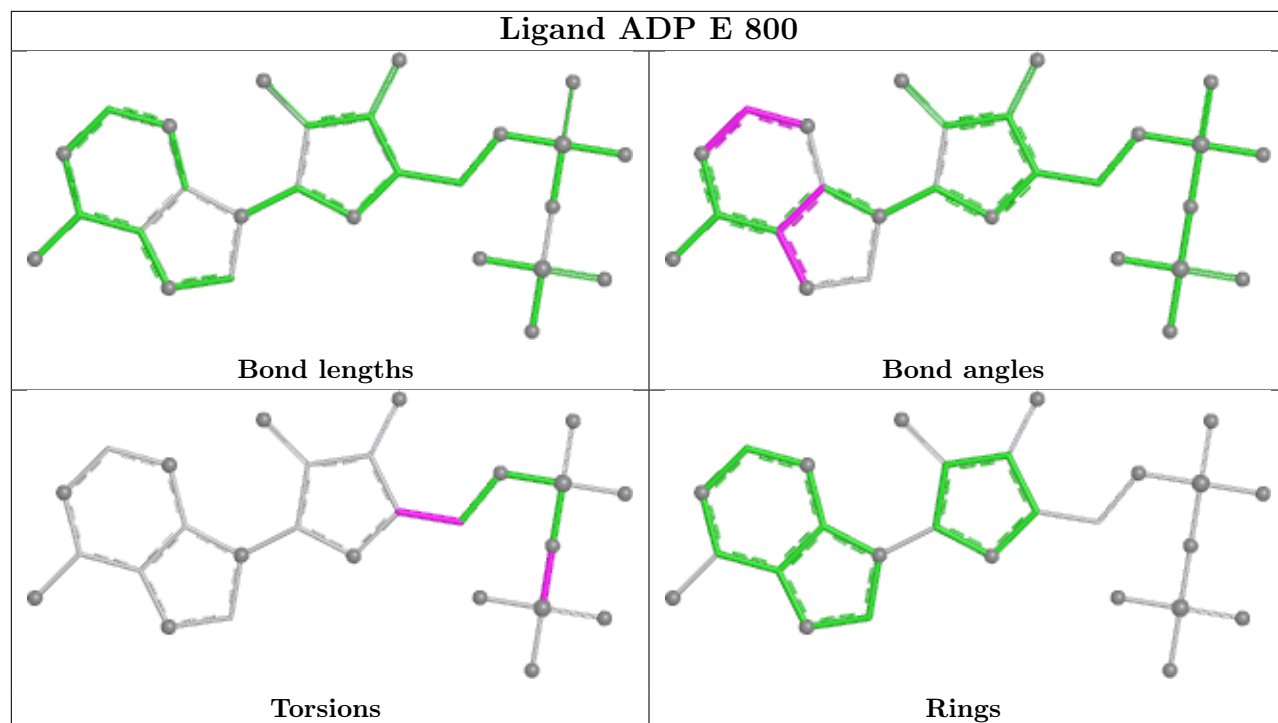
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	G	800	ADP	1	0
14	C	800	ADP	2	0
15	H	401	ATP	8	0
14	D	800	ADP	3	0
14	J	800	ADP	1	0
14	B	800	ADP	1	0
14	F	800	ADP	1	0
14	A	800	ADP	2	0

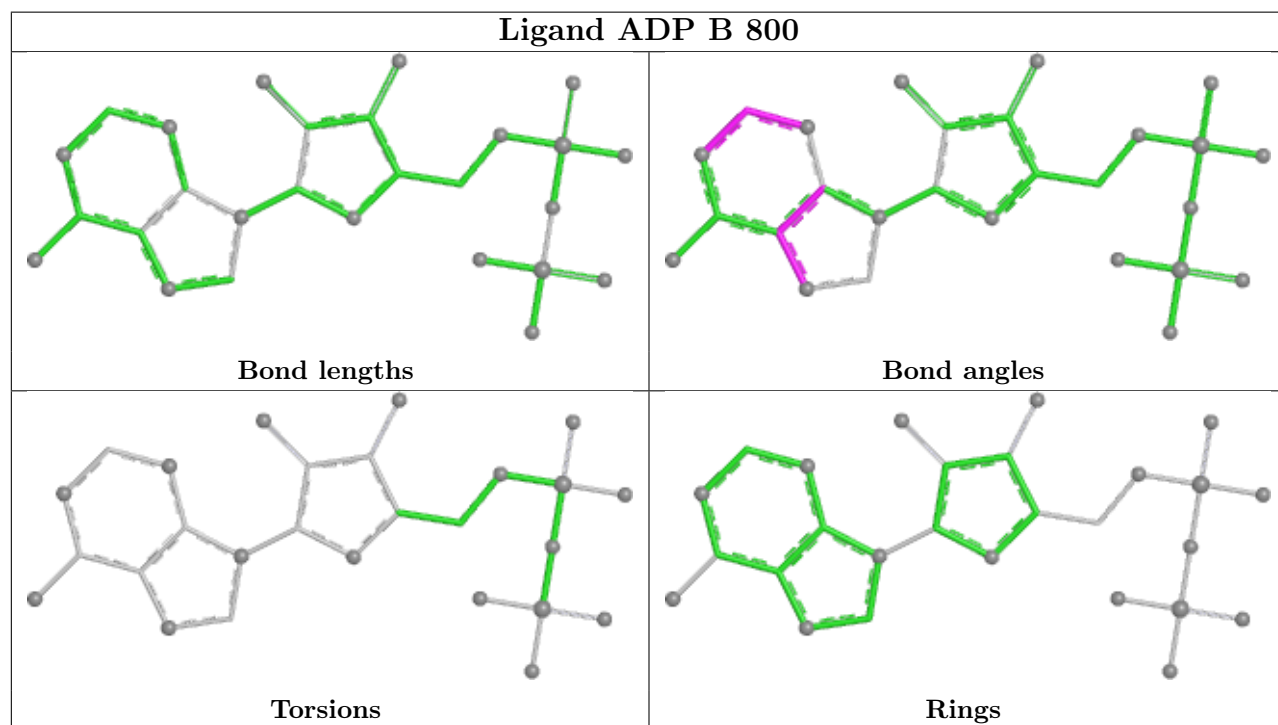
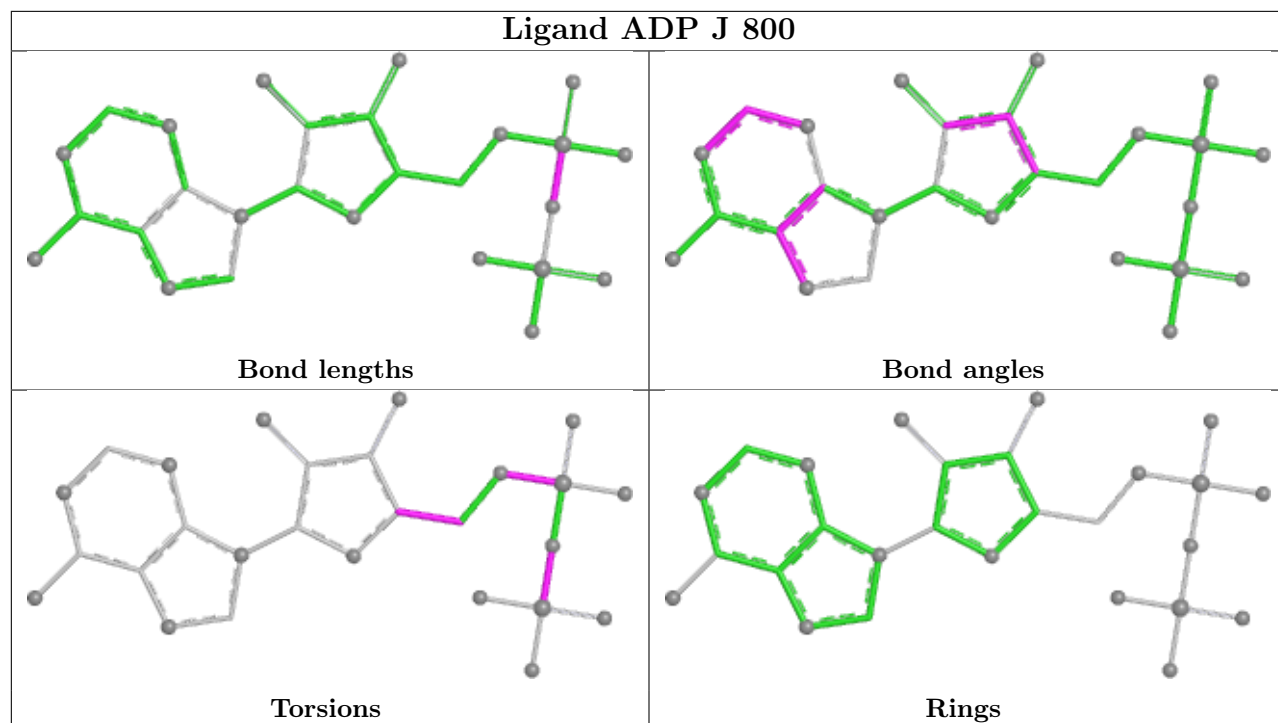
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

