



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 08:44 AM UTC

PDB ID : 9KI1 / pdb_00009ki1
EMDB ID : EMD-62362
Title : Baseplate structure of Escherichia phage Mu
Authors : Zhou, J.Q.; Liu, H.R.
Deposited on : 2024-11-11
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

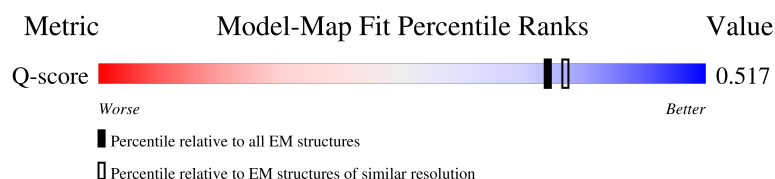
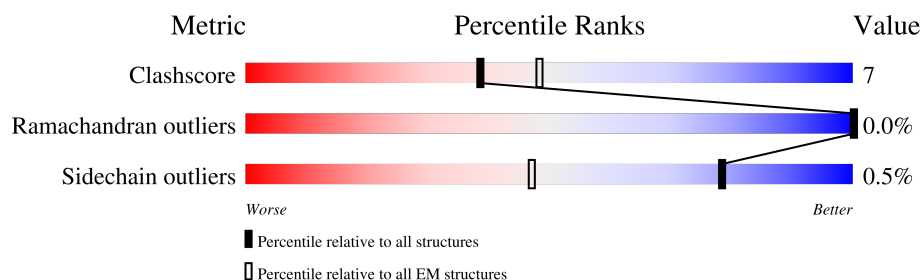
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.30 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.



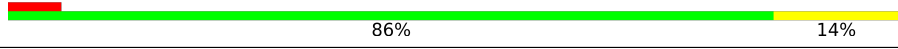
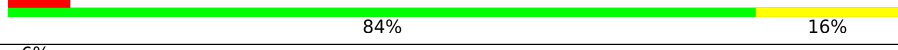
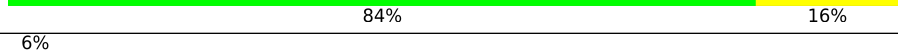
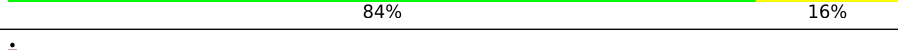
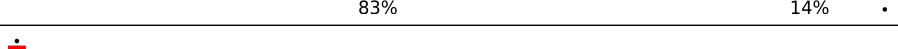
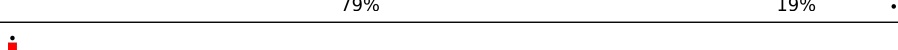
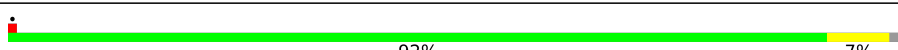
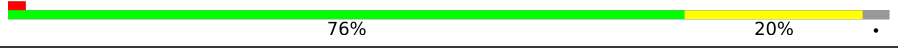
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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

Mol	Chain	Length	Quality of chain
1	0	495	
1	s	495	
1	t	495	
1	u	495	

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Mol	Chain	Length	Quality of chain
1	v	495	
1	w	495	
2	1	495	
2	2	495	
2	3	495	
2	x	495	
2	y	495	
2	z	495	
3	4	118	
3	5	118	
3	6	118	
3	7	118	
3	8	118	
3	9	118	
4	A	145	
4	B	145	
4	C	145	
4	D	145	
4	E	145	
4	F	145	
5	G	379	
5	N	379	
5	U	379	
6	H	360	
6	I	360	

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Mol	Chain	Length	Quality of chain
6	J	360	
6	K	360	
6	L	360	
6	M	360	
6	O	360	
6	P	360	
6	Q	360	
6	R	360	
6	S	360	
6	T	360	
7	V	197	
7	W	197	
7	X	197	
8	a	180	
8	b	180	
8	c	180	
8	d	180	
8	e	180	
8	f	180	
9	g	690	
9	h	690	
9	i	690	
10	j	504	
10	k	504	
10	l	504	

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Mol	Chain	Length	Quality of chain
10	m	504	17%5%79%
10	n	504	5%18%79%
10	o	504	19%79%
10	p	504	17%79%
10	q	504	5%17%79%
10	r	504	19%79%

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 114473 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 DNA circularization protein N.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	446	Total	C	N	O	S	0	0
			3294	2035	579	666	14		
1	s	446	Total	C	N	O	S	0	0
			3294	2035	579	666	14		
1	t	446	Total	C	N	O	S	0	0
			3294	2035	579	666	14		
1	u	419	Total	C	N	O	S	0	0
			3119	1935	553	617	14		
1	v	419	Total	C	N	O	S	0	0
			3119	1935	553	617	14		
1	w	419	Total	C	N	O	S	0	0
			3119	1935	553	617	14		

- Molecule 2 is a protein called Tail sheath protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	493	Total	C	N	O	S	0	0
			3719	2340	638	727	14		
2	2	493	Total	C	N	O	S	0	0
			3719	2340	638	727	14		
2	3	493	Total	C	N	O	S	0	0
			3719	2340	638	727	14		
2	x	493	Total	C	N	O	S	0	0
			3719	2340	638	727	14		
2	y	493	Total	C	N	O	S	0	0
			3719	2340	638	727	14		
2	z	493	Total	C	N	O	S	0	0
			3719	2340	638	727	14		

- Molecule 3 is a protein called Tail tube protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	115	Total	C	N	O	S	0	0
			880	549	154	172	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	5	115	Total	C	N	O	S	0	0
			880	549	154	172	5		
3	6	115	Total	C	N	O	S	0	0
			880	549	154	172	5		
3	7	115	Total	C	N	O	S	0	0
			880	549	154	172	5		
3	8	115	Total	C	N	O	S	0	0
			880	549	154	172	5		
3	9	115	Total	C	N	O	S	0	0
			880	549	154	172	5		

- Molecule 4 is a protein called Baseplate protein gp46.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	143	Total	C	N	O	S	0	0
			1137	714	199	223	1		
4	B	143	Total	C	N	O	S	0	0
			1137	714	199	223	1		
4	C	143	Total	C	N	O	S	0	0
			1137	714	199	223	1		
4	D	143	Total	C	N	O	S	0	0
			1137	714	199	223	1		
4	E	143	Total	C	N	O	S	0	0
			1137	714	199	223	1		
4	F	143	Total	C	N	O	S	0	0
			1137	714	199	223	1		

- Molecule 5 is a protein called Baseplate hub protein gp44.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	366	Total	C	N	O	S	0	0
			2830	1769	499	554	8		
5	N	366	Total	C	N	O	S	0	0
			2830	1769	499	554	8		
5	U	366	Total	C	N	O	S	0	0
			2830	1769	499	554	8		

- Molecule 6 is a protein called Baseplate protein gp47.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	356	Total	C	N	O	S	0	0
			2694	1699	471	517	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	356	Total	C	N	O	S	0	0
			2694	1699	471	517	7		
6	J	356	Total	C	N	O	S	0	0
			2694	1699	471	517	7		
6	K	356	Total	C	N	O	S	0	0
			2694	1699	471	517	7		
6	L	356	Total	C	N	O	S	0	0
			2694	1699	471	517	7		
6	M	356	Total	C	N	O	S	0	0
			2694	1699	471	517	7		
6	O	359	Total	C	N	O	S	0	0
			2712	1711	474	520	7		
6	P	359	Total	C	N	O	S	0	0
			2712	1711	474	520	7		
6	Q	359	Total	C	N	O	S	0	0
			2712	1711	474	520	7		
6	R	343	Total	C	N	O	S	0	0
			2609	1652	455	495	7		
6	S	343	Total	C	N	O	S	0	0
			2609	1652	455	495	7		
6	T	343	Total	C	N	O	S	0	0
			2609	1652	455	495	7		

- Molecule 7 is a protein called Baseplate puncturing device gp45.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	V	194	Total	C	N	O	S	0	0
			1486	911	278	290	7		
7	W	194	Total	C	N	O	S	0	0
			1486	911	278	290	7		
7	X	194	Total	C	N	O	S	0	0
			1486	911	278	290	7		

- Molecule 8 is a protein called Baseplate protein gp48.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	a	174	Total	C	N	O	S	0	0
			1401	891	244	261	5		
8	b	150	Total	C	N	O	S	0	0
			1208	770	210	223	5		
8	c	174	Total	C	N	O	S	0	0
			1401	891	244	261	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	d	150	Total	C	N	O	S	0	0
			1208	770	210	223	5		
8	e	174	Total	C	N	O	S	0	0
			1401	891	244	261	5		
8	f	150	Total	C	N	O	S	0	0
			1208	770	210	223	5		

