Full wwPDB EM Validation Report

Mar 8, 2026 – 05:36 AM UTC

PDB ID	:	8IYK / pdb_00008iyk
EMDB ID	:	EMD-35824
Title	:	Tail tip conformation 1 of phage lambda tail
Authors	:	Wang, J.W.; Wang, C.
Deposited on	:	2023-04-05
Resolution	:	2.95 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 (i) 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 (1)) were used in the production of this report:

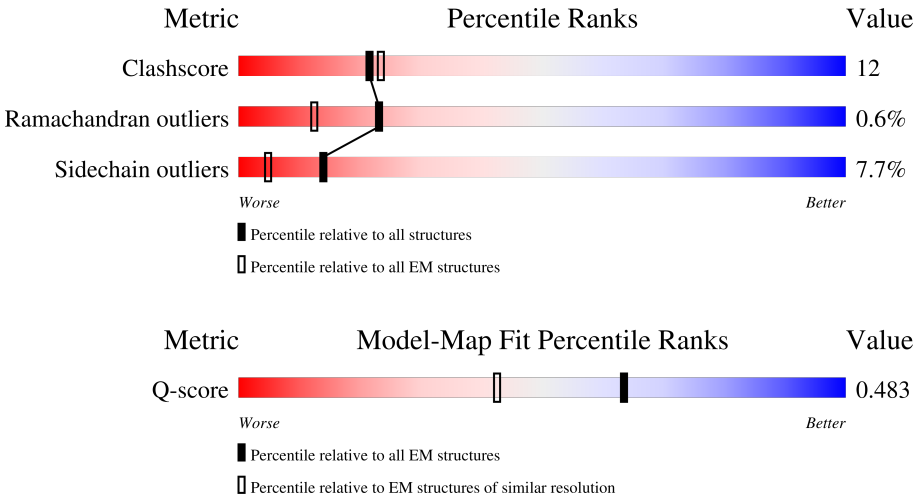
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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 2.95 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	13114 (2.45 - 3.45)

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	246	11% 69% 28%
1	B	246	13% 63% 32%
1	C	246	30% 63% 34%
1	D	246	12% 72% 26%

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Mol	Chain	Length	Quality of chain
1	G	246	14% 73% 25%
1	Q	246	13% 68% 29%
1	R	246	16% 69% 28%
1	S	246	12% 67% 29%
1	T	246	14% 74% 22%
1	U	246	31% 58% 39%
1	V	246	12% 70% 28%
1	W	246	34% 61% 36%
1	X	246	12% 71% 26%
1	a	246	13% 68% 28%
1	b	246	16% 66% 31%
1	c	246	35% 65% 33%
1	d	246	14% 71% 27%
1	i	246	14% 63% 33%
1	j	246	17% 67% 29%
1	k	246	11% 70% 27%
1	l	246	13% 72% 25%
1	n	246	32% 62% 35%
1	o	246	34% 65% 31%
1	v	246	14% 69% 28%
2	E	109	68% 28% 5%
2	K	109	70% 28%
2	M	109	67% 30%
2	Y	109	65% 31%
2	e	109	69% 30%

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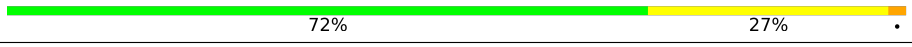
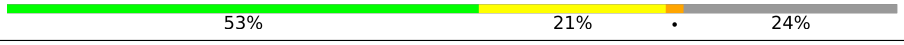
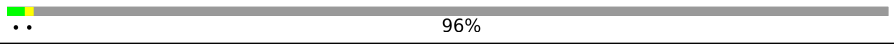
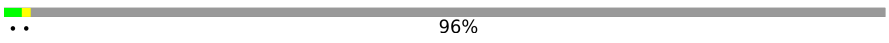
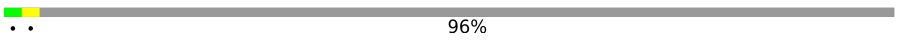
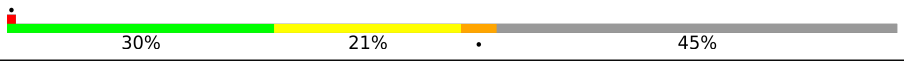
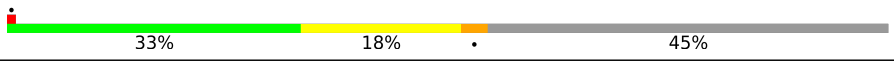
Mol	Chain	Length	Quality of chain
2	m	109	
3	F	1132	
3	J	1132	
3	Z	1132	
4	L	232	
4	N	232	
4	f	232	
5	H	853	
5	O	853	
5	g	853	
6	I	223	
6	P	223	
6	h	223	

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 tube protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	V	243	Total	C	N	O	S	0	0
			1792	1119	302	366	5		
1	v	243	Total	C	N	O	S	0	0
			1792	1119	302	366	5		
1	B	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
1	b	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
1	A	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
1	a	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
1	C	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
1	c	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
1	D	243	Total	C	N	O	S	0	0
			1792	1119	302	366	5		
1	G	243	Total	C	N	O	S	0	0
			1792	1119	302	366	5		
1	Q	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
1	R	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
1	S	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
1	T	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
1	U	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
1	W	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
1	X	243	Total	C	N	O	S	0	0
			1792	1119	302	366	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	d	243	Total	C	N	O	S	0	0
			1792	1119	302	366	5		
1	i	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
1	j	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
1	k	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
1	l	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
1	n	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
1	o	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		

- Molecule 2 is a protein called Tail tip protein M.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	109	Total	C	N	O	S	0	0
			884	569	154	157	4		
2	m	109	Total	C	N	O	S	0	0
			884	569	154	157	4		
2	E	109	Total	C	N	O	S	0	0
			884	569	154	157	4		
2	K	109	Total	C	N	O	S	0	0
			884	569	154	157	4		
2	Y	109	Total	C	N	O	S	0	0
			884	569	154	157	4		
2	e	109	Total	C	N	O	S	0	0
			884	569	154	157	4		

- Molecule 3 is a protein called Tip attachment protein J.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	861	Total	C	N	O	S	0	0
			6720	4212	1171	1317	20		
3	F	861	Total	C	N	O	S	0	0
			6720	4212	1171	1317	20		
3	Z	861	Total	C	N	O	S	0	0
			6720	4212	1171	1317	20		

- Molecule 4 is a protein called Tail tip protein L.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	232	Total	C	N	O	S	0	0
			1801	1117	309	362	13		
4	N	232	Total	C	N	O	S	0	0
			1801	1117	309	362	13		
4	f	232	Total	C	N	O	S	0	0
			1801	1117	309	362	13		

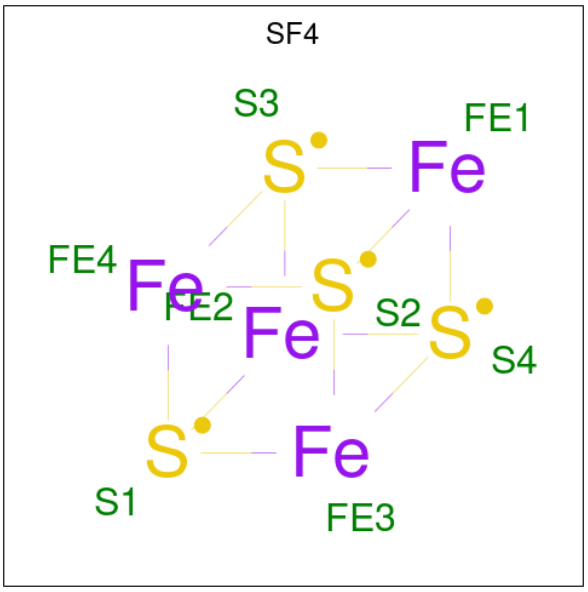
- Molecule 5 is a protein called Tape measure protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	33	Total	C	N	O	S	0	0
			250	154	47	47	2		
5	O	33	Total	C	N	O	S	0	0
			250	154	47	47	2		
5	g	33	Total	C	N	O	S	0	0
			250	154	47	47	2		

- Molecule 6 is a protein called Tail tip assembly protein I.

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

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

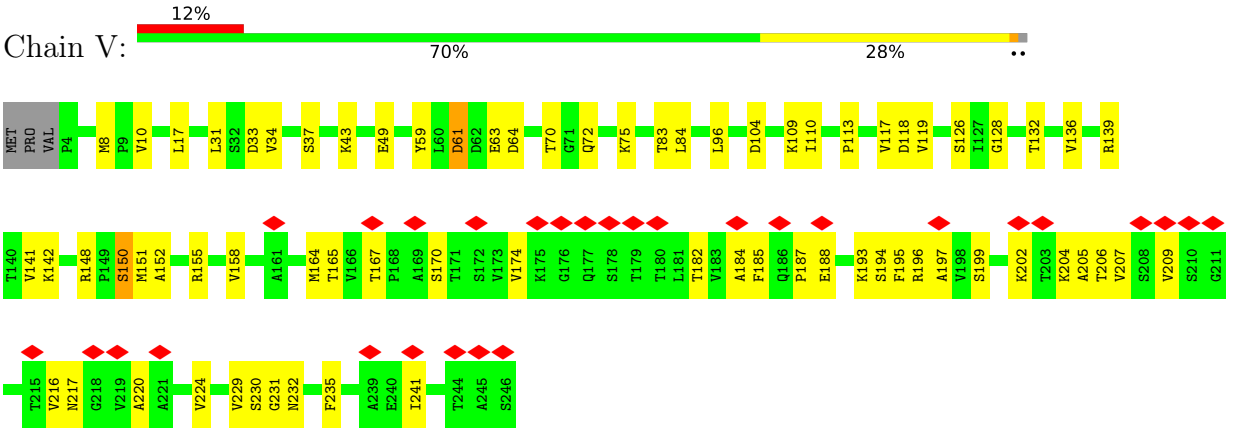


Mol	Chain	Residues	Atoms			AltConf
7	L	1	Total	Fe	S	0
			8	4	4	
7	N	1	Total	Fe	S	0
			8	4	4	
7	f	1	Total	Fe	S	0
			8	4	4	

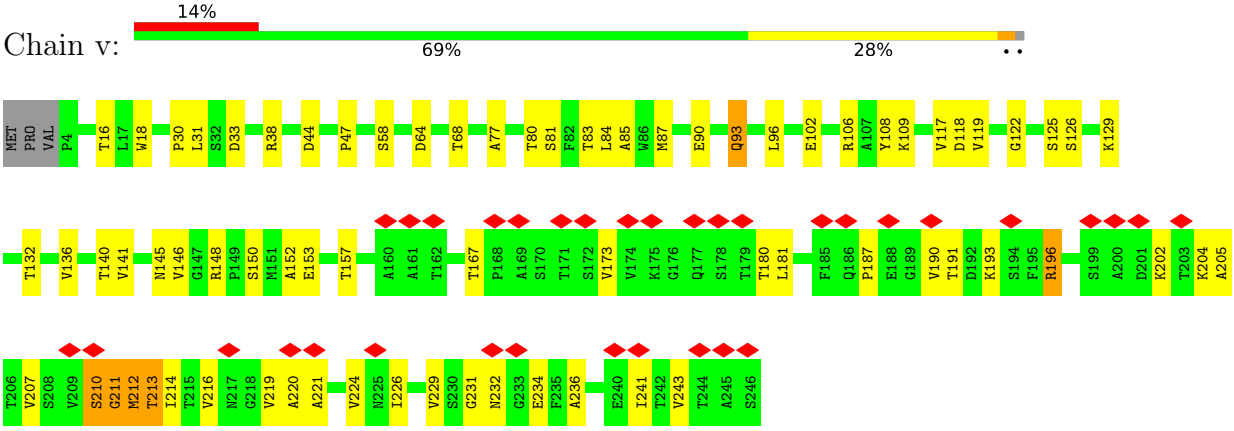
3 Residue-property plots (i)

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.

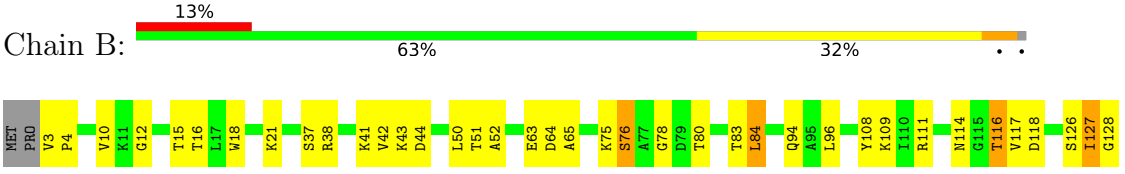
• Molecule 1: Tail tube protein

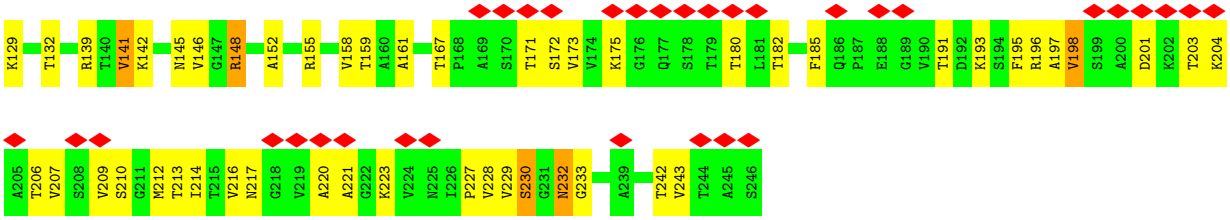


• Molecule 1: Tail tube protein

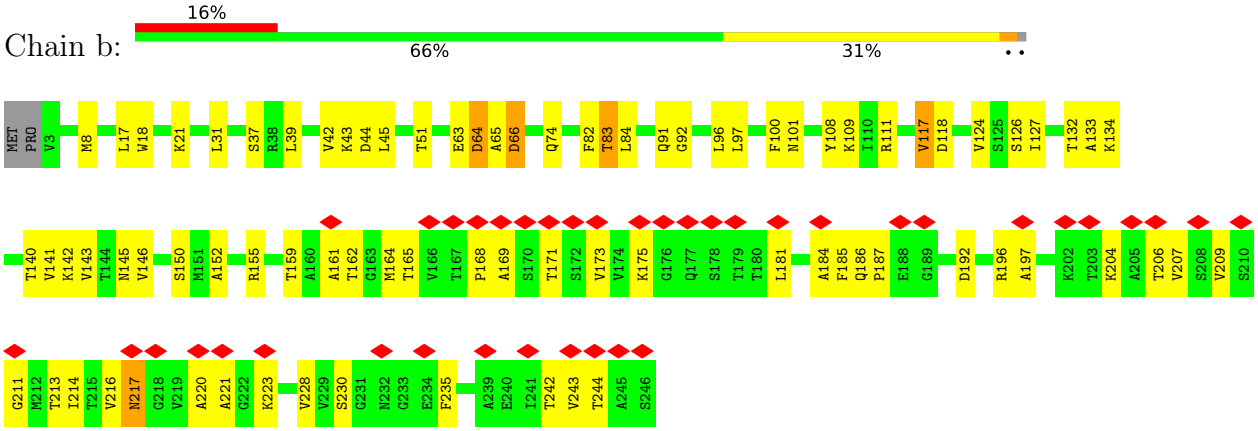


• Molecule 1: Tail tube protein

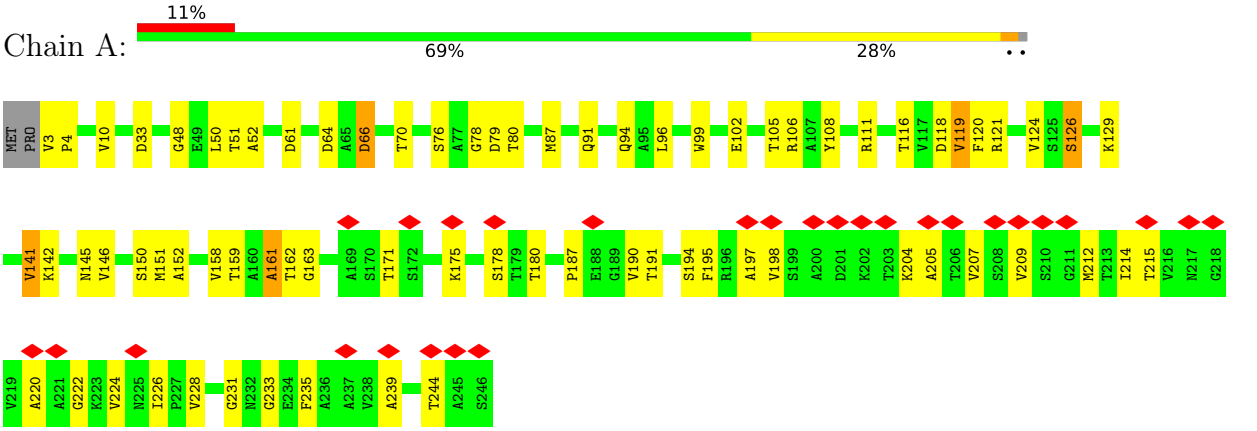




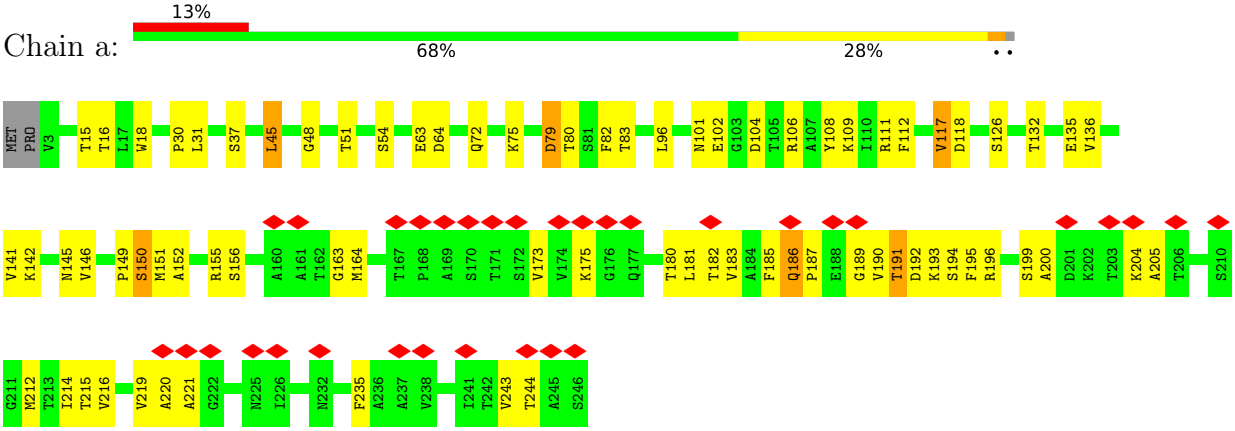
• Molecule 1: Tail tube protein



• Molecule 1: Tail tube protein

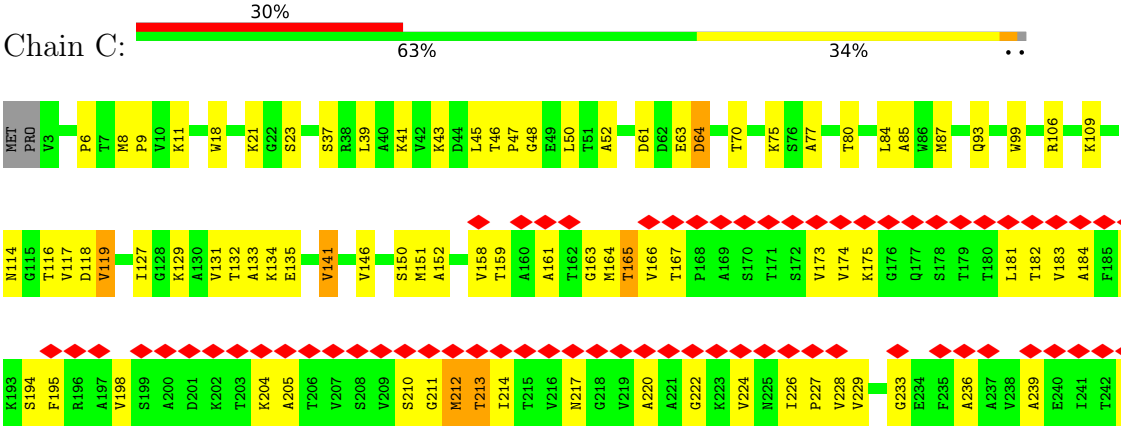


• Molecule 1: Tail tube protein



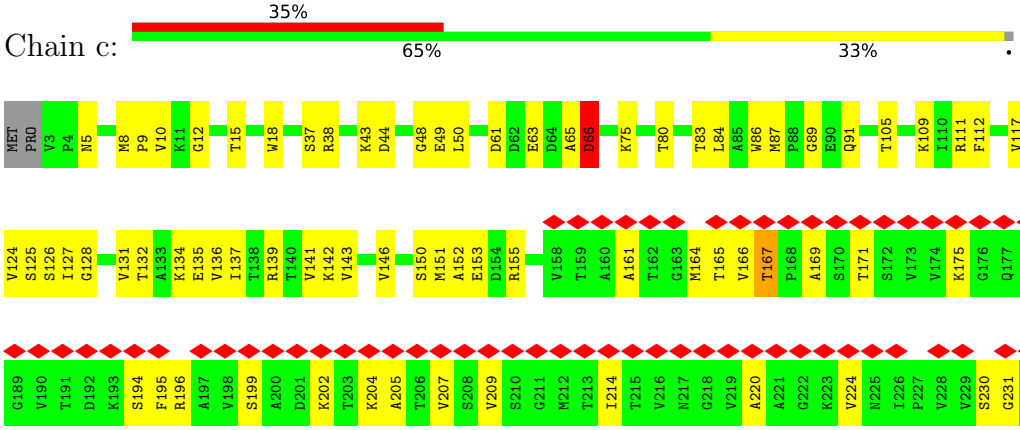
• Molecule 1: Tail tube protein

Chain C:



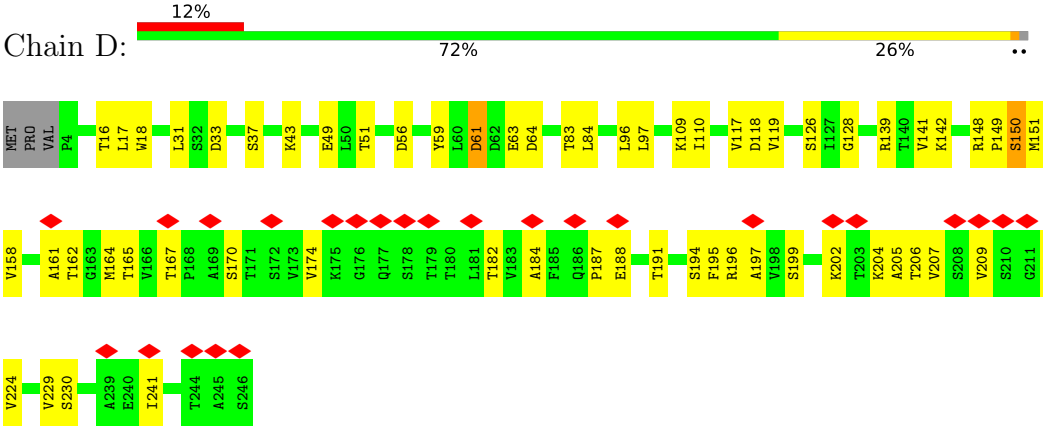
• Molecule 1: Tail tube protein

Chain c:



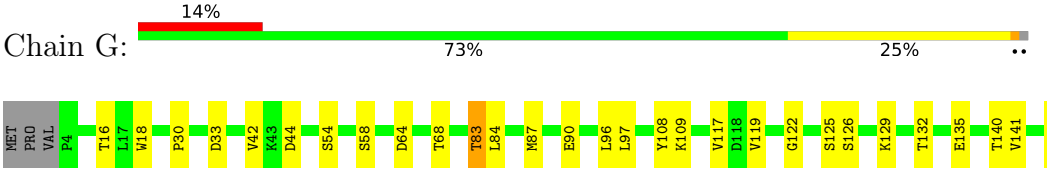
• Molecule 1: Tail tube protein

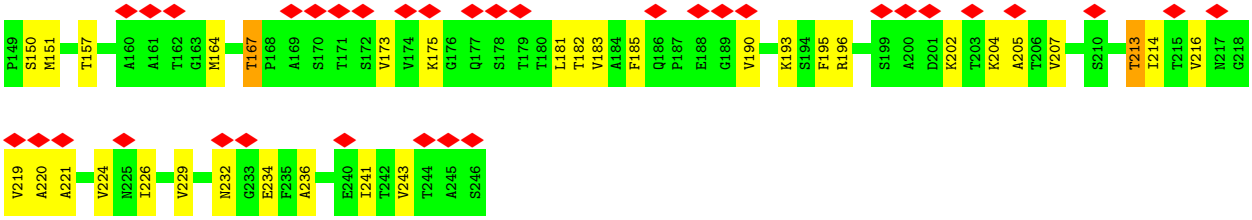
Chain D:



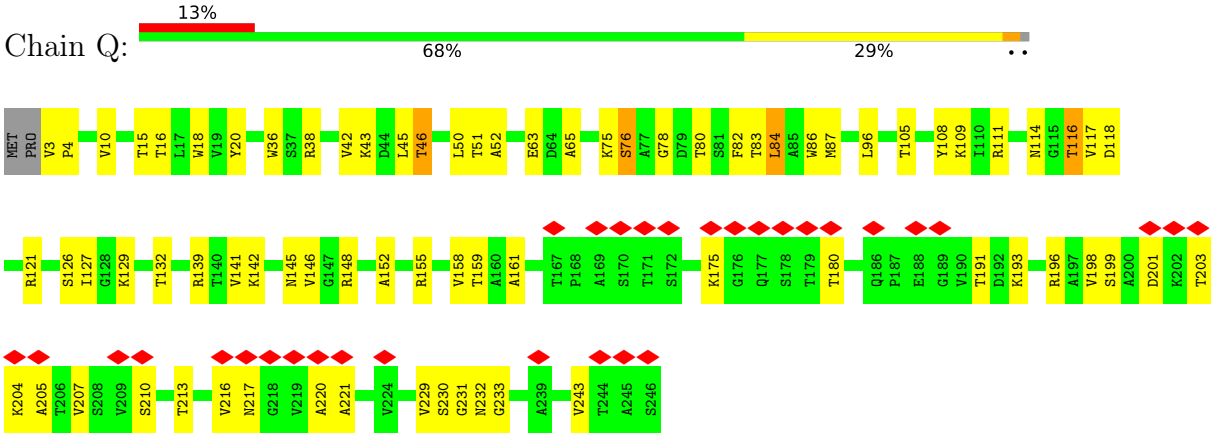
• Molecule 1: Tail tube protein

Chain G:

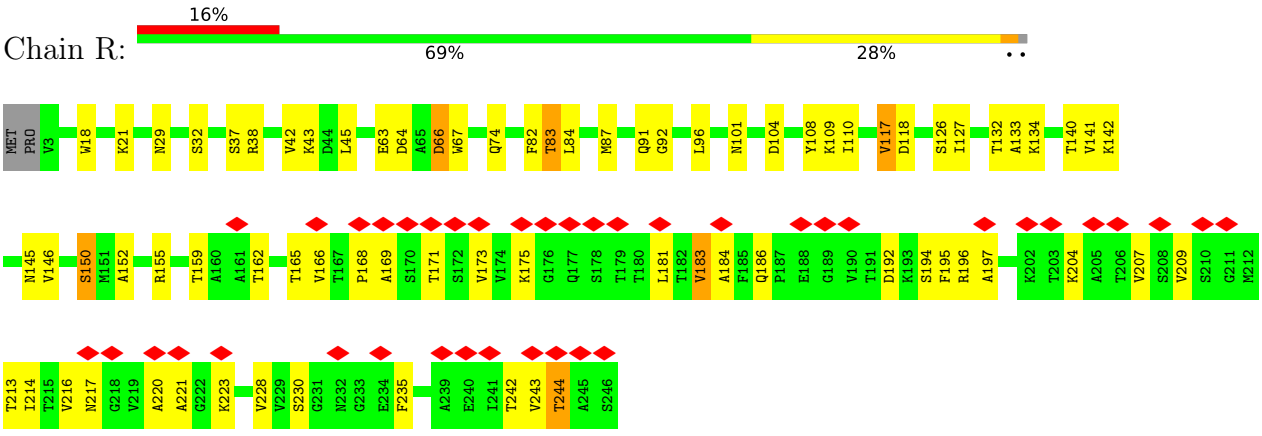




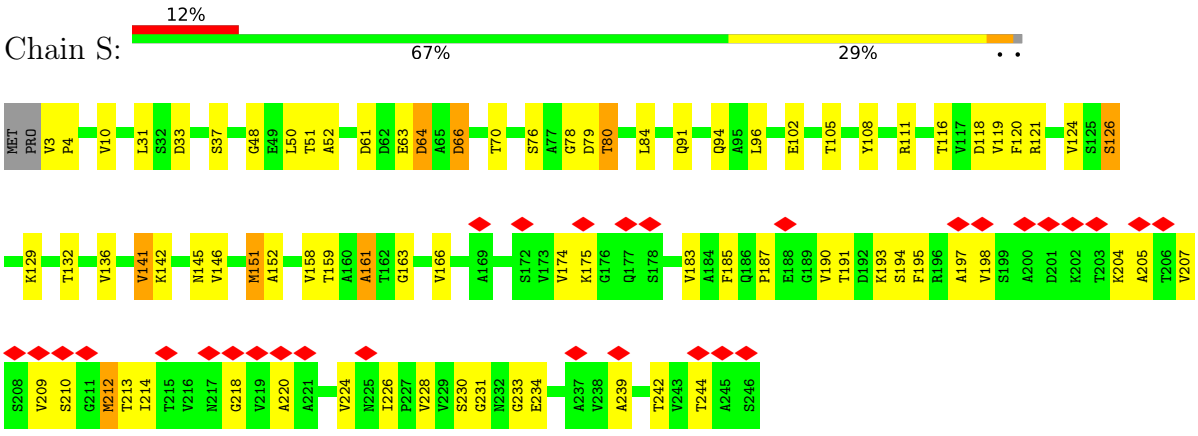
• Molecule 1: Tail tube protein



• Molecule 1: Tail tube protein

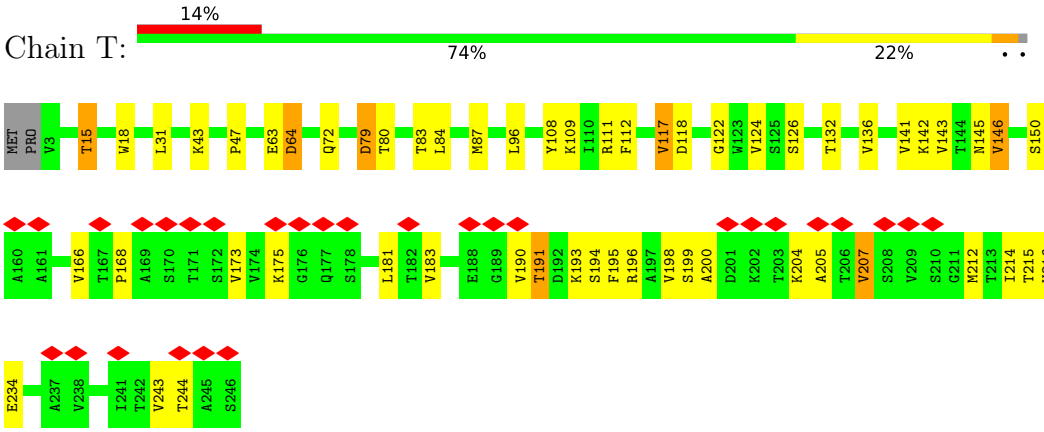


• Molecule 1: Tail tube protein



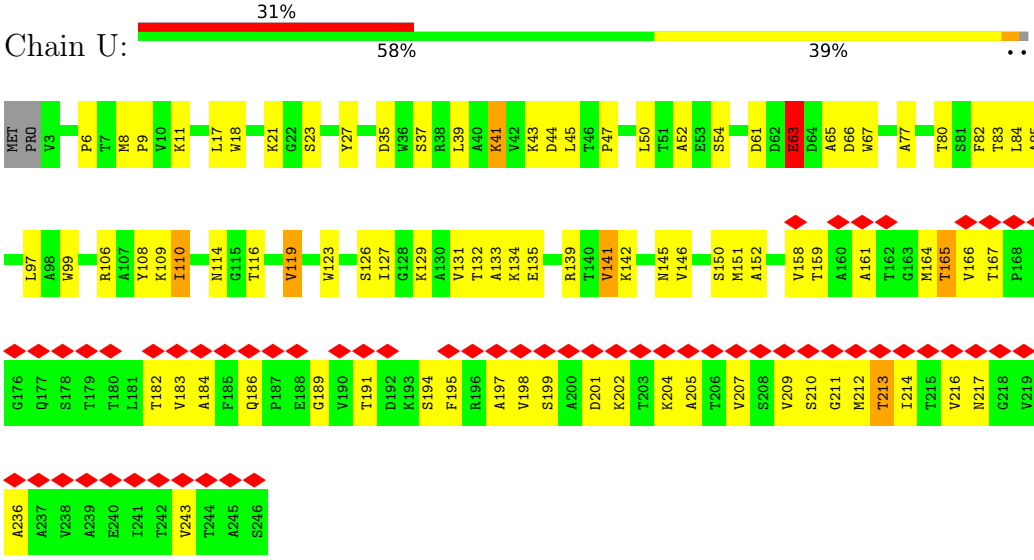
• Molecule 1: Tail tube protein

Chain T:



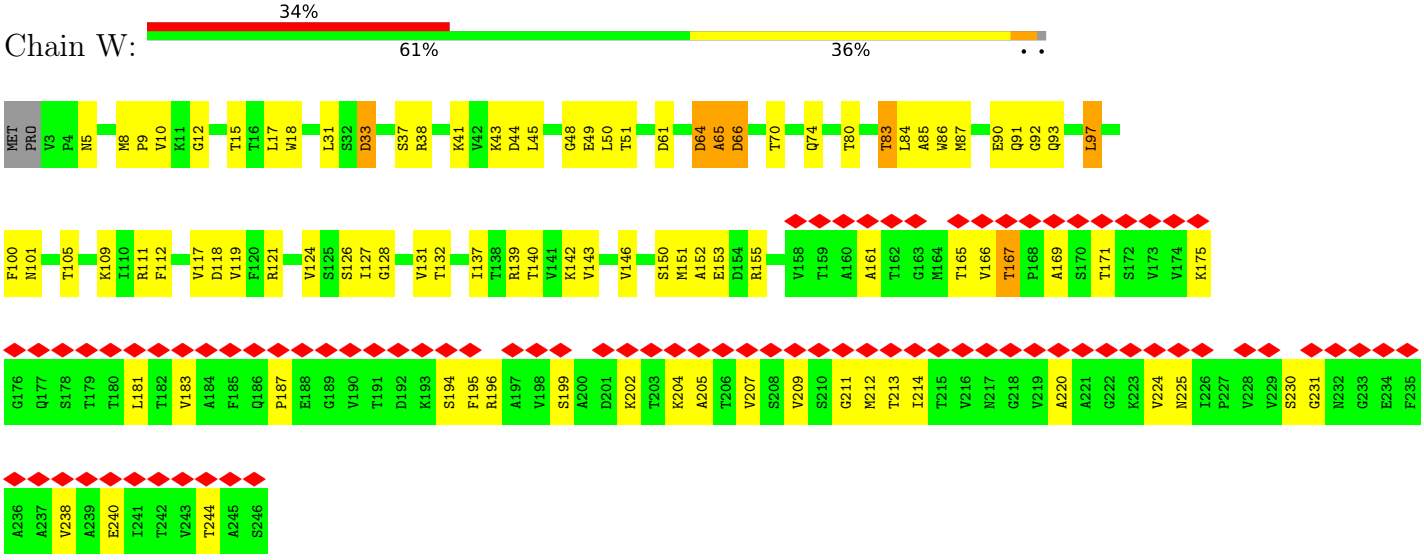
• Molecule 1: Tail tube protein

Chain U:



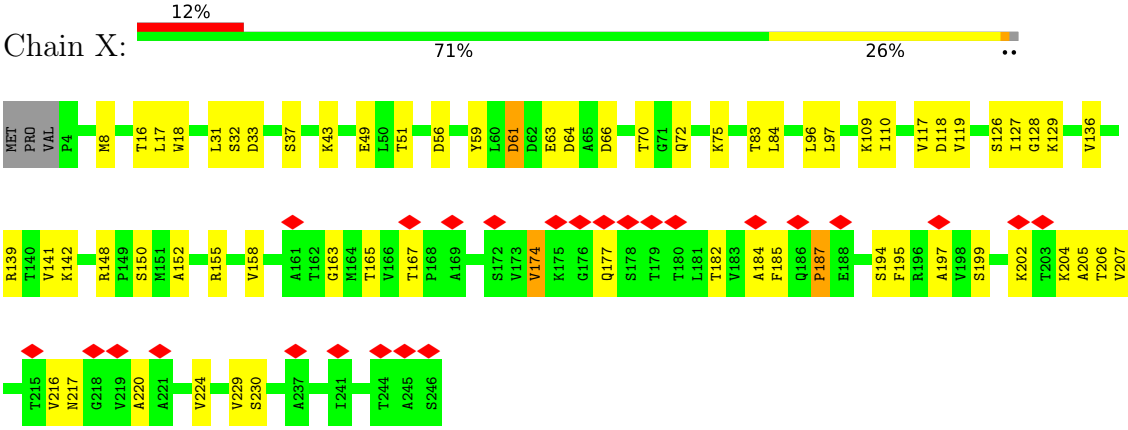
• Molecule 1: Tail tube protein

Chain W:



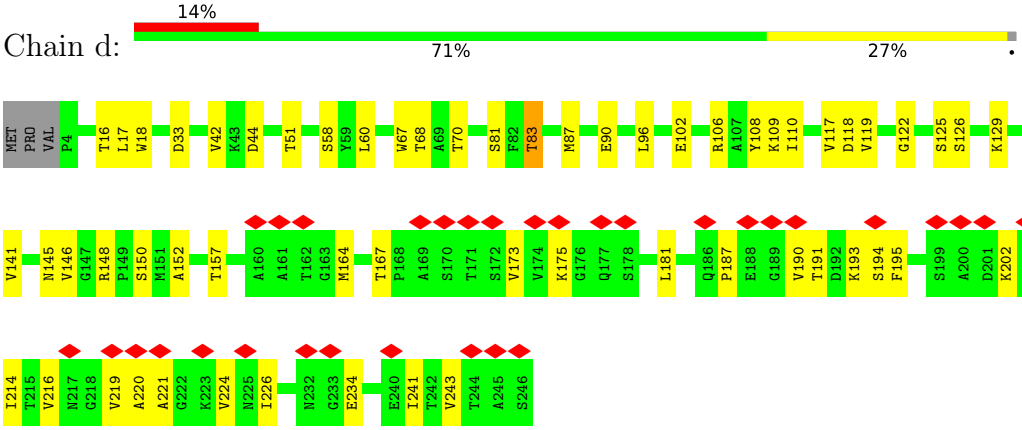
• Molecule 1: Tail tube protein

Chain X:



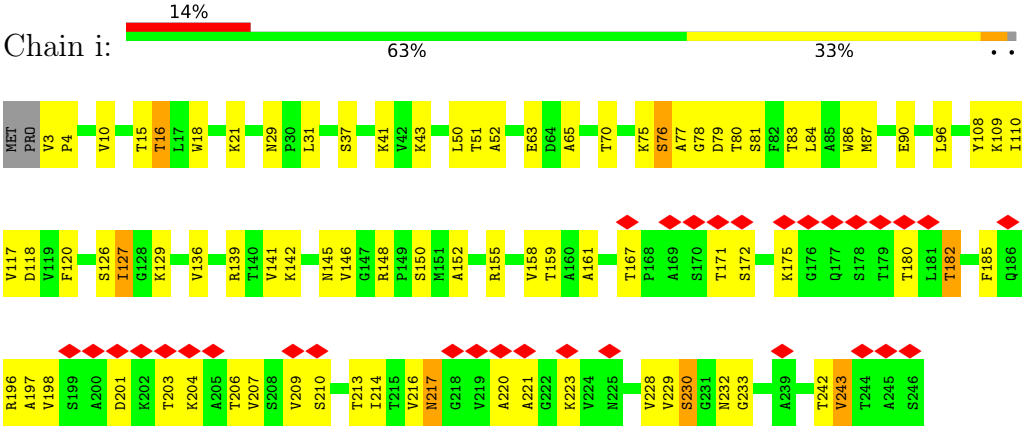
• Molecule 1: Tail tube protein

Chain d:



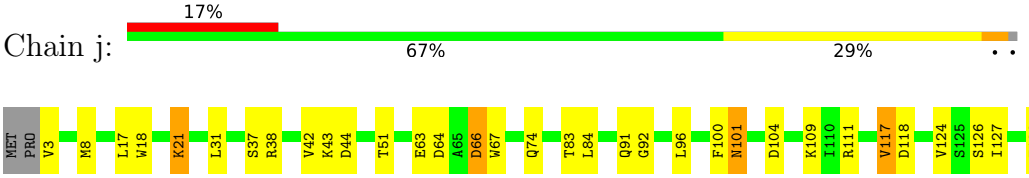
• Molecule 1: Tail tube protein

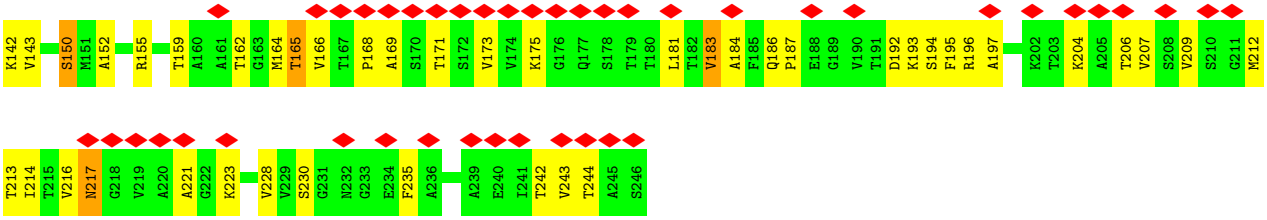
Chain i:



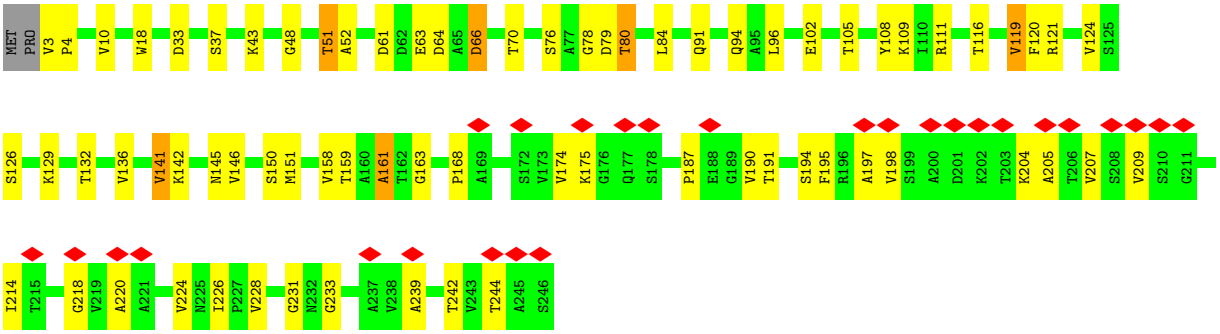
• Molecule 1: Tail tube protein

Chain j:

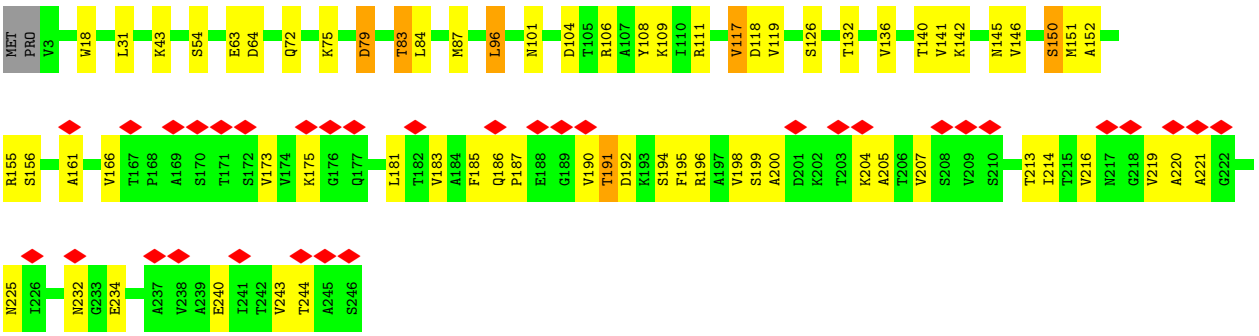




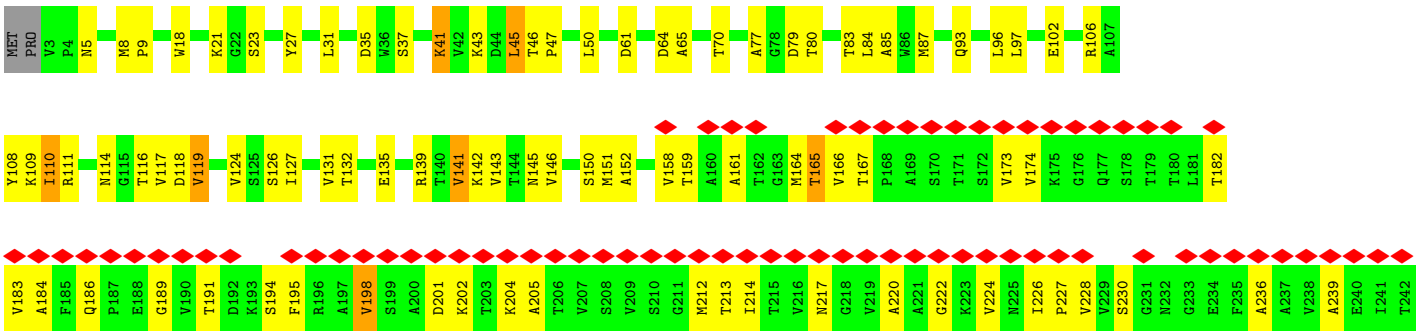
• Molecule 1: Tail tube protein



• Molecule 1: Tail tube protein

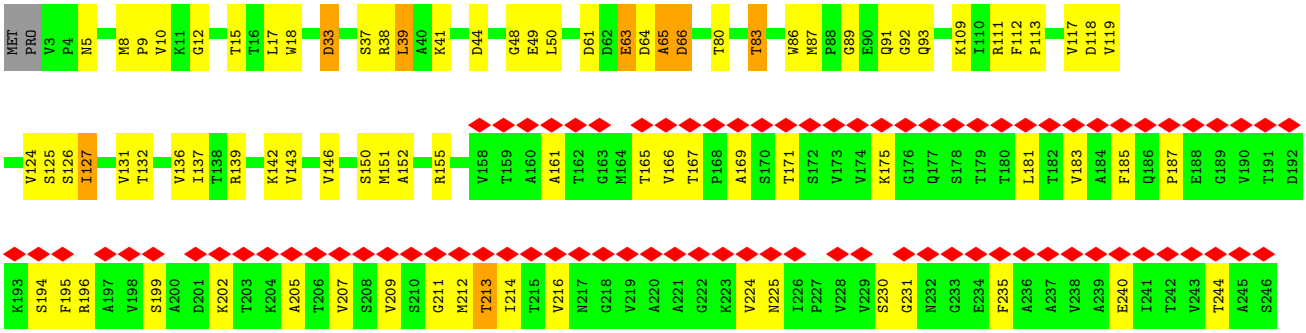


• Molecule 1: Tail tube protein



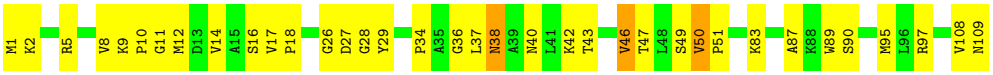
• Molecule 1: Tail tube protein

Chain o:



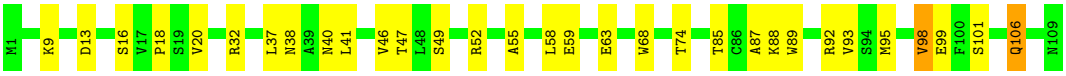
• Molecule 2: Tail tip protein M

Chain M:



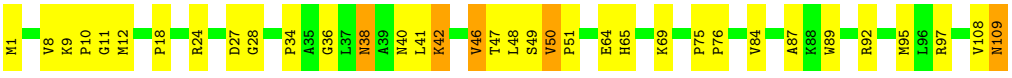
• Molecule 2: Tail tip protein M

Chain m:



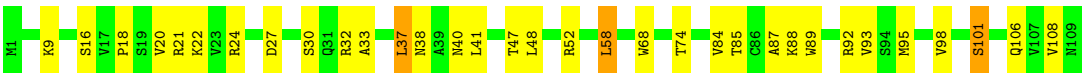
• Molecule 2: Tail tip protein M

Chain E:



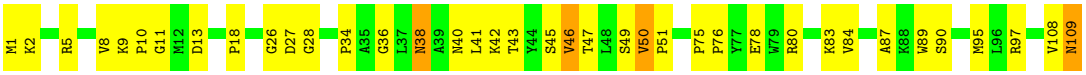
• Molecule 2: Tail tip protein M

Chain K:



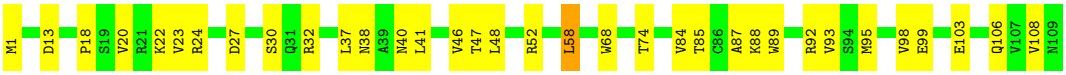
• Molecule 2: Tail tip protein M

Chain Y:



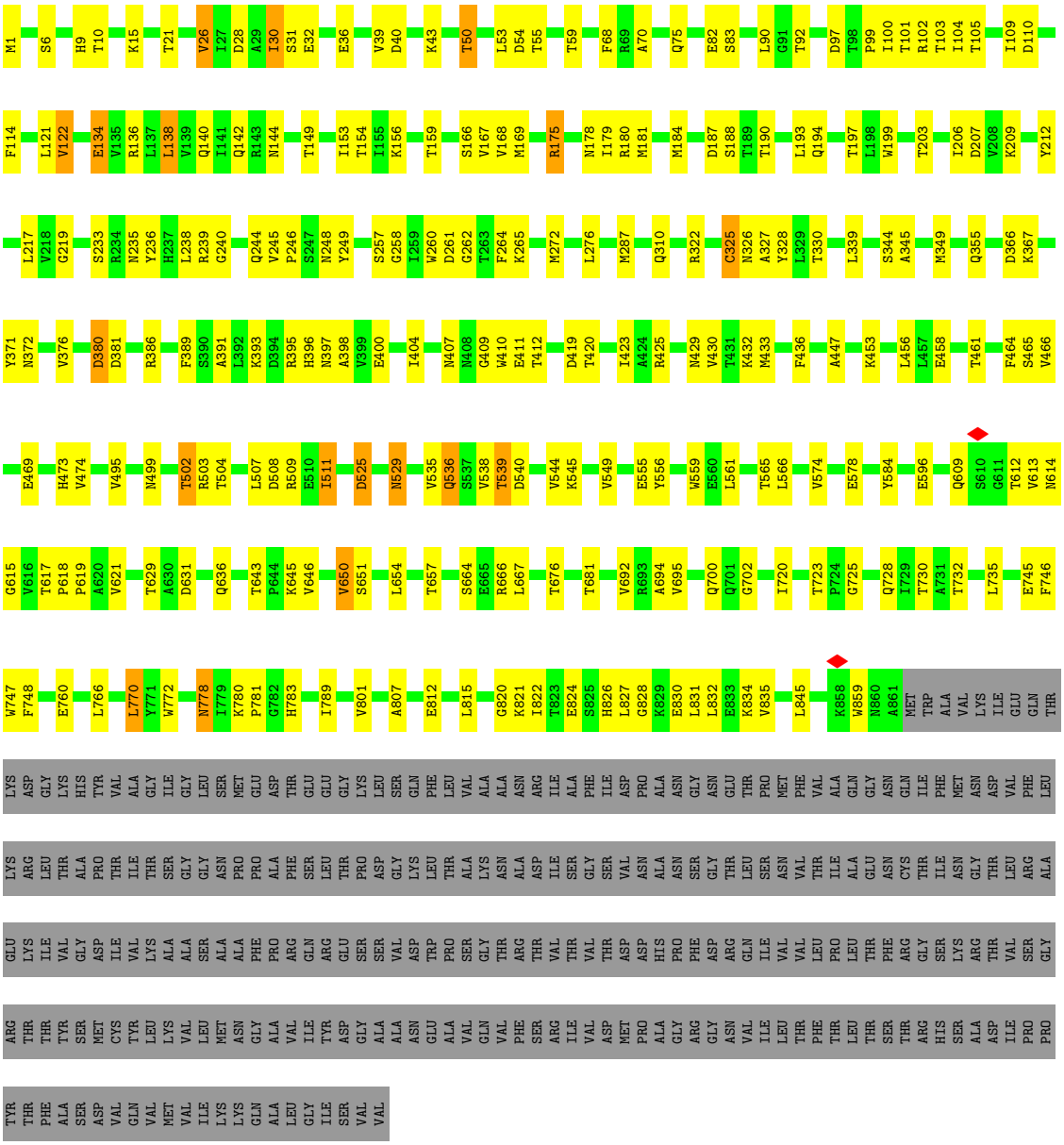
• Molecule 2: Tail tip protein M

Chain e:



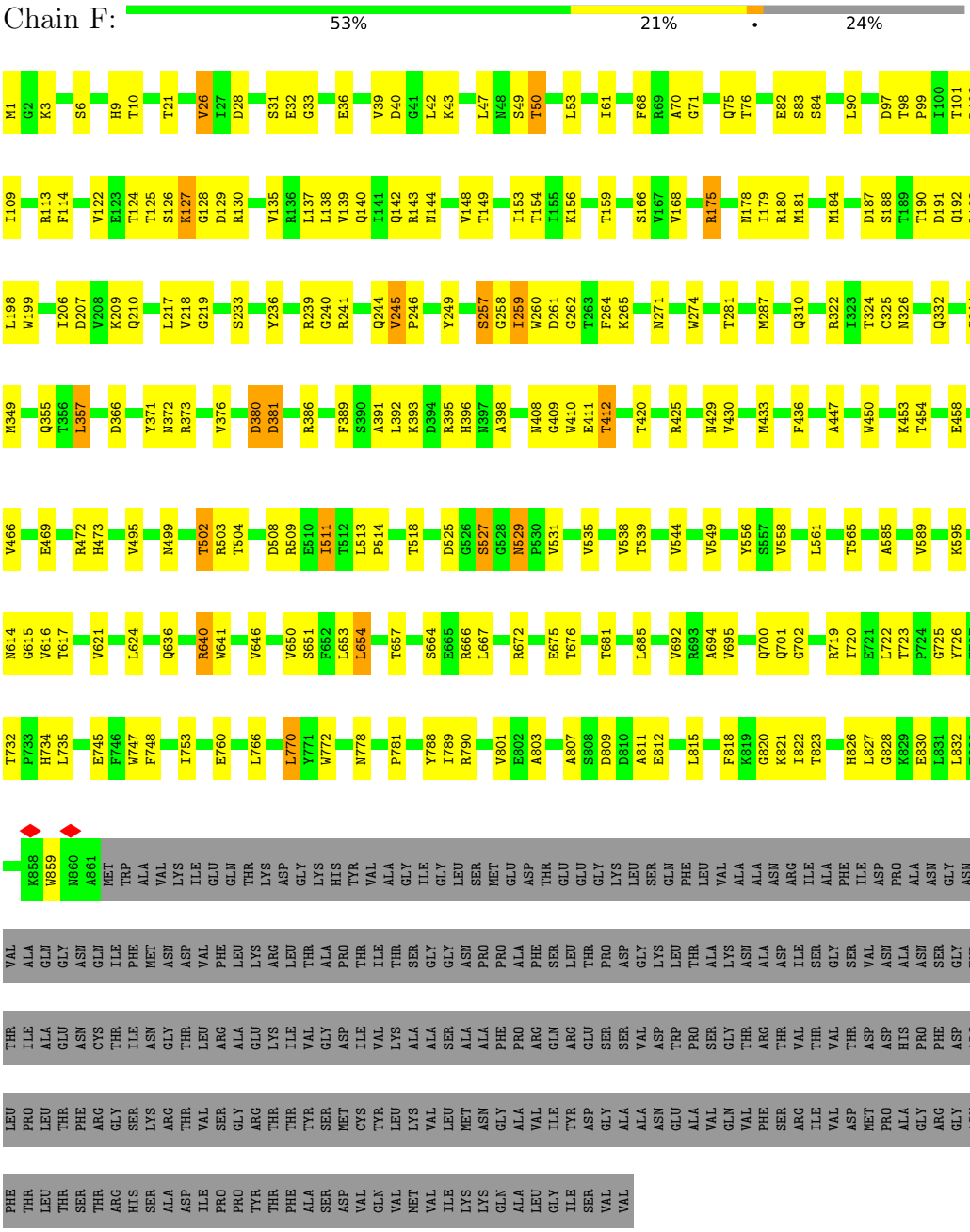
• Molecule 3: Tip attachment protein J

Chain J:



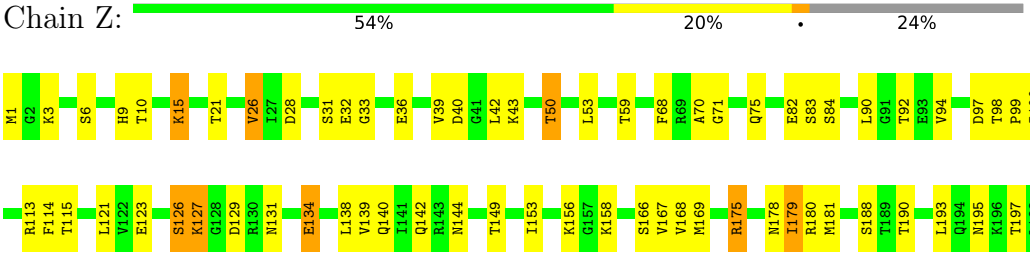
• Molecule 3: Tip attachment protein J

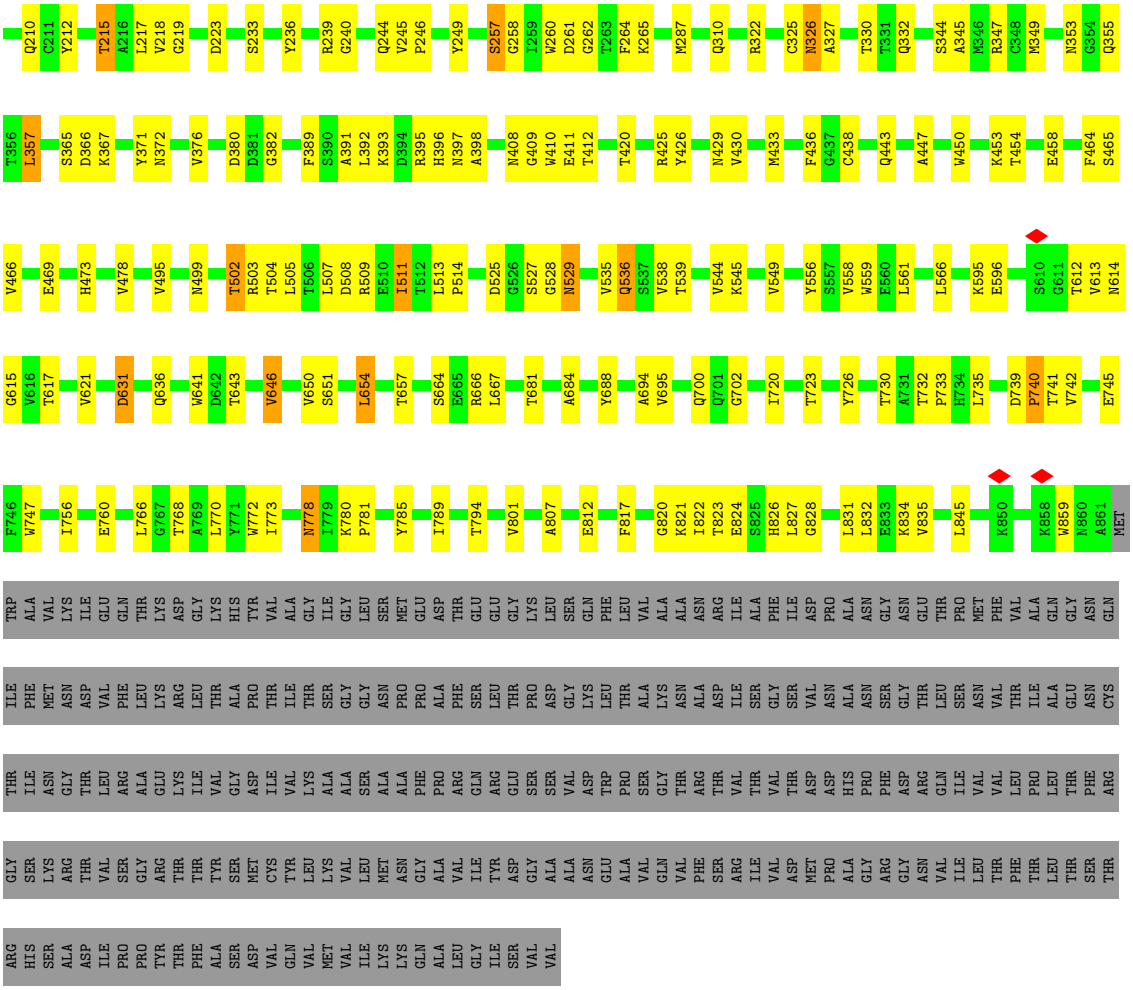
Chain F:



• Molecule 3: Tip attachment protein J

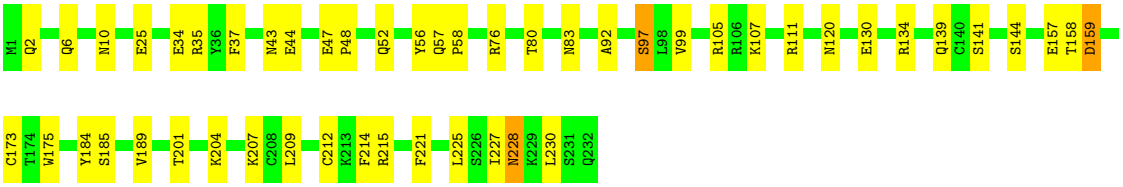
Chain Z:





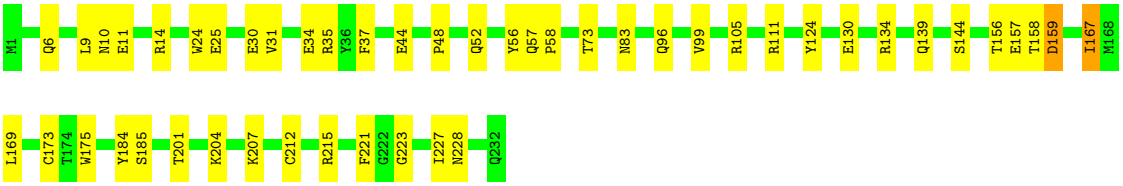
• Molecule 4: Tail tip protein L

Chain L:



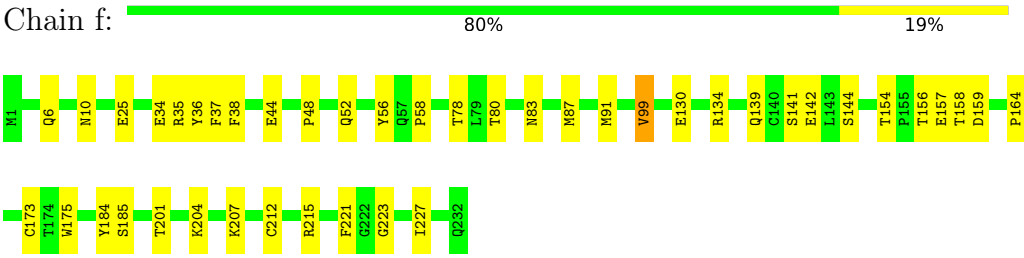
• Molecule 4: Tail tip protein L

Chain N:



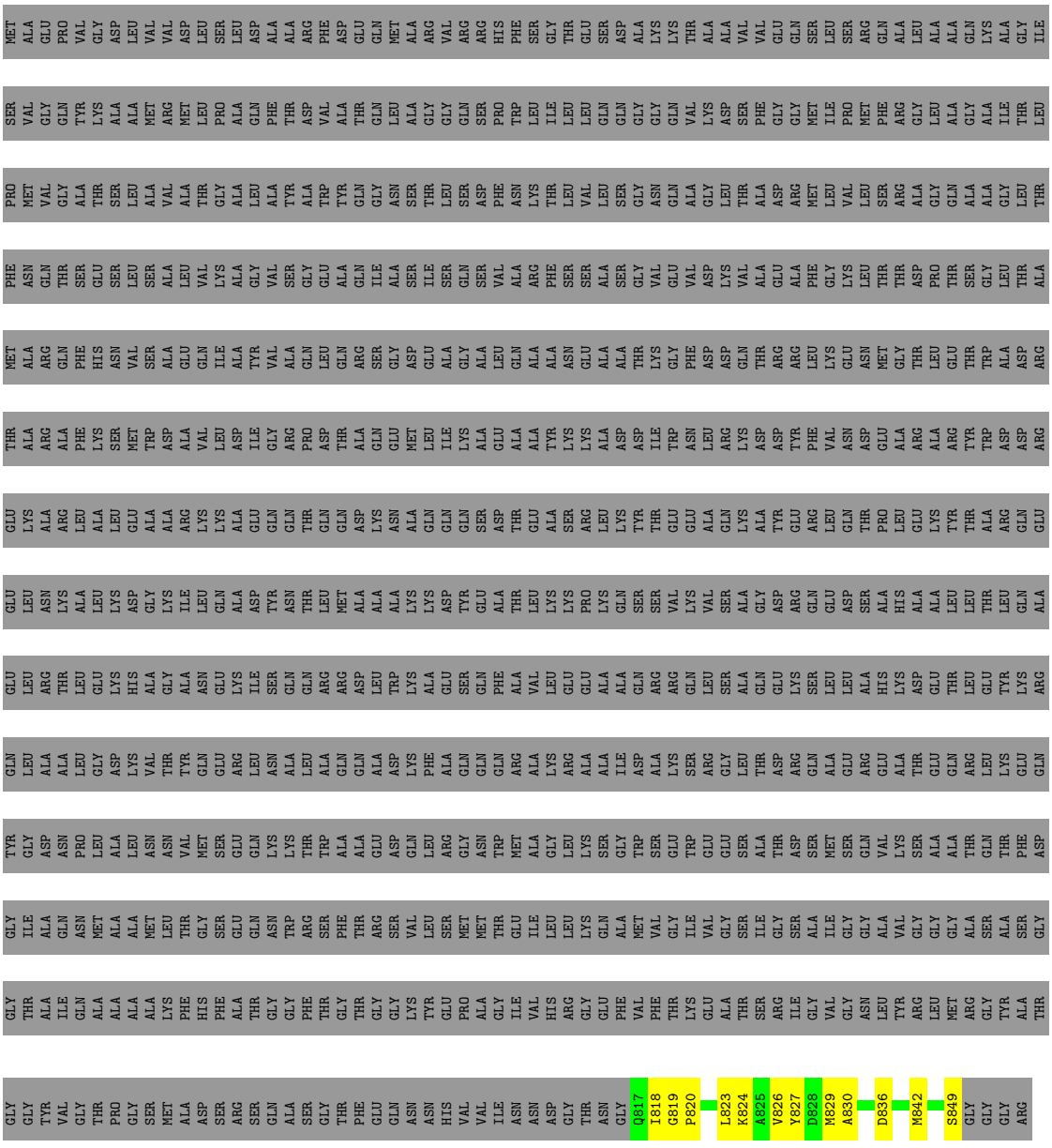
• Molecule 4: Tail tip protein L

Chain f:



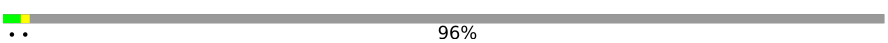
• Molecule 5: Tape measure protein

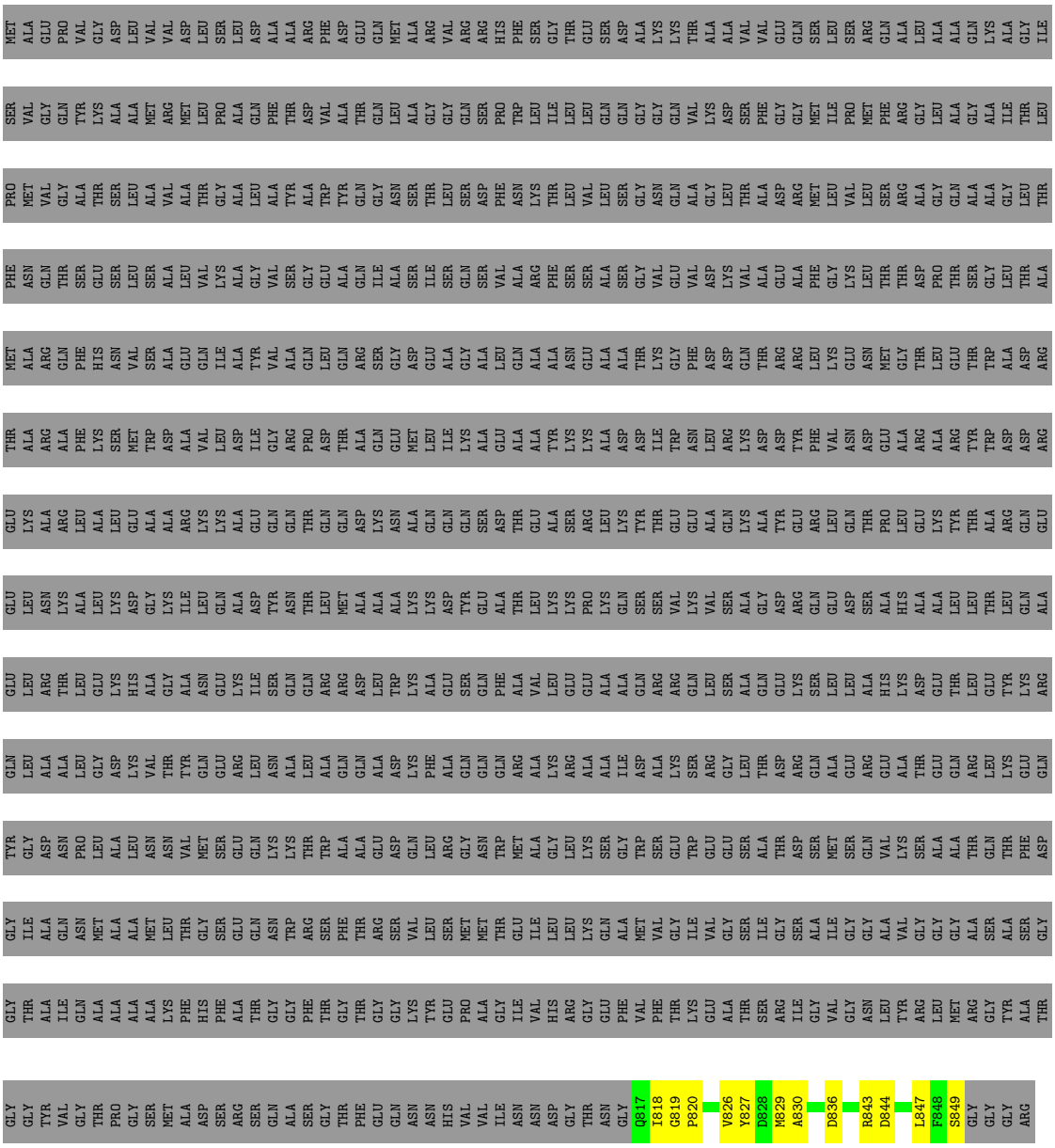
Chain H:



• Molecule 5: Tape measure protein

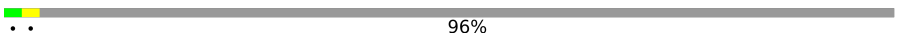
Chain O:

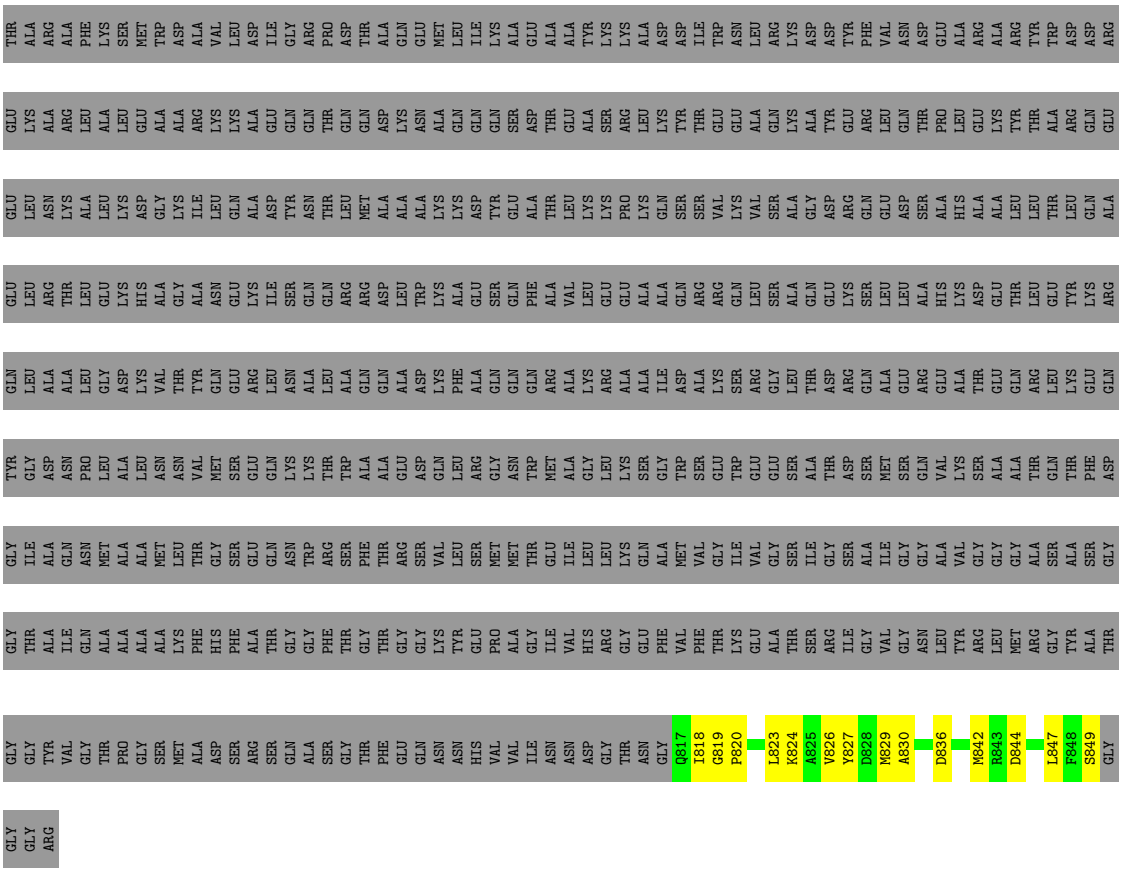




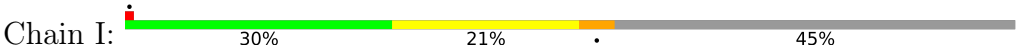
• Molecule 5: Tape measure protein

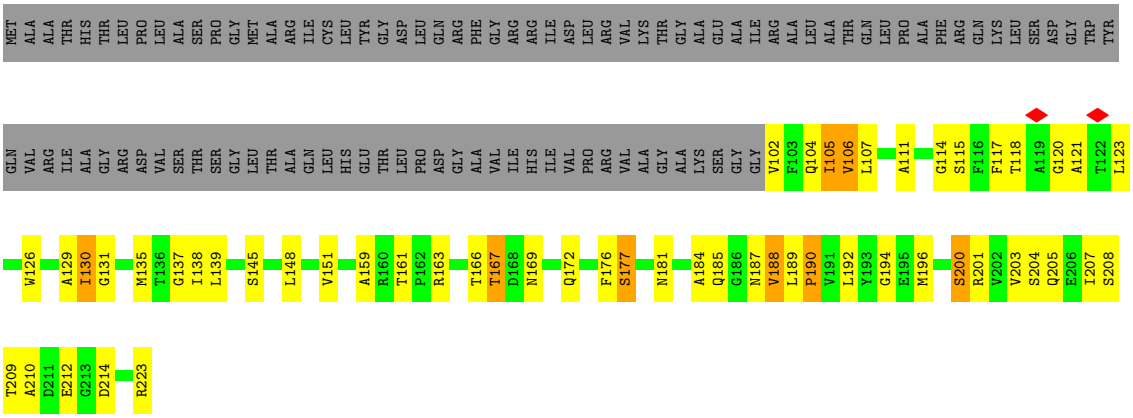
Chain g:



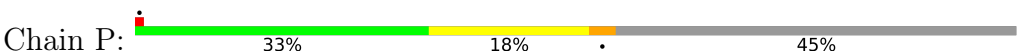


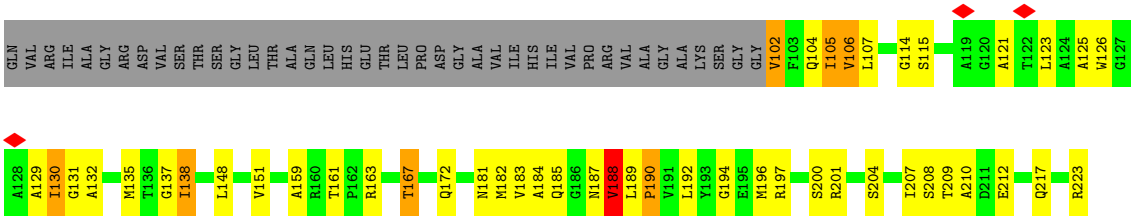
• Molecule 6: Tail tip assembly protein I





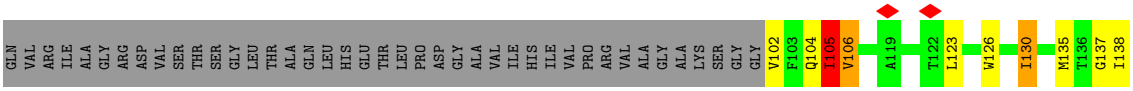
• Molecule 6: Tail tip assembly protein I





• Molecule 6: Tail tip assembly protein I

Chain h:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	57290	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 ($e^-/Å^2$)	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	4.086	Depositor
Minimum map value	-1.793	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.090	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	515.616, 515.616, 515.616	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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	A	0.13	0/1834	0.36	0/2505
1	B	0.17	0/1834	0.38	0/2505
1	C	0.20	0/1834	0.41	0/2505
1	D	0.11	0/1827	0.29	0/2494
1	G	0.12	0/1827	0.31	0/2494
1	Q	0.13	0/1834	0.33	0/2505
1	R	0.12	0/1834	0.33	0/2505
1	S	0.13	0/1834	0.33	0/2505
1	T	0.16	0/1834	0.35	0/2505
1	U	0.20	0/1834	0.43	0/2505
1	V	0.12	0/1827	0.30	0/2494
1	W	0.16	0/1834	0.36	0/2505
1	X	0.13	0/1827	0.34	1/2494 (0.0%)
1	a	0.16	0/1834	0.32	0/2505
1	b	0.17	0/1834	0.36	0/2505
1	c	0.17	0/1834	0.40	1/2505 (0.0%)
1	d	0.12	0/1827	0.31	0/2494
1	i	0.13	0/1834	0.34	0/2505
1	j	0.16	0/1834	0.32	0/2505
1	k	0.13	0/1834	0.36	0/2505
1	l	0.16	0/1834	0.32	0/2505
1	n	0.14	0/1834	0.40	0/2505
1	o	0.16	0/1834	0.37	0/2505
1	v	0.17	0/1827	0.32	0/2494
2	E	0.16	0/909	0.43	0/1231
2	K	0.14	0/909	0.38	0/1231
2	M	0.15	0/909	0.41	0/1231
2	Y	0.16	0/909	0.42	0/1231
2	e	0.15	0/909	0.40	0/1231
2	m	0.14	0/909	0.38	0/1231
3	F	0.16	0/6866	0.36	0/9348
3	J	0.16	0/6866	0.38	1/9348 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
3	Z	0.15	0/6866	0.39	2/9348 (0.0%)
4	L	0.12	0/1836	0.27	0/2487
4	N	0.12	0/1836	0.27	0/2487
4	f	0.12	0/1836	0.28	0/2487
5	H	0.11	0/252	0.33	0/335
5	O	0.14	0/252	0.38	0/335
5	g	0.13	0/252	0.33	0/335
6	I	0.31	1/876 (0.1%)	0.59	2/1186 (0.2%)
6	P	0.31	1/876 (0.1%)	0.53	0/1186
6	h	0.14	0/876	0.44	0/1186
All	All	0.15	2/78918 (0.0%)	0.36	7/107508 (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
3	F	0	1
3	J	0	1
3	Z	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	190	PRO	C-O	-6.27	1.16	1.23
6	P	190	PRO	C-O	-5.44	1.17	1.23

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	I	190	PRO	N-CA-CB	-6.44	97.75	103.35
1	X	187	PRO	N-CA-C	-6.21	99.67	112.47
3	Z	740	PRO	CB-CA-C	-5.90	101.83	111.56
3	Z	134	GLU	CB-CG-CD	5.39	121.76	112.60
3	J	134	GLU	CB-CG-CD	5.37	121.72	112.60
6	I	190	PRO	CA-C-O	-5.09	115.65	121.56
1	c	66	ASP	N-CA-C	-5.04	106.98	113.23