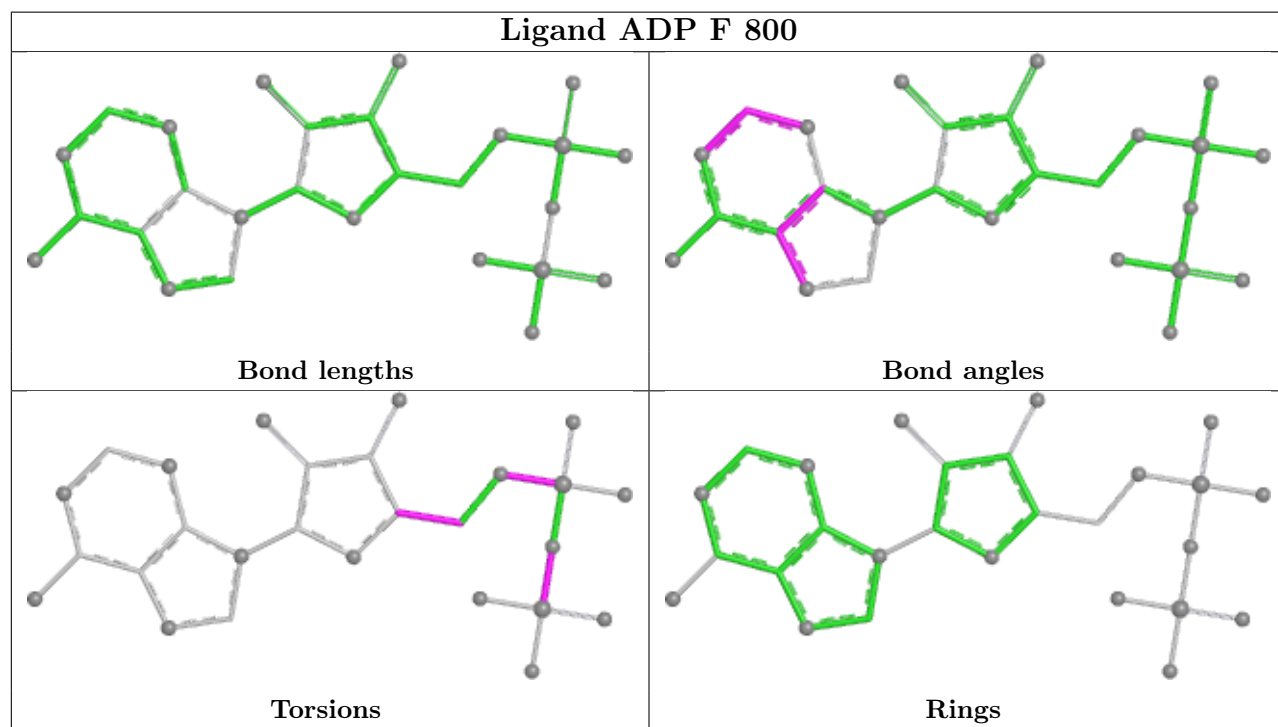
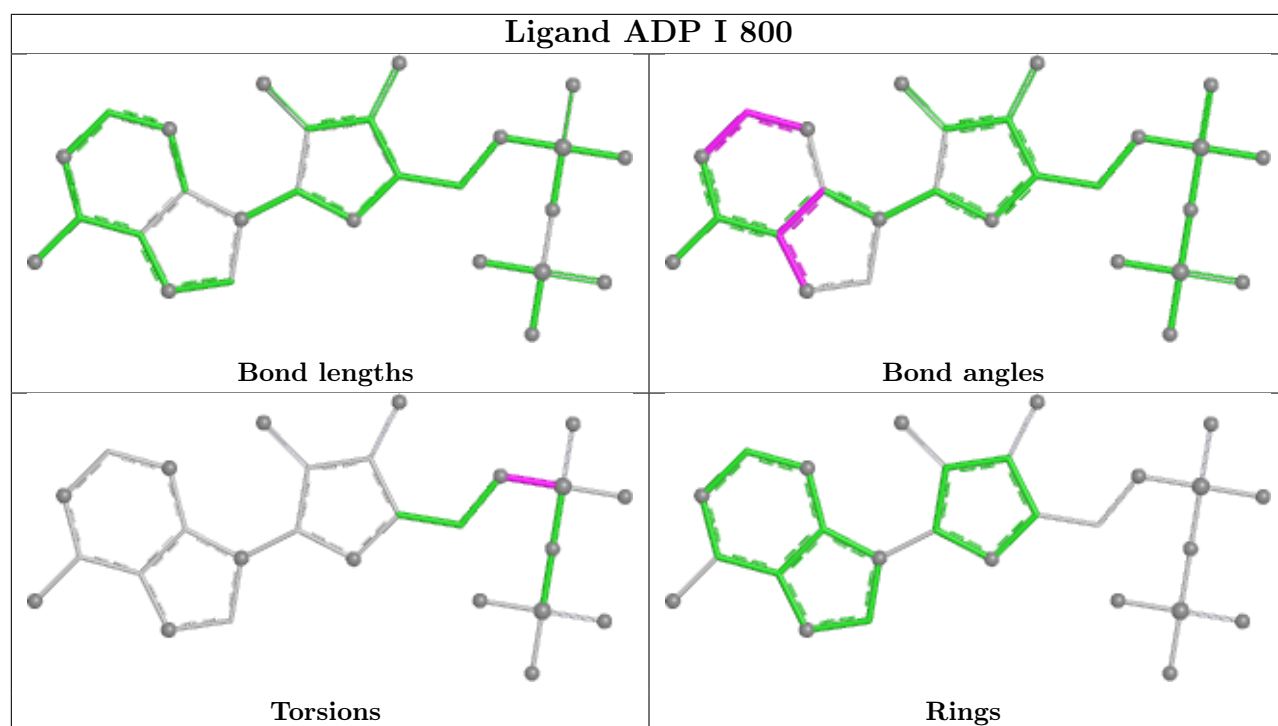