- Molecule 9 is a protein called Probable tape measure protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	g	17	Total	C	N	O	S	0	0
			130	83	20	26	1		
9	h	17	Total	C	N	O	S	0	0
			130	83	20	26	1		
9	i	17	Total	C	N	O	S	0	0
			130	83	20	26	1		

- Molecule 10 is a protein called Tail fiber protein S.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	108	Total	C	N	O	S	0	0
			836	529	142	162	3		
10	k	108	Total	C	N	O	S	0	0
			836	529	142	162	3		
10	l	108	Total	C	N	O	S	0	0
			836	529	142	162	3		
10	m	108	Total	C	N	O	S	0	0
			836	529	142	162	3		
10	n	108	Total	C	N	O	S	0	0
			836	529	142	162	3		
10	o	108	Total	C	N	O	S	0	0
			836	529	142	162	3		
10	p	108	Total	C	N	O	S	0	0
			836	529	142	162	3		
10	q	108	Total	C	N	O	S	0	0
			836	529	142	162	3		
10	r	108	Total	C	N	O	S	0	0
			836	529	142	162	3		

- Molecule 11 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
11	V	1	Total	Ca	0
			1	1	

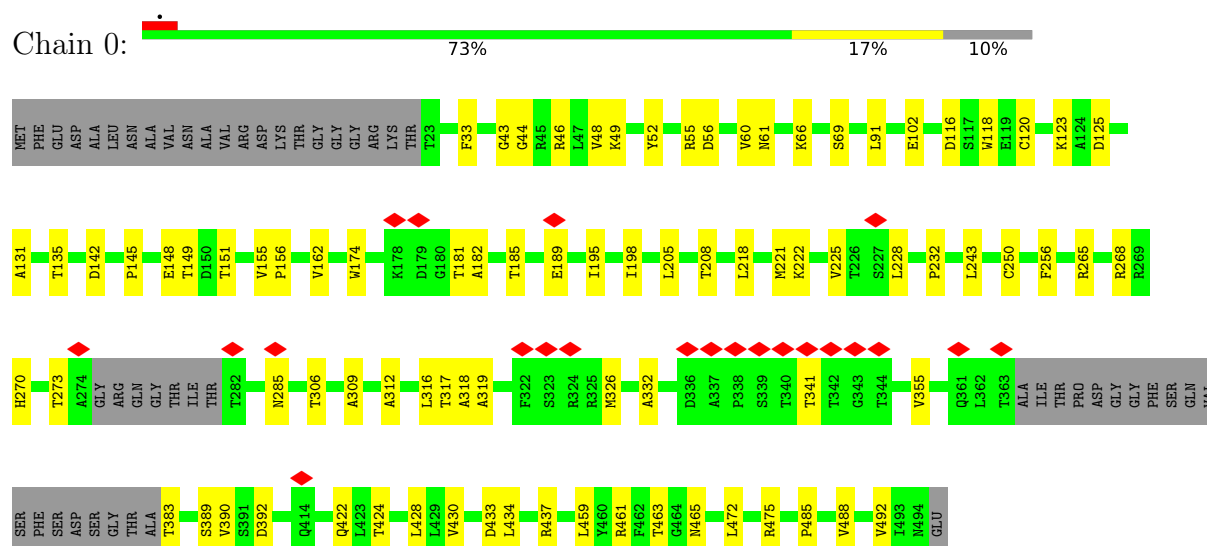
- Molecule 12 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
12	V	1	Total	Fe	0
			1	1	

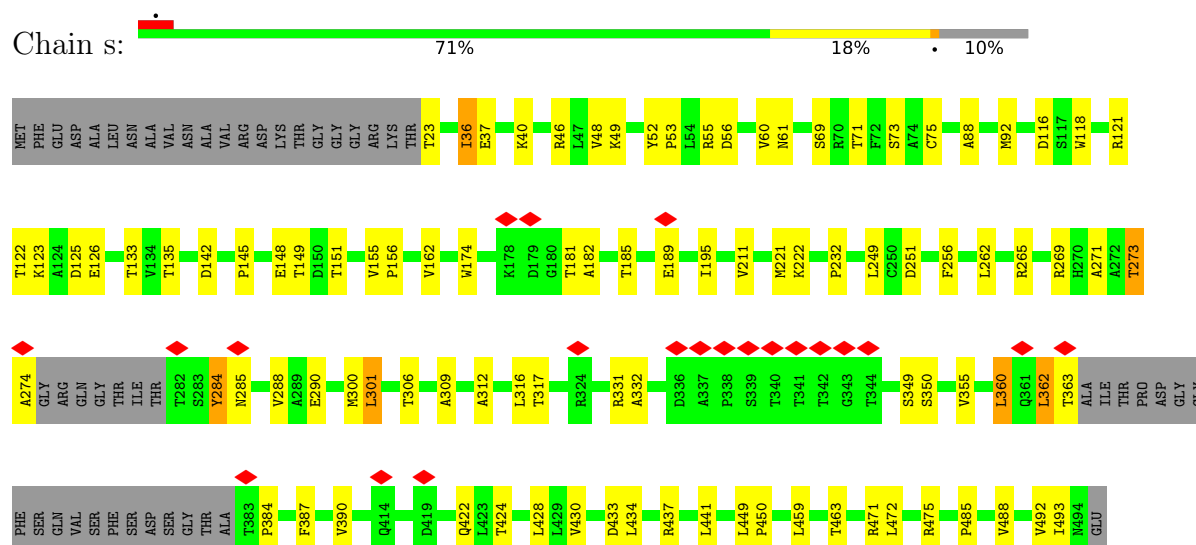
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

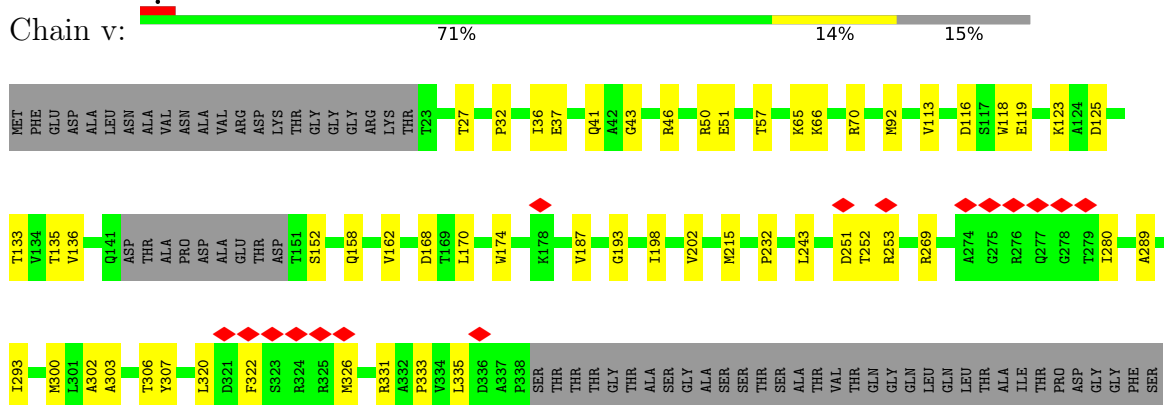
• Molecule 1: DNA circularization protein N



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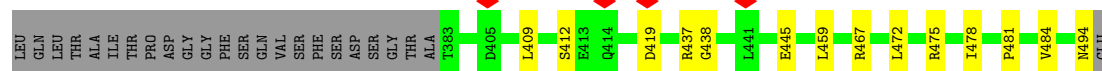
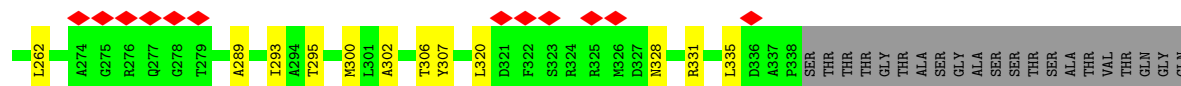
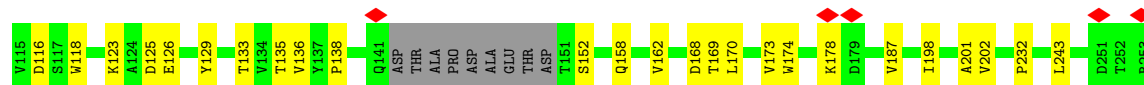


• Molecule 1: DNA circularization protein N

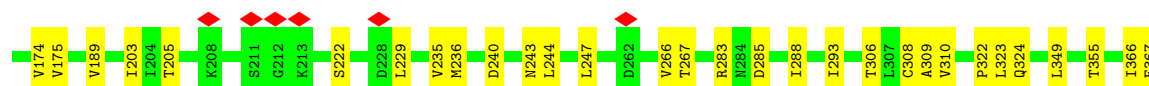
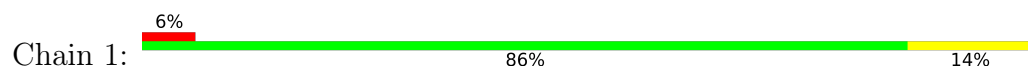