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	F	175	ARG	Peptide
3	J	175	ARG	Peptide
3	Z	175	ARG	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	A	1799	0	1768	43	0
1	B	1799	0	1768	55	0
1	C	1799	0	1768	60	0
1	D	1792	0	1760	36	0
1	G	1792	0	1760	45	0
1	Q	1799	0	1768	44	0
1	R	1799	0	1768	47	0
1	S	1799	0	1768	40	0
1	T	1799	0	1768	37	0
1	U	1799	0	1768	66	0
1	V	1792	0	1760	41	0
1	W	1799	0	1768	66	0
1	X	1792	0	1760	33	0
1	a	1799	0	1768	43	0
1	b	1799	0	1768	51	0
1	c	1799	0	1768	58	0
1	d	1792	0	1760	44	0
1	i	1799	0	1768	55	0
1	j	1799	0	1768	49	0
1	k	1799	0	1768	40	0
1	l	1799	0	1768	41	0
1	n	1799	0	1768	57	0
1	o	1799	0	1768	57	0
1	v	1792	0	1760	46	0
2	E	884	0	881	27	0
2	K	884	0	881	21	0
2	M	884	0	881	28	0
2	Y	884	0	881	31	0
2	e	884	0	881	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	m	884	0	881	20	0
3	F	6720	0	6558	176	0
3	J	6720	0	6558	158	0
3	Z	6720	0	6558	168	0
4	L	1801	0	1715	38	0
4	N	1801	0	1715	33	0
4	f	1801	0	1715	30	0
5	H	250	0	251	16	0
5	O	250	0	251	16	0
5	g	250	0	251	17	0
6	I	865	0	874	49	0
6	P	865	0	874	46	0
6	h	865	0	874	42	0
7	L	8	0	0	0	0
7	N	8	0	0	0	0
7	f	8	0	0	0	0
All	All	77370	0	75864	1793	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 (1793) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:v:180:THR:HG23	1:v:213:THR:HG23	1.43	1.00
3:Z:240:GLY:HA3	6:h:194:GLY:H	1.36	0.89
3:F:240:GLY:HA3	6:P:194:GLY:H	1.37	0.89
3:J:240:GLY:HA3	6:I:194:GLY:H	1.38	0.89
1:U:167:THR:O	1:U:182:THR:HB	1.73	0.88
3:F:332:GLN:HB2	6:P:188:VAL:HG11	1.59	0.84
1:n:167:THR:O	1:n:182:THR:HB	1.78	0.82
1:C:167:THR:O	1:C:182:THR:HB	1.79	0.82
3:J:835:VAL:HG13	3:F:834:LYS:HE2	1.64	0.79
3:J:36:GLU:HG2	3:J:239:ARG:HD2	1.65	0.79
3:F:815:LEU:HD21	3:Z:821:LYS:HB3	1.65	0.79
3:F:36:GLU:HG2	3:F:239:ARG:HD2	1.65	0.78
1:C:21:LYS:HD2	1:C:37:SER:HB3	1.66	0.78
2:E:95:MET:HE3	1:G:58:SER:HB3	1.66	0.78
3:F:380:ASP:OD1	3:F:380:ASP:N	2.18	0.77
3:J:380:ASP:OD1	3:J:380:ASP:N	2.17	0.76
3:Z:36:GLU:HG2	3:Z:239:ARG:HD2	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:95:MET:HE3	1:v:58:SER:HB3	1.69	0.75
2:K:37:LEU:HB3	2:Y:27:ASP:HB3	1.69	0.75
3:J:720:ILE:HD12	3:J:789:ILE:HD11	1.67	0.75
5:O:819:GLY:HA3	6:h:123:LEU:HD22	1.69	0.74
1:j:63:GLU:HG2	1:j:64:ASP:H	1.52	0.74
3:J:287:MET:HE1	4:L:158:THR:HG22	1.68	0.74
2:K:92:ARG:NH1	2:Y:13:ASP:OD1	2.21	0.73
3:Z:134:GLU:HG2	3:Z:156:LYS:HE3	1.68	0.73
1:C:198:VAL:HG23	1:C:227:PRO:HG2	1.71	0.73
3:Z:43:LYS:HG2	3:Z:53:LEU:HB2	1.71	0.73
3:Z:287:MET:HE1	4:f:158:THR:HG22	1.70	0.73
3:J:134:GLU:HG2	3:J:156:LYS:HE3	1.68	0.73
1:W:66:ASP:OD1	1:W:66:ASP:N	2.20	0.73
2:M:1:MET:HE1	2:M:5:ARG:HH12	1.54	0.72
2:M:27:ASP:OD2	3:J:509:ARG:NH2	2.22	0.72
1:T:63:GLU:HG2	1:T:64:ASP:H	1.54	0.72
1:U:21:LYS:HD2	1:U:37:SER:HB3	1.71	0.72
3:Z:396:HIS:HA	3:Z:429:ASN:HB2	1.71	0.72
1:b:126:SER:HB3	1:b:142:LYS:HB3	1.71	0.72
2:Y:95:MET:HE3	1:d:58:SER:HB3	1.72	0.72
2:M:38:ASN:OD1	2:M:38:ASN:N	2.23	0.72
1:B:210:SER:O	1:B:213:THR:OG1	2.07	0.72
3:F:249:TYR:O	3:F:265:LYS:NZ	2.23	0.72
1:l:185:PHE:O	1:l:191:THR:OG1	2.08	0.72
1:Q:210:SER:O	1:Q:213:THR:OG1	2.08	0.71
3:F:287:MET:HE1	4:N:158:THR:HG22	1.71	0.71
2:Y:38:ASN:N	2:Y:38:ASN:OD1	2.24	0.71
3:F:149:THR:O	6:P:217:GLN:NE2	2.24	0.71
1:a:204:LYS:HA	1:a:220:ALA:HB3	1.72	0.71
3:F:114:PHE:O	3:F:166:SER:HA	1.89	0.71
1:a:126:SER:HB3	1:a:142:LYS:HB3	1.72	0.71
3:Z:720:ILE:HD12	3:Z:789:ILE:HD11	1.73	0.71
1:T:204:LYS:HA	1:T:220:ALA:HB3	1.73	0.71
3:J:380:ASP:HB2	6:I:121:ALA:HB1	1.73	0.71
1:b:42:VAL:HG22	1:U:61:ASP:HB2	1.73	0.71
4:L:157:GLU:HG2	3:F:393:LYS:HE3	1.73	0.70
1:i:209:VAL:HG12	1:i:214:ILE:HG12	1.73	0.70
3:F:380:ASP:HB2	6:P:121:ALA:HB1	1.72	0.70
1:V:167:THR:O	1:V:182:THR:HB	1.92	0.70
3:F:127:LYS:HG2	3:F:128:GLY:H	1.56	0.70
2:E:27:ASP:OD2	3:F:509:ARG:NH2	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:l:150:SER:OG	1:l:155:ARG:NH2	2.24	0.70
3:Z:114:PHE:O	3:Z:166:SER:HA	1.92	0.70
1:l:204:LYS:HA	1:l:220:ALA:HB3	1.74	0.70
2:E:24:ARG:NH1	6:P:102:VAL:O	2.25	0.70
1:i:210:SER:O	1:i:213:THR:OG1	2.08	0.70
1:R:96:LEU:HD21	1:R:141:VAL:HG21	1.72	0.69
3:F:9:HIS:ND1	3:F:9:HIS:O	2.26	0.69
1:T:150:SER:OG	1:T:155:ARG:NH2	2.26	0.69
2:m:37:LEU:HB3	2:E:27:ASP:HB3	1.74	0.69
1:b:63:GLU:HG2	1:b:64:ASP:H	1.58	0.69
1:j:126:SER:HB3	1:j:142:LYS:HB3	1.74	0.69
1:R:126:SER:HB3	1:R:142:LYS:HB3	1.74	0.69
1:n:198:VAL:HG23	1:n:227:PRO:HG2	1.73	0.69
2:E:38:ASN:OD1	2:E:38:ASN:N	2.25	0.69
1:R:127:ILE:HB	1:i:50:LEU:HB2	1.75	0.69
1:U:151:MET:HE3	1:U:152:ALA:H	1.57	0.68
1:o:49:GLU:OE2	1:o:49:GLU:N	2.21	0.68
1:D:167:THR:O	1:D:182:THR:HB	1.93	0.68
1:U:198:VAL:HG23	1:U:227:PRO:HG2	1.76	0.68
1:X:96:LEU:HD11	1:X:141:VAL:HG11	1.75	0.68
3:J:538:VAL:HG22	3:J:544:VAL:HG22	1.75	0.68
3:F:396:HIS:HA	3:F:429:ASN:HB2	1.75	0.68
1:Q:126:SER:HB3	1:Q:142:LYS:HB3	1.75	0.68
1:W:49:GLU:N	1:W:49:GLU:OE2	2.27	0.68
3:Z:70:ALA:O	3:Z:75:GLN:NE2	2.26	0.68
1:l:126:SER:HB3	1:l:142:LYS:HB3	1.75	0.68
1:B:209:VAL:HG12	1:B:214:ILE:HG12	1.73	0.68
1:d:187:PRO:HD2	1:d:191:THR:HG22	1.76	0.68
1:c:8:MET:SD	1:c:8:MET:N	2.67	0.68
1:D:96:LEU:HD11	1:D:141:VAL:HG11	1.76	0.68
1:G:16:THR:OG1	1:G:18:TRP:NE1	2.27	0.68
1:S:175:LYS:NZ	1:S:244:THR:O	2.27	0.68
1:U:205:ALA:HA	1:U:217:ASN:O	1.94	0.68
1:i:96:LEU:HD21	1:i:141:VAL:HG21	1.76	0.68
1:k:175:LYS:NZ	1:k:244:THR:O	2.27	0.68
1:n:165:THR:HG23	1:n:184:ALA:HB3	1.76	0.68
1:n:205:ALA:HA	1:n:217:ASN:O	1.93	0.68
3:F:745:GLU:O	3:F:789:ILE:HA	1.94	0.68
1:v:210:SER:O	1:v:211:GLY:C	2.37	0.67
1:d:102:GLU:OE2	1:d:106:ARG:NH2	2.27	0.67
1:S:195:PHE:HE2	1:S:214:ILE:HD11	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:245:VAL:HG22	3:Z:246:PRO:HD2	1.74	0.67
1:A:175:LYS:NZ	1:A:244:THR:O	2.27	0.67
1:D:126:SER:HB3	1:D:142:LYS:HB3	1.76	0.67
1:i:126:SER:HB3	1:i:142:LYS:HB3	1.76	0.67
1:k:126:SER:HB3	1:k:142:LYS:HB3	1.77	0.67
1:C:205:ALA:HA	1:C:217:ASN:O	1.94	0.67
1:G:148:ARG:NH1	1:X:64:ASP:OD1	2.26	0.67
4:N:34:GLU:N	4:N:34:GLU:OE2	2.28	0.67
2:Y:27:ASP:OD2	3:Z:509:ARG:NH2	2.27	0.67
3:J:245:VAL:HG22	3:J:246:PRO:HD2	1.74	0.67
1:V:204:LYS:HA	1:V:220:ALA:HB3	1.76	0.67
3:J:723:THR:HG22	3:J:730:THR:HB	1.77	0.67
3:F:43:LYS:HG2	3:F:53:LEU:HB2	1.77	0.67
1:c:49:GLU:OE2	1:c:49:GLU:N	2.24	0.66
1:D:59:TYR:HA	2:E:9:LYS:HA	1.78	0.66
3:Z:100:ILE:HG22	3:Z:102:ARG:HH21	1.59	0.66
1:D:204:LYS:HA	1:D:220:ALA:HB3	1.77	0.66
3:F:245:VAL:HG22	3:F:246:PRO:HD2	1.77	0.66
2:Y:8:VAL:HG11	2:Y:46:VAL:HG22	1.77	0.66
1:C:61:ASP:HB2	1:j:42:VAL:HG22	1.76	0.66
1:C:165:THR:HG23	1:C:184:ALA:HB3	1.76	0.66
3:F:70:ALA:O	3:F:75:GLN:NE2	2.28	0.66
1:R:42:VAL:HG22	1:n:61:ASP:HB2	1.76	0.66
2:Y:78:GLU:OE2	2:Y:80:ARG:NH2	2.28	0.66
3:Z:723:THR:HG22	3:Z:730:THR:HB	1.78	0.66
3:J:834:LYS:HE2	3:Z:835:VAL:HG13	1.77	0.66
1:R:117:VAL:O	1:R:155:ARG:NH1	2.28	0.66
3:J:822:ILE:HG23	3:F:827:LEU:HA	1.78	0.66
1:a:63:GLU:HG2	1:a:64:ASP:H	1.60	0.66
1:V:197:ALA:HB3	1:V:209:VAL:HG21	1.77	0.66
3:J:43:LYS:HG2	3:J:53:LEU:HB2	1.76	0.66
1:S:102:GLU:N	1:S:102:GLU:OE2	2.29	0.66
1:U:8:MET:HE3	1:U:9:PRO:HD2	1.77	0.66
1:T:166:VAL:HG22	1:T:183:VAL:HG22	1.78	0.65
3:Z:140:GLN:HG2	3:Z:149:THR:HA	1.77	0.65
3:F:142:GLN:NE2	3:F:144:ASN:O	2.29	0.65
4:L:34:GLU:N	4:L:34:GLU:OE2	2.30	0.65
1:v:216:VAL:HG11	1:v:241:ILE:HG13	1.78	0.65
3:F:723:THR:HG22	3:F:730:THR:HB	1.76	0.65
1:V:126:SER:HB3	1:V:142:LYS:HB3	1.76	0.65
1:n:151:MET:HA	1:n:151:MET:HE3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:l:96:LEU:HD11	1:l:141:VAL:HG11	1.79	0.65
1:C:226:ILE:HD11	1:C:239:ALA:HB3	1.79	0.65
1:o:5:ASN:HD21	1:o:8:MET:HE1	1.60	0.65
1:a:181:LEU:HB2	1:a:214:ILE:HB	1.77	0.65
1:W:127:ILE:O	1:n:50:LEU:N	2.30	0.65
3:J:184:MET:HA	3:J:184:MET:HE3	1.79	0.65
6:I:189:LEU:HD12	6:I:190:PRO:HD2	1.77	0.65
3:J:396:HIS:HA	3:J:429:ASN:HB2	1.79	0.64
1:C:8:MET:HE3	1:C:9:PRO:HD2	1.79	0.64
1:U:165:THR:HG23	1:U:184:ALA:HB3	1.78	0.64
4:f:34:GLU:N	4:f:34:GLU:OE2	2.30	0.64
1:i:196:ARG:HH22	1:j:196:ARG:HD2	1.63	0.64
1:b:117:VAL:O	1:b:155:ARG:NH1	2.31	0.64
1:D:199:SER:HB3	1:D:202:LYS:HD3	1.77	0.64
1:G:96:LEU:HD11	1:G:141:VAL:HG11	1.80	0.64
1:X:59:TYR:HA	2:Y:9:LYS:HA	1.78	0.64
2:M:27:ASP:HB3	2:e:37:LEU:HB3	1.79	0.64
3:J:745:GLU:O	3:J:789:ILE:HA	1.97	0.64
1:a:150:SER:OG	1:a:155:ARG:NH2	2.29	0.64
1:U:17:LEU:HD23	1:U:39:LEU:HD12	1.80	0.64
3:Z:538:VAL:HG22	3:Z:544:VAL:HG22	1.79	0.64
3:J:70:ALA:O	3:J:75:GLN:NE2	2.30	0.64
1:V:195:PHE:HA	1:V:230:SER:HA	1.79	0.64
3:F:1:MET:HE2	3:F:6:SER:HB3	1.79	0.64
1:G:202:LYS:HZ1	1:G:207:VAL:HG22	1.63	0.64
1:R:66:ASP:OD1	1:R:66:ASP:N	2.30	0.64
1:j:117:VAL:O	1:j:155:ARG:NH1	2.30	0.64
1:o:17:LEU:HD11	1:o:39:LEU:HD11	1.80	0.64
1:V:64:ASP:OD1	1:d:148:ARG:NH1	2.30	0.64
1:v:181:LEU:HB2	1:v:214:ILE:HB	1.80	0.64
1:X:199:SER:HB3	1:X:202:LYS:HD3	1.78	0.64
1:d:164:MET:HA	1:d:164:MET:HE3	1.80	0.64
3:J:827:LEU:HA	3:Z:822:ILE:HG23	1.80	0.64
1:X:204:LYS:HA	1:X:220:ALA:HB3	1.77	0.64
6:h:105:ILE:HD12	6:h:106:VAL:H	1.63	0.64
1:V:96:LEU:HD11	1:V:141:VAL:HG11	1.80	0.64
1:v:148:ARG:NH1	1:D:64:ASP:OD1	2.27	0.64
1:D:195:PHE:HA	1:D:230:SER:HA	1.79	0.64
3:J:142:GLN:NE2	3:J:144:ASN:O	2.31	0.64
3:J:391:ALA:HA	4:f:139:GLN:HB2	1.78	0.64
1:B:43:LYS:HB2	1:B:83:THR:HG23	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:VAL:HG11	1:A:226:ILE:HD13	1.78	0.64
1:T:126:SER:HB3	1:T:142:LYS:HB3	1.79	0.64
3:J:1:MET:HE2	3:J:6:SER:HB3	1.79	0.63
1:X:167:THR:O	1:X:182:THR:HB	1.97	0.63
1:X:197:ALA:HB3	1:X:209:VAL:HG21	1.80	0.63
1:k:102:GLU:OE1	1:k:102:GLU:N	2.30	0.63
1:b:127:ILE:HB	1:Q:50:LEU:HB2	1.78	0.63
4:f:175:TRP:O	4:f:207:LYS:NZ	2.32	0.63
6:h:189:LEU:HD12	6:h:190:PRO:HD2	1.79	0.63
1:b:66:ASP:OD1	1:b:66:ASP:N	2.31	0.63
1:T:79:ASP:N	1:T:79:ASP:OD1	2.29	0.63
3:Z:636:GLN:HG2	3:Z:681:THR:HG22	1.79	0.63
1:Q:196:ARG:HH22	1:R:196:ARG:HD2	1.63	0.63
1:c:161:ALA:HB3	1:c:187:PRO:HB2	1.81	0.63
4:f:48:PRO:HB3	4:f:58:PRO:HD3	1.80	0.63
3:J:109:ILE:HG22	3:J:175:ARG:HD3	1.81	0.63
5:H:829:MET:HG2	5:g:826:VAL:HG12	1.81	0.63
3:F:820:GLY:H	3:Z:826:HIS:HA	1.64	0.63
1:j:66:ASP:OD1	1:j:66:ASP:N	2.30	0.63
1:k:207:VAL:HG11	1:k:226:ILE:HD13	1.80	0.63
1:S:207:VAL:HG11	1:S:226:ILE:HD13	1.79	0.63
1:V:199:SER:HB3	1:V:202:LYS:HD3	1.79	0.63
1:B:63:GLU:HG2	1:B:64:ASP:N	2.13	0.63
5:H:819:GLY:HA3	6:P:123:LEU:HD22	1.81	0.62
3:Z:142:GLN:NE2	3:Z:144:ASN:O	2.32	0.62
3:J:114:PHE:O	3:J:166:SER:HA	1.98	0.62
1:U:207:VAL:HG12	1:U:216:VAL:HG22	1.81	0.62
6:h:105:ILE:HD11	6:h:137:GLY:HA2	1.81	0.62
1:i:223:LYS:HG3	1:i:242:THR:HG23	1.81	0.62
3:J:140:GLN:HG2	3:J:149:THR:HA	1.80	0.62
3:J:249:TYR:O	3:J:265:LYS:NZ	2.32	0.62
1:c:164:MET:HG2	1:c:185:PHE:HA	1.81	0.62
3:Z:109:ILE:HG22	3:Z:175:ARG:HD3	1.80	0.62
1:l:225:ASN:ND2	1:l:240:GLU:OE1	2.33	0.62
1:V:165:THR:HG23	1:V:184:ALA:HB3	1.81	0.62
3:F:109:ILE:HG22	3:F:175:ARG:HD3	1.81	0.62
1:d:96:LEU:HD11	1:d:141:VAL:HG11	1.81	0.62
6:P:129:ALA:O	6:P:131:GLY:N	2.32	0.62
1:Q:96:LEU:HD21	1:Q:141:VAL:HG21	1.80	0.62
4:L:175:TRP:O	4:L:207:LYS:NZ	2.33	0.62
1:U:108:TYR:OH	1:U:145:ASN:ND2	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:l:108:TYR:OH	1:l:145:ASN:OD1	2.16	0.62
1:c:196:ARG:NH1	1:c:231:GLY:O	2.32	0.62
1:R:209:VAL:HG22	1:R:214:ILE:HG13	1.81	0.62
3:F:140:GLN:HG2	3:F:149:THR:HA	1.80	0.61
4:N:139:GLN:HB2	3:Z:391:ALA:HA	1.81	0.61
6:P:104:GLN:O	6:P:106:VAL:N	2.33	0.61
1:G:164:MET:HE3	1:G:164:MET:HA	1.82	0.61
1:R:21:LYS:HD3	1:R:37:SER:HB3	1.81	0.61
4:L:139:GLN:HB2	3:F:391:ALA:HA	1.81	0.61
1:G:216:VAL:HG11	1:G:241:ILE:HG13	1.82	0.61
1:X:195:PHE:HA	1:X:230:SER:HA	1.82	0.61
1:d:216:VAL:HG11	1:d:241:ILE:HG13	1.81	0.61
1:W:161:ALA:HB3	1:W:187:PRO:HB2	1.81	0.61
1:d:16:THR:OG1	1:d:18:TRP:NE1	2.30	0.61
3:J:636:GLN:HG2	3:J:681:THR:HG22	1.83	0.61
3:J:646:VAL:HG21	3:J:650:VAL:HB	1.81	0.61
2:m:52:ARG:NH1	2:m:95:MET:O	2.33	0.61
5:H:818:ILE:HG12	6:I:130:ILE:HG21	1.83	0.61
3:F:815:LEU:HB3	3:Z:826:HIS:HE2	1.65	0.61
1:U:87:MET:N	1:U:93:GLN:OE1	2.32	0.61
1:o:161:ALA:HB3	1:o:187:PRO:HB2	1.82	0.61
4:N:83:ASN:ND2	4:N:144:SER:O	2.25	0.61
4:N:175:TRP:O	4:N:207:LYS:NZ	2.34	0.61
1:k:195:PHE:HE2	1:k:214:ILE:HD11	1.64	0.61
1:l:79:ASP:N	1:l:79:ASP:OD1	2.33	0.61
4:L:83:ASN:ND2	4:L:144:SER:O	2.26	0.61
1:A:197:ALA:HB1	1:A:226:ILE:HD11	1.83	0.61
1:C:50:LEU:HD13	1:C:77:ALA:HB2	1.81	0.61
1:C:163:GLY:C	1:C:164:MET:HE3	2.26	0.61
3:F:538:VAL:HG22	3:F:544:VAL:HG22	1.83	0.61
1:v:221:ALA:HA	1:v:243:VAL:HB	1.83	0.61
2:e:52:ARG:NH1	2:e:95:MET:O	2.34	0.61
3:J:9:HIS:ND1	3:J:9:HIS:O	2.34	0.60
1:a:108:TYR:OH	1:a:145:ASN:OD1	2.15	0.60
1:W:83:THR:HG22	1:W:140:THR:HG23	1.82	0.60
1:a:79:ASP:N	1:a:79:ASP:OD1	2.32	0.60
1:a:164:MET:HE2	1:a:235:PHE:HB3	1.82	0.60
1:d:202:LYS:HZ1	1:d:207:VAL:HG22	1.66	0.60
1:C:43:LYS:H	1:C:84:LEU:HA	1.65	0.60
3:F:815:LEU:HA	3:F:818:PHE:HB2	1.84	0.60
1:S:33:ASP:OD1	1:S:111:ARG:NH1	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:127:ILE:HB	1:W:50:LEU:HB2	1.83	0.60
4:f:25:GLU:OE2	4:f:35:ARG:NH1	2.34	0.60
6:P:129:ALA:C	6:P:131:GLY:H	2.09	0.60
1:S:204:LYS:HA	1:S:220:ALA:HB3	1.83	0.60
4:f:83:ASN:ND2	4:f:144:SER:O	2.29	0.60
1:V:151:MET:HE2	1:V:151:MET:HA	1.84	0.60
3:F:646:VAL:HG21	3:F:650:VAL:HB	1.84	0.60
1:W:10:VAL:HG13	1:W:12:GLY:H	1.67	0.60
1:k:204:LYS:HA	1:k:220:ALA:HB3	1.83	0.60
1:B:96:LEU:HD21	1:B:141:VAL:HG21	1.82	0.60
1:C:50:LEU:N	1:o:127:ILE:O	2.33	0.60
2:K:52:ARG:NH1	2:K:95:MET:O	2.33	0.60
1:l:63:GLU:HG2	1:l:64:ASP:H	1.66	0.60
1:V:164:MET:HE2	1:V:230:SER:HB2	1.84	0.60
3:J:821:LYS:NZ	3:Z:812:GLU:OE2	2.34	0.60
1:v:196:ARG:NH2	1:v:231:GLY:O	2.34	0.60
1:B:63:GLU:HG2	1:B:64:ASP:H	1.66	0.60
1:c:135:GLU:N	1:c:135:GLU:OE2	2.35	0.60
3:F:636:GLN:HG2	3:F:681:THR:HG22	1.82	0.60
1:B:223:LYS:HG3	1:B:242:THR:HG23	1.83	0.60
1:Q:193:LYS:HZ3	1:Q:231:GLY:HA3	1.67	0.60
1:v:193:LYS:NZ	1:v:234:GLU:OE2	2.35	0.59
6:I:104:GLN:O	6:I:106:VAL:N	2.36	0.59
1:A:204:LYS:HA	1:A:220:ALA:HB3	1.83	0.59
1:G:221:ALA:HA	1:G:243:VAL:HB	1.83	0.59
1:l:221:ALA:HA	1:l:243:VAL:HB	1.84	0.59
1:V:59:TYR:HA	2:M:9:LYS:HA	1.82	0.59
1:v:96:LEU:HD11	1:v:141:VAL:HG11	1.84	0.59
1:W:86:TRP:HB3	1:W:137:ILE:HG23	1.84	0.59
3:Z:355:GLN:O	4:f:134:ARG:NH1	2.35	0.59
1:v:16:THR:OG1	1:v:18:TRP:NE1	2.30	0.59
1:B:197:ALA:HB3	1:B:209:VAL:HG11	1.84	0.59
1:A:195:PHE:HE2	1:A:214:ILE:HD11	1.65	0.59
3:Z:745:GLU:O	3:Z:789:ILE:HA	2.02	0.59
1:T:221:ALA:HA	1:T:243:VAL:HB	1.85	0.59
1:j:207:VAL:HG12	1:j:216:VAL:HG22	1.83	0.59
2:K:41:LEU:O	2:K:106:GLN:HG2	2.02	0.59
1:R:74:GLN:NE2	1:i:65:ALA:O	2.36	0.59
1:U:43:LYS:H	1:U:84:LEU:HA	1.67	0.59
1:X:126:SER:HB3	1:X:142:LYS:HB3	1.85	0.59
3:F:179:ILE:HD13	3:F:199:TRP:HH2	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:167:THR:HG23	1:G:182:THR:HB	1.83	0.59
3:Z:249:TYR:O	3:Z:265:LYS:NZ	2.34	0.59
1:B:50:LEU:HB2	1:j:127:ILE:HB	1.84	0.59
1:B:196:ARG:HH22	1:b:196:ARG:HD2	1.68	0.59
1:D:197:ALA:HB3	1:D:209:VAL:HG21	1.83	0.59
1:Q:86:TRP:CD1	1:Q:139:ARG:HE	2.21	0.59
1:R:18:TRP:HB2	1:R:109:LYS:HG2	1.84	0.59
1:n:204:LYS:HD2	1:n:222:GLY:HA3	1.84	0.59
1:o:181:LEU:HB2	1:o:214:ILE:HB	1.84	0.59
1:b:74:GLN:NE2	1:Q:65:ALA:O	2.36	0.59
1:a:221:ALA:HA	1:a:243:VAL:HB	1.85	0.58
3:Z:142:GLN:HB2	3:Z:178:ASN:HB2	1.83	0.58
3:Z:215:THR:HG22	4:f:166:ARG:HH22	1.66	0.58
1:v:202:LYS:HZ1	1:v:207:VAL:HG22	1.68	0.58
4:N:25:GLU:OE2	4:N:35:ARG:NH1	2.36	0.58
4:N:228:ASN:ND2	3:Z:408:ASN:OD1	2.36	0.58
1:i:221:ALA:HA	1:i:243:VAL:HB	1.85	0.58
1:v:30:PRO:HB2	1:v:117:VAL:HG11	1.84	0.58
6:P:187:ASN:HD21	6:h:170:GLY:HA3	1.68	0.58
1:W:127:ILE:HB	1:n:50:LEU:HB2	1.85	0.58
3:F:376:VAL:HG12	3:F:466:VAL:HG12	1.85	0.58
3:Z:657:THR:HG22	3:Z:667:LEU:HA	1.84	0.58
1:o:86:TRP:HB3	1:o:137:ILE:HG23	1.84	0.58
3:J:657:THR:HG22	3:J:667:LEU:HA	1.86	0.58
1:Q:45:LEU:HD12	1:Q:82:PHE:HB3	1.85	0.58
1:X:63:GLU:N	1:X:63:GLU:OE2	2.37	0.58
3:J:142:GLN:HB2	3:J:178:ASN:HB2	1.85	0.58
1:c:86:TRP:HB3	1:c:137:ILE:HG23	1.86	0.58
2:E:24:ARG:NH1	2:E:24:ARG:HB2	2.19	0.58
1:T:15:THR:HG23	1:T:112:PHE:HA	1.85	0.58
1:T:96:LEU:HD11	1:T:141:VAL:HG11	1.85	0.58
1:B:221:ALA:HA	1:B:243:VAL:HB	1.86	0.58
1:A:66:ASP:OD1	1:A:66:ASP:N	2.34	0.58
1:C:119:VAL:HG13	1:C:150:SER:HB3	1.85	0.58
1:W:87:MET:HG2	1:n:9:PRO:HD3	1.85	0.58
1:X:33:ASP:OD1	1:X:109:LYS:NZ	2.32	0.58
1:i:117:VAL:O	1:i:155:ARG:NH2	2.36	0.58
1:k:197:ALA:HB1	1:k:226:ILE:HD11	1.86	0.58
1:l:117:VAL:O	1:l:155:ARG:NH1	2.37	0.58
1:l:175:LYS:NZ	1:l:244:THR:O	2.36	0.58
1:c:127:ILE:O	1:U:50:LEU:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:148:ARG:NH2	1:v:64:ASP:OD1	2.37	0.58
4:L:48:PRO:HB3	4:L:58:PRO:HD3	1.86	0.58
1:A:209:VAL:HG22	1:A:214:ILE:HG12	1.86	0.58
1:c:151:MET:O	1:c:155:ARG:NH1	2.36	0.58
3:J:21:THR:HB	6:I:210:ALA:HB3	1.85	0.58
3:J:407:ASN:ND2	3:J:609:GLN:O	2.36	0.58
1:a:31:LEU:O	1:a:111:ARG:NH1	2.37	0.58
1:a:183:VAL:HB	1:a:212:MET:HE1	1.86	0.58
3:F:184:MET:HA	3:F:184:MET:HE3	1.84	0.58
1:G:16:THR:HG1	1:G:18:TRP:HE1	1.52	0.58
1:U:85:ALA:HB1	1:W:9:PRO:HB3	1.86	0.58
3:Z:525:ASP:OD2	3:Z:529:ASN:ND2	2.37	0.58
1:j:18:TRP:HB2	1:j:109:LYS:HG2	1.85	0.58
1:Q:63:GLU:CD	1:Q:63:GLU:H	2.12	0.57
1:c:126:SER:HB3	1:c:142:LYS:HB3	1.86	0.57
1:W:44:ASP:OD1	1:W:83:THR:OG1	2.15	0.57
1:X:194:SER:OG	1:X:195:PHE:N	2.37	0.57
1:n:119:VAL:HG13	1:n:150:SER:HB3	1.86	0.57
1:B:117:VAL:O	1:B:155:ARG:NH2	2.37	0.57
3:F:6:SER:HB2	3:F:68:PHE:HB3	1.86	0.57
1:o:196:ARG:NH1	1:o:231:GLY:O	2.36	0.57
3:J:179:ILE:HD13	3:J:199:TRP:HH2	1.69	0.57
3:J:345:ALA:HB2	3:J:436:PHE:HB3	1.86	0.57
3:J:376:VAL:HG12	3:J:466:VAL:HG12	1.86	0.57
1:k:209:VAL:HG22	1:k:214:ILE:HG12	1.85	0.57
1:n:50:LEU:HD13	1:n:77:ALA:HB2	1.86	0.57
1:n:85:ALA:HB1	1:o:9:PRO:HB3	1.87	0.57
1:n:127:ILE:HD13	1:n:141:VAL:HB	1.86	0.57
1:V:63:GLU:N	1:V:63:GLU:OE2	2.37	0.57
5:H:827:TYR:OH	5:O:836:ASP:OD2	2.22	0.57
1:C:129:LYS:NZ	1:c:118:ASP:OD2	2.38	0.57
6:h:104:GLN:O	6:h:106:VAL:N	2.38	0.57
2:M:8:VAL:HG11	2:M:46:VAL:HG22	1.86	0.57
1:c:127:ILE:HG22	1:U:50:LEU:HD23	1.87	0.57
3:F:345:ALA:HB2	3:F:436:PHE:HB3	1.87	0.57
1:R:175:LYS:NZ	1:R:244:THR:O	2.36	0.57
1:S:197:ALA:HB1	1:S:226:ILE:HD11	1.86	0.57
1:j:184:ALA:HB1	1:j:186:GLN:HE22	1.68	0.57
1:o:8:MET:SD	1:o:8:MET:N	2.66	0.57
1:C:204:LYS:HA	1:C:220:ALA:HB3	1.87	0.57
1:c:10:VAL:HG13	1:c:12:GLY:H	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:194:SER:OG	1:D:195:PHE:N	2.38	0.57
3:F:409:GLY:O	3:F:411:GLU:HG3	2.05	0.57
1:U:159:THR:HG23	1:U:161:ALA:H	1.70	0.57
1:c:181:LEU:HB2	1:c:214:ILE:HB	1.86	0.57
4:N:48:PRO:HB3	4:N:58:PRO:HD3	1.87	0.57
1:S:63:GLU:H	1:S:63:GLU:CD	2.12	0.57
3:J:409:GLY:O	3:J:411:GLU:HG3	2.05	0.57
3:J:629:THR:OG1	3:J:631:ASP:OD1	2.23	0.57
4:L:25:GLU:OE2	4:L:35:ARG:NH1	2.38	0.57
3:F:381:ASP:OD2	3:F:386:ARG:NH2	2.31	0.57
1:Q:204:LYS:HA	1:Q:220:ALA:HB3	1.87	0.57
3:Z:612:THR:OG1	3:Z:614:ASN:ND2	2.37	0.57
1:o:166:VAL:HG22	1:o:183:VAL:HG22	1.87	0.57
3:F:139:VAL:HG22	3:F:181:MET:HG3	1.87	0.56
1:j:168:PRO:HA	1:j:181:LEU:HG	1.87	0.56
1:j:221:ALA:HA	1:j:243:VAL:HB	1.87	0.56
1:l:166:VAL:HG22	1:l:183:VAL:HG22	1.87	0.56
1:c:128:GLY:O	1:c:139:ARG:NH1	2.39	0.56
3:F:433:MET:HE1	3:F:447:ALA:HB1	1.86	0.56
1:o:151:MET:O	1:o:155:ARG:NH1	2.38	0.56
3:J:6:SER:HB2	3:J:68:PHE:HB3	1.87	0.56
3:J:502:THR:O	3:J:502:THR:OG1	2.24	0.56
6:I:123:LEU:HD22	5:g:819:GLY:HA3	1.88	0.56
1:C:50:LEU:HB2	1:o:127:ILE:HB	1.87	0.56
1:G:181:LEU:O	1:G:213:THR:OG1	2.23	0.56
1:T:108:TYR:OH	1:T:145:ASN:OD1	2.19	0.56
1:T:175:LYS:NZ	1:T:244:THR:O	2.38	0.56
1:W:166:VAL:HG22	1:W:183:VAL:HG22	1.87	0.56
3:Z:244:GLN:HG3	3:Z:264:PHE:HB3	1.88	0.56
1:k:124:VAL:O	1:l:72:GLN:NE2	2.38	0.56
1:n:108:TYR:OH	1:n:145:ASN:ND2	2.30	0.56
5:H:826:VAL:HG12	5:O:829:MET:HG2	1.86	0.56
5:O:818:ILE:HG12	6:P:130:ILE:HG21	1.86	0.56
1:B:204:LYS:HA	1:B:220:ALA:HB3	1.86	0.56
1:b:207:VAL:HG12	1:b:216:VAL:HG22	1.87	0.56
3:F:31:SER:OG	3:F:32:GLU:N	2.39	0.56
1:U:119:VAL:HG13	1:U:150:SER:HB3	1.87	0.56
3:Z:179:ILE:HD13	3:Z:199:TRP:HH2	1.70	0.56
1:b:18:TRP:HB2	1:b:109:LYS:HG2	1.88	0.56
1:W:74:GLN:NE2	1:n:65:ALA:O	2.35	0.56
2:e:88:LYS:NZ	2:e:103:GLU:OE2	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:j:175:LYS:NZ	1:j:244:THR:O	2.39	0.56
1:v:207:VAL:HG11	1:v:226:ILE:HG21	1.86	0.56
1:A:126:SER:HB3	1:A:142:LYS:HB3	1.88	0.56
1:C:132:THR:HG23	1:C:135:GLU:HB3	1.87	0.56
3:Z:380:ASP:N	3:Z:380:ASP:OD1	2.33	0.56
1:n:43:LYS:H	1:n:84:LEU:HA	1.70	0.56
3:F:142:GLN:HB2	3:F:178:ASN:HB2	1.88	0.56
1:G:193:LYS:NZ	1:G:234:GLU:OE2	2.39	0.56
3:Z:614:ASN:OD1	3:Z:615:GLY:N	2.39	0.56
3:J:395:ARG:O	3:J:429:ASN:ND2	2.34	0.55
3:J:409:GLY:O	3:J:411:GLU:N	2.39	0.55
3:F:26:VAL:O	3:F:219:GLY:HA2	2.07	0.55
3:F:371:TYR:OH	3:F:473:HIS:NE2	2.28	0.55
1:S:76:SER:O	1:S:76:SER:OG	2.24	0.55
1:W:205:ALA:HB3	1:W:224:VAL:HG21	1.89	0.55
4:f:167:ILE:HA	6:h:188:VAL:HA	1.87	0.55
1:l:199:SER:OG	1:l:200:ALA:N	2.39	0.55
1:n:102:GLU:OE1	1:n:102:GLU:N	2.39	0.55
1:a:175:LYS:NZ	1:a:244:THR:O	2.38	0.55
1:C:186:GLN:NE2	1:C:189:GLY:O	2.39	0.55
3:F:21:THR:HB	6:P:210:ALA:HB3	1.87	0.55
1:Q:118:ASP:OD1	1:Q:152:ALA:N	2.39	0.55
6:h:177:SER:HB2	6:h:196:MET:HE1	1.88	0.55
1:i:204:LYS:HA	1:i:220:ALA:HB3	1.88	0.55
1:k:91:GLN:NE2	1:l:192:ASP:HB3	2.21	0.55
1:a:199:SER:OG	1:a:200:ALA:N	2.39	0.55
1:G:122:GLY:HA2	1:G:146:VAL:HG22	1.88	0.55
1:d:221:ALA:HA	1:d:243:VAL:HB	1.88	0.55
1:o:15:THR:HG23	1:o:112:PHE:HA	1.88	0.55
1:B:118:ASP:OD1	1:B:152:ALA:N	2.40	0.55
3:F:409:GLY:O	3:F:411:GLU:N	2.39	0.55
1:S:124:VAL:O	1:T:72:GLN:NE2	2.40	0.55
3:J:612:THR:OG1	3:J:614:ASN:ND2	2.40	0.55
3:F:82:GLU:HA	3:F:207:ASP:HA	1.87	0.55
1:T:63:GLU:CD	1:T:63:GLU:H	2.13	0.55
1:T:109:LYS:HD2	1:T:117:VAL:HG21	1.89	0.55
1:T:117:VAL:O	1:T:155:ARG:NH1	2.39	0.55
3:Z:409:GLY:O	3:Z:411:GLU:HG3	2.05	0.55
1:o:109:LYS:HE3	1:o:111:ARG:HD2	1.87	0.55
1:b:96:LEU:HD11	1:b:141:VAL:HG11	1.89	0.55
1:c:48:GLY:N	1:c:80:THR:OG1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:614:ASN:OD1	3:F:615:GLY:N	2.40	0.55
2:Y:1:MET:HE1	2:Y:5:ARG:NH1	2.21	0.55
1:a:15:THR:HG23	1:a:112:PHE:HA	1.88	0.55
3:F:612:THR:OG1	3:F:614:ASN:ND2	2.39	0.55
6:P:189:LEU:HD12	6:P:190:PRO:HD2	1.86	0.55
1:W:8:MET:N	1:W:8:MET:SD	2.73	0.55
3:Z:26:VAL:O	3:Z:219:GLY:HA2	2.07	0.55
3:Z:50:THR:HG22	3:Z:700:GLN:HA	1.87	0.55
3:Z:511:ILE:HD12	3:Z:561:LEU:HD22	1.87	0.55
5:g:818:ILE:HG12	6:h:130:ILE:HG21	1.89	0.55
1:j:63:GLU:HG2	1:j:64:ASP:N	2.22	0.55
3:J:393:LYS:HZ1	4:f:157:GLU:HG2	1.72	0.55
2:Y:9:LYS:HG2	2:Y:10:PRO:HD3	1.88	0.55
3:Z:345:ALA:HB2	3:Z:436:PHE:HB3	1.89	0.55
5:H:820:PRO:HD3	6:P:123:LEU:HB3	1.89	0.55
1:C:61:ASP:OD1	1:j:38:ARG:NH1	2.40	0.55
1:C:114:ASN:OD1	1:C:116:THR:OG1	2.24	0.55
1:R:207:VAL:HG12	1:R:216:VAL:HG22	1.87	0.55
1:W:109:LYS:HE3	1:W:111:ARG:HD2	1.88	0.55
1:d:181:LEU:O	1:d:213:THR:OG1	2.24	0.55
1:W:151:MET:O	1:W:155:ARG:NH1	2.39	0.55
1:V:194:SER:OG	1:V:195:PHE:N	2.39	0.54
1:c:166:VAL:HG22	1:c:183:VAL:HG22	1.89	0.54
3:J:812:GLU:OE2	3:F:821:LYS:NZ	2.33	0.54
1:B:126:SER:HB3	1:B:142:LYS:HB3	1.89	0.54
3:F:50:THR:HG22	3:F:700:GLN:HA	1.89	0.54
5:O:826:VAL:HG12	5:g:829:MET:HG2	1.90	0.54
1:Q:117:VAL:O	1:Q:155:ARG:NH2	2.39	0.54
2:e:24:ARG:NH2	2:e:27:ASP:OD1	2.40	0.54
1:i:118:ASP:OD1	1:i:152:ALA:N	2.40	0.54
1:i:207:VAL:HG12	1:i:216:VAL:HG22	1.89	0.54
3:J:244:GLN:HG3	3:J:264:PHE:HB3	1.89	0.54
3:J:664:SER:OG	6:I:223:ARG:NH2	2.38	0.54
4:L:228:ASN:OD1	3:F:408:ASN:ND2	2.40	0.54
1:c:136:VAL:HA	1:U:11:LYS:HA	1.89	0.54
1:D:16:THR:OG1	1:D:18:TRP:NE1	2.39	0.54
6:P:132:ALA:HB3	6:P:135:MET:HG3	1.88	0.54
1:U:47:PRO:HA	1:U:80:THR:HG23	1.90	0.54
3:J:614:ASN:OD1	3:J:615:GLY:N	2.41	0.54
1:B:129:LYS:NZ	1:b:118:ASP:OD2	2.41	0.54
3:F:244:GLN:HG3	3:F:264:PHE:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:657:THR:HG22	3:F:667:LEU:HA	1.88	0.54
6:P:182:MET:HA	6:h:169:ASN:HB3	1.89	0.54
1:V:33:ASP:OD1	1:V:109:LYS:NZ	2.31	0.54
1:a:109:LYS:HD2	1:a:117:VAL:HG21	1.90	0.54
1:S:51:THR:HG22	1:S:52:ALA:H	1.70	0.54
1:v:212:MET:O	1:v:214:ILE:N	2.40	0.54
1:A:178:SER:HB2	1:A:215:THR:HG23	1.88	0.54
1:D:196:ARG:HH21	1:G:196:ARG:HE	1.56	0.54
1:G:83:THR:HG22	1:G:140:THR:HG23	1.90	0.54
1:k:96:LEU:HD21	1:k:141:VAL:HG21	1.88	0.54
3:J:26:VAL:O	3:J:219:GLY:HA2	2.08	0.54
3:J:31:SER:OG	3:J:32:GLU:N	2.41	0.54
3:J:400:GLU:OE1	3:J:432:LYS:NZ	2.40	0.54
6:I:115:SER:HB3	5:g:824:LYS:HB2	1.89	0.54
1:b:83:THR:HG22	1:b:140:THR:HG23	1.88	0.54
2:E:8:VAL:HG11	2:E:46:VAL:HG22	1.89	0.54
1:T:205:ALA:HB1	1:T:216:VAL:HG13	1.90	0.54
1:U:132:THR:HG23	1:U:135:GLU:HB3	1.88	0.54
1:W:48:GLY:N	1:W:80:THR:OG1	2.40	0.54
1:X:207:VAL:HG12	1:X:216:VAL:HG22	1.90	0.54
1:i:43:LYS:HB2	1:i:83:THR:HG23	1.90	0.54
3:J:371:TYR:OH	3:J:473:HIS:NE2	2.28	0.54
3:J:529:ASN:OD1	3:J:529:ASN:N	2.40	0.54
1:C:85:ALA:HB1	1:c:9:PRO:HB3	1.89	0.54
1:T:173:VAL:HG13	1:T:243:VAL:HG13	1.90	0.54
3:J:393:LYS:NZ	4:f:157:GLU:HG2	2.23	0.54
1:B:111:ARG:HG2	1:B:117:VAL:HG22	1.90	0.54
1:c:194:SER:OG	1:c:195:PHE:N	2.40	0.54
3:F:822:ILE:HG23	3:Z:827:LEU:HA	1.90	0.54
1:R:83:THR:HG22	1:R:140:THR:HG23	1.90	0.54
1:W:196:ARG:NH1	1:W:231:GLY:O	2.41	0.54
1:k:48:GLY:N	1:k:80:THR:OG1	2.41	0.54
3:J:82:GLU:HA	3:J:207:ASP:HA	1.90	0.54
3:J:381:ASP:OD2	3:J:386:ARG:NH2	2.32	0.54
1:B:65:ALA:O	1:j:74:GLN:NE2	2.40	0.54
1:B:207:VAL:HG12	1:B:216:VAL:HG22	1.89	0.54
1:R:184:ALA:HB1	1:R:186:GLN:HE22	1.73	0.54
1:U:204:LYS:HA	1:U:220:ALA:HB3	1.90	0.54
2:Y:109:ASN:OD1	2:e:32:ARG:NH2	2.41	0.54
1:l:185:PHE:HD1	1:l:191:THR:HG21	1.73	0.54
1:n:159:THR:HG23	1:n:161:ALA:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:o:195:PHE:HA	1:o:230:SER:HA	1.89	0.54
1:a:63:GLU:HG2	1:a:64:ASP:N	2.22	0.53
1:C:159:THR:HG23	1:C:161:ALA:H	1.72	0.53
1:G:207:VAL:HG11	1:G:226:ILE:HG21	1.89	0.53
1:j:197:ALA:HB3	1:j:214:ILE:HG12	1.90	0.53
1:T:181:LEU:HB2	1:T:214:ILE:HB	1.91	0.53
1:U:127:ILE:HD13	1:U:141:VAL:HB	1.89	0.53
3:Z:527:SER:OG	3:Z:528:GLY:N	2.40	0.53
1:d:109:LYS:HD2	1:d:117:VAL:HG21	1.91	0.53
1:n:97:LEU:HD21	1:n:139:ARG:HH12	1.73	0.53
1:n:127:ILE:HB	1:o:50:LEU:HB2	1.90	0.53
1:W:194:SER:OG	1:W:195:PHE:N	2.41	0.53
1:i:197:ALA:HB3	1:i:209:VAL:HG11	1.89	0.53
1:j:206:THR:OG1	1:j:217:ASN:ND2	2.30	0.53
3:J:508:ASP:OD1	3:J:508:ASP:N	2.42	0.53
6:I:187:ASN:O	6:I:188:VAL:HG22	2.09	0.53
1:A:91:GLN:HE22	1:a:192:ASP:HB2	1.73	0.53
1:D:61:ASP:OD1	1:D:61:ASP:N	2.36	0.53
3:F:525:ASP:OD2	3:F:529:ASN:HB2	2.08	0.53
1:R:221:ALA:HA	1:R:243:VAL:HB	1.90	0.53
1:U:114:ASN:OD1	1:U:116:THR:OG1	2.21	0.53
3:J:212:TYR:HB2	3:J:217:LEU:HD11	1.89	0.53
3:J:826:HIS:HA	3:Z:820:GLY:H	1.72	0.53
1:A:51:THR:HG22	1:A:52:ALA:H	1.72	0.53
1:C:9:PRO:HD3	1:o:87:MET:HG2	1.89	0.53
1:D:196:ARG:HH12	1:G:229:VAL:HG11	1.72	0.53
1:Q:111:ARG:HG2	1:Q:117:VAL:HG22	1.89	0.53
1:d:207:VAL:HG11	1:d:226:ILE:HG21	1.89	0.53
1:v:122:GLY:HA2	1:v:146:VAL:HG22	1.91	0.53
5:H:842:MET:HE2	5:O:847:LEU:HD22	1.90	0.53
1:c:87:MET:HG2	1:U:9:PRO:HD3	1.89	0.53
1:l:63:GLU:HG2	1:l:64:ASP:N	2.23	0.53
3:J:748:PHE:HB2	3:J:766:LEU:HG	1.91	0.53
1:A:102:GLU:N	1:A:102:GLU:OE1	2.42	0.53
1:C:127:ILE:HD13	1:C:141:VAL:HB	1.89	0.53
1:C:195:PHE:HE2	1:C:214:ILE:HD11	1.74	0.53
1:c:127:ILE:HG12	1:c:141:VAL:HG22	1.89	0.53
3:F:126:SER:O	3:F:128:GLY:N	2.42	0.53
1:W:175:LYS:NZ	1:W:244:THR:O	2.42	0.53
1:i:63:GLU:H	1:i:63:GLU:CD	2.16	0.53
1:v:129:LYS:NZ	1:D:118:ASP:OD2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:ARG:NH1	1:j:101:ASN:OD1	2.25	0.53
1:a:212:MET:O	1:a:212:MET:HE3	2.08	0.53
3:F:28:ASP:OD2	3:F:236:TYR:OH	2.21	0.53
3:F:815:LEU:HB3	3:Z:826:HIS:NE2	2.24	0.53
3:F:835:VAL:HB	3:Z:834:LYS:HE2	1.91	0.53
3:F:845:LEU:HD13	3:Z:845:LEU:HD11	1.91	0.53
1:T:31:LEU:O	1:T:111:ARG:NH1	2.41	0.53
1:j:44:ASP:OD1	1:j:44:ASP:N	2.41	0.53
1:S:126:SER:HB3	1:S:142:LYS:HB3	1.91	0.53
1:W:225:ASN:ND2	1:W:240:GLU:OE1	2.43	0.53
2:e:18:PRO:HB3	2:e:40:ASN:HB3	1.90	0.53
1:l:63:GLU:CD	1:l:63:GLU:H	2.17	0.53
1:V:118:ASP:OD1	1:V:152:ALA:N	2.42	0.52
1:b:175:LYS:NZ	1:b:244:THR:O	2.40	0.52
3:F:499:ASN:HB3	3:F:504:THR:HG22	1.90	0.52
1:W:131:VAL:HG22	1:W:137:ILE:HD11	1.91	0.52
2:Y:87:ALA:O	2:e:18:PRO:HD2	2.08	0.52
3:Z:502:THR:O	3:Z:502:THR:OG1	2.25	0.52
3:J:272:MET:HE1	3:J:345:ALA:HB1	1.90	0.52
1:b:197:ALA:HB3	1:b:214:ILE:HG12	1.90	0.52
1:D:118:ASP:OD1	1:D:152:ALA:N	2.43	0.52
2:E:87:ALA:O	2:K:18:PRO:HD2	2.09	0.52
1:Q:159:THR:HG23	1:Q:161:ALA:H	1.74	0.52
1:R:173:VAL:HG23	1:R:243:VAL:HG13	1.90	0.52
1:o:48:GLY:N	1:o:80:THR:OG1	2.42	0.52
3:J:355:GLN:O	4:L:134:ARG:NH1	2.42	0.52
3:F:458:GLU:HB3	6:P:151:VAL:HG11	1.91	0.52
1:Q:129:LYS:NZ	1:R:118:ASP:OD2	2.42	0.52
1:T:212:MET:HG3	1:T:212:MET:O	2.09	0.52
3:Z:31:SER:OG	3:Z:32:GLU:N	2.42	0.52
1:B:159:THR:HG23	1:B:161:ALA:H	1.74	0.52
1:D:206:THR:OG1	1:D:217:ASN:ND2	2.37	0.52
3:F:834:LYS:HZ2	3:F:834:LYS:C	2.16	0.52
6:P:167:THR:HG21	6:h:167:THR:HB	1.91	0.52
1:S:209:VAL:HG22	1:S:214:ILE:HG12	1.91	0.52
4:f:6:GLN:NE2	4:f:10:ASN:OD1	2.34	0.52
1:n:186:GLN:NE2	1:n:189:GLY:O	2.42	0.52
1:n:201:ASP:C	1:n:202:LYS:HG2	2.33	0.52
1:n:204:LYS:HA	1:n:220:ALA:HB3	1.91	0.52
1:o:63:GLU:HG3	1:o:64:ASP:N	2.24	0.52
1:B:128:GLY:O	1:B:139:ARG:NH1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:6:GLN:NE2	4:N:10:ASN:OD1	2.42	0.52
4:N:167:ILE:HG12	4:N:169:LEU:HG	1.92	0.52
1:R:166:VAL:HG22	1:R:183:VAL:HG13	1.90	0.52
1:T:63:GLU:HG2	1:T:64:ASP:N	2.23	0.52
2:Y:1:MET:HE1	2:Y:5:ARG:HH12	1.73	0.52
1:i:195:PHE:HE2	1:i:214:ILE:HD11	1.74	0.52
2:K:24:ARG:NH2	2:K:27:ASP:OD1	2.41	0.52
1:T:199:SER:OG	1:T:200:ALA:N	2.41	0.52
1:U:123:TRP:NE1	1:W:70:THR:O	2.42	0.52
1:U:204:LYS:HD2	1:U:222:GLY:HA3	1.92	0.52
1:X:118:ASP:OD1	1:X:152:ALA:N	2.43	0.52
3:Z:646:VAL:HG21	3:Z:650:VAL:HB	1.92	0.52
1:j:209:VAL:HG22	1:j:214:ILE:HG13	1.92	0.52
1:o:64:ASP:O	1:o:65:ALA:HB2	2.09	0.52
1:b:118:ASP:OD1	1:b:152:ALA:N	2.43	0.52
1:A:33:ASP:OD1	1:A:111:ARG:NH1	2.41	0.52
1:D:33:ASP:OD1	1:D:109:LYS:NZ	2.32	0.52
2:Y:13:ASP:HB2	2:Y:45:SER:HB2	1.91	0.52
1:l:173:VAL:HG13	1:l:243:VAL:HG13	1.92	0.52
3:J:525:ASP:HB3	3:J:529:ASN:OD1	2.10	0.52
1:A:226:ILE:HG23	1:A:239:ALA:HB3	1.92	0.52
1:n:132:THR:HG23	1:n:135:GLU:HB3	1.90	0.52
3:J:748:PHE:HD2	3:J:766:LEU:HD11	1.74	0.52
6:I:123:LEU:HB3	5:g:820:PRO:HD3	1.91	0.52
1:B:63:GLU:H	1:B:63:GLU:CD	2.18	0.52
1:C:181:LEU:HB2	1:C:214:ILE:HB	1.91	0.52
1:G:151:MET:HE2	1:G:151:MET:HA	1.91	0.52
1:Q:221:ALA:HA	1:Q:243:VAL:HB	1.92	0.52
1:k:76:SER:O	1:k:76:SER:OG	2.24	0.52
1:k:78:GLY:HA2	1:k:145:ASN:HB2	1.92	0.52
1:B:108:TYR:OH	1:B:145:ASN:OD1	2.28	0.52
1:c:66:ASP:N	1:c:66:ASP:OD1	2.41	0.52
1:V:206:THR:OG1	1:V:217:ASN:ND2	2.39	0.51
1:B:21:LYS:HE3	1:B:37:SER:HB2	1.92	0.51
1:b:206:THR:OG1	1:b:217:ASN:ND2	2.30	0.51
1:S:194:SER:O	1:S:231:GLY:N	2.44	0.51
1:U:129:LYS:NZ	1:W:118:ASP:OD2	2.43	0.51
1:U:210:SER:O	1:U:213:THR:HG22	2.10	0.51
1:k:226:ILE:HG23	1:k:239:ALA:HB3	1.92	0.51
1:o:66:ASP:OD1	1:o:66:ASP:N	2.43	0.51
1:S:48:GLY:N	1:S:80:THR:OG1	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:205:ALA:HB3	1:U:224:VAL:HG11	1.92	0.51
4:L:44:GLU:OE1	4:L:44:GLU:N	2.43	0.51
1:b:21:LYS:HD2	1:b:37:SER:HB3	1.92	0.51
1:A:119:VAL:HG13	1:A:150:SER:HB3	1.92	0.51
1:A:124:VAL:O	1:a:72:GLN:NE2	2.43	0.51
1:D:207:VAL:HG12	1:D:216:VAL:HG22	1.92	0.51
5:O:827:TYR:OH	5:g:836:ASP:OD2	2.29	0.51
1:k:63:GLU:H	1:k:63:GLU:CD	2.18	0.51
3:J:28:ASP:OD2	3:J:236:TYR:OH	2.22	0.51
1:D:148:ARG:NH2	1:G:64:ASP:OD1	2.43	0.51
1:S:94:GLN:OE1	1:T:156:SER:OG	2.26	0.51
3:Z:82:GLU:OE2	3:Z:113:ARG:NH2	2.43	0.51
3:Z:330:THR:HA	6:h:190:PRO:HB3	1.92	0.51
3:Z:409:GLY:O	3:Z:411:GLU:N	2.40	0.51
1:d:122:GLY:HA2	1:d:146:VAL:HG22	1.91	0.51
3:J:503:ARG:HB2	3:J:549:VAL:HG23	1.91	0.51
1:B:195:PHE:HE2	1:B:214:ILE:HD11	1.75	0.51
1:b:108:TYR:OH	1:b:145:ASN:OD1	2.27	0.51
3:Z:212:TYR:HB2	3:Z:217:LEU:HD11	1.92	0.51
1:o:10:VAL:HG22	1:o:12:GLY:H	1.74	0.51
1:v:109:LYS:HD2	1:v:117:VAL:HG21	1.92	0.51
1:b:221:ALA:HA	1:b:243:VAL:HB	1.91	0.51
1:C:47:PRO:HA	1:C:80:THR:HG23	1.92	0.51
1:d:16:THR:HG1	1:d:18:TRP:HE1	1.55	0.51
1:i:18:TRP:HB2	1:i:109:LYS:HG2	1.93	0.51
1:j:173:VAL:HG23	1:j:243:VAL:HG13	1.92	0.51
1:o:194:SER:OG	1:o:195:PHE:N	2.42	0.51
1:v:173:VAL:HG13	1:v:243:VAL:HG13	1.93	0.51
6:I:184:ALA:HB2	6:I:201:ARG:HB3	1.92	0.51
1:T:18:TRP:HB2	1:T:109:LYS:HG2	1.93	0.51
3:Z:139:VAL:HG22	3:Z:181:MET:HG3	1.92	0.51
3:Z:380:ASP:OD1	6:h:105:ILE:HA	2.11	0.51
1:l:109:LYS:HD2	1:l:117:VAL:HG21	1.92	0.51
1:o:131:VAL:HG22	1:o:137:ILE:HD11	1.93	0.51
3:J:100:ILE:HG22	3:J:102:ARG:HH21	1.75	0.51
6:I:106:VAL:HA	6:I:139:LEU:HB2	1.92	0.51
1:b:173:VAL:HG23	1:b:243:VAL:HG13	1.91	0.51
1:G:229:VAL:HG13	1:G:236:ALA:HB2	1.93	0.51
1:Q:108:TYR:OH	1:Q:145:ASN:OD1	2.27	0.51
1:R:165:THR:HB	1:R:184:ALA:HB3	1.92	0.51
1:S:205:ALA:HB3	1:S:224:VAL:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:631:ASP:OD1	3:Z:631:ASP:N	2.43	0.51
6:h:184:ALA:HB2	6:h:201:ARG:HB3	1.93	0.51
1:l:31:LEU:O	1:l:111:ARG:NH1	2.44	0.51
1:o:124:VAL:HG22	1:o:143:VAL:HG22	1.93	0.51
2:M:87:ALA:O	2:m:18:PRO:HD2	2.10	0.51
1:v:102:GLU:OE2	1:v:106:ARG:NH2	2.44	0.51
1:B:167:THR:O	1:B:182:THR:OG1	2.28	0.51
1:c:175:LYS:NZ	1:c:244:THR:O	2.43	0.51
1:T:47:PRO:HA	1:T:80:THR:HG23	1.92	0.51
1:W:18:TRP:CZ3	1:W:38:ARG:HB2	2.46	0.51
1:X:205:ALA:HB3	1:X:224:VAL:HG11	1.93	0.51
3:Z:9:HIS:O	3:Z:9:HIS:CG	2.64	0.51
3:Z:508:ASP:OD2	3:Z:509:ARG:NH1	2.44	0.51
1:j:166:VAL:HG22	1:j:183:VAL:HG13	1.93	0.51
1:k:119:VAL:HG13	1:k:150:SER:HB3	1.93	0.51
1:n:226:ILE:HD11	1:n:239:ALA:HB3	1.93	0.51
1:v:229:VAL:HG13	1:v:236:ALA:HB2	1.92	0.51
1:A:96:LEU:HD21	1:A:141:VAL:HG21	1.93	0.51
1:R:133:ALA:O	1:R:134:LYS:HG2	2.11	0.51
1:X:128:GLY:O	1:X:139:ARG:NH1	2.40	0.51
3:Z:233:SER:O	3:Z:233:SER:OG	2.29	0.51
3:Z:398:ALA:O	3:Z:430:VAL:HA	2.11	0.51
3:J:260:TRP:NE1	3:J:262:GLY:O	2.44	0.50
1:b:168:PRO:HA	1:b:181:LEU:HG	1.92	0.50
3:F:233:SER:O	3:F:233:SER:OG	2.29	0.50
1:S:226:ILE:HG23	1:S:239:ALA:HB3	1.91	0.50
3:J:389:PHE:O	4:f:139:GLN:NE2	2.41	0.50
2:m:38:ASN:HB2	2:E:28:GLY:HA3	1.93	0.50
1:A:76:SER:O	1:A:76:SER:OG	2.24	0.50
1:G:173:VAL:HG13	1:G:243:VAL:HG13	1.93	0.50
4:N:48:PRO:HB3	4:N:57:GLN:HA	1.92	0.50
1:S:129:LYS:NZ	1:T:118:ASP:OD2	2.45	0.50
1:k:194:SER:O	1:k:231:GLY:N	2.44	0.50
2:M:18:PRO:HD2	2:e:87:ALA:O	2.11	0.50
2:M:29:TYR:OH	3:J:508:ASP:OD2	2.28	0.50
5:H:849:SER:OG	5:O:849:SER:O	2.27	0.50
4:N:44:GLU:OE1	4:N:44:GLU:N	2.43	0.50
1:W:128:GLY:O	1:W:139:ARG:NH1	2.44	0.50
3:Z:326:ASN:HB3	6:h:196:MET:HG2	1.93	0.50
1:k:51:THR:HG22	1:k:52:ALA:H	1.76	0.50
1:o:109:LYS:HD2	1:o:117:VAL:HG21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:17:VAL:O	2:M:17:VAL:HG12	2.10	0.50
1:D:128:GLY:O	1:D:139:ARG:NH1	2.41	0.50
3:J:327:ALA:HB1	6:I:176:PHE:HB2	1.94	0.50
3:J:845:LEU:HD13	3:F:845:LEU:HD11	1.93	0.50
1:v:87:MET:HB2	1:v:90:GLU:HG2	1.93	0.50
1:A:194:SER:O	1:A:231:GLY:N	2.45	0.50
3:F:125:THR:OG1	3:F:129:ASP:OD1	2.28	0.50
3:F:811:ALA:O	3:F:815:LEU:HD13	2.12	0.50
1:X:129:LYS:NZ	1:d:118:ASP:OD2	2.44	0.50
3:Z:433:MET:HE1	3:Z:447:ALA:HB1	1.93	0.50
2:e:41:LEU:O	2:e:106:GLN:HG2	2.10	0.50
1:n:118:ASP:OD1	1:n:152:ALA:N	2.44	0.50
1:v:83:THR:HG22	1:v:140:THR:HG23	1.94	0.50
4:L:48:PRO:HB3	4:L:57:GLN:HA	1.93	0.50
1:b:133:ALA:O	1:b:134:LYS:HG2	2.11	0.50
3:F:508:ASP:OD2	3:F:509:ARG:NH1	2.45	0.50
4:f:44:GLU:OE1	4:f:44:GLU:N	2.44	0.50
3:J:134:GLU:O	3:J:134:GLU:OE2	2.30	0.50
1:B:50:LEU:HD12	1:j:100:PHE:HE2	1.77	0.50
1:C:127:ILE:HB	1:c:50:LEU:HB2	1.93	0.50
1:c:91:GLN:OE1	1:c:91:GLN:N	2.45	0.50
3:F:127:LYS:HG2	3:F:128:GLY:N	2.25	0.50
1:G:181:LEU:HB2	1:G:214:ILE:HB	1.93	0.50
1:U:65:ALA:O	1:U:67:TRP:N	2.44	0.50
1:j:133:ALA:O	1:j:134:LYS:HG2	2.11	0.50
1:n:47:PRO:HA	1:n:80:THR:HG23	1.93	0.50
3:J:828:GLY:HA3	3:Z:823:THR:HA	1.93	0.50
5:H:824:LYS:HB2	6:P:115:SER:HB3	1.94	0.50
1:A:78:GLY:HA2	1:A:145:ASN:HB2	1.93	0.50
1:Q:199:SER:HB2	1:Q:207:VAL:HG22	1.94	0.50
1:R:43:LYS:H	1:R:84:LEU:HA	1.77	0.50
1:R:168:PRO:HA	1:R:181:LEU:HG	1.93	0.50
1:X:163:GLY:O	1:X:187:PRO:HG3	2.12	0.50
1:a:186:GLN:HB3	1:a:189:GLY:HA2	1.93	0.50
1:R:108:TYR:OH	1:R:145:ASN:OD1	2.26	0.50
1:j:96:LEU:HD21	1:j:141:VAL:HG21	1.93	0.50
1:A:79:ASP:OD1	1:A:142:LYS:NZ	2.37	0.49
6:P:126:TRP:CD1	6:P:135:MET:HE1	2.47	0.49
6:P:212:GLU:H	6:P:212:GLU:CD	2.20	0.49
1:n:205:ALA:HB3	1:n:224:VAL:HG11	1.94	0.49
3:J:815:LEU:HD11	3:F:821:LYS:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:181:ASN:OD1	6:I:200:SER:OG	2.29	0.49
2:E:109:ASN:HB2	2:K:32:ARG:HH22	1.77	0.49
3:F:355:GLN:O	4:N:134:ARG:NH1	2.45	0.49
1:R:38:ARG:NH1	1:n:61:ASP:OD1	2.45	0.49
1:W:87:MET:H	1:W:93:GLN:NE2	2.09	0.49
1:V:207:VAL:HG12	1:V:216:VAL:HG22	1.93	0.49
3:J:233:SER:O	3:J:233:SER:OG	2.29	0.49
3:F:102:ARG:HB3	3:F:179:ILE:HD11	1.94	0.49
1:W:199:SER:H	1:W:207:VAL:HG21	1.77	0.49
3:Z:21:THR:HB	6:h:210:ALA:HB3	1.95	0.49
1:d:173:VAL:HG13	1:d:243:VAL:HG13	1.94	0.49
1:i:86:TRP:CD1	1:i:139:ARG:HE	2.30	0.49
6:P:187:ASN:O	6:P:188:VAL:HG22	2.11	0.49
1:W:202:LYS:HZ3	1:W:207:VAL:H	1.60	0.49
1:X:61:ASP:OD1	1:X:61:ASP:N	2.41	0.49
1:n:18:TRP:HA	1:n:37:SER:O	2.11	0.49
1:n:114:ASN:OD1	1:n:116:THR:OG1	2.24	0.49
1:o:199:SER:H	1:o:207:VAL:HG21	1.77	0.49
3:J:420:THR:OG1	4:f:204:LYS:NZ	2.45	0.49
6:P:137:GLY:O	6:P:138:ILE:HD12	2.13	0.49
1:d:87:MET:HB2	1:d:90:GLU:HG2	1.93	0.49
1:j:31:LEU:O	1:j:111:ARG:NH1	2.43	0.49
1:k:205:ALA:HB3	1:k:224:VAL:HG21	1.93	0.49
2:K:48:LEU:HD22	2:K:58:LEU:HD21	1.94	0.49
1:c:199:SER:H	1:c:207:VAL:HG21	1.77	0.49
4:N:204:LYS:NZ	3:Z:420:THR:OG1	2.45	0.49
1:S:96:LEU:HD21	1:S:141:VAL:HG21	1.95	0.49
3:Z:508:ASP:OD1	3:Z:508:ASP:N	2.45	0.49
1:l:18:TRP:HB2	1:l:109:LYS:HG2	1.94	0.49
3:Z:458:GLU:HB3	6:h:151:VAL:HG11	1.95	0.49
1:i:159:THR:HG23	1:i:161:ALA:H	1.78	0.49
1:G:204:LYS:HA	1:G:220:ALA:HB3	1.94	0.49
4:N:204:LYS:HB3	4:N:204:LYS:HE3	1.63	0.49
1:X:17:LEU:HD12	1:X:110:ILE:HG12	1.94	0.49
6:h:181:ASN:OD1	6:h:200:SER:OG	2.30	0.49
1:i:111:ARG:HG2	1:i:117:VAL:HG22	1.93	0.49
2:M:50:VAL:HG13	2:M:51:PRO:O	2.12	0.49
1:A:205:ALA:HB3	1:A:224:VAL:HG21	1.94	0.49
1:a:173:VAL:HG13	1:a:243:VAL:HG13	1.95	0.49
1:c:44:ASP:N	1:c:44:ASP:OD1	2.45	0.49
1:W:33:ASP:OD1	1:W:33:ASP:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:119:VAL:HB	1:W:150:SER:HB3	1.95	0.49
3:Z:310:GLN:OE1	3:Z:322:ARG:NH1	2.33	0.49
1:n:212:MET:HE2	1:n:212:MET:O	2.13	0.49
2:M:9:LYS:HZ3	2:M:9:LYS:HB2	1.78	0.48
1:v:204:LYS:HA	1:v:220:ALA:HB3	1.95	0.48
1:b:162:THR:HB	1:b:235:PHE:CZ	2.48	0.48
1:b:209:VAL:HG22	1:b:214:ILE:HG13	1.94	0.48
3:F:82:GLU:OE2	3:F:113:ARG:NH2	2.45	0.48
1:R:118:ASP:OD1	1:R:152:ALA:N	2.46	0.48
6:I:114:GLY:H	5:g:824:LYS:HE3	1.78	0.48
1:b:63:GLU:HG2	1:b:64:ASP:N	2.28	0.48
1:C:6:PRO:HB2	1:o:89:GLY:HA3	1.95	0.48
1:C:181:LEU:HD21	1:C:226:ILE:CD1	2.43	0.48
1:U:186:GLN:NE2	1:U:189:GLY:O	2.45	0.48
1:l:181:LEU:HB2	1:l:214:ILE:HB	1.94	0.48
2:M:11:GLY:HA2	2:e:93:VAL:O	2.13	0.48
1:v:108:TYR:OH	1:v:145:ASN:OD1	2.26	0.48
1:B:76:SER:O	1:B:76:SER:OG	2.28	0.48
1:A:48:GLY:N	1:A:80:THR:OG1	2.46	0.48
1:c:127:ILE:HG23	1:c:139:ARG:NH1	2.28	0.48
2:E:1:MET:N	2:E:64:GLU:OE2	2.47	0.48
1:T:191:THR:HG23	1:T:193:LYS:HG2	1.95	0.48
1:v:212:MET:O	1:v:213:THR:C	2.56	0.48
1:c:124:VAL:HG22	1:c:143:VAL:HG22	1.95	0.48
1:W:109:LYS:HD2	1:W:117:VAL:HG21	1.94	0.48
3:Z:453:LYS:HD3	3:Z:453:LYS:HA	1.60	0.48
2:e:84:VAL:HA	2:e:106:GLN:HA	1.94	0.48
4:N:37:PHE:HB3	4:N:56:TYR:CD2	2.49	0.48
1:d:119:VAL:HG13	1:d:150:SER:HB3	1.95	0.48
1:i:52:ALA:HA	1:i:75:LYS:HA	1.95	0.48
1:i:127:ILE:HG23	1:i:139:ARG:HH12	1.79	0.48
1:j:43:LYS:H	1:j:84:LEU:HA	1.79	0.48
1:k:94:GLN:OE1	1:l:156:SER:OG	2.26	0.48
1:V:17:LEU:HD12	1:V:110:ILE:HG12	1.95	0.48
1:V:118:ASP:OD2	1:d:129:LYS:NZ	2.47	0.48
1:S:50:LEU:HD11	1:S:151:MET:HE3	1.95	0.48
1:S:78:GLY:HA2	1:S:145:ASN:HB2	1.96	0.48
1:X:150:SER:OG	1:X:155:ARG:NH1	2.39	0.48
1:j:124:VAL:HG22	1:j:143:VAL:HG22	1.96	0.48
4:L:37:PHE:HB3	4:L:56:TYR:CD2	2.48	0.48
1:A:61:ASP:OD2	1:d:42:VAL:HB	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:672:ARG:HH22	3:F:701:GLN:HE21	1.62	0.48
1:G:146:VAL:HG12	1:X:70:THR:H	1.79	0.48
1:Q:207:VAL:HG12	1:Q:216:VAL:HG22	1.95	0.48
3:Z:83:SER:OG	3:Z:207:ASP:O	2.27	0.48
1:i:127:ILE:HG23	1:i:139:ARG:NH1	2.29	0.48
3:J:54:ASP:OD1	3:J:55:THR:N	2.46	0.48
3:J:643:THR:O	6:h:209:THR:OG1	2.32	0.48
1:D:17:LEU:HD12	1:D:110:ILE:HG12	1.94	0.48
4:N:139:GLN:NE2	3:Z:389:PHE:O	2.37	0.48
1:Q:51:THR:HG22	1:Q:52:ALA:H	1.78	0.48
1:R:197:ALA:HB3	1:R:214:ILE:HG12	1.94	0.48
1:U:65:ALA:O	1:U:66:ASP:C	2.54	0.48
1:W:44:ASP:OD1	1:W:44:ASP:N	2.46	0.48
3:Z:1:MET:HE3	3:Z:6:SER:HB3	1.95	0.48
3:Z:82:GLU:HA	3:Z:207:ASP:HA	1.96	0.48
3:Z:99:PRO:HB2	3:Z:180:ARG:HH11	1.79	0.48
1:i:167:THR:HB	1:i:182:THR:HG22	1.96	0.48
1:k:66:ASP:OD1	1:k:66:ASP:N	2.33	0.48
1:n:41:LYS:HA	1:n:41:LYS:HD2	1.60	0.48
2:M:14:VAL:HG12	2:M:42:LYS:HG2	1.95	0.48
3:J:90:LEU:O	3:J:92:THR:HG23	2.14	0.48
3:F:745:GLU:OE1	3:F:790:ARG:NE	2.35	0.48
3:F:766:LEU:HD13	3:F:772:TRP:CD1	2.49	0.48
1:G:126:SER:OG	1:X:49:GLU:OE2	2.32	0.48
1:S:159:THR:HG23	1:S:161:ALA:H	1.79	0.48
1:U:41:LYS:HD2	1:U:41:LYS:HA	1.63	0.48
3:Z:495:VAL:O	3:Z:556:TYR:N	2.40	0.48
1:i:150:SER:OG	1:i:155:ARG:NH1	2.45	0.48
1:o:118:ASP:OD1	1:o:152:ALA:N	2.47	0.48