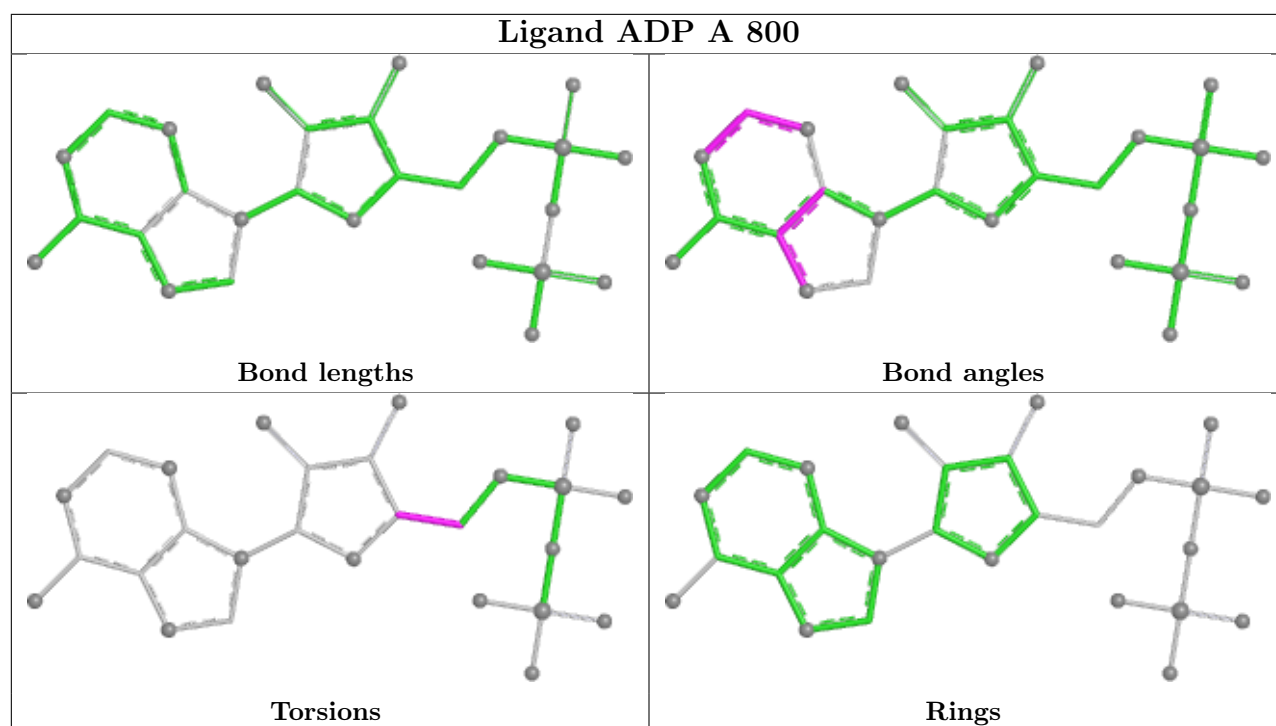












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

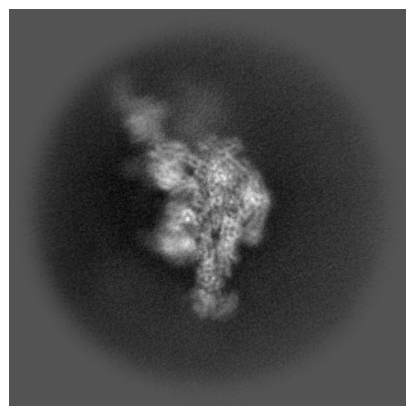
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46846. These allow visual inspection of the internal detail of the map and identification of artifacts.

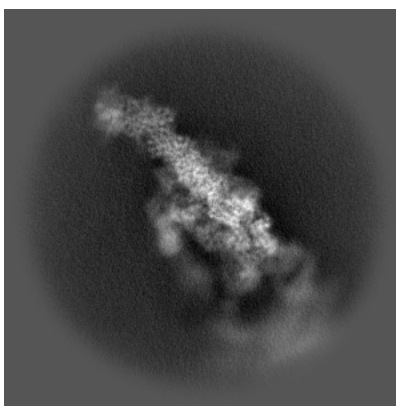
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

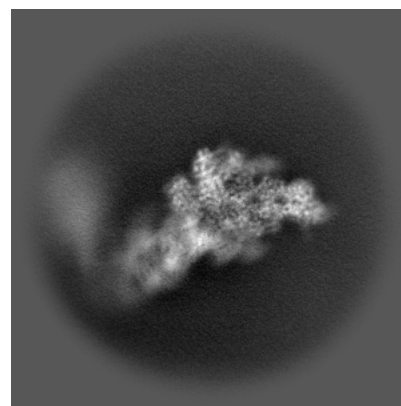
#### 6.1.1 Primary map



X

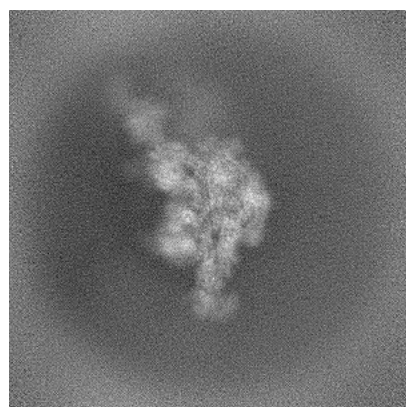


Y

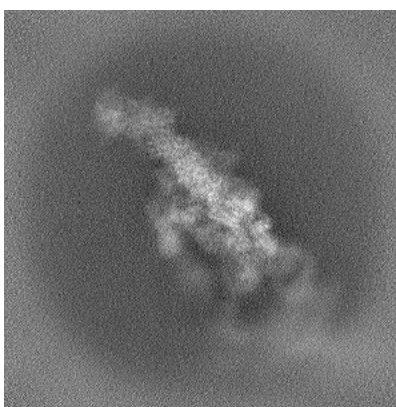


Z

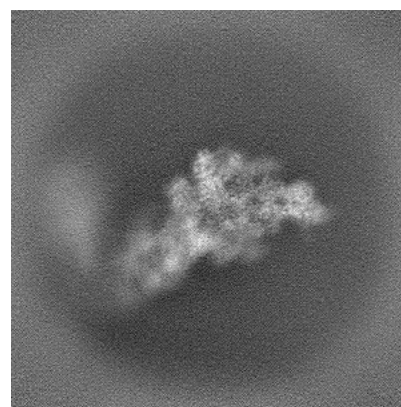
#### 6.1.2 Raw map



X



Y

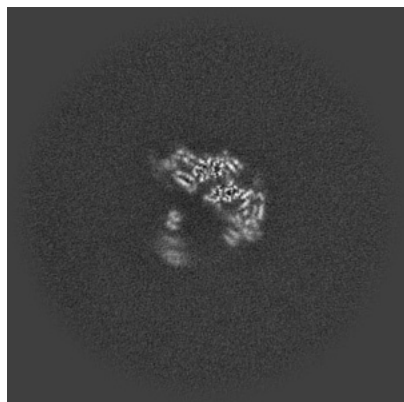


Z

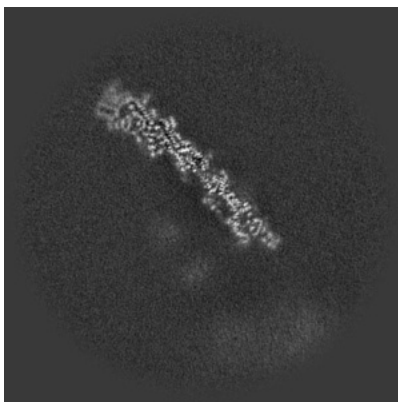
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