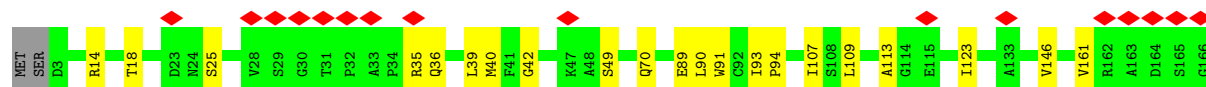
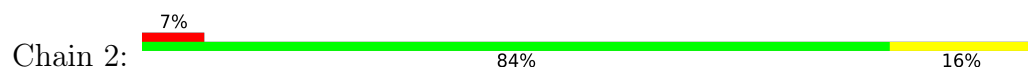
• Molecule 1: DNA circularization protein N



• Molecule 2: Tail sheath protein

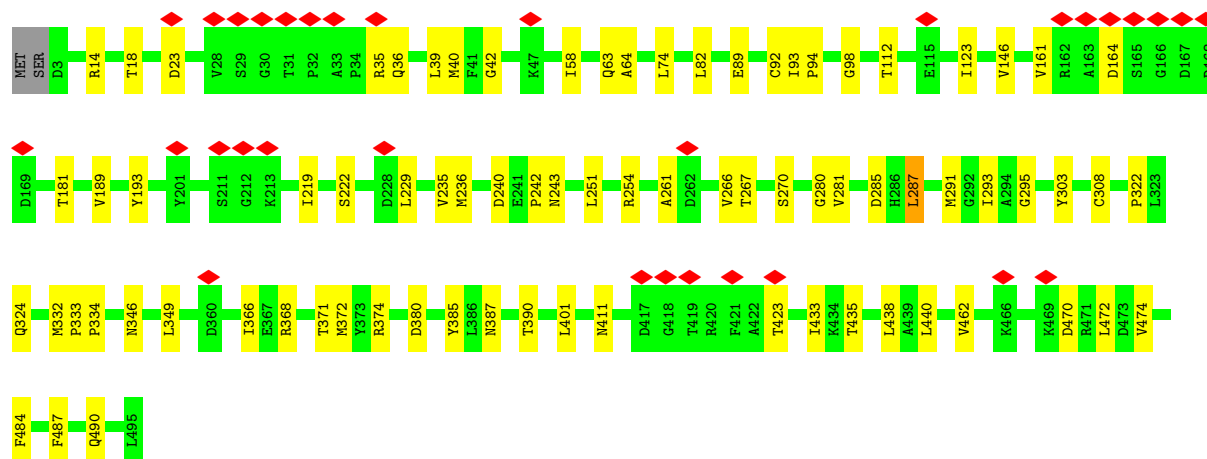
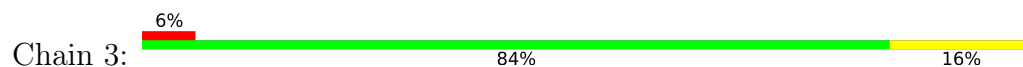


• Molecule 2: Tail sheath protein

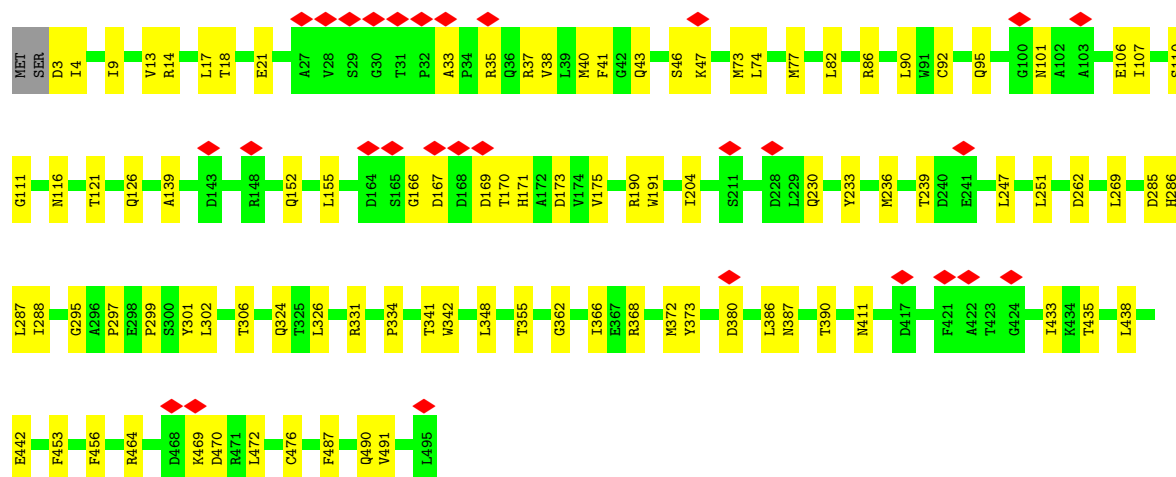
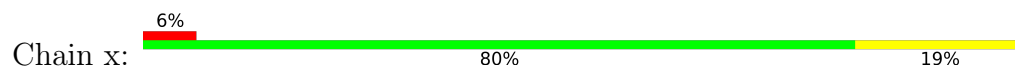




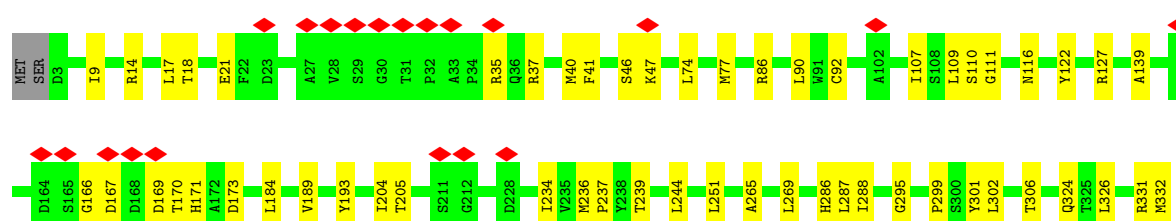
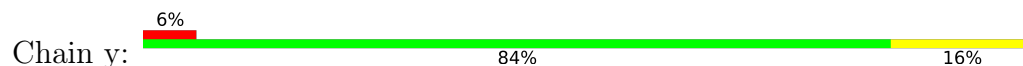
• Molecule 2: Tail sheath protein

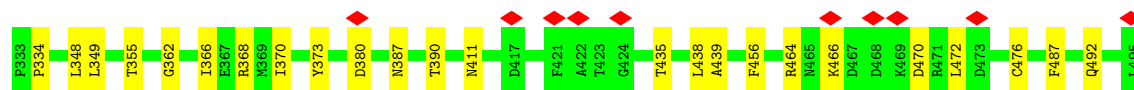


• Molecule 2: Tail sheath protein

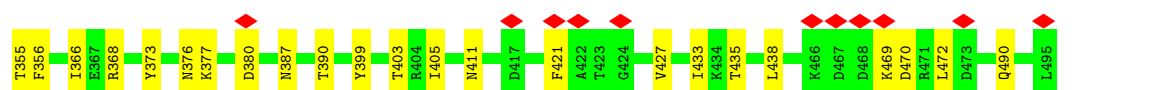
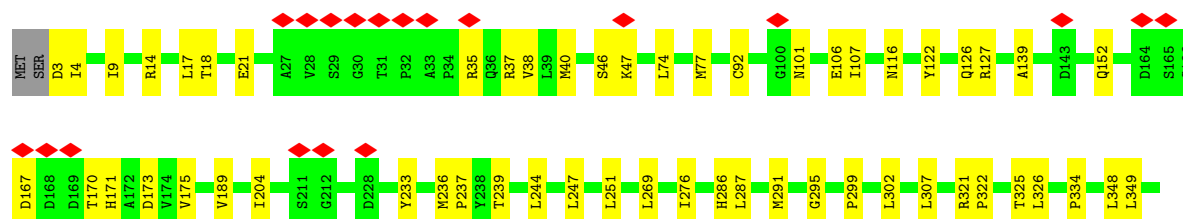
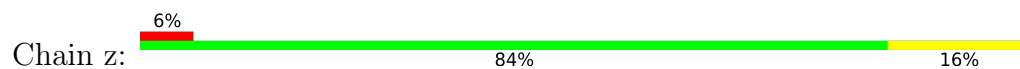


