



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 03:37 PM UTC

PDB ID : 8IYL / pdb_00008iyl
EMDB ID : EMD-35825
Title : Tail tip conformation 2 of phage lambda tail
Authors : Wang, J.W.; Wang, C.
Deposited on : 2023-04-05
Resolution : 3.00 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

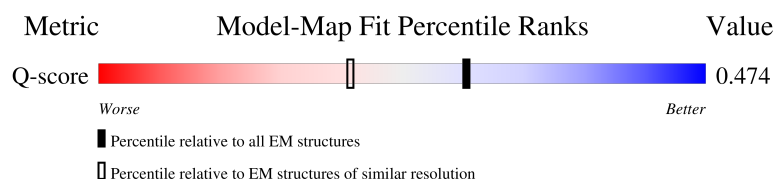
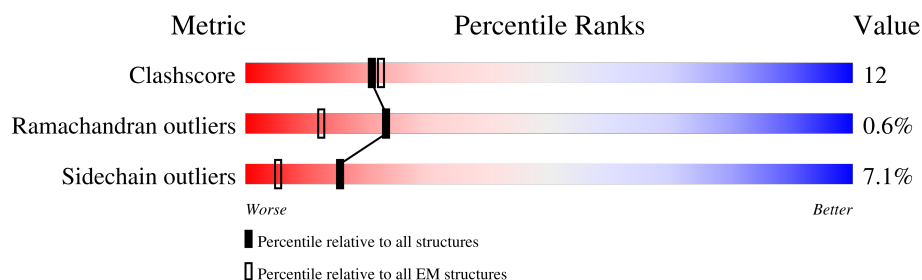
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.00 Å.

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



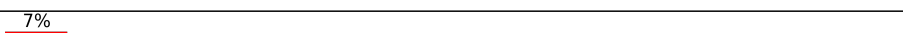
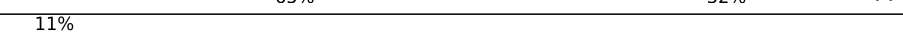
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 (2.50 - 3.50)

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

Mol	Chain	Length	Quality of chain
1	D	109	
1	F	109	
1	M	109	
1	X	109	

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Mol	Chain	Length	Quality of chain
1	Z	109	
1	m	109	
2	E	1132	
2	J	1132	
2	Y	1132	
3	G	232	
3	L	232	
3	d	232	
4	H	853	
4	K	853	
4	e	853	
5	I	223	
5	N	223	
5	f	223	
6	A	246	
6	B	246	
6	C	246	
6	O	246	
6	P	246	
6	Q	246	
6	R	246	
6	S	246	
6	T	246	
6	U	246	
6	V	246	

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Mol	Chain	Length	Quality of chain
6	W	246	
6	a	246	
6	b	246	
6	c	246	
6	g	246	
6	h	246	
6	i	246	
6	j	246	
6	k	246	
6	l	246	
6	n	246	
6	o	246	
6	v	246	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 77370 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 Tail tip protein M.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	M	109	Total	C	N	O	S	0	0
			884	569	154	157	4		
1	m	109	Total	C	N	O	S	0	0
			884	569	154	157	4		
1	D	109	Total	C	N	O	S	0	0
			884	569	154	157	4		
1	F	109	Total	C	N	O	S	0	0
			884	569	154	157	4		
1	X	109	Total	C	N	O	S	0	0
			884	569	154	157	4		
1	Z	109	Total	C	N	O	S	0	0
			884	569	154	157	4		

- Molecule 2 is a protein called Tip attachment protein J.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	J	861	Total	C	N	O	S	0	0
			6720	4212	1171	1317	20		
2	E	861	Total	C	N	O	S	0	0
			6720	4212	1171	1317	20		
2	Y	861	Total	C	N	O	S	0	0
			6720	4212	1171	1317	20		

- Molecule 3 is a protein called Tail tip protein L.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	232	Total	C	N	O	S	0	0
			1801	1117	309	362	13		
3	G	232	Total	C	N	O	S	0	0
			1801	1117	309	362	13		
3	d	232	Total	C	N	O	S	0	0
			1801	1117	309	362	13		

- Molecule 4 is a protein called Tape measure protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	33	Total	C	N	O	S	0	0
			250	154	47	47	2		
4	K	33	Total	C	N	O	S	0	0
			250	154	47	47	2		
4	e	33	Total	C	N	O	S	0	0
			250	154	47	47	2		

- Molecule 5 is a protein called Tail tip assembly protein I.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	122	Total	C	N	O	S	0	0
			865	544	151	165	5		
5	N	122	Total	C	N	O	S	0	0
			865	544	151	165	5		
5	f	122	Total	C	N	O	S	0	0
			865	544	151	165	5		

- Molecule 6 is a protein called Tail tube protein.

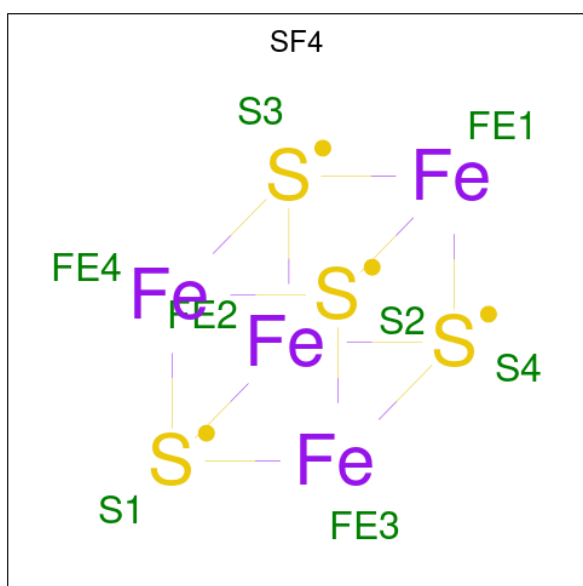
Mol	Chain	Residues	Atoms					AltConf	Trace
6	V	243	Total	C	N	O	S	0	0
			1792	1119	302	366	5		
6	v	243	Total	C	N	O	S	0	0
			1792	1119	302	366	5		
6	B	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
6	b	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
6	A	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
6	a	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
6	C	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
6	c	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
6	O	243	Total	C	N	O	S	0	0
			1792	1119	302	366	5		
6	P	243	Total	C	N	O	S	0	0
			1792	1119	302	366	5		
6	Q	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
6	R	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	S	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
6	T	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
6	U	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
6	W	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
6	g	243	Total	C	N	O	S	0	0
			1792	1119	302	366	5		
6	h	243	Total	C	N	O	S	0	0
			1792	1119	302	366	5		
6	i	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
6	j	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
6	k	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
6	l	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
6	n	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
6	o	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		

- Molecule 7 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
7	L	1	Total 8	Fe 4	S 4	0
7	G	1	Total 8	Fe 4	S 4	0
7	d	1	Total 8	Fe 4	S 4	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.

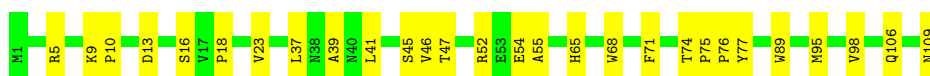
- Molecule 1: Tail tip protein M

Chain M: 



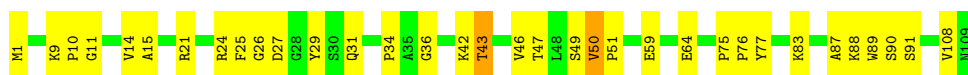
- Molecule 1: Tail tip protein M

Chain m: 



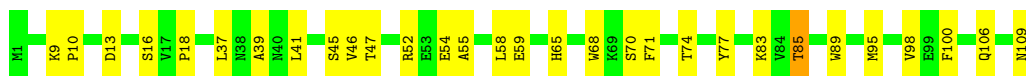
- Molecule 1: Tail tip protein M

Chain D: 



- Molecule 1: Tail tip protein M

Chain F: 



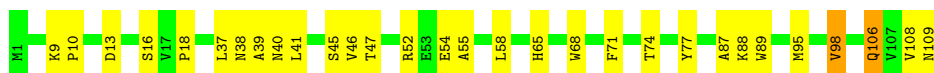
- Molecule 1: Tail tip protein M

Chain X: 



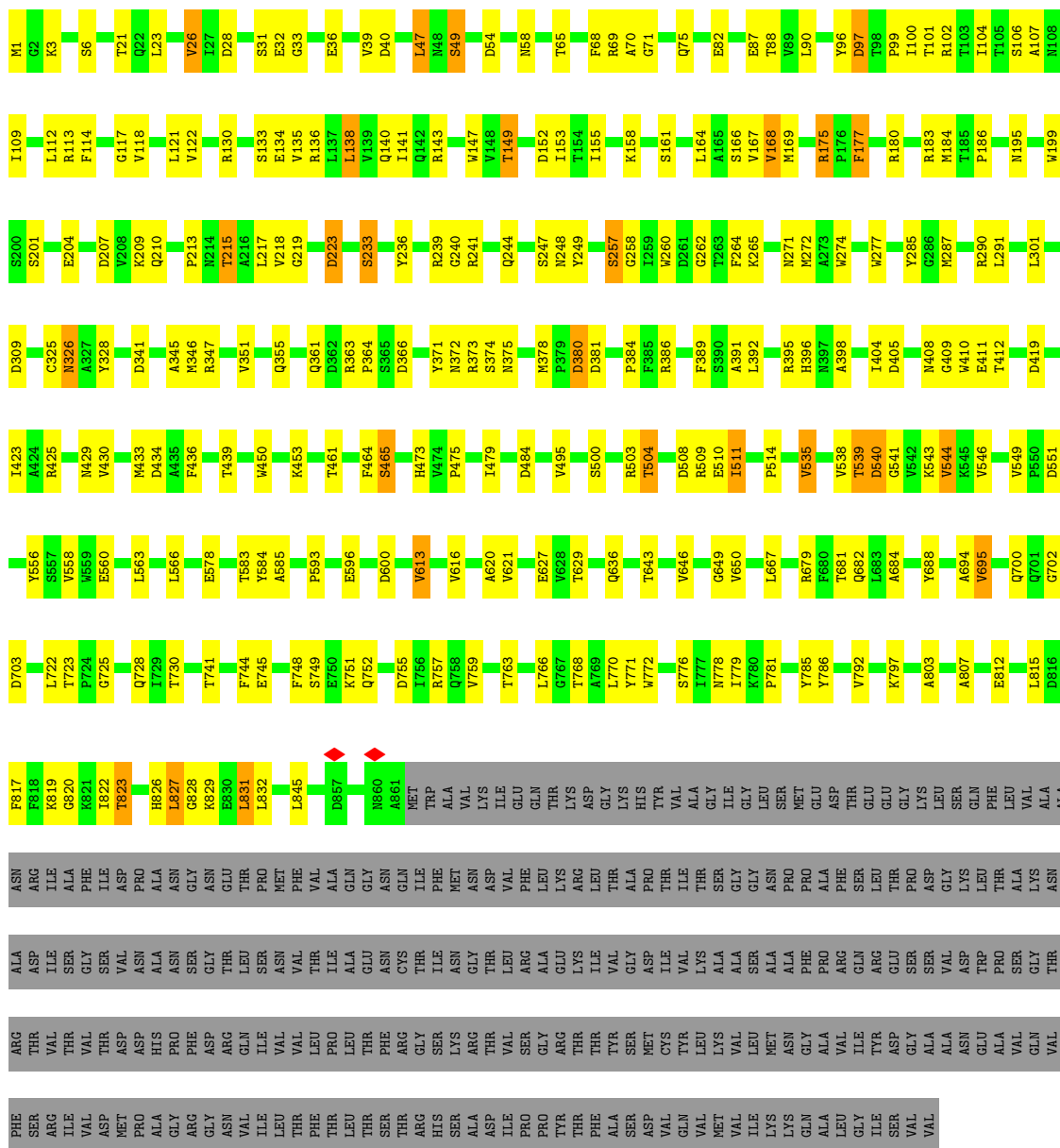
- Molecule 1: Tail tip protein M

Chain Z:  72% 26% .



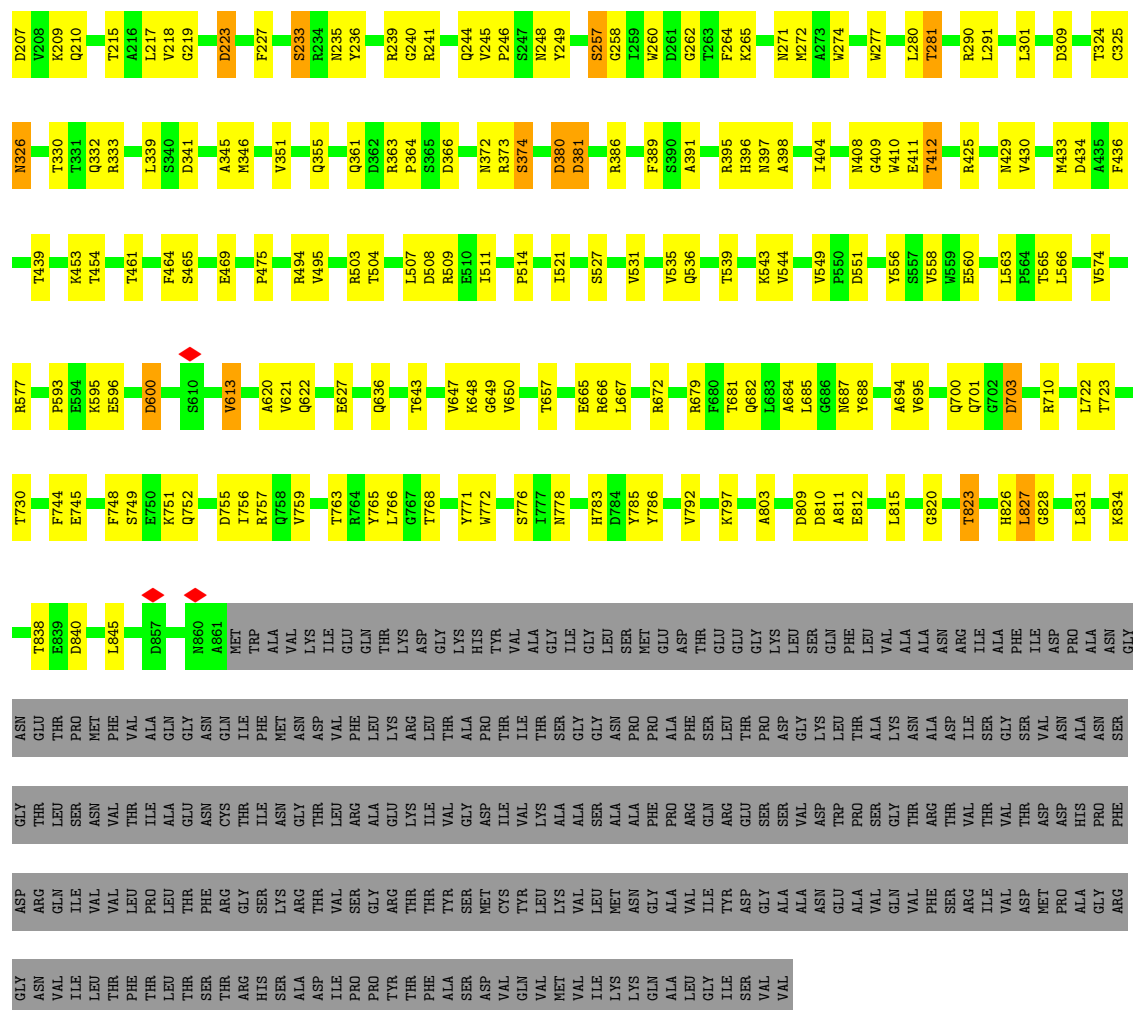
• Molecule 2: Tip attachment protein J

Chain J:  53% 21% . 24%



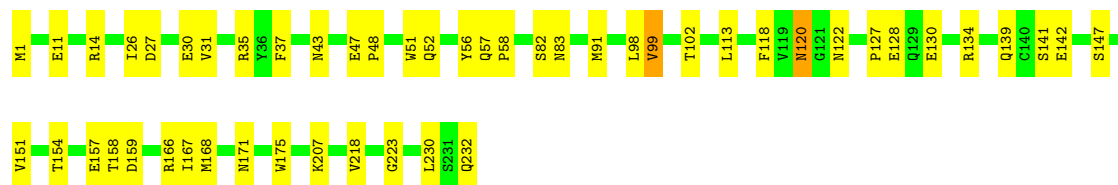
• Molecule 2: Tip attachment protein J

Chain E:  52% 22% . 24%



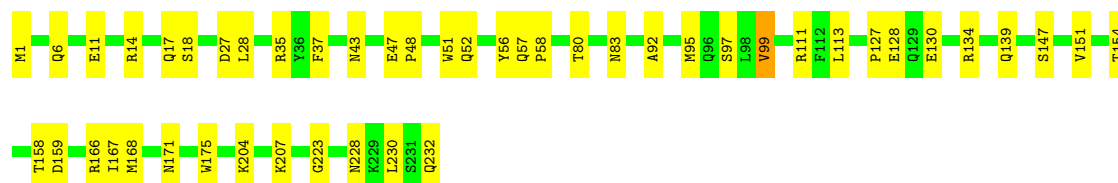
• Molecule 3: Tail tip protein L

Chain L: 78% 21% .

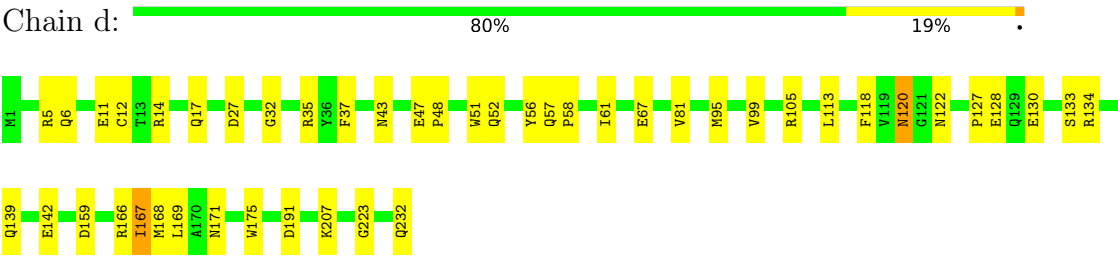


• Molecule 3: Tail tip protein L

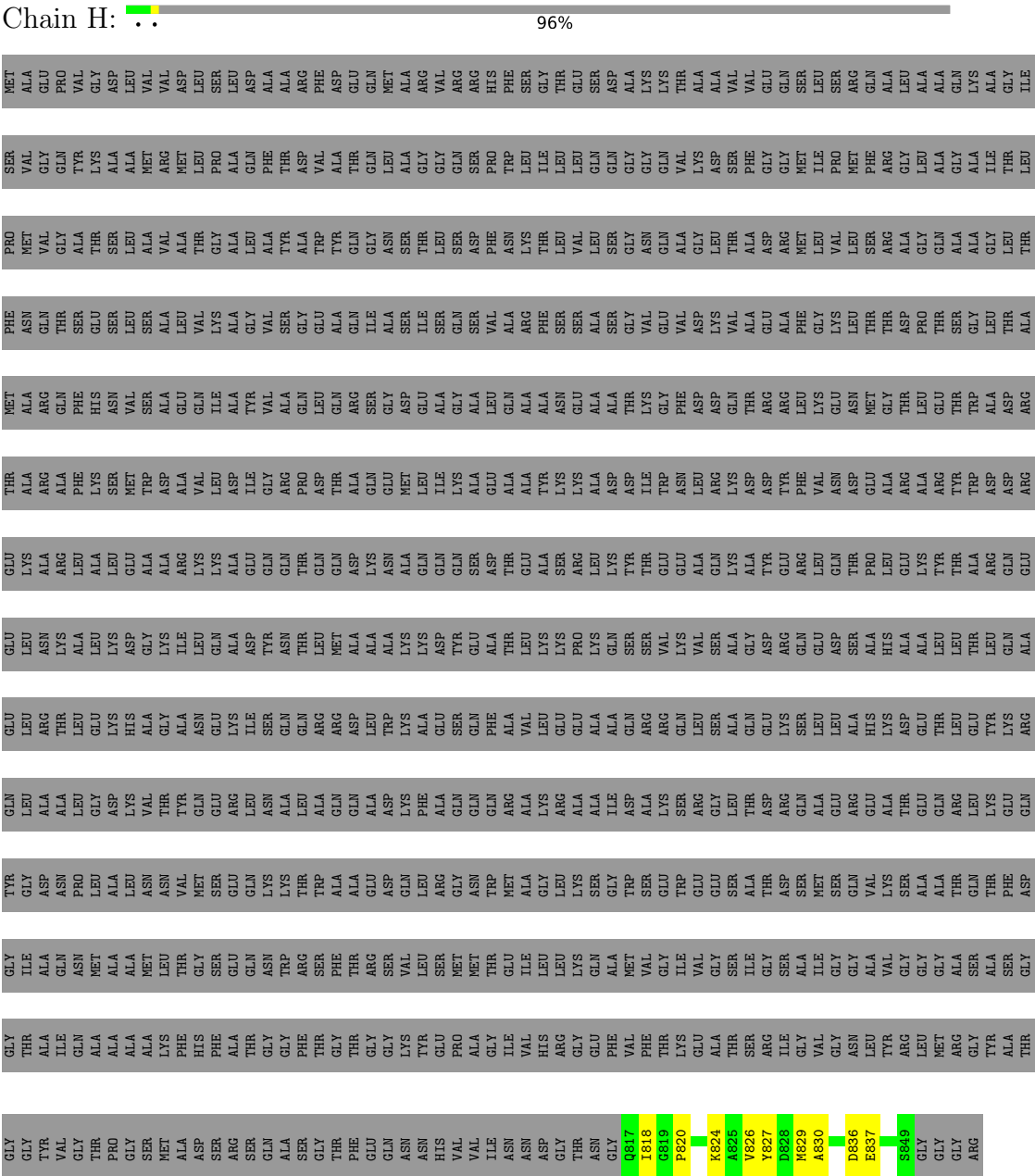
Chain G: 80% 20%



• Molecule 3: Tail tip protein L



• Molecule 4: Tape measure protein



• Molecule 4: Tape measure protein

96%

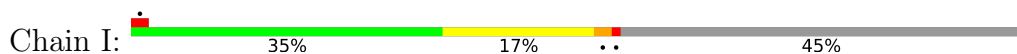
- Molecule 4: Tape measure protein

96%

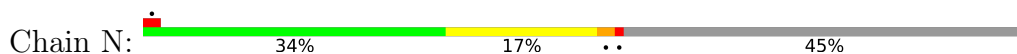
[illegible]

[illegible]

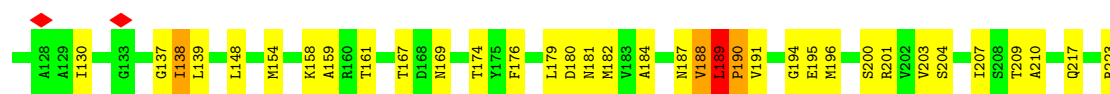
- Molecule 5: Tail tip assembly protein I

[illegible]

- Molecule 5: Tail tip assembly protein I

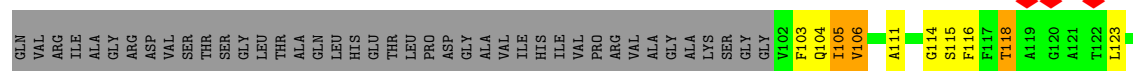


Gln	Val	Arg	Ile	Ala	Gly	Arg	Asp	Val	Ser	Thr	Ser	Gly	Leu	Thr	Gln	Pro	Phe	Arg	Gln	Lys	Leu	Ser	Asp	Gly	Tyr
Met	Ala	Arg	Ile	Ala	His	Leu	Pro	Val	Ala	Thr	Ser	Gly	Leu	Thr	Gln	Pro	Phe	Arg	Gln	Lys	Leu	Ser	Asp	Gly	Tyr



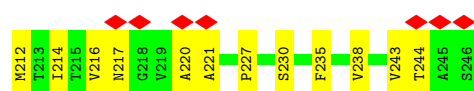
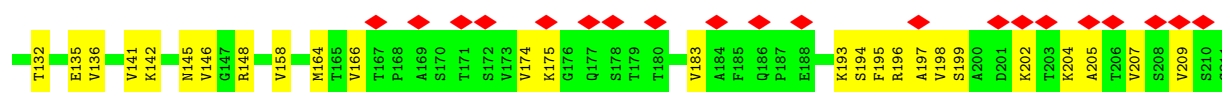
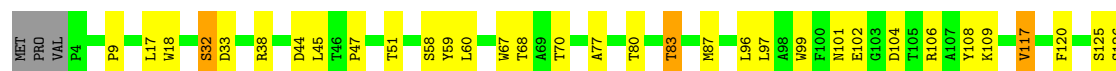
• Molecule 5: Tail tip assembly protein I

Chain f: 33% 18% 45%



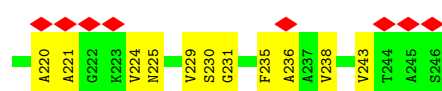
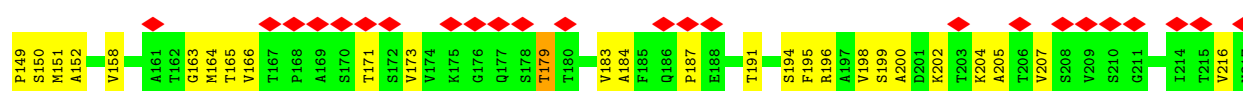
• Molecule 6: Tail tube protein