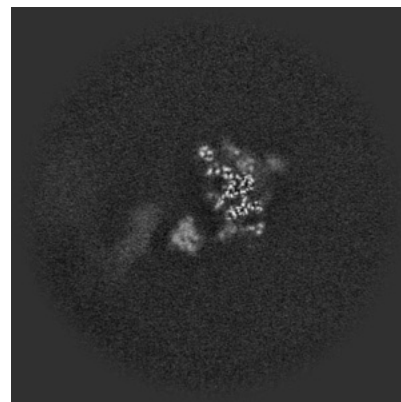
### 6.2.1 Primary map



X Index: 256



Y Index: 256

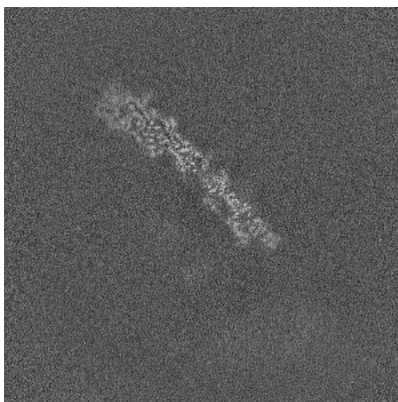


Z Index: 256

### 6.2.2 Raw map



X Index: 256



Y Index: 256



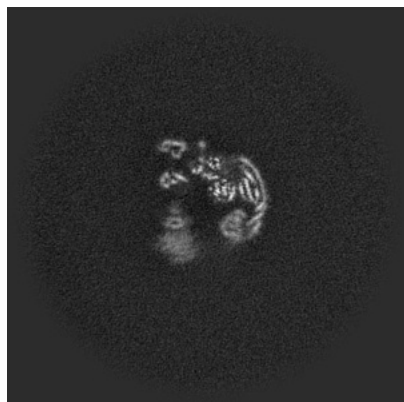
Z Index: 256

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

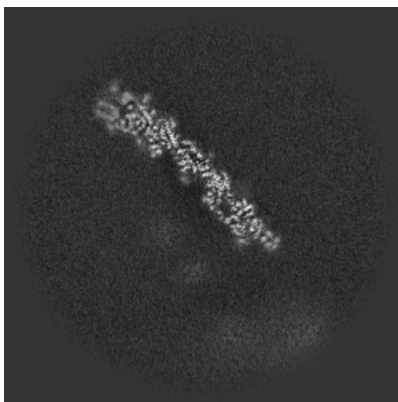


## 6.3 Largest variance slices [i](#)

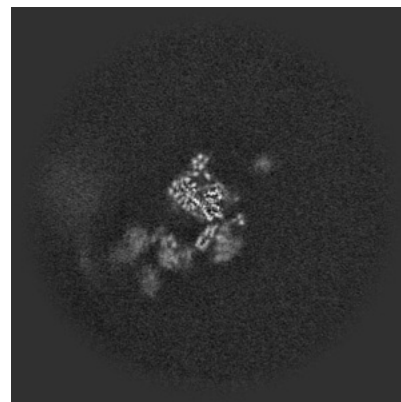
### 6.3.1 Primary map



X Index: 244

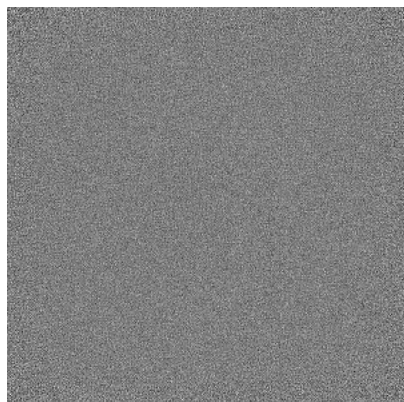


Y Index: 258

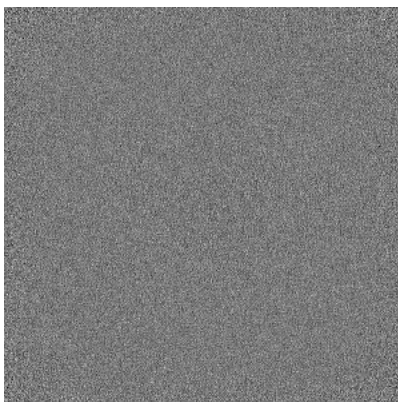


Z Index: 298

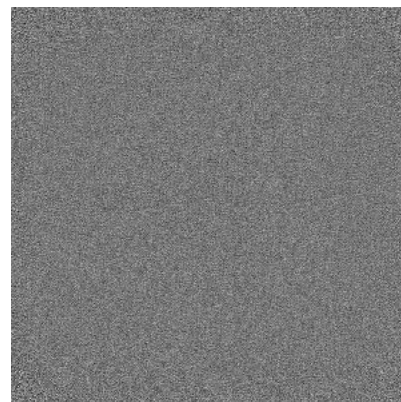
### 6.3.2 Raw map



X Index: 0



Y Index: 0

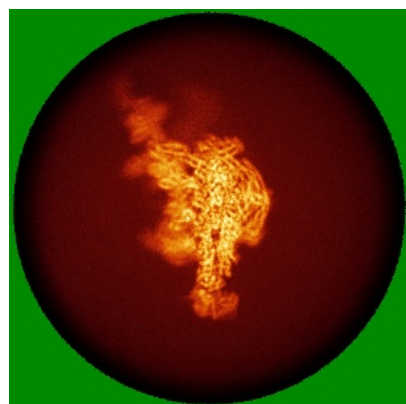


Z Index: 0

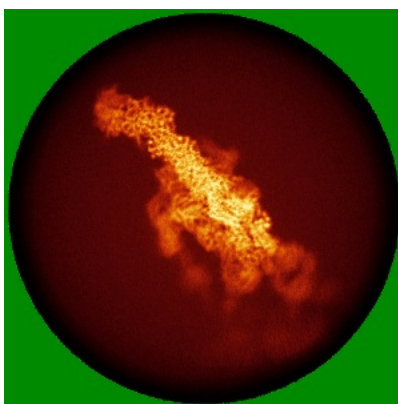
The images above show the largest variance slices of the map in three orthogonal directions.