• Molecule 2: Tail sheath protein

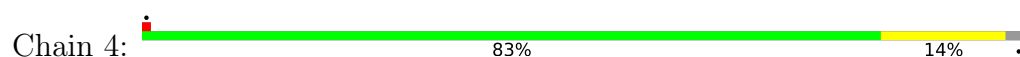




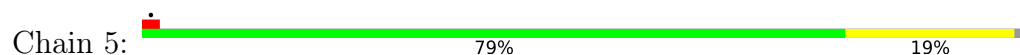
- Molecule 2: Tail sheath protein



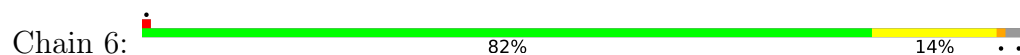
- Molecule 3: Tail tube protein



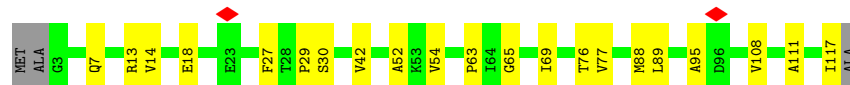
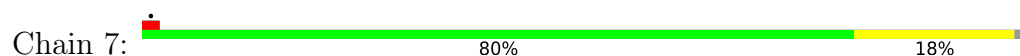
- Molecule 3: Tail tube protein



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- Molecule 3: Tail tube protein



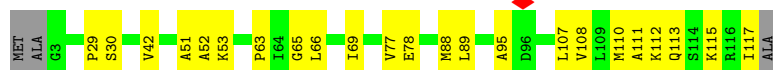
- Molecule 3: Tail tube protein

Chain 8:  76% 21%



- Molecule 3: Tail tube protein

Chain 9:  78% 19%



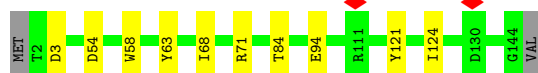
- Molecule 4: Baseplate protein gp46

Chain A:  81% 17%



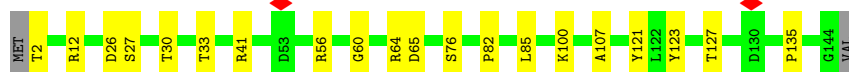
- Molecule 4: Baseplate protein gp46

Chain B:  92% 7%



- Molecule 4: Baseplate protein gp46

Chain C:  85% 14%



- Molecule 4: Baseplate protein gp46

Chain D:  86% 13%



- Molecule 4: Baseplate protein gp46

Chain E:  82% 17%



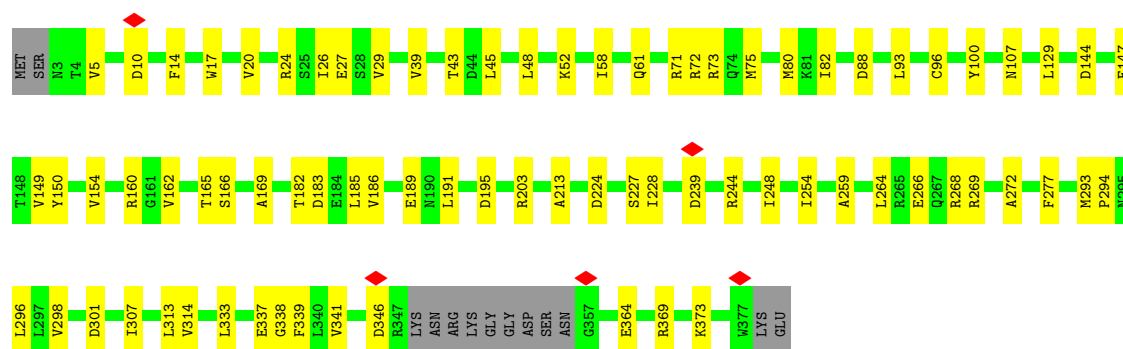
- Molecule 4: Baseplate protein gp46

Chain F:  84% 14%



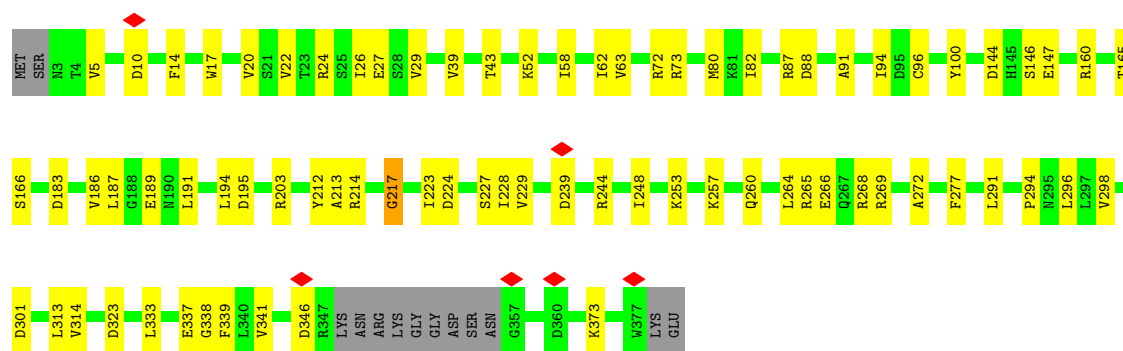
- Molecule 5: Baseplate hub protein gp44

Chain G:  76% 21%



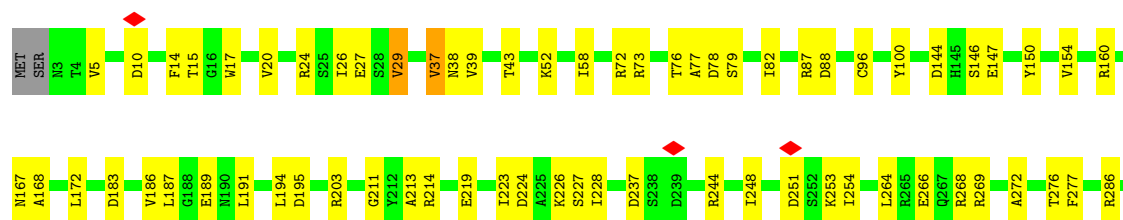
- Molecule 5: Baseplate hub protein gp44

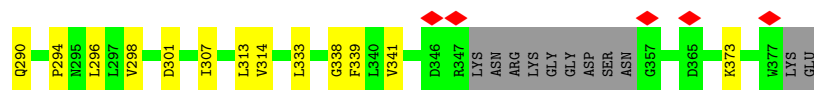
Chain N:  76% 20%



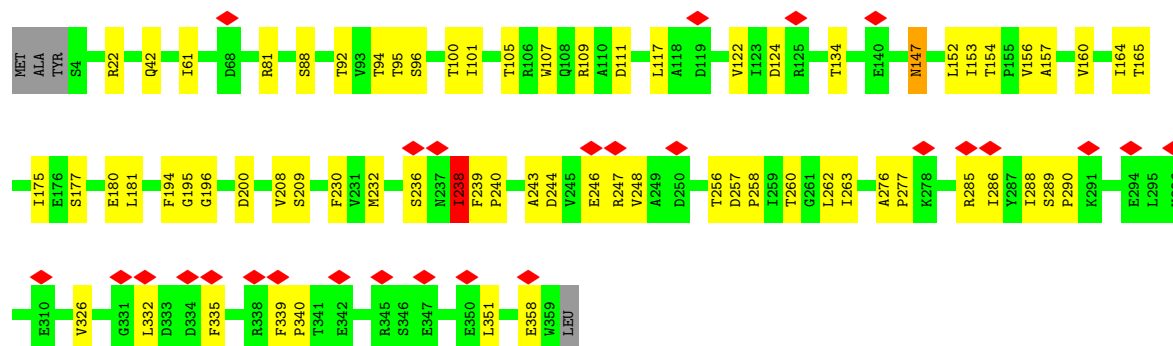
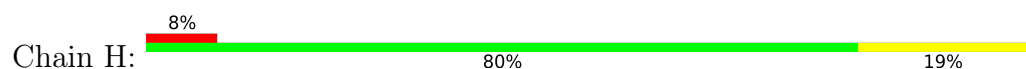
- Molecule 5: Baseplate hub protein gp44