Chain V: 11% 70% 28%

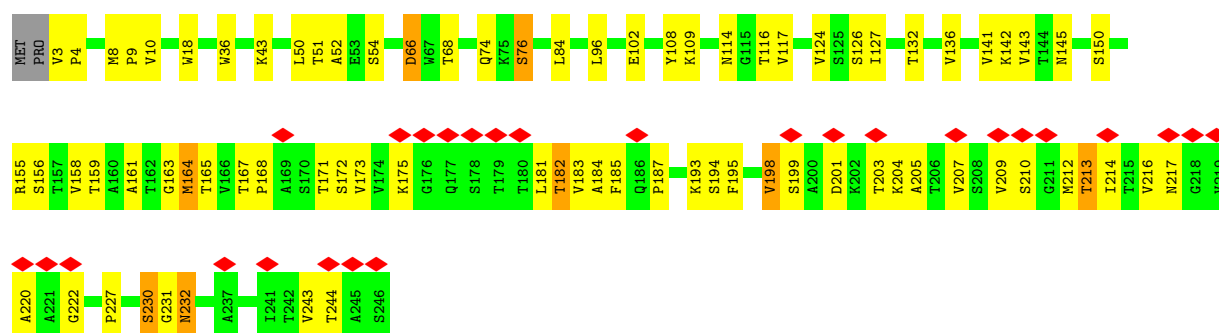


• Molecule 6: Tail tube protein

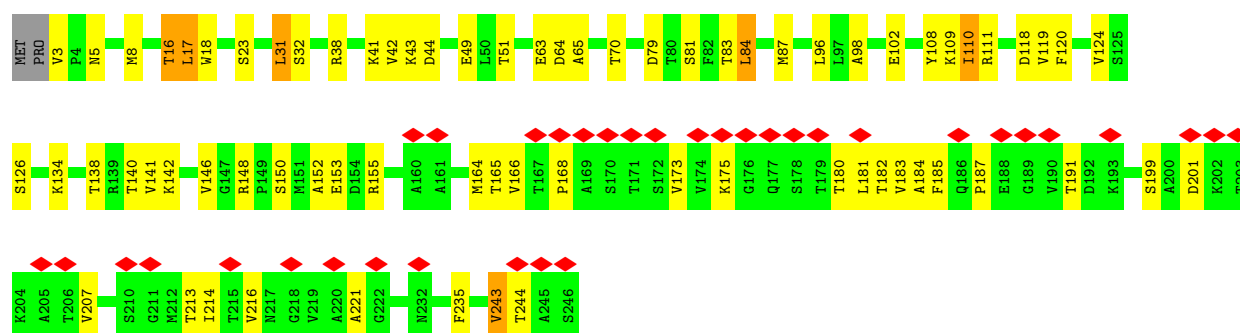
Chain v: 13% 69% 28%



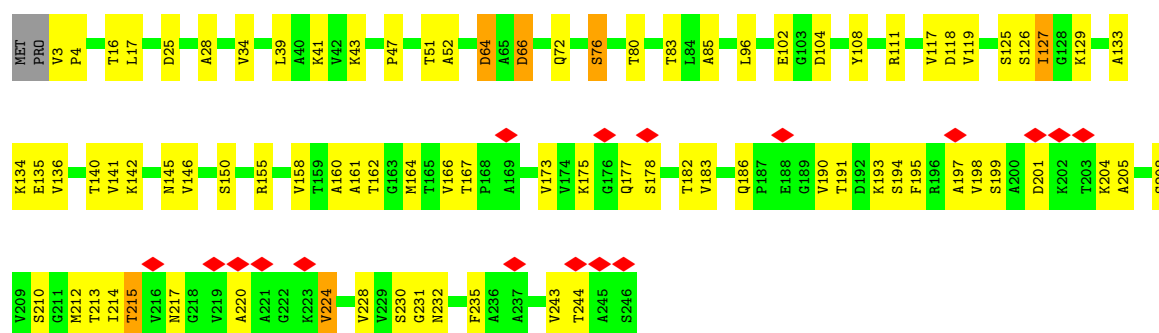
• Molecule 6: Tail tube protein



• Molecule 6: Tail tube protein

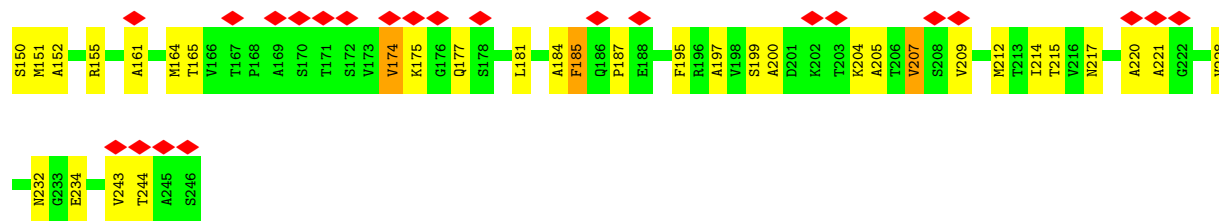


• Molecule 6: Tail tube protein

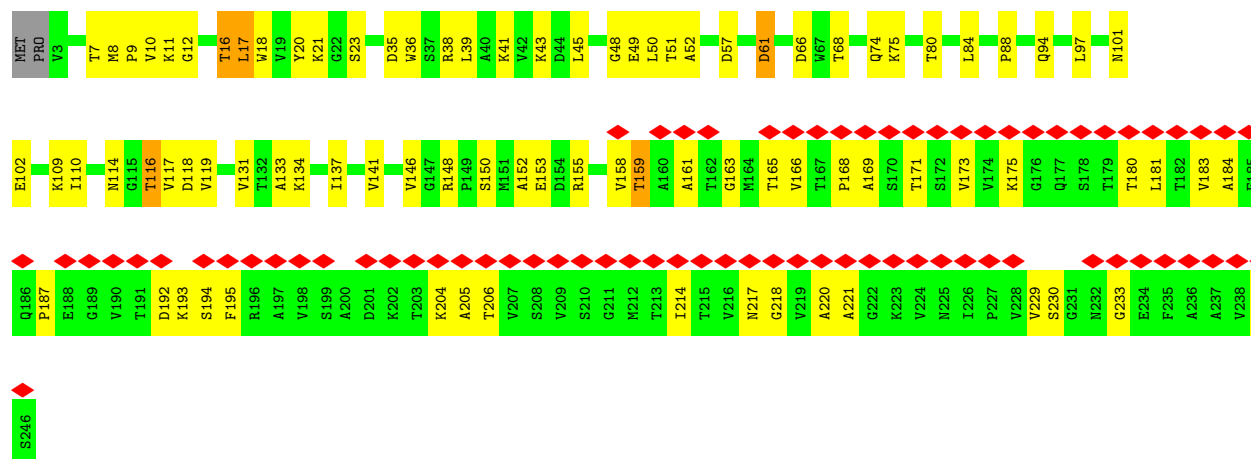


• Molecule 6: Tail tube protein

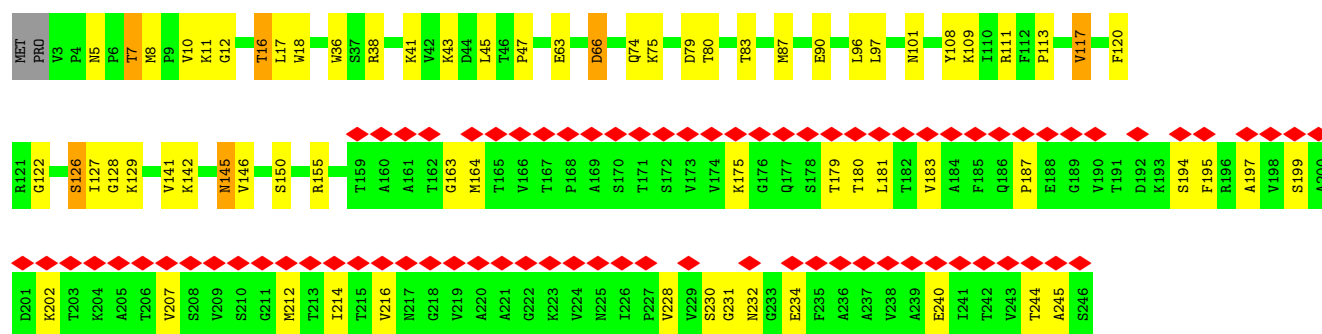




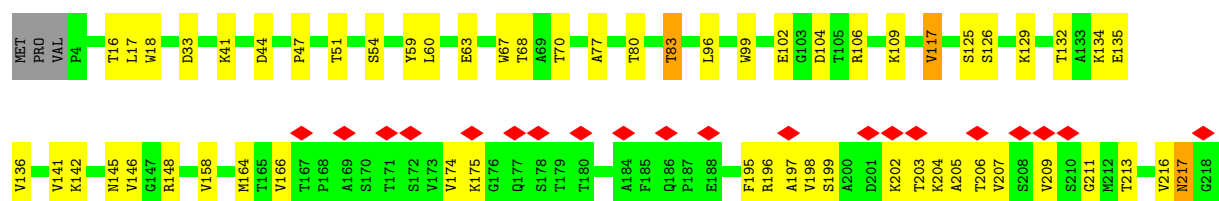
• Molecule 6: Tail tube protein



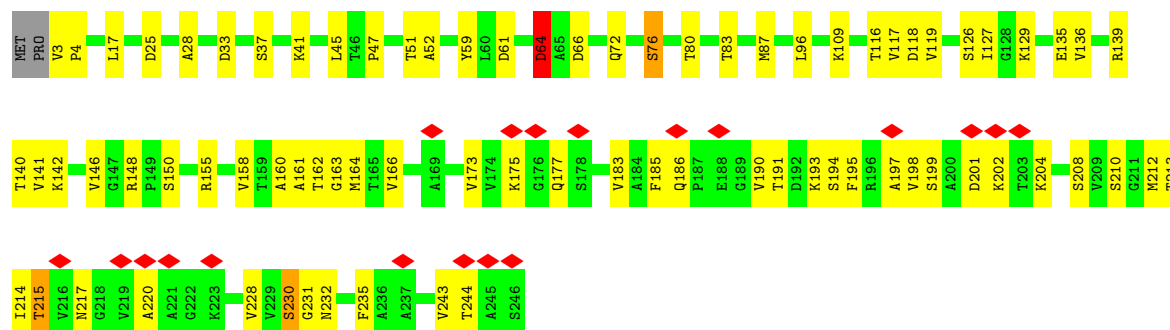
• Molecule 6: Tail tube protein



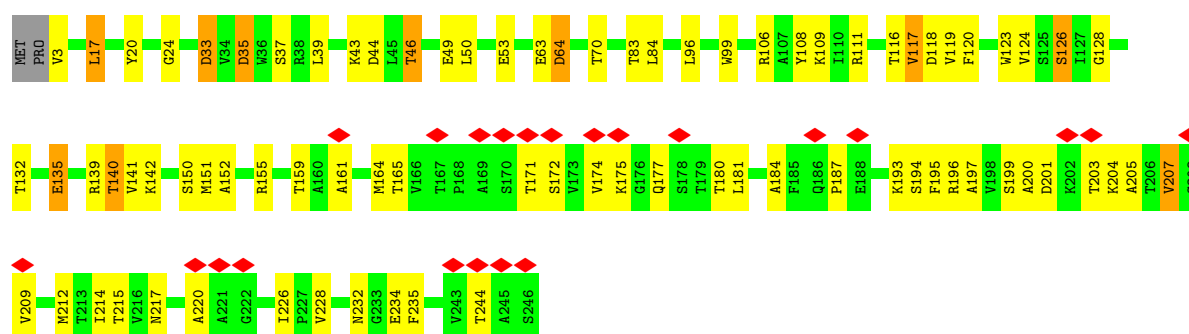
• Molecule 6: Tail tube protein



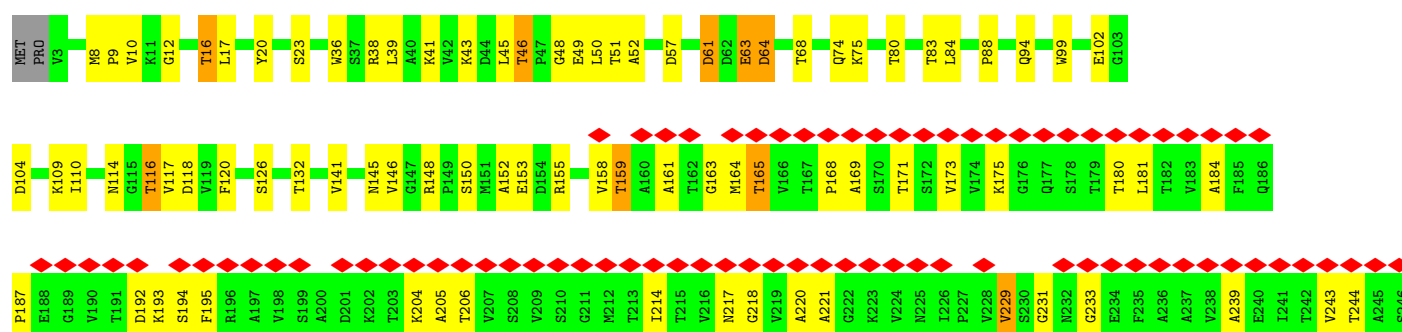




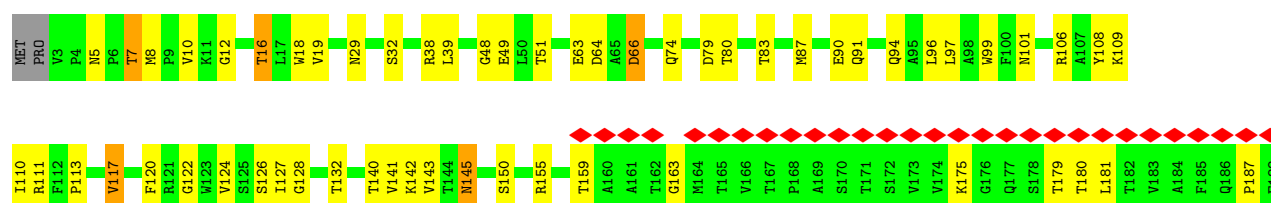
• Molecule 6: Tail tube protein



• Molecule 6: Tail tube protein

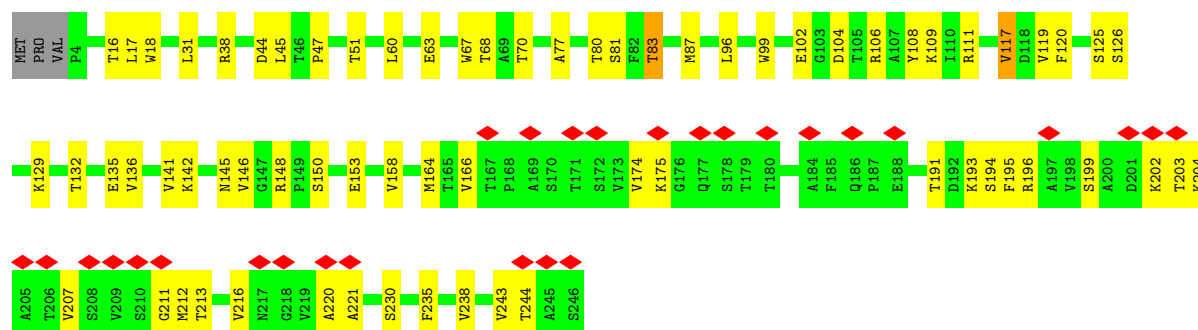


• Molecule 6: Tail tube protein

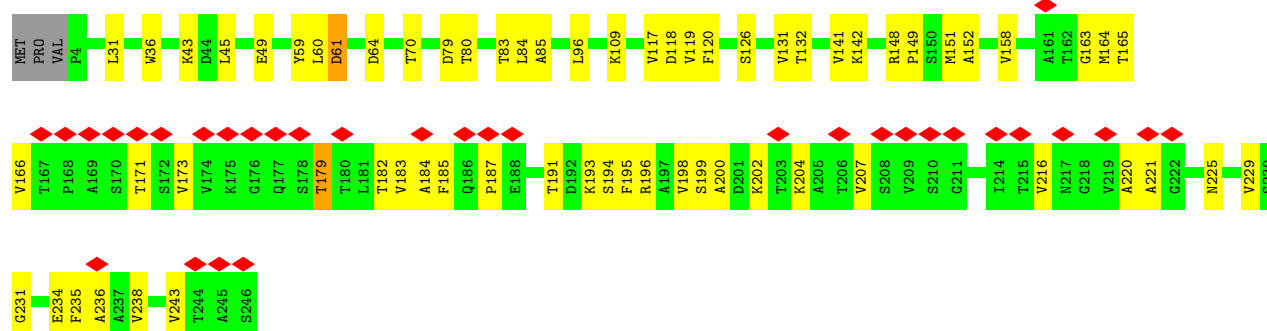
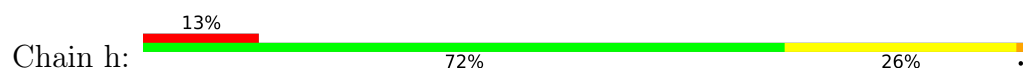




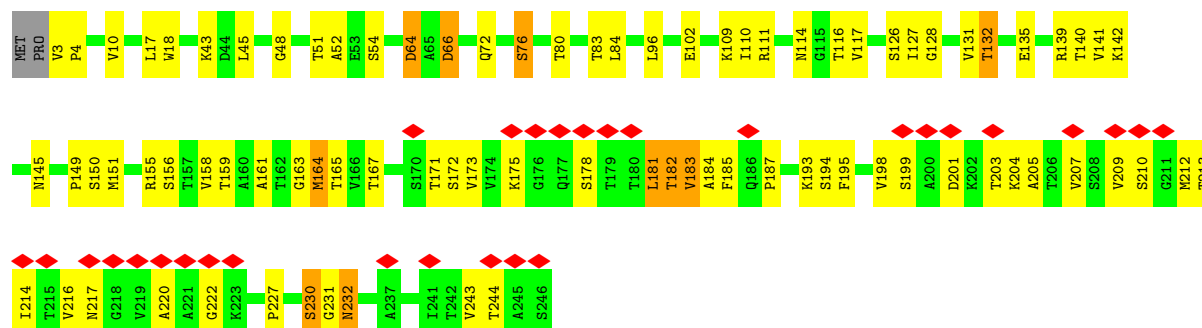
• Molecule 6: Tail tube protein



• Molecule 6: Tail tube protein

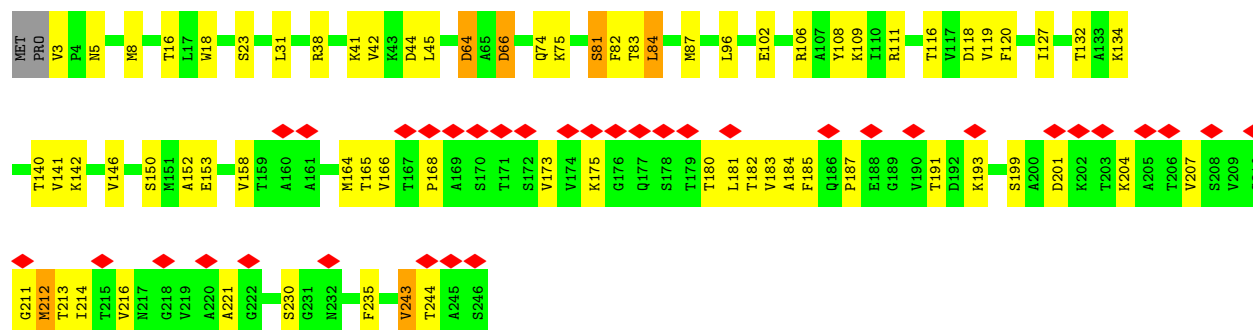


• Molecule 6: Tail tube protein

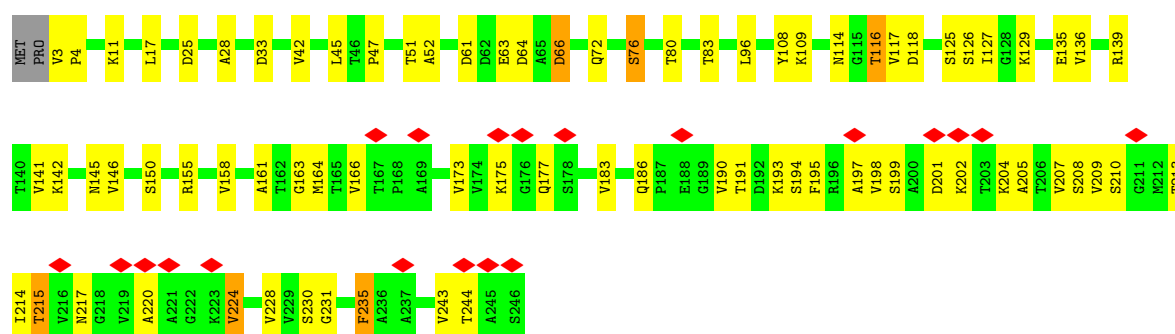


• Molecule 6: Tail tube protein

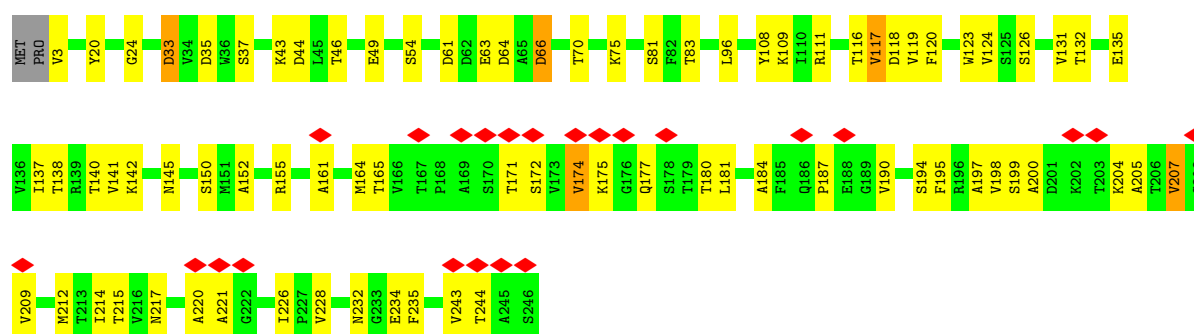




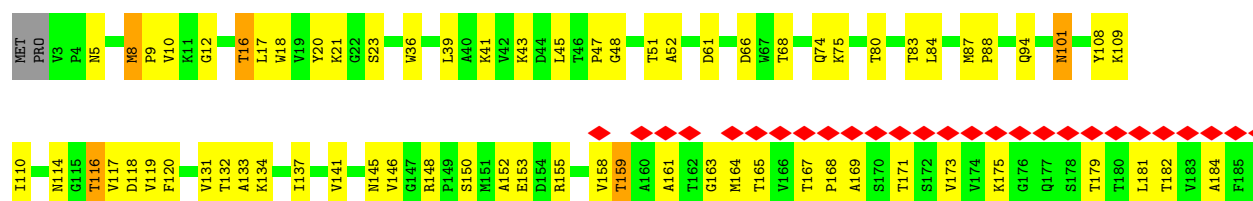
• Molecule 6: Tail tube protein

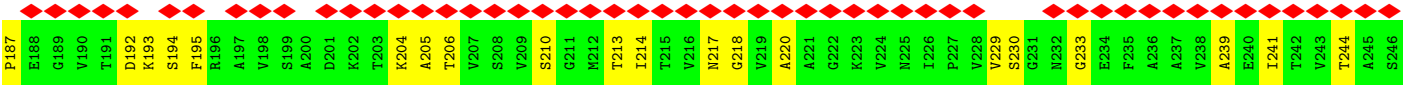


• Molecule 6: Tail tube protein

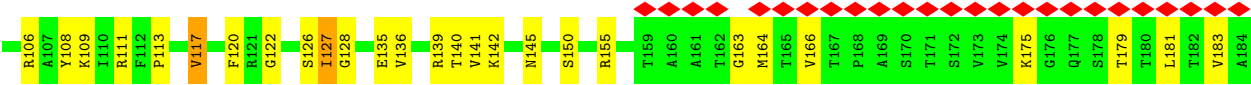


• Molecule 6: Tail tube protein





• Molecule 6: Tail tube protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	54547	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.471	Depositor
Minimum map value	-1.590	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.082	Depositor
Recommended contour level	0.25	Depositor
Map size ($\text{\AA}$)	515.616, 515.616, 515.616	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0742, 1.0742, 1.0742	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SF4

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	D	0.19	0/909	0.42	0/1231
1	F	0.18	0/909	0.41	0/1231
1	M	0.19	0/909	0.41	0/1231
1	X	0.19	0/909	0.41	0/1231
1	Z	0.19	0/909	0.41	0/1231
1	m	0.18	0/909	0.39	0/1231
2	E	0.16	0/6866	0.36	0/9348
2	J	0.16	0/6866	0.36	0/9348
2	Y	0.16	0/6866	0.37	0/9348
3	G	0.16	0/1836	0.27	0/2487
3	L	0.16	0/1836	0.28	0/2487
3	d	0.16	0/1836	0.29	0/2487
4	H	0.18	0/252	0.42	0/335
4	K	0.21	0/252	0.45	0/335
4	e	0.23	0/252	0.43	0/335
5	I	0.20	0/876	0.57	0/1186
5	N	0.19	0/876	0.55	0/1186
5	f	0.19	0/876	0.53	0/1186
6	A	0.17	0/1834	0.39	0/2505
6	B	0.16	0/1834	0.37	0/2505
6	C	0.14	0/1834	0.37	0/2505
6	O	0.16	0/1827	0.34	0/2494
6	P	0.16	0/1827	0.29	0/2494
6	Q	0.16	0/1834	0.38	0/2505
6	R	0.16	0/1834	0.37	1/2505 (0.0%)
6	S	0.17	0/1834	0.40	0/2505
6	T	0.17	0/1834	0.35	0/2505
6	U	0.13	0/1834	0.37	2/2505 (0.1%)
6	V	0.16	0/1827	0.34	0/2494
6	W	0.14	0/1834	0.34	0/2505
6	a	0.17	0/1834	0.36	2/2505 (0.1%)
6	b	0.16	0/1834	0.37	0/2505

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	c	0.15	0/1834	0.37	0/2505
6	g	0.16	0/1827	0.33	0/2494
6	h	0.16	0/1827	0.29	0/2494
6	i	0.16	0/1834	0.38	0/2505
6	j	0.16	0/1834	0.37	1/2505 (0.0%)
6	k	0.17	0/1834	0.40	0/2505
6	l	0.17	0/1834	0.34	0/2505
6	n	0.14	0/1834	0.36	0/2505
6	o	0.14	0/1834	0.35	0/2505
6	v	0.16	0/1827	0.29	0/2494
All	All	0.16	0/78918	0.37	6/107508 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	E	0	1
2	J	0	1
2	Y	0	1
5	I	0	1
5	N	0	1
5	f	0	1
All	All	0	6

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	a	63	GLU	CA-C-N	5.53	132.10	121.54
6	a	63	GLU	C-N-CA	5.53	132.10	121.54
6	j	212	MET	CA-CB-CG	5.19	124.47	114.10
6	U	63	GLU	CA-C-N	5.16	131.40	121.54
6	U	63	GLU	C-N-CA	5.16	131.40	121.54
6	R	212	MET	CA-CB-CG	5.03	124.15	114.10

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	175	ARG	Peptide
5	I	189	LEU	Peptide
2	J	175	ARG	Peptide
5	N	189	LEU	Peptide
2	Y	175	ARG	Peptide
5	f	189	LEU	Peptide

5.2 Too-close contacts [i](#)

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	D	884	0	881	24	0
1	F	884	0	881	20	0
1	M	884	0	881	23	0
1	X	884	0	881	20	0
1	Z	884	0	881	21	0
1	m	884	0	881	22	0
2	E	6720	0	6558	206	0
2	J	6720	0	6558	178	0
2	Y	6720	0	6558	177	0
3	G	1801	0	1715	30	0
3	L	1801	0	1715	32	0
3	d	1801	0	1715	34	0
4	H	250	0	251	11	0
4	K	250	0	251	11	0
4	e	250	0	251	14	0
5	I	865	0	874	42	0
5	N	865	0	874	45	0
5	f	865	0	874	49	0
6	A	1799	0	1768	49	0
6	B	1799	0	1768	48	0
6	C	1799	0	1768	57	0
6	O	1792	0	1760	32	0
6	P	1792	0	1760	39	0
6	Q	1799	0	1768	54	0
6	R	1799	0	1768	42	0
6	S	1799	0	1768	48	0
6	T	1799	0	1768	50	0
6	U	1799	0	1768	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	V	1792	0	1760	44	0
6	W	1799	0	1768	52	0
6	a	1799	0	1768	41	0
6	b	1799	0	1768	47	0
6	c	1799	0	1768	52	0
6	g	1792	0	1760	35	0
6	h	1792	0	1760	39	0
6	i	1799	0	1768	51	0
6	j	1799	0	1768	45	0
6	k	1799	0	1768	50	0
6	l	1799	0	1768	47	0
6	n	1799	0	1768	62	0
6	o	1799	0	1768	59	0
6	v	1792	0	1760	44	0
7	G	8	0	0	0	0
7	L	8	0	0	0	0
7	d	8	0	0	0	0
All	All	77370	0	75864	1837	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 12.