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

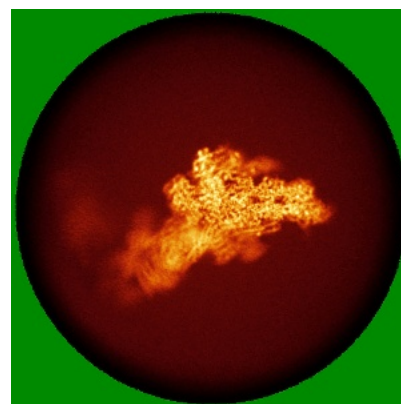
### 6.4.1 Primary map



X

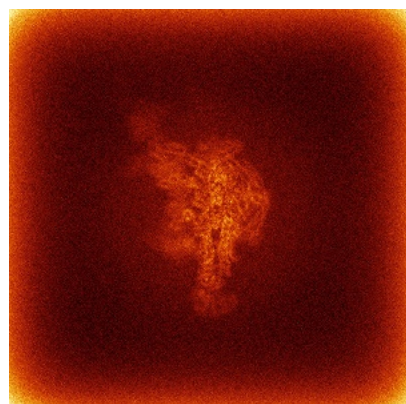


Y

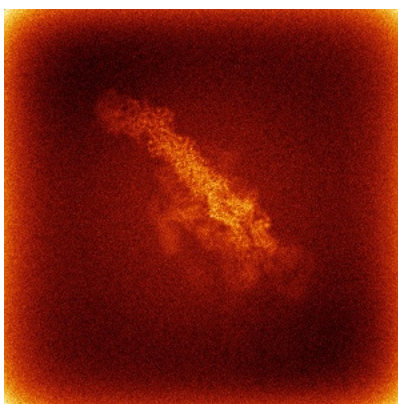


Z

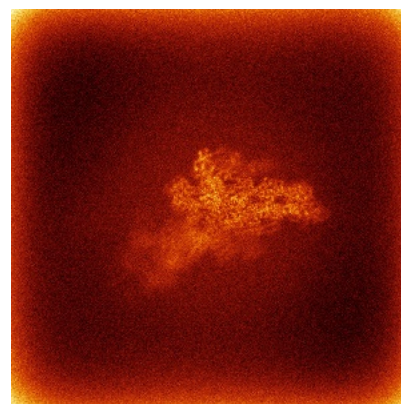
### 6.4.2 Raw map



X



Y



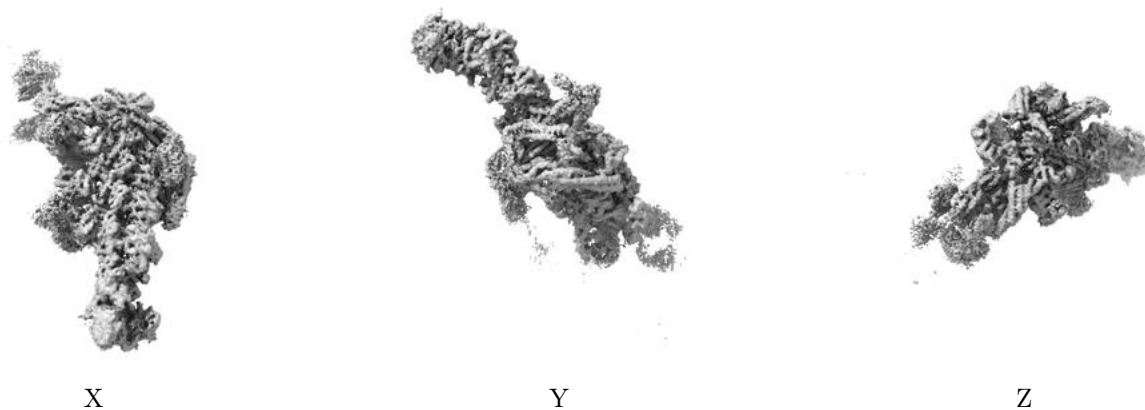
Z

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.



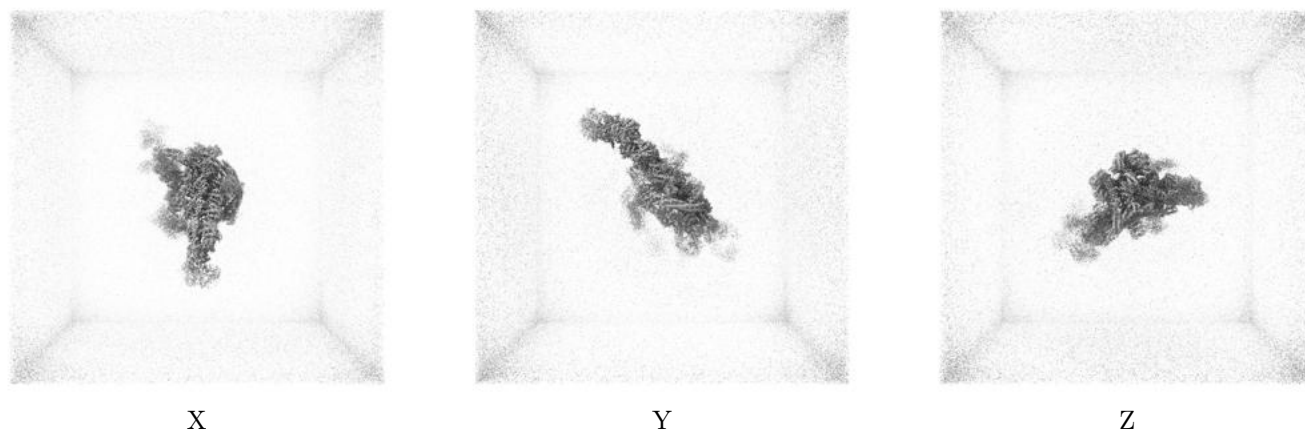
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.13. 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.

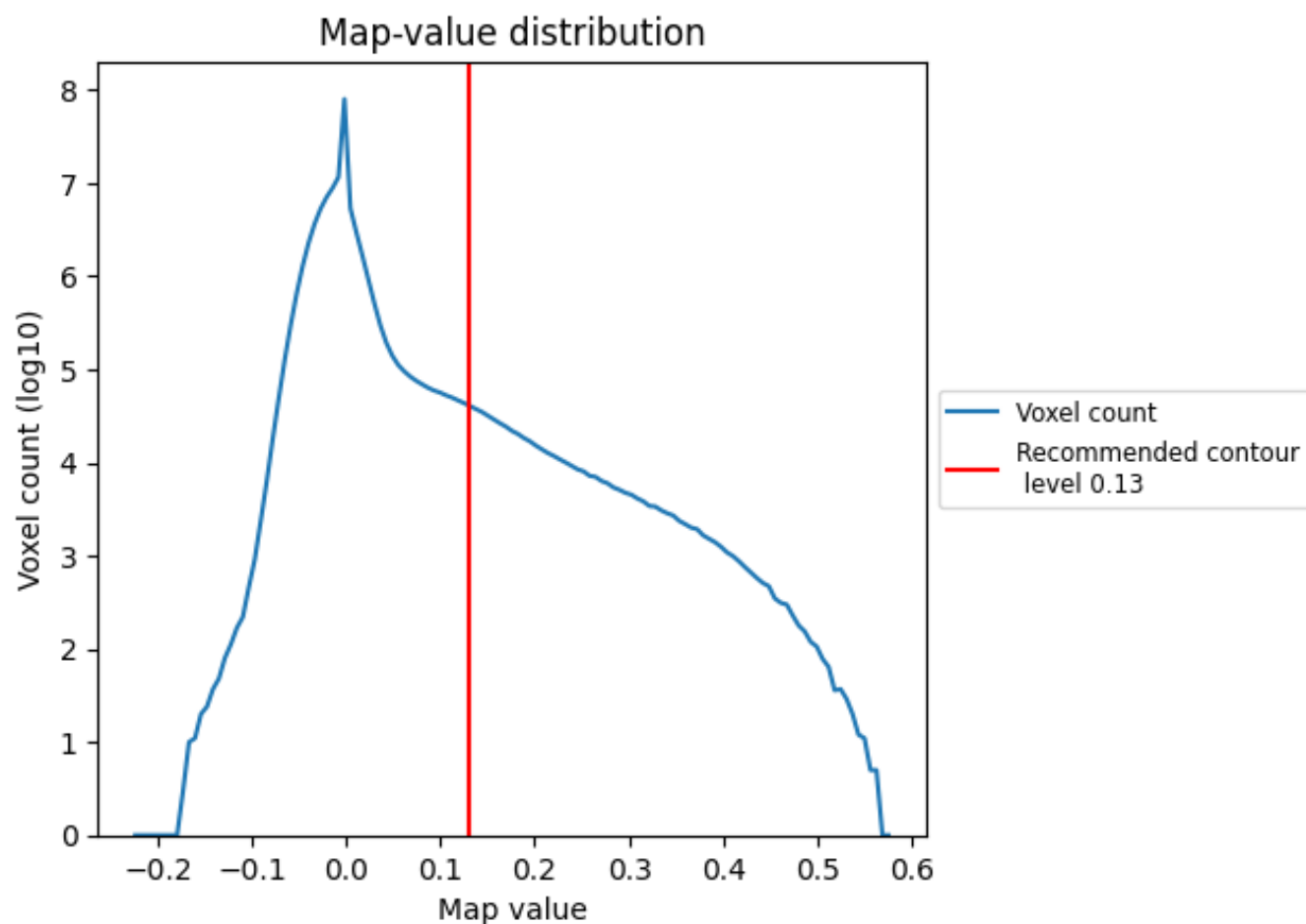
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