Chain U:  75% 21%

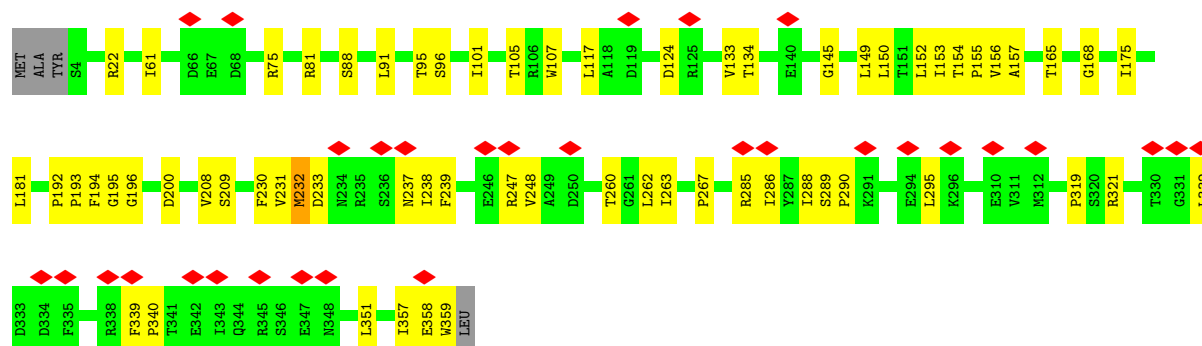
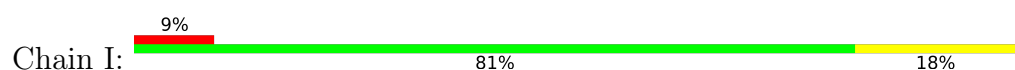




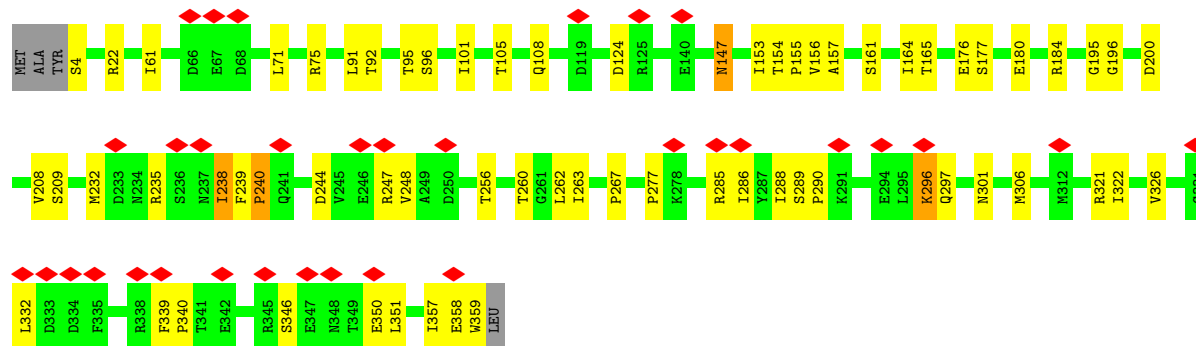
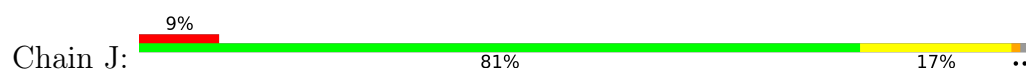
• Molecule 6: Baseplate protein gp47



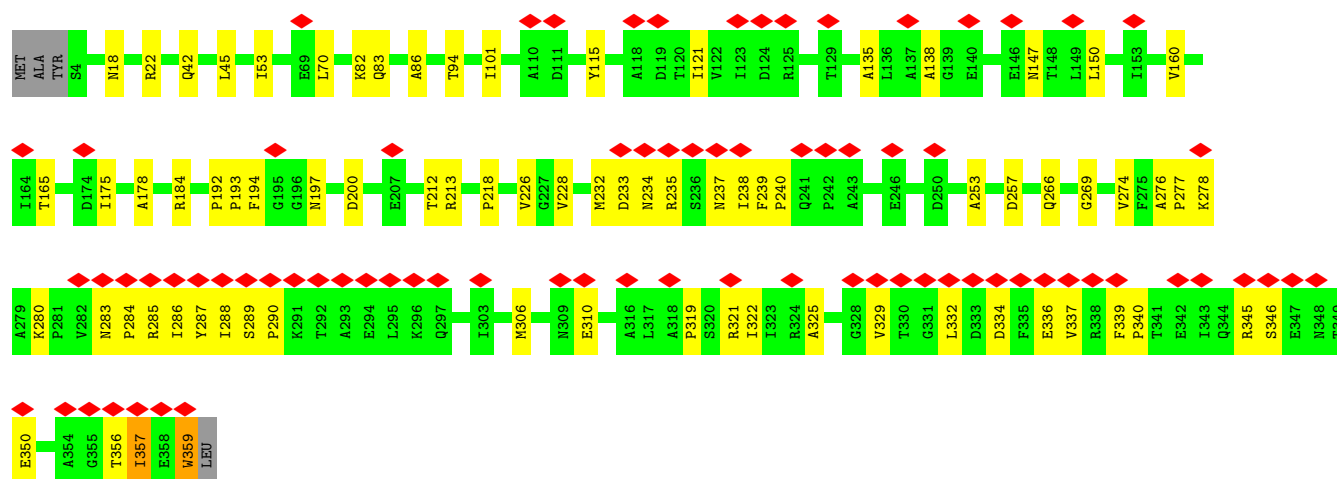
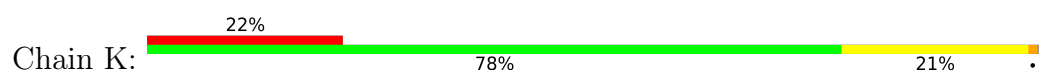
• Molecule 6: Baseplate protein gp47



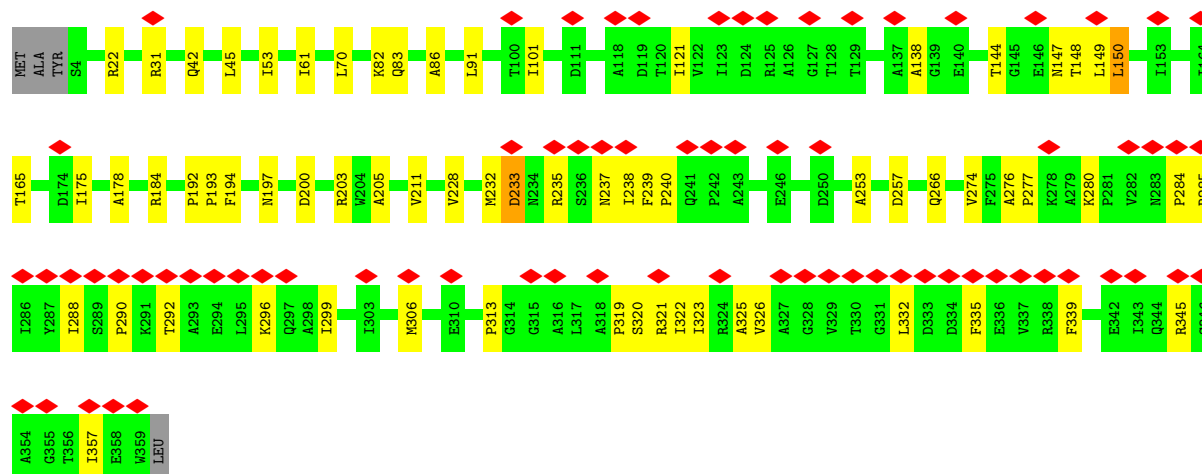
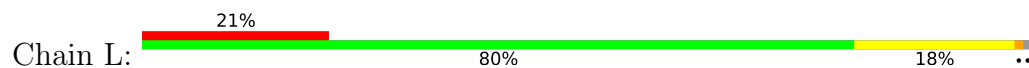
• Molecule 6: Baseplate protein gp47



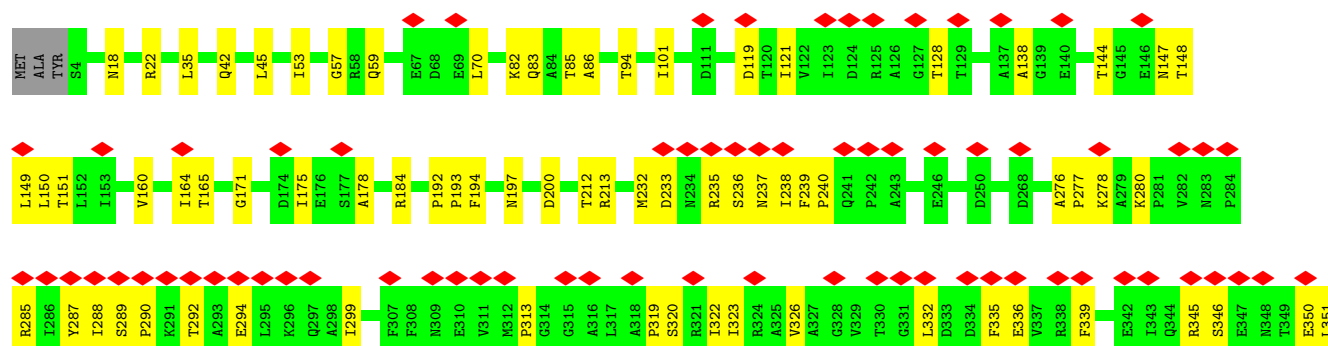
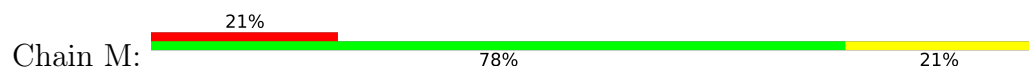
• Molecule 6: Baseplate protein gp47