All (1837) 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)
6:Q:183:VAL:HB	6:Q:212:MET:HE1	1.58	0.86
6:B:96:LEU:HD21	6:B:141:VAL:HG21	1.59	0.84
6:W:87:MET:HB3	6:W:90:GLU:HG2	1.59	0.84
2:J:240:GLY:HA3	5:I:194:GLY:H	1.43	0.83
1:Z:55:ALA:HB2	1:Z:98:VAL:HG11	1.60	0.83
2:J:36:GLU:HG2	2:J:239:ARG:HD2	1.61	0.82
2:E:240:GLY:HA3	5:N:194:GLY:H	1.44	0.82
2:Y:240:GLY:HA3	5:f:194:GLY:H	1.44	0.82
1:F:55:ALA:HB2	1:F:98:VAL:HG11	1.63	0.81
4:H:826:VAL:HG12	4:K:829:MET:HG2	1.63	0.81
2:Y:36:GLU:HG2	2:Y:239:ARG:HD2	1.62	0.81
2:E:36:GLU:HG2	2:E:239:ARG:HD2	1.63	0.81
6:B:183:VAL:HB	6:B:212:MET:HE1	1.61	0.80
6:P:126:SER:HB3	6:P:142:LYS:HB3	1.65	0.78
6:c:74:GLN:HE21	6:U:68:THR:HG22	1.47	0.78
6:i:96:LEU:HD21	6:i:141:VAL:HG21	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:U:10:VAL:HG21	6:U:114:ASN:HB3	1.65	0.77
6:C:10:VAL:HG21	6:C:114:ASN:HB3	1.66	0.76
6:Q:66:ASP:OD1	6:Q:66:ASP:N	2.17	0.76
6:v:126:SER:HB3	6:v:142:LYS:HB3	1.67	0.76
6:W:74:GLN:HE21	6:n:68:THR:HG22	1.50	0.75
6:C:68:THR:HG22	6:o:74:GLN:HE21	1.51	0.75
6:i:210:SER:O	6:i:213:THR:OG1	2.04	0.75
6:Q:102:GLU:N	6:Q:102:GLU:OE1	2.20	0.74
6:i:66:ASP:OD1	6:i:66:ASP:N	2.21	0.74
6:j:66:ASP:OD1	6:j:66:ASP:N	2.21	0.74
6:n:8:MET:HG3	6:n:9:PRO:HD2	1.70	0.74
6:U:165:THR:HG22	6:U:184:ALA:HB3	1.69	0.74
6:B:102:GLU:OE1	6:B:102:GLU:N	2.21	0.73
5:N:182:MET:HA	5:f:169:ASN:HB3	1.70	0.73
6:Q:210:SER:O	6:Q:213:THR:OG1	2.04	0.73
2:J:118:VAL:HG11	2:J:121:LEU:HD13	1.71	0.73
6:Q:209:VAL:HG12	6:Q:214:ILE:HG12	1.71	0.73
6:o:128:GLY:N	6:o:140:THR:O	2.21	0.73
6:R:102:GLU:OE2	6:R:106:ARG:NH2	2.22	0.73
3:d:128:GLU:N	3:d:128:GLU:OE2	2.22	0.72
1:M:27:ASP:OD2	2:J:509:ARG:NH2	2.22	0.72
2:J:97:ASP:N	2:J:97:ASP:OD1	2.22	0.72
2:E:118:VAL:HG11	2:E:121:LEU:HD13	1.71	0.72
6:i:102:GLU:N	6:i:102:GLU:OE1	2.22	0.72
6:j:102:GLU:OE2	6:j:106:ARG:NH2	2.23	0.72
6:Q:212:MET:HE2	6:Q:212:MET:HA	1.71	0.72
6:B:210:SER:O	6:B:213:THR:OG1	2.05	0.72
2:E:149:THR:O	5:N:217:GLN:NE2	2.23	0.71
6:b:164:MET:HE2	6:b:164:MET:HA	1.71	0.71
6:l:199:SER:H	6:l:207:VAL:HG21	1.55	0.71
6:o:11:LYS:HE2	6:o:11:LYS:HA	1.72	0.71
6:B:165:THR:HG23	6:B:184:ALA:HB3	1.72	0.71
6:B:212:MET:HA	6:B:212:MET:HE2	1.72	0.71
5:I:158:LYS:HE2	5:I:158:LYS:HA	1.70	0.71
6:c:5:ASN:ND2	6:c:8:MET:SD	2.63	0.71
6:B:164:MET:HE1	6:B:183:VAL:HG13	1.72	0.71
2:Y:396:HIS:HA	2:Y:429:ASN:HB2	1.72	0.71
6:B:66:ASP:OD1	6:B:66:ASP:N	2.18	0.71
2:Y:97:ASP:OD1	2:Y:97:ASP:N	2.22	0.71
6:i:183:VAL:HG22	6:i:212:MET:HE1	1.72	0.71
6:n:10:VAL:HG21	6:n:114:ASN:HB3	1.71	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:W:5:ASN:ND2	6:W:8:MET:SD	2.64	0.70
6:V:193:LYS:HE2	6:V:193:LYS:HA	1.71	0.70
2:E:97:ASP:N	2:E:97:ASP:OD1	2.22	0.70
6:b:16:THR:OG1	6:b:18:TRP:NE1	2.25	0.70
2:Y:812:GLU:HA	2:Y:815:LEU:HD23	1.73	0.70
1:m:37:LEU:HB3	1:D:27:ASP:HB3	1.71	0.70
6:c:87:MET:HE1	6:U:9:PRO:HD3	1.74	0.70
6:T:199:SER:H	6:T:207:VAL:HG21	1.57	0.70
6:o:5:ASN:ND2	6:o:8:MET:SD	2.63	0.70
2:E:43:LYS:HG2	2:E:53:LEU:HB2	1.74	0.70
6:A:66:ASP:OD1	6:A:66:ASP:N	2.21	0.70
6:R:164:MET:HE2	6:R:164:MET:HA	1.74	0.70
2:E:372:ASN:ND2	2:E:560:GLU:OE2	2.24	0.69
2:Y:372:ASN:ND2	2:Y:560:GLU:OE2	2.24	0.69
3:L:128:GLU:N	3:L:128:GLU:OE1	2.26	0.69
6:c:87:MET:HB3	6:c:90:GLU:HG2	1.74	0.69
1:M:27:ASP:HB3	1:Z:37:LEU:HB3	1.73	0.69
6:b:42:VAL:N	6:U:61:ASP:OD1	2.24	0.69
6:T:204:LYS:HA	6:T:220:ALA:HB3	1.75	0.69
1:Z:52:ARG:NH1	1:Z:95:MET:O	2.26	0.69
6:i:164:MET:HE1	6:i:183:VAL:HB	1.75	0.69
6:j:164:MET:HE2	6:j:164:MET:HA	1.75	0.69
6:Q:204:LYS:HA	6:Q:220:ALA:HB3	1.75	0.69
5:N:189:LEU:HD22	5:N:190:PRO:HD3	1.74	0.68
1:F:9:LYS:HB2	1:F:47:THR:HG23	1.76	0.68
6:v:30:PRO:HB2	6:v:117:VAL:HG21	1.74	0.68
2:E:140:GLN:HG2	2:E:149:THR:HA	1.75	0.68
6:U:88:PRO:O	6:U:94:GLN:NE2	2.27	0.68
6:a:175:LYS:NZ	6:a:244:THR:O	2.27	0.68
6:Q:96:LEU:HD21	6:Q:141:VAL:HG21	1.76	0.68
2:J:380:ASP:N	2:J:380:ASP:OD1	2.26	0.68
1:F:37:LEU:HB3	1:X:27:ASP:HB3	1.74	0.68
6:V:196:ARG:HH22	6:v:196:ARG:HD2	1.59	0.68
6:a:204:LYS:HA	6:a:220:ALA:HB3	1.74	0.68
6:C:88:PRO:O	6:C:94:GLN:NE2	2.26	0.68
6:k:166:VAL:HG22	6:k:183:VAL:HG13	1.76	0.68
2:J:247:SER:O	2:J:248:ASN:ND2	2.27	0.68
3:G:128:GLU:N	3:G:128:GLU:OE1	2.27	0.68
6:l:204:LYS:HA	6:l:220:ALA:HB3	1.75	0.68
6:g:196:ARG:HH22	6:h:196:ARG:HD2	1.58	0.68
6:c:207:VAL:HG12	6:c:216:VAL:HG22	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:372:ASN:ND2	2:J:560:GLU:OE2	2.27	0.67
5:I:182:MET:HA	5:N:169:ASN:HB3	1.74	0.67
6:a:63:GLU:N	6:a:63:GLU:OE1	2.23	0.67
1:m:9:LYS:HB2	1:m:47:THR:HG23	1.77	0.67
6:a:165:THR:HB	6:a:184:ALA:HB3	1.76	0.67
6:O:196:ARG:HH22	6:P:196:ARG:HD2	1.60	0.67
6:T:175:LYS:NZ	6:T:244:THR:O	2.27	0.67
6:j:153:GLU:OE1	6:j:153:GLU:N	2.23	0.67
6:j:199:SER:OG	6:j:201:ASP:OD1	2.13	0.67
6:l:175:LYS:NZ	6:l:244:THR:O	2.27	0.67
2:Y:118:VAL:HG11	2:Y:121:LEU:HD13	1.75	0.67
2:J:392:LEU:HB2	3:d:99:VAL:HG13	1.76	0.67
2:Y:620:ALA:HB2	2:Y:703:ASP:HB2	1.76	0.67
6:i:51:THR:HG22	6:i:52:ALA:H	1.60	0.67
6:i:209:VAL:HG12	6:i:214:ILE:HG12	1.77	0.67
6:S:166:VAL:HG21	6:S:228:VAL:HG21	1.77	0.67
1:M:9:LYS:HD2	1:M:49:SER:HB3	1.77	0.67
6:C:9:PRO:HD3	6:o:87:MET:HE1	1.75	0.67
5:N:180:ASP:OD2	5:f:169:ASN:ND2	2.28	0.67
6:b:126:SER:HB3	6:b:142:LYS:HB3	1.77	0.66
6:W:94:GLN:HG3	6:n:153:GLU:HB3	1.77	0.66
6:W:207:VAL:HG12	6:W:216:VAL:HG22	1.76	0.66
2:J:826:HIS:HA	2:Y:820:GLY:H	1.60	0.66
6:i:204:LYS:HA	6:i:220:ALA:HB3	1.77	0.66
6:A:166:VAL:HG21	6:A:228:VAL:HG21	1.77	0.66
1:D:27:ASP:OD2	2:E:509:ARG:NH2	2.28	0.66
3:d:27:ASP:OD2	3:d:35:ARG:NH1	2.29	0.66
6:b:153:GLU:OE1	6:b:153:GLU:N	2.28	0.66
6:A:72:GLN:NE2	6:l:124:VAL:O	2.29	0.66
6:o:207:VAL:HG12	6:o:216:VAL:HG22	1.76	0.66
6:V:183:VAL:H	6:V:212:MET:HE1	1.61	0.66
2:E:748:PHE:HB2	2:E:766:LEU:HD11	1.78	0.66
3:L:27:ASP:OD2	3:L:35:ARG:NH1	2.29	0.66
6:b:124:VAL:O	6:Q:72:GLN:NE2	2.29	0.65
1:X:1:MET:HE1	1:X:5:ARG:HH22	1.61	0.65
6:Q:167:THR:HB	6:Q:182:THR:HG22	1.79	0.65
6:i:165:THR:HG23	6:i:184:ALA:HB3	1.77	0.65
3:G:27:ASP:OD2	3:G:35:ARG:NH1	2.30	0.65
6:P:30:PRO:HB2	6:P:117:VAL:HG21	1.78	0.65
6:k:66:ASP:N	6:k:66:ASP:OD1	2.24	0.65
6:k:204:LYS:HA	6:k:220:ALA:HB3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:126:SER:HB3	6:B:142:LYS:HB3	1.79	0.65
6:o:83:THR:HG22	6:o:140:THR:HG23	1.77	0.65
6:o:212:MET:HE2	6:o:212:MET:HA	1.77	0.65
5:I:189:LEU:HD22	5:I:190:PRO:HD3	1.78	0.65
6:v:164:MET:HE1	6:v:183:VAL:HG13	1.76	0.65
6:a:124:VAL:O	6:S:72:GLN:NE2	2.30	0.65
6:T:124:VAL:O	6:k:72:GLN:NE2	2.28	0.65
6:g:204:LYS:HA	6:g:220:ALA:HB3	1.78	0.65
6:n:88:PRO:O	6:n:94:GLN:NE2	2.29	0.65
6:o:66:ASP:OD1	6:o:66:ASP:N	2.27	0.65
2:J:822:ILE:HG13	2:E:827:LEU:HA	1.78	0.65
2:Y:748:PHE:HE1	2:Y:785:TYR:HB3	1.61	0.65
6:j:109:LYS:HB2	6:j:119:VAL:HG12	1.79	0.65
5:N:209:THR:OG1	2:Y:643:THR:O	2.15	0.65
6:T:165:THR:HB	6:T:184:ALA:HB3	1.79	0.65
6:R:126:SER:HB3	6:R:142:LYS:HB3	1.79	0.65
6:T:174:VAL:HG12	6:T:177:GLN:HE21	1.62	0.65
5:I:180:ASP:OD2	5:N:169:ASN:ND2	2.29	0.64
6:V:204:LYS:HA	6:V:220:ALA:HB3	1.79	0.64
6:B:209:VAL:HG12	6:B:214:ILE:HG12	1.79	0.64
6:h:204:LYS:HA	6:h:220:ALA:HB3	1.79	0.64
6:W:91:GLN:HA	6:W:91:GLN:HE21	1.62	0.64
6:O:204:LYS:HA	6:O:220:ALA:HB3	1.79	0.64
6:S:96:LEU:HD21	6:S:141:VAL:HG21	1.80	0.64
3:d:175:TRP:O	3:d:207:LYS:NZ	2.31	0.64
6:B:204:LYS:HA	6:B:220:ALA:HB3	1.79	0.64
6:A:204:LYS:HA	6:A:220:ALA:HB3	1.78	0.64
6:S:126:SER:HB3	6:S:142:LYS:HB3	1.78	0.64
2:Y:1:MET:HE3	2:Y:6:SER:HB3	1.79	0.64
6:c:11:LYS:HE2	6:c:11:LYS:HA	1.80	0.64
6:W:87:MET:HE1	6:n:9:PRO:HD3	1.79	0.64
6:l:165:THR:HB	6:l:184:ALA:HB3	1.80	0.64
5:I:209:THR:OG1	2:E:643:THR:O	2.15	0.64
6:C:102:GLU:OE1	6:C:102:GLU:N	2.29	0.64
6:j:16:THR:OG1	6:j:18:TRP:NE1	2.28	0.64
3:L:175:TRP:O	3:L:207:LYS:NZ	2.30	0.64
1:D:88:LYS:O	1:F:16:SER:OG	2.16	0.64
2:E:210:GLN:NE2	3:G:223:GLY:O	2.28	0.64
2:Y:223:ASP:OD1	2:Y:223:ASP:N	2.29	0.64
6:o:128:GLY:HA3	6:o:140:THR:HB	1.78	0.64
1:M:9:LYS:HA	6:v:59:TYR:HA	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:199:SER:OG	6:A:201:ASP:OD1	2.15	0.64
6:i:167:THR:HB	6:i:182:THR:HG22	1.80	0.64
6:k:195:PHE:HA	6:k:230:SER:HA	1.80	0.64
1:m:52:ARG:NH1	1:m:95:MET:O	2.31	0.64
2:E:745:GLU:HG3	2:E:768:THR:HG22	1.80	0.64
6:P:38:ARG:NH2	6:k:61:ASP:OD1	2.28	0.64
2:Y:745:GLU:HG3	2:Y:768:THR:HG22	1.79	0.64
2:J:748:PHE:HE1	2:J:785:TYR:HB3	1.63	0.63
2:E:620:ALA:HB2	2:E:703:ASP:HB2	1.78	0.63
6:S:204:LYS:HA	6:S:220:ALA:HB3	1.78	0.63
6:W:128:GLY:N	6:W:140:THR:O	2.26	0.63
6:W:202:LYS:HZ3	6:W:207:VAL:H	1.45	0.63
2:J:223:ASP:N	2:J:223:ASP:OD1	2.30	0.63
2:J:396:HIS:HA	2:J:429:ASN:HB2	1.80	0.63
6:b:199:SER:OG	6:b:201:ASP:OD1	2.15	0.63
6:a:199:SER:H	6:a:207:VAL:HG21	1.63	0.63
6:R:16:THR:OG1	6:R:18:TRP:NE1	2.27	0.63
2:J:643:THR:O	5:f:209:THR:OG1	2.15	0.63
2:E:822:ILE:HD12	2:Y:827:LEU:HA	1.80	0.63
2:J:745:GLU:HG3	2:J:768:THR:HG22	1.79	0.63
2:E:32:GLU:OE1	3:G:166:ARG:NH1	2.31	0.63
4:K:818:ILE:HG12	5:N:130:ILE:HG21	1.81	0.63
2:Y:70:ALA:O	2:Y:75:GLN:NE2	2.32	0.63
3:L:157:GLU:HG2	2:E:393:LYS:HE3	1.81	0.63
2:E:695:VAL:HG12	2:E:701:GLN:HA	1.79	0.63
2:E:223:ASP:OD1	2:E:223:ASP:N	2.31	0.63
6:R:207:VAL:HG12	6:R:216:VAL:HG22	1.80	0.63
6:i:126:SER:HB3	6:i:142:LYS:HB3	1.81	0.63
2:E:96:TYR:HD2	2:E:186:PRO:HA	1.64	0.62
6:k:96:LEU:HD21	6:k:141:VAL:HG21	1.81	0.62
2:J:620:ALA:HB2	2:J:703:ASP:HB2	1.80	0.62
6:V:164:MET:HB3	6:V:235:PHE:HD2	1.63	0.62
6:b:207:VAL:HG12	6:b:216:VAL:HG22	1.80	0.62
6:W:63:GLU:CD	6:W:63:GLU:H	2.07	0.62
1:X:38:ASN:O	1:X:38:ASN:ND2	2.32	0.62
6:j:212:MET:O	6:j:212:MET:HE3	1.98	0.62
2:J:96:TYR:HD2	2:J:186:PRO:HA	1.64	0.62
6:a:96:LEU:HD21	6:a:141:VAL:HG21	1.80	0.62
6:c:97:LEU:HG	6:U:153:GLU:HG3	1.81	0.62
6:A:133:ALA:O	6:A:134:LYS:HG2	1.99	0.62
6:c:128:GLY:HA2	6:U:49:GLU:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:748:PHE:HE1	2:E:785:TYR:HB3	1.64	0.62
6:R:42:VAL:N	6:n:61:ASP:OD1	2.26	0.62
6:l:118:ASP:OD1	6:l:152:ALA:N	2.32	0.62
6:n:175:LYS:NZ	6:n:244:THR:O	2.33	0.62
6:V:96:LEU:HD21	6:V:141:VAL:HG21	1.81	0.62
2:E:371:TYR:OH	2:E:473:HIS:NE2	2.23	0.62
2:J:70:ALA:O	2:J:75:GLN:NE2	2.32	0.62
6:c:150:SER:OG	6:c:155:ARG:NH2	2.33	0.62
6:O:96:LEU:HD21	6:O:141:VAL:HG21	1.82	0.62
6:a:197:ALA:HB3	6:a:209:VAL:HG21	1.82	0.62
6:P:198:VAL:HA	6:P:207:VAL:HG21	1.82	0.62
6:T:126:SER:HB3	6:T:142:LYS:HB3	1.82	0.62
3:L:139:GLN:HB2	2:E:391:ALA:HA	1.81	0.62
4:K:820:PRO:HA	5:f:118:THR:HB	1.80	0.62
6:T:197:ALA:HB3	6:T:209:VAL:HG21	1.82	0.62
6:W:16:THR:OG1	6:W:18:TRP:NE1	2.33	0.62
2:Y:744:PHE:O	2:Y:768:THR:HA	2.00	0.62
2:E:396:HIS:HA	2:E:429:ASN:HB2	1.82	0.62
6:j:207:VAL:HG12	6:j:216:VAL:HG22	1.81	0.62
2:J:391:ALA:HA	3:d:139:GLN:HB2	1.82	0.62
2:E:70:ALA:O	2:E:75:GLN:NE2	2.33	0.62
6:k:166:VAL:HG21	6:k:228:VAL:HG21	1.82	0.62
2:J:32:GLU:OE1	3:L:166:ARG:NH1	2.33	0.61
3:G:175:TRP:O	3:G:207:LYS:NZ	2.31	0.61
2:J:820:GLY:H	2:E:826:HIS:HA	1.64	0.61
5:I:169:ASN:HB3	5:f:182:MET:HA	1.80	0.61
6:v:198:VAL:HA	6:v:207:VAL:HG21	1.81	0.61
6:B:167:THR:HB	6:B:182:THR:HG22	1.81	0.61
2:J:215:THR:HB	5:I:189:LEU:HD11	1.83	0.61
6:A:150:SER:O	6:A:155:ARG:NH2	2.34	0.61
2:E:539:THR:OG1	2:E:540:ASP:OD1	2.18	0.61
6:T:118:ASP:OD1	6:T:152:ALA:N	2.33	0.61
6:U:43:LYS:H	6:U:84:LEU:HA	1.65	0.61
1:X:9:LYS:HA	6:h:59:TYR:HA	1.82	0.61
6:V:58:SER:HB2	1:X:95:MET:HE3	1.82	0.61
2:E:766:LEU:HD23	2:E:772:TRP:CD1	2.35	0.61
6:g:96:LEU:HD21	6:g:141:VAL:HG21	1.82	0.61
6:S:150:SER:OG	6:S:155:ARG:NH1	2.31	0.61
6:U:175:LYS:NZ	6:U:244:THR:O	2.34	0.61
6:l:197:ALA:HB3	6:l:209:VAL:HG21	1.82	0.61
2:J:361:GLN:OE1	2:J:363:ARG:NH1	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:o:202:LYS:HZ3	6:o:207:VAL:H	1.47	0.61
2:J:389:PHE:O	3:d:139:GLN:NE2	2.34	0.61
3:L:120:ASN:OD1	3:L:120:ASN:N	2.34	0.61
6:l:66:ASP:OD1	6:l:66:ASP:N	2.26	0.61
6:o:63:GLU:CD	6:o:63:GLU:H	2.09	0.61
5:I:118:THR:HB	4:e:820:PRO:HA	1.82	0.61
6:a:118:ASP:OD1	6:a:152:ALA:N	2.34	0.61
6:h:198:VAL:HA	6:h:207:VAL:HG21	1.82	0.61
6:v:204:LYS:HA	6:v:220:ALA:HB3	1.82	0.61
3:G:139:GLN:HB2	2:Y:391:ALA:HA	1.82	0.61
6:U:117:VAL:O	6:U:155:ARG:NH1	2.34	0.61
6:g:47:PRO:HA	6:g:80:THR:HG23	1.83	0.61
6:Q:207:VAL:HG11	6:Q:226:ILE:HD13	1.82	0.60
6:R:221:ALA:HA	6:R:243:VAL:HB	1.83	0.60
6:k:199:SER:OG	6:k:201:ASP:OD1	2.19	0.60
6:o:16:THR:OG1	6:o:18:TRP:NE1	2.34	0.60
6:C:175:LYS:NZ	6:C:244:THR:O	2.34	0.60
6:c:16:THR:HG23	6:c:111:ARG:HB2	1.83	0.60
6:v:164:MET:HE2	6:v:166:VAL:HG23	1.82	0.60
6:A:164:MET:SD	6:A:230:SER:OG	2.54	0.60
6:c:16:THR:OG1	6:c:18:TRP:NE1	2.34	0.60
3:G:48:PRO:HB3	3:G:58:PRO:HD3	1.83	0.60
3:d:120:ASN:N	3:d:120:ASN:OD1	2.34	0.60
6:g:175:LYS:NZ	6:g:244:THR:O	2.34	0.60
6:A:126:SER:HB3	6:A:142:LYS:HB3	1.81	0.60
2:E:744:PHE:O	2:E:768:THR:HA	2.02	0.60
6:T:50:LEU:HD11	6:T:151:MET:HE3	1.83	0.60
6:b:109:LYS:HB2	6:b:119:VAL:HG12	1.83	0.60
1:D:9:LYS:HD2	1:D:49:SER:HB3	1.84	0.60
2:E:215:THR:HB	5:N:189:LEU:HD11	1.82	0.60
6:A:76:SER:O	6:A:76:SER:OG	2.16	0.60
1:D:9:LYS:HA	6:P:59:TYR:HA	1.83	0.60
6:Q:164:MET:HE1	6:Q:183:VAL:HG13	1.84	0.60
6:R:109:LYS:HB2	6:R:119:VAL:HG12	1.83	0.60
6:S:51:THR:HG22	6:S:52:ALA:H	1.67	0.60
6:S:117:VAL:O	6:S:155:ARG:NH2	2.32	0.60
6:i:178:SER:HB3	6:i:217:ASN:HB3	1.84	0.60
6:j:31:LEU:O	6:j:111:ARG:NH1	2.35	0.60
6:k:76:SER:O	6:k:76:SER:OG	2.16	0.60
2:J:6:SER:HB2	2:J:68:PHE:HB3	1.84	0.60
6:W:212:MET:HE2	6:W:212:MET:HA	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:695:VAL:HG12	2:Y:701:GLN:HA	1.82	0.60
6:n:117:VAL:O	6:n:155:ARG:NH1	2.35	0.60
6:b:79:ASP:OD2	6:b:142:LYS:NZ	2.34	0.60
6:c:195:PHE:HA	6:c:230:SER:HA	1.84	0.60
6:S:195:PHE:HA	6:S:230:SER:HA	1.82	0.60
6:k:135:GLU:OE1	6:k:135:GLU:N	2.35	0.60
6:l:33:ASP:OD1	6:l:111:ARG:NH1	2.34	0.60
3:G:99:VAL:O	2:Y:425:ARG:NH2	2.28	0.59
2:Y:766:LEU:HD23	2:Y:772:TRP:CD1	2.37	0.59
2:J:744:PHE:O	2:J:768:THR:HA	2.02	0.59
1:M:88:LYS:O	1:m:16:SER:OG	2.19	0.59
4:H:820:PRO:HA	5:N:118:THR:HB	1.83	0.59
6:R:165:THR:HB	6:R:184:ALA:HB3	1.84	0.59
6:k:126:SER:HB3	6:k:142:LYS:HB3	1.82	0.59
1:M:59:GLU:OE1	1:m:77:TYR:OH	2.16	0.59
6:c:63:GLU:H	6:c:63:GLU:CD	2.11	0.59
6:R:96:LEU:HD21	6:R:141:VAL:HG21	1.83	0.59
6:o:88:PRO:O	6:o:94:GLN:NE2	2.35	0.59
2:J:371:TYR:OH	2:J:473:HIS:NE2	2.23	0.59
6:Q:117:VAL:O	6:Q:155:ARG:NH2	2.35	0.59
6:Q:178:SER:HB3	6:Q:217:ASN:HB3	1.85	0.59
6:W:195:PHE:HA	6:W:230:SER:HA	1.85	0.59
6:b:165:THR:HB	6:b:184:ALA:HB3	1.85	0.59
6:Q:159:THR:HG23	6:Q:161:ALA:H	1.66	0.59
6:R:212:MET:O	6:R:212:MET:HE3	2.02	0.59
6:S:135:GLU:N	6:S:135:GLU:OE2	2.35	0.59
1:X:88:LYS:O	1:Z:16:SER:OG	2.21	0.59
2:Y:32:GLU:OE1	3:d:166:ARG:NH1	2.35	0.59
6:i:159:THR:HG23	6:i:161:ALA:H	1.68	0.59
2:J:249:TYR:O	2:J:265:LYS:NZ	2.35	0.59
2:J:341:ASP:HA	5:I:159:ALA:HB2	1.84	0.59
6:j:96:LEU:HD21	6:j:141:VAL:HG21	1.83	0.59
6:b:221:ALA:HA	6:b:243:VAL:HB	1.83	0.59
6:A:51:THR:HG22	6:A:52:ALA:H	1.68	0.59
6:A:210:SER:O	6:A:213:THR:OG1	2.20	0.59
6:k:51:THR:HG22	6:k:52:ALA:H	1.67	0.59
6:B:159:THR:HG23	6:B:161:ALA:H	1.68	0.59
2:E:341:ASP:HA	5:N:159:ALA:HB2	1.85	0.59
3:G:139:GLN:NE2	2:Y:389:PHE:O	2.35	0.59
6:n:43:LYS:H	6:n:84:LEU:HA	1.67	0.59
6:v:38:ARG:NH2	6:S:61:ASP:OD2	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:o:195:PHE:HA	6:o:230:SER:HA	1.85	0.58
4:H:818:ILE:HG12	5:I:130:ILE:HG21	1.84	0.58
6:a:50:LEU:HD11	6:a:151:MET:HE3	1.85	0.58
5:f:111:ALA:HB1	5:f:118:THR:HG23	1.85	0.58
3:L:232:GLN:HA	2:E:411:GLU:HG2	1.85	0.58
5:I:105:ILE:HG22	5:I:123:LEU:HD22	1.84	0.58
6:A:195:PHE:HA	6:A:230:SER:HA	1.83	0.58
2:Y:169:MET:N	2:Y:169:MET:SD	2.76	0.58
6:b:118:ASP:OD1	6:b:152:ALA:N	2.35	0.58
2:E:822:ILE:HA	2:E:826:HIS:CD2	2.38	0.58
6:P:96:LEU:HD11	6:P:141:VAL:HG11	1.84	0.58
6:Q:206:THR:OG1	6:Q:217:ASN:OD1	2.16	0.58
1:m:41:LEU:O	1:m:106:GLN:HB3	2.04	0.58
6:C:165:THR:HG22	6:C:184:ALA:HB3	1.84	0.58
5:f:105:ILE:HG22	5:f:123:LEU:HD22	1.85	0.58
6:i:76:SER:O	6:i:76:SER:OG	2.20	0.58
6:l:197:ALA:HB2	6:l:228:VAL:HG13	1.86	0.58
2:J:682:GLN:OE1	2:E:679:ARG:NH1	2.36	0.58
6:C:43:LYS:H	6:C:84:LEU:HA	1.69	0.58
6:n:108:TYR:OH	6:n:145:ASN:ND2	2.36	0.58
2:J:141:ILE:HG23	2:J:143:ARG:HB2	1.85	0.58
6:c:181:LEU:HB2	6:c:214:ILE:HB	1.86	0.58
6:U:16:THR:HB	6:U:38:ARG:HE	1.68	0.58
6:i:117:VAL:O	6:i:155:ARG:NH2	2.37	0.58
6:O:175:LYS:NZ	6:O:244:THR:O	2.37	0.58
6:j:221:ALA:HA	6:j:243:VAL:HB	1.85	0.58
5:N:105:ILE:HG22	5:N:123:LEU:HD22	1.86	0.58
6:R:175:LYS:NZ	6:R:244:THR:O	2.37	0.58
6:W:16:THR:HG23	6:W:111:ARG:HB2	1.86	0.58
6:j:165:THR:HB	6:j:184:ALA:HB3	1.85	0.58
3:L:52:GLN:NE2	3:L:130:GLU:OE1	2.37	0.57
6:v:16:THR:OG1	6:v:18:TRP:NE1	2.37	0.57
6:C:117:VAL:O	6:C:155:ARG:NH1	2.37	0.57
6:R:31:LEU:O	6:R:111:ARG:NH1	2.36	0.57
1:Z:65:HIS:CE1	1:Z:71:PHE:HB3	2.39	0.57
6:j:175:LYS:NZ	6:j:244:THR:O	2.37	0.57
6:k:47:PRO:HA	6:k:80:THR:HG23	1.85	0.57
6:v:164:MET:HG2	6:v:235:PHE:HB3	1.86	0.57
6:C:131:VAL:HG22	6:C:137:ILE:HD12	1.85	0.57
1:F:65:HIS:CE1	1:F:71:PHE:HB3	2.40	0.57
6:V:175:LYS:NZ	6:V:244:THR:O	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Q:175:LYS:NZ	6:Q:244:THR:O	2.36	0.57
6:T:96:LEU:HD21	6:T:141:VAL:HG21	1.86	0.57
6:U:150:SER:HG	6:U:155:ARG:HH21	1.51	0.57
6:a:197:ALA:HB2	6:a:228:VAL:HG13	1.85	0.57
2:E:361:GLN:OE1	2:E:363:ARG:NH1	2.37	0.57
6:R:118:ASP:OD1	6:R:152:ALA:N	2.36	0.57
2:Y:249:TYR:O	2:Y:265:LYS:NZ	2.37	0.57
6:o:150:SER:OG	6:o:155:ARG:NH2	2.34	0.57
3:L:48:PRO:HB3	3:L:57:GLN:HA	1.87	0.57
6:b:31:LEU:O	6:b:111:ARG:NH1	2.37	0.57
6:S:166:VAL:HG22	6:S:183:VAL:HG13	1.85	0.57
6:i:204:LYS:HD2	6:i:222:GLY:HA3	1.86	0.57
2:J:636:GLN:HG2	2:J:681:THR:HG22	1.85	0.57
6:B:10:VAL:HG11	6:B:114:ASN:HB3	1.85	0.57
6:B:51:THR:HG22	6:B:52:ALA:H	1.69	0.57
6:W:150:SER:OG	6:W:155:ARG:NH2	2.35	0.57
2:E:333:ARG:NH2	2:E:341:ASP:OD2	2.37	0.57
3:G:52:GLN:NE2	3:G:127:PRO:O	2.28	0.57
1:m:65:HIS:CE1	1:m:71:PHE:HB3	2.40	0.57
6:S:210:SER:O	6:S:213:THR:OG1	2.21	0.57
2:Y:6:SER:HB2	2:Y:68:PHE:HB3	1.86	0.57
6:k:175:LYS:NZ	6:k:244:THR:O	2.37	0.57
6:o:16:THR:HG23	6:o:111:ARG:HB2	1.85	0.57
2:E:636:GLN:HG2	2:E:681:THR:HG22	1.86	0.57
2:E:822:ILE:HA	2:E:826:HIS:HD2	1.69	0.57
6:n:131:VAL:HG22	6:n:137:ILE:HD12	1.86	0.57
5:I:181:ASN:OD1	5:I:200:SER:OG	2.22	0.56
6:B:108:TYR:OH	6:B:145:ASN:OD1	2.22	0.56
6:B:127:ILE:HD13	6:B:141:VAL:HG22	1.87	0.56
6:A:175:LYS:NZ	6:A:244:THR:O	2.37	0.56
2:E:351:VAL:HG11	2:E:475:PRO:HG2	1.87	0.56
6:Q:51:THR:HG22	6:Q:52:ALA:H	1.70	0.56
6:R:173:VAL:HG23	6:R:243:VAL:HG13	1.87	0.56
6:S:175:LYS:NZ	6:S:244:THR:O	2.38	0.56
2:Y:636:GLN:HG2	2:Y:681:THR:HG22	1.86	0.56
3:d:48:PRO:HB3	3:d:58:PRO:HD3	1.86	0.56
5:f:104:GLN:O	5:f:106:VAL:N	2.38	0.56
6:o:10:VAL:HG22	6:o:12:GLY:H	1.70	0.56
2:J:130:ARG:HG3	2:J:158:LYS:HD3	1.86	0.56
6:O:47:PRO:HA	6:O:80:THR:HG23	1.87	0.56
6:Q:126:SER:HB3	6:Q:142:LYS:HB3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:124:VAL:O	6:i:72:GLN:NE2	2.37	0.56
6:T:197:ALA:HB2	6:T:228:VAL:HG13	1.87	0.56
6:k:150:SER:O	6:k:155:ARG:NH2	2.38	0.56
6:n:5:ASN:HD21	6:n:8:MET:HB2	1.70	0.56
2:J:26:VAL:O	2:J:219:GLY:HA2	2.06	0.56
3:L:91:MET:HE3	3:L:98:LEU:HD21	1.87	0.56
6:V:126:SER:HB3	6:V:142:LYS:HB3	1.87	0.56
6:b:175:LYS:NZ	6:b:244:THR:O	2.38	0.56
4:K:826:VAL:HG12	4:e:829:MET:HG2	1.87	0.56
6:R:83:THR:HG22	6:R:140:THR:HG23	1.86	0.56
6:j:118:ASP:OD1	6:j:152:ALA:N	2.38	0.56
6:n:159:THR:OG1	6:n:192:ASP:OD2	2.23	0.56
6:o:175:LYS:NZ	6:o:244:THR:O	2.38	0.56
6:A:166:VAL:HG22	6:A:183:VAL:HG13	1.86	0.56
6:Q:132:THR:OG1	6:Q:135:GLU:OE1	2.21	0.56
2:Y:127:LYS:NZ	2:Y:745:GLU:OE2	2.37	0.56
6:o:7:THR:HG23	6:o:8:MET:SD	2.45	0.56
6:v:166:VAL:HG22	6:v:183:VAL:HG22	1.88	0.56
6:O:16:THR:OG1	6:O:18:TRP:NE1	2.30	0.56
6:P:221:ALA:HA	6:P:243:VAL:HB	1.87	0.56
6:W:10:VAL:HG22	6:W:12:GLY:H	1.71	0.56
2:Y:140:GLN:HG2	2:Y:149:THR:HA	1.86	0.56
6:j:16:THR:HG1	6:j:18:TRP:HE1	1.53	0.56
2:J:99:PRO:HB2	2:J:180:ARG:HH11	1.69	0.56
2:E:682:GLN:OE1	2:Y:679:ARG:NH1	2.37	0.56
6:g:16:THR:OG1	6:g:18:TRP:NE1	2.30	0.56
6:i:207:VAL:HG12	6:i:216:VAL:HG22	1.88	0.56
6:V:47:PRO:HA	6:V:80:THR:HG23	1.87	0.56
2:E:503:ARG:HB2	2:E:549:VAL:HG23	1.88	0.56
1:F:9:LYS:HD3	1:F:10:PRO:HD2	1.88	0.56
1:Z:41:LEU:HB3	1:Z:106:GLN:HG2	1.87	0.56
6:v:221:ALA:HA	6:v:243:VAL:HB	1.87	0.56
6:B:117:VAL:O	6:B:155:ARG:NH2	2.39	0.56
6:c:10:VAL:HG22	6:c:12:GLY:H	1.70	0.56
6:c:66:ASP:OD1	6:c:66:ASP:N	2.25	0.56
6:T:128:GLY:O	6:T:139:ARG:NH1	2.35	0.56
6:h:118:ASP:OD1	6:h:152:ALA:N	2.39	0.56
6:j:83:THR:HG22	6:j:140:THR:HG23	1.87	0.56
1:M:1:MET:HE1	1:M:5:ARG:HH21	1.71	0.56
6:A:47:PRO:HA	6:A:80:THR:HG23	1.88	0.56
2:E:26:VAL:O	2:E:219:GLY:HA2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:239:ARG:NH1	5:N:195:GLU:OE2	2.39	0.56
6:T:63:GLU:CD	6:T:63:GLU:H	2.14	0.56
2:Y:341:ASP:HA	5:f:159:ALA:HB2	1.87	0.56
6:g:44:ASP:HB3	6:g:83:THR:HG23	1.87	0.56
5:I:104:GLN:O	5:I:106:VAL:N	2.39	0.56
2:E:244:GLN:HG3	2:E:264:PHE:HB3	1.88	0.56
6:h:165:THR:HB	6:h:184:ALA:HB3	1.88	0.56
2:J:239:ARG:NH1	5:I:195:GLU:OE2	2.39	0.55
6:v:131:VAL:HG22	6:v:137:ILE:HD13	1.88	0.55
6:a:209:VAL:HG22	6:a:214:ILE:HG12	1.87	0.55
2:E:31:SER:OG	2:E:32:GLU:N	2.38	0.55
2:E:99:PRO:HB2	2:E:180:ARG:HH11	1.70	0.55
2:E:366:ASP:OD1	2:E:366:ASP:N	2.36	0.55
6:S:129:LYS:NZ	6:T:118:ASP:OD2	2.39	0.55
6:W:7:THR:HG23	6:W:8:MET:SD	2.45	0.55
2:Y:666:ARG:HG2	5:f:223:ARG:NH2	2.22	0.55
2:E:86:SER:OG	2:E:204:GLU:OE1	2.23	0.55
5:N:111:ALA:HB1	5:N:118:THR:HG23	1.87	0.55
6:n:51:THR:HG22	6:n:52:ALA:H	1.71	0.55
2:J:161:SER:OG	2:E:627:GLU:OE1	2.24	0.55
1:m:9:LYS:HD3	1:m:10:PRO:HD2	1.88	0.55
2:E:823:THR:HB	2:Y:828:GLY:HA3	1.88	0.55
3:G:43:ASN:ND2	3:G:47:GLU:O	2.39	0.55
2:Y:121:LEU:O	2:Y:133:SER:OG	2.22	0.55
6:c:175:LYS:NZ	6:c:244:THR:O	2.39	0.55
2:E:127:LYS:NZ	2:E:745:GLU:OE2	2.37	0.55
2:E:574:VAL:HG21	5:N:154:MET:HE3	1.88	0.55
6:W:66:ASP:OD1	6:W:66:ASP:N	2.24	0.55
1:M:29:TYR:HD1	1:Z:109:ASN:ND2	2.04	0.55
2:J:49:SER:HB3	2:J:700:GLN:HG3	1.87	0.55
2:Y:26:VAL:O	2:Y:219:GLY:HA2	2.07	0.55
3:d:11:GLU:OE1	3:d:14:ARG:NH1	2.39	0.55
6:k:126:SER:OG	6:l:49:GLU:OE2	2.23	0.55
6:l:96:LEU:HD21	6:l:141:VAL:HG21	1.88	0.55
2:J:326:ASN:HB3	5:I:196:MET:HG2	1.89	0.55
2:J:828:GLY:HA3	2:Y:823:THR:HB	1.88	0.55
2:E:664:SER:OG	5:N:223:ARG:NH2	2.39	0.55
6:S:197:ALA:HB2	6:S:228:VAL:HG12	1.88	0.55
6:U:150:SER:OG	6:U:155:ARG:NH2	2.33	0.55
2:Y:109:ILE:HG13	2:Y:204:GLU:HB3	1.89	0.55
6:B:207:VAL:HG12	6:B:216:VAL:HG22	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:W:181:LEU:HB2	6:W:214:ILE:HB	1.89	0.55
2:Y:355:GLN:O	3:d:134:ARG:NH1	2.39	0.55
3:d:52:GLN:NE2	3:d:130:GLU:OE1	2.38	0.55
6:g:164:MET:HB3	6:g:235:PHE:HD2	1.71	0.55
6:n:45:LEU:HD21	6:n:110:ILE:HD13	1.89	0.55
6:C:159:THR:OG1	6:C:192:ASP:OD2	2.24	0.55
6:C:229:VAL:HG13	6:C:233:GLY:HA2	1.88	0.55
6:k:210:SER:O	6:k:213:THR:OG1	2.24	0.55
4:H:829:MET:HG2	4:e:826:VAL:HG12	1.88	0.55
6:v:96:LEU:HD11	6:v:141:VAL:HG11	1.87	0.55
6:b:96:LEU:HD21	6:b:141:VAL:HG21	1.87	0.55
1:F:41:LEU:O	1:F:106:GLN:HG2	2.07	0.55
6:S:76:SER:O	6:S:76:SER:OG	2.16	0.55
2:Y:210:GLN:NE2	3:d:223:GLY:O	2.34	0.55
6:j:173:VAL:HG23	6:j:243:VAL:HG13	1.88	0.55
6:n:163:GLY:HA3	6:n:187:PRO:HB3	1.89	0.55
2:J:409:GLY:O	2:J:411:GLU:N	2.38	0.55
6:c:7:THR:HG23	6:c:8:MET:SD	2.46	0.55
2:E:820:GLY:HA2	2:Y:827:LEU:O	2.07	0.55
3:G:52:GLN:NE2	3:G:130:GLU:OE1	2.40	0.55
5:f:183:VAL:O	5:f:187:ASN:ND2	2.40	0.55
2:J:140:GLN:HG2	2:J:149:THR:HA	1.90	0.54
2:Y:351:VAL:HG11	2:Y:475:PRO:HG2	1.89	0.54
2:Y:361:GLN:OE1	2:Y:363:ARG:NH1	2.40	0.54
3:L:43:ASN:ND2	3:L:47:GLU:O	2.39	0.54
2:E:116:PHE:HE2	2:E:167:VAL:HG13	1.73	0.54
2:E:759:VAL:O	2:E:763:THR:OG1	2.25	0.54
6:S:126:SER:OG	6:T:49:GLU:OE2	2.24	0.54
6:W:91:GLN:HA	6:W:91:GLN:NE2	2.22	0.54
2:Y:142:GLN:NE2	2:Y:144:ASN:O	2.41	0.54
2:Y:332:GLN:HB2	5:f:188:VAL:HG11	1.89	0.54
2:Y:395:ARG:O	2:Y:429:ASN:ND2	2.35	0.54
1:Z:9:LYS:HB2	1:Z:47:THR:HG23	1.90	0.54
6:o:87:MET:HB3	6:o:90:GLU:HG3	1.89	0.54
6:A:129:LYS:NZ	6:a:118:ASP:OD2	2.41	0.54
6:P:148:ARG:HG2	6:g:67:TRP:CD1	2.42	0.54
6:U:193:LYS:HE2	6:U:231:GLY:HA3	1.88	0.54
6:A:96:LEU:HD21	6:A:141:VAL:HG21	1.89	0.54
2:E:130:ARG:HG3	2:E:158:LYS:HD3	1.87	0.54
6:R:166:VAL:HG22	6:R:183:VAL:HG22	1.90	0.54
6:S:139:ARG:HH11	6:S:139:ARG:HG3	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:g:102:GLU:HG2	6:g:104:ASP:H	1.72	0.54
6:i:201:ASP:OD2	6:i:203:THR:OG1	2.21	0.54
6:b:5:ASN:HD21	6:b:8:MET:HB2	1.72	0.54
6:Q:173:VAL:HB	6:Q:243:VAL:HG22	1.89	0.54
6:U:102:GLU:N	6:U:102:GLU:OE2	2.41	0.54
6:U:114:ASN:OD1	6:U:116:THR:OG1	2.26	0.54
6:o:179:THR:HG22	6:o:216:VAL:HB	1.90	0.54
6:o:181:LEU:HB2	6:o:214:ILE:HB	1.89	0.54
6:B:36:TRP:CG	6:B:109:LYS:HZ3	2.26	0.54
6:C:204:LYS:HA	6:C:220:ALA:HB3	1.90	0.54
6:O:33:ASP:OD1	6:O:109:LYS:NZ	2.30	0.54
6:W:10:VAL:HG21	6:W:113:PRO:HG2	1.89	0.54
2:Y:244:GLN:HG3	2:Y:264:PHE:HB3	1.90	0.54
6:i:18:TRP:HB2	6:i:109:LYS:HG2	1.89	0.54
6:o:117:VAL:O	6:o:155:ARG:NH1	2.40	0.54
2:J:351:VAL:HG11	2:J:475:PRO:HG2	1.90	0.54
6:v:229:VAL:HG13	6:v:236:ALA:HB2	1.90	0.54
6:b:173:VAL:HG23	6:b:243:VAL:HG13	1.87	0.54
6:C:49:GLU:HG3	6:C:50:LEU:N	2.23	0.54
6:c:109:LYS:HD2	6:c:117:VAL:HG21	1.89	0.54
6:P:118:ASP:OD1	6:P:152:ALA:N	2.40	0.54
6:T:159:THR:O	6:T:193:LYS:NZ	2.40	0.54
6:l:199:SER:HA	6:l:226:ILE:HA	1.90	0.54
2:J:107:ALA:O	2:J:175:ARG:NH2	2.41	0.54
6:B:175:LYS:NZ	6:B:244:THR:O	2.40	0.54
2:E:49:SER:HB3	2:E:700:GLN:HG3	1.89	0.54
5:I:111:ALA:HB1	5:I:118:THR:HG23	1.89	0.54
2:E:1:MET:HE3	2:E:6:SER:HB3	1.89	0.54
1:X:9:LYS:HD2	1:X:49:SER:HB3	1.89	0.54
6:n:204:LYS:HA	6:n:220:ALA:HB3	1.89	0.54
6:P:204:LYS:HA	6:P:220:ALA:HB3	1.89	0.54
6:Q:108:TYR:OH	6:Q:145:ASN:OD1	2.26	0.54
6:U:204:LYS:HA	6:U:220:ALA:HB3	1.90	0.54
2:Y:23:LEU:HB2	5:f:210:ALA:HB2	1.89	0.54
2:Y:233:SER:O	2:Y:233:SER:OG	2.26	0.54
6:b:17:LEU:HD12	6:b:110:ILE:HG23	1.90	0.53
2:E:139:VAL:HB	2:E:181:MET:HG3	1.90	0.53
6:i:194:SER:O	6:i:231:GLY:N	2.41	0.53
6:c:202:LYS:HZ3	6:c:207:VAL:H	1.55	0.53
2:E:6:SER:HB2	2:E:68:PHE:HB3	1.89	0.53
2:E:104:ILE:HD12	2:E:106:SER:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:181:ASN:OD1	5:N:200:SER:OG	2.25	0.53
6:W:179:THR:HG22	6:W:216:VAL:HB	1.90	0.53
2:J:109:ILE:HG13	2:J:204:GLU:HB3	1.89	0.53
6:T:20:TYR:OH	6:T:24:GLY:N	2.42	0.53
3:d:48:PRO:HB3	3:d:57:GLN:HA	1.90	0.53
6:g:109:LYS:HD2	6:g:117:VAL:HG21	1.90	0.53
6:i:173:VAL:HB	6:i:243:VAL:HG22	1.89	0.53
2:J:503:ARG:HB2	2:J:549:VAL:HG23	1.90	0.53
6:V:108:TYR:OH	6:V:145:ASN:OD1	2.22	0.53
6:v:118:ASP:OD1	6:v:152:ALA:N	2.41	0.53
6:b:42:VAL:HG12	6:b:84:LEU:HD23	1.90	0.53
1:F:52:ARG:NH1	1:F:95:MET:O	2.41	0.53
6:Q:76:SER:O	6:Q:76:SER:OG	2.20	0.53
6:n:118:ASP:OD1	6:n:152:ALA:N	2.42	0.53
2:J:169:MET:N	2:J:169:MET:SD	2.81	0.53
2:J:845:LEU:HD13	2:E:845:LEU:HD13	1.90	0.53
2:J:845:LEU:HD13	2:Y:845:LEU:HD13	1.90	0.53
6:V:33:ASP:OD1	6:V:109:LYS:NZ	2.37	0.53
6:a:33:ASP:OD1	6:a:111:ARG:NH1	2.41	0.53
6:c:117:VAL:O	6:c:155:ARG:NH1	2.42	0.53
6:c:179:THR:HG22	6:c:216:VAL:HB	1.89	0.53
6:U:159:THR:OG1	6:U:192:ASP:OD2	2.26	0.53
1:M:24:ARG:NH2	1:M:26:GLY:O	2.39	0.53
2:J:121:LEU:HD11	2:J:135:VAL:HG23	1.91	0.53
6:B:76:SER:OG	6:B:76:SER:O	2.20	0.53
6:B:198:VAL:HG13	6:B:227:PRO:HG2	1.89	0.53
6:C:114:ASN:OD1	6:C:116:THR:OG1	2.26	0.53
2:E:121:LEU:HD11	2:E:135:VAL:HG23	1.91	0.53
2:Y:49:SER:HB3	2:Y:700:GLN:HG3	1.91	0.53
2:J:410:TRP:CZ3	5:I:196:MET:HA	2.44	0.53
6:B:193:LYS:NZ	6:B:232:ASN:OD1	2.42	0.53
2:E:109:ILE:HG13	2:E:204:GLU:HB3	1.91	0.53
6:Q:164:MET:HG2	6:Q:235:PHE:HB3	1.89	0.53
6:Q:164:MET:HB2	6:Q:235:PHE:HD2	1.73	0.53
2:Y:99:PRO:HB2	2:Y:180:ARG:HH11	1.74	0.53
6:l:43:LYS:HB2	6:l:83:THR:HG23	1.90	0.53
6:l:199:SER:OG	6:l:200:ALA:N	2.42	0.53
6:n:164:MET:HE2	6:n:164:MET:HA	1.91	0.53