3:J:458:GLU:HB3	6:I:151:VAL:HG11	1.96	0.48
4:L:92:ALA:HA	4:L:97:SER:HA	1.96	0.48
1:b:124:VAL:HG22	1:b:143:VAL:HG22	1.95	0.48
1:a:63:GLU:H	1:a:63:GLU:CD	2.22	0.48
1:C:18:TRP:HB2	1:C:109:LYS:HG2	1.96	0.48
4:N:99:VAL:HG13	3:Z:392:LEU:HB2	1.96	0.48
1:W:118:ASP:OD1	1:W:152:ALA:N	2.47	0.48
1:W:126:SER:HB3	1:W:142:LYS:HB3	1.94	0.48
1:i:16:THR:HB	1:i:18:TRP:HE1	1.79	0.48
1:V:61:ASP:OD1	1:V:61:ASP:N	2.33	0.47
2:M:34:PRO:O	2:M:36:GLY:N	2.45	0.47
1:v:38:ARG:HH21	1:S:61:ASP:HB3	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:43:ASN:ND2	4:L:47:GLU:O	2.47	0.47
6:I:129:ALA:C	6:I:131:GLY:H	2.22	0.47
1:C:133:ALA:O	1:C:134:LYS:HG2	2.14	0.47
2:E:49:SER:OG	2:E:97:ARG:NH1	2.46	0.47
5:O:830:ALA:HB1	5:g:830:ALA:HA	1.96	0.47
3:Z:332:GLN:NE2	4:f:164:PRO:O	2.42	0.47
1:i:87:MET:HE2	1:i:90:GLU:HG3	1.96	0.47
1:o:44:ASP:OD1	1:o:44:ASP:N	2.47	0.47
1:o:202:LYS:HZ3	1:o:207:VAL:H	1.61	0.47
3:J:820:GLY:H	3:F:826:HIS:HA	1.78	0.47
6:I:126:TRP:CD1	6:I:135:MET:HE1	2.49	0.47
3:Z:694:ALA:O	3:Z:702:GLY:N	2.45	0.47
1:n:228:VAL:O	1:n:236:ALA:HA	2.14	0.47
4:L:52:GLN:NE2	4:L:130:GLU:OE1	2.47	0.47
1:B:201:ASP:OD2	1:B:203:THR:OG1	2.24	0.47
1:b:31:LEU:O	1:b:111:ARG:NH1	2.47	0.47
1:c:15:THR:HG23	1:c:112:PHE:HA	1.95	0.47
3:F:198:LEU:HD12	3:F:199:TRP:N	2.29	0.47
6:P:209:THR:OG1	3:Z:643:THR:O	2.32	0.47
1:d:207:VAL:HG12	1:d:216:VAL:HG22	1.96	0.47
6:h:105:ILE:CD1	6:h:106:VAL:H	2.25	0.47
1:k:79:ASP:OD1	1:k:142:LYS:NZ	2.36	0.47
1:l:205:ALA:HB1	1:l:216:VAL:HG13	1.96	0.47
1:n:45:LEU:HD11	1:n:110:ILE:HD12	1.95	0.47
2:M:16:SER:HB3	2:M:40:ASN:ND2	2.29	0.47
3:J:845:LEU:HD11	3:Z:845:LEU:HD13	1.96	0.47
2:E:50:VAL:HG13	2:E:51:PRO:O	2.14	0.47
3:F:104:ILE:HD12	3:F:105:THR:N	2.29	0.47
2:Y:50:VAL:HG13	2:Y:51:PRO:O	2.14	0.47
1:j:165:THR:HB	1:j:184:ALA:HB3	1.95	0.47
1:B:114:ASN:OD1	1:B:116:THR:OG1	2.32	0.47
1:b:100:PHE:HE2	1:Q:50:LEU:HD12	1.79	0.47
1:G:129:LYS:NZ	1:X:118:ASP:OD2	2.48	0.47
4:N:227:ILE:HD12	6:P:185:GLN:HA	1.97	0.47
1:Q:42:VAL:HA	1:Q:84:LEU:HB3	1.96	0.47
1:i:201:ASP:OD2	1:i:203:THR:OG1	2.23	0.47
1:k:91:GLN:HE22	1:l:192:ASP:HB3	1.78	0.47
1:o:202:LYS:HD3	1:o:202:LYS:HA	1.71	0.47
1:V:205:ALA:HB3	1:V:224:VAL:HG11	1.96	0.47
1:v:126:SER:OG	1:D:49:GLU:OE2	2.32	0.47
2:m:9:LYS:HB2	2:m:47:THR:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:18:TRP:HB2	1:a:109:LYS:HG2	1.96	0.47
1:X:206:THR:OG1	1:X:217:ASN:ND2	2.45	0.47
3:Z:739:ASP:OD1	3:Z:741:THR:HG22	2.14	0.47
1:o:127:ILE:HG23	1:o:139:ARG:NH1	2.30	0.47
3:J:654:LEU:HD23	3:J:692:VAL:HG22	1.96	0.47
4:L:204:LYS:HE3	4:L:204:LYS:HB3	1.59	0.47
6:I:212:GLU:CD	6:I:212:GLU:H	2.23	0.47
1:B:206:THR:HG22	1:B:217:ASN:HD21	1.79	0.47
2:E:34:PRO:O	2:E:36:GLY:N	2.45	0.47
3:F:398:ALA:O	3:F:430:VAL:HA	2.15	0.47
3:F:453:LYS:HD3	3:F:453:LYS:HA	1.59	0.47
1:G:42:VAL:HB	1:k:61:ASP:OD1	2.15	0.47
4:N:157:GLU:HG2	3:Z:393:LYS:HZ1	1.80	0.47
6:P:181:ASN:OD1	6:P:200:SER:OG	2.32	0.47
3:Z:6:SER:HB2	3:Z:68:PHE:HB3	1.97	0.47
6:h:212:GLU:H	6:h:212:GLU:CD	2.23	0.47
1:l:151:MET:HA	1:l:151:MET:HE2	1.97	0.47
1:o:5:ASN:ND2	1:o:8:MET:HE1	2.29	0.47
1:o:33:ASP:N	1:o:33:ASP:OD1	2.47	0.47
3:F:495:VAL:O	3:F:556:TYR:N	2.39	0.47
1:G:109:LYS:HD2	1:G:117:VAL:HG21	1.97	0.47
2:K:93:VAL:O	2:Y:11:GLY:HA2	2.15	0.47
1:W:124:VAL:HG22	1:W:143:VAL:HG22	1.97	0.47
1:W:127:ILE:HG23	1:W:139:ARG:NH1	2.30	0.47
2:Y:9:LYS:HE3	2:Y:49:SER:HB3	1.96	0.47
1:d:205:ALA:HB3	1:d:224:VAL:HG11	1.95	0.47
1:j:183:VAL:HB	1:j:212:MET:HE2	1.95	0.47
1:V:49:GLU:OE2	1:d:126:SER:OG	2.33	0.47
1:V:128:GLY:O	1:V:139:ARG:NH1	2.42	0.47
2:m:18:PRO:HB3	2:m:40:ASN:HB3	1.96	0.47
1:a:185:PHE:CD1	1:a:191:THR:HG21	2.50	0.47
1:C:63:GLU:OE1	1:C:63:GLU:N	2.41	0.47
1:D:196:ARG:NH2	1:G:196:ARG:HE	2.13	0.47
3:F:31:SER:HB2	6:P:192:LEU:HB3	1.97	0.47
1:Q:43:LYS:HB2	1:Q:83:THR:HG23	1.97	0.47
1:S:120:PHE:CE2	1:S:151:MET:HE1	2.49	0.47
1:W:15:THR:HG23	1:W:112:PHE:HA	1.96	0.47
1:l:83:THR:HB	1:l:140:THR:HG22	1.97	0.47
1:n:164:MET:N	1:n:164:MET:SD	2.88	0.47
3:J:240:GLY:HA2	6:I:192:LEU:HG	1.96	0.47
1:v:202:LYS:HD3	1:v:202:LYS:HA	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:97:SER:O	4:L:97:SER:OG	2.30	0.47
4:L:139:GLN:NE2	3:F:389:PHE:O	2.38	0.47
1:b:223:LYS:HG3	1:b:242:THR:HG22	1.97	0.47
2:K:38:ASN:ND2	2:K:108:VAL:HG21	2.30	0.47
1:Q:114:ASN:OD1	1:Q:116:THR:OG1	2.33	0.47
1:T:168:PRO:HB3	1:T:181:LEU:HD23	1.97	0.47
6:h:123:LEU:O	6:h:123:LEU:HD23	2.15	0.47
6:h:187:ASN:O	6:h:188:VAL:HG22	2.14	0.47
3:J:122:VAL:HG23	3:J:194:GLN:HE21	1.80	0.46
1:C:11:LYS:HA	1:o:136:VAL:HA	1.96	0.46
3:F:310:GLN:OE1	3:F:322:ARG:NH1	2.36	0.46
3:Z:210:GLN:NE2	4:f:223:GLY:O	2.30	0.46
1:n:31:LEU:O	1:n:111:ARG:NH1	2.45	0.46
1:o:126:SER:HB3	1:o:142:LYS:HB3	1.98	0.46
3:J:694:ALA:O	3:J:702:GLY:N	2.47	0.46
1:v:119:VAL:HG13	1:v:150:SER:HB3	1.97	0.46
6:I:107:LEU:HD11	5:g:823:LEU:HD13	1.97	0.46
6:I:129:ALA:O	6:I:131:GLY:N	2.48	0.46
1:b:43:LYS:H	1:b:84:LEU:HA	1.81	0.46
1:c:131:VAL:HG22	1:c:137:ILE:HD11	1.98	0.46
1:D:165:THR:HG23	1:D:184:ALA:HB3	1.97	0.46
5:O:849:SER:OG	5:g:849:SER:O	2.30	0.46
1:R:150:SER:O	1:R:150:SER:OG	2.31	0.46
1:T:122:GLY:HA2	1:T:146:VAL:HG13	1.97	0.46
1:W:91:GLN:OE1	1:W:92:GLY:N	2.48	0.46
2:Y:109:ASN:HB2	2:e:32:ARG:HH22	1.80	0.46
3:Z:97:ASP:OD1	3:Z:98:THR:HG23	2.15	0.46
3:Z:733:PRO:HB3	3:Z:789:ILE:HD12	1.96	0.46
4:f:36:TYR:CZ	4:f:91:MET:HE2	2.50	0.46
1:j:91:GLN:OE1	1:j:92:GLY:N	2.46	0.46
3:J:433:MET:HE1	3:J:447:ALA:HB1	1.97	0.46
3:J:666:ARG:HG2	6:I:223:ARG:HB2	1.96	0.46
6:I:117:PHE:HZ	2:e:23:VAL:HG13	1.80	0.46
1:B:44:ASP:OD1	1:B:83:THR:HG22	2.14	0.46
1:b:91:GLN:OE1	1:b:92:GLY:N	2.48	0.46
1:C:211:GLY:O	1:C:213:THR:N	2.48	0.46
1:c:118:ASP:OD1	1:c:152:ALA:N	2.49	0.46
3:F:781:PRO:HG2	3:Z:817:PHE:CD2	2.50	0.46
1:U:211:GLY:O	1:U:213:THR:N	2.48	0.46
3:Z:28:ASP:OD2	3:Z:236:TYR:OH	2.23	0.46
1:o:205:ALA:HB3	1:o:224:VAL:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:m:59:GLU:O	2:m:63:GLU:HB2	2.15	0.46
1:B:51:THR:HG22	1:B:52:ALA:H	1.79	0.46
1:B:78:GLY:HA2	1:B:145:ASN:ND2	2.29	0.46
1:c:109:LYS:HD2	1:c:117:VAL:HG21	1.96	0.46
1:R:204:LYS:HB3	1:R:220:ALA:HB3	1.98	0.46
3:Z:349:MET:HE2	3:Z:349:MET:HB2	1.88	0.46
1:n:21:LYS:NZ	1:n:37:SER:HB3	2.31	0.46
1:n:124:VAL:HG22	1:n:143:VAL:HG22	1.97	0.46
1:o:225:ASN:ND2	1:o:240:GLU:OE1	2.47	0.46
3:J:83:SER:OG	3:J:207:ASP:O	2.26	0.46
1:v:33:ASP:OD1	1:v:109:LYS:NZ	2.39	0.46
3:F:260:TRP:NE1	3:F:262:GLY:O	2.48	0.46
2:K:18:PRO:HB3	2:K:40:ASN:HB3	1.98	0.46
1:Q:201:ASP:OD2	1:Q:203:THR:OG1	2.23	0.46
1:U:126:SER:HB3	1:U:142:LYS:HB3	1.97	0.46
2:Y:34:PRO:O	2:Y:36:GLY:N	2.49	0.46
3:Z:664:SER:OG	6:h:223:ARG:NH2	2.46	0.46
1:d:108:TYR:OH	1:d:145:ASN:OD1	2.30	0.46
1:d:202:LYS:HA	1:d:202:LYS:HD3	1.79	0.46
4:f:204:LYS:HB3	4:f:204:LYS:HE3	1.61	0.46
1:i:195:PHE:CE2	1:i:214:ILE:HD11	2.50	0.46
3:J:425:ARG:NH2	4:f:99:VAL:O	2.37	0.46
3:J:766:LEU:HD13	3:J:772:TRP:CD1	2.50	0.46
3:J:781:PRO:HA	3:J:807:ALA:HB3	1.98	0.46
5:H:824:LYS:HZ2	6:P:114:GLY:HA2	1.80	0.46
1:b:184:ALA:HB1	1:b:186:GLN:HE22	1.79	0.46
1:C:228:VAL:O	1:C:236:ALA:HA	2.15	0.46
1:G:87:MET:HB2	1:G:90:GLU:HG2	1.98	0.46
2:K:40:ASN:OD1	2:K:40:ASN:N	2.48	0.46
1:R:197:ALA:HB2	1:R:228:VAL:HG13	1.96	0.46
1:U:166:VAL:HG22	1:U:183:VAL:HG22	1.97	0.46
1:W:195:PHE:HA	1:W:230:SER:HA	1.97	0.46
1:i:206:THR:HG22	1:i:217:ASN:HD21	1.80	0.46
1:o:119:VAL:HB	1:o:150:SER:HB3	1.98	0.46
1:o:139:ARG:HH11	1:o:139:ARG:HG3	1.79	0.46
3:J:31:SER:HA	6:I:190:PRO:O	2.16	0.46
6:I:137:GLY:O	6:I:138:ILE:HD12	2.16	0.46
6:I:167:THR:HG22	6:h:167:THR:HG21	1.96	0.46
1:B:185:PHE:HE2	1:B:230:SER:HB2	1.79	0.46
1:c:167:THR:HG1	1:c:182:THR:HG1	1.62	0.46
3:F:465:SER:HB2	3:F:585:ALA:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:508:ASP:N	3:F:508:ASP:OD1	2.47	0.46
1:U:213:THR:C	1:U:214:ILE:HG13	2.40	0.46
2:Y:83:LYS:HE3	2:Y:83:LYS:HB3	1.50	0.46
3:Z:395:ARG:O	3:Z:429:ASN:ND2	2.35	0.46
1:l:198:VAL:HA	1:l:207:VAL:HG21	1.98	0.46
5:H:836:ASP:OD2	5:g:827:TYR:OH	2.33	0.46
6:I:117:PHE:HD1	6:I:120:GLY:HA3	1.80	0.46
1:B:52:ALA:HA	1:B:75:LYS:HA	1.98	0.46
1:c:43:LYS:H	1:c:84:LEU:HA	1.81	0.46
3:F:395:ARG:O	3:F:429:ASN:ND2	2.37	0.46
3:F:664:SER:OG	6:P:223:ARG:NH2	2.49	0.46
1:S:105:THR:HG22	1:S:121:ARG:HG2	1.96	0.46
1:W:17:LEU:HD22	1:W:45:LEU:HD12	1.98	0.46
1:W:202:LYS:HD3	1:W:202:LYS:HA	1.72	0.46
1:k:233:GLY:HA3	1:l:196:ARG:CZ	2.46	0.46
1:o:175:LYS:NZ	1:o:244:THR:O	2.49	0.46
3:J:536:GLN:HG3	3:J:545:LYS:HG2	1.97	0.46
1:a:118:ASP:OD1	1:a:152:ALA:N	2.49	0.46
3:F:781:PRO:HA	3:F:807:ALA:HB3	1.98	0.46
1:Q:76:SER:O	1:Q:76:SER:OG	2.28	0.46
3:Z:3:LYS:HE2	3:Z:3:LYS:HB3	1.80	0.46
1:d:83:THR:HG22	1:d:140:THR:HG23	1.96	0.46
4:L:99:VAL:HG13	3:F:392:LEU:HB2	1.97	0.46
1:A:163:GLY:O	1:A:187:PRO:HG3	2.15	0.46
2:E:109:ASN:OD1	2:K:32:ARG:NH2	2.49	0.46
1:G:44:ASP:C	1:G:44:ASP:OD2	2.59	0.46
1:W:85:ALA:HB1	1:n:9:PRO:HB3	1.97	0.46
1:d:33:ASP:OD1	1:d:109:LYS:NZ	2.38	0.46
1:n:195:PHE:HE2	1:n:214:ILE:HD11	1.80	0.46
1:B:193:LYS:NZ	1:B:232:ASN:OD1	2.48	0.45
1:b:45:LEU:HD12	1:b:82:PHE:HB3	1.98	0.45
1:A:197:ALA:HB2	1:A:228:VAL:HG13	1.98	0.45
1:c:105:THR:HG22	1:c:121:ARG:HG2	1.98	0.45
1:G:33:ASP:OD1	1:G:109:LYS:NZ	2.37	0.45
1:U:229:VAL:HG13	1:U:233:GLY:HA2	1.98	0.45
1:W:139:ARG:HH11	1:W:139:ARG:HG3	1.81	0.45
3:Z:90:LEU:O	3:Z:92:THR:HG23	2.17	0.45
3:Z:745:GLU:HG3	3:Z:768:THR:HG22	1.98	0.45
2:m:93:VAL:O	2:E:11:GLY:HA2	2.15	0.45
1:B:12:GLY:O	1:B:15:THR:OG1	2.35	0.45
1:A:87:MET:HE3	1:A:87:MET:HB2	1.88	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:MET:O	1:A:212:MET:HE3	2.15	0.45
3:F:32:GLU:HG2	6:P:189:LEU:HD23	1.98	0.45
3:F:83:SER:OG	3:F:207:ASP:O	2.30	0.45
3:F:726:TYR:HE2	3:Z:726:TYR:CG	2.34	0.45
4:N:184:TYR:CZ	4:N:215:ARG:HG2	2.51	0.45
1:R:91:GLN:OE1	1:R:92:GLY:N	2.49	0.45
3:Z:260:TRP:NE1	3:Z:262:GLY:O	2.49	0.45
3:Z:566:LEU:HD23	3:Z:566:LEU:HA	1.81	0.45
4:f:173:CYS:HB2	4:f:221:PHE:CE1	2.51	0.45
1:i:51:THR:HG22	1:i:52:ALA:H	1.81	0.45
1:i:229:VAL:HG13	1:i:233:GLY:HA2	1.98	0.45
5:H:830:ALA:HA	5:g:830:ALA:HB1	1.97	0.45
6:I:126:TRP:NE1	6:I:135:MET:HE1	2.32	0.45
1:a:102:GLU:OE2	1:a:106:ARG:NH2	2.44	0.45
1:c:127:ILE:HB	1:U:50:LEU:HB2	1.98	0.45
3:F:349:MET:HE2	3:F:349:MET:HB2	1.91	0.45
3:F:502:THR:O	3:F:502:THR:OG1	2.25	0.45
2:K:21:ARG:HB2	2:K:33:ALA:HB3	1.99	0.45
4:N:173:CYS:HB2	4:N:221:PHE:CE1	2.51	0.45
3:Z:410:TRP:CZ3	6:h:196:MET:HA	2.52	0.45
3:Z:499:ASN:HB3	3:Z:504:THR:HG22	1.98	0.45
1:d:44:ASP:OD2	1:d:44:ASP:C	2.60	0.45
2:e:92:ARG:HB3	2:e:99:GLU:HG3	1.99	0.45
1:V:34:VAL:HG13	1:V:196:ARG:HD3	1.99	0.45
3:J:584:TYR:OH	4:L:107:LYS:NZ	2.49	0.45
2:m:55:ALA:HB2	2:m:98:VAL:HG11	1.99	0.45
5:H:824:LYS:HE3	6:P:114:GLY:H	1.80	0.45
3:F:28:ASP:HB3	6:P:200:SER:CB	2.46	0.45
3:F:719:ARG:C	3:F:720:ILE:HD13	2.41	0.45
2:K:87:ALA:O	2:Y:18:PRO:HD2	2.16	0.45
1:Q:78:GLY:HA2	1:Q:145:ASN:ND2	2.32	0.45
1:R:213:THR:C	1:R:214:ILE:HD12	2.41	0.45
1:U:201:ASP:C	1:U:202:LYS:HG2	2.41	0.45
1:B:195:PHE:CE2	1:B:214:ILE:HD11	2.51	0.45
1:C:194:SER:OG	1:C:195:PHE:N	2.49	0.45
1:D:205:ALA:HB3	1:D:224:VAL:HG11	1.99	0.45
1:R:87:MET:HE3	1:R:87:MET:HB2	1.79	0.45
3:Z:121:LEU:HD12	3:Z:121:LEU:HA	1.84	0.45
3:Z:376:VAL:HG12	3:Z:466:VAL:HG12	1.99	0.45
1:i:31:LEU:HD22	1:i:31:LEU:H	1.81	0.45
1:i:129:LYS:NZ	1:j:118:ASP:OD1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:k:197:ALA:HB2	1:k:228:VAL:HG13	1.98	0.45
4:L:204:LYS:NZ	3:F:420:THR:OG1	2.50	0.45
1:c:167:THR:O	1:c:167:THR:OG1	2.34	0.45
2:E:9:LYS:HG2	2:E:10:PRO:HD3	1.98	0.45
1:G:129:LYS:HB2	1:G:129:LYS:HE3	1.77	0.45
6:P:129:ALA:C	6:P:131:GLY:N	2.74	0.45
1:U:18:TRP:HB2	1:U:109:LYS:HG2	1.99	0.45
3:Z:134:GLU:OE1	3:Z:134:GLU:O	2.35	0.45
6:h:104:GLN:O	6:h:105:ILE:HD12	2.17	0.45
1:i:78:GLY:HA2	1:i:145:ASN:ND2	2.32	0.45
1:i:185:PHE:HE2	1:i:230:SER:HB2	1.81	0.45
1:o:44:ASP:OD1	1:o:83:THR:OG1	2.27	0.45
3:J:398:ALA:O	3:J:430:VAL:HA	2.16	0.45
3:J:830:GLU:HB3	3:Z:824:GLU:OE2	2.17	0.45
3:F:513:LEU:HD22	3:F:514:PRO:HD2	1.99	0.45
3:F:748:PHE:HB2	3:F:766:LEU:HG	1.97	0.45
3:F:822:ILE:HG13	3:F:826:HIS:CG	2.52	0.45
1:Q:52:ALA:HA	1:Q:75:LYS:HA	1.98	0.45
1:V:70:THR:H	1:d:146:VAL:HG12	1.81	0.45
1:v:207:VAL:HG12	1:v:216:VAL:HG22	1.97	0.45
1:B:42:VAL:HA	1:B:84:LEU:HB3	1.99	0.45
1:a:205:ALA:HB1	1:a:216:VAL:HG13	1.98	0.45
2:K:21:ARG:HD3	3:Z:382:GLY:HA3	1.99	0.45
1:S:79:ASP:OD1	1:S:142:LYS:NZ	2.43	0.45
1:S:118:ASP:OD2	1:S:152:ALA:N	2.50	0.45
1:U:50:LEU:HD13	1:U:77:ALA:HB2	1.97	0.45
3:Z:100:ILE:HG22	3:Z:102:ARG:NH2	2.29	0.45
4:f:37:PHE:HB3	4:f:56:TYR:CD2	2.52	0.45
1:i:175:LYS:HD3	1:i:175:LYS:HA	1.78	0.45
1:j:164:MET:HE3	1:j:187:PRO:HG3	1.99	0.45
3:J:366:ASP:OD1	3:J:366:ASP:N	2.38	0.45
1:v:44:ASP:OD2	1:v:44:ASP:C	2.60	0.45
1:v:232:ASN:N	1:v:234:GLU:OE1	2.50	0.45
6:I:117:PHE:CD1	6:I:120:GLY:HA3	2.51	0.45
1:b:164:MET:HE2	1:b:164:MET:HA	1.99	0.45
1:a:117:VAL:O	1:a:155:ARG:NH1	2.50	0.45
1:W:100:PHE:HE2	1:n:50:LEU:HD12	1.82	0.45
3:Z:223:ASP:OD1	3:Z:223:ASP:N	2.50	0.45
2:e:48:LEU:HD22	2:e:58:LEU:HD11	1.99	0.45
1:i:43:LYS:H	1:i:84:LEU:HA	1.81	0.45
3:J:110:ASP:OD2	3:J:209:LYS:NZ	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:175:LYS:NZ	1:C:244:THR:O	2.50	0.45
1:D:212:MET:HG3	1:D:212:MET:O	2.16	0.45
3:F:828:GLY:O	3:F:832:LEU:HG	2.17	0.45
1:R:204:LYS:HB2	1:R:204:LYS:HE2	1.71	0.45
1:k:129:LYS:NZ	1:l:118:ASP:OD1	2.50	0.45
1:o:18:TRP:CZ3	1:o:38:ARG:HB2	2.52	0.45
3:J:828:GLY:O	3:J:832:LEU:HG	2.17	0.44
1:B:41:LYS:N	1:c:61:ASP:OD2	2.50	0.44
1:A:94:GLN:OE1	1:a:156:SER:OG	2.33	0.44
1:D:161:ALA:O	1:D:162:THR:OG1	2.34	0.44
1:S:163:GLY:O	1:S:187:PRO:HG3	2.17	0.44
1:l:194:SER:OG	1:l:195:PHE:N	2.50	0.44
1:n:18:TRP:HB2	1:n:109:LYS:HG2	1.98	0.44
1:n:79:ASP:OD1	1:n:142:LYS:NZ	2.40	0.44
1:c:195:PHE:HA	1:c:230:SER:HA	1.99	0.44
3:F:188:SER:HB2	3:F:193:LEU:O	2.18	0.44
1:G:119:VAL:HG13	1:G:150:SER:HB3	1.98	0.44
1:G:207:VAL:HG12	1:G:216:VAL:HG22	1.99	0.44
1:U:195:PHE:HE2	1:U:214:ILE:HD11	1.82	0.44
3:Z:684:ALA:O	3:Z:688:TYR:OH	2.31	0.44
3:Z:831:LEU:HA	3:Z:831:LEU:HD23	1.83	0.44
1:j:169:ALA:HB1	1:j:171:THR:HG22	1.99	0.44
2:M:89:TRP:O	2:M:89:TRP:CD1	2.70	0.44
1:C:99:TRP:CE2	1:C:106:ARG:HG2	2.52	0.44
2:E:50:VAL:HG22	2:E:51:PRO:HD2	1.99	0.44
2:K:68:TRP:CD1	2:K:68:TRP:H	2.36	0.44
1:Q:229:VAL:HG13	1:Q:233:GLY:HA2	1.98	0.44
1:W:5:ASN:OD1	1:W:5:ASN:C	2.61	0.44
3:Z:536:GLN:HG3	3:Z:545:LYS:HG2	1.99	0.44
1:d:129:LYS:HB2	1:d:129:LYS:HE3	1.74	0.44
1:i:206:THR:HG22	1:i:217:ASN:ND2	2.33	0.44
1:o:211:GLY:O	1:o:212:MET:HB3	2.18	0.44
1:V:194:SER:O	1:V:230:SER:OG	2.30	0.44
3:J:240:GLY:HA3	6:I:194:GLY:N	2.20	0.44
3:J:828:GLY:N	3:Z:822:ILE:O	2.46	0.44
4:L:227:ILE:HD12	6:I:185:GLN:HA	1.99	0.44
1:B:229:VAL:HG13	1:B:233:GLY:HA2	1.98	0.44
1:C:181:LEU:HD21	1:C:226:ILE:HD13	1.98	0.44
1:X:185:PHE:C	1:X:187:PRO:HD3	2.43	0.44
3:Z:366:ASP:OD1	3:Z:366:ASP:N	2.35	0.44
3:Z:513:LEU:HD13	3:Z:514:PRO:HD2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:f:38:PHE:CZ	4:f:87:MET:HE1	2.52	0.44
1:k:33:ASP:OD1	1:k:111:ARG:NH1	2.47	0.44
1:l:64:ASP:N	1:l:64:ASP:OD2	2.49	0.44
2:M:28:GLY:HA3	2:e:38:ASN:HB2	1.99	0.44
2:m:87:ALA:O	2:E:18:PRO:HD2	2.17	0.44
1:c:86:TRP:HE3	1:c:137:ILE:HG21	1.82	0.44
3:F:722:LEU:HD11	3:F:803:ALA:HB1	1.99	0.44
5:O:820:PRO:HD3	6:h:123:LEU:HB3	1.99	0.44
1:R:162:THR:HB	1:R:235:PHE:CZ	2.53	0.44
1:U:99:TRP:CE2	1:U:106:ARG:HG2	2.53	0.44
1:W:64:ASP:O	1:W:65:ALA:HB2	2.16	0.44
1:W:211:GLY:O	1:W:212:MET:HB3	2.17	0.44
2:Y:41:LEU:O	2:Y:42:LYS:HB3	2.18	0.44
3:Z:169:MET:HE3	3:Z:169:MET:HB3	1.78	0.44
1:j:162:THR:HB	1:j:235:PHE:CZ	2.52	0.44
1:n:87:MET:HE3	1:n:93:GLN:HG3	1.98	0.44
1:o:185:PHE:CD1	1:o:212:MET:HE3	2.52	0.44
1:V:96:LEU:HD21	1:V:141:VAL:HG21	1.99	0.44
6:I:111:ALA:HB1	6:I:118:THR:HG23	1.99	0.44
1:b:150:SER:O	1:b:150:SER:OG	2.34	0.44
1:C:205:ALA:HB3	1:C:224:VAL:HG11	1.98	0.44
1:c:18:TRP:CZ3	1:c:38:ARG:HB2	2.53	0.44
3:F:859:TRP:HB3	3:Z:859:TRP:HZ2	1.83	0.44
1:T:232:ASN:N	1:T:234:GLU:OE1	2.51	0.44
1:X:16:THR:OG1	1:X:18:TRP:NE1	2.46	0.44
2:e:13:ASP:OD2	2:e:13:ASP:N	2.51	0.44
3:J:499:ASN:HB3	3:J:504:THR:HG22	1.98	0.44
2:m:13:ASP:OD1	2:m:13:ASP:N	2.51	0.44
1:b:96:LEU:HD21	1:b:141:VAL:HG21	2.00	0.44
1:a:16:THR:OG1	1:a:111:ARG:HB2	2.17	0.44
1:D:63:GLU:OE1	1:D:63:GLU:N	2.50	0.44
2:E:92:ARG:HH11	2:E:92:ARG:HG3	1.81	0.44
4:N:96:GLN:OE1	3:Z:425:ARG:NE	2.39	0.44
6:P:183:VAL:O	6:P:187:ASN:ND2	2.47	0.44
1:R:223:LYS:HG3	1:R:242:THR:HG22	2.00	0.44
1:i:129:LYS:HE2	1:i:139:ARG:HH21	1.83	0.44
1:i:171:THR:OG1	1:i:172:SER:N	2.51	0.44
1:i:193:LYS:HA	1:i:193:LYS:HD3	1.81	0.44
3:J:50:THR:HG22	3:J:700:GLN:HA	2.00	0.44
3:J:328:TYR:HB3	6:I:177:SER:HA	2.00	0.44
3:J:539:THR:OG1	3:J:540:ASP:OD2	2.34	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:165:THR:HB	1:b:184:ALA:HB3	2.00	0.44
1:A:108:TYR:CZ	1:A:120:PHE:HB2	2.52	0.44
3:F:209:LYS:HB2	3:F:209:LYS:HE2	1.83	0.44
3:F:527:SER:O	3:F:529:ASN:ND2	2.51	0.44
1:d:204:LYS:HA	1:d:220:ALA:HB3	2.00	0.44
1:j:197:ALA:HB2	1:j:228:VAL:HG13	1.99	0.44
3:J:257:SER:OG	3:J:258:GLY:N	2.51	0.44
4:L:173:CYS:HB2	4:L:221:PHE:CE1	2.52	0.44
3:F:666:ARG:HG2	6:P:223:ARG:HB2	1.98	0.44
1:Q:16:THR:HG23	1:Q:38:ARG:NH1	2.33	0.44
1:U:145:ASN:OD1	1:U:145:ASN:N	2.50	0.44
3:Z:828:GLY:O	3:Z:832:LEU:HG	2.16	0.44
1:d:175:LYS:HE3	1:d:220:ALA:HA	2.00	0.44
1:i:108:TYR:OH	1:i:145:ASN:OD1	2.30	0.44
1:k:163:GLY:O	1:k:187:PRO:HG3	2.18	0.44
2:M:83:LYS:HB3	2:M:83:LYS:HE3	1.62	0.43
3:J:310:GLN:OE1	3:J:322:ARG:NH1	2.36	0.43
2:m:41:LEU:HB3	2:m:106:GLN:HG2	1.99	0.43
1:B:16:THR:HG23	1:B:38:ARG:NH1	2.33	0.43
1:B:127:ILE:HG23	1:B:139:ARG:NH1	2.33	0.43
1:b:211:GLY:O	1:b:213:THR:HG23	2.17	0.43
1:C:211:GLY:C	1:C:213:THR:N	2.76	0.43
3:F:99:PRO:HB2	3:F:180:ARG:HH11	1.83	0.43
3:F:503:ARG:HB2	3:F:549:VAL:HG23	1.99	0.43
1:R:29:ASN:OD1	1:R:32:SER:OG	2.27	0.43
1:R:169:ALA:HB1	1:R:171:THR:HG22	2.00	0.43
1:T:194:SER:OG	1:T:195:PHE:N	2.51	0.43
1:n:194:SER:OG	1:n:195:PHE:N	2.51	0.43
2:M:10:PRO:HG3	2:M:47:THR:OG1	2.17	0.43
2:M:50:VAL:HG22	2:M:51:PRO:HD2	2.00	0.43
2:M:109:ASN:OD1	2:m:32:ARG:NH2	2.51	0.43
3:J:453:LYS:HD3	3:J:453:LYS:HA	1.59	0.43
3:J:859:TRP:HZ2	3:Z:859:TRP:HB3	1.83	0.43
5:H:823:LEU:HD13	6:P:107:LEU:HD11	2.00	0.43
2:E:40:ASN:OD1	2:E:40:ASN:N	2.50	0.43
4:N:52:GLN:NE2	4:N:130:GLU:OE1	2.51	0.43
1:Q:175:LYS:HA	1:Q:175:LYS:HD3	1.84	0.43
1:S:197:ALA:HB2	1:S:228:VAL:HG13	1.98	0.43
1:U:63:GLU:N	1:U:63:GLU:CD	2.76	0.43
1:U:133:ALA:O	1:U:134:LYS:HG2	2.17	0.43
1:U:164:MET:N	1:U:164:MET:SD	2.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:31:LEU:HD13	1:W:31:LEU:HA	1.91	0.43
1:W:43:LYS:H	1:W:84:LEU:HA	1.83	0.43
1:b:169:ALA:HB1	1:b:171:THR:HG22	2.00	0.43
1:D:149:PRO:HG2	1:D:151:MET:HE3	2.01	0.43
3:F:154:THR:HB	3:F:156:LYS:HZ3	1.82	0.43
3:F:454:THR:OG1	3:F:595:LYS:NZ	2.41	0.43
5:O:829:MET:HE2	5:O:829:MET:HB2	1.84	0.43
1:i:84:LEU:HD12	1:i:139:ARG:HB3	2.00	0.43
1:i:114:ASN:OD1	1:i:116:THR:OG1	2.35	0.43
1:n:8:MET:HE3	1:n:9:PRO:HD2	2.00	0.43
1:n:126:SER:HB3	1:n:142:LYS:HB3	2.00	0.43
1:v:196:ARG:NH1	1:v:229:VAL:O	2.51	0.43
1:c:150:SER:HG	1:c:155:ARG:HH22	1.65	0.43
3:F:809:ASP:OD1	3:F:809:ASP:N	2.52	0.43
1:R:109:LYS:HD2	1:R:117:VAL:HG21	2.00	0.43
1:S:183:VAL:HB	1:S:212:MET:HE1	2.00	0.43
1:k:43:LYS:H	1:k:84:LEU:HA	1.83	0.43
1:l:87:MET:HB2	1:l:87:MET:HE3	1.77	0.43
1:V:150:SER:OG	1:V:155:ARG:NH1	2.34	0.43
3:J:169:MET:HE3	3:J:169:MET:HB3	1.74	0.43
1:b:8:MET:HE3	1:b:8:MET:HB3	1.82	0.43
1:b:44:ASP:OD1	1:b:44:ASP:N	2.51	0.43
1:C:204:LYS:HD2	1:C:222:GLY:HA3	2.00	0.43
1:c:202:LYS:HZ3	1:c:207:VAL:H	1.65	0.43
3:F:823:THR:HA	3:Z:828:GLY:HA3	1.99	0.43
1:S:210:SER:O	1:S:213:THR:OG1	2.30	0.43
1:T:198:VAL:HA	1:T:207:VAL:HG21	2.01	0.43
1:W:49:GLU:HG2	1:W:51:THR:HG23	2.00	0.43
3:Z:123:GLU:OE1	3:Z:131:ASN:ND2	2.48	0.43
3:Z:766:LEU:HD13	3:Z:772:TRP:CD1	2.53	0.43
1:k:120:PHE:CZ	1:k:151:MET:HE1	2.54	0.43
1:o:41:LYS:HA	1:o:41:LYS:HD2	1.73	0.43
2:M:26:GLY:O	2:M:28:GLY:N	2.48	0.43
3:J:859:TRP:HB3	3:F:859:TRP:HZ2	1.84	0.43
1:b:64:ASP:N	1:b:64:ASP:OD1	2.51	0.43
1:W:86:TRP:HA	1:W:93:GLN:HE22	1.83	0.43
3:Z:747:TRP:CZ3	3:Z:760:GLU:HA	2.54	0.43
3:Z:778:ASN:OD1	3:Z:778:ASN:N	2.51	0.43
1:o:91:GLN:HG3	1:o:92:GLY:N	2.34	0.43
3:J:495:VAL:O	3:J:556:TYR:N	2.41	0.43
3:J:566:LEU:HD23	3:J:566:LEU:HA	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:631:ASP:OD1	3:J:631:ASP:N	2.51	0.43
2:m:92:ARG:HA	2:E:12:MET:O	2.18	0.43
6:I:117:PHE:CZ	2:e:23:VAL:HG13	2.52	0.43
1:B:206:THR:HG22	1:B:217:ASN:ND2	2.33	0.43
1:b:109:LYS:HD2	1:b:117:VAL:HG21	2.00	0.43
1:b:204:LYS:HB3	1:b:220:ALA:HB3	2.01	0.43
1:A:50:LEU:HD11	1:A:151:MET:HE3	2.00	0.43
1:c:109:LYS:HE3	1:c:111:ARG:HD2	2.00	0.43
1:D:164:MET:HE3	1:D:164:MET:HB2	1.82	0.43
3:F:9:HIS:O	3:F:9:HIS:CG	2.71	0.43
3:F:31:SER:HA	6:P:190:PRO:O	2.18	0.43
3:F:357:LEU:HB2	4:N:156:THR:HG21	2.00	0.43
3:Z:240:GLY:HA2	6:h:192:LEU:HG	2.00	0.43
3:Z:344:SER:OG	6:h:159:ALA:HB2	2.19	0.43
3:Z:511:ILE:HD13	3:Z:511:ILE:HA	1.81	0.43
3:Z:641:TRP:CH2	3:Z:654:LEU:HD21	2.54	0.43
3:Z:735:LEU:HD11	3:Z:742:VAL:HG11	2.01	0.43
4:f:87:MET:HE2	4:f:91:MET:HE1	2.01	0.43
1:i:129:LYS:HE3	1:i:129:LYS:HB2	1.79	0.43
1:j:109:LYS:HD2	1:j:117:VAL:HG21	1.99	0.43
1:l:104:ASP:CG	1:l:106:ARG:HE	2.27	0.43
1:V:43:LYS:H	1:V:84:LEU:HA	1.84	0.43
3:J:9:HIS:O	3:J:9:HIS:CG	2.71	0.43
1:v:211:GLY:O	1:v:212:MET:HB2	2.19	0.43
1:C:151:MET:HA	1:C:151:MET:HE3	2.01	0.43
2:E:89:TRP:O	2:E:89:TRP:CD1	2.71	0.43
3:F:469:GLU:H	3:F:469:GLU:HG3	1.67	0.43
1:U:211:GLY:C	1:U:213:THR:H	2.26	0.43
1:d:118:ASP:OD1	1:d:152:ALA:N	2.51	0.43
2:M:49:SER:OG	2:M:97:ARG:NH1	2.51	0.43
3:J:770:LEU:HD22	3:J:770:LEU:HA	1.88	0.43
1:v:187:PRO:HD2	1:v:191:THR:HB	2.01	0.43
1:v:205:ALA:HB3	1:v:224:VAL:HG11	2.01	0.43
4:L:76:ARG:HG3	5:O:843:ARG:NH1	2.33	0.43
4:L:76:ARG:HG3	5:O:843:ARG:HH12	1.84	0.43
1:C:211:GLY:C	1:C:213:THR:H	2.27	0.43
1:D:43:LYS:H	1:D:84:LEU:HA	1.84	0.43
6:P:184:ALA:HB2	6:P:201:ARG:HB3	2.01	0.43
1:U:194:SER:OG	1:U:195:PHE:N	2.52	0.43
3:Z:84:SER:HB3	3:Z:206:ILE:HD12	2.00	0.43
3:Z:412:THR:OG1	6:h:172:GLN:O	2.29	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:17:LEU:HD12	1:d:110:ILE:HG12	2.01	0.43
1:d:193:LYS:NZ	1:d:234:GLU:OE2	2.52	0.43
1:i:50:LEU:HD13	1:i:77:ALA:CB	2.48	0.43
1:o:169:ALA:HB1	1:o:171:THR:HG22	2.01	0.43
3:J:778:ASN:OD1	3:J:778:ASN:N	2.52	0.43
1:v:77:ALA:HB3	1:v:145:ASN:HB2	2.01	0.43
2:m:88:LYS:HE3	2:m:88:LYS:HB3	1.79	0.43
4:L:209:LEU:HD22	4:L:225:LEU:HD22	2.01	0.43
1:b:197:ALA:HB2	1:b:228:VAL:HG13	1.99	0.43
1:A:105:THR:HG22	1:A:121:ARG:HG2	1.99	0.43
1:A:159:THR:HG23	1:A:161:ALA:H	1.84	0.43
1:U:175:LYS:HA	1:U:175:LYS:HD3	1.74	0.43
3:Z:28:ASP:HB3	6:h:200:SER:CB	2.49	0.43
3:Z:218:VAL:HG11	3:Z:236:TYR:CE1	2.53	0.43
1:d:60:LEU:HD23	1:d:60:LEU:HA	1.91	0.43
1:k:3:VAL:HB	1:k:4:PRO:HD3	2.01	0.43
1:k:108:TYR:CZ	1:k:120:PHE:HB2	2.54	0.43
3:J:511:ILE:HD12	3:J:561:LEU:HD22	2.01	0.42
1:C:64:ASP:OD2	1:C:64:ASP:C	2.61	0.42
1:c:125:SER:HA	1:U:52:ALA:HB3	2.00	0.42
1:W:196:ARG:HH22	1:W:231:GLY:N	2.17	0.42
1:X:148:ARG:HG3	1:d:67:TRP:CD1	2.53	0.42
1:d:18:TRP:HB2	1:d:109:LYS:HG2	2.01	0.42
1:o:207:VAL:HG12	1:o:216:VAL:HG22	2.01	0.42
3:J:349:MET:HE2	3:J:349:MET:HB2	1.86	0.42
1:v:118:ASP:OD1	1:v:152:ALA:N	2.52	0.42
1:C:229:VAL:HG13	1:C:233:GLY:HA2	2.01	0.42
4:N:159:ASP:HA	5:g:844:ASP:OD1	2.19	0.42
1:U:45:LEU:HB2	1:U:82:PHE:HB3	2.01	0.42
2:Y:41:LEU:HD23	2:Y:41:LEU:HA	1.85	0.42
2:Y:89:TRP:CD1	2:Y:89:TRP:O	2.72	0.42
3:Z:357:LEU:HB2	4:f:156:THR:HG21	2.00	0.42
3:Z:511:ILE:HD11	3:Z:559:TRP:HH2	1.84	0.42
1:j:118:ASP:OD2	1:j:152:ALA:N	2.52	0.42
1:j:194:SER:OG	1:j:195:PHE:N	2.52	0.42
1:o:10:VAL:HG21	1:o:113:PRO:HG2	2.01	0.42
1:o:87:MET:H	1:o:93:GLN:NE2	2.17	0.42
1:V:164:MET:HE3	1:V:235:PHE:HB3	2.01	0.42
3:J:845:LEU:HD13	3:F:845:LEU:HD21	2.02	0.42
1:v:153:GLU:OE1	1:v:153:GLU:N	2.47	0.42
6:I:214:ASP:OD1	6:I:214:ASP:N	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:VAL:HB	1:A:4:PRO:HD3	2.00	0.42
1:c:5:ASN:OD1	1:c:5:ASN:C	2.62	0.42
1:D:150:SER:HG	1:D:155:ARG:HH12	1.63	0.42
3:F:344:SER:OG	6:P:159:ALA:HB2	2.19	0.42
1:G:175:LYS:HE3	1:G:220:ALA:HA	2.01	0.42
1:G:232:ASN:N	1:G:234:GLU:OE1	2.52	0.42
1:Q:205:ALA:HA	1:Q:217:ASN:O	2.19	0.42
1:U:211:GLY:C	1:U:213:THR:N	2.76	0.42
1:W:169:ALA:HB1	1:W:171:THR:HG22	2.01	0.42
1:X:8:MET:HE3	1:X:8:MET:HB3	1.79	0.42
2:Y:49:SER:OG	2:Y:97:ARG:NH1	2.51	0.42
3:Z:32:GLU:OE1	4:f:166:ARG:NH1	2.52	0.42
3:Z:142:GLN:CD	3:Z:178:ASN:HD22	2.27	0.42
3:Z:666:ARG:HG2	6:h:223:ARG:HB2	2.01	0.42
3:Z:781:PRO:HA	3:Z:807:ALA:HB3	2.01	0.42
1:d:211:GLY:O	1:d:212:MET:HB3	2.19	0.42
3:J:827:LEU:HD23	3:J:831:LEU:HD13	2.02	0.42
5:H:829:MET:HE2	5:H:829:MET:HB2	1.79	0.42
5:H:830:ALA:HB1	5:O:830:ALA:HA	2.01	0.42
1:A:162:THR:HA	1:A:235:PHE:HE2	1.85	0.42
1:A:233:GLY:HA3	1:a:196:ARG:CZ	2.49	0.42
1:a:149:PRO:HB2	1:a:151:MET:HE3	2.00	0.42
1:c:204:LYS:HA	1:c:220:ALA:HB3	2.01	0.42
3:F:259:ILE:H	3:F:259:ILE:HG12	1.64	0.42
4:N:157:GLU:HG2	3:Z:393:LYS:NZ	2.34	0.42
1:R:45:LEU:HD12	1:R:82:PHE:HB3	2.02	0.42
1:S:3:VAL:HB	1:S:4:PRO:HD3	2.00	0.42
1:X:72:GLN:OE1	1:X:75:LYS:HE3	2.20	0.42
3:Z:371:TYR:OH	3:Z:473:HIS:NE2	2.29	0.42
1:j:8:MET:HE3	1:j:8:MET:HB3	1.78	0.42
2:M:109:ASN:HB2	2:m:32:ARG:HH22	1.85	0.42
4:L:6:GLN:NE2	4:L:10:ASN:OD1	2.51	0.42
4:L:184:TYR:CZ	4:L:215:ARG:HG2	2.55	0.42
1:a:163:GLY:HA3	1:a:187:PRO:HG3	2.01	0.42
1:C:211:GLY:C	1:C:212:MET:HG3	2.45	0.42
1:G:185:PHE:HZ	1:G:195:PHE:CD1	2.37	0.42
1:T:87:MET:HE3	1:T:87:MET:HB2	1.79	0.42
1:T:124:VAL:HG22	1:T:143:VAL:HG22	2.01	0.42
1:W:153:GLU:OE1	1:W:153:GLU:N	2.52	0.42
2:Y:50:VAL:HG22	2:Y:51:PRO:HD2	2.00	0.42
1:j:21:LYS:HD2	1:j:37:SER:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:j:164:MET:HE2	1:j:164:MET:HA	2.01	0.42
1:k:168:PRO:HG3	1:k:239:ALA:HB1	2.02	0.42
1:n:195:PHE:HA	1:n:230:SER:HA	2.01	0.42
2:M:2:LYS:HA	2:M:2:LYS:HD2	1.83	0.42
3:J:99:PRO:HB2	3:J:180:ARG:HH11	1.84	0.42
2:m:89:TRP:O	2:m:89:TRP:CD1	2.73	0.42
6:I:169:ASN:HB3	6:h:182:MET:HA	2.01	0.42
1:B:18:TRP:HB2	1:B:109:LYS:HG2	2.00	0.42
1:C:166:VAL:HG22	1:C:183:VAL:HG22	2.02	0.42
1:G:30:PRO:HB2	1:G:117:VAL:HG11	2.01	0.42
2:K:88:LYS:HE3	2:K:88:LYS:HB3	1.90	0.42
1:Q:193:LYS:HD2	1:Q:231:GLY:HA3	2.02	0.42
6:h:126:TRP:CD1	6:h:135:MET:HE1	2.54	0.42
3:J:618:PRO:HA	3:J:619:PRO:HD3	1.95	0.42
4:L:99:VAL:O	3:F:425:ARG:NH2	2.43	0.42
1:a:194:SER:OG	1:a:195:PHE:N	2.53	0.42
1:C:41:LYS:HA	1:C:41:LYS:HD2	1.79	0.42
3:F:412:THR:OG1	6:P:172:GLN:O	2.25	0.42
1:G:202:LYS:HA	1:G:202:LYS:HD3	1.78	0.42
1:R:194:SER:OG	1:R:195:PHE:N	2.53	0.42
1:S:175:LYS:HD3	1:S:218:GLY:O	2.20	0.42
1:U:173:VAL:HB	1:U:243:VAL:HG22	2.02	0.42
1:X:43:LYS:H	1:X:84:LEU:HA	1.85	0.42
1:d:181:LEU:HB2	1:d:214:ILE:HB	2.02	0.42
4:f:184:TYR:CZ	4:f:215:ARG:HG2	2.54	0.42
1:l:232:ASN:N	1:l:234:GLU:OE1	2.53	0.42
3:J:32:GLU:CD	6:I:189:LEU:HD23	2.45	0.42
1:b:127:ILE:O	1:Q:50:LEU:N	2.45	0.42
3:F:3:LYS:HE2	3:F:3:LYS:HB3	1.77	0.42
3:F:654:LEU:HD23	3:F:692:VAL:HG22	2.01	0.42
3:F:694:ALA:O	3:F:702:GLY:N	2.52	0.42
3:F:719:ARG:HG2	3:F:734:HIS:HB2	2.02	0.42
1:G:234:GLU:OE1	1:G:234:GLU:N	2.37	0.42
1:Q:46:THR:O	1:Q:46:THR:OG1	2.34	0.42
1:U:199:SER:HB2	1:U:207:VAL:HG13	2.01	0.42
1:W:97:LEU:HD21	1:n:151:MET:HG3	2.02	0.42
3:Z:126:SER:O	3:Z:127:LYS:HG2	2.20	0.42
2:e:89:TRP:O	2:e:89:TRP:CD1	2.72	0.42
1:i:21:LYS:HE3	1:i:37:SER:HB2	2.01	0.42
2:M:37:LEU:HD12	2:M:37:LEU:HA	1.91	0.42
3:J:103:THR:HG23	3:J:178:ASN:ND2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:747:TRP:CZ3	3:J:760:GLU:HA	2.55	0.42
1:A:66:ASP:O	1:l:75:LYS:N	2.49	0.42
1:C:213:THR:C	1:C:214:ILE:HG13	2.45	0.42
3:F:766:LEU:HD22	3:F:772:TRP:HE1	1.82	0.42
1:G:205:ALA:HB3	1:G:224:VAL:HG11	2.01	0.42
2:Y:40:ASN:OD1	2:Y:40:ASN:N	2.53	0.42
5:g:847:LEU:HD23	5:g:847:LEU:HA	1.85	0.42
1:i:41:LYS:N	1:o:61:ASP:OD2	2.53	0.42
1:i:76:SER:O	1:i:76:SER:OG	2.28	0.42
1:n:106:ARG:HE	1:n:106:ARG:HB3	1.68	0.42
1:o:211:GLY:C	1:o:213:THR:H	2.27	0.42
3:J:381:ASP:OD1	3:J:381:ASP:N	2.48	0.42
2:m:68:TRP:CD1	2:m:68:TRP:H	2.38	0.42
1:a:30:PRO:O	1:a:109:LYS:NZ	2.53	0.42
1:a:45:LEU:HD12	1:a:82:PHE:HB3	2.01	0.42
1:C:8:MET:HE3	1:C:9:PRO:CD	2.48	0.42
3:F:191:ASP:OD2	3:F:191:ASP:C	2.62	0.42
2:K:9:LYS:HB2	2:K:47:THR:HG23	2.02	0.42
1:R:45:LEU:HD21	1:R:110:ILE:HD13	2.02	0.42
1:W:167:THR:O	1:W:167:THR:OG1	2.37	0.42
3:Z:525:ASP:OD1	3:Z:529:ASN:N	2.42	0.42
1:d:204:LYS:HB2	1:d:204:LYS:HE2	1.74	0.42
6:h:138:ILE:HD12	6:h:138:ILE:O	2.19	0.42
1:i:197:ALA:HB2	1:i:228:VAL:HG22	2.02	0.42
1:j:223:LYS:HG3	1:j:242:THR:HG22	2.01	0.42
1:l:118:ASP:OD2	1:l:152:ALA:N	2.53	0.42
3:J:30:ILE:HD13	3:J:238:LEU:HD11	2.01	0.41
2:E:75:PRO:HA	2:E:76:PRO:HD3	1.94	0.41
3:F:84:SER:HB3	3:F:206:ILE:HD12	2.01	0.41
3:F:366:ASP:OD1	3:F:366:ASP:N	2.37	0.41
3:F:624:LEU:HA	3:F:640:ARG:O	2.19	0.41
3:F:747:TRP:CZ3	3:F:760:GLU:HA	2.54	0.41
6:P:102:VAL:HG11	6:P:125:ALA:HB1	2.02	0.41
1:R:150:SER:OG	1:R:155:ARG:NH2	2.43	0.41
1:W:181:LEU:HB2	1:W:214:ILE:HB	2.00	0.41
3:Z:327:ALA:HB1	6:h:176:PHE:HB2	2.02	0.41
1:k:105:THR:HG22	1:k:121:ARG:HG2	2.02	0.41
1:n:173:VAL:HB	1:n:243:VAL:HG22	2.02	0.41
3:J:121:LEU:HD12	3:J:121:LEU:HA	1.86	0.41
3:J:824:GLU:OE2	3:F:830:GLU:HB3	2.20	0.41
1:b:185:PHE:C	1:b:187:PRO:HD3	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:SER:O	1:C:213:THR:HG22	2.20	0.41
1:c:153:GLU:N	1:c:153:GLU:OE1	2.53	0.41
1:c:169:ALA:HB1	1:c:171:THR:HG22	2.02	0.41
3:Z:365:SER:HB2	3:Z:478:VAL:HG21	2.02	0.41
3:J:15:LYS:HE3	3:J:15:LYS:HB2	1.90	0.41
4:L:228:ASN:HD22	4:L:228:ASN:HA	1.61	0.41
6:I:129:ALA:C	6:I:131:GLY:N	2.77	0.41
1:B:173:VAL:HG12	1:B:243:VAL:HG13	2.03	0.41
1:A:204:LYS:HD2	1:A:222:GLY:HA3	2.02	0.41
1:c:205:ALA:HB3	1:c:224:VAL:HG21	2.02	0.41
3:F:589:VAL:HG21	6:P:151:VAL:HG13	2.02	0.41
4:N:11:GLU:HA	4:N:14:ARG:HH11	1.86	0.41
1:Q:148:ARG:HG3	1:R:67:TRP:CE2	2.55	0.41
1:W:204:LYS:HA	1:W:220:ALA:HB3	2.02	0.41
1:W:211:GLY:C	1:W:213:THR:H	2.28	0.41
3:Z:245:VAL:CG2	3:Z:246:PRO:HD2	2.49	0.41
3:Z:464:PHE:O	3:Z:465:SER:C	2.63	0.41
3:J:344:SER:OG	6:I:159:ALA:HB2	2.21	0.41
3:J:511:ILE:HD11	3:J:559:TRP:HH2	1.86	0.41
3:J:725:GLY:HA3	3:J:728:GLN:NE2	2.35	0.41
1:a:96:LEU:HD21	1:a:141:VAL:HG21	2.01	0.41
1:D:170:SER:HA	1:D:241:ILE:HD13	2.02	0.41
3:F:124:THR:O	3:F:192:GLN:HB3	2.20	0.41
3:F:410:TRP:CD1	6:P:197:ARG:HD3	2.55	0.41
3:F:410:TRP:HZ3	6:P:196:MET:HE2	1.85	0.41
1:Q:20:TYR:HB2	1:Q:36:TRP:CZ3	2.55	0.41
1:Q:105:THR:HG22	1:Q:121:ARG:HG2	2.03	0.41
1:U:44:ASP:OD2	1:U:44:ASP:C	2.63	0.41
3:Z:257:SER:OG	3:Z:258:GLY:N	2.51	0.41
3:Z:353:ASN:OD1	3:Z:353:ASN:C	2.64	0.41
4:f:170:ALA:HB2	4:f:227:ILE:HG12	2.02	0.41
6:h:105:ILE:HD11	6:h:137:GLY:CA	2.48	0.41
1:i:108:TYR:CZ	1:i:120:PHE:HB2	2.55	0.41
3:J:28:ASP:HB3	6:I:200:SER:CB	2.50	0.41
3:J:138:LEU:O	3:J:181:MET:HA	2.21	0.41
6:I:163:ARG:NH1	6:P:163:ARG:HD3	2.35	0.41
1:b:161:ALA:HB3	1:b:187:PRO:HB2	2.02	0.41
1:A:118:ASP:OD2	1:A:152:ALA:N	2.53	0.41
1:C:48:GLY:N	1:C:80:THR:OG1	2.40	0.41
1:c:134:LYS:HB3	1:c:134:LYS:HE3	1.75	0.41
3:F:188:SER:HB3	3:F:195:ASN:OD1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:210:GLN:NE2	4:N:223:GLY:O	2.30	0.41
3:F:218:VAL:HG11	3:F:236:TYR:CE1	2.55	0.41
3:F:822:ILE:HG13	3:F:826:HIS:ND1	2.36	0.41
1:S:166:VAL:HG22	1:S:183:VAL:HG22	2.02	0.41
1:T:63:GLU:CD	1:T:63:GLU:N	2.78	0.41
1:W:85:ALA:O	1:W:93:GLN:NE2	2.53	0.41
3:Z:823:THR:OG1	3:Z:824:GLU:N	2.54	0.41
1:i:3:VAL:HB	1:i:4:PRO:HD3	2.01	0.41
1:i:148:ARG:HG3	1:j:67:TRP:CZ2	2.55	0.41
1:j:193:LYS:HB2	1:j:193:LYS:HE2	1.89	0.41
1:V:170:SER:HA	1:V:241:ILE:HD13	2.03	0.41
3:J:831:LEU:HD12	3:Z:823:THR:O	2.19	0.41
1:A:120:PHE:CE2	1:A:151:MET:HE1	2.56	0.41
3:F:47:LEU:HD12	3:F:61:ILE:HD13	2.03	0.41
3:F:90:LEU:HD12	3:F:102:ARG:HE	1.85	0.41
3:F:357:LEU:HD13	4:N:156:THR:HG21	2.03	0.41
3:F:511:ILE:HD12	3:F:561:LEU:HD22	2.01	0.41
1:W:105:THR:HG22	1:W:121:ARG:HG2	2.01	0.41
3:Z:15:LYS:HE3	3:Z:15:LYS:HB2	1.85	0.41
3:Z:454:THR:OG1	3:Z:595:LYS:NZ	2.38	0.41
2:e:38:ASN:ND2	2:e:108:VAL:HG21	2.35	0.41
1:V:167:THR:O	1:V:182:THR:CB	2.67	0.41
3:J:248:ASN:OD1	3:J:248:ASN:C	2.63	0.41
3:J:464:PHE:O	3:J:465:SER:C	2.63	0.41
1:v:84:LEU:HD12	1:v:85:ALA:O	2.21	0.41
1:B:129:LYS:HB2	1:B:129:LYS:HE3	1.77	0.41
1:a:75:LYS:N	1:S:66:ASP:O	2.48	0.41
1:a:191:THR:HG23	1:a:193:LYS:H	1.86	0.41
1:C:52:ALA:HB3	1:o:125:SER:HA	2.02	0.41
3:F:464:PHE:O	3:F:465:SER:C	2.63	0.41
3:F:641:TRP:CH2	3:F:654:LEU:HD21	2.55	0.41
3:F:748:PHE:HD2	3:F:766:LEU:HD11	1.85	0.41
2:K:84:VAL:HA	2:K:106:GLN:HA	2.02	0.41
1:Q:3:VAL:HB	1:Q:4:PRO:HD3	2.02	0.41
1:S:193:LYS:HZ1	1:S:234:GLU:H	1.67	0.41
1:S:233:GLY:HA3	1:T:196:ARG:CZ	2.50	0.41
3:Z:503:ARG:HB2	3:Z:549:VAL:HG23	2.02	0.41
3:Z:780:LYS:H	3:Z:785:TYR:HH	1.68	0.41
1:j:150:SER:OG	1:j:155:ARG:NH2	2.40	0.41
1:l:161:ALA:HB3	1:l:187:PRO:HB2	2.01	0.41
1:n:166:VAL:HG22	1:n:183:VAL:HG22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:104:ILE:HD12	3:J:105:THR:N	2.36	0.41
4:L:120:ASN:OD1	4:L:120:ASN:N	2.54	0.41
4:L:230:LEU:HD21	6:I:205:GLN:HB3	2.02	0.41
1:B:198:VAL:O	1:B:227:PRO:HD2	2.21	0.41
3:F:135:VAL:CG2	3:F:195:ASN:HB2	2.51	0.41
3:F:472:ARG:NH1	4:N:9:LEU:HD22	2.36	0.41
1:G:108:TYR:OH	1:G:145:ASN:OD1	2.22	0.41
1:Q:148:ARG:HG3	1:R:67:TRP:CZ2	2.56	0.41
1:d:210:SER:O	1:d:213:THR:HG22	2.21	0.41
2:e:68:TRP:CD1	2:e:68:TRP:H	2.38	0.41
6:h:106:VAL:HG22	6:h:139:LEU:HB2	2.03	0.41
3:J:36:GLU:HB3	3:J:239:ARG:HB3	2.03	0.41
3:J:136:ARG:HD2	3:J:154:THR:HG22	2.03	0.41
3:J:410:TRP:HZ3	6:I:196:MET:HE2	1.86	0.41
3:J:474:VAL:HG22	4:L:2:GLN:HG3	2.02	0.41
3:J:645:LYS:HG2	6:h:206:GLU:OE2	2.21	0.41
6:I:172:GLN:NE2	6:h:186:GLY:O	2.53	0.41
1:B:175:LYS:HA	1:B:175:LYS:HD3	1.79	0.41
1:C:118:ASP:OD1	1:C:152:ALA:N	2.53	0.41
1:C:173:VAL:HB	1:C:243:VAL:HG22	2.02	0.41
1:c:89:GLY:HA3	1:U:6:PRO:HB2	2.03	0.41
1:c:119:VAL:HB	1:c:150:SER:HB3	2.03	0.41
1:D:187:PRO:O	1:D:188:GLU:HB2	2.21	0.41
2:E:41:LEU:O	2:E:42:LYS:HB3	2.21	0.41
3:F:257:SER:OG	3:F:258:GLY:N	2.53	0.41
3:F:381:ASP:OD1	3:F:381:ASP:N	2.43	0.41
3:F:410:TRP:CZ3	6:P:196:MET:HE2	2.55	0.41
3:F:770:LEU:HD22	3:F:770:LEU:HA	1.88	0.41
3:F:778:ASN:OD1	3:F:778:ASN:N	2.54	0.41
3:F:812:GLU:OE2	3:Z:821:LYS:NZ	2.39	0.41
1:G:202:LYS:NZ	1:G:207:VAL:HG22	2.34	0.41
2:K:89:TRP:HA	2:K:101:SER:O	2.21	0.41
1:S:108:TYR:CZ	1:S:120:PHE:HB2	2.56	0.41
1:S:185:PHE:CE2	1:S:230:SER:HB2	2.56	0.41
1:U:27:TYR:HE2	1:U:119:VAL:HG22	1.86	0.41
3:Z:33:GLY:O	3:Z:71:GLY:HA3	2.20	0.41
4:f:52:GLN:NE2	4:f:130:GLU:OE1	2.54	0.41
1:k:175:LYS:HD3	1:k:218:GLY:O	2.20	0.41
1:n:5:ASN:OD1	1:n:8:MET:HB2	2.21	0.41
1:n:27:TYR:HE1	1:n:119:VAL:HG22	1.85	0.41
1:V:104:ASP:OD1	1:V:104:ASP:N	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:187:PRO:O	1:V:188:GLU:HB2	2.21	0.41
3:J:780:LYS:HB2	3:J:783:HIS:CD2	2.56	0.41
4:L:159:ASP:HA	5:O:844:ASP:OD1	2.21	0.41
4:L:189:VAL:HG11	4:L:214:PHE:HB3	2.03	0.41
6:I:118:THR:C	5:g:820:PRO:HB3	2.46	0.41
1:B:197:ALA:HB2	1:B:228:VAL:HG22	2.03	0.41
3:F:33:GLY:O	3:F:71:GLY:HA3	2.21	0.41
2:Y:2:LYS:HD2	2:Y:2:LYS:HA	1.88	0.41
3:Z:94:VAL:HG22	3:Z:100:ILE:HD11	2.03	0.41
3:Z:188:SER:HB3	3:Z:195:ASN:OD1	2.21	0.41
3:Z:438:CYS:SG	3:Z:443:GLN:HB3	2.61	0.41
1:j:183:VAL:HG21	1:j:195:PHE:CE2	2.56	0.41
1:V:10:VAL:HG21	1:V:113:PRO:O	2.21	0.40
1:V:193:LYS:HE2	1:V:231:GLY:HA3	2.03	0.40
3:J:188:SER:HB2	3:J:193:LEU:O	2.21	0.40
1:v:93:GLN:HE21	1:v:93:GLN:HB3	1.74	0.40
1:B:3:VAL:HB	1:B:4:PRO:HD3	2.02	0.40
1:b:17:LEU:HD23	1:b:39:LEU:HD12	2.01	0.40
2:E:65:HIS:CD2	2:E:69:LYS:HG2	2.55	0.40
3:F:154:THR:HB	3:F:156:LYS:NZ	2.35	0.40
4:N:24:TRP:CZ3	4:N:105:ARG:HB2	2.56	0.40
1:Q:43:LYS:H	1:Q:84:LEU:HA	1.84	0.40
1:X:174:VAL:HG22	1:X:177:GLN:HB2	2.02	0.40
3:Z:372:ASN:HD21	3:Z:558:VAL:CG1	2.34	0.40
1:d:194:SER:OG	1:d:195:PHE:N	2.54	0.40
1:n:96:LEU:HD12	1:n:96:LEU:HA	1.90	0.40
1:V:8:MET:HE3	1:V:8:MET:HB3	1.77	0.40
1:V:72:GLN:OE1	1:V:75:LYS:HE3	2.22	0.40
3:J:746:PHE:HA	3:J:789:ILE:HG22	2.02	0.40
1:v:47:PRO:HA	1:v:80:THR:HG23	2.02	0.40
1:B:212:MET:HE3	1:B:212:MET:O	2.21	0.40
1:C:87:MET:HE3	1:C:93:GLN:HG3	2.03	0.40
1:c:202:LYS:HA	1:c:202:LYS:HD3	1.71	0.40
3:F:271:ASN:HD22	3:F:274:TRP:CD1	2.38	0.40
3:F:372:ASN:HD21	3:F:558:VAL:CG1	2.33	0.40
3:F:725:GLY:HA3	3:F:728:GLN:NE2	2.36	0.40
1:G:204:LYS:HE2	1:G:204:LYS:HB2	1.75	0.40
1:Q:18:TRP:HB2	1:Q:109:LYS:HG2	2.02	0.40
2:Y:42:LYS:HB2	2:Y:42:LYS:HE3	1.77	0.40
3:Z:188:SER:HB2	3:Z:193:LEU:O	2.21	0.40
3:Z:347:ARG:HG2	3:Z:450:TRP:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:g:842:MET:HE3	5:g:842:MET:HB3	1.95	0.40
1:k:108:TYR:OH	1:k:145:ASN:OD1	2.19	0.40
1:k:159:THR:HG23	1:k:161:ALA:H	1.85	0.40
1:o:137:ILE:HD12	1:o:137:ILE:HA	1.94	0.40
3:J:276:LEU:HD11	3:J:339:LEU:HD12	2.03	0.40
3:J:412:THR:OG1	6:I:172:GLN:O	2.29	0.40
3:J:419:ASP:O	3:J:423:ILE:HG13	2.20	0.40
3:J:578:GLU:OE2	4:L:105:ARG:NH2	2.54	0.40
2:m:40:ASN:OD1	2:m:40:ASN:N	2.52	0.40
2:m:92:ARG:HB3	2:m:99:GLU:HG2	2.02	0.40
1:B:171:THR:OG1	1:B:172:SER:N	2.54	0.40
1:b:42:VAL:HA	1:b:84:LEU:HB3	2.03	0.40
1:A:91:GLN:HE22	1:a:192:ASP:CB	2.33	0.40
1:A:99:TRP:CE2	1:A:106:ARG:HB2	2.56	0.40
1:a:48:GLY:N	1:a:80:THR:OG1	2.53	0.40
1:a:104:ASP:CG	1:a:106:ARG:HE	2.29	0.40
1:D:150:SER:OG	1:D:155:ARG:NH1	2.41	0.40
3:F:726:TYR:HE2	3:Z:726:TYR:CD2	2.39	0.40
3:F:753:ILE:HG12	3:F:788:TYR:OH	2.21	0.40
4:N:30:GLU:HG2	4:N:31:VAL:HG13	2.03	0.40
1:U:45:LEU:HD11	1:U:110:ILE:HD12	2.02	0.40
1:U:228:VAL:O	1:U:236:ALA:HA	2.21	0.40
2:Y:26:GLY:O	2:Y:28:GLY:N	2.48	0.40
3:Z:826:HIS:ND1	3:Z:826:HIS:N	2.70	0.40
1:l:43:LYS:H	1:l:84:LEU:HA	1.86	0.40
3:J:32:GLU:HG2	6:I:189:LEU:HD23	2.03	0.40
4:L:43:ASN:HD21	4:L:47:GLU:HB2	1.85	0.40
1:C:151:MET:HE3	1:C:152:ALA:H	1.87	0.40
1:C:175:LYS:HA	1:C:175:LYS:HD3	1.72	0.40
1:c:75:LYS:HE2	1:c:75:LYS:HB2	1.96	0.40
3:F:97:ASP:OD1	3:F:98:THR:HG23	2.21	0.40
3:F:124:THR:HA	3:F:130:ARG:HG3	2.03	0.40
3:F:143:ARG:HE	3:F:148:VAL:HG11	1.86	0.40
3:F:347:ARG:HG2	3:F:450:TRP:CE2	2.56	0.40
1:U:197:ALA:H	1:U:209:VAL:HG21	1.86	0.40
1:W:41:LYS:HA	1:W:41:LYS:HD2	1.59	0.40
2:Y:75:PRO:HA	2:Y:76:PRO:HD3	1.94	0.40
1:V:185:PHE:C	1:V:187:PRO:HD3	2.47	0.40
3:J:845:LEU:HD21	3:Z:845:LEU:HD13	2.03	0.40
1:v:16:THR:HG1	1:v:18:TRP:HE1	1.62	0.40
1:A:129:LYS:NZ	1:a:118:ASP:OD2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:5:ASN:HD21	1:c:8:MET:HE1	1.86	0.40
3:F:47:LEU:HD23	3:F:47:LEU:HA	1.79	0.40
1:Q:42:VAL:H	1:W:61:ASP:CG	2.30	0.40
1:R:63:GLU:HG2	1:R:63:GLU:O	2.22	0.40
1:R:64:ASP:OD1	1:R:64:ASP:C	2.64	0.40
1:T:43:LYS:H	1:T:84:LEU:HA	1.86	0.40
1:U:65:ALA:C	1:U:67:TRP:N	2.79	0.40
1:U:97:LEU:HD21	1:U:139:ARG:HH12	1.86	0.40
1:X:165:THR:HG23	1:X:184:ALA:HB3	2.04	0.40
3:Z:505:LEU:N	3:Z:544:VAL:O	2.50	0.40
2:e:88:LYS:HE3	2:e:88:LYS:HB2	1.88	0.40
1:j:204:LYS:HE2	1:j:204:LYS:HB2	1.69	0.40
1:k:18:TRP:HB2	1:k:109:LYS:HG2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	242/246 (98%)	224 (93%)	15 (6%)	3 (1%)	10 28
1	B	242/246 (98%)	226 (93%)	15 (6%)	1 (0%)	30 53
1	C	242/246 (98%)	221 (91%)	19 (8%)	2 (1%)	16 37
1	D	241/246 (98%)	226 (94%)	14 (6%)	1 (0%)	30 53
1	G	241/246 (98%)	226 (94%)	15 (6%)	0	100 100
1	Q	242/246 (98%)	224 (93%)	17 (7%)	1 (0%)	30 53
1	R	242/246 (98%)	231 (96%)	11 (4%)	0	100 100
1	S	242/246 (98%)	224 (93%)	15 (6%)	3 (1%)	10 28
1	T	242/246 (98%)	233 (96%)	9 (4%)	0	100 100
1	U	242/246 (98%)	222 (92%)	17 (7%)	3 (1%)	10 28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	V	241/246 (98%)	228 (95%)	12 (5%)	1 (0%)	30 53
1	W	242/246 (98%)	231 (96%)	10 (4%)	1 (0%)	30 53
1	X	241/246 (98%)	228 (95%)	12 (5%)	1 (0%)	30 53
1	a	242/246 (98%)	231 (96%)	11 (4%)	0	100 100
1	b	242/246 (98%)	226 (93%)	15 (6%)	1 (0%)	30 53
1	c	242/246 (98%)	230 (95%)	11 (4%)	1 (0%)	30 53
1	d	241/246 (98%)	228 (95%)	13 (5%)	0	100 100
1	i	242/246 (98%)	225 (93%)	16 (7%)	1 (0%)	30 53
1	j	242/246 (98%)	225 (93%)	17 (7%)	0	100 100
1	k	242/246 (98%)	225 (93%)	14 (6%)	3 (1%)	10 28
1	l	242/246 (98%)	231 (96%)	11 (4%)	0	100 100
1	n	242/246 (98%)	222 (92%)	19 (8%)	1 (0%)	30 53
1	o	242/246 (98%)	231 (96%)	10 (4%)	1 (0%)	30 53
1	v	241/246 (98%)	225 (93%)	13 (5%)	3 (1%)	10 28
2	E	107/109 (98%)	93 (87%)	13 (12%)	1 (1%)	14 34
2	K	107/109 (98%)	91 (85%)	16 (15%)	0	100 100
2	M	107/109 (98%)	93 (87%)	14 (13%)	0	100 100
2	Y	107/109 (98%)	93 (87%)	14 (13%)	0	100 100
2	e	107/109 (98%)	93 (87%)	14 (13%)	0	100 100
2	m	107/109 (98%)	95 (89%)	12 (11%)	0	100 100
3	F	859/1132 (76%)	780 (91%)	73 (8%)	6 (1%)	18 40
3	J	859/1132 (76%)	776 (90%)	77 (9%)	6 (1%)	18 40
3	Z	859/1132 (76%)	779 (91%)	76 (9%)	4 (0%)	24 49
4	L	230/232 (99%)	221 (96%)	9 (4%)	0	100 100
4	N	230/232 (99%)	222 (96%)	8 (4%)	0	100 100
4	f	230/232 (99%)	222 (96%)	8 (4%)	0	100 100
5	H	31/853 (4%)	27 (87%)	4 (13%)	0	100 100
5	O	31/853 (4%)	26 (84%)	5 (16%)	0	100 100
5	g	31/853 (4%)	26 (84%)	5 (16%)	0	100 100
6	I	120/223 (54%)	101 (84%)	15 (12%)	4 (3%)	3 7
6	P	120/223 (54%)	101 (84%)	14 (12%)	5 (4%)	2 5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
6	h	120/223 (54%)	100 (83%)	16 (13%)	4 (3%)	3 7
All	All	10164/13878 (73%)	9382 (92%)	724 (7%)	58 (1%)	23 45