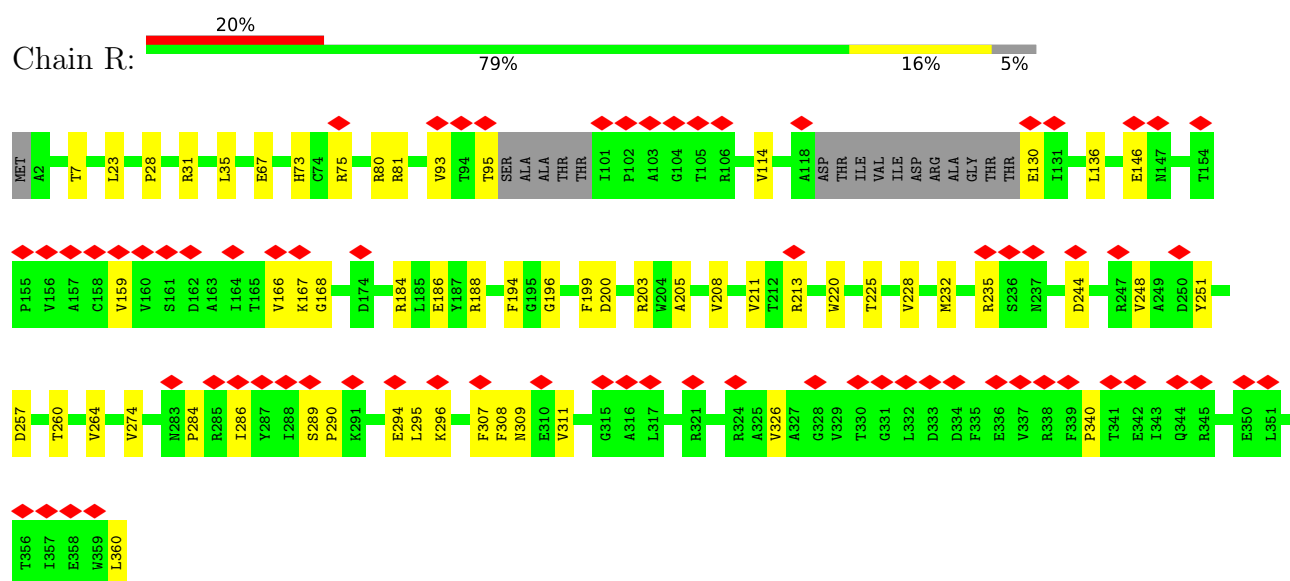
• Molecule 6: Baseplate protein gp47



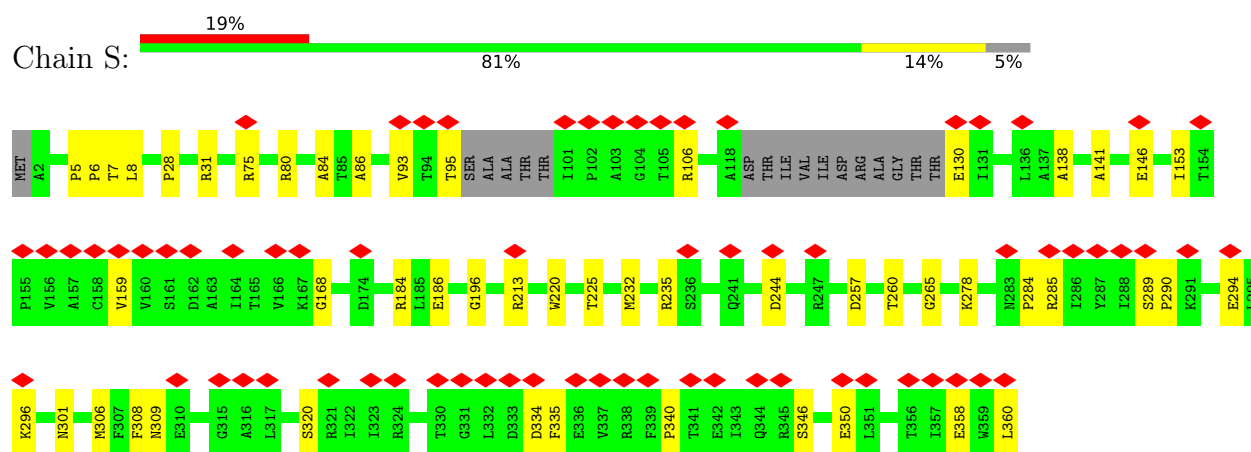
• Molecule 6: Baseplate protein gp47



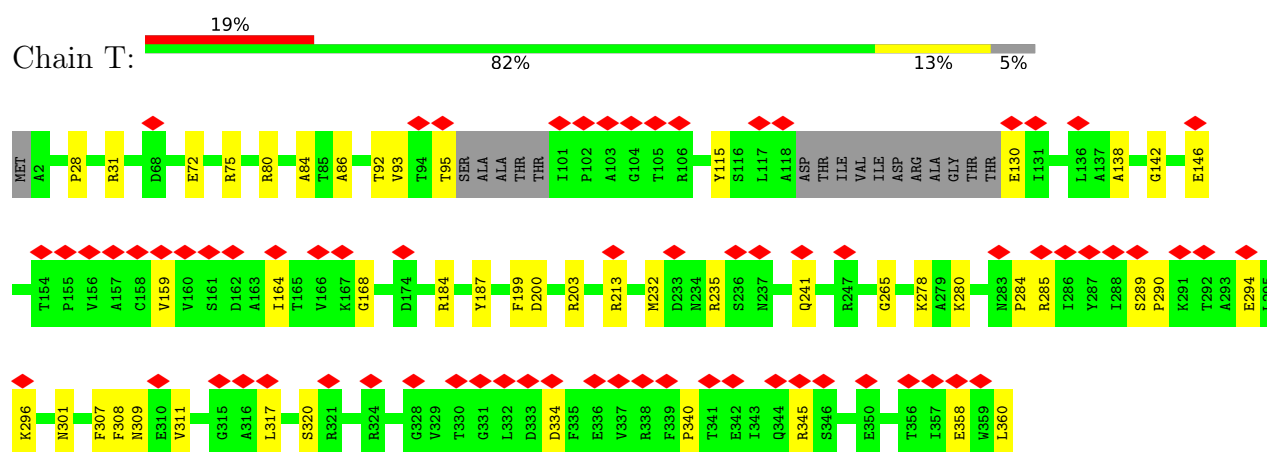




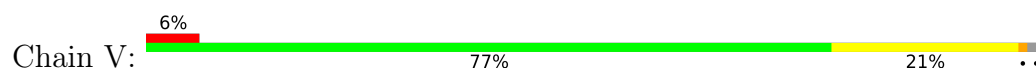
• Molecule 6: Baseplate protein gp47

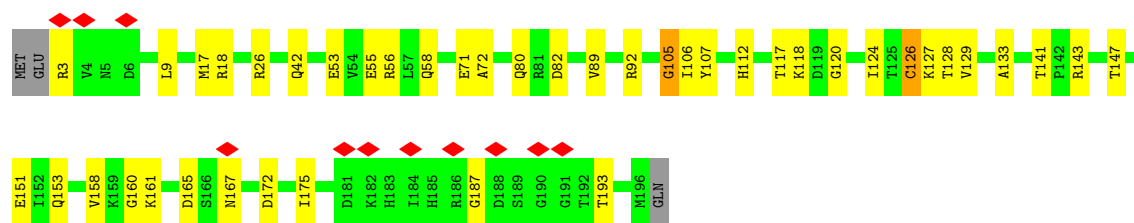


• Molecule 6: Baseplate protein gp47

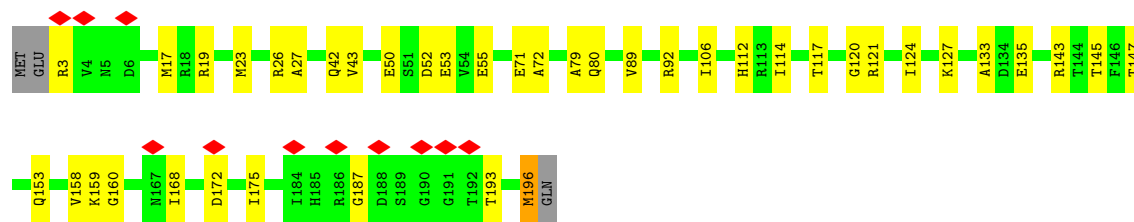
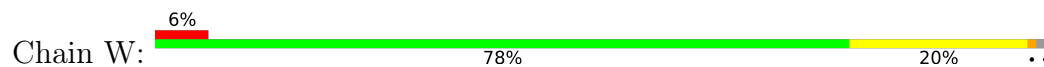