6:c:127:ILE:HG22	6:c:141:VAL:HA	1.91	0.53
2:E:121:LEU:O	2:E:133:SER:OG	2.24	0.53
5:N:187:ASN:O	5:N:188:VAL:HG22	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:130:ARG:H	2:Y:130:ARG:HD2	1.74	0.53
6:o:10:VAL:HG21	6:o:113:PRO:HG2	1.90	0.53
6:C:61:ASP:OD1	6:j:42:VAL:N	2.30	0.53
2:E:845:LEU:HD13	2:Y:845:LEU:HD13	1.90	0.53
6:T:33:ASP:OD2	6:T:111:ARG:NH1	2.42	0.53
2:Y:503:ARG:HB2	2:Y:549:VAL:HG23	1.89	0.53
5:f:189:LEU:HG	5:f:190:PRO:HD3	1.90	0.53
6:B:205:ALA:HA	6:B:217:ASN:O	2.08	0.53
6:A:197:ALA:HB2	6:A:228:VAL:HG12	1.91	0.53
6:a:181:LEU:HB2	6:a:214:ILE:HB	1.91	0.53
6:c:43:LYS:HE2	6:c:43:LYS:HA	1.90	0.53
6:U:118:ASP:OD1	6:U:152:ALA:N	2.42	0.53
6:h:221:ALA:HA	6:h:243:VAL:HB	1.89	0.53
6:j:5:ASN:HD21	6:j:8:MET:HB2	1.74	0.53
2:J:759:VAL:O	2:J:763:THR:OG1	2.23	0.52
6:B:9:PRO:HD3	6:j:87:MET:HE1	1.91	0.52
1:D:11:GLY:HA2	6:P:60:LEU:HD11	1.91	0.52
5:N:189:LEU:CD2	5:N:190:PRO:HD3	2.38	0.52
6:i:175:LYS:NZ	6:i:244:THR:O	2.42	0.52
6:l:108:TYR:OH	6:l:145:ASN:OD1	2.24	0.52
2:J:1:MET:HE3	2:J:6:SER:HB3	1.89	0.52
6:C:48:GLY:H	6:C:80:THR:HA	1.73	0.52
2:E:395:ARG:O	2:E:429:ASN:ND2	2.39	0.52
1:X:27:ASP:OD1	1:X:27:ASP:N	2.42	0.52
6:h:164:MET:HG2	6:h:235:PHE:HB3	1.91	0.52
6:n:36:TRP:CD1	6:n:109:LYS:HZ3	2.28	0.52
6:v:179:THR:HG22	6:v:216:VAL:HB	1.91	0.52
6:B:173:VAL:HB	6:B:243:VAL:HG22	1.91	0.52
6:A:135:GLU:OE1	6:A:135:GLU:N	2.42	0.52
6:a:43:LYS:HB2	6:a:83:THR:HG23	1.92	0.52
6:W:109:LYS:HD2	6:W:117:VAL:HG21	1.91	0.52
2:Y:650:VAL:HA	2:Y:695:VAL:O	2.10	0.52
6:j:81:SER:HB3	6:j:142:LYS:HG3	1.91	0.52
5:N:104:GLN:O	5:N:106:VAL:N	2.43	0.52
2:Y:136:ARG:HG2	2:Y:184:MET:HG3	1.91	0.52
6:o:164:MET:HA	6:o:164:MET:HE2	1.90	0.52
6:b:63:GLU:OE1	6:b:63:GLU:N	2.43	0.52
6:a:20:TYR:OH	6:a:24:GLY:N	2.42	0.52
3:G:11:GLU:OE1	3:G:14:ARG:NH1	2.42	0.52
6:O:44:ASP:HB3	6:O:83:THR:HG23	1.91	0.52
2:Y:759:VAL:O	2:Y:763:THR:OG1	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:16:THR:HB	6:C:38:ARG:HE	1.74	0.52
6:i:10:VAL:HG11	6:i:114:ASN:HB3	1.91	0.52
6:c:41:LYS:HA	6:c:41:LYS:HE2	1.92	0.52
2:E:245:VAL:HG22	2:E:246:PRO:HD2	1.90	0.52
2:E:398:ALA:O	2:E:430:VAL:HA	2.10	0.52
2:E:666:ARG:HG2	5:N:223:ARG:CZ	2.40	0.52
6:U:8:MET:HG3	6:U:9:PRO:HD2	1.91	0.52
2:Y:121:LEU:HD11	2:Y:135:VAL:HG23	1.92	0.52
2:J:272:MET:HG2	2:J:346:MET:SD	2.50	0.52
2:J:395:ARG:O	2:J:429:ASN:ND2	2.39	0.52
5:I:137:GLY:O	5:I:138:ILE:HD12	2.09	0.52
2:E:233:SER:O	2:E:233:SER:OG	2.25	0.52
3:G:232:GLN:HA	2:Y:411:GLU:HG2	1.92	0.52
6:Q:10:VAL:HG11	6:Q:114:ASN:HB3	1.92	0.52
6:Q:165:THR:OG1	6:Q:184:ALA:HB3	2.08	0.52
6:R:42:VAL:HA	6:R:84:LEU:HB3	1.92	0.52
6:W:175:LYS:NZ	6:W:244:THR:O	2.42	0.52
6:g:126:SER:HB3	6:g:142:LYS:HB3	1.91	0.52
6:l:81:SER:HB2	6:l:142:LYS:HG3	1.90	0.52
1:M:11:GLY:HA2	6:v:60:LEU:HD11	1.92	0.52
2:J:776:SER:OG	2:J:778:ASN:OD1	2.27	0.52
3:L:48:PRO:HB3	3:L:58:PRO:HD3	1.92	0.52
3:L:52:GLN:NE2	3:L:127:PRO:O	2.29	0.52
3:L:99:VAL:O	2:E:425:ARG:NH2	2.35	0.52
3:L:139:GLN:NE2	2:E:389:PHE:O	2.40	0.52
6:V:32:SER:HB2	6:V:193:LYS:NZ	2.25	0.52
2:E:271:ASN:HD22	2:E:274:TRP:CD1	2.28	0.52
2:E:409:GLY:O	2:E:411:GLU:N	2.40	0.52
6:T:209:VAL:HG22	6:T:214:ILE:HG12	1.92	0.52
6:h:43:LYS:HB3	6:h:83:THR:HG23	1.92	0.52
2:E:249:TYR:O	2:E:265:LYS:NZ	2.42	0.52
6:R:213:THR:OG1	6:R:214:ILE:N	2.43	0.52
2:Y:245:VAL:HG22	2:Y:246:PRO:HD2	1.91	0.52
2:Y:412:THR:OG1	5:f:172:GLN:O	2.20	0.52
2:Y:757:ARG:NH1	2:Y:757:ARG:HB2	2.25	0.52
4:e:817:GLN:HA	5:f:130:ILE:HD12	1.92	0.52
6:j:213:THR:OG1	6:j:214:ILE:N	2.43	0.52
6:n:114:ASN:OD1	6:n:116:THR:OG1	2.27	0.52
6:b:42:VAL:HA	6:b:84:LEU:HB3	1.92	0.51
6:a:108:TYR:CZ	6:a:120:PHE:HB2	2.46	0.51
1:F:13:ASP:HB2	1:F:45:SER:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:748:PHE:CE1	2:Y:785:TYR:HB3	2.43	0.51
2:J:121:LEU:O	2:J:133:SER:OG	2.23	0.51
6:V:17:LEU:HD11	6:V:45:LEU:HD13	1.92	0.51
6:R:63:GLU:OE1	6:R:63:GLU:N	2.43	0.51
6:i:198:VAL:HG13	6:i:227:PRO:HG2	1.91	0.51
2:J:410:TRP:HB2	5:I:179:LEU:HD11	1.92	0.51
6:V:148:ARG:NH2	6:v:64:ASP:OD1	2.44	0.51
2:E:169:MET:SD	2:E:169:MET:N	2.84	0.51
6:R:16:THR:HG1	6:R:18:TRP:HE1	1.51	0.51
6:T:35:ASP:OD1	6:T:35:ASP:N	2.29	0.51
5:f:189:LEU:HG	5:f:190:PRO:CD	2.40	0.51
6:i:212:MET:HE2	6:i:212:MET:HA	1.92	0.51
6:V:132:THR:HG23	6:V:135:GLU:HB2	1.91	0.51
6:B:8:MET:HA	6:B:8:MET:HE2	1.92	0.51
6:b:213:THR:OG1	6:b:214:ILE:N	2.44	0.51
6:C:118:ASP:OD1	6:C:152:ALA:N	2.43	0.51
2:E:831:LEU:HA	2:E:834:LYS:HE2	1.92	0.51
6:O:126:SER:HB3	6:O:142:LYS:HB3	1.92	0.51
1:X:59:GLU:OE1	1:Z:77:TYR:OH	2.17	0.51
2:Y:107:ALA:O	2:Y:175:ARG:NH2	2.43	0.51
6:h:166:VAL:HG22	6:h:183:VAL:HG22	1.92	0.51
6:k:127:ILE:HG23	6:k:139:ARG:HE	1.76	0.51
2:J:380:ASP:HB2	5:I:121:ALA:HB1	1.91	0.51
6:b:98:ALA:O	6:b:102:GLU:HG2	2.10	0.51
6:C:51:THR:HG22	6:C:52:ALA:H	1.75	0.51
6:C:193:LYS:NZ	6:C:230:SER:O	2.38	0.51
1:D:50:VAL:HG22	1:D:51:PRO:HD2	1.92	0.51
2:E:514:PRO:HG3	2:E:563:LEU:HD22	1.92	0.51
2:E:812:GLU:O	2:E:816:ASP:N	2.44	0.51
6:U:52:ALA:HA	6:U:75:LYS:HA	1.93	0.51
3:d:43:ASN:ND2	3:d:47:GLU:O	2.42	0.51
1:M:95:MET:HE1	6:O:59:TYR:O	2.11	0.51
2:E:410:TRP:CZ3	5:N:196:MET:HA	2.46	0.51
5:N:137:GLY:O	5:N:138:ILE:HD12	2.11	0.51
6:P:229:VAL:HG13	6:P:236:ALA:HB2	1.92	0.51
2:Y:404:ILE:HD12	5:f:176:PHE:CE2	2.45	0.51
5:f:137:GLY:O	5:f:138:ILE:HD12	2.10	0.51
2:J:355:GLN:O	3:L:134:ARG:NH1	2.43	0.51
2:J:405:ASP:OD2	2:J:408:ASN:ND2	2.44	0.51
2:J:679:ARG:NH1	2:Y:682:GLN:OE1	2.40	0.51
4:H:837:GLU:OE1	4:e:835:ARG:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:138:LEU:HD21	2:E:149:THR:HB	1.91	0.51
2:E:495:VAL:O	2:E:556:TYR:N	2.35	0.51
6:T:232:ASN:N	6:T:234:GLU:OE1	2.43	0.51
2:Y:277:TRP:HB2	2:Y:301:LEU:HD13	1.93	0.51
2:J:627:GLU:HG2	2:Y:160:THR:HB	1.93	0.51
2:E:657:THR:OG1	2:E:665:GLU:OE1	2.27	0.51
6:O:132:THR:HG23	6:O:135:GLU:HB2	1.93	0.51
6:P:153:GLU:N	6:P:153:GLU:OE1	2.44	0.51
6:T:199:SER:OG	6:T:200:ALA:N	2.44	0.51
2:Y:409:GLY:O	2:Y:411:GLU:N	2.42	0.51
2:Y:410:TRP:CZ3	5:f:196:MET:HA	2.45	0.51
6:k:129:LYS:NZ	6:l:118:ASP:OD2	2.44	0.51
6:v:165:THR:HB	6:v:184:ALA:HB3	1.93	0.51
6:C:206:THR:O	6:C:217:ASN:ND2	2.44	0.51
6:O:109:LYS:HD2	6:O:117:VAL:HG21	1.93	0.51
2:Y:96:TYR:HD2	2:Y:186:PRO:HA	1.74	0.51
6:l:116:THR:HB	6:l:152:ALA:HB1	1.92	0.51
2:J:149:THR:OG1	5:I:217:GLN:OE1	2.23	0.51
6:C:153:GLU:OE2	6:o:139:ARG:NH2	2.44	0.51
2:E:600:ASP:OD1	2:E:600:ASP:N	2.44	0.51
3:G:37:PHE:HB3	3:G:56:TYR:CD2	2.46	0.51
6:R:183:VAL:HB	6:R:212:MET:HE1	1.92	0.51
6:U:48:GLY:N	6:U:80:THR:OG1	2.40	0.51
6:k:17:LEU:HD11	6:k:45:LEU:HD13	1.92	0.51
6:k:197:ALA:HB2	6:k:228:VAL:HG12	1.91	0.51
6:o:127:ILE:HA	6:o:141:VAL:HA	1.93	0.51
4:H:827:TYR:OH	4:K:836:ASP:OD2	2.30	0.50
6:v:79:ASP:N	6:v:79:ASP:OD1	2.43	0.50
6:A:39:LEU:HD21	6:A:96:LEU:HD13	1.92	0.50
6:a:199:SER:OG	6:a:200:ALA:N	2.44	0.50
2:E:404:ILE:HD12	5:N:176:PHE:CE2	2.47	0.50
6:o:18:TRP:HB2	6:o:109:LYS:HG2	1.93	0.50
6:V:193:LYS:HD3	6:V:194:SER:O	2.12	0.50
6:b:164:MET:HB3	6:b:235:PHE:CD1	2.46	0.50
1:D:59:GLU:OE1	1:F:77:TYR:OH	2.13	0.50
2:E:410:TRP:HB2	5:N:179:LEU:HD11	1.92	0.50
6:U:10:VAL:HG12	6:U:12:GLY:H	1.75	0.50
6:h:61:ASP:OD1	6:h:61:ASP:N	2.44	0.50
2:J:241:ARG:NH1	2:J:285:TYR:OH	2.38	0.50
6:V:102:GLU:OE1	6:V:106:ARG:NH2	2.34	0.50
6:C:119:VAL:HG22	6:C:150:SER:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:c:18:TRP:HB2	6:c:109:LYS:HG2	1.93	0.50
2:E:114:PHE:HD2	2:E:181:MET:HE2	1.76	0.50
6:P:163:GLY:HA3	6:P:187:PRO:HA	1.93	0.50
6:Q:18:TRP:HB2	6:Q:109:LYS:HG2	1.94	0.50
6:T:161:ALA:HB3	6:T:187:PRO:HB2	1.93	0.50
1:X:11:GLY:HA2	6:h:60:LEU:HD11	1.94	0.50
2:Y:748:PHE:HB2	2:Y:766:LEU:HD11	1.92	0.50
6:l:108:TYR:CZ	6:l:120:PHE:HB2	2.46	0.50
3:G:48:PRO:HB3	3:G:57:GLN:HA	1.93	0.50
2:Y:748:PHE:HB2	2:Y:766:LEU:HD21	1.94	0.50
6:h:229:VAL:HG13	6:h:236:ALA:HB2	1.92	0.50
6:o:96:LEU:HD11	6:o:141:VAL:HG21	1.93	0.50
2:E:272:MET:HG2	2:E:346:MET:SD	2.51	0.50
2:E:281:THR:O	2:E:281:THR:OG1	2.26	0.50
6:T:108:TYR:CZ	6:T:120:PHE:HB2	2.46	0.50
6:T:116:THR:HB	6:T:152:ALA:HB1	1.94	0.50
6:U:205:ALA:HA	6:U:217:ASN:O	2.11	0.50
6:U:206:THR:O	6:U:217:ASN:ND2	2.44	0.50
6:h:126:SER:HB3	6:h:142:LYS:HB3	1.92	0.50
6:n:8:MET:HA	6:n:8:MET:HE3	1.92	0.50
6:n:194:SER:OG	6:n:195:PHE:N	2.44	0.50
2:J:722:LEU:HD11	2:J:803:ALA:HB1	1.94	0.50
6:B:204:LYS:HD2	6:B:222:GLY:HA3	1.93	0.50
6:C:45:LEU:HD21	6:C:110:ILE:HD13	1.93	0.50
2:E:355:GLN:O	3:G:134:ARG:NH1	2.43	0.50
5:N:167:THR:HG21	5:f:167:THR:HG21	1.92	0.50
6:P:179:THR:HG22	6:P:216:VAL:HB	1.94	0.50
6:W:117:VAL:O	6:W:155:ARG:NH1	2.44	0.50
6:h:179:THR:HG22	6:h:216:VAL:HB	1.92	0.50
6:i:193:LYS:NZ	6:i:232:ASN:OD1	2.41	0.50
2:J:104:ILE:HD12	2:J:106:SER:H	1.77	0.50
6:c:10:VAL:HG21	6:c:113:PRO:HG2	1.93	0.50
6:O:207:VAL:HG12	6:O:216:VAL:HG22	1.94	0.50
6:Q:193:LYS:NZ	6:Q:232:ASN:OD1	2.43	0.50
6:i:205:ALA:HA	6:i:217:ASN:O	2.11	0.50
5:I:167:THR:HG21	5:f:167:THR:HG21	1.93	0.50
6:a:232:ASN:N	6:a:234:GLU:OE1	2.45	0.50
6:c:101:ASN:OD1	6:U:148:ARG:NH2	2.44	0.50
6:c:111:ARG:HG2	6:c:117:VAL:HB	1.94	0.50
6:P:61:ASP:OD1	6:P:61:ASP:N	2.43	0.50
6:U:45:LEU:HD21	6:U:110:ILE:HD13	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:f:181:ASN:OD1	5:f:200:SER:OG	2.30	0.50
1:M:50:VAL:HG22	1:M:51:PRO:HD2	1.94	0.50
2:J:827:LEU:HD12	2:J:831:LEU:HD12	1.92	0.50
6:P:207:VAL:HG12	6:P:216:VAL:HG22	1.94	0.50
6:W:96:LEU:HD23	6:W:97:LEU:HD22	1.93	0.50
2:J:535:VAL:HA	2:J:546:VAL:HA	1.94	0.49
2:E:114:PHE:O	2:E:166:SER:HA	2.10	0.49
6:S:47:PRO:HA	6:S:80:THR:HG23	1.93	0.49
6:k:108:TYR:OH	6:k:145:ASN:OD1	2.24	0.49
2:J:244:GLN:HG3	2:J:264:PHE:HB3	1.94	0.49
2:E:405:ASP:OD2	2:E:408:ASN:ND2	2.45	0.49
6:P:43:LYS:HB3	6:P:83:THR:HG23	1.94	0.49
2:J:684:ALA:O	2:J:688:TYR:OH	2.30	0.49
2:J:741:THR:O	2:J:741:THR:OG1	2.28	0.49
6:b:83:THR:HG22	6:b:140:THR:HG23	1.92	0.49
6:C:21:LYS:HD2	6:C:35:ASP:HA	1.94	0.49
6:O:198:VAL:HG13	6:O:227:PRO:HG2	1.94	0.49
6:Q:164:MET:HE1	6:Q:183:VAL:CG1	2.41	0.49
6:Q:204:LYS:HD2	6:Q:222:GLY:HA3	1.92	0.49
6:T:164:MET:HA	6:T:164:MET:HE2	1.93	0.49
2:Y:54:ASP:OD1	2:Y:55:THR:N	2.44	0.49
2:Y:621:VAL:HG23	2:Y:694:ALA:HB2	1.94	0.49
6:h:207:VAL:HG12	6:h:216:VAL:HG22	1.94	0.49
6:n:150:SER:OG	6:n:155:ARG:NH2	2.38	0.49
6:o:96:LEU:HD23	6:o:97:LEU:HD22	1.94	0.49
6:V:109:LYS:HD2	6:V:117:VAL:HG21	1.94	0.49
2:E:23:LEU:HB2	5:N:210:ALA:HB2	1.93	0.49
1:X:87:ALA:O	1:Z:18:PRO:HD2	2.13	0.49
6:l:232:ASN:N	6:l:234:GLU:OE1	2.45	0.49
1:M:6:TRP:NE1	1:M:54:GLU:OE1	2.33	0.49
6:V:32:SER:HB2	6:V:193:LYS:HZ3	1.77	0.49
6:V:198:VAL:HG13	6:V:227:PRO:HG2	1.93	0.49
6:v:148:ARG:HB3	6:O:67:TRP:CD1	2.47	0.49
2:E:160:THR:HB	2:Y:627:GLU:HG2	1.93	0.49
6:T:181:LEU:HB2	6:T:214:ILE:HB	1.94	0.49
1:X:50:VAL:HG22	1:X:51:PRO:HD2	1.95	0.49
3:d:105:ARG:HG2	3:d:133:SER:HB2	1.93	0.49
6:l:161:ALA:HB3	6:l:187:PRO:HB2	1.94	0.49
6:n:48:GLY:H	6:n:80:THR:HG1	1.57	0.49
2:J:411:GLU:HG2	3:d:232:GLN:HA	1.93	0.49
1:m:5:ARG:HH11	1:m:5:ARG:HG3	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:830:ALA:HB1	4:K:830:ALA:HA	1.93	0.49
6:V:44:ASP:HB3	6:V:83:THR:HG23	1.94	0.49
6:B:50:LEU:HD23	6:j:127:ILE:HG22	1.94	0.49
6:A:108:TYR:OH	6:A:145:ASN:OD1	2.23	0.49
6:Q:194:SER:O	6:Q:231:GLY:N	2.46	0.49
3:L:37:PHE:HB3	3:L:56:TYR:CD2	2.48	0.49
6:b:16:THR:HG1	6:b:18:TRP:HE1	1.55	0.49
2:Y:173:PRO:HD2	2:Y:177:PHE:HZ	1.77	0.49
6:i:45:LEU:HD21	6:i:110:ILE:HD13	1.95	0.49
6:i:48:GLY:H	6:i:80:THR:HG22	1.78	0.49
6:n:206:THR:O	6:n:217:ASN:ND2	2.46	0.49
2:J:134:GLU:HA	2:J:155:ILE:O	2.13	0.49
6:C:20:TYR:OH	6:C:23:SER:O	2.21	0.49
6:P:131:VAL:HG22	6:P:137:ILE:HD13	1.95	0.49
6:l:164:MET:HA	6:l:164:MET:HE2	1.95	0.49
6:n:133:ALA:O	6:n:134:LYS:HG2	2.12	0.49
1:M:87:ALA:O	1:m:18:PRO:HD2	2.12	0.49
2:J:398:ALA:O	2:J:430:VAL:HA	2.12	0.49
5:I:189:LEU:CD2	5:I:190:PRO:HD3	2.42	0.49
6:A:183:VAL:HG21	6:A:214:ILE:HD12	1.95	0.49
1:D:34:PRO:O	1:D:36:GLY:N	2.45	0.49
1:D:87:ALA:O	1:F:18:PRO:HD2	2.12	0.49
2:E:326:ASN:HB3	5:N:196:MET:HG2	1.95	0.49
6:S:17:LEU:HD11	6:S:45:LEU:HD13	1.94	0.49
2:J:23:LEU:HB2	5:I:210:ALA:HB2	1.96	0.48
6:C:205:ALA:HA	6:C:217:ASN:O	2.13	0.48
6:c:175:LYS:HZ3	6:c:245:ALA:HA	1.77	0.48
1:D:21:ARG:NH2	3:G:17:GLN:OE1	2.46	0.48
6:R:5:ASN:HD21	6:R:8:MET:HB2	1.78	0.48
2:Y:149:THR:OG1	5:f:217:GLN:OE1	2.24	0.48
2:Y:227:PHE:HA	2:Y:672:ARG:HH11	1.78	0.48
6:g:132:THR:HG23	6:g:135:GLU:HB2	1.94	0.48
6:n:20:TYR:OH	6:n:23:SER:O	2.24	0.48
6:o:109:LYS:HD2	6:o:117:VAL:HG21	1.94	0.48
2:J:404:ILE:HD12	5:I:176:PHE:CE2	2.47	0.48
2:J:772:TRP:CE3	2:J:772:TRP:HA	2.48	0.48
6:B:201:ASP:OD2	6:B:203:THR:OG1	2.22	0.48
6:S:41:LYS:HB2	6:S:87:MET:HE2	1.95	0.48
6:S:164:MET:HE1	6:S:230:SER:HB2	1.94	0.48
2:J:819:LYS:HA	2:E:826:HIS:HA	1.94	0.48
6:A:72:GLN:HE21	6:l:123:TRP:HE3	1.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:748:PHE:CE1	2:E:785:TYR:HB3	2.46	0.48
6:U:229:VAL:HG13	6:U:233:GLY:HA2	1.95	0.48
6:n:205:ALA:HA	6:n:217:ASN:O	2.13	0.48
3:L:168:MET:SD	5:I:184:ALA:HB1	2.53	0.48
6:C:101:ASN:O	6:c:75:LYS:NZ	2.43	0.48
6:W:111:ARG:HG2	6:W:117:VAL:HB	1.95	0.48
2:Y:776:SER:OG	2:Y:778:ASN:OD1	2.31	0.48
6:V:67:TRP:NE1	6:h:148:ARG:HG3	2.28	0.48
6:a:116:THR:HB	6:a:152:ALA:HB1	1.96	0.48
2:E:513:LEU:HD21	2:E:535:VAL:HG11	1.95	0.48
3:G:168:MET:SD	5:N:184:ALA:HB1	2.53	0.48
6:U:50:LEU:H	6:U:50:LEU:HD12	1.78	0.48
6:W:194:SER:O	6:W:231:GLY:N	2.42	0.48
2:Y:333:ARG:NH2	2:Y:341:ASP:OD2	2.43	0.48
6:h:120:PHE:CE2	6:h:151:MET:HE1	2.48	0.48
6:o:175:LYS:HZ3	6:o:245:ALA:HA	1.79	0.48
3:L:30:GLU:OE2	3:L:102:THR:OG1	2.32	0.48
2:E:651:SER:OG	2:E:673:THR:O	2.28	0.48
6:Q:126:SER:OG	6:R:49:GLU:OE1	2.22	0.48
6:U:194:SER:OG	6:U:195:PHE:N	2.45	0.48
6:W:159:THR:OG1	6:W:192:ASP:OD2	2.28	0.48
1:X:34:PRO:O	1:X:36:GLY:N	2.46	0.48
5:f:184:ALA:HB2	5:f:201:ARG:HB3	1.96	0.48
5:f:212:GLU:H	5:f:212:GLU:CD	2.19	0.48
2:J:82:GLU:HA	2:J:207:ASP:HA	1.96	0.48
2:E:776:SER:OG	2:E:778:ASN:OD1	2.28	0.48
6:S:199:SER:OG	6:S:201:ASP:OD1	2.32	0.48
6:T:43:LYS:HB2	6:T:83:THR:HG23	1.95	0.48
2:Y:722:LEU:HD11	2:Y:803:ALA:HB1	1.96	0.48
6:o:111:ARG:HG2	6:o:117:VAL:HB	1.96	0.48
6:U:51:THR:HG22	6:U:52:ALA:H	1.79	0.48
2:Y:28:ASP:OD2	5:f:200:SER:OG	2.31	0.48
2:Y:271:ASN:HD22	2:Y:274:TRP:CD1	2.32	0.48
6:n:193:LYS:NZ	6:n:230:SER:O	2.44	0.48
2:J:649:GLY:HA2	5:f:207:ILE:HD12	1.95	0.48
6:V:197:ALA:HB3	6:V:209:VAL:HG21	1.95	0.48
6:B:194:SER:O	6:B:231:GLY:N	2.46	0.48
6:g:195:PHE:HA	6:g:230:SER:HA	1.95	0.48
6:i:48:GLY:N	6:i:80:THR:HG22	2.29	0.48
6:l:150:SER:OG	6:l:155:ARG:NH2	2.39	0.48
2:J:621:VAL:HG23	2:J:694:ALA:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:V:195:PHE:HA	6:V:230:SER:HA	1.96	0.48
6:a:63:GLU:O	6:a:64:ASP:OD2	2.32	0.48
6:Q:43:LYS:HB2	6:Q:83:THR:HG23	1.96	0.48
2:Y:345:ALA:HB2	2:Y:436:PHE:HB3	1.96	0.48
6:j:166:VAL:HG22	6:j:183:VAL:HG22	1.95	0.48
6:k:17:LEU:HD12	6:k:42:VAL:HG21	1.95	0.48
2:Y:272:MET:HG2	2:Y:346:MET:SD	2.54	0.47
5:I:114:GLY:H	4:e:824:LYS:HE3	1.79	0.47
6:b:41:LYS:HD2	6:b:87:MET:HE1	1.95	0.47
6:b:150:SER:OG	6:b:155:ARG:NH2	2.42	0.47
6:C:194:SER:OG	6:C:195:PHE:N	2.44	0.47
6:W:175:LYS:HZ3	6:W:245:ALA:HA	1.79	0.47
2:Y:657:THR:OG1	2:Y:665:GLU:OE1	2.31	0.47
2:J:249:TYR:OH	2:J:309:ASP:OD2	2.30	0.47
2:J:650:VAL:HA	2:J:695:VAL:O	2.14	0.47
6:v:43:LYS:HB3	6:v:83:THR:HG23	1.96	0.47
6:Q:201:ASP:OD2	6:Q:203:THR:OG1	2.26	0.47
6:S:119:VAL:HG13	6:S:150:SER:HB3	1.95	0.47
6:l:20:TYR:OH	6:l:24:GLY:N	2.46	0.47
1:m:54:GLU:OE1	1:m:54:GLU:N	2.46	0.47
6:A:117:VAL:O	6:A:155:ARG:NH1	2.36	0.47
2:E:52:VAL:O	2:E:60:ASN:N	2.45	0.47
2:E:136:ARG:HG2	2:E:184:MET:HG3	1.95	0.47
4:K:835:ARG:NE	4:e:837:GLU:OE1	2.47	0.47
5:N:158:LYS:HA	5:N:158:LYS:HE3	1.96	0.47
6:P:199:SER:H	6:P:202:LYS:HZ3	1.61	0.47
6:U:41:LYS:HD2	6:U:41:LYS:HA	1.66	0.47
1:Z:13:ASP:HB2	1:Z:45:SER:HB2	1.95	0.47
6:i:171:THR:OG1	6:i:172:SER:N	2.48	0.47
6:j:41:LYS:HE2	6:j:41:LYS:HB2	1.69	0.47
6:j:168:PRO:HA	6:j:181:LEU:HG	1.97	0.47
2:J:508:ASP:OD2	2:J:509:ARG:NH1	2.47	0.47
6:A:208:SER:HB2	6:A:215:THR:HG23	1.97	0.47
6:C:166:VAL:HG22	6:C:183:VAL:HG22	1.96	0.47
6:P:173:VAL:HG13	6:P:243:VAL:HG13	1.97	0.47
3:d:118:PHE:CD2	3:d:122:ASN:HB2	2.49	0.47
6:n:16:THR:OG1	6:n:18:TRP:NE1	2.47	0.47
6:n:119:VAL:HG22	6:n:150:SER:HB3	1.97	0.47
6:B:18:TRP:HB2	6:B:109:LYS:HG2	1.96	0.47
1:D:83:LYS:HB3	1:D:83:LYS:HE3	1.54	0.47
6:T:109:LYS:HD2	6:T:117:VAL:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:37:PHE:HB3	3:d:56:TYR:CD2	2.49	0.47
5:f:163:ARG:HG2	5:f:163:ARG:HH11	1.79	0.47
2:J:453:LYS:HD3	2:J:453:LYS:HA	1.59	0.47
2:J:829:LYS:HA	2:J:832:LEU:HD13	1.97	0.47
6:v:61:ASP:OD1	6:v:61:ASP:N	2.44	0.47
6:b:38:ARG:HH12	6:U:61:ASP:HB3	1.79	0.47
6:a:164:MET:HE2	6:a:164:MET:HA	1.97	0.47
2:E:142:GLN:HB2	2:E:178:ASN:HB2	1.97	0.47
2:E:409:GLY:O	2:E:411:GLU:HG3	2.15	0.47
1:F:54:GLU:OE1	1:F:54:GLU:N	2.46	0.47
1:F:59:GLU:HG3	1:F:100:PHE:HE2	1.79	0.47
6:P:185:PHE:HZ	6:P:195:PHE:HB3	1.79	0.47
2:Y:21:THR:OG1	5:f:210:ALA:HB3	2.15	0.47
2:Y:326:ASN:HB3	5:f:196:MET:HG2	1.95	0.47
2:Y:600:ASP:OD1	2:Y:600:ASP:N	2.43	0.47
2:J:104:ILE:HG13	2:J:177:PHE:HB3	1.97	0.47
2:J:121:LEU:HD12	2:J:121:LEU:HA	1.74	0.47
2:J:210:GLN:NE2	3:L:223:GLY:O	2.31	0.47
6:A:127:ILE:HD13	6:A:141:VAL:HG22	1.95	0.47
6:C:48:GLY:N	6:C:80:THR:HA	2.29	0.47
2:E:621:VAL:HG23	2:E:694:ALA:HB2	1.97	0.47
6:P:7:THR:C	6:P:8:MET:HE2	2.39	0.47
2:Y:31:SER:OG	5:f:192:LEU:HB3	2.15	0.47
2:J:277:TRP:HB2	2:J:301:LEU:HD13	1.97	0.47
5:I:187:ASN:O	5:I:188:VAL:HG22	2.14	0.47
6:V:38:ARG:HH12	6:a:61:ASP:HB2	1.80	0.47
6:A:126:SER:OG	6:a:49:GLU:OE2	2.30	0.47
6:S:127:ILE:HD13	6:S:141:VAL:HG22	1.97	0.47
6:h:164:MET:HE2	6:h:166:VAL:HG23	1.97	0.47
6:i:195:PHE:HA	6:i:230:SER:HA	1.96	0.47
3:L:11:GLU:OE1	3:L:14:ARG:NH1	2.46	0.47
3:L:51:TRP:CE3	3:L:113:LEU:HD23	2.49	0.47
6:V:77:ALA:HB3	6:V:145:ASN:HB2	1.97	0.47
6:v:202:LYS:HD3	6:v:202:LYS:HA	1.79	0.47
2:E:287:MET:HE1	3:G:158:THR:HG22	1.96	0.47
2:E:551:ASP:OD1	2:E:551:ASP:N	2.47	0.47
2:E:772:TRP:HA	2:E:772:TRP:CE3	2.51	0.47
6:Q:195:PHE:HA	6:Q:230:SER:HA	1.97	0.47
6:S:193:LYS:HE2	6:S:231:GLY:HA3	1.97	0.47
2:Y:454:THR:OG1	2:Y:595:LYS:NZ	2.35	0.47
6:V:45:LEU:HD23	6:h:131:VAL:HG11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:a:150:SER:OG	6:a:155:ARG:NH2	2.42	0.46
6:c:197:ALA:HB2	6:c:228:VAL:HG13	1.97	0.46
6:Q:171:THR:OG1	6:Q:172:SER:N	2.47	0.46
2:Y:104:ILE:HD12	2:Y:106:SER:H	1.81	0.46
5:f:146:MET:HG2	5:f:154:MET:HE3	1.96	0.46
6:i:132:THR:OG1	6:i:135:GLU:OE2	2.30	0.46
6:l:181:LEU:HB2	6:l:214:ILE:HB	1.96	0.46
6:b:164:MET:HB3	6:b:235:PHE:HD1	1.80	0.46
2:E:54:ASP:OD1	2:E:55:THR:N	2.46	0.46
2:E:134:GLU:HA	2:E:155:ILE:O	2.15	0.46
6:U:20:TYR:OH	6:U:23:SER:O	2.18	0.46
6:W:197:ALA:HB2	6:W:228:VAL:HG13	1.97	0.46
6:h:200:ALA:N	6:h:225:ASN:O	2.47	0.46
6:k:63:GLU:N	6:k:63:GLU:OE2	2.48	0.46
2:J:114:PHE:O	2:J:166:SER:HA	2.15	0.46
6:A:43:LYS:HA	6:A:43:LYS:HD2	1.75	0.46
6:A:102:GLU:OE2	6:A:104:ASP:HB2	2.14	0.46
2:E:3:LYS:HB3	2:E:3:LYS:HE2	1.69	0.46
2:E:21:THR:OG1	5:N:210:ALA:HB3	2.15	0.46
3:G:51:TRP:CE3	3:G:113:LEU:HD23	2.50	0.46
6:l:174:VAL:HG12	6:l:177:GLN:HE21	1.81	0.46
4:H:824:LYS:HA	4:H:824:LYS:HD2	1.66	0.46
6:a:161:ALA:HB3	6:a:187:PRO:HB2	1.98	0.46
2:E:257:SER:OG	2:E:258:GLY:N	2.49	0.46
2:E:260:TRP:NE1	2:E:262:GLY:O	2.49	0.46
6:O:195:PHE:HA	6:O:230:SER:HA	1.97	0.46
6:S:164:MET:HB2	6:S:185:PHE:HA	1.96	0.46
6:T:132:THR:HG23	6:T:135:GLU:HB3	1.96	0.46
3:d:12:CYS:O	3:d:17:GLN:NE2	2.49	0.46
6:n:210:SER:O	6:n:213:THR:HB	2.16	0.46
1:M:34:PRO:O	1:M:36:GLY:N	2.46	0.46
2:J:425:ARG:NH2	3:d:99:VAL:O	2.29	0.46
6:V:207:VAL:HG12	6:V:216:VAL:HG22	1.97	0.46
6:b:108:TYR:CE1	6:b:120:PHE:HB2	2.51	0.46
2:E:820:GLY:H	2:Y:826:HIS:HA	1.79	0.46
6:Q:204:LYS:HE2	6:Q:204:LYS:HB2	1.74	0.46
6:R:168:PRO:HA	6:R:181:LEU:HG	1.97	0.46
6:U:57:ASP:OD1	6:U:57:ASP:N	2.47	0.46
1:X:83:LYS:HB3	1:X:83:LYS:HE3	1.54	0.46
2:Y:96:TYR:CD2	2:Y:186:PRO:HA	2.50	0.46
2:Y:647:VAL:HG12	2:Y:648:LYS:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:54:GLU:OE1	1:Z:54:GLU:N	2.47	0.46
6:g:199:SER:HB3	6:g:202:LYS:HD3	1.98	0.46
6:o:127:ILE:HG22	6:o:141:VAL:HG22	1.98	0.46
6:o:194:SER:O	6:o:231:GLY:N	2.43	0.46
6:v:207:VAL:HG12	6:v:216:VAL:HG22	1.97	0.46
6:C:41:LYS:HD2	6:C:41:LYS:HA	1.66	0.46
6:C:51:THR:HG22	6:C:52:ALA:N	2.30	0.46
6:R:18:TRP:HB3	6:R:36:TRP:HB3	1.98	0.46
6:b:134:LYS:HE3	6:U:74:GLN:HG3	1.98	0.46
2:E:845:LEU:HB3	2:Y:845:LEU:HD21	1.98	0.46
6:W:106:ARG:HE	6:W:106:ARG:HB3	1.59	0.46
6:h:199:SER:H	6:h:202:LYS:HZ3	1.64	0.46
6:h:204:LYS:HB2	6:h:204:LYS:HE2	1.71	0.46
6:l:131:VAL:HG22	6:l:137:ILE:HD13	1.98	0.46
6:n:17:LEU:HD11	6:n:39:LEU:HD12	1.97	0.46
2:J:271:ASN:HD22	2:J:274:TRP:CD1	2.33	0.46
6:a:75:LYS:N	6:S:66:ASP:O	2.49	0.46
2:E:218:VAL:HG11	2:E:236:TYR:CE1	2.51	0.46
6:i:204:LYS:HE2	6:i:204:LYS:HB2	1.74	0.46
6:k:208:SER:HB2	6:k:215:THR:HG23	1.98	0.46
6:V:60:LEU:HG	1:Z:10:PRO:HA	1.97	0.46
2:E:520:LEU:HD23	2:E:534:GLU:HA	1.98	0.46
2:E:722:LEU:HD11	2:E:803:ALA:HB1	1.97	0.46
2:E:827:LEU:CD2	2:E:827:LEU:H	2.29	0.46
2:E:829:LYS:HA	2:E:832:LEU:HD13	1.98	0.46
6:R:108:TYR:CZ	6:R:120:PHE:HB2	2.51	0.46
6:W:97:LEU:HG	6:n:153:GLU:HG3	1.97	0.46
2:Y:90:LEU:O	2:Y:90:LEU:HD12	2.16	0.46
6:i:43:LYS:HB2	6:i:83:THR:HG23	1.98	0.46
1:M:9:LYS:HB2	1:M:9:LYS:NZ	2.31	0.46
2:J:409:GLY:O	2:J:411:GLU:HG3	2.16	0.46
2:J:812:GLU:HA	2:J:815:LEU:HB2	1.97	0.46
3:L:43:ASN:HD21	3:L:47:GLU:HB2	1.80	0.46
6:V:102:GLU:HG2	6:V:104:ASP:H	1.80	0.46
2:E:752:GLN:HB2	2:E:786:TYR:CZ	2.51	0.46
1:X:27:ASP:CG	2:Y:373:ARG:HH12	2.24	0.46
6:i:128:GLY:O	6:i:139:ARG:NH1	2.48	0.46
6:l:46:THR:O	6:l:46:THR:OG1	2.34	0.46
6:n:87:MET:HE3	6:n:87:MET:HB2	1.82	0.46
6:n:229:VAL:HG13	6:n:233:GLY:HA2	1.97	0.46
2:J:287:MET:HE1	3:L:158:THR:HG22	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:287:MET:HE3	2:J:287:MET:HB3	1.86	0.45
2:J:347:ARG:HG2	2:J:450:TRP:CE2	2.52	0.45
2:J:433:MET:HG2	2:J:434:ASP:N	2.31	0.45
1:m:13:ASP:HB2	1:m:45:SER:HB2	1.96	0.45
6:A:194:SER:OG	6:A:195:PHE:N	2.50	0.45
2:E:141:ILE:HG23	2:E:143:ARG:HB2	1.98	0.45
2:E:345:ALA:HB2	2:E:436:PHE:HB3	1.98	0.45
2:Y:83:SER:OG	2:Y:207:ASP:O	2.26	0.45
2:J:21:THR:OG1	5:I:210:ALA:HB3	2.16	0.45
2:J:218:VAL:HG11	2:J:236:TYR:CE1	2.52	0.45
2:J:748:PHE:CE1	2:J:785:TYR:HB3	2.48	0.45
2:J:823:THR:HB	2:E:828:GLY:HA3	1.98	0.45
5:I:195:GLU:HB3	5:I:196:MET:H	1.49	0.45
6:v:150:SER:O	6:v:150:SER:OG	2.34	0.45
1:D:42:LYS:HB2	1:D:42:LYS:HE3	1.75	0.45
2:E:100:ILE:HG22	2:E:102:ARG:HH21	1.81	0.45
2:E:117:GLY:HA3	2:E:164:LEU:HD23	1.97	0.45
6:W:202:LYS:NZ	6:W:207:VAL:H	2.12	0.45
2:Y:409:GLY:O	2:Y:411:GLU:HG3	2.15	0.45
2:Y:755:ASP:CG	2:Y:757:ARG:H	2.24	0.45
6:o:163:GLY:H	6:o:187:PRO:HB3	1.80	0.45
2:J:755:ASP:CG	2:J:757:ARG:H	2.25	0.45
5:I:167:THR:HG21	5:N:167:THR:HG21	1.98	0.45
6:V:97:LEU:O	6:V:101:ASN:ND2	2.47	0.45
6:a:109:LYS:HD2	6:a:117:VAL:HG21	1.99	0.45
3:G:228:ASN:ND2	2:Y:408:ASN:OD1	2.49	0.45
5:N:116:PHE:N	5:N:116:PHE:CD2	2.85	0.45
6:S:195:PHE:HZ	6:S:212:MET:HA	1.81	0.45
6:T:123:TRP:HE3	6:k:72:GLN:HE21	1.64	0.45
6:k:117:VAL:O	6:k:155:ARG:NH1	2.30	0.45
6:k:183:VAL:HG21	6:k:214:ILE:HD12	1.97	0.45
3:L:118:PHE:CD2	3:L:122:ASN:HB2	2.52	0.45
6:c:164:MET:HE2	6:c:164:MET:HA	1.99	0.45
6:c:194:SER:O	6:c:231:GLY:N	2.42	0.45
2:E:755:ASP:CG	2:E:757:ARG:H	2.24	0.45
6:g:99:TRP:CD1	6:g:106:ARG:HG3	2.51	0.45
6:g:193:LYS:HD3	6:g:194:SER:H	1.81	0.45
6:n:41:LYS:HA	6:n:41:LYS:HD2	1.65	0.45
2:J:152:ASP:OD1	2:J:152:ASP:N	2.49	0.45
4:H:837:GLU:OE2	4:e:831:ARG:NH1	2.50	0.45
6:b:168:PRO:HA	6:b:181:LEU:HG	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:c:127:ILE:HD11	6:U:50:LEU:HD13	1.98	0.45
6:c:202:LYS:HA	6:c:202:LYS:HD3	1.75	0.45
6:W:101:ASN:OD1	6:n:148:ARG:NH2	2.50	0.45
2:Y:218:VAL:HG11	2:Y:236:TYR:CE1	2.52	0.45
6:g:212:MET:O	6:g:212:MET:HE3	2.17	0.45
1:M:27:ASP:HB3	1:Z:37:LEU:H	1.82	0.45
6:C:150:SER:OG	6:C:155:ARG:NH2	2.41	0.45
2:E:684:ALA:O	2:E:688:TYR:OH	2.31	0.45
4:K:830:ALA:HB1	4:e:830:ALA:HA	1.97	0.45
6:O:77:ALA:HB3	6:O:145:ASN:HB2	1.98	0.45
6:O:148:ARG:NH2	6:P:64:ASP:OD1	2.49	0.45
6:O:238:VAL:HG11	6:P:238:VAL:HG11	1.99	0.45
6:U:43:LYS:HA	6:U:43:LYS:HD3	1.76	0.45
6:U:63:GLU:O	6:U:64:ASP:OD1	2.34	0.45
2:Y:134:GLU:HA	2:Y:155:ILE:O	2.17	0.45
6:g:148:ARG:NH2	6:h:64:ASP:OD1	2.50	0.45
6:g:207:VAL:HG12	6:g:216:VAL:HG22	1.99	0.45
2:J:274:TRP:HA	2:J:277:TRP:HB3	1.99	0.45
2:J:748:PHE:HE2	2:J:779:ILE:HD11	1.81	0.45
3:L:230:LEU:HD23	2:E:648:LYS:HG3	1.98	0.45
6:V:199:SER:HB3	6:V:202:LYS:HD3	1.99	0.45
6:a:42:VAL:H	6:Q:61:ASP:CG	2.25	0.45
2:E:277:TRP:HB2	2:E:301:LEU:HD13	1.99	0.45
2:E:378:MET:HE2	2:E:378:MET:HB2	1.85	0.45
2:E:650:VAL:HA	2:E:695:VAL:O	2.16	0.45
1:F:65:HIS:HE1	1:F:71:PHE:HB3	1.81	0.45
6:P:150:SER:OG	6:P:155:ARG:NH1	2.43	0.45
6:Q:207:VAL:HG12	6:Q:216:VAL:HG22	1.99	0.45
6:g:126:SER:OG	6:h:49:GLU:OE2	2.35	0.45
6:n:120:PHE:HB3	6:n:145:ASN:HD22	1.82	0.45
1:M:89:TRP:O	1:M:89:TRP:CD1	2.70	0.45
2:J:694:ALA:O	2:J:702:GLY:N	2.49	0.45
3:L:142:GLU:HB2	5:N:109:ALA:HB3	1.98	0.45
6:C:61:ASP:HB3	6:j:38:ARG:HH12	1.82	0.45
1:D:1:MET:N	1:D:64:GLU:OE2	2.47	0.45
2:E:274:TRP:HA	2:E:277:TRP:HB3	1.99	0.45
2:E:380:ASP:OD1	2:E:380:ASP:N	2.48	0.45
2:E:741:THR:O	2:E:741:THR:OG1	2.28	0.45
2:Y:752:GLN:HB2	2:Y:786:TYR:CZ	2.51	0.45
6:o:225:ASN:ND2	6:o:240:GLU:OE1	2.50	0.45
2:J:822:ILE:HA	2:J:826:HIS:ND1	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:170:GLY:HA3	5:f:187:ASN:HD21	1.81	0.45
6:C:133:ALA:O	6:C:134:LYS:HG2	2.16	0.45
6:c:47:PRO:HA	6:c:80:THR:HG23	1.99	0.45
2:E:121:LEU:HD12	2:E:121:LEU:HA	1.76	0.45
6:O:205:ALA:HA	6:O:217:ASN:O	2.17	0.45
6:Q:198:VAL:O	6:Q:227:PRO:HD2	2.16	0.45
2:Y:380:ASP:OD2	5:f:103:PHE:HB3	2.17	0.45
6:l:209:VAL:HG22	6:l:214:ILE:HG12	1.99	0.45
6:n:10:VAL:HG12	6:n:12:GLY:H	1.82	0.45
6:n:168:PRO:HB3	6:n:239:ALA:HB1	1.99	0.45
2:J:54:ASP:N	2:J:58:ASN:O	2.43	0.45
2:J:233:SER:O	2:J:233:SER:OG	2.26	0.45
2:J:364:PRO:HB3	2:J:593:PRO:HB3	1.99	0.45
4:H:830:ALA:HA	4:e:830:ALA:HB1	1.98	0.45
6:B:204:LYS:HE2	6:B:204:LYS:HB2	1.74	0.45
6:A:119:VAL:HG13	6:A:150:SER:HB3	1.99	0.45
6:C:221:ALA:HA	6:C:243:VAL:HB	1.99	0.45
2:E:139:VAL:HG13	2:E:151:LYS:HB2	1.99	0.45
2:E:508:ASP:OD2	2:E:509:ARG:NH1	2.50	0.45
4:K:827:TYR:OH	4:e:836:ASP:OD2	2.29	0.45
6:R:42:VAL:HA	6:R:84:LEU:HA	1.98	0.45
6:S:208:SER:HB2	6:S:215:THR:HG23	1.99	0.45
6:U:168:PRO:HA	6:U:181:LEU:HG	1.98	0.45
2:Y:135:VAL:HA	2:Y:185:THR:HG21	1.98	0.45
2:Y:239:ARG:NH1	5:f:195:GLU:OE2	2.50	0.45
2:Y:398:ALA:O	2:Y:430:VAL:HA	2.17	0.45
3:d:51:TRP:CE3	3:d:113:LEU:HD23	2.52	0.45
6:a:205:ALA:HA	6:a:217:ASN:O	2.18	0.44
6:U:164:MET:N	6:U:164:MET:SD	2.90	0.44
6:j:204:LYS:HB2	6:j:204:LYS:HE2	1.84	0.44
6:l:44:ASP:OD1	6:l:44:ASP:C	2.60	0.44
6:n:168:PRO:HA	6:n:181:LEU:HG	1.99	0.44
2:J:100:ILE:HG22	2:J:102:ARG:HH21	1.83	0.44
2:J:113:ARG:HB2	2:J:168:VAL:HG13	2.00	0.44
2:J:381:ASP:OD2	2:J:386:ARG:NH2	2.45	0.44
6:V:238:VAL:HG11	6:v:238:VAL:HG11	2.00	0.44
6:C:11:LYS:HD3	6:C:11:LYS:HA	1.70	0.44
2:E:83:SER:OG	2:E:207:ASP:O	2.29	0.44
6:W:48:GLY:N	6:W:80:THR:OG1	2.50	0.44
2:Y:152:ASP:N	2:Y:152:ASP:OD1	2.49	0.44
2:Y:257:SER:OG	2:Y:258:GLY:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:j:42:VAL:HA	6:j:84:LEU:HB3	1.99	0.44
6:V:59:TYR:O	1:X:95:MET:HE1	2.18	0.44
6:C:10:VAL:HG12	6:C:12:GLY:H	1.81	0.44
6:c:8:MET:SD	6:c:8:MET:N	2.90	0.44
1:D:31:GLN:OE1	3:G:17:GLN:NE2	2.47	0.44
2:E:819:LYS:HB2	2:E:819:LYS:HE3	1.70	0.44
2:Y:834:LYS:HB2	2:Y:834:LYS:HE3	1.69	0.44
1:Z:9:LYS:HD3	1:Z:10:PRO:HD2	1.99	0.44
6:j:45:LEU:HD12	6:j:82:PHE:HB3	1.98	0.44
6:n:21:LYS:O	6:n:21:LYS:HG2	2.17	0.44
2:J:117:GLY:HA3	2:J:164:LEU:HD23	2.00	0.44
6:V:209:VAL:HG13	6:V:214:ILE:HG12	1.98	0.44