All (58) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	V	158	VAL
1	v	213	THR
6	I	105	ILE
6	I	188	VAL
1	B	158	VAL
1	A	158	VAL
1	C	158	VAL
1	D	158	VAL
3	F	127	LYS
6	P	105	ILE
6	P	130	ILE
1	Q	158	VAL
1	S	158	VAL
1	U	158	VAL
1	W	65	ALA
1	X	158	VAL
3	Z	129	ASP
6	h	105	ILE
6	h	188	VAL
1	i	158	VAL
1	k	158	VAL
1	n	158	VAL
1	o	65	ALA
3	J	525	ASP
1	v	211	GLY
1	C	212	MET
6	P	188	VAL
1	S	64	ASP
1	U	63	GLU
1	U	212	MET
3	J	101	THR
3	J	326	ASN
6	I	130	ILE
1	b	65	ALA
1	A	64	ASP
3	F	101	THR

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Mol	Chain	Res	Type
3	F	326	ASN
3	Z	101	THR
3	Z	326	ASN
1	k	64	ASP
1	v	212	MET
1	A	161	ALA
1	c	65	ALA
6	h	106	VAL
3	J	159	THR
3	J	325	CYS
2	E	42	LYS
3	F	159	THR
6	P	106	VAL
1	S	161	ALA
1	k	161	ALA
6	I	106	VAL
3	J	613	VAL
6	P	138	ILE
3	Z	613	VAL
6	h	130	ILE
3	F	613	VAL
3	F	616	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	194/196 (99%)	181 (93%)	13 (7%)	15	36
1	B	194/196 (99%)	178 (92%)	16 (8%)	10	27
1	C	194/196 (99%)	178 (92%)	16 (8%)	10	27
1	D	193/196 (98%)	180 (93%)	13 (7%)	15	36
1	G	193/196 (98%)	179 (93%)	14 (7%)	13	33
1	Q	194/196 (99%)	178 (92%)	16 (8%)	10	27
1	R	194/196 (99%)	180 (93%)	14 (7%)	13	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	S	194/196 (99%)	171 (88%)	23 (12%)	5 15
1	T	194/196 (99%)	182 (94%)	12 (6%)	16 39
1	U	194/196 (99%)	179 (92%)	15 (8%)	12 30
1	V	193/196 (98%)	181 (94%)	12 (6%)	16 39
1	W	194/196 (99%)	180 (93%)	14 (7%)	13 33
1	X	193/196 (98%)	177 (92%)	16 (8%)	10 27
1	a	194/196 (99%)	174 (90%)	20 (10%)	7 19
1	b	194/196 (99%)	181 (93%)	13 (7%)	15 36
1	c	194/196 (99%)	185 (95%)	9 (5%)	24 50
1	d	193/196 (98%)	181 (94%)	12 (6%)	16 39
1	i	194/196 (99%)	172 (89%)	22 (11%)	5 17
1	j	194/196 (99%)	176 (91%)	18 (9%)	8 23
1	k	194/196 (99%)	177 (91%)	17 (9%)	9 24
1	l	194/196 (99%)	178 (92%)	16 (8%)	10 27
1	n	194/196 (99%)	175 (90%)	19 (10%)	7 21
1	o	194/196 (99%)	180 (93%)	14 (7%)	13 33
1	v	193/196 (98%)	180 (93%)	13 (7%)	15 36
2	E	96/96 (100%)	88 (92%)	8 (8%)	10 27
2	K	96/96 (100%)	86 (90%)	10 (10%)	7 19
2	M	96/96 (100%)	89 (93%)	7 (7%)	13 33
2	Y	96/96 (100%)	87 (91%)	9 (9%)	8 22
2	e	96/96 (100%)	86 (90%)	10 (10%)	7 19
2	m	96/96 (100%)	86 (90%)	10 (10%)	7 19
3	F	734/958 (77%)	679 (92%)	55 (8%)	12 31
3	J	734/958 (77%)	682 (93%)	52 (7%)	13 33
3	Z	734/958 (77%)	683 (93%)	51 (7%)	14 35
4	L	198/198 (100%)	189 (96%)	9 (4%)	24 50
4	N	198/198 (100%)	190 (96%)	8 (4%)	28 53
4	f	198/198 (100%)	188 (95%)	10 (5%)	21 47
5	H	24/648 (4%)	24 (100%)	0	100 100
5	O	24/648 (4%)	24 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	g	24/648 (4%)	24 (100%)	0	100 100
6	I	86/162 (53%)	72 (84%)	14 (16%)	2 7
6	P	86/162 (53%)	77 (90%)	9 (10%)	6 19
6	h	86/162 (53%)	75 (87%)	11 (13%)	4 13
All	All	8352/11178 (75%)	7712 (92%)	640 (8%)	14 30