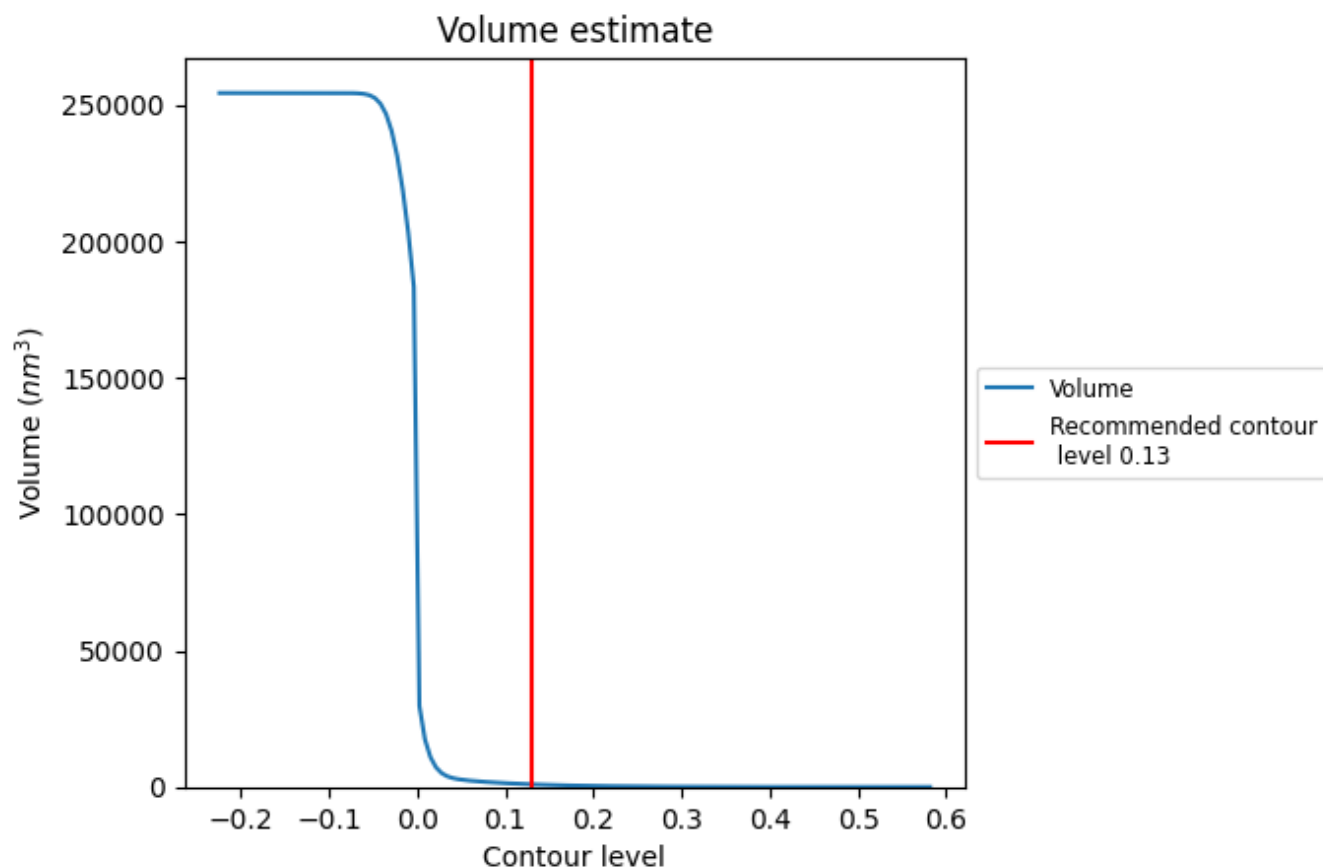
This section contains the results of statistical analysis of the map.

### 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.

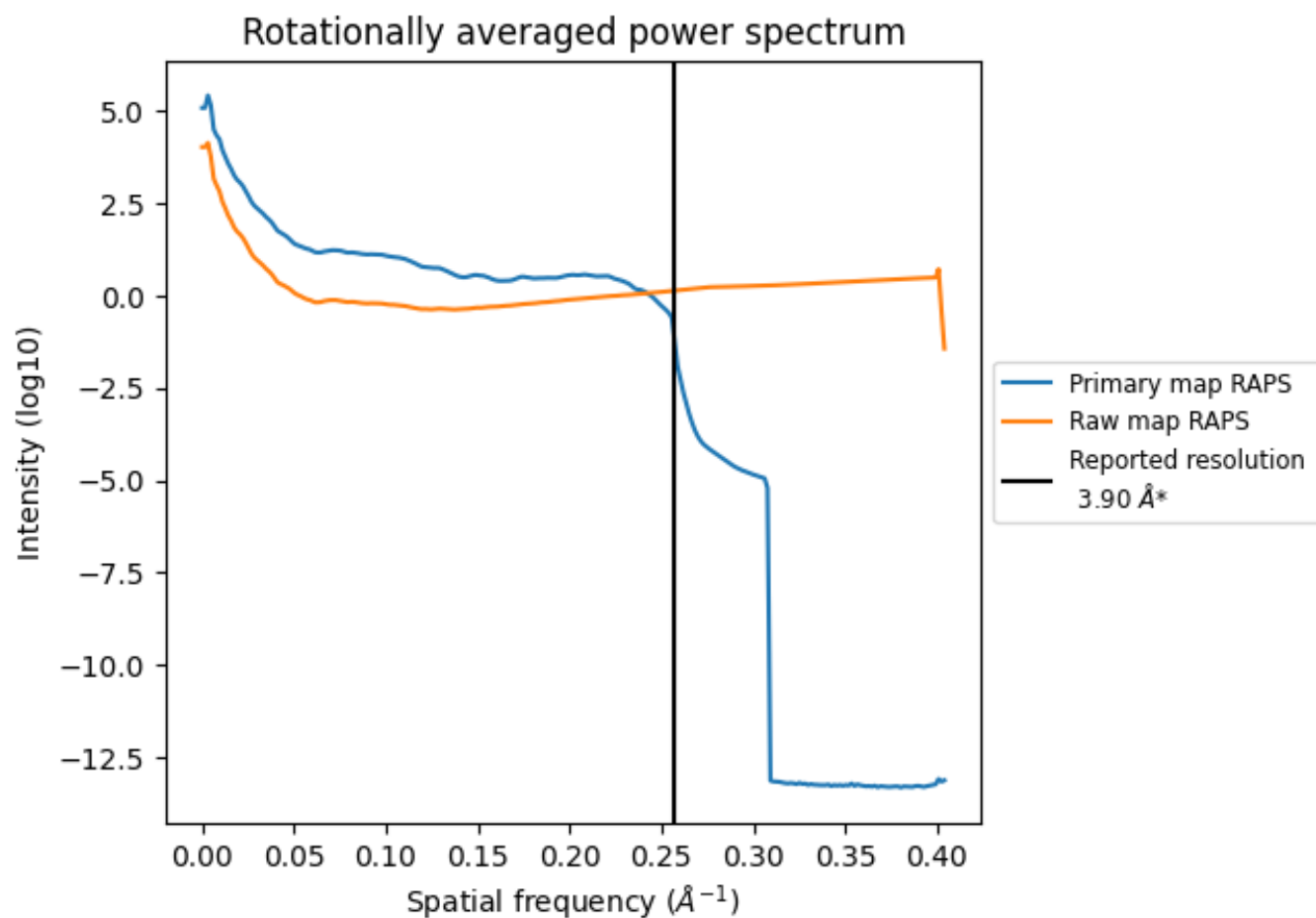
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 955  $\text{nm}^3$ ; this corresponds to an approximate mass of 863 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 ⓘ