1:F:89:TRP:CD1	1:F:89:TRP:O	2.71	0.44
6:P:193:LYS:NZ	6:P:234:GLU:OE2	2.50	0.44
6:k:194:SER:OG	6:k:195:PHE:N	2.51	0.44
6:n:165:THR:CG2	6:n:184:ALA:HB3	2.47	0.44
2:J:749:SER:OG	2:J:751:LYS:O	2.33	0.44
6:b:44:ASP:C	6:b:44:ASP:OD1	2.60	0.44
6:b:187:PRO:HG2	6:b:191:THR:HB	1.99	0.44
6:C:173:VAL:HG11	6:C:218:GLY:H	1.83	0.44
2:E:364:PRO:HB3	2:E:593:PRO:HB3	1.99	0.44
6:S:202:LYS:HE3	6:T:235:PHE:HA	1.99	0.44
6:U:120:PHE:HB3	6:U:145:ASN:ND2	2.32	0.44
5:f:136:THR:HG23	5:f:139:LEU:HD11	2.00	0.44
6:j:187:PRO:HG2	6:j:191:THR:HB	1.99	0.44
6:l:111:ARG:HE	6:l:111:ARG:HB3	1.64	0.44
6:B:43:LYS:H	6:B:84:LEU:HA	1.83	0.44
6:C:148:ARG:NH2	6:o:101:ASN:OD1	2.50	0.44
2:E:771:TYR:C	2:E:771:TYR:CD2	2.95	0.44
6:R:108:TYR:CE1	6:R:120:PHE:HB2	2.53	0.44
6:S:3:VAL:HB	6:S:4:PRO:HD3	2.00	0.44
6:W:18:TRP:HB2	6:W:109:LYS:HG2	1.98	0.44
2:Y:52:VAL:O	2:Y:60:ASN:N	2.47	0.44
2:Y:281:THR:O	2:Y:281:THR:OG1	2.27	0.44
5:f:163:ARG:HG2	5:f:163:ARG:NH1	2.33	0.44
6:k:164:MET:HE1	6:k:235:PHE:HB3	1.99	0.44
2:J:257:SER:OG	2:J:258:GLY:N	2.51	0.44
2:J:511:ILE:HG23	2:J:538:VAL:HG21	2.00	0.44
2:J:766:LEU:HD23	2:J:772:TRP:CD1	2.53	0.44
1:m:89:TRP:O	1:m:89:TRP:CD1	2.71	0.44
6:B:195:PHE:HA	6:B:230:SER:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:347:ARG:HG2	2:E:450:TRP:CE2	2.53	0.44
5:N:190:PRO:O	5:N:191:VAL:HG23	2.17	0.44
6:O:221:ALA:HA	6:O:243:VAL:HB	1.99	0.44
2:Y:687:ASN:CG	2:Y:710:ARG:HE	2.25	0.44
6:k:202:LYS:HE3	6:l:235:PHE:HA	1.99	0.44
6:v:17:LEU:HD12	6:v:110:ILE:HG12	2.00	0.44
6:A:177:GLN:O	6:A:217:ASN:ND2	2.51	0.44
6:C:7:THR:O	6:C:8:MET:HE2	2.18	0.44
6:C:168:PRO:HA	6:C:181:LEU:HG	1.99	0.44
6:S:163:GLY:HA2	6:S:235:PHE:CD2	2.53	0.44
6:U:99:TRP:NE1	6:U:104:ASP:O	2.47	0.44
2:Y:114:PHE:CD1	2:Y:169:MET:HE1	2.53	0.44
2:Y:127:LYS:HB2	2:Y:127:LYS:HE3	1.85	0.44
6:k:205:ALA:HA	6:k:217:ASN:O	2.17	0.44
6:o:202:LYS:NZ	6:o:207:VAL:H	2.14	0.44
2:J:260:TRP:NE1	2:J:262:GLY:O	2.51	0.44
2:E:401:VAL:HG22	2:E:433:MET:HE3	2.00	0.44
6:O:164:MET:HB3	6:O:235:PHE:HD2	1.83	0.44
6:O:211:GLY:C	6:O:213:THR:H	2.26	0.44
6:Q:86:TRP:HE1	6:Q:139:ARG:HH21	1.66	0.44
6:U:221:ALA:HA	6:U:243:VAL:HB	2.00	0.44
2:Y:121:LEU:HA	2:Y:121:LEU:HD12	1.76	0.44
2:Y:771:TYR:C	2:Y:771:TYR:CD2	2.96	0.44
6:h:164:MET:HE1	6:h:183:VAL:HG13	2.00	0.44
6:k:25:ASP:OD1	6:k:28:ALA:N	2.50	0.44
6:a:119:VAL:HG13	6:a:150:SER:HB3	2.00	0.43
6:C:17:LEU:HD11	6:C:39:LEU:HD12	2.00	0.43
6:C:52:ALA:HA	6:C:75:LYS:HA	2.00	0.43
2:E:104:ILE:HG22	2:E:202:TYR:CZ	2.53	0.43
6:P:205:ALA:HB3	6:P:224:VAL:HG21	1.99	0.43
6:R:196:ARG:NH2	6:R:231:GLY:O	2.38	0.43
2:Y:372:ASN:HD21	2:Y:558:VAL:HG13	1.83	0.43
6:g:18:TRP:CZ3	6:g:38:ARG:HB2	2.53	0.43
6:g:38:ARG:HH12	6:l:61:ASP:HB2	1.83	0.43
6:g:221:ALA:HA	6:g:243:VAL:HB	2.00	0.43
6:i:149:PRO:HB2	6:i:151:MET:HE3	2.00	0.43
6:j:183:VAL:HB	6:j:212:MET:HE1	2.00	0.43
6:n:167:THR:HB	6:n:182:THR:HB	2.00	0.43
2:J:495:VAL:O	2:J:556:TYR:N	2.40	0.43
6:v:199:SER:H	6:v:202:LYS:HZ3	1.66	0.43
6:B:163:GLY:HA3	6:B:187:PRO:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:193:LYS:HE2	6:A:231:GLY:HA3	2.00	0.43
2:E:245:VAL:CG2	2:E:246:PRO:HD2	2.47	0.43
6:U:163:GLY:HA3	6:U:187:PRO:HB3	1.99	0.43
2:Y:248:ASN:ND2	2:Y:258:GLY:O	2.51	0.43
2:Y:274:TRP:HA	2:Y:277:TRP:HB3	2.00	0.43
2:Y:453:LYS:HD3	2:Y:453:LYS:HA	1.59	0.43
2:Y:685:LEU:HD23	2:Y:685:LEU:H	1.83	0.43
6:h:96:LEU:HD11	6:h:141:VAL:HG11	2.01	0.43
6:n:43:LYS:HD3	6:n:43:LYS:HA	1.77	0.43
1:m:10:PRO:HA	6:O:60:LEU:HG	2.00	0.43
6:A:52:ALA:HB1	6:A:72:GLN:HG3	2.01	0.43
6:a:185:PHE:HZ	6:a:195:PHE:HB3	1.82	0.43
6:C:74:GLN:HG3	6:j:134:LYS:HE3	2.00	0.43
6:C:153:GLU:HG3	6:o:97:LEU:HG	2.00	0.43
2:E:566:LEU:HD23	2:E:566:LEU:HA	1.83	0.43
6:R:204:LYS:HB2	6:R:204:LYS:HE2	1.84	0.43
6:h:36:TRP:CD1	6:h:109:LYS:HZ3	2.36	0.43
6:h:193:LYS:NZ	6:h:234:GLU:OE2	2.51	0.43
1:m:13:ASP:OD2	1:m:13:ASP:N	2.52	0.43
6:v:164:MET:HE3	6:v:165:THR:N	2.33	0.43
6:A:25:ASP:OD1	6:A:28:ALA:N	2.51	0.43
6:a:174:VAL:HG12	6:a:177:GLN:HE21	1.83	0.43
6:c:183:VAL:HB	6:c:212:MET:HE1	2.00	0.43
2:E:102:ARG:HB3	2:E:179:ILE:HD11	2.00	0.43
2:Y:381:ASP:OD2	2:Y:386:ARG:NH2	2.44	0.43
2:Y:766:LEU:HD23	2:Y:772:TRP:NE1	2.34	0.43
2:J:31:SER:OG	5:I:192:LEU:HB3	2.17	0.43
2:J:183:ARG:NH2	2:J:195:ASN:O	2.51	0.43
1:m:23:VAL:HG13	5:N:117:PHE:HZ	1.83	0.43
6:c:108:TYR:CZ	6:c:120:PHE:HB2	2.54	0.43
3:G:83:ASN:H	3:G:147:SER:HA	1.83	0.43
5:N:148:LEU:HA	5:N:148:LEU:HD12	1.77	0.43
6:R:185:PHE:CD1	6:R:191:THR:HG21	2.53	0.43
6:T:193:LYS:N	6:T:193:LYS:HD2	2.34	0.43
2:Y:827:LEU:HB2	2:Y:831:LEU:HD12	2.01	0.43
3:d:43:ASN:HD21	3:d:47:GLU:HB2	1.82	0.43
6:g:129:LYS:HB2	6:g:129:LYS:HE2	1.92	0.43
6:g:238:VAL:HG11	6:h:238:VAL:HG11	2.00	0.43
6:n:195:PHE:HE2	6:n:214:ILE:HD11	1.82	0.43
2:J:3:LYS:HE2	2:J:3:LYS:HB3	1.67	0.43
2:J:378:MET:SD	2:J:384:PRO:HG3	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:771:TYR:C	2:J:771:TYR:CD2	2.97	0.43
5:I:148:LEU:HD12	5:I:148:LEU:HA	1.82	0.43
6:V:18:TRP:HB2	6:V:109:LYS:HG2	2.00	0.43
6:b:43:LYS:N	6:b:83:THR:O	2.52	0.43
6:c:122:GLY:HA3	6:c:145:ASN:HA	2.01	0.43
6:T:83:THR:HB	6:T:140:THR:HG23	2.01	0.43
2:Y:380:ASP:OD2	2:Y:380:ASP:N	2.50	0.43
6:g:77:ALA:HB3	6:g:145:ASN:HB2	2.01	0.43
6:g:108:TYR:CZ	6:g:120:PHE:HB2	2.53	0.43
6:i:43:LYS:H	6:i:84:LEU:HA	1.83	0.43
6:o:197:ALA:HB2	6:o:228:VAL:HG13	2.01	0.43
6:v:72:GLN:OE1	6:v:75:LYS:HE3	2.18	0.43
6:v:205:ALA:HB3	6:v:224:VAL:HG21	2.00	0.43
6:T:43:LYS:H	6:T:84:LEU:HA	1.83	0.43
6:T:205:ALA:HA	6:T:217:ASN:O	2.19	0.43
6:U:36:TRP:CD1	6:U:109:LYS:HZ3	2.36	0.43
2:Y:749:SER:OG	2:Y:751:LYS:O	2.30	0.43
6:i:127:ILE:HD13	6:i:141:VAL:HG22	2.00	0.43
6:o:43:LYS:HA	6:o:43:LYS:HD3	1.77	0.43
6:o:99:TRP:CD2	6:o:106:ARG:HD2	2.54	0.43
6:v:173:VAL:HG13	6:v:243:VAL:HG13	2.00	0.43
6:b:31:LEU:HD13	6:b:31:LEU:HA	1.87	0.43
6:A:41:LYS:HB3	6:A:85:ALA:HB3	2.01	0.43
6:c:129:LYS:HB2	6:c:129:LYS:HE3	1.76	0.43
2:E:33:GLY:O	2:E:71:GLY:HA3	2.19	0.43
2:E:134:GLU:HG3	2:E:156:LYS:HG2	2.00	0.43
2:E:464:PHE:O	2:E:465:SER:C	2.61	0.43
6:O:206:THR:O	6:O:217:ASN:ND2	2.52	0.43
6:P:204:LYS:HE2	6:P:204:LYS:HB2	1.74	0.43
6:W:19:VAL:HG23	6:W:39:LEU:HD11	2.00	0.43
2:Y:209:LYS:HB2	2:Y:209:LYS:HE2	1.87	0.43
6:i:193:LYS:HE3	6:i:231:GLY:HA3	2.00	0.43
6:n:173:VAL:HG11	6:n:218:GLY:H	1.83	0.43
1:M:42:LYS:HE3	1:M:42:LYS:HB2	1.72	0.43
2:J:138:LEU:HD21	2:J:149:THR:HB	2.01	0.43
2:J:845:LEU:HB3	2:E:845:LEU:HD21	2.00	0.43
6:A:3:VAL:HB	6:A:4:PRO:HD3	2.00	0.43
6:C:163:GLY:HA3	6:C:187:PRO:HB3	2.01	0.43
6:c:202:LYS:NZ	6:c:207:VAL:H	2.17	0.43
1:D:9:LYS:HG3	1:D:10:PRO:HD3	2.01	0.43
1:D:14:VAL:HG21	1:D:77:TYR:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:766:LEU:HD23	2:E:772:TRP:NE1	2.33	0.43
4:K:824:LYS:HD3	5:f:114:GLY:C	2.43	0.43
1:X:89:TRP:O	1:X:89:TRP:CD1	2.71	0.43
2:Y:464:PHE:O	2:Y:465:SER:C	2.61	0.43
2:Y:723:THR:OG1	2:Y:730:THR:HB	2.19	0.43
5:f:116:PHE:N	5:f:116:PHE:CD1	2.86	0.43
6:i:198:VAL:O	6:i:227:PRO:HD2	2.18	0.43
6:j:211:GLY:O	6:j:212:MET:HB3	2.18	0.43
6:n:241:ILE:HD13	6:n:241:ILE:HA	1.86	0.43
6:o:87:MET:HB2	6:o:93:GLN:CD	2.43	0.43
2:J:47:LEU:HD22	2:J:47:LEU:HA	1.81	0.43
2:J:827:LEU:CD2	2:J:827:LEU:H	2.31	0.43
2:J:828:GLY:O	2:J:832:LEU:HD12	2.19	0.43
6:b:185:PHE:CD1	6:b:191:THR:HG21	2.53	0.43
1:D:89:TRP:O	1:D:89:TRP:CD1	2.72	0.43
1:F:10:PRO:HA	6:g:60:LEU:HG	2.01	0.43
6:Q:43:LYS:H	6:Q:84:LEU:HA	1.84	0.43
6:Q:45:LEU:HD21	6:Q:110:ILE:HD13	2.00	0.43
6:S:51:THR:HG22	6:S:52:ALA:N	2.31	0.43
6:S:173:VAL:O	6:S:243:VAL:HG13	2.19	0.43
6:W:127:ILE:HG22	6:W:141:VAL:HG22	2.01	0.43
2:Y:543:LYS:HE3	2:Y:543:LYS:HB3	1.74	0.43
3:d:61:ILE:HB	3:d:81:VAL:HG23	1.99	0.43
6:j:108:TYR:CE1	6:j:120:PHE:HB2	2.53	0.43
2:J:752:GLN:HB2	2:J:786:TYR:CZ	2.54	0.42
2:J:845:LEU:HD21	2:Y:845:LEU:HB3	2.01	0.42
6:V:99:TRP:CD1	6:V:106:ARG:HG3	2.54	0.42
6:V:205:ALA:HA	6:V:217:ASN:O	2.19	0.42
6:B:198:VAL:O	6:B:227:PRO:HD2	2.18	0.42
6:b:108:TYR:CZ	6:b:120:PHE:HB2	2.54	0.42
6:b:148:ARG:NH1	6:b:148:ARG:HG2	2.34	0.42
2:E:96:TYR:CD2	2:E:186:PRO:HA	2.49	0.42
6:W:122:GLY:HA3	6:W:145:ASN:HA	2.01	0.42
5:f:115:SER:C	5:f:116:PHE:HD1	2.27	0.42
6:o:91:GLN:OE1	6:o:91:GLN:HA	2.18	0.42
6:B:126:SER:OG	6:b:49:GLU:OE2	2.22	0.42
6:B:171:THR:OG1	6:B:172:SER:N	2.47	0.42
6:C:57:ASP:OD1	6:C:57:ASP:N	2.51	0.42
1:D:75:PRO:HA	1:D:76:PRO:HD3	1.94	0.42
2:E:109:ILE:HD11	2:E:112:LEU:HD13	2.01	0.42
2:E:290:ARG:HG2	2:E:291:LEU:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:207:ILE:HD12	2:Y:649:GLY:HA2	2.01	0.42
6:O:129:LYS:HB2	6:O:129:LYS:HE2	1.90	0.42
6:R:134:LYS:HE3	6:n:74:GLN:HG3	2.01	0.42
6:T:99:TRP:CE2	6:T:106:ARG:HB2	2.54	0.42
2:Y:433:MET:HG2	2:Y:434:ASP:N	2.34	0.42
6:j:108:TYR:CZ	6:j:120:PHE:HB2	2.53	0.42
2:J:112:LEU:HD12	2:J:112:LEU:HA	1.90	0.42
2:J:138:LEU:HD23	2:J:140:GLN:HG3	2.01	0.42
6:b:41:LYS:HE2	6:b:41:LYS:HB2	1.92	0.42
6:A:16:THR:OG1	6:A:111:ARG:HB2	2.19	0.42
6:a:111:ARG:HE	6:a:111:ARG:HB3	1.62	0.42
6:C:36:TRP:CD1	6:C:109:LYS:HZ3	2.36	0.42
2:E:113:ARG:HB2	2:E:168:VAL:HG13	2.01	0.42
6:Q:185:PHE:O	6:Q:187:PRO:HD3	2.19	0.42
2:J:464:PHE:O	2:J:465:SER:C	2.61	0.42
2:J:822:ILE:HA	2:J:826:HIS:CE1	2.54	0.42
1:m:23:VAL:HG11	3:L:82:SER:HB2	2.01	0.42
1:m:68:TRP:CD1	1:m:68:TRP:H	2.37	0.42
6:v:200:ALA:N	6:v:225:ASN:O	2.48	0.42
2:E:510:GLU:HA	2:E:541:GLY:O	2.20	0.42
3:G:43:ASN:HD21	3:G:47:GLU:HB2	1.83	0.42
6:S:177:GLN:O	6:S:217:ASN:ND2	2.52	0.42
6:U:173:VAL:HG11	6:U:218:GLY:H	1.84	0.42
6:W:29:ASN:OD1	6:W:32:SER:HB3	2.19	0.42
2:Y:9:HIS:O	2:Y:9:HIS:CG	2.72	0.42
2:Y:227:PHE:HA	2:Y:672:ARG:NH1	2.34	0.42
2:Y:249:TYR:OH	2:Y:309:ASP:OD2	2.37	0.42
6:h:202:LYS:HD3	6:h:202:LYS:HA	1.79	0.42
6:i:80:THR:HG23	6:i:145:ASN:HD21	1.84	0.42
6:k:118:ASP:OD1	6:k:118:ASP:C	2.62	0.42
6:k:209:VAL:HG22	6:k:214:ILE:HG12	2.01	0.42
2:J:69:ARG:HD3	2:J:69:ARG:HA	1.83	0.42
1:m:37:LEU:H	1:D:27:ASP:HB3	1.84	0.42
5:I:117:PHE:C	5:I:120:GLY:H	2.27	0.42
6:V:9:PRO:HB3	6:h:85:ALA:HB1	2.02	0.42
6:B:124:VAL:HG22	6:B:143:VAL:HG22	2.01	0.42
6:b:42:VAL:HA	6:b:84:LEU:HA	2.00	0.42
6:b:166:VAL:HG22	6:b:183:VAL:HG22	2.01	0.42
2:E:578:GLU:HG2	2:E:584:TYR:CE2	2.54	0.42
1:F:109:ASN:ND2	1:X:29:TYR:HD1	2.18	0.42
6:R:44:ASP:OD1	6:R:44:ASP:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:9:LYS:HB2	1:X:9:LYS:NZ	2.34	0.42
2:Y:260:TRP:NE1	2:Y:262:GLY:O	2.52	0.42
2:Y:364:PRO:HB3	2:Y:593:PRO:HB3	2.00	0.42
6:h:163:GLY:HA3	6:h:187:PRO:HA	2.01	0.42
6:j:164:MET:HB3	6:j:235:PHE:CD2	2.55	0.42
2:J:28:ASP:OD1	2:J:236:TYR:OH	2.32	0.42
4:H:836:ASP:OD2	4:e:827:TYR:OH	2.31	0.42
6:c:18:TRP:HB3	6:c:36:TRP:HB3	2.01	0.42
6:P:165:THR:HB	6:P:184:ALA:HB3	2.00	0.42
6:S:25:ASP:OD1	6:S:28:ALA:N	2.51	0.42
6:U:195:PHE:HE2	6:U:214:ILE:HD11	1.85	0.42
2:Y:141:ILE:HG23	2:Y:143:ARG:HB2	2.01	0.42
2:Y:280:LEU:HD21	2:Y:339:LEU:HD13	2.01	0.42
2:Y:566:LEU:HD23	2:Y:566:LEU:HA	1.81	0.42
6:l:44:ASP:CG	6:l:83:THR:HG22	2.45	0.42
6:n:47:PRO:HA	6:n:80:THR:HG23	2.02	0.42
6:n:181:LEU:HD11	6:n:241:ILE:HD11	2.01	0.42
2:J:465:SER:HB2	2:J:585:ALA:HA	2.01	0.42
2:J:514:PRO:HG3	2:J:563:LEU:HD22	2.00	0.42
2:J:551:ASP:OD1	2:J:551:ASP:N	2.52	0.42
6:A:66:ASP:O	6:l:75:LYS:N	2.52	0.42
6:A:205:ALA:HA	6:A:217:ASN:O	2.19	0.42
1:D:15:ALA:HB3	1:D:43:THR:HG23	2.02	0.42
2:E:213:PRO:HG2	3:G:175:TRP:HZ2	1.85	0.42
3:G:92:ALA:HA	3:G:97:SER:HA	2.01	0.42
6:P:43:LYS:H	6:P:84:LEU:HA	1.85	0.42
6:S:139:ARG:HG3	6:S:139:ARG:NH1	2.35	0.42
6:T:196:ARG:HA	6:T:196:ARG:HH11	1.85	0.42
6:W:163:GLY:H	6:W:187:PRO:HB3	1.85	0.42
2:J:33:GLY:O	2:J:71:GLY:HA3	2.19	0.42
2:J:504:THR:OG1	2:J:544:VAL:O	2.28	0.42
2:J:792:VAL:HG12	2:J:797:LYS:HG3	2.02	0.42
6:c:18:TRP:CZ3	6:c:38:ARG:HB2	2.55	0.42
6:c:127:ILE:HG22	6:c:141:VAL:HG13	2.01	0.42
2:E:116:PHE:HB3	2:E:181:MET:HE1	2.02	0.42
2:E:116:PHE:CZ	2:E:153:ILE:HD13	2.55	0.42
2:E:127:LYS:HE3	2:E:127:LYS:HB2	1.88	0.42
2:E:161:SER:OG	2:Y:627:GLU:OE2	2.29	0.42
2:E:508:ASP:OD1	2:E:508:ASP:N	2.53	0.42
6:Q:27:TYR:HE1	6:Q:119:VAL:HG22	1.85	0.42
6:Q:237:ALA:HA	6:R:200:ALA:HB1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:199:SER:HA	6:T:226:ILE:HA	2.02	0.42
6:U:168:PRO:HB3	6:U:239:ALA:HB1	2.01	0.42
3:d:168:MET:HE2	5:f:184:ALA:HB1	2.02	0.42
4:e:829:MET:HE2	4:e:829:MET:HB2	1.83	0.42
6:l:221:ALA:HA	6:l:243:VAL:HB	2.01	0.42
6:o:18:TRP:HB3	6:o:36:TRP:HB3	2.02	0.42
2:J:419:ASP:O	2:J:423:ILE:HG13	2.19	0.42
2:J:781:PRO:HA	2:J:807:ALA:HB3	2.01	0.42
6:V:87:MET:HE3	6:V:87:MET:HB2	1.80	0.42
6:v:163:GLY:HA3	6:v:187:PRO:HA	2.01	0.42
2:E:112:LEU:HD12	2:E:112:LEU:HA	1.90	0.42
2:E:252:GLN:H	2:E:252:GLN:HG2	1.69	0.42
2:E:296:VAL:HG12	2:E:357:LEU:HD23	2.02	0.42
3:G:28:LEU:HD13	3:G:95:MET:HG2	2.02	0.42
6:O:99:TRP:CD1	6:O:106:ARG:HG3	2.55	0.42
6:P:200:ALA:N	6:P:225:ASN:O	2.48	0.42
6:Q:238:VAL:HG11	6:R:238:VAL:HG11	2.02	0.42
2:Y:622:GLN:H	2:Y:622:GLN:HG2	1.69	0.42
5:f:187:ASN:O	5:f:188:VAL:HG22	2.20	0.42
6:j:185:PHE:CD1	6:j:191:THR:HG21	2.55	0.42
6:l:109:LYS:HD2	6:l:117:VAL:HG21	2.02	0.42
6:n:20:TYR:HD2	6:n:36:TRP:CE2	2.38	0.42
1:M:41:LEU:HD13	1:M:41:LEU:HA	1.82	0.42
2:J:723:THR:OG1	2:J:730:THR:HB	2.20	0.42
6:C:168:PRO:HB3	6:C:239:ALA:HB1	2.02	0.42
1:D:24:ARG:NH2	1:D:25:PHE:O	2.53	0.42
2:E:249:TYR:OH	2:E:309:ASP:OD2	2.37	0.42
6:T:201:ASP:OD2	6:T:203:THR:OG1	2.36	0.42
2:Y:33:GLY:O	2:Y:71:GLY:HA3	2.20	0.42
2:Y:114:PHE:O	2:Y:166:SER:HA	2.20	0.42
2:Y:577:ARG:HA	3:d:67:GLU:HB3	2.02	0.42
1:Z:89:TRP:O	1:Z:89:TRP:CD1	2.73	0.42
6:l:205:ALA:HA	6:l:217:ASN:O	2.19	0.42
6:o:18:TRP:CZ3	6:o:38:ARG:HB2	2.55	0.42
2:J:109:ILE:HD11	2:J:112:LEU:HD13	2.02	0.41
2:J:209:LYS:HB2	2:J:209:LYS:HE2	1.89	0.41
2:J:345:ALA:HB2	2:J:436:PHE:HB3	2.00	0.41
2:J:404:ILE:HD11	5:I:174:THR:OG1	2.19	0.41
2:J:510:GLU:HA	2:J:541:GLY:O	2.19	0.41
2:E:30:ILE:HD13	2:E:238:LEU:HD11	2.01	0.41
2:E:40:ASP:OD2	2:E:40:ASP:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:70:SER:OG	1:F:83:LYS:NZ	2.52	0.41
6:Q:124:VAL:HG22	6:Q:143:VAL:HG22	2.02	0.41
6:S:118:ASP:C	6:S:118:ASP:OD2	2.63	0.41
6:S:183:VAL:HG21	6:S:214:ILE:HD12	2.02	0.41
6:W:18:TRP:CZ3	6:W:38:ARG:HB2	2.55	0.41
6:W:79:ASP:OD2	6:W:142:LYS:NZ	2.52	0.41
6:W:128:GLY:HA3	6:W:140:THR:HB	2.01	0.41
2:Y:138:LEU:HD23	2:Y:140:GLN:HG3	2.02	0.41
2:Y:173:PRO:HD2	2:Y:177:PHE:CZ	2.54	0.41
2:Y:245:VAL:CG2	2:Y:246:PRO:HD2	2.50	0.41
2:Y:684:ALA:O	2:Y:688:TYR:OH	2.31	0.41
6:h:194:SER:O	6:h:231:GLY:N	2.52	0.41
6:k:3:VAL:HB	6:k:4:PRO:HD3	2.01	0.41
6:k:177:GLN:O	6:k:217:ASN:ND2	2.53	0.41
2:J:96:TYR:CD2	2:J:186:PRO:HA	2.51	0.41
2:J:845:LEU:HD22	2:E:845:LEU:HD22	2.01	0.41
5:I:116:PHE:N	5:I:116:PHE:CD2	2.87	0.41
6:A:173:VAL:O	6:A:243:VAL:HG13	2.20	0.41
2:E:69:ARG:HD3	2:E:69:ARG:HA	1.93	0.41
2:E:101:THR:HA	2:E:179:ILE:O	2.20	0.41
2:E:643:THR:HG21	2:E:650:VAL:HG11	2.02	0.41
1:F:70:SER:HB3	1:F:85:THR:HG22	2.02	0.41
6:O:77:ALA:O	6:O:145:ASN:ND2	2.50	0.41
6:Q:3:VAL:HB	6:Q:4:PRO:HD3	2.02	0.41
6:S:194:SER:OG	6:S:195:PHE:N	2.52	0.41
6:T:46:THR:O	6:T:46:THR:OG1	2.34	0.41
6:U:49:GLU:OE1	6:U:49:GLU:N	2.39	0.41
2:Y:495:VAL:O	2:Y:556:TYR:N	2.37	0.41
1:Z:88:LYS:HB3	1:Z:88:LYS:NZ	2.35	0.41
6:g:31:LEU:O	6:g:111:ARG:NH1	2.53	0.41
6:i:163:GLY:HA3	6:i:187:PRO:HB3	2.02	0.41
6:k:173:VAL:O	6:k:243:VAL:HG13	2.21	0.41
6:o:106:ARG:HE	6:o:106:ARG:HB3	1.57	0.41
6:o:108:TYR:CZ	6:o:120:PHE:HB2	2.55	0.41
6:o:122:GLY:HA3	6:o:145:ASN:HA	2.01	0.41
2:J:40:ASP:C	2:J:40:ASP:OD1	2.63	0.41
3:L:83:ASN:H	3:L:147:SER:HA	1.86	0.41
6:a:46:THR:O	6:a:46:THR:OG1	2.35	0.41
1:D:24:ARG:NH2	1:D:26:GLY:O	2.46	0.41
2:E:373:ARG:H	2:E:373:ARG:HG2	1.64	0.41
1:F:68:TRP:CD1	1:F:68:TRP:H	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:33:ASP:OD1	6:S:109:LYS:NZ	2.40	0.41
6:T:150:SER:OG	6:T:155:ARG:NH2	2.39	0.41
6:U:48:GLY:H	6:U:80:THR:HA	1.85	0.41
2:Y:90:LEU:HD22	2:Y:102:ARG:HG3	2.03	0.41
3:d:52:GLN:NE2	3:d:127:PRO:O	2.28	0.41
6:h:149:PRO:HG2	6:h:151:MET:HE2	2.03	0.41
6:i:51:THR:HG22	6:i:52:ALA:N	2.30	0.41
6:k:201:ASP:OD2	6:k:204:LYS:HE2	2.21	0.41
2:J:114:PHE:CD1	2:J:169:MET:HE1	2.54	0.41
5:I:109:ALA:HB3	3:d:142:GLU:HB2	2.02	0.41
5:I:163:ARG:HH11	5:f:163:ARG:NH2	2.18	0.41
6:V:18:TRP:CZ3	6:V:38:ARG:HB2	2.56	0.41
6:B:9:PRO:CD	6:j:87:MET:HE1	2.50	0.41
6:C:43:LYS:HA	6:C:43:LYS:HD3	1.76	0.41
2:E:127:LYS:HB2	2:E:128:GLY:H	1.71	0.41
2:E:152:ASP:OD1	2:E:152:ASP:N	2.53	0.41
2:E:206:ILE:O	2:E:209:LYS:NZ	2.45	0.41
6:Q:163:GLY:HA3	6:Q:187:PRO:HB3	2.02	0.41
6:T:194:SER:OG	6:T:195:PHE:N	2.53	0.41
2:Y:290:ARG:HG2	2:Y:291:LEU:H	1.84	0.41
2:Y:792:VAL:HG12	2:Y:797:LYS:HG3	2.03	0.41
6:i:3:VAL:HB	6:i:4:PRO:HD3	2.01	0.41
6:o:79:ASP:OD2	6:o:142:LYS:NZ	2.53	0.41
2:J:845:LEU:HD22	2:Y:845:LEU:HD22	2.02	0.41
2:E:465:SER:HB2	2:E:585:ALA:HA	2.01	0.41
6:O:134:LYS:NZ	6:T:53:GLU:OE2	2.54	0.41
6:Q:116:THR:H	6:Q:116:THR:HG1	1.58	0.41
6:T:63:GLU:O	6:T:64:ASP:OD2	2.37	0.41
6:W:108:TYR:CZ	6:W:120:PHE:HB2	2.55	0.41
2:Y:410:TRP:HB2	5:f:179:LEU:HD11	2.02	0.41
3:d:166:ARG:O	5:f:188:VAL:HA	2.20	0.41
6:g:87:MET:HE3	6:g:87:MET:HB2	1.86	0.41
6:h:43:LYS:H	6:h:84:LEU:HA	1.85	0.41
6:k:195:PHE:HB3	6:k:230:SER:OG	2.20	0.41
6:l:126:SER:HB3	6:l:142:LYS:HB3	2.02	0.41
2:J:87:GLU:OE2	2:J:201:SER:OG	2.35	0.41
2:J:539:THR:OG1	2:J:540:ASP:OD2	2.38	0.41
1:m:109:ASN:ND2	1:D:29:TYR:HD1	2.18	0.41
6:B:185:PHE:O	6:B:187:PRO:HD3	2.20	0.41
6:A:167:THR:O	6:A:182:THR:OG1	2.36	0.41
6:a:90:GLU:OE1	6:a:93:GLN:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:404:ILE:HD11	5:N:174:THR:OG1	2.21	0.41
2:E:453:LYS:HA	2:E:453:LYS:HD3	1.59	0.41
2:E:827:LEU:HD12	2:E:831:LEU:HD12	2.03	0.41
6:R:43:LYS:N	6:R:83:THR:O	2.52	0.41
6:R:164:MET:HB3	6:R:235:PHE:CD2	2.56	0.41
6:T:171:THR:OG1	6:T:172:SER:N	2.52	0.41
2:Y:374:SER:HG	2:Y:494:ARG:HE	1.67	0.41
2:Y:772:TRP:CE3	2:Y:772:TRP:HA	2.56	0.41
6:k:163:GLY:HA2	6:k:235:PHE:CD2	2.55	0.41
6:n:18:TRP:HB2	6:n:109:LYS:HG2	2.02	0.41
2:J:375:ASN:ND2	2:J:558:VAL:HG21	2.36	0.41
6:v:195:PHE:HB2	6:v:230:SER:HA	2.02	0.41
6:A:118:ASP:OD1	6:A:118:ASP:C	2.63	0.41
2:E:845:LEU:HD22	2:Y:845:LEU:HD22	2.01	0.41
6:W:99:TRP:CD2	6:W:106:ARG:HD2	2.55	0.41
1:Z:16:SER:HB2	1:Z:40:ASN:HD22	1.85	0.41
1:Z:68:TRP:CD1	1:Z:68:TRP:H	2.39	0.41
6:h:185:PHE:HZ	6:h:195:PHE:HB3	1.86	0.41
6:k:52:ALA:HB1	6:k:72:GLN:HG3	2.03	0.41
6:k:129:LYS:HB2	6:k:129:LYS:HE3	1.81	0.41
1:M:83:LYS:HB3	1:M:83:LYS:HE3	1.56	0.41
5:I:184:ALA:HB2	5:I:201:ARG:HB3	2.03	0.41
6:B:68:THR:HG23	6:j:75:LYS:O	2.20	0.41
2:E:135:VAL:HA	2:E:185:THR:HG21	2.02	0.41
2:E:147:TRP:NE1	2:E:180:ARG:HH21	2.19	0.41
6:Q:63:GLU:O	6:Q:64:ASP:OD1	2.38	0.41
6:R:193:LYS:HE2	6:R:193:LYS:HB2	1.93	0.41
6:R:211:GLY:O	6:R:212:MET:HB3	2.19	0.41
6:T:44:ASP:OD1	6:T:44:ASP:C	2.63	0.41
2:Y:102:ARG:HA	2:Y:102:ARG:HD3	1.83	0.41
2:Y:551:ASP:OD1	2:Y:551:ASP:N	2.51	0.41
6:i:181:LEU:O	6:i:214:ILE:HB	2.21	0.41
6:l:155:ARG:H	6:l:155:ARG:HG2	1.74	0.41
2:J:328:TYR:CD1	5:I:192:LEU:HB2	2.56	0.41
2:J:366:ASP:OD1	2:J:366:ASP:N	2.37	0.41
2:J:578:GLU:HG2	2:J:584:TYR:CE2	2.56	0.41
2:J:748:PHE:HB2	2:J:766:LEU:HD21	2.03	0.41
6:V:221:ALA:HA	6:V:243:VAL:HB	2.02	0.41
6:v:18:TRP:NE1	6:v:111:ARG:HG3	2.35	0.41
6:v:194:SER:O	6:v:231:GLY:N	2.53	0.41
6:A:205:ALA:HB3	6:A:224:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:a:175:LYS:HE3	6:a:220:ALA:HA	2.02	0.41
6:a:221:ALA:HA	6:a:243:VAL:HB	2.03	0.41
6:C:152:ALA:HA	6:C:155:ARG:HH12	1.86	0.41
6:C:195:PHE:HE2	6:C:214:ILE:HD11	1.85	0.41
6:c:199:SER:N	6:c:207:VAL:HG21	2.36	0.41
2:E:130:ARG:H	2:E:130:ARG:HG2	1.72	0.41
2:E:248:ASN:OD1	2:E:248:ASN:C	2.64	0.41
2:E:291:LEU:HD21	2:E:296:VAL:HG13	2.03	0.41
2:E:822:ILE:HG22	2:E:826:HIS:CD2	2.56	0.41
4:K:829:MET:HE2	4:K:829:MET:HB2	1.76	0.41
5:N:117:PHE:C	5:N:120:GLY:H	2.28	0.41
6:P:148:ARG:HE	6:P:148:ARG:HB3	1.72	0.41
6:Q:185:PHE:C	6:Q:187:PRO:HD3	2.46	0.41
6:T:17:LEU:HD23	6:T:39:LEU:HD12	2.03	0.41
6:U:46:THR:O	6:U:46:THR:OG1	2.37	0.41
6:W:8:MET:SD	6:W:8:MET:N	2.94	0.41
6:W:202:LYS:HA	6:W:202:LYS:HD3	1.79	0.41
2:Y:404:ILE:HD11	5:f:174:THR:OG1	2.21	0.41
2:Y:527:SER:O	3:d:6:GLN:NE2	2.53	0.41
6:j:18:TRP:HB2	6:j:109:LYS:HG2	2.03	0.41
6:k:11:LYS:HD3	6:k:11:LYS:HA	1.95	0.41
6:k:205:ALA:HB3	6:k:224:VAL:HG21	2.02	0.41
6:k:209:VAL:HG13	6:k:214:ILE:HG12	2.03	0.41
6:l:132:THR:HG23	6:l:135:GLU:HB3	2.03	0.41
6:n:165:THR:HG22	6:n:184:ALA:HB3	2.02	0.41
6:n:169:ALA:HB1	6:n:171:THR:HG22	2.03	0.41
6:o:166:VAL:HG22	6:o:183:VAL:HG22	2.03	0.41
2:J:147:TRP:NE1	2:J:180:ARG:HE	2.19	0.41
2:J:213:PRO:HG2	3:L:175:TRP:HZ2	1.86	0.41
6:V:108:TYR:CZ	6:V:120:PHE:HB2	2.56	0.41
6:v:42:VAL:O	6:S:59:TYR:HB3	2.21	0.41
6:B:74:GLN:HG2	6:b:65:ALA:O	2.21	0.41
6:B:168:PRO:HA	6:B:181:LEU:HG	2.03	0.41
6:A:201:ASP:OD2	6:A:204:LYS:HE2	2.21	0.41
6:C:16:THR:OG1	6:C:18:TRP:NE1	2.52	0.41
6:c:163:GLY:H	6:c:187:PRO:HB3	1.86	0.41
6:c:232:ASN:N	6:c:234:GLU:OE1	2.54	0.41
2:E:141:ILE:HB	2:E:150:GLU:CD	2.46	0.41
2:E:265:LYS:HE2	2:E:265:LYS:HB3	1.86	0.41
2:E:372:ASN:HD21	2:E:558:VAL:HG13	1.86	0.41
2:E:410:TRP:CH2	5:N:196:MET:HA	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:527:SER:O	3:G:6:GLN:NE2	2.54	0.41
2:E:589:VAL:HB	5:N:154:MET:HE1	2.04	0.41
6:O:102:GLU:HG2	6:O:104:ASP:H	1.86	0.41
6:O:199:SER:HB3	6:O:202:LYS:HD3	2.03	0.41
6:P:194:SER:O	6:P:231:GLY:N	2.53	0.41
6:S:129:LYS:HB2	6:S:129:LYS:HE3	1.77	0.41
6:S:160:ALA:O	6:S:162:THR:N	2.54	0.41
6:U:126:SER:OG	6:W:49:GLU:OE2	2.26	0.41
1:Z:38:ASN:ND2	1:Z:108:VAL:HG21	2.36	0.41
3:d:32:GLY:O	3:d:95:MET:HE1	2.20	0.41
6:g:211:GLY:C	6:g:213:THR:H	2.28	0.41
6:k:33:ASP:OD1	6:k:109:LYS:NZ	2.49	0.41
6:k:114:ASN:OD1	6:k:116:THR:OG1	2.38	0.41
6:l:63:GLU:HA	6:l:63:GLU:OE1	2.21	0.41
6:l:171:THR:OG1	6:l:172:SER:N	2.53	0.41
6:o:199:SER:N	6:o:207:VAL:HG21	2.35	0.41
2:J:290:ARG:HG2	2:J:291:LEU:H	1.85	0.40
2:J:725:GLY:HA3	2:J:728:GLN:HG2	2.02	0.40
6:v:164:MET:HG2	6:v:235:PHE:CB	2.48	0.40
6:B:3:VAL:HB	6:B:4:PRO:HD3	2.02	0.40
6:c:79:ASP:OD2	6:c:142:LYS:NZ	2.53	0.40
6:c:96:LEU:HD23	6:c:97:LEU:HD22	2.03	0.40
2:E:124:THR:N	2:E:192:GLN:O	2.54	0.40
5:N:184:ALA:HB2	5:N:201:ARG:HB3	2.03	0.40
6:T:44:ASP:CG	6:T:83:THR:HG22	2.45	0.40
6:W:124:VAL:HG22	6:W:143:VAL:HG22	2.03	0.40
3:d:191:ASP:OD1	3:d:191:ASP:N	2.53	0.40
6:o:135:GLU:OE1	6:o:136:VAL:N	2.54	0.40
6:o:202:LYS:HA	6:o:202:LYS:HD3	1.77	0.40
2:J:90:LEU:HD11	2:J:199:TRP:CD2	2.56	0.40
2:J:627:GLU:OE2	2:Y:161:SER:OG	2.28	0.40
6:C:169:ALA:HB1	6:C:171:THR:HG22	2.02	0.40
2:E:828:GLY:O	2:E:832:LEU:HD12	2.22	0.40
6:P:202:LYS:HD3	6:P:202:LYS:HA	1.82	0.40
6:U:17:LEU:HD11	6:U:39:LEU:HD12	2.04	0.40
6:U:169:ALA:HB1	6:U:171:THR:HG22	2.03	0.40
1:X:26:GLY:O	1:X:28:GLY:N	2.53	0.40
2:Y:366:ASP:OD1	2:Y:366:ASP:N	2.34	0.40
6:g:17:LEU:HD11	6:g:45:LEU:HD13	2.03	0.40
6:g:119:VAL:HG13	6:g:150:SER:HB3	2.04	0.40
6:g:153:GLU:OE1	6:g:153:GLU:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:h:79:ASP:OD1	6:h:79:ASP:N	2.54	0.40
6:i:185:PHE:C	6:i:187:PRO:HD3	2.47	0.40
6:j:44:ASP:OD1	6:j:83:THR:OG1	2.32	0.40
6:l:194:SER:OG	6:l:195:PHE:N	2.53	0.40
6:n:101:ASN:O	6:o:75:LYS:NZ	2.47	0.40
2:J:566:LEU:HD23	2:J:566:LEU:HA	1.81	0.40
1:m:75:PRO:HA	1:m:76:PRO:HD3	1.91	0.40
6:v:43:LYS:H	6:v:84:LEU:HA	1.86	0.40
6:A:195:PHE:HZ	6:A:212:MET:HA	1.86	0.40
6:a:123:TRP:HE3	6:S:72:GLN:HE21	1.70	0.40
6:a:126:SER:HB3	6:a:142:LYS:HB3	2.04	0.40
6:c:126:SER:HB2	6:U:51:THR:HA	2.03	0.40
2:E:16:ASP:OD1	2:E:666:ARG:NH1	2.54	0.40
2:E:748:PHE:HB2	2:E:766:LEU:HD21	2.02	0.40
6:P:36:TRP:CD1	6:P:109:LYS:HZ3	2.40	0.40
6:P:119:VAL:HG13	6:P:150:SER:HB3	2.02	0.40
6:P:168:PRO:HA	6:P:181:LEU:HG	2.03	0.40
6:S:64:ASP:OD1	6:S:64:ASP:C	2.64	0.40
6:i:111:ARG:HG2	6:i:117:VAL:HG22	2.02	0.40
6:o:29:ASN:OD1	6:o:32:SER:HB3	2.21	0.40
1:M:18:PRO:HD2	1:Z:87:ALA:O	2.22	0.40
2:J:817:PHE:CZ	2:Y:810:ASP:HA	2.57	0.40
1:m:55:ALA:HB2	1:m:98:VAL:HG21	2.04	0.40
3:L:26:ILE:O	3:L:35:ARG:HA	2.22	0.40
6:b:32:SER:O	6:b:109:LYS:NZ	2.54	0.40
6:A:160:ALA:O	6:A:162:THR:HG23	2.21	0.40
6:A:178:SER:HB3	6:A:217:ASN:HB2	2.03	0.40
2:E:28:ASP:OD1	2:E:236:TYR:OH	2.36	0.40
2:E:622:GLN:H	2:E:622:GLN:HG2	1.70	0.40
6:R:150:SER:OG	6:R:155:ARG:NH2	2.44	0.40
6:W:199:SER:N	6:W:207:VAL:HG21	2.36	0.40
2:Y:3:LYS:HE2	2:Y:3:LYS:HB3	1.69	0.40
2:Y:127:LYS:HB2	2:Y:128:GLY:H	1.70	0.40
2:Y:508:ASP:OD2	2:Y:509:ARG:NH1	2.54	0.40
4:e:818:ILE:HG12	5:f:130:ILE:HG21	2.04	0.40
6:h:173:VAL:HG13	6:h:243:VAL:HG13	2.03	0.40
6:j:193:LYS:HE2	6:j:193:LYS:HB2	1.92	0.40
6:n:21:LYS:HZ2	6:n:36:TRP:C	2.30	0.40
6:n:164:MET:SD	6:n:165:THR:N	2.94	0.40
6:o:47:PRO:HA	6:o:80:THR:HG23	2.03	0.40
1:M:29:TYR:OH	2:J:508:ASP:OD2	2.31	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:136:ARG:NH1	2:J:184:MET:HG3	2.36	0.40
6:v:149:PRO:HG2	6:v:151:MET:HE3	2.03	0.40
6:B:185:PHE:C	6:B:187:PRO:HD3	2.47	0.40
3:G:204:LYS:HB3	3:G:204:LYS:HE2	1.54	0.40
5:N:137:GLY:O	5:N:139:LEU:HD22	2.21	0.40
6:O:197:ALA:HB3	6:O:209:VAL:HG21	2.02	0.40
2:Y:69:ARG:HA	2:Y:69:ARG:HD3	1.89	0.40
2:Y:514:PRO:HG3	2:Y:563:LEU:HD22	2.03	0.40
2:Y:745:GLU:HG2	2:Y:765:TYR:HE1	1.87	0.40
2:Y:809:ASP:O	2:Y:811:ALA:N	2.54	0.40
3:d:5:ARG:H	3:d:5:ARG:HG2	1.72	0.40
3:d:167:ILE:HG12	3:d:169:LEU:HG	2.04	0.40
6:i:64:ASP:C	6:i:64:ASP:OD1	2.65	0.40
6:j:42:VAL:HG22	6:j:84:LEU:HD23	2.03	0.40
6:k:193:LYS:HE2	6:k:231:GLY:HA3	2.03	0.40
6:l:175:LYS:HE3	6:l:220:ALA:HA	2.04	0.40
6:n:52:ALA:HA	6:n:75:LYS:HA	2.02	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	D	107/109 (98%)	94 (88%)	13 (12%)	0	100	100
1	F	107/109 (98%)	93 (87%)	13 (12%)	1 (1%)	14	48
1	M	107/109 (98%)	94 (88%)	13 (12%)	0	100	100
1	X	107/109 (98%)	94 (88%)	13 (12%)	0	100	100
1	Z	107/109 (98%)	95 (89%)	11 (10%)	1 (1%)	14	48
1	m	107/109 (98%)	92 (86%)	14 (13%)	1 (1%)	14	48
2	E	859/1132 (76%)	780 (91%)	75 (9%)	4 (0%)	24	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	J	859/1132 (76%)	773 (90%)	82 (10%)	4 (0%)	24	60
2	Y	859/1132 (76%)	775 (90%)	81 (9%)	3 (0%)	36	70
3	G	230/232 (99%)	222 (96%)	8 (4%)	0	100	100
3	L	230/232 (99%)	222 (96%)	8 (4%)	0	100	100
3	d	230/232 (99%)	224 (97%)	6 (3%)	0	100	100
4	H	31/853 (4%)	25 (81%)	6 (19%)	0	100	100
4	K	31/853 (4%)	25 (81%)	6 (19%)	0	100	100
4	e	31/853 (4%)	26 (84%)	5 (16%)	0	100	100
5	I	120/223 (54%)	97 (81%)	17 (14%)	6 (5%)	1	10
5	N	120/223 (54%)	97 (81%)	17 (14%)	6 (5%)	1	10
5	f	120/223 (54%)	97 (81%)	17 (14%)	6 (5%)	1	10
6	A	242/246 (98%)	225 (93%)	14 (6%)	3 (1%)	10	40
6	B	242/246 (98%)	223 (92%)	18 (7%)	1 (0%)	30	65
6	C	242/246 (98%)	224 (93%)	16 (7%)	2 (1%)	16	50
6	O	241/246 (98%)	227 (94%)	13 (5%)	1 (0%)	30	65
6	P	241/246 (98%)	229 (95%)	12 (5%)	0	100	100
6	Q	242/246 (98%)	223 (92%)	18 (7%)	1 (0%)	30	65
6	R	242/246 (98%)	228 (94%)	13 (5%)	1 (0%)	30	65
6	S	242/246 (98%)	224 (93%)	15 (6%)	3 (1%)	10	40
6	T	242/246 (98%)	231 (96%)	10 (4%)	1 (0%)	30	65
6	U	242/246 (98%)	225 (93%)	14 (6%)	3 (1%)	10	40
6	V	241/246 (98%)	228 (95%)	12 (5%)	1 (0%)	30	65
6	W	242/246 (98%)	228 (94%)	14 (6%)	0	100	100
6	a	242/246 (98%)	232 (96%)	9 (4%)	1 (0%)	30	65
6	b	242/246 (98%)	230 (95%)	11 (4%)	1 (0%)	30	65
6	c	242/246 (98%)	230 (95%)	12 (5%)	0	100	100
6	g	241/246 (98%)	229 (95%)	11 (5%)	1 (0%)	30	65
6	h	241/246 (98%)	228 (95%)	13 (5%)	0	100	100
6	i	242/246 (98%)	224 (93%)	17 (7%)	1 (0%)	30	65
6	j	242/246 (98%)	229 (95%)	12 (5%)	1 (0%)	30	65
6	k	242/246 (98%)	224 (93%)	15 (6%)	3 (1%)	10	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	l	242/246 (98%)	230 (95%)	11 (4%)	1 (0%)	30	65
6	n	242/246 (98%)	225 (93%)	15 (6%)	2 (1%)	16	50
6	o	242/246 (98%)	229 (95%)	12 (5%)	1 (0%)	30	65
6	v	241/246 (98%)	228 (95%)	13 (5%)	0	100	100
All	All	10164/13878 (73%)	9378 (92%)	725 (7%)	61 (1%)	23	56