All (640) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	V	31	LEU
1	V	37	SER
1	V	61	ASP
1	V	83	THR
1	V	117	VAL
1	V	119	VAL
1	V	132	THR
1	V	136	VAL
1	V	150	SER
1	V	174	VAL
1	V	229	VAL
1	V	232	ASN
2	M	12	MET
2	M	38	ASN
2	M	43	THR
2	M	46	VAL
2	M	50	VAL
2	M	90	SER
2	M	108	VAL
3	J	10	THR
3	J	26	VAL
3	J	30	ILE
3	J	39	VAL
3	J	40	ASP
3	J	50	THR
3	J	59	THR
3	J	97	ASP
3	J	122	VAL
3	J	138	LEU
3	J	153	ILE
3	J	167	VAL
3	J	168	VAL

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Mol	Chain	Res	Type
3	J	187	ASP
3	J	190	THR
3	J	197	THR
3	J	203	THR
3	J	206	ILE
3	J	235	ASN
3	J	261	ASP
3	J	325	CYS
3	J	330	THR
3	J	367	LYS
3	J	372	ASN
3	J	380	ASP
3	J	397	ASN
3	J	404	ILE
3	J	456	LEU
3	J	461	THR
3	J	469	GLU
3	J	502	THR
3	J	507	LEU
3	J	511	ILE
3	J	529	ASN
3	J	535	VAL
3	J	536	GLN
3	J	539	THR
3	J	555	GLU
3	J	565	THR
3	J	574	VAL
3	J	596	GLU
3	J	617	THR
3	J	621	VAL
3	J	650	VAL
3	J	651	SER
3	J	676	THR
3	J	695	VAL
3	J	732	THR
3	J	735	LEU
3	J	770	LEU
3	J	778	ASN
3	J	801	VAL
1	v	31	LEU
1	v	68	THR
1	v	81	SER

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Mol	Chain	Res	Type
1	v	93	GLN
1	v	125	SER
1	v	132	THR
1	v	136	VAL
1	v	157	THR
1	v	167	THR
1	v	190	VAL
1	v	196	ARG
1	v	210	SER
1	v	219	VAL
2	m	16	SER
2	m	20	VAL
2	m	46	VAL
2	m	49	SER
2	m	58	LEU
2	m	74	THR
2	m	85	THR
2	m	98	VAL
2	m	101	SER
2	m	106	GLN
4	L	80	THR
4	L	97	SER
4	L	111	ARG
4	L	141	SER
4	L	159	ASP
4	L	185	SER
4	L	201	THR
4	L	212	CYS
4	L	228	ASN
6	I	102	VAL
6	I	105	ILE
6	I	145	SER
6	I	148	LEU
6	I	161	THR
6	I	166	THR
6	I	167	THR
6	I	177	SER
6	I	200	SER
6	I	203	VAL
6	I	204	SER
6	I	207	ILE
6	I	208	SER

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Mol	Chain	Res	Type
6	I	209	THR
1	B	10	VAL
1	B	76	SER
1	B	80	THR
1	B	84	LEU
1	B	94	GLN
1	B	116	THR
1	B	127	ILE
1	B	132	THR
1	B	141	VAL
1	B	146	VAL
1	B	148	ARG
1	B	180	THR
1	B	191	THR
1	B	198	VAL
1	B	230	SER
1	B	232	ASN
1	b	51	THR
1	b	64	ASP
1	b	66	ASP
1	b	83	THR
1	b	97	LEU
1	b	101	ASN
1	b	117	VAL
1	b	132	THR
1	b	146	VAL
1	b	159	THR
1	b	192	ASP
1	b	217	ASN
1	b	230	SER
1	A	10	VAL
1	A	66	ASP
1	A	70	THR
1	A	116	THR
1	A	119	VAL
1	A	126	SER
1	A	141	VAL
1	A	146	VAL
1	A	171	THR
1	A	180	THR
1	A	190	VAL
1	A	191	THR

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Mol	Chain	Res	Type
1	A	198	VAL
1	a	37	SER
1	a	45	LEU
1	a	51	THR
1	a	54	SER
1	a	79	ASP
1	a	83	THR
1	a	101	ASN
1	a	117	VAL
1	a	132	THR
1	a	135	GLU
1	a	136	VAL
1	a	146	VAL
1	a	150	SER
1	a	180	THR
1	a	182	THR
1	a	186	GLN
1	a	190	VAL
1	a	191	THR
1	a	215	THR
1	a	219	VAL
1	C	23	SER
1	C	39	LEU
1	C	45	LEU
1	C	46	THR
1	C	64	ASP
1	C	70	THR
1	C	75	LYS
1	C	117	VAL
1	C	119	VAL
1	C	131	VAL
1	C	141	VAL
1	C	146	VAL
1	C	165	THR
1	C	174	VAL
1	C	191	THR
1	C	213	THR
1	c	37	SER
1	c	63	GLU
1	c	66	ASP
1	c	83	THR
1	c	132	THR

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Mol	Chain	Res	Type
1	c	146	VAL
1	c	165	THR
1	c	167	THR
1	c	209	VAL
1	D	31	LEU
1	D	37	SER
1	D	51	THR
1	D	56	ASP
1	D	61	ASP
1	D	83	THR
1	D	97	LEU
1	D	117	VAL
1	D	119	VAL
1	D	150	SER
1	D	174	VAL
1	D	191	THR
1	D	229	VAL
2	E	38	ASN
2	E	46	VAL
2	E	47	THR
2	E	48	LEU
2	E	50	VAL
2	E	84	VAL
2	E	108	VAL
2	E	109	ASN
3	F	10	THR
3	F	26	VAL
3	F	39	VAL
3	F	40	ASP
3	F	42	LEU
3	F	49	SER
3	F	50	THR
3	F	76	THR
3	F	122	VAL
3	F	137	LEU
3	F	138	LEU
3	F	153	ILE
3	F	168	VAL
3	F	187	ASP
3	F	190	THR
3	F	197	THR
3	F	217	LEU

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Mol	Chain	Res	Type
3	F	241	ARG
3	F	245	VAL
3	F	257	SER
3	F	259	ILE
3	F	261	ASP
3	F	281	THR
3	F	324	THR
3	F	325	CYS
3	F	357	LEU
3	F	373	ARG
3	F	380	ASP
3	F	381	ASP
3	F	412	THR
3	F	461	THR
3	F	465	SER
3	F	502	THR
3	F	511	ILE
3	F	518	THR
3	F	527	SER
3	F	529	ASN
3	F	531	VAL
3	F	535	VAL
3	F	539	THR
3	F	565	THR
3	F	617	THR
3	F	621	VAL
3	F	640	ARG
3	F	651	SER
3	F	653	LEU
3	F	654	LEU
3	F	675	GLU
3	F	676	THR
3	F	685	LEU
3	F	695	VAL
3	F	732	THR
3	F	735	LEU
3	F	770	LEU
3	F	801	VAL
1	G	54	SER
1	G	68	THR
1	G	83	THR
1	G	84	LEU

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Mol	Chain	Res	Type
1	G	97	LEU
1	G	125	SER
1	G	132	THR
1	G	135	GLU
1	G	157	THR
1	G	167	THR
1	G	183	VAL
1	G	190	VAL
1	G	213	THR
1	G	219	VAL
2	K	16	SER
2	K	20	VAL
2	K	22	LYS
2	K	30	SER
2	K	37	LEU
2	K	58	LEU
2	K	74	THR
2	K	85	THR
2	K	98	VAL
2	K	101	SER
4	N	73	THR
4	N	111	ARG
4	N	124	TYR
4	N	159	ASP
4	N	167	ILE
4	N	185	SER
4	N	201	THR
4	N	212	CYS
6	P	102	VAL
6	P	105	ILE
6	P	148	LEU
6	P	161	THR
6	P	167	THR
6	P	188	VAL
6	P	204	SER
6	P	207	ILE
6	P	208	SER
1	Q	10	VAL
1	Q	15	THR
1	Q	46	THR
1	Q	76	SER
1	Q	80	THR

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Mol	Chain	Res	Type
1	Q	84	LEU
1	Q	87	MET
1	Q	116	THR
1	Q	127	ILE
1	Q	132	THR
1	Q	146	VAL
1	Q	180	THR
1	Q	191	THR
1	Q	198	VAL
1	Q	230	SER
1	Q	232	ASN
1	R	66	ASP
1	R	83	THR
1	R	101	ASN
1	R	104	ASP
1	R	117	VAL
1	R	132	THR
1	R	146	VAL
1	R	150	SER
1	R	159	THR
1	R	183	VAL
1	R	192	ASP
1	R	217	ASN
1	R	230	SER
1	R	244	THR
1	S	10	VAL
1	S	31	LEU
1	S	37	SER
1	S	64	ASP
1	S	66	ASP
1	S	70	THR
1	S	80	THR
1	S	84	LEU
1	S	91	GLN
1	S	116	THR
1	S	119	VAL
1	S	126	SER
1	S	132	THR
1	S	136	VAL
1	S	141	VAL
1	S	146	VAL
1	S	151	MET

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Mol	Chain	Res	Type
1	S	174	VAL
1	S	190	VAL
1	S	191	THR
1	S	198	VAL
1	S	212	MET
1	S	242	THR
1	T	15	THR
1	T	64	ASP
1	T	79	ASP
1	T	83	THR
1	T	117	VAL
1	T	132	THR
1	T	136	VAL
1	T	146	VAL
1	T	190	VAL
1	T	191	THR
1	T	207	VAL
1	T	215	THR
1	U	23	SER
1	U	35	ASP
1	U	41	LYS
1	U	54	SER
1	U	63	GLU
1	U	83	THR
1	U	110	ILE
1	U	119	VAL
1	U	131	VAL
1	U	141	VAL
1	U	146	VAL
1	U	165	THR
1	U	174	VAL
1	U	191	THR
1	U	213	THR
1	W	33	ASP
1	W	37	SER
1	W	64	ASP
1	W	66	ASP
1	W	83	THR
1	W	90	GLU
1	W	97	LEU
1	W	101	ASN
1	W	132	THR

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Mol	Chain	Res	Type
1	W	146	VAL
1	W	165	THR
1	W	167	THR
1	W	209	VAL
1	W	238	VAL
1	X	31	LEU
1	X	32	SER
1	X	37	SER
1	X	51	THR
1	X	56	ASP
1	X	61	ASP
1	X	66	ASP
1	X	83	THR
1	X	97	LEU
1	X	117	VAL
1	X	119	VAL
1	X	127	ILE
1	X	136	VAL
1	X	174	VAL
1	X	208	SER
1	X	229	VAL
2	Y	38	ASN
2	Y	43	THR
2	Y	46	VAL
2	Y	47	THR
2	Y	50	VAL
2	Y	84	VAL
2	Y	90	SER
2	Y	108	VAL
2	Y	109	ASN
3	Z	10	THR
3	Z	15	LYS
3	Z	26	VAL
3	Z	39	VAL
3	Z	40	ASP
3	Z	42	LEU
3	Z	50	THR
3	Z	59	THR
3	Z	115	THR
3	Z	126	SER
3	Z	127	LYS
3	Z	138	LEU

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Mol	Chain	Res	Type
3	Z	153	ILE
3	Z	158	LYS
3	Z	167	VAL
3	Z	168	VAL
3	Z	179	ILE
3	Z	190	THR
3	Z	197	THR
3	Z	215	THR
3	Z	257	SER
3	Z	261	ASP
3	Z	325	CYS
3	Z	357	LEU
3	Z	367	LYS
3	Z	397	ASN
3	Z	426	TYR
3	Z	469	GLU
3	Z	502	THR
3	Z	507	LEU
3	Z	511	ILE
3	Z	529	ASN
3	Z	535	VAL
3	Z	536	GLN
3	Z	539	THR
3	Z	596	GLU
3	Z	617	THR
3	Z	621	VAL
3	Z	631	ASP
3	Z	646	VAL
3	Z	651	SER
3	Z	654	LEU
3	Z	695	VAL
3	Z	732	THR
3	Z	740	PRO
3	Z	756	ILE
3	Z	770	LEU
3	Z	773	ILE
3	Z	778	ASN
3	Z	794	THR
3	Z	801	VAL
1	d	51	THR
1	d	68	THR
1	d	70	THR

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Mol	Chain	Res	Type
1	d	81	SER
1	d	83	THR
1	d	125	SER
1	d	132	THR
1	d	135	GLU
1	d	157	THR
1	d	167	THR
1	d	190	VAL
1	d	219	VAL
2	e	1	MET
2	e	20	VAL
2	e	22	LYS
2	e	30	SER
2	e	46	VAL
2	e	47	THR
2	e	58	LEU
2	e	74	THR
2	e	85	THR
2	e	98	VAL
4	f	78	THR
4	f	80	THR
4	f	99	VAL
4	f	141	SER
4	f	142	GLU
4	f	154	THR
4	f	159	ASP
4	f	185	SER
4	f	201	THR
4	f	212	CYS
6	h	102	VAL
6	h	105	ILE
6	h	145	SER
6	h	148	LEU
6	h	161	THR
6	h	167	THR
6	h	177	SER
6	h	204	SER
6	h	207	ILE
6	h	208	SER
6	h	217	GLN
1	i	10	VAL
1	i	15	THR

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Mol	Chain	Res	Type
1	i	16	THR
1	i	29	ASN
1	i	70	THR
1	i	76	SER
1	i	79	ASP
1	i	80	THR
1	i	81	SER
1	i	110	ILE
1	i	116	THR
1	i	127	ILE
1	i	136	VAL
1	i	146	VAL
1	i	180	THR
1	i	182	THR
1	i	191	THR
1	i	198	VAL
1	i	217	ASN
1	i	230	SER
1	i	232	ASN
1	i	243	VAL
1	j	3	VAL
1	j	17	LEU
1	j	21	LYS
1	j	51	THR
1	j	66	ASP
1	j	83	THR
1	j	101	ASN
1	j	104	ASP
1	j	117	VAL
1	j	132	THR
1	j	150	SER
1	j	159	THR
1	j	165	THR
1	j	183	VAL
1	j	192	ASP
1	j	213	THR
1	j	217	ASN
1	j	230	SER
1	k	10	VAL
1	k	37	SER
1	k	51	THR
1	k	66	ASP

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Mol	Chain	Res	Type
1	k	70	THR
1	k	80	THR
1	k	116	THR
1	k	119	VAL
1	k	132	THR
1	k	136	VAL
1	k	141	VAL
1	k	146	VAL
1	k	174	VAL
1	k	190	VAL
1	k	191	THR
1	k	198	VAL
1	k	242	THR
1	l	54	SER
1	l	79	ASP
1	l	83	THR
1	l	96	LEU
1	l	101	ASN
1	l	117	VAL
1	l	119	VAL
1	l	132	THR
1	l	136	VAL
1	l	146	VAL
1	l	150	SER
1	l	186	GLN
1	l	190	VAL
1	l	191	THR
1	l	213	THR
1	l	219	VAL
1	n	23	SER
1	n	35	ASP
1	n	41	LYS
1	n	45	LEU
1	n	46	THR
1	n	64	ASP
1	n	70	THR
1	n	83	THR
1	n	110	ILE
1	n	117	VAL
1	n	119	VAL
1	n	131	VAL
1	n	141	VAL

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Mol	Chain	Res	Type
1	n	146	VAL
1	n	165	THR
1	n	174	VAL
1	n	191	THR
1	n	198	VAL
1	n	213	THR
1	o	33	ASP
1	o	37	SER
1	o	39	LEU
1	o	63	GLU
1	o	66	ASP
1	o	83	THR
1	o	127	ILE
1	o	132	THR
1	o	146	VAL
1	o	165	THR
1	o	167	THR
1	o	209	VAL
1	o	213	THR
1	o	235	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	V	91	GLN
1	V	177	GLN
1	V	232	ASN
3	J	75	GLN
3	J	237	HIS
3	J	407	ASN
3	J	783	HIS
4	L	55	GLN
5	H	841	GLN
6	I	104	GLN
1	b	177	GLN
1	A	232	ASN
1	a	72	GLN
1	a	232	ASN
1	D	177	GLN
1	D	232	ASN
3	F	75	GLN
3	F	192	GLN

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Mol	Chain	Res	Type
3	F	221	GLN
3	F	237	HIS
3	F	250	ASN
3	F	408	ASN
3	F	701	GLN
4	N	2	GLN
4	N	55	GLN
5	O	841	GLN
6	P	172	GLN
1	R	177	GLN
1	R	186	GLN
1	S	29	ASN
1	U	94	GLN
1	U	225	ASN
1	W	93	GLN
1	W	94	GLN
1	X	177	GLN
1	X	232	ASN
3	Z	460	GLN
3	Z	734	HIS
4	f	228	ASN
4	f	232	GLN
6	h	172	GLN
6	h	185	GLN
1	i	5	ASN
1	j	94	GLN
1	j	186	GLN
1	l	72	GLN
1	l	225	ASN
1	n	94	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	N	301	4	0,12,12	-	-	-		
7	SF4	f	301	4	0,12,12	-	-	-		
7	SF4	L	301	4	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	N	301	4	-	-	0/6/5/5
7	SF4	f	301	4	-	-	0/6/5/5
7	SF4	L	301	4	-	-	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.

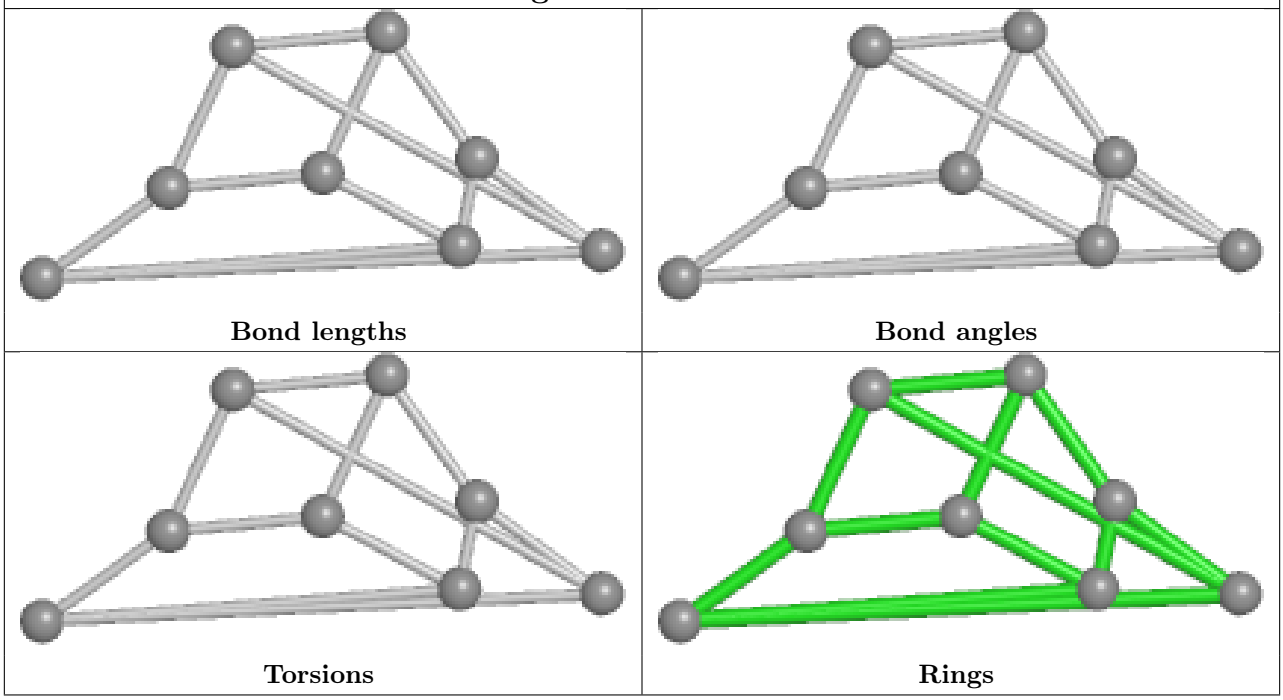
There are no ring outliers.

No monomer is involved in short contacts.

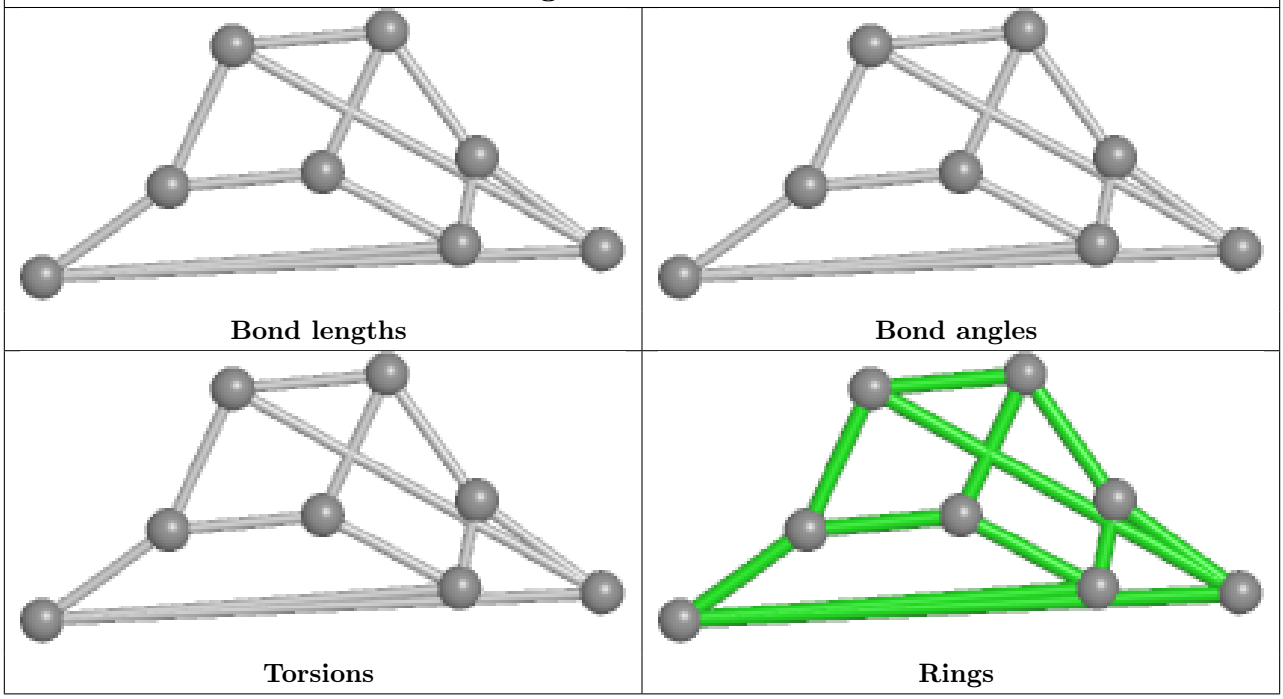
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

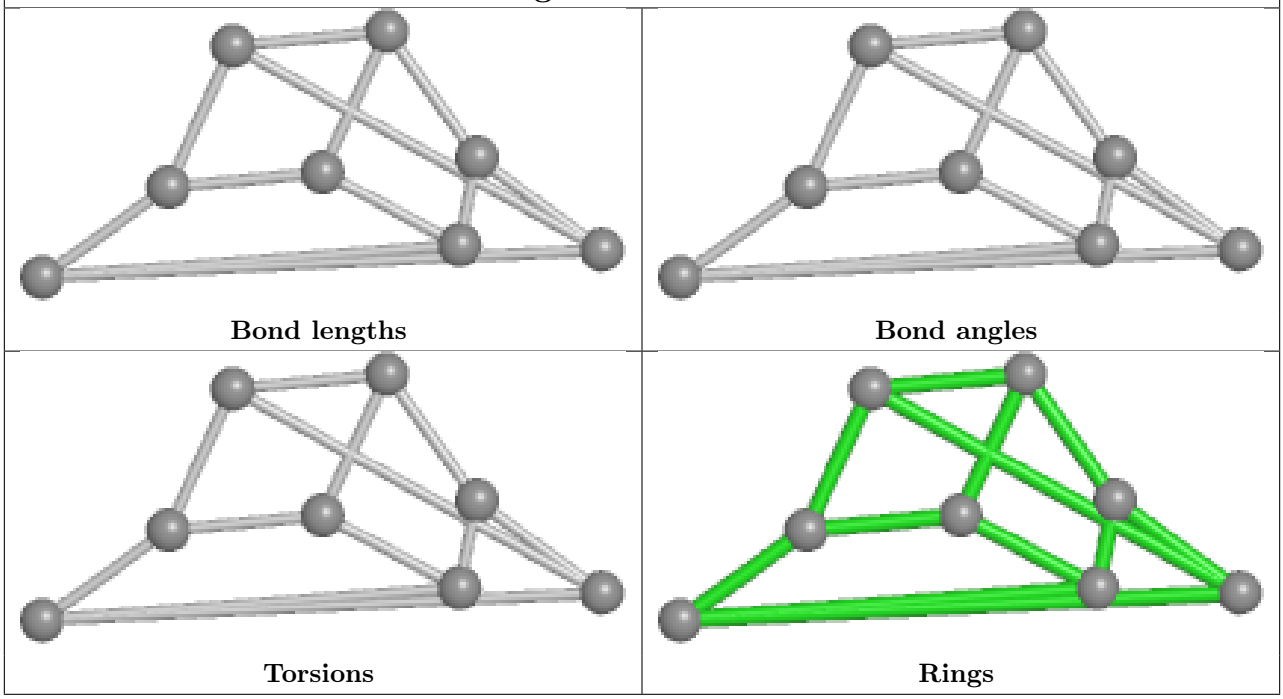
Ligand SF4 N 301



Ligand SF4 f 301



Ligand SF4 L 301



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

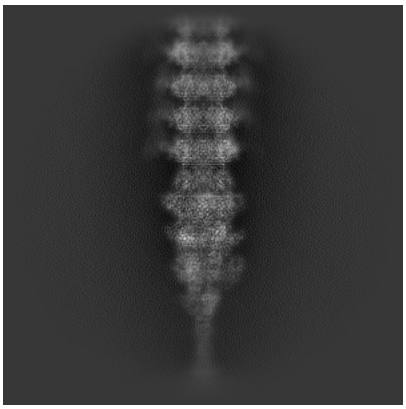
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-35824. These allow visual inspection of the internal detail of the map and identification of artifacts.