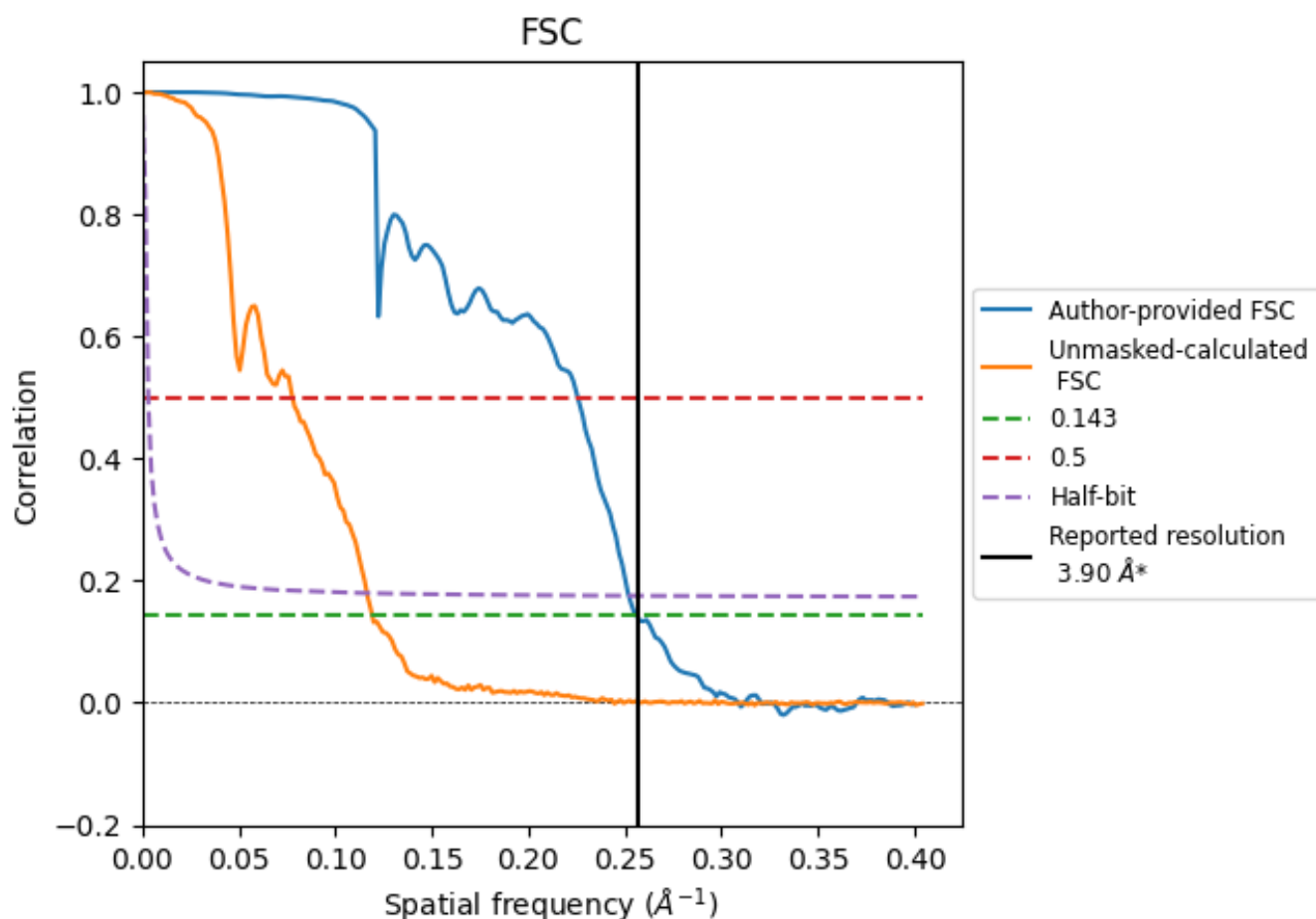


\*Reported resolution corresponds to spatial frequency of 0.256 Å<sup>-1</sup>

## 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 0.256  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

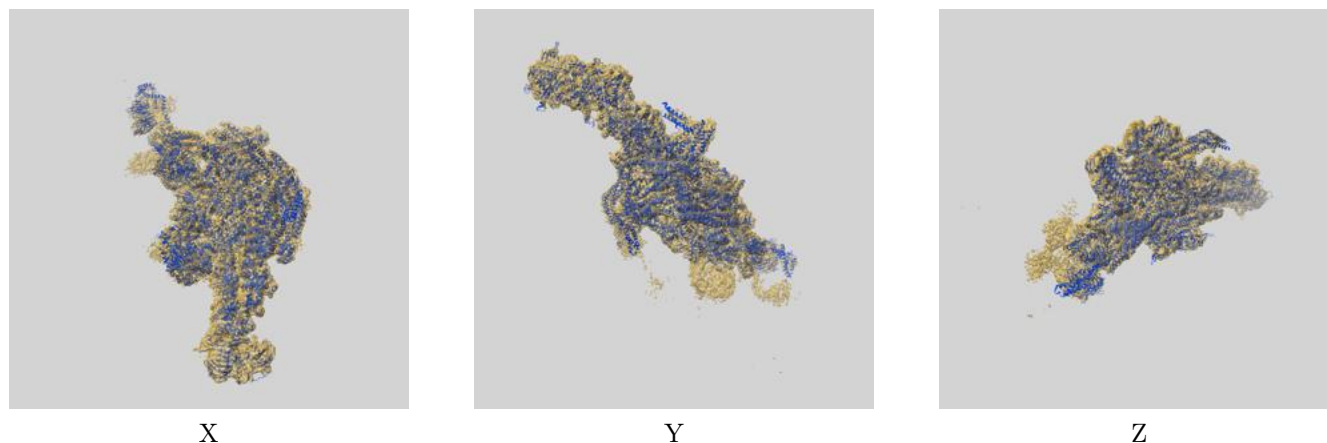
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.91	4.43	3.97
Unmasked-calculated*	8.40	12.84	8.59

\*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 8.40 differs from the reported value 3.9 by more than 10 %

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

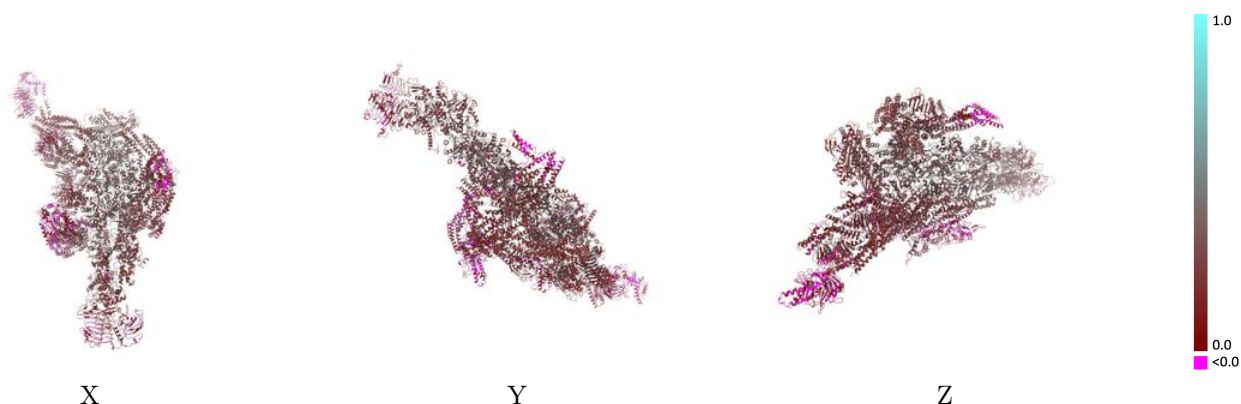
This section contains information regarding the fit between EMDB map EMD-46846 and PDB model 9DGS. Per-residue inclusion information can be found in section 3 on page 10.