• Molecule 7: Baseplate puncturing device gp45

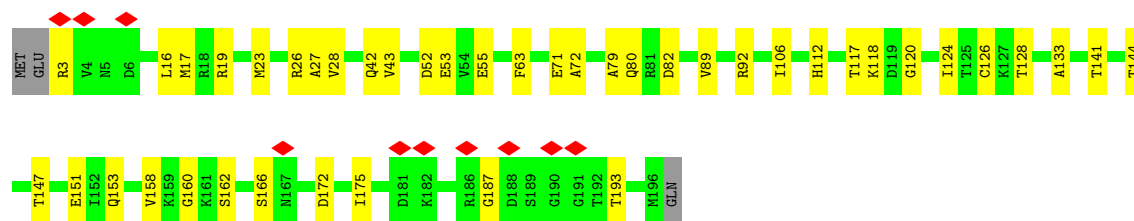
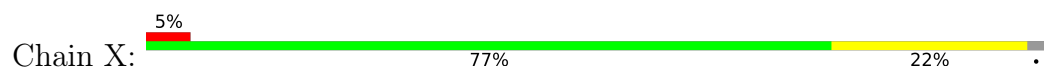




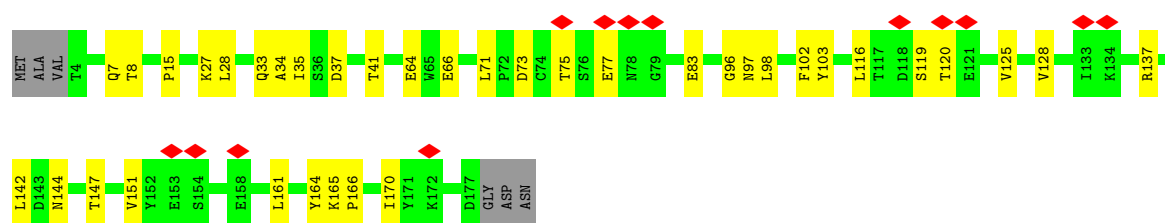
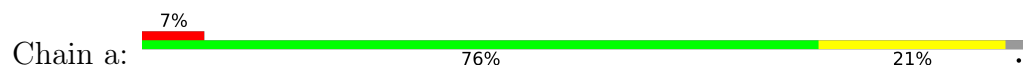
• Molecule 7: Baseplate puncturing device gp45



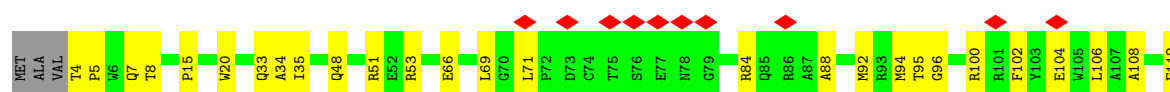
• Molecule 7: Baseplate puncturing device gp45

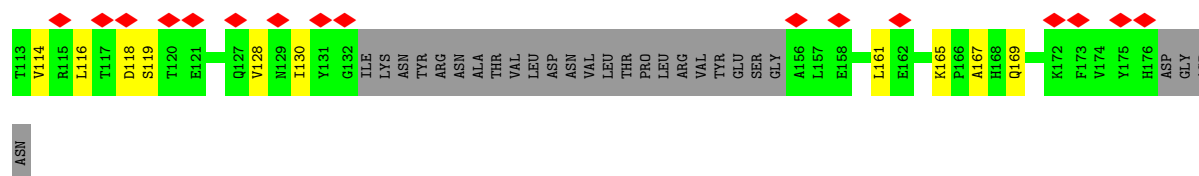


• Molecule 8: Baseplate protein gp48

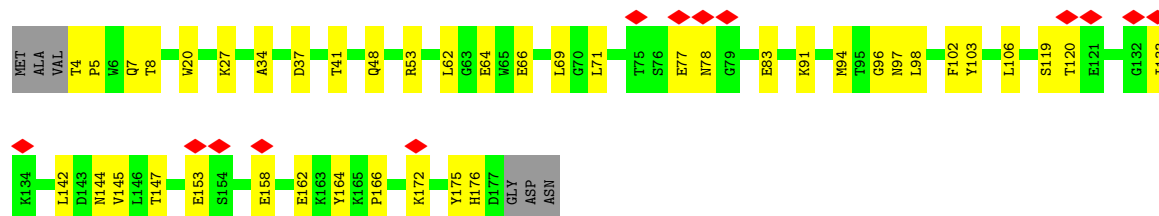


• Molecule 8: Baseplate protein gp48

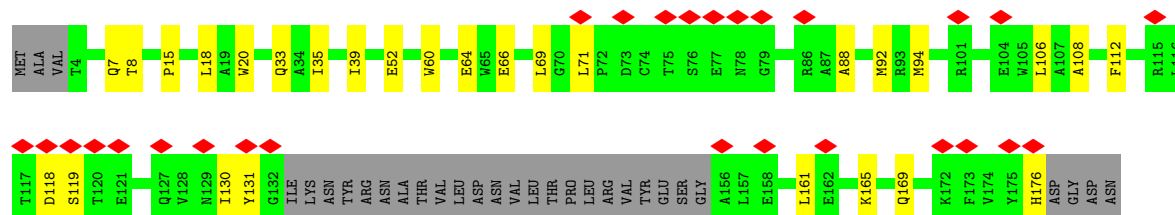




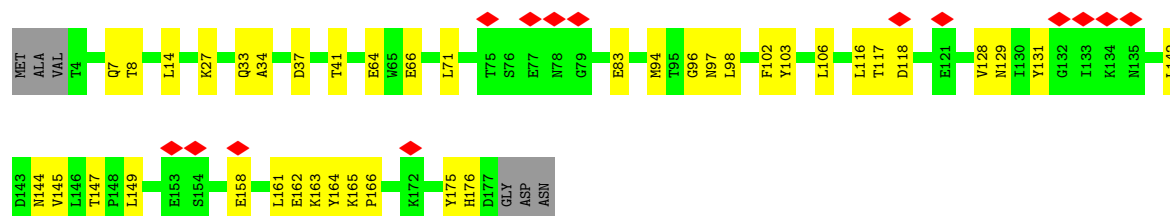
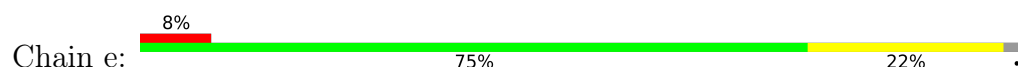
• Molecule 8: Baseplate protein gp48



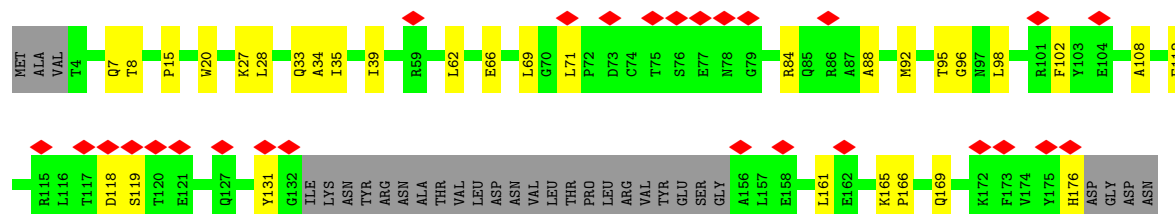
• Molecule 8: Baseplate protein gp48



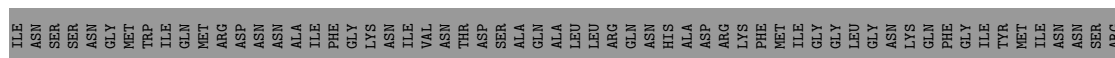
• Molecule 8: Baseplate protein gp48



• Molecule 8: Baseplate protein gp48







[illegible]