All (61) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	I	105	ILE
5	I	188	VAL
5	I	190	PRO
6	V	158	VAL
6	B	158	VAL
6	A	158	VAL
6	C	158	VAL
5	N	105	ILE
5	N	188	VAL
5	N	190	PRO
6	O	158	VAL
6	Q	158	VAL
6	S	158	VAL
6	U	158	VAL
5	f	105	ILE
5	f	188	VAL
5	f	190	PRO
6	g	158	VAL
6	i	158	VAL
6	k	158	VAL
6	n	158	VAL
2	J	101	THR
2	E	101	THR
2	J	326	ASN
2	E	326	ASN
6	R	64	ASP
6	S	161	ALA
2	Y	101	THR
2	Y	326	ASN
6	k	161	ALA
6	l	64	ASP
5	I	189	LEU

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Mol	Chain	Res	Type
6	a	64	ASP
5	N	189	LEU
6	T	64	ASP
6	j	64	ASP
1	m	39	ALA
5	I	106	VAL
6	A	64	ASP
6	C	161	ALA
1	F	39	ALA
5	N	106	VAL
5	N	138	ILE
5	f	106	VAL
5	f	138	ILE
5	f	189	LEU
6	k	64	ASP
6	b	64	ASP
6	A	161	ALA
2	E	325	CYS
6	S	64	ASP
6	U	64	ASP
6	U	161	ALA
1	Z	39	ALA
6	n	161	ALA
6	o	64	ASP
2	J	613	VAL
2	E	613	VAL
2	Y	613	VAL
5	I	138	ILE
2	J	616	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	96/96 (100%)	89 (93%)	7 (7%)	13	42
1	F	96/96 (100%)	92 (96%)	4 (4%)	26	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	96/96 (100%)	88 (92%)	8 (8%)	10	37
1	X	96/96 (100%)	86 (90%)	10 (10%)	7	28
1	Z	96/96 (100%)	91 (95%)	5 (5%)	21	55
1	m	96/96 (100%)	94 (98%)	2 (2%)	47	75
2	E	734/958 (77%)	683 (93%)	51 (7%)	14	45
2	J	734/958 (77%)	685 (93%)	49 (7%)	15	46
2	Y	734/958 (77%)	676 (92%)	58 (8%)	11	39
3	G	198/198 (100%)	187 (94%)	11 (6%)	19	52
3	L	198/198 (100%)	187 (94%)	11 (6%)	19	52
3	d	198/198 (100%)	194 (98%)	4 (2%)	48	76
4	H	24/648 (4%)	24 (100%)	0	100	100
4	K	24/648 (4%)	24 (100%)	0	100	100
4	e	24/648 (4%)	24 (100%)	0	100	100
5	I	86/162 (53%)	81 (94%)	5 (6%)	18	51
5	N	86/162 (53%)	80 (93%)	6 (7%)	14	44
5	f	86/162 (53%)	79 (92%)	7 (8%)	11	38
6	A	194/196 (99%)	175 (90%)	19 (10%)	7	30
6	B	194/196 (99%)	179 (92%)	15 (8%)	12	40
6	C	194/196 (99%)	184 (95%)	10 (5%)	21	55
6	O	193/196 (98%)	176 (91%)	17 (9%)	9	35
6	P	193/196 (98%)	175 (91%)	18 (9%)	8	32
6	Q	194/196 (99%)	173 (89%)	21 (11%)	6	26
6	R	194/196 (99%)	179 (92%)	15 (8%)	12	40
6	S	194/196 (99%)	178 (92%)	16 (8%)	10	37
6	T	194/196 (99%)	178 (92%)	16 (8%)	10	37
6	U	194/196 (99%)	182 (94%)	12 (6%)	16	49
6	V	193/196 (98%)	182 (94%)	11 (6%)	18	52
6	W	194/196 (99%)	182 (94%)	12 (6%)	16	49
6	a	194/196 (99%)	181 (93%)	13 (7%)	15	46
6	b	194/196 (99%)	179 (92%)	15 (8%)	12	40
6	c	194/196 (99%)	182 (94%)	12 (6%)	16	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	g	193/196 (98%)	179 (93%)	14 (7%)	13	42
6	h	193/196 (98%)	180 (93%)	13 (7%)	15	46
6	i	194/196 (99%)	176 (91%)	18 (9%)	8	32
6	j	194/196 (99%)	178 (92%)	16 (8%)	10	37
6	k	194/196 (99%)	179 (92%)	15 (8%)	12	40
6	l	194/196 (99%)	176 (91%)	18 (9%)	8	32
6	n	194/196 (99%)	183 (94%)	11 (6%)	18	52
6	o	194/196 (99%)	184 (95%)	10 (5%)	21	55
6	v	193/196 (98%)	177 (92%)	16 (8%)	10	37
All	All	8352/11178 (75%)	7761 (93%)	591 (7%)	15	43