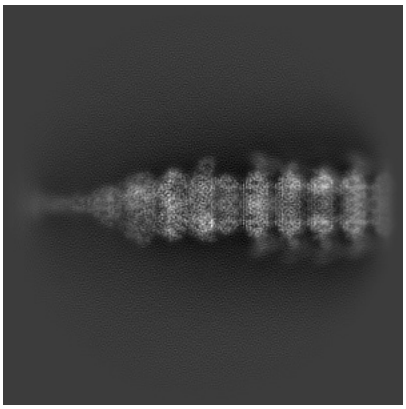
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

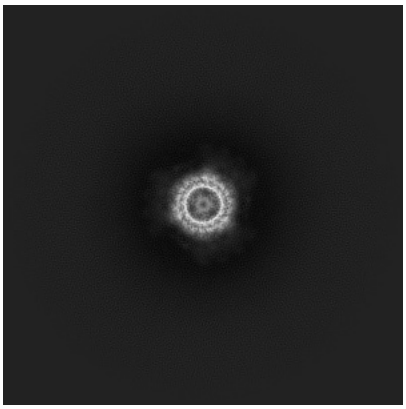
6.1.1 Primary map



X

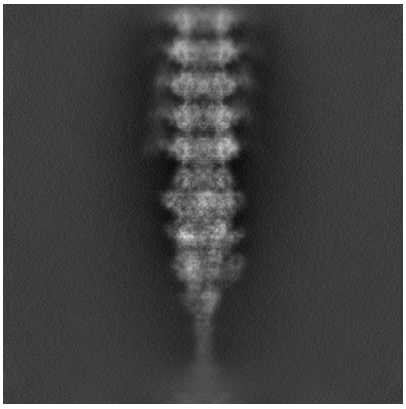


Y

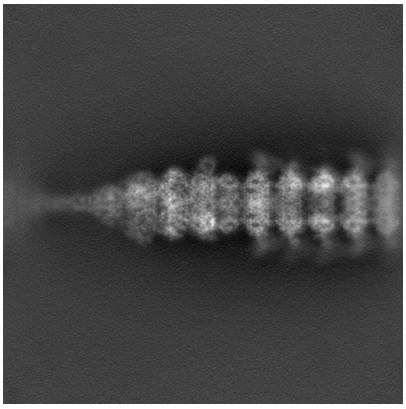


Z

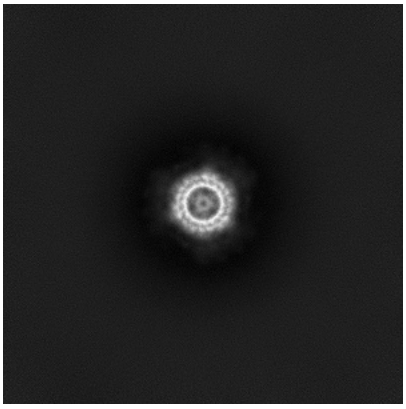
6.1.2 Raw map



X



Y

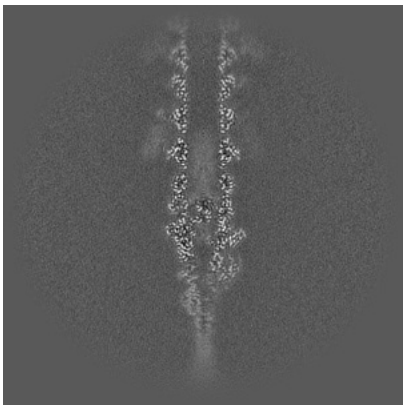


Z

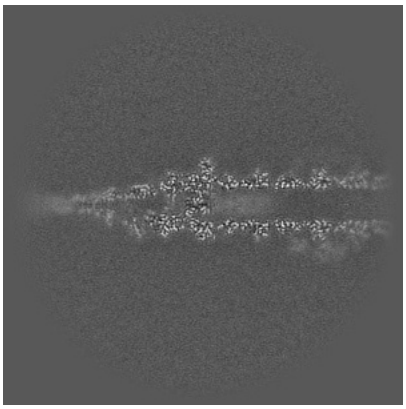
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

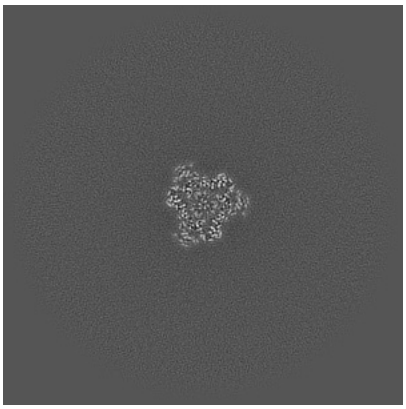
6.2.1 Primary map



X Index: 240

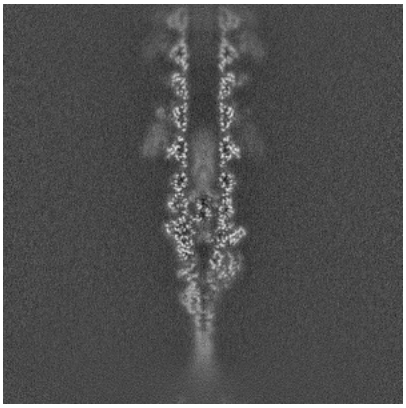


Y Index: 240

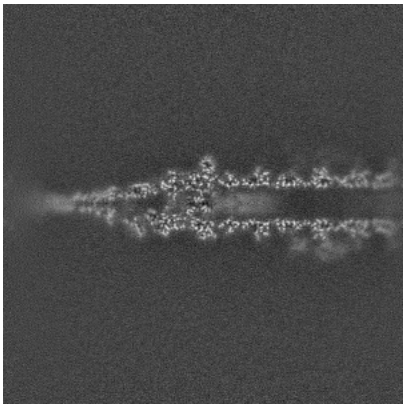


Z Index: 240

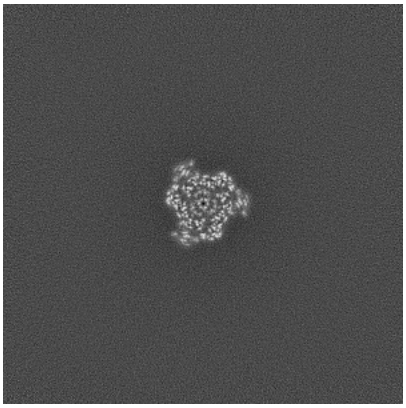
6.2.2 Raw map



X Index: 240



Y Index: 240

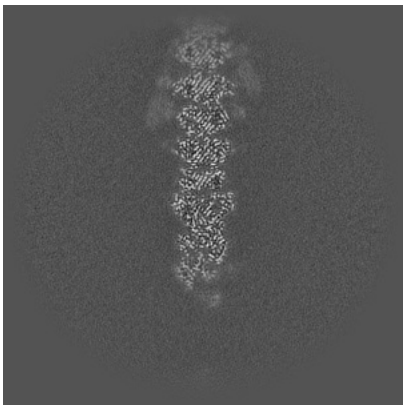


Z Index: 240

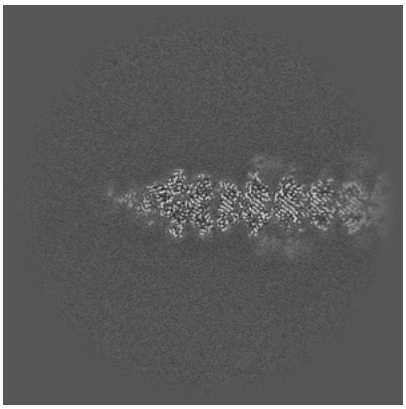
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

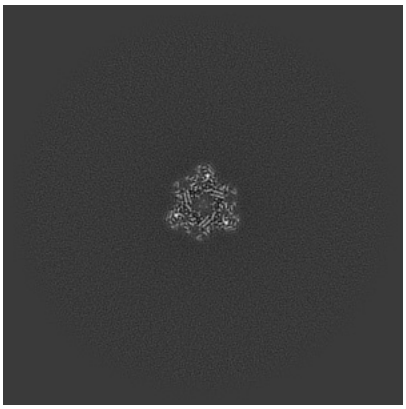
6.3.1 Primary map



X Index: 261

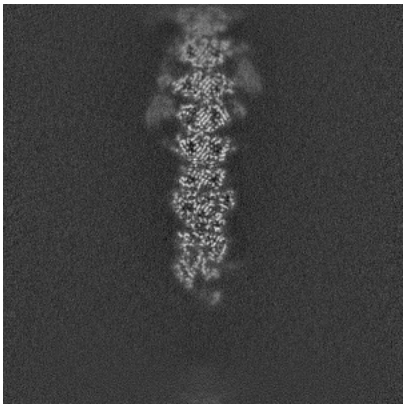


Y Index: 261

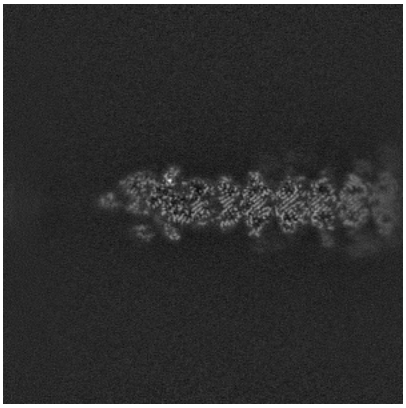


Z Index: 199

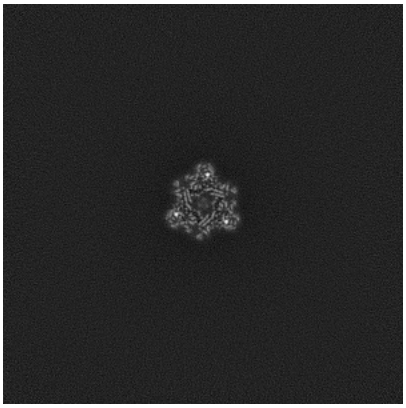
6.3.2 Raw map



X Index: 262



Y Index: 219

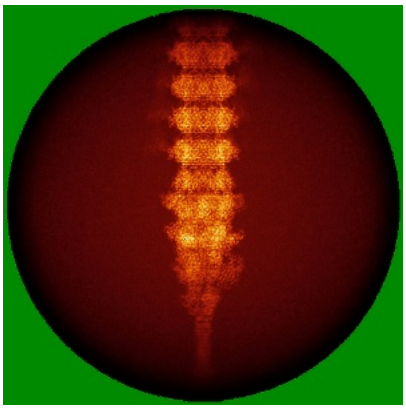


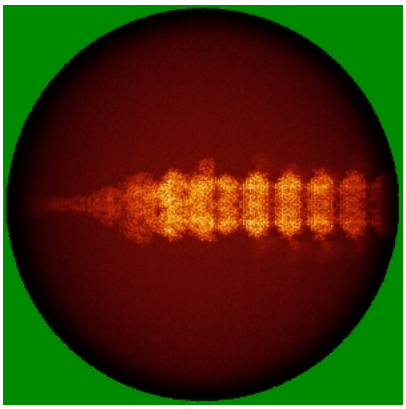
Z Index: 200

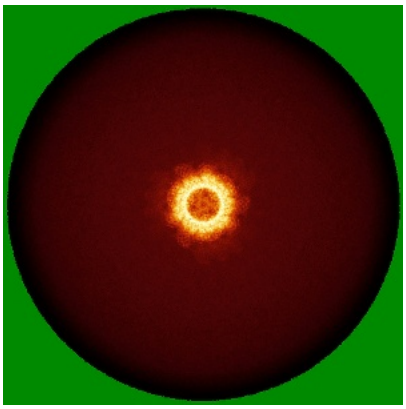
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

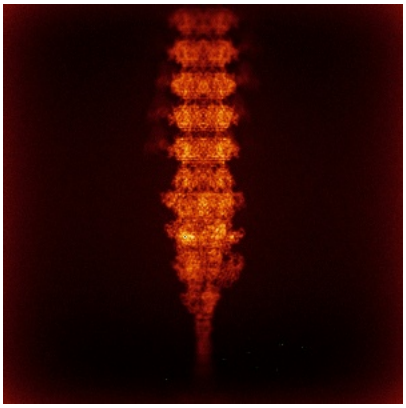
6.4.1 Primary map

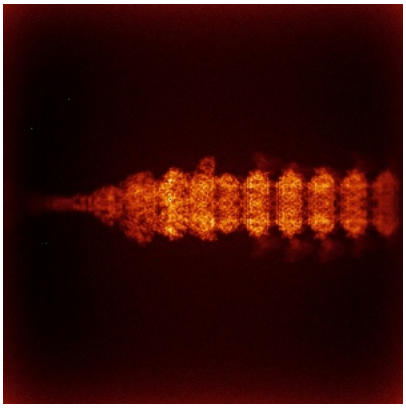

X

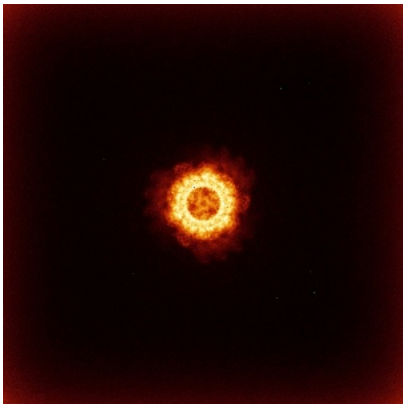

Y


Z

6.4.2 Raw map


X

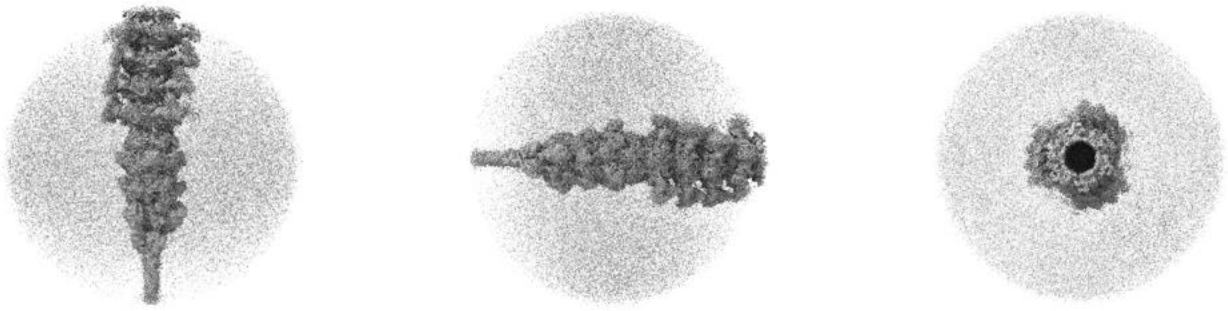

Y


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



X Y Z

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

X Y Z

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.

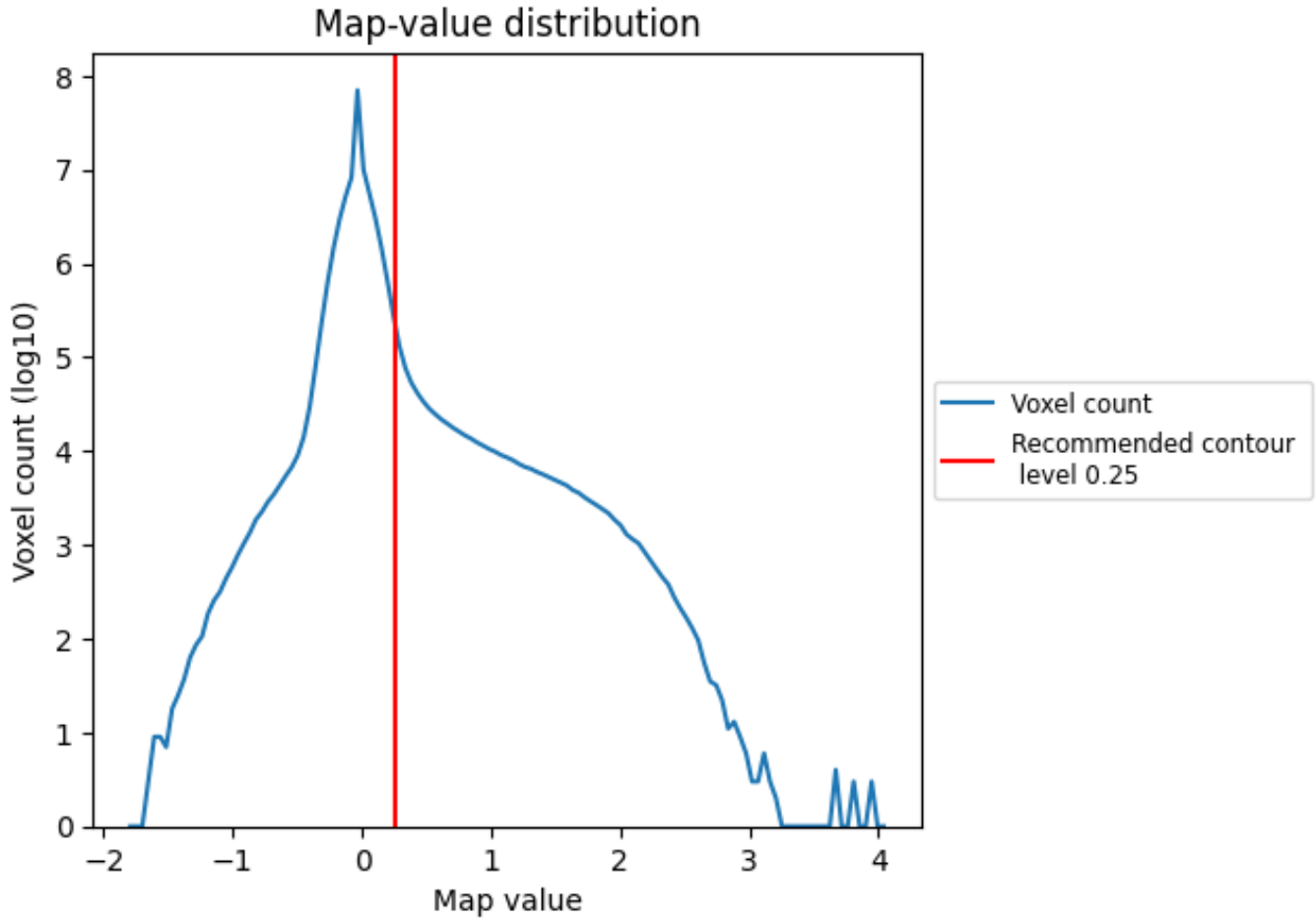
6.6 Mask visualisation (i)

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

7 Map analysis

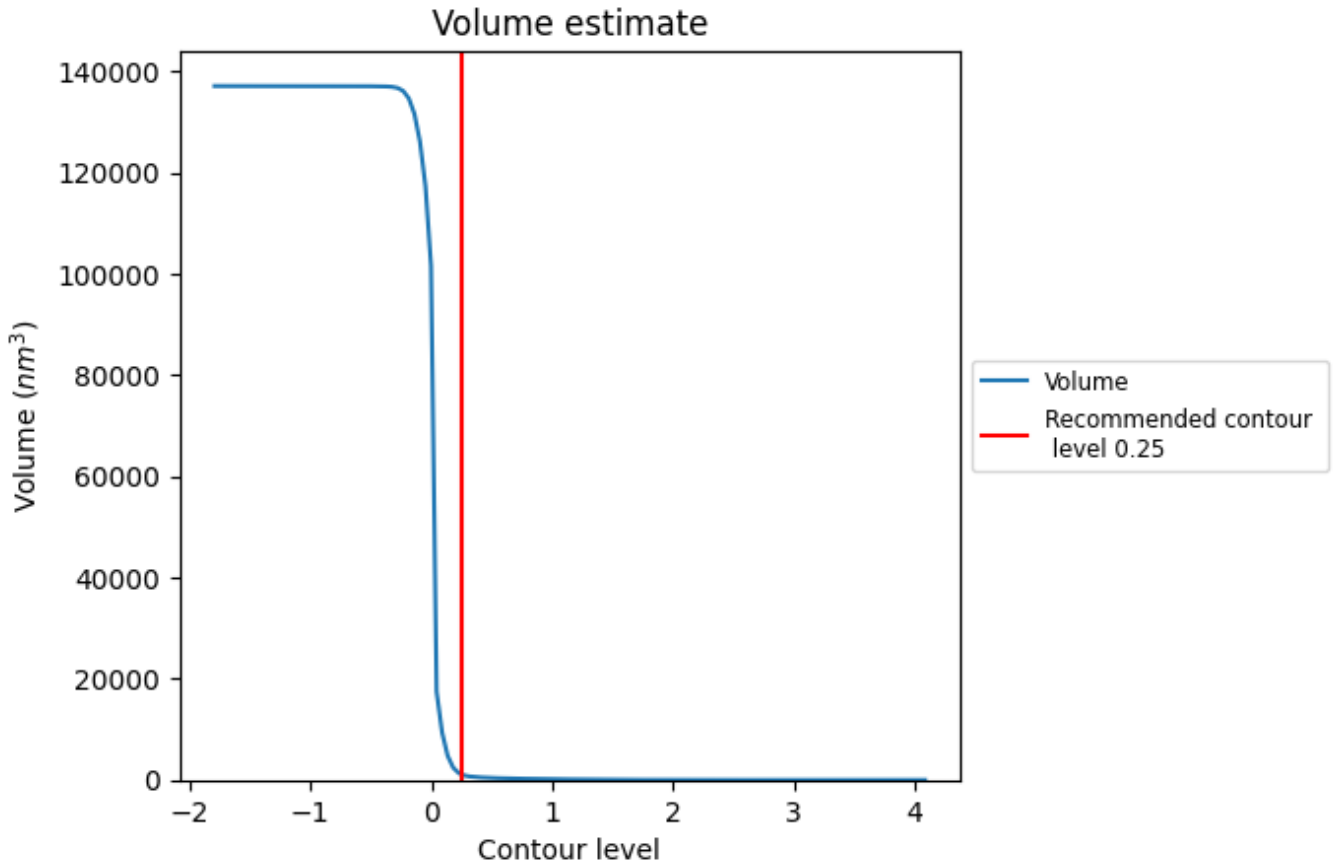
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

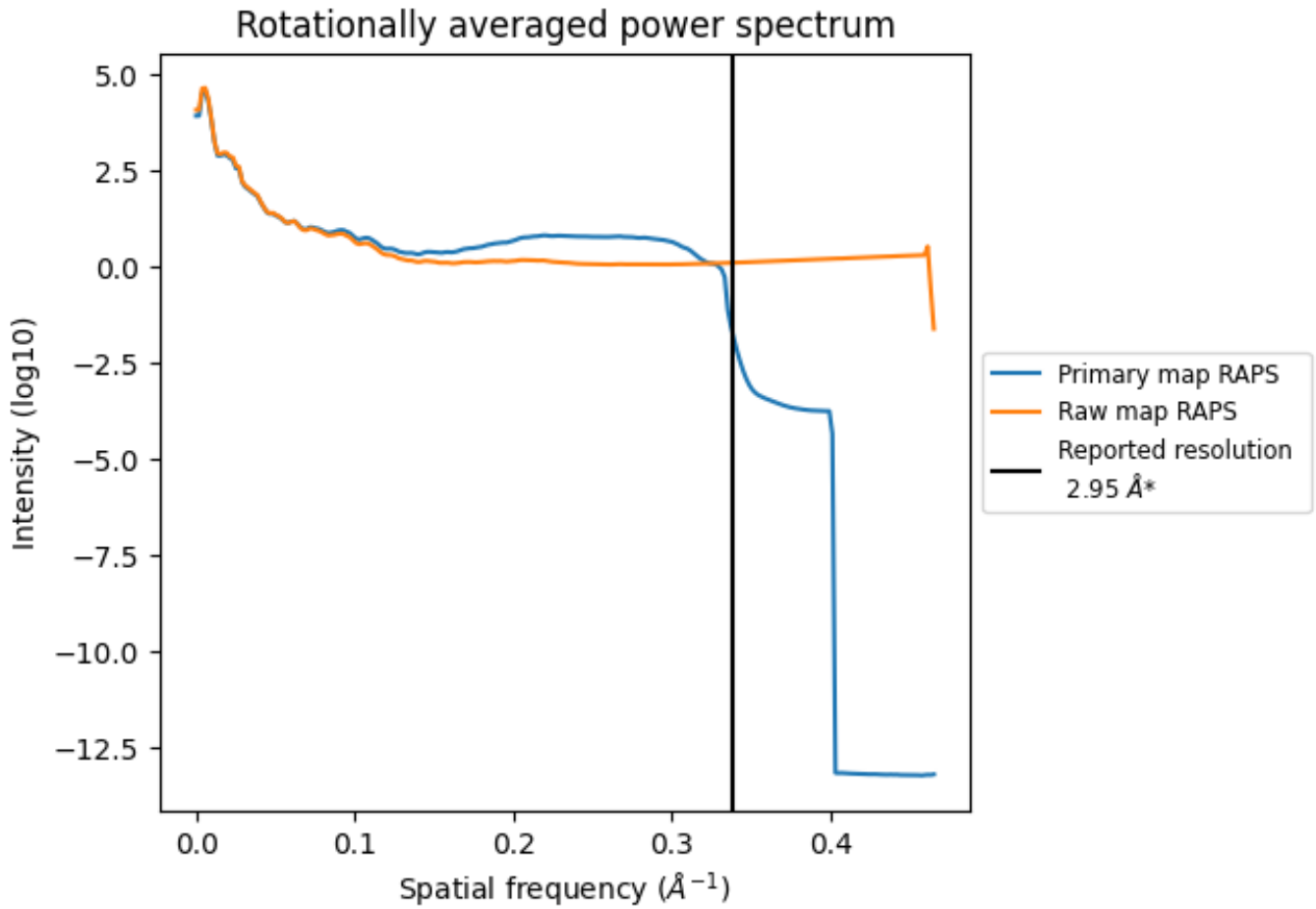
7.2 Volume estimate



The volume at the recommended contour level is 1130 nm^3; this corresponds to an approximate mass of 1021 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 (i)

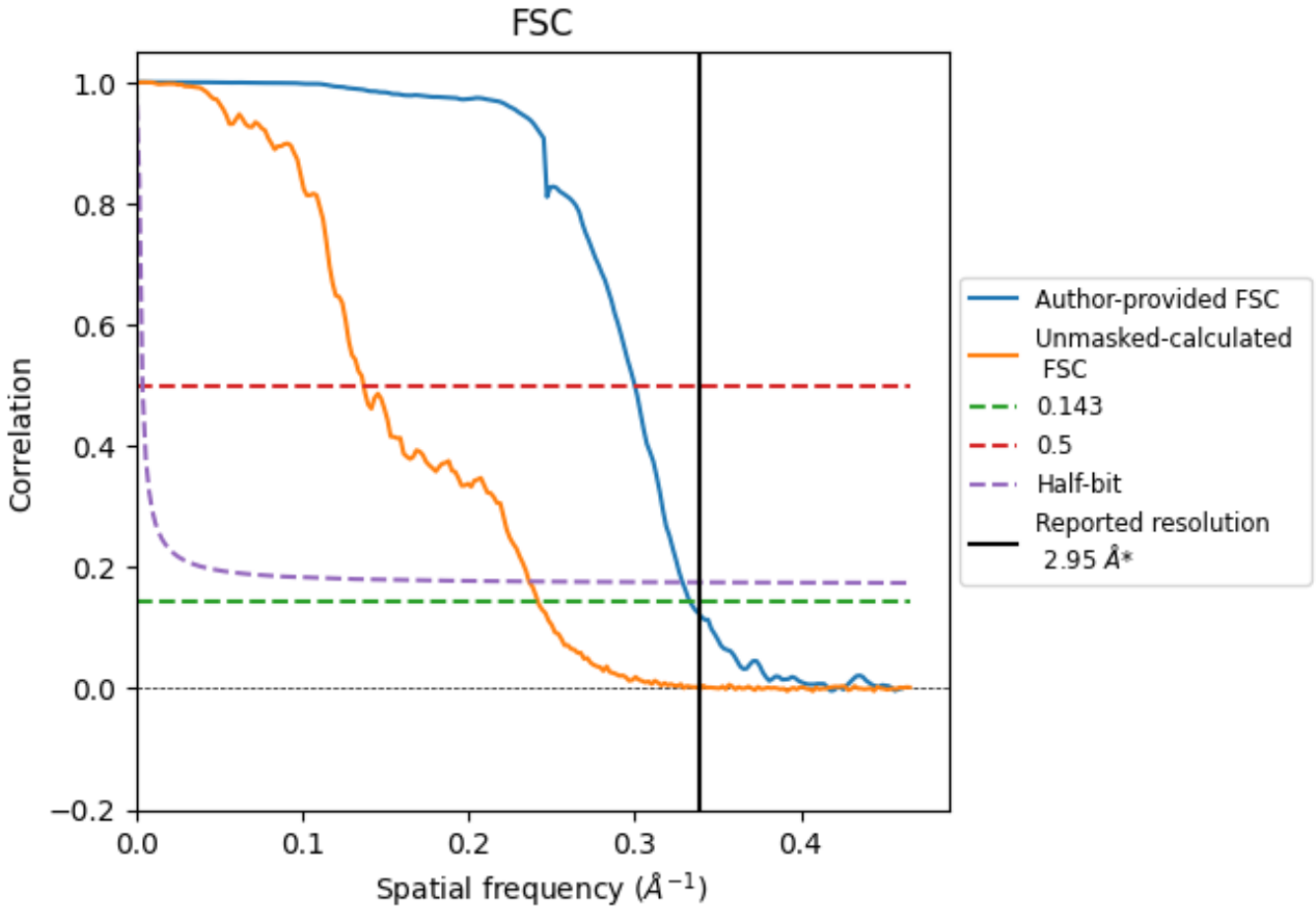


*Reported resolution corresponds to spatial frequency of 0.339 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.339 $Å^{-1}$

8.2 Resolution estimates (i)

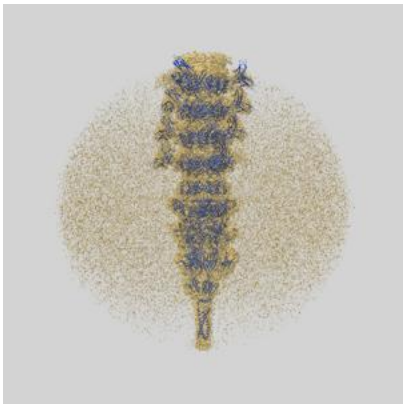
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.95	-	-
Author-provided FSC curve	3.00	3.33	3.04
Unmasked-calculated*	4.14	7.30	4.23

*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 4.14 differs from the reported value 2.95 by more than 10 %

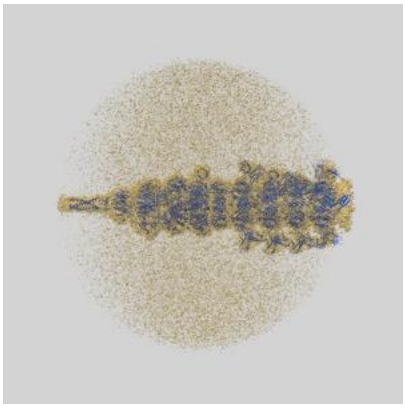
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-35824 and PDB model 8IYK. Per-residue inclusion information can be found in section 3 on page 9.

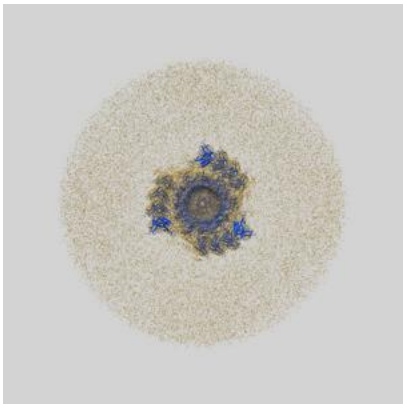
9.1 Map-model overlay



X



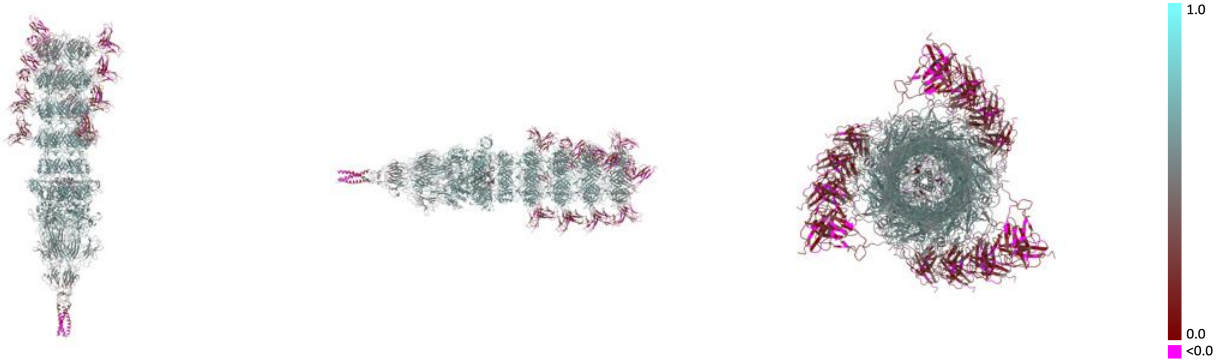
Y



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.

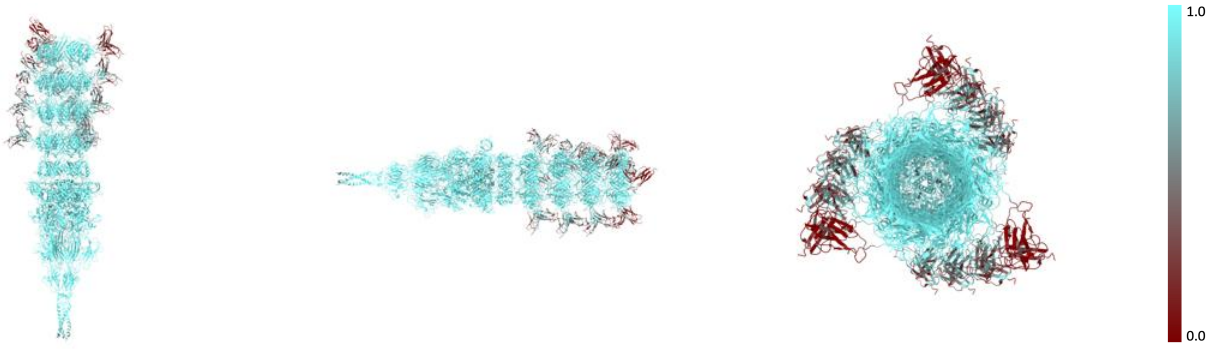
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

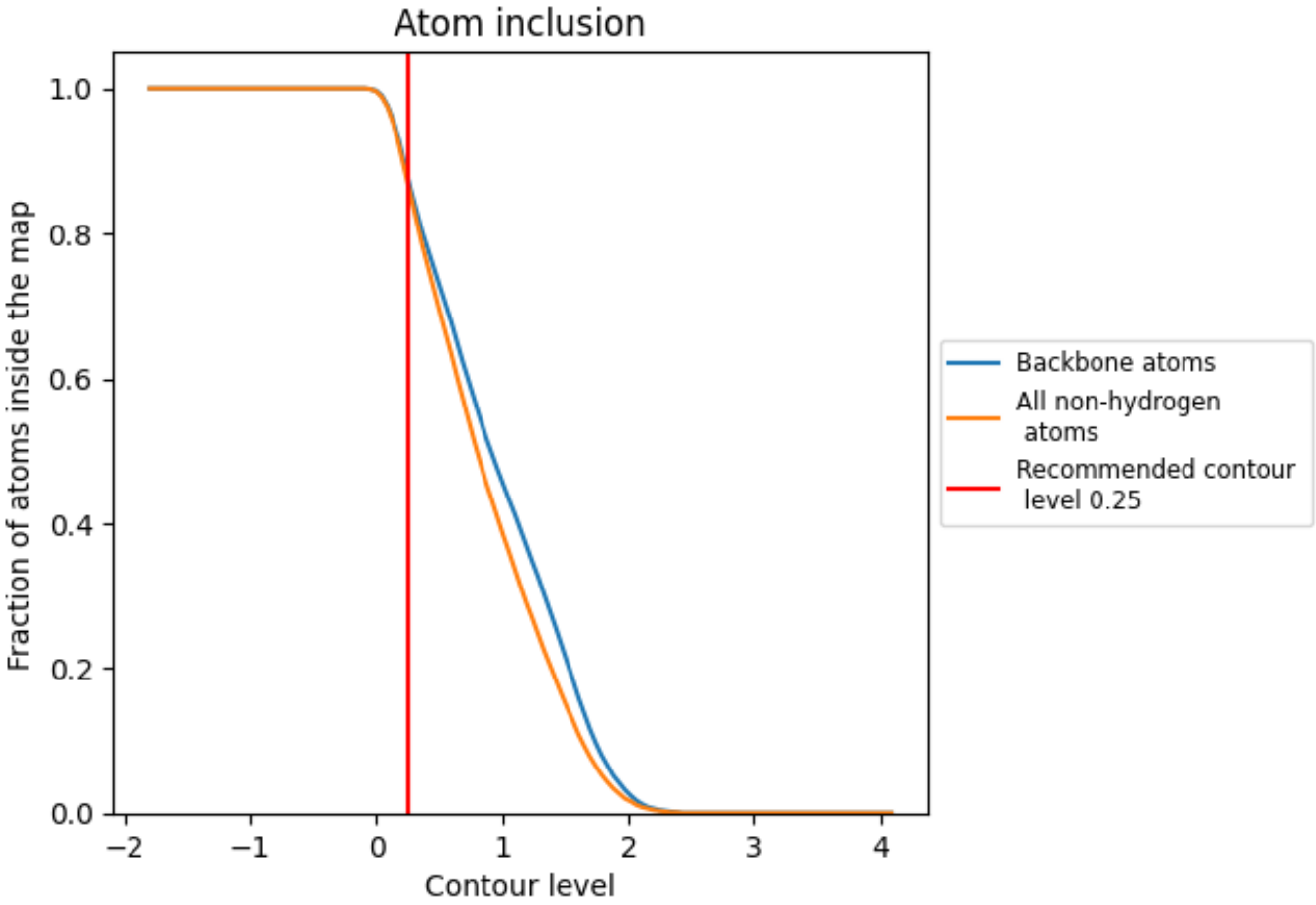
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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, 87% 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	0.8710	0.4830
A	0.8390	0.4680
B	0.8250	0.4430
C	0.7010	0.3850
D	0.8260	0.4750
E	0.9840	0.5740
F	0.9780	0.5190
G	0.8130	0.4670
H	0.9470	0.5420
I	0.9260	0.5000
J	0.9760	0.5200
K	0.9780	0.5830
L	0.9920	0.5810
M	0.9870	0.5790
N	0.9920	0.5810
O	0.9470	0.5330
P	0.9210	0.5020
Q	0.8210	0.4420
R	0.8060	0.4440
S	0.8380	0.4710
T	0.8300	0.4660
U	0.7020	0.3850
V	0.8270	0.4770
W	0.6780	0.3780
X	0.8280	0.4720
Y	0.9800	0.5730
Z	0.9770	0.5200
a	0.8320	0.4680
b	0.8050	0.4450
c	0.6720	0.3760
d	0.8150	0.4670
e	0.9770	0.5780
f	0.9920	0.5810
g	0.9510	0.5390
h	0.9180	0.5000

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Chain	Atom inclusion	Q-score
i	0.8260	0.4420
j	0.8030	0.4470
k	0.8390	0.4680
l	0.8280	0.4660
m	0.9800	0.5840
n	0.7010	0.3860
o	0.6740	0.3780
v	0.8140	0.4650