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



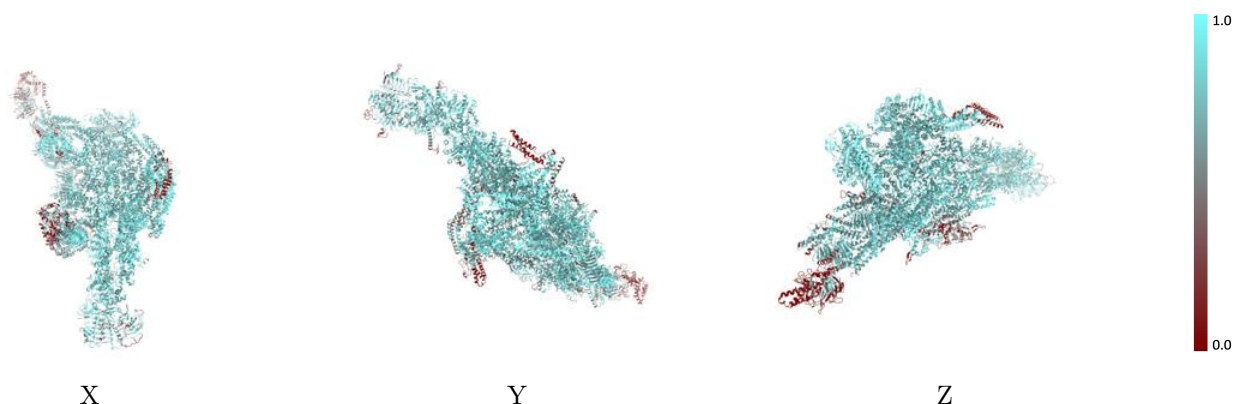
The images above show the 3D surface view of the map at the recommended contour level 0.13 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



The images above show the model with each residue coloured according 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.

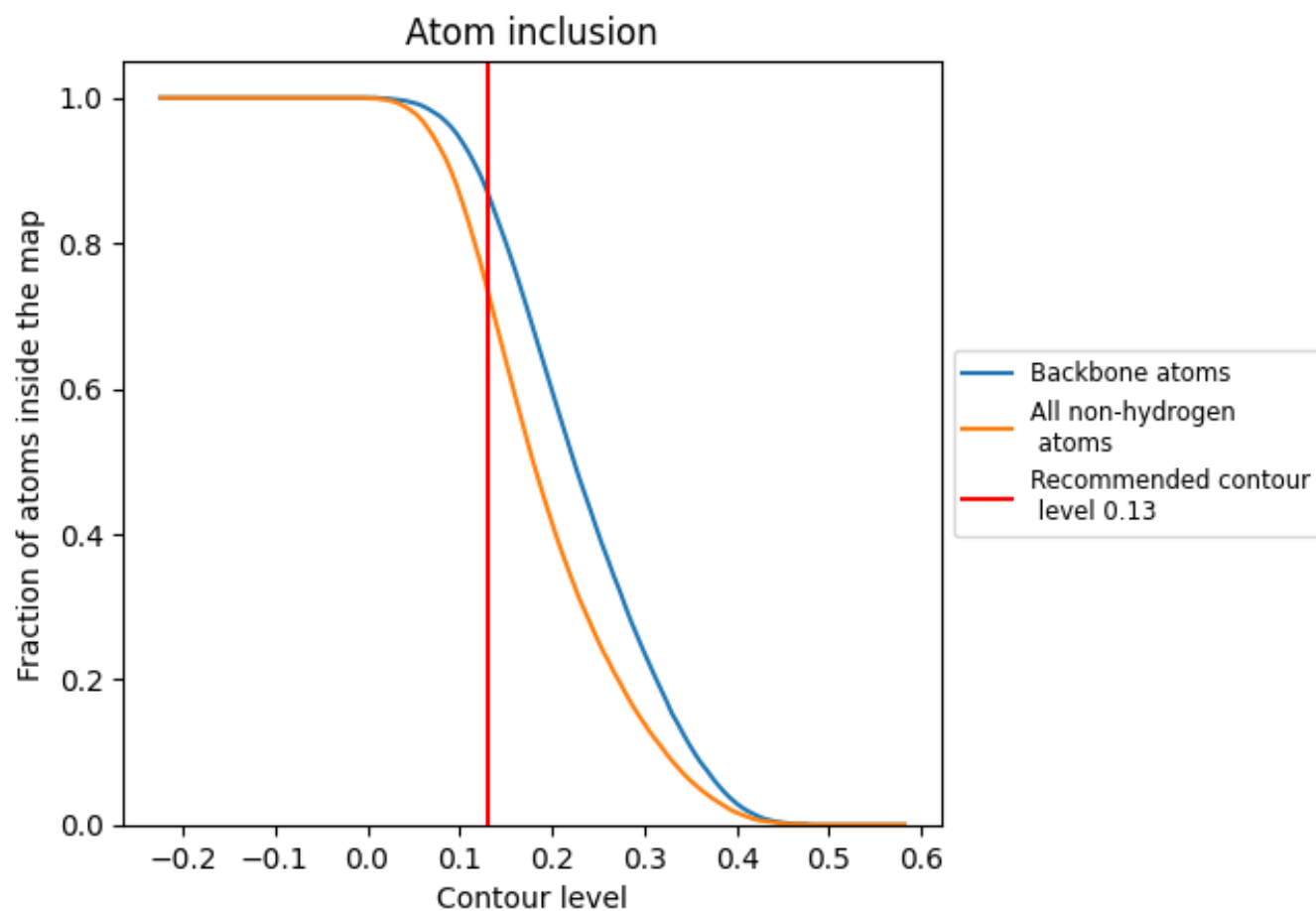
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.13).



































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 74% 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 (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7370	 0.2500
A	 0.8350	 0.3150
B	 0.8510	 0.3500
C	 0.8500	 0.3670
D	 0.8590	 0.3650
E	 0.8420	 0.3610
F	 0.8570	 0.3590
G	 0.8420	 0.3440
H	 0.8420	 0.3470
I	 0.8150	 0.2910
J	 0.7850	 0.2860
K	 0.8150	 0.2520
L	 0.8190	 0.2630
M	 0.7450	 0.2350
N	 0.6990	 0.2060
O	 0.8200	 0.2050
P	 0.8050	 0.2670
Q	 0.7700	 0.2570
R	 0.8270	 0.2240
U	 0.6650	 0.1530
V	 0.7160	 0.1860
W	 0.7700	 0.2050
Y	 0.6720	 0.2130
Z	 0.8170	 0.2780
e	 0.5260	 0.1590
f	 0.6400	 0.1700
g	 0.5720	 0.1210
h	 0.8050	 0.1880
m	 0.7460	 0.2430
n	 0.6100	 0.1950
o	 0.7350	 0.2260
p	 0.3350	 0.0830