All (591) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	41	LEU
1	M	46	VAL
1	M	47	THR
1	M	50	VAL
1	M	84	VAL
1	M	91	SER
1	M	99	GLU
1	M	108	VAL
2	J	26	VAL
2	J	39	VAL
2	J	47	LEU
2	J	49	SER
2	J	65	THR
2	J	88	THR
2	J	97	ASP
2	J	122	VAL
2	J	138	LEU
2	J	149	THR
2	J	153	ILE
2	J	167	VAL
2	J	168	VAL
2	J	177	PHE
2	J	215	THR
2	J	217	LEU
2	J	223	ASP

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Mol	Chain	Res	Type
2	J	233	SER
2	J	257	SER
2	J	325	CYS
2	J	373	ARG
2	J	374	SER
2	J	380	ASP
2	J	412	THR
2	J	439	THR
2	J	461	THR
2	J	465	SER
2	J	479	ILE
2	J	484	ASP
2	J	500	SER
2	J	504	THR
2	J	511	ILE
2	J	535	VAL
2	J	539	THR
2	J	540	ASP
2	J	543	LYS
2	J	544	VAL
2	J	583	THR
2	J	596	GLU
2	J	600	ASP
2	J	613	VAL
2	J	629	THR
2	J	646	VAL
2	J	667	LEU
2	J	695	VAL
2	J	770	LEU
2	J	823	THR
2	J	827	LEU
2	J	831	LEU
1	m	46	VAL
1	m	74	THR
3	L	1	MET
3	L	31	VAL
3	L	99	VAL
3	L	120	ASN
3	L	141	SER
3	L	151	VAL
3	L	154	THR
3	L	159	ASP

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Mol	Chain	Res	Type
3	L	167	ILE
3	L	171	ASN
3	L	218	VAL
5	I	105	ILE
5	I	107	LEU
5	I	118	THR
5	I	161	THR
5	I	207	ILE
6	V	32	SER
6	V	51	THR
6	V	68	THR
6	V	70	THR
6	V	83	THR
6	V	117	VAL
6	V	125	SER
6	V	136	VAL
6	V	146	VAL
6	V	166	VAL
6	V	174	VAL
6	v	10	VAL
6	v	16	THR
6	v	32	SER
6	v	33	ASP
6	v	61	ASP
6	v	70	THR
6	v	79	ASP
6	v	80	THR
6	v	84	LEU
6	v	119	VAL
6	v	127	ILE
6	v	132	THR
6	v	158	VAL
6	v	171	THR
6	v	179	THR
6	v	191	THR
6	B	54	SER
6	B	66	ASP
6	B	76	SER
6	B	116	THR
6	B	132	THR
6	B	136	VAL
6	B	150	SER

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Mol	Chain	Res	Type
6	B	156	SER
6	B	164	MET
6	B	182	THR
6	B	198	VAL
6	B	199	SER
6	B	213	THR
6	B	230	SER
6	B	232	ASN
6	b	3	VAL
6	b	16	THR
6	b	17	LEU
6	b	23	SER
6	b	31	LEU
6	b	51	THR
6	b	70	THR
6	b	81	SER
6	b	84	LEU
6	b	110	ILE
6	b	138	THR
6	b	146	VAL
6	b	180	THR
6	b	182	THR
6	b	243	VAL
6	A	17	LEU
6	A	34	VAL
6	A	64	ASP
6	A	66	ASP
6	A	76	SER
6	A	83	THR
6	A	125	SER
6	A	127	ILE
6	A	136	VAL
6	A	140	THR
6	A	146	VAL
6	A	186	GLN
6	A	190	VAL
6	A	191	THR
6	A	198	VAL
6	A	215	THR
6	A	224	VAL
6	A	232	ASN
6	A	235	PHE

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Mol	Chain	Res	Type
6	a	33	ASP
6	a	37	SER
6	a	70	THR
6	a	117	VAL
6	a	119	VAL
6	a	126	SER
6	a	132	THR
6	a	138	THR
6	a	174	VAL
6	a	185	PHE
6	a	207	VAL
6	a	212	MET
6	a	215	THR
6	C	16	THR
6	C	17	LEU
6	C	61	ASP
6	C	66	ASP
6	C	97	LEU
6	C	116	THR
6	C	141	VAL
6	C	146	VAL
6	C	159	THR
6	C	180	THR
6	c	7	THR
6	c	16	THR
6	c	17	LEU
6	c	45	LEU
6	c	66	ASP
6	c	83	THR
6	c	117	VAL
6	c	126	SER
6	c	145	ASN
6	c	146	VAL
6	c	180	THR
6	c	240	GLU
1	D	43	THR
1	D	46	VAL
1	D	47	THR
1	D	50	VAL
1	D	90	SER
1	D	91	SER
1	D	108	VAL

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Mol	Chain	Res	Type
2	E	10	THR
2	E	21	THR
2	E	26	VAL
2	E	30	ILE
2	E	39	VAL
2	E	49	SER
2	E	64	VAL
2	E	65	THR
2	E	97	ASP
2	E	115	THR
2	E	122	VAL
2	E	124	THR
2	E	138	LEU
2	E	139	VAL
2	E	149	THR
2	E	153	ILE
2	E	168	VAL
2	E	177	PHE
2	E	204	GLU
2	E	215	THR
2	E	217	LEU
2	E	223	ASP
2	E	233	SER
2	E	241	ARG
2	E	257	SER
2	E	281	THR
2	E	324	THR
2	E	325	CYS
2	E	330	THR
2	E	397	ASN
2	E	412	THR
2	E	439	THR
2	E	465	SER
2	E	502	THR
2	E	504	THR
2	E	511	ILE
2	E	531	VAL
2	E	540	ASP
2	E	544	VAL
2	E	566	LEU
2	E	596	GLU
2	E	600	ASP

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Mol	Chain	Res	Type
2	E	613	VAL
2	E	648	LYS
2	E	653	LEU
2	E	656	LEU
2	E	667	LEU
2	E	703	ASP
2	E	823	THR
2	E	827	LEU
2	E	840	ASP
1	F	46	VAL
1	F	58	LEU
1	F	74	THR
1	F	85	THR
3	G	1	MET
3	G	18	SER
3	G	80	THR
3	G	99	VAL
3	G	111	ARG
3	G	151	VAL
3	G	154	THR
3	G	159	ASP
3	G	167	ILE
3	G	171	ASN
3	G	230	LEU
5	N	105	ILE
5	N	107	LEU
5	N	118	THR
5	N	161	THR
5	N	203	VAL
5	N	204	SER
6	O	17	LEU
6	O	41	LYS
6	O	51	THR
6	O	54	SER
6	O	63	GLU
6	O	68	THR
6	O	70	THR
6	O	83	THR
6	O	117	VAL
6	O	125	SER
6	O	136	VAL
6	O	146	VAL

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Mol	Chain	Res	Type
6	O	166	VAL
6	O	174	VAL
6	O	203	THR
6	O	217	ASN
6	O	232	ASN
6	P	31	LEU
6	P	32	SER
6	P	33	ASP
6	P	53	GLU
6	P	61	ASP
6	P	66	ASP
6	P	70	THR
6	P	80	THR
6	P	97	LEU
6	P	117	VAL
6	P	119	VAL
6	P	127	ILE
6	P	132	THR
6	P	158	VAL
6	P	171	THR
6	P	179	THR
6	P	191	THR
6	P	219	VAL
6	Q	64	ASP
6	Q	66	ASP
6	Q	76	SER
6	Q	97	LEU
6	Q	116	THR
6	Q	119	VAL
6	Q	126	SER
6	Q	131	VAL
6	Q	132	THR
6	Q	136	VAL
6	Q	150	SER
6	Q	156	SER
6	Q	165	THR
6	Q	166	VAL
6	Q	180	THR
6	Q	181	LEU
6	Q	182	THR
6	Q	191	THR
6	Q	198	VAL

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Mol	Chain	Res	Type
6	Q	199	SER
6	Q	230	SER
6	R	16	THR
6	R	17	LEU
6	R	42	VAL
6	R	51	THR
6	R	64	ASP
6	R	70	THR
6	R	81	SER
6	R	84	LEU
6	R	132	THR
6	R	138	THR
6	R	158	VAL
6	R	180	THR
6	R	199	SER
6	R	213	THR
6	R	243	VAL
6	S	37	SER
6	S	64	ASP
6	S	76	SER
6	S	83	THR
6	S	116	THR
6	S	136	VAL
6	S	140	THR
6	S	146	VAL
6	S	148	ARG
6	S	186	GLN
6	S	190	VAL
6	S	191	THR
6	S	198	VAL
6	S	215	THR
6	S	230	SER
6	S	232	ASN
6	T	3	VAL
6	T	17	LEU
6	T	33	ASP
6	T	35	ASP
6	T	37	SER
6	T	46	THR
6	T	70	THR
6	T	117	VAL
6	T	119	VAL

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Mol	Chain	Res	Type
6	T	126	SER
6	T	135	GLU
6	T	140	THR
6	T	180	THR
6	T	207	VAL
6	T	212	MET
6	T	215	THR
6	U	16	THR
6	U	46	THR
6	U	61	ASP
6	U	83	THR
6	U	116	THR
6	U	132	THR
6	U	141	VAL
6	U	146	VAL
6	U	159	THR
6	U	165	THR
6	U	180	THR
6	U	229	VAL
6	W	7	THR
6	W	16	THR
6	W	51	THR
6	W	64	ASP
6	W	66	ASP
6	W	83	THR
6	W	110	ILE
6	W	117	VAL
6	W	126	SER
6	W	132	THR
6	W	145	ASN
6	W	180	THR
1	X	27	ASP
1	X	43	THR
1	X	46	VAL
1	X	47	THR
1	X	50	VAL
1	X	53	GLU
1	X	64	GLU
1	X	91	SER
1	X	103	GLU
1	X	108	VAL
2	Y	26	VAL

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Mol	Chain	Res	Type
2	Y	30	ILE
2	Y	39	VAL
2	Y	49	SER
2	Y	50	THR
2	Y	88	THR
2	Y	97	ASP
2	Y	109	ILE
2	Y	115	THR
2	Y	122	VAL
2	Y	138	LEU
2	Y	149	THR
2	Y	153	ILE
2	Y	167	VAL
2	Y	168	VAL
2	Y	177	PHE
2	Y	197	THR
2	Y	215	THR
2	Y	217	LEU
2	Y	223	ASP
2	Y	233	SER
2	Y	235	ASN
2	Y	241	ARG
2	Y	257	SER
2	Y	281	THR
2	Y	324	THR
2	Y	325	CYS
2	Y	330	THR
2	Y	374	SER
2	Y	380	ASP
2	Y	381	ASP
2	Y	397	ASN
2	Y	412	THR
2	Y	439	THR
2	Y	461	THR
2	Y	469	GLU
2	Y	504	THR
2	Y	507	LEU
2	Y	511	ILE
2	Y	521	ILE
2	Y	531	VAL
2	Y	535	VAL
2	Y	536	GLN

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Mol	Chain	Res	Type
2	Y	539	THR
2	Y	544	VAL
2	Y	565	THR
2	Y	574	VAL
2	Y	596	GLU
2	Y	600	ASP
2	Y	613	VAL
2	Y	667	LEU
2	Y	703	ASP
2	Y	756	ILE
2	Y	783	HIS
2	Y	823	THR
2	Y	827	LEU
2	Y	838	THR
2	Y	840	ASP
1	Z	46	VAL
1	Z	58	LEU
1	Z	74	THR
1	Z	98	VAL
1	Z	106	GLN
3	d	120	ASN
3	d	159	ASP
3	d	167	ILE
3	d	171	ASN
5	f	118	THR
5	f	161	THR
5	f	188	VAL
5	f	191	VAL
5	f	203	VAL
5	f	204	SER
5	f	217	GLN
6	g	51	THR
6	g	63	GLU
6	g	68	THR
6	g	70	THR
6	g	81	SER
6	g	83	THR
6	g	117	VAL
6	g	125	SER
6	g	136	VAL
6	g	146	VAL
6	g	166	VAL

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Mol	Chain	Res	Type
6	g	174	VAL
6	g	191	THR
6	g	203	THR
6	h	31	LEU
6	h	45	LEU
6	h	61	ASP
6	h	70	THR
6	h	80	THR
6	h	117	VAL
6	h	119	VAL
6	h	132	THR
6	h	158	VAL
6	h	171	THR
6	h	179	THR
6	h	182	THR
6	h	191	THR
6	i	17	LEU
6	i	54	SER
6	i	64	ASP
6	i	66	ASP
6	i	76	SER
6	i	116	THR
6	i	131	VAL
6	i	132	THR
6	i	140	THR
6	i	150	SER
6	i	156	SER
6	i	164	MET
6	i	181	LEU
6	i	182	THR
6	i	183	VAL
6	i	199	SER
6	i	230	SER
6	i	232	ASN
6	j	3	VAL
6	j	23	SER
6	j	64	ASP
6	j	66	ASP
6	j	74	GLN
6	j	81	SER
6	j	84	LEU
6	j	116	THR

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Mol	Chain	Res	Type
6	j	132	THR
6	j	146	VAL
6	j	150	SER
6	j	158	VAL
6	j	180	THR
6	j	182	THR
6	j	230	SER
6	j	243	VAL
6	k	66	ASP
6	k	76	SER
6	k	83	THR
6	k	116	THR
6	k	125	SER
6	k	136	VAL
6	k	146	VAL
6	k	186	GLN
6	k	190	VAL
6	k	191	THR
6	k	198	VAL
6	k	207	VAL
6	k	215	THR
6	k	224	VAL
6	k	235	PHE
6	l	3	VAL
6	l	33	ASP
6	l	35	ASP
6	l	37	SER
6	l	54	SER
6	l	66	ASP
6	l	70	THR
6	l	117	VAL
6	l	119	VAL
6	l	138	THR
6	l	140	THR
6	l	174	VAL
6	l	180	THR
6	l	190	VAL
6	l	198	VAL
6	l	207	VAL
6	l	212	MET
6	l	215	THR
6	n	8	MET

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Mol	Chain	Res	Type
6	n	16	THR
6	n	66	ASP
6	n	83	THR
6	n	101	ASN
6	n	116	THR
6	n	132	THR
6	n	141	VAL
6	n	146	VAL
6	n	159	THR
6	n	179	THR
6	o	7	THR
6	o	16	THR
6	o	51	THR
6	o	64	ASP
6	o	66	ASP
6	o	83	THR
6	o	84	LEU
6	o	117	VAL
6	o	126	SER
6	o	127	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
2	J	75	GLN
2	J	144	ASN
2	J	282	HIS
2	J	407	ASN
2	J	408	ASN
2	J	568	GLN
2	J	609	GLN
2	J	623	HIS
3	L	17	GLN
3	L	43	ASN
3	L	55	GLN
3	L	57	GLN
3	L	228	ASN
3	L	232	GLN
5	I	169	ASN
5	I	185	GLN
6	v	74	GLN
6	B	101	ASN

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Mol	Chain	Res	Type
6	b	94	GLN
6	A	29	ASN
6	a	94	GLN
6	a	225	ASN
6	C	94	GLN
6	c	74	GLN
6	c	177	GLN
2	E	75	GLN
2	E	237	HIS
2	E	310	GLN
2	E	407	ASN
2	E	408	ASN
2	E	623	HIS
2	E	826	HIS
3	G	2	GLN
3	G	55	GLN
5	N	169	ASN
5	N	185	GLN
6	O	101	ASN
6	Q	101	ASN
6	S	29	ASN
6	S	217	ASN
6	U	94	GLN
6	W	74	GLN
6	W	91	GLN
6	W	177	GLN
6	W	225	ASN
1	X	38	ASN
2	Y	75	GLN
2	Y	396	HIS
2	Y	568	GLN
2	Y	623	HIS
1	Z	31	GLN
1	Z	38	ASN
3	d	55	GLN
3	d	228	ASN
4	e	841	GLN
5	f	169	ASN
5	f	185	GLN
6	k	29	ASN
6	l	94	GLN
6	l	225	ASN

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Mol	Chain	Res	Type
6	n	94	GLN
6	o	74	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

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	$\# Z > 2$
7	SF4	L	301	3	0,12,12	-	-	-		
7	SF4	d	301	3	0,12,12	-	-	-		
7	SF4	G	301	3	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	SF4	L	301	3	-	-	0/6/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	SF4	d	301	3	-	-	0/6/5/5
7	SF4	G	301	3	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

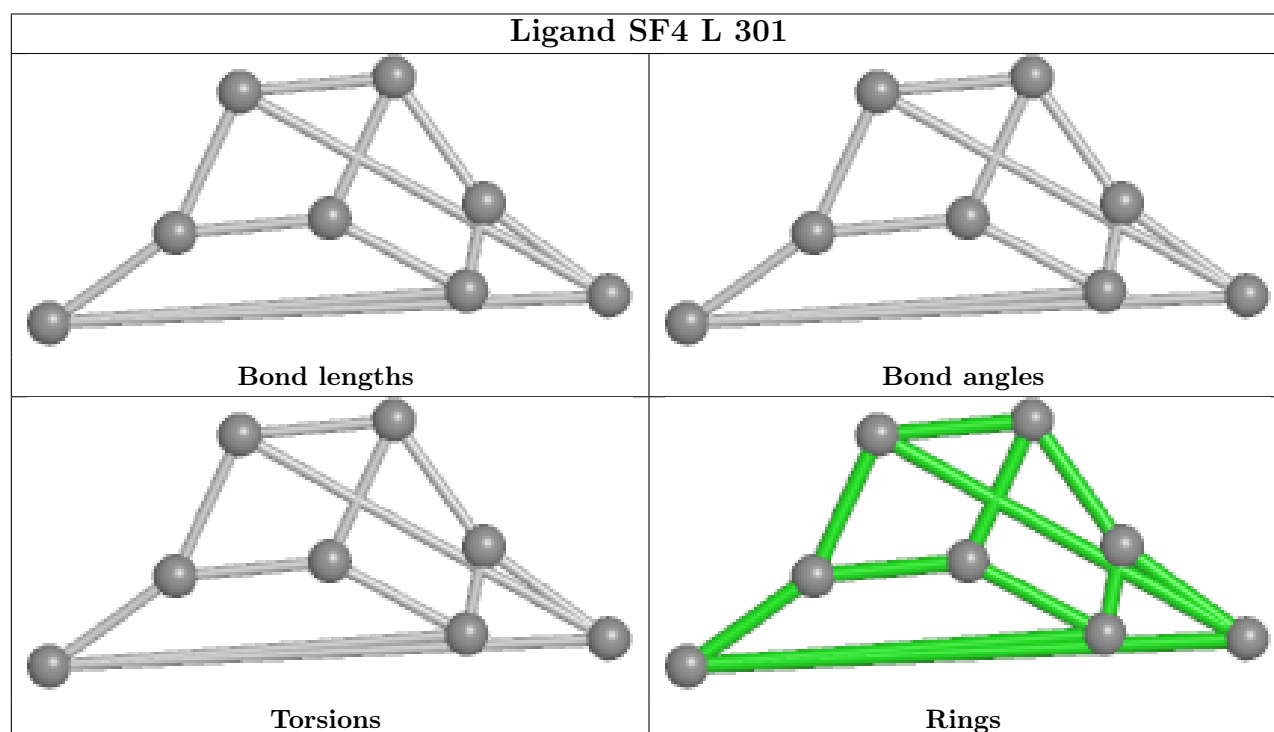
There are no chirality outliers.

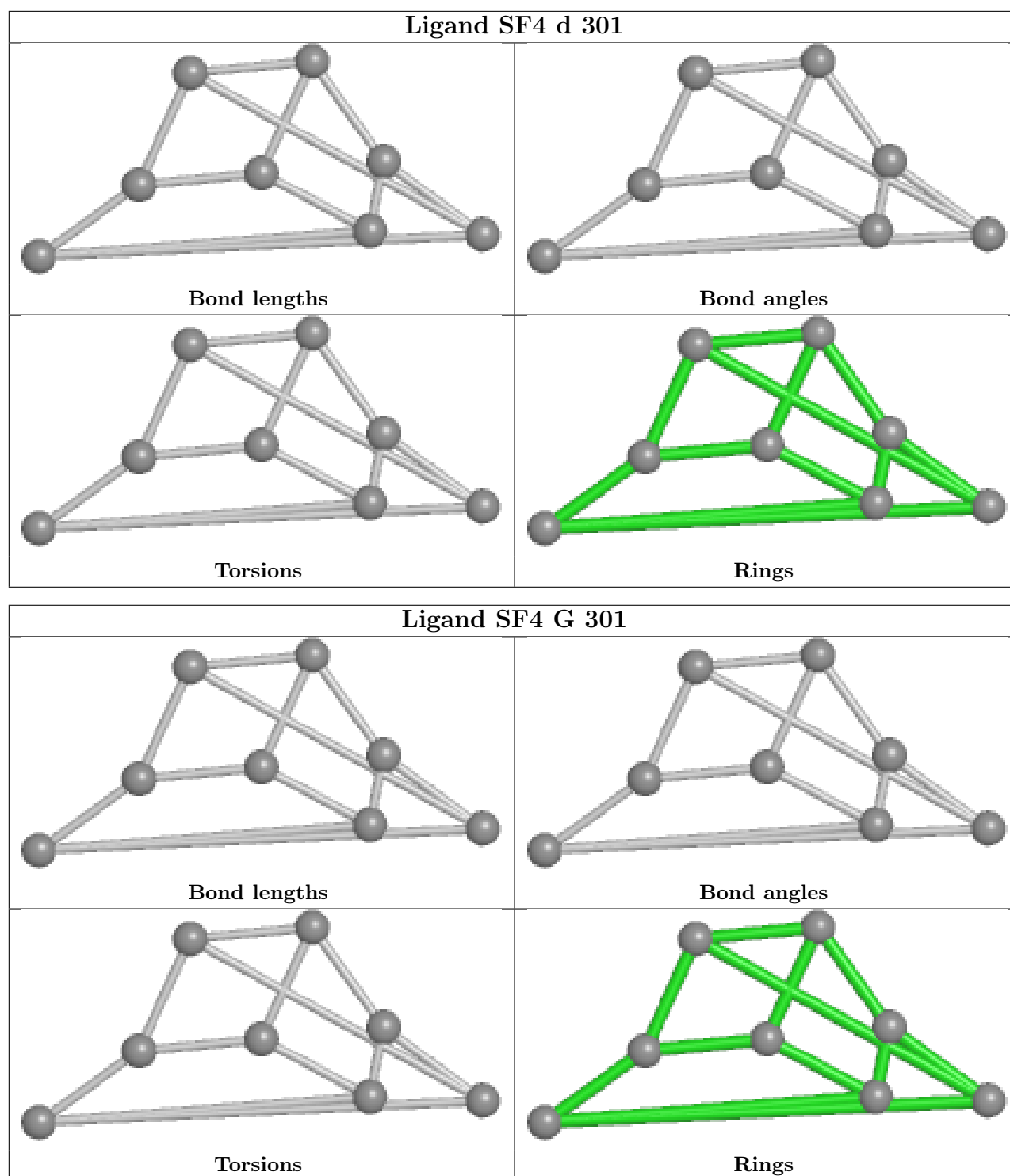
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

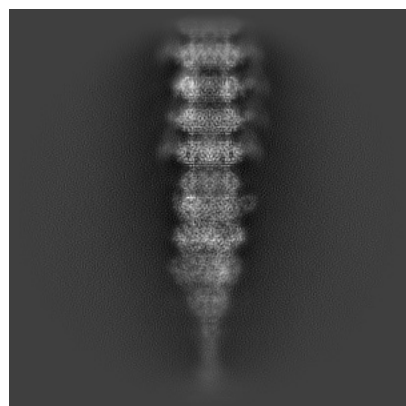
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35825. These allow visual inspection of the internal detail of the map and identification of artifacts.

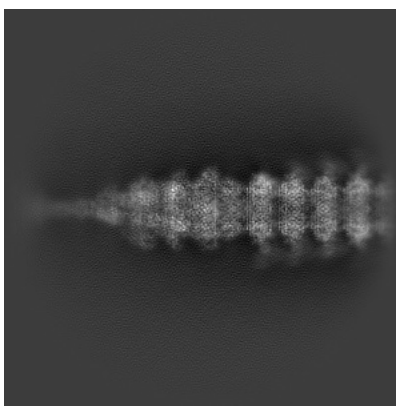
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

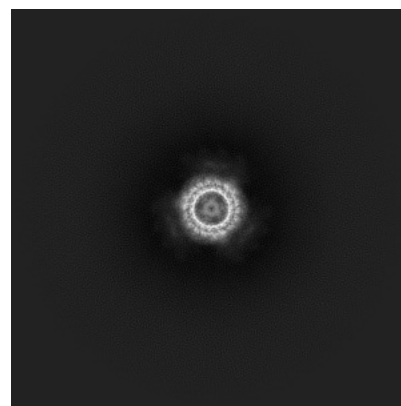
6.1.1 Primary map



X

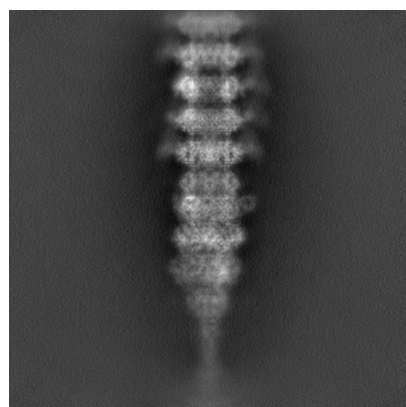


Y

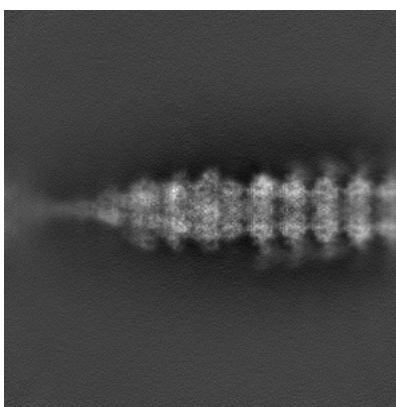


Z

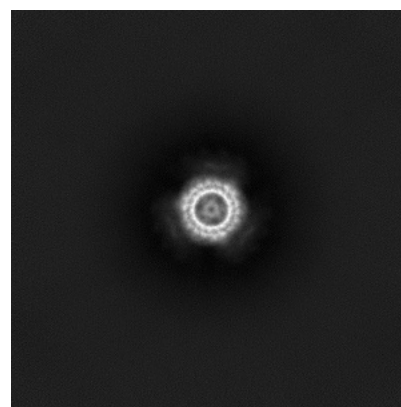
6.1.2 Raw map



X



Y

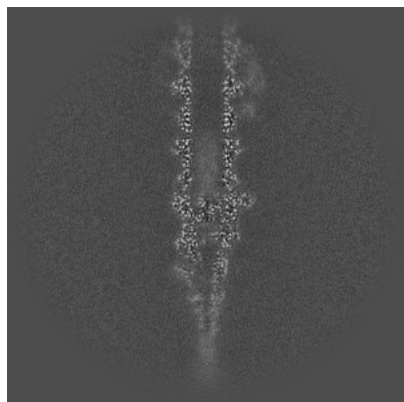


Z

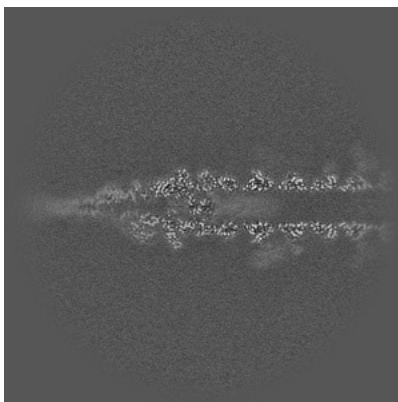
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

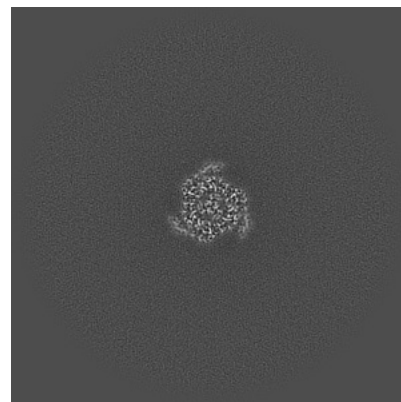
6.2.1 Primary map



X Index: 240

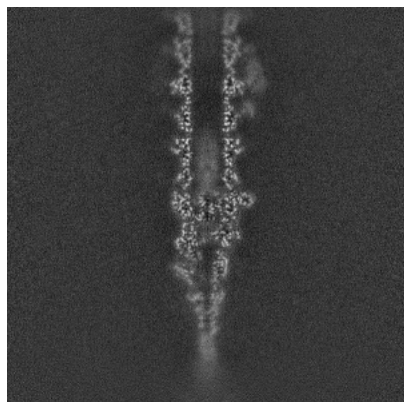


Y Index: 240

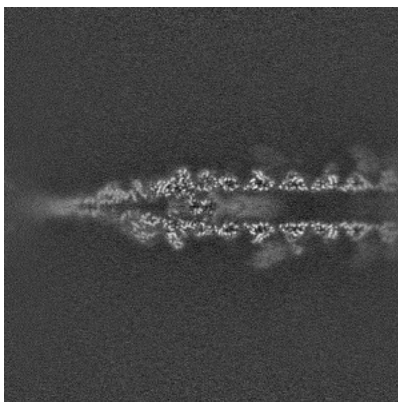


Z Index: 240

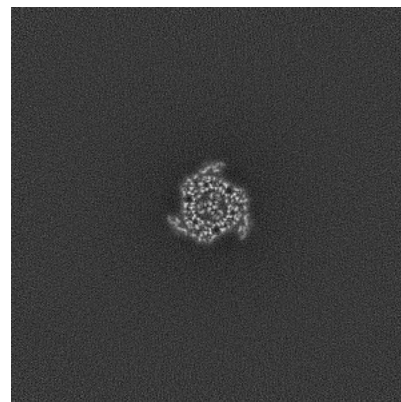
6.2.2 Raw map



X Index: 240



Y Index: 240

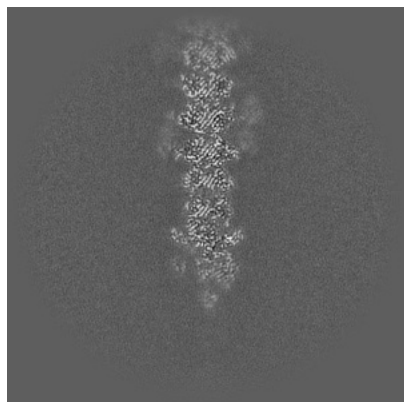


Z Index: 240

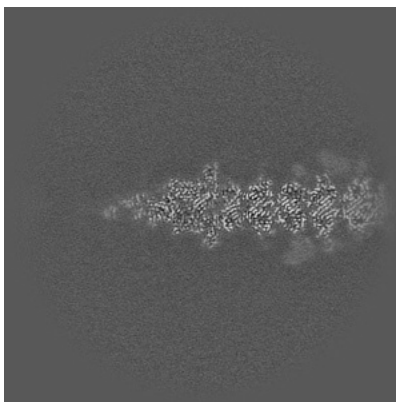
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

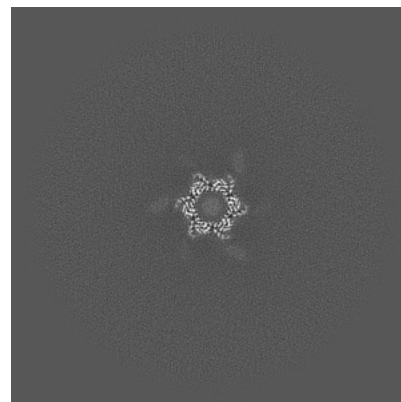
6.3.1 Primary map



X Index: 261

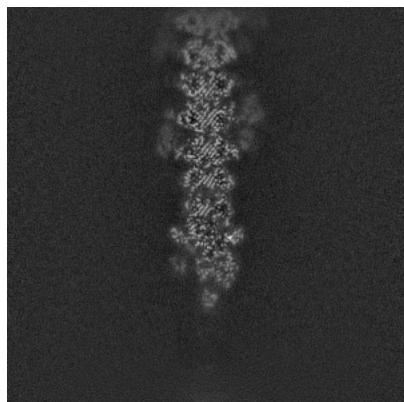


Y Index: 219

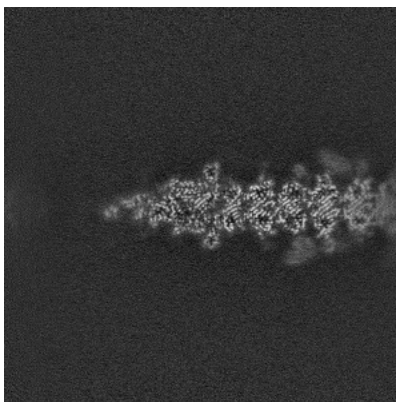


Z Index: 299

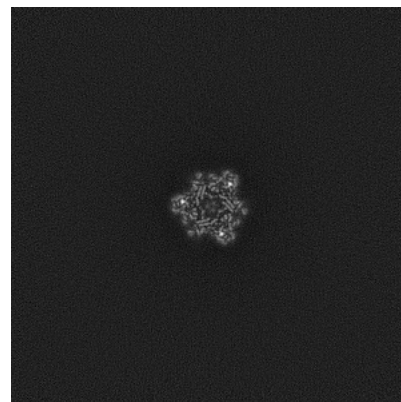
6.3.2 Raw map



X Index: 261



Y Index: 219

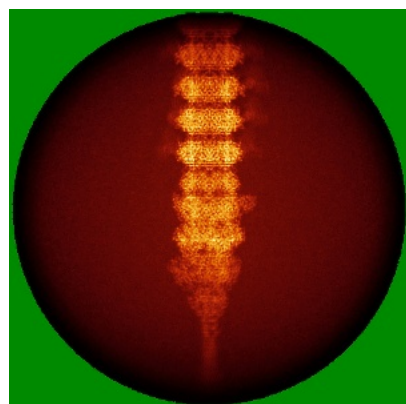


Z Index: 203

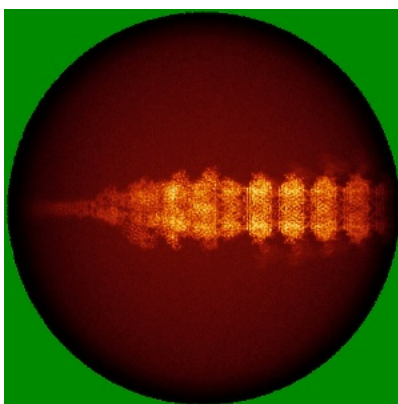
The images above show the largest variance slices of the map in three orthogonal directions.

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

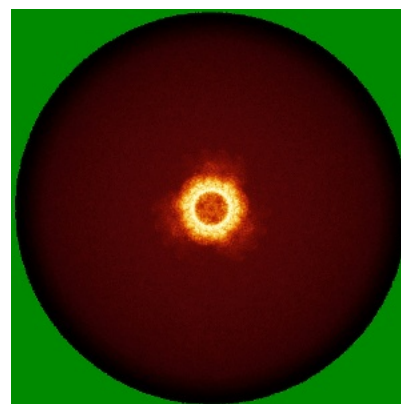
6.4.1 Primary map



X

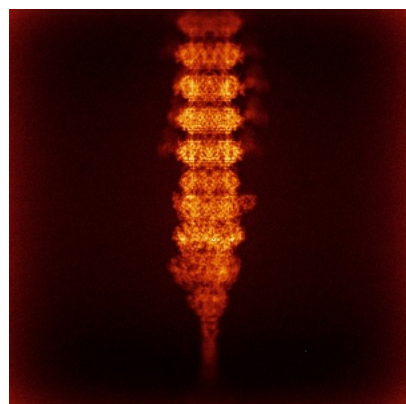


Y

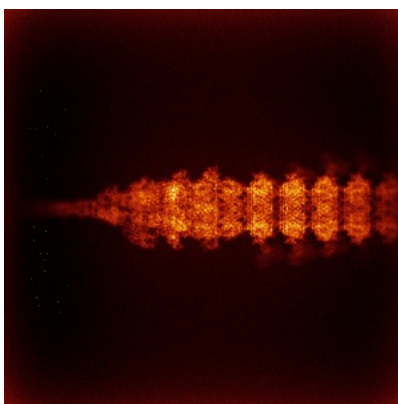


Z

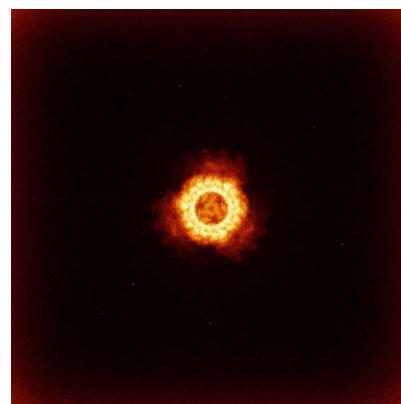
6.4.2 Raw map



X



Y

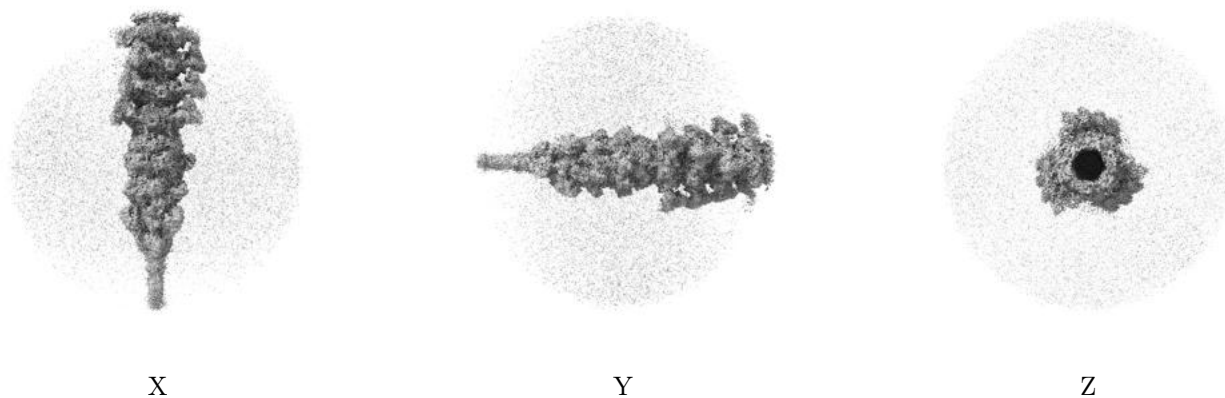


Z

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.

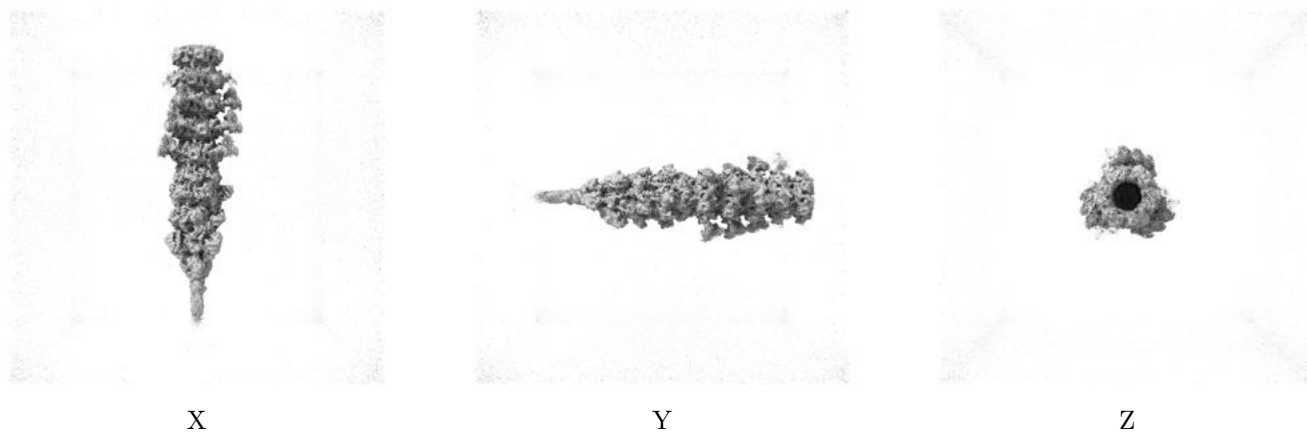
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.25. 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.

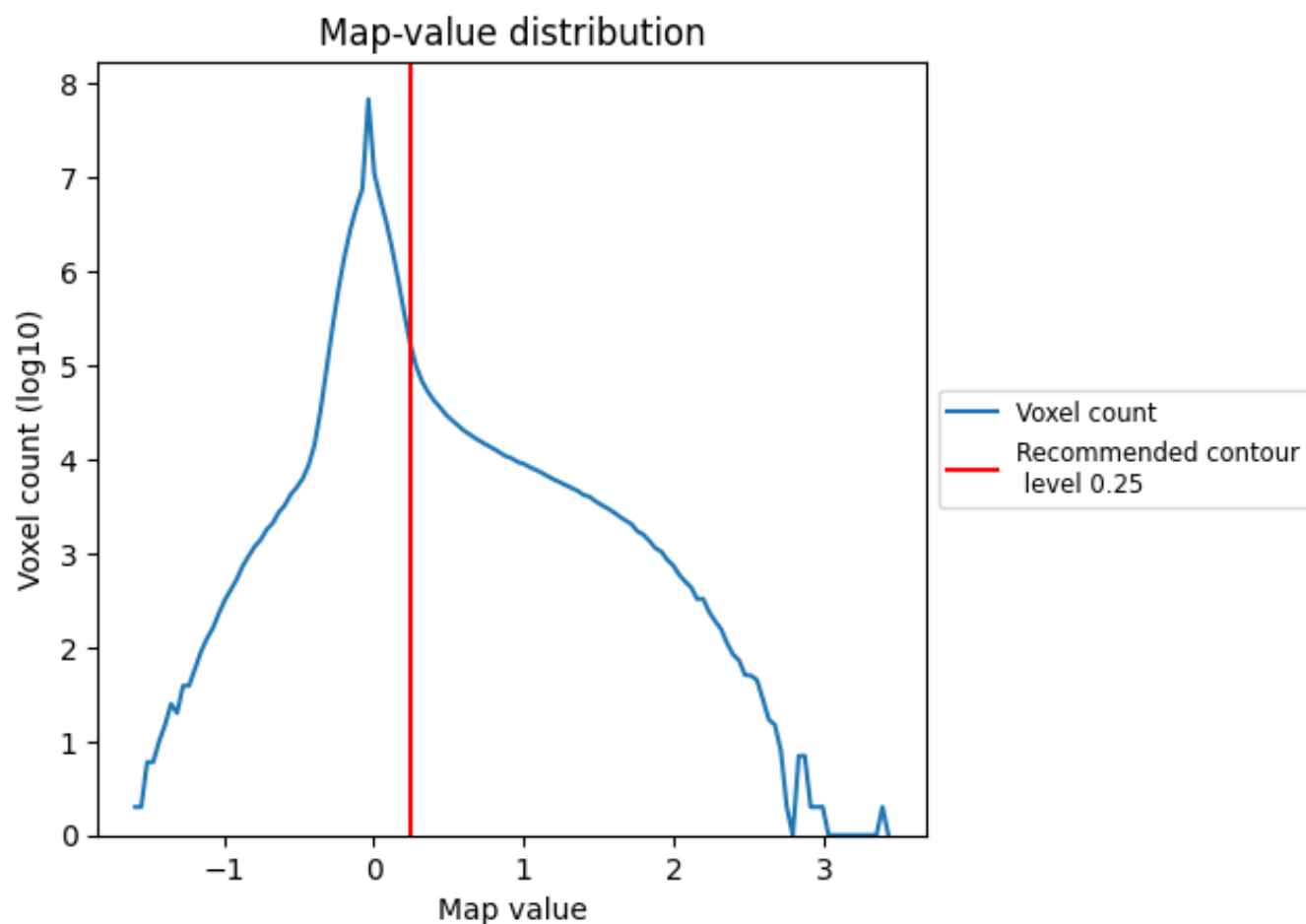
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

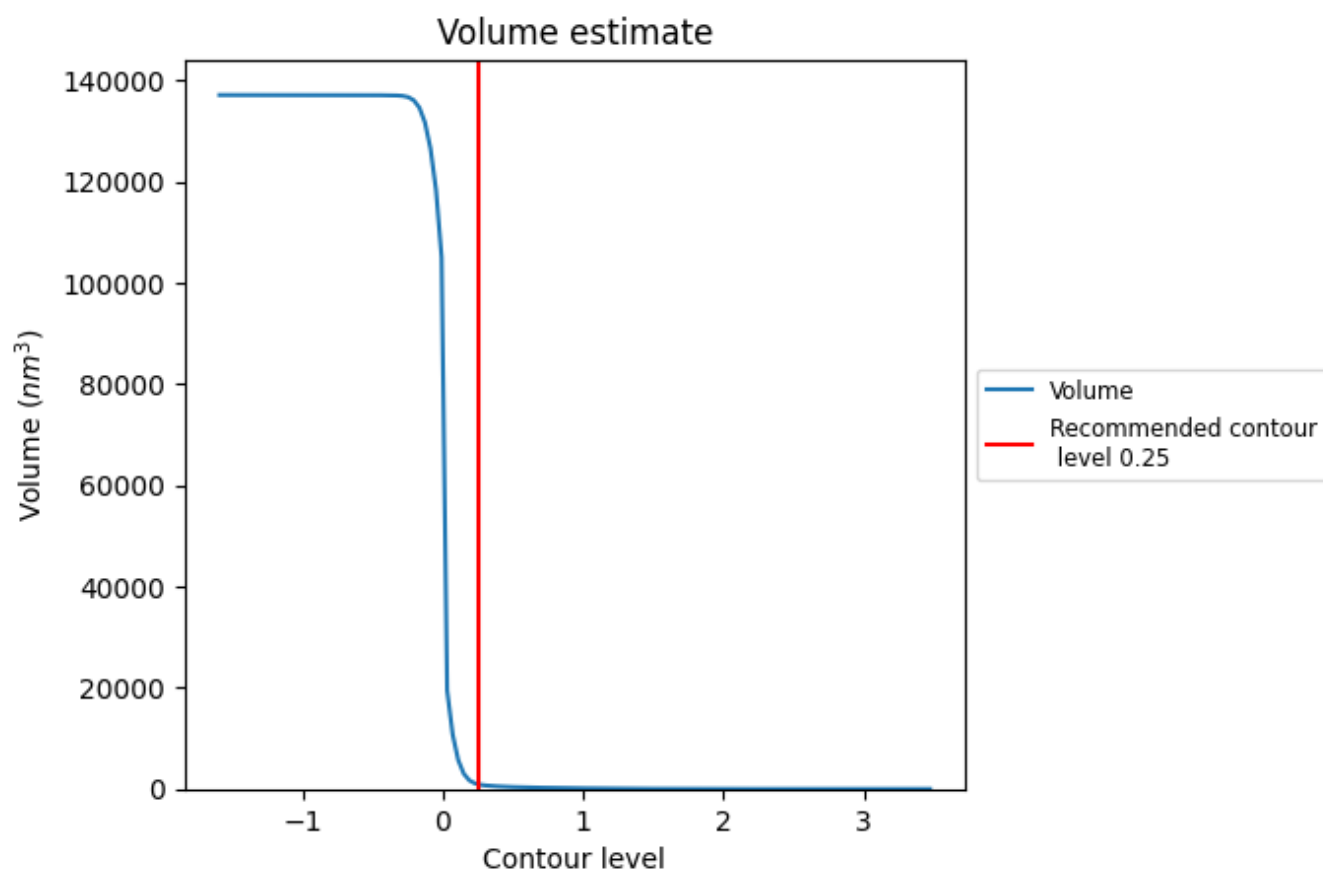
This section contains the results of statistical analysis of the map.

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.

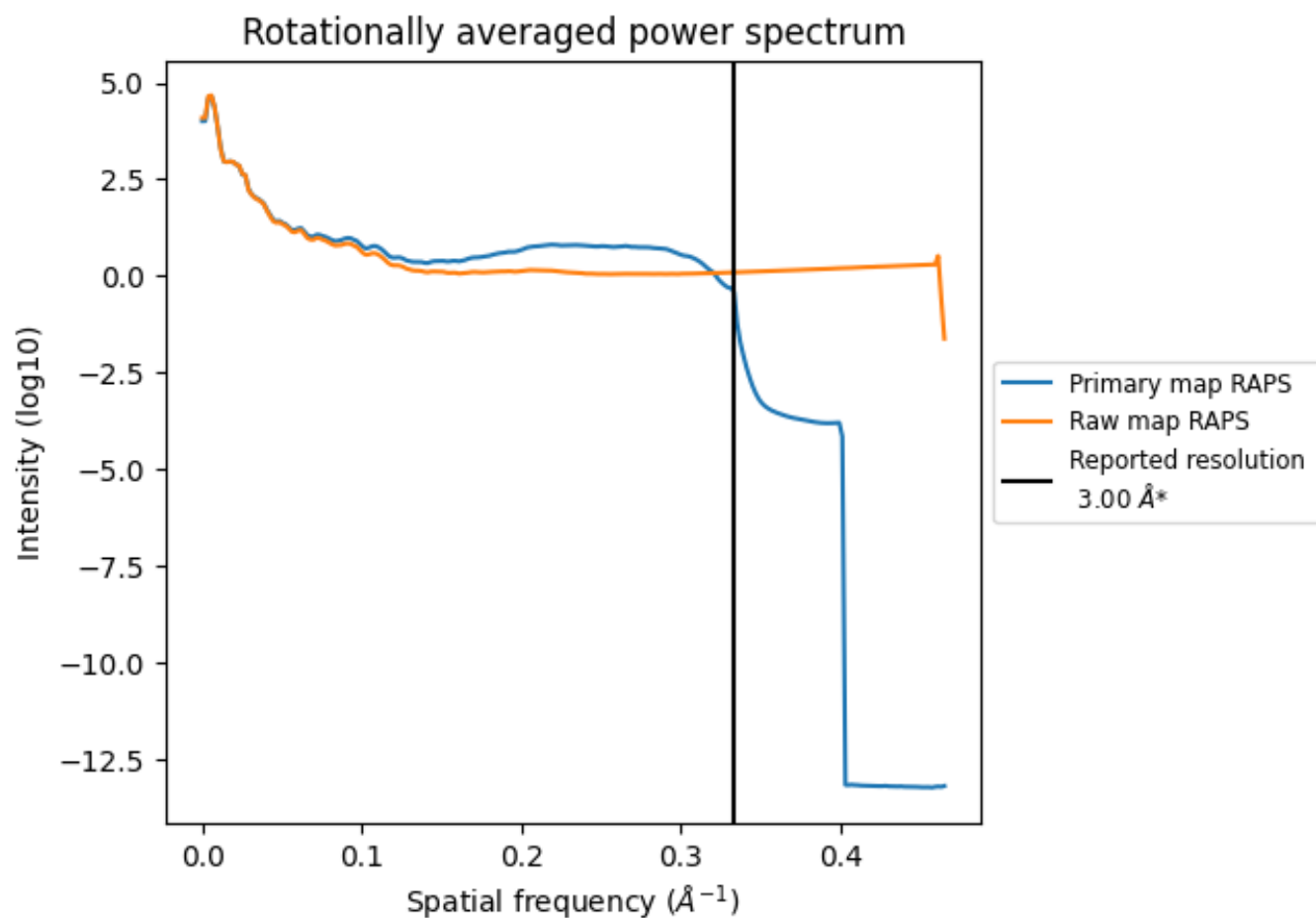
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 959 nm^3 ; this corresponds to an approximate mass of 867 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 ⓘ

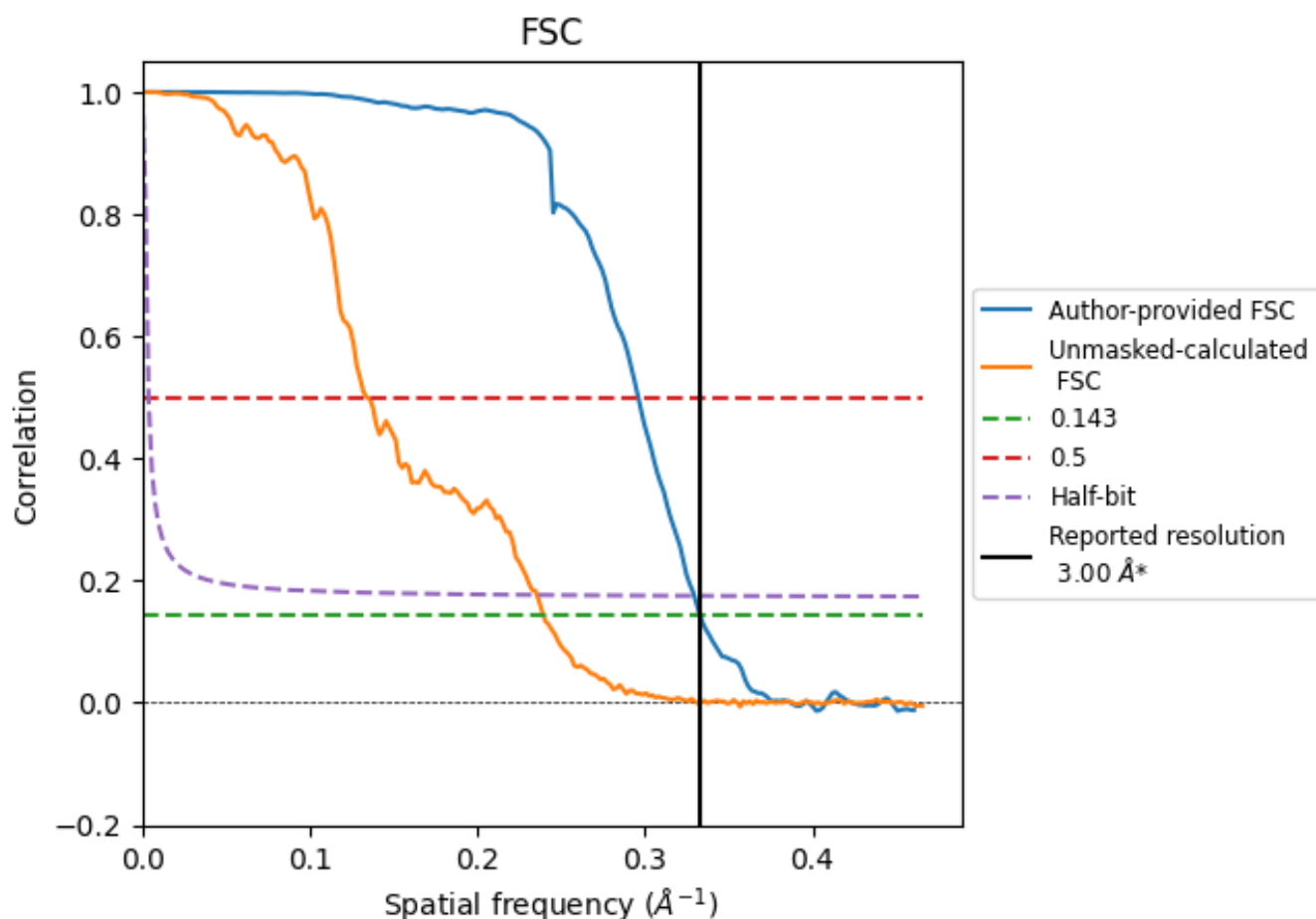


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

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 0.333 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.00	3.38	3.04
Unmasked-calculated*	4.18	7.46	4.24

*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 4.18 differs from the reported value 3.0 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-35825 and PDB model 8IYL. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

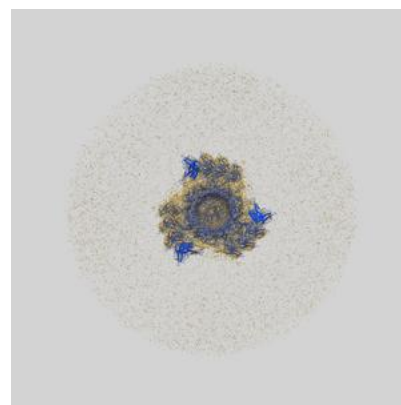
9.1 Map-model overlay [i](#)



X



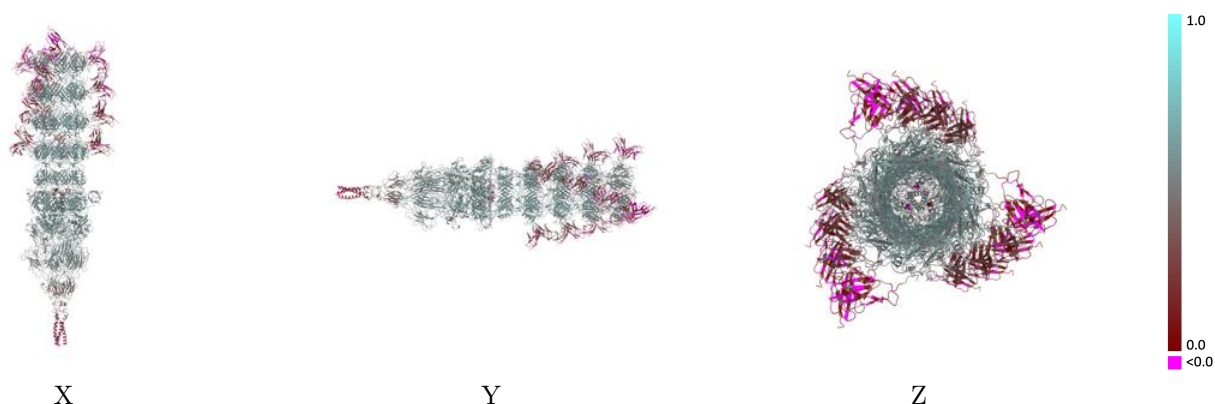
Y



Z

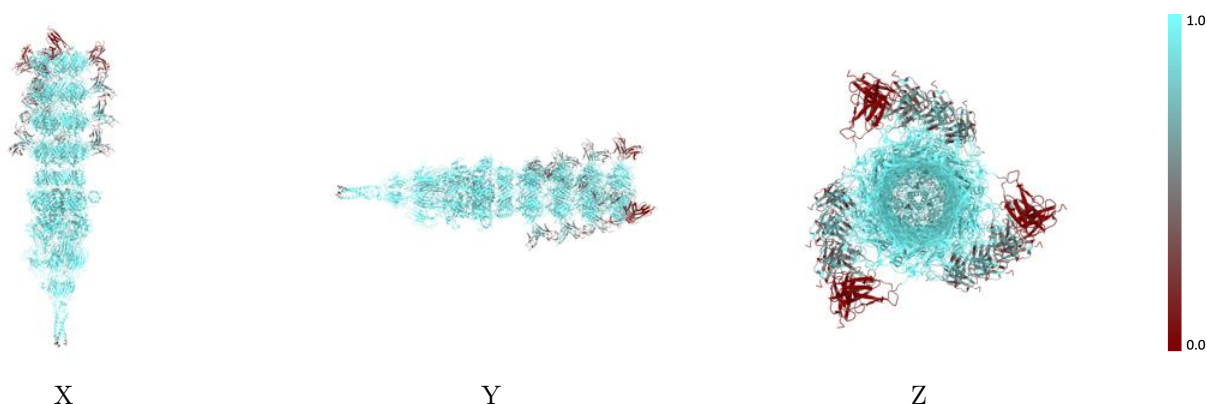
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



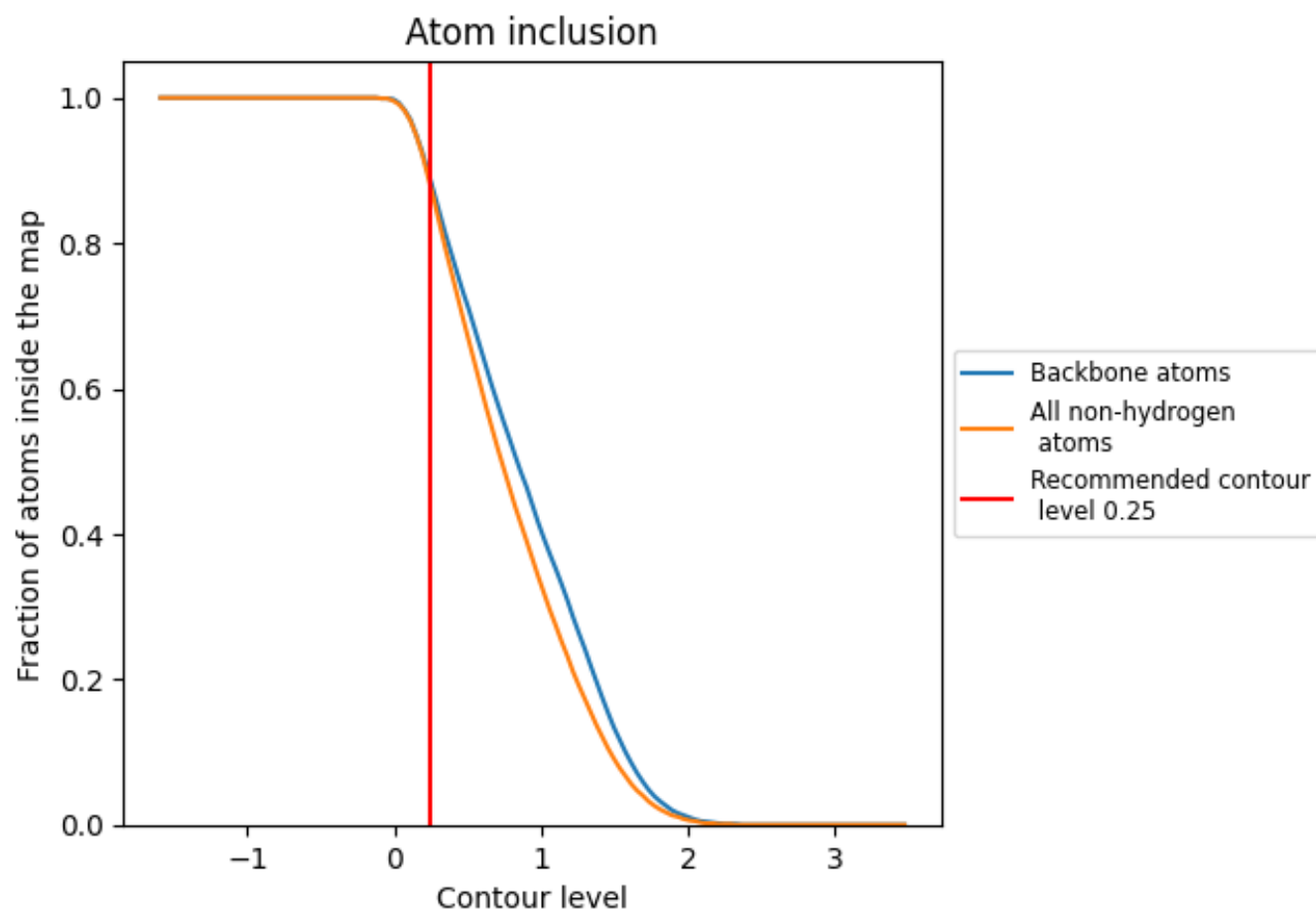
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.25).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 88% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8760	 0.4740
A	 0.8720	 0.4660
B	 0.8360	 0.4360
C	 0.6960	 0.3720
D	 0.9880	 0.5630
E	 0.9700	 0.5070
F	 0.9860	 0.5690
G	 0.9840	 0.5690
H	 0.9470	 0.5320
I	 0.9150	 0.4910
J	 0.9720	 0.5070
K	 0.9510	 0.5240
L	 0.9840	 0.5670
M	 0.9910	 0.5640
N	 0.9050	 0.4850
O	 0.8370	 0.4680
P	 0.8230	 0.4600
Q	 0.8330	 0.4370
R	 0.8270	 0.4420
S	 0.8660	 0.4650
T	 0.8530	 0.4610
U	 0.6920	 0.3750
V	 0.8360	 0.4650
W	 0.6700	 0.3730
X	 0.9910	 0.5650
Y	 0.9730	 0.5070
Z	 0.9830	 0.5700
a	 0.8570	 0.4600
b	 0.8320	 0.4420
c	 0.6710	 0.3720
d	 0.9860	 0.5650
e	 0.9550	 0.5260
f	 0.9070	 0.4880
g	 0.8350	 0.4680
h	 0.8230	 0.4600



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Chain	Atom inclusion	Q-score
i	 0.8320	 0.4350
j	 0.8310	 0.4410
k	 0.8670	 0.4650
l	 0.8540	 0.4590
m	 0.9800	 0.5710
n	 0.6880	 0.3710
o	 0.6690	 0.3710
v	 0.8200	 0.4620