- Molecule 10: Tail fiber protein S



R101	E105	N106	D107	D108	D109	Y110	D111	ALA	SER	LEU	ASN	LYS	GLY	LEU	VAL	GLN	LEU	THR	SER	ALA	THR	ASP	SER	PRO	SER	GLU	THR	LEU	ALA	ALA	THR	ALA	LYS	VAL	LYS	ILE	ALA	MET	ASP	ASN	ASN	ALA	ALA	ARG	LEU	ALA	LYS	ASP	ARG	ASN	GLY	ALA	ASP	ILE	PRO	GLN
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LYS PRO LEU LEU PHE ILE GLN ASN ASN LEU LEU GLY GLN GLN THR VAL ASN ARG ARG ASN ALA VAL GLN LYS ASN GLY ASP THR LEU SER LEU GLY GLY LEU LEU THR PHE GLU ASN ASP ASP SER ILE LEU LEU ALA ALA TRP TRP ILE ILE ARG ASN THR THR ASP ALA ALA TRP LYS ASN ASP ASP ALA SER

THR	ASP	SER	TYR	MET	TRP	PHE	GLU	THR	GLY	ASP	ASN	GLY	ASN	GLU	GLU	TYR	PHE	LYS	TRP	ARG	ASN	GLN	LYS	SER	THR	THR	ASP	LYS	LEU	MET	ASN	ASN	LEU	LEU	LYS	TRP	ASP	VAL	VAL	ASN	VAL	ASN	ALA	ALA	ILE	VAL	VAL	ASN	GLY	GLY	GLU	VAL	ILE	VAL	SER	SER	LYS	SER	ALA	ASN	ASN	GLY	LEU	LEU	ARG	THR
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[illegible]

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

ASN	SER	ARG	THR	ALA	ASN	GLY	THR	ASP	GLN	GLY	ALA	ASN	ASN	ASN	GLY	ASN	TRP	LEU	CYS	GLY	ALA	GLN	ILE	VAL	PRO	GLY	ASN	TYR	ALA	ASN	PHE	ASP	SER	ARG	THR	VAL	ARG	ASP	VAL	ARG	LEU	GLY	THR	GLN	SER	LEU	THR	GLY	GLY	LEU	SER	ASP	ASP	TYR	LYS	ALA	PRO
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SER	GLY	HIS	VAL	ILE	THR	GLY	PHE	HIS	THR	ASN	GLY	ASP	TRP	GLU	MET	GLN	GLY	GLY	ASP	ASP	LYS	VAL	TYR	ILE	ARG	PRO	VAL	VAL	GLN	LYS	ASN	ILE	ASN	GLY	THR	TRP	TYR	ASN	VAL	ALA	SER	ALA
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- Molecule 10: Tail fiber protein S



M1	I4	V12	F27	S28	E29	G30	ASP	GLY	ASN	N34	V35	I36	F44	E57	I60	D63	K66	M78	L83	L84	I85	K86	N87	N88	L89	S90	E91	I92	K93	T94	A95	G96	A97	Q100	R101	E105	D108	I109	Y110	D111	ALA	SER	LEU	ASN	LYS
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GLY VAL LEU VAL GLN THR SER ALA THR ASP ASP PRO SER GLU THR LEU LEU ALA ALA THR ALA LYS VAL LYS ILE LEU MET ASP ASN ALA ASN ALA ALA ARG ARG ASN GLY GLY LYS ASP ASP PRO ASN LYS PRO LEU PHE ILE GLN ASN LEU LEU GLY LEU GLN GLU THR VAL ASN

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

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

MET	GLN	GLY	GLY	ASP	ASP	LYS	VAL	TYR	TLE	ARG	PRO	VAL	GLN	ASN	LYS	ASN	TLE	ASN	GLY	THR	THR	TYR	ASN	VAL	ALA	SER	ALA
ASN	ASN	ASN	TRP	LEU	CYS	GLY	ALA	GLN	VAL	IIE	PRO	GLY	ASN	TYR	ALA	ASN	PHE	ASP	SER	ARG	VAL	THR	GLY	LEU	THR	GLY	LEU
ASN	GLY	ASN	TRP	LEU	CYS	GLY	ALA	GLN	VAL	IIE	PRO	GLY	ASN	TYR	ALA	ASN	PHE	ASP	SER	ARG	VAL	THR	GLY	LEU	THR	GLY	LEU

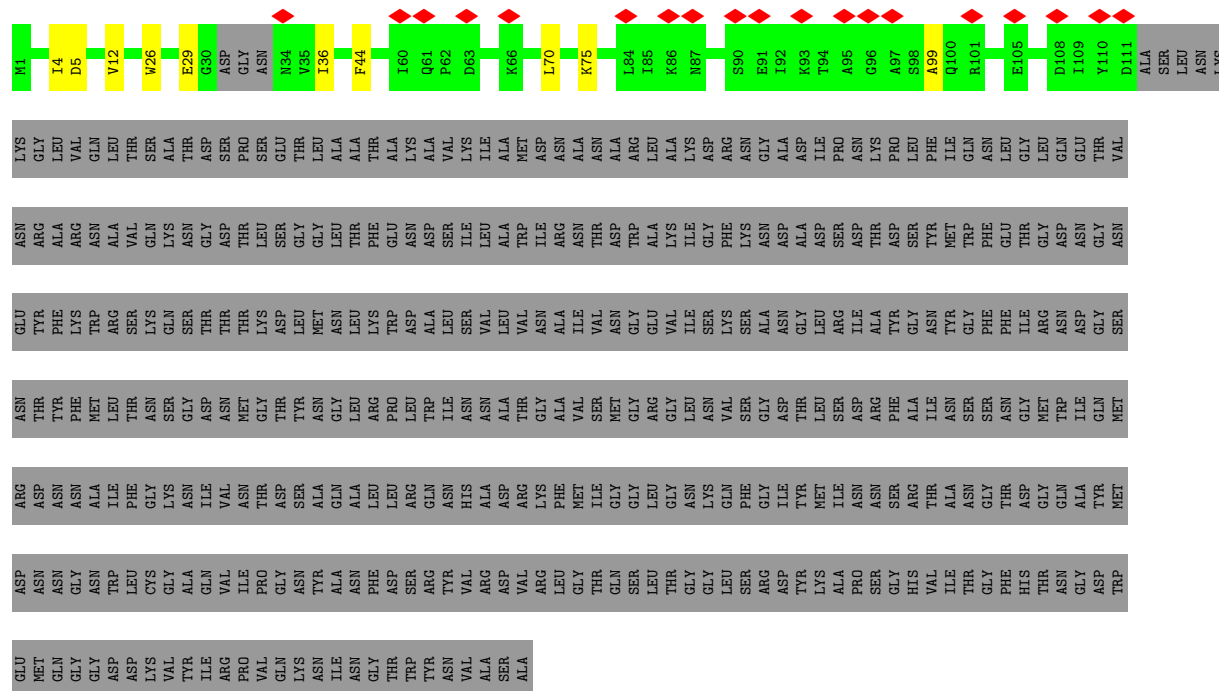
- Molecule 10: Tail fiber protein S

[illegible]

- Molecule 10: Tail fiber protein S

[illegible]

- Molecule 10: Tail fiber protein S



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	46000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	35	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.111	Depositor
Minimum map value	-0.054	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.025	Depositor
Map size ($\text{\AA}$)	408.0, 408.0, 408.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.36, 1.36, 1.36	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0	0.33	0/3340	0.49	0/4545
1	s	0.47	1/3340 (0.0%)	0.65	1/4545 (0.0%)
1	t	0.43	0/3340	0.64	1/4545 (0.0%)
1	u	0.30	0/3164	0.45	0/4300
1	v	0.26	0/3164	0.40	0/4300
1	w	0.23	0/3164	0.39	0/4300
2	1	0.13	0/3793	0.30	0/5166
2	2	0.13	0/3793	0.30	0/5166
2	3	0.20	0/3793	0.35	0/5166
2	x	0.17	0/3793	0.35	0/5166
2	y	0.19	0/3793	0.36	0/5166
2	z	0.22	0/3793	0.38	0/5166
3	4	0.13	0/896	0.37	0/1208
3	5	0.13	0/896	0.34	0/1208
3	6	0.13	0/896	0.36	0/1208
3	7	0.13	0/896	0.33	0/1208
3	8	0.13	0/896	0.33	0/1208
3	9	0.14	0/896	0.36	0/1208
4	A	0.33	0/1162	0.46	0/1582
4	B	0.39	0/1162	0.52	0/1582
4	C	0.25	0/1162	0.38	0/1582
4	D	0.13	0/1162	0.30	0/1582
4	E	0.30	0/1162	0.45	0/1582
4	F	0.24	0/1162	0.37	0/1582
5	G	0.23	0/2876	0.38	0/3895
5	N	0.23	0/2876	0.42	1/3895 (0.0%)
5	U	0.24	0/2876	0.42	0/3895
6	H	0.37	0/2754	0.53	0/3766
6	I	0.34	0/2754	0.50	0/3766
6	J	0.31	0/2754	0.49	1/3766 (0.0%)
6	K	0.27	0/2754	0.44	0/3766
6	L	0.29	0/2754	0.46	0/3766

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	M	0.24	0/2754	0.41	0/3766
6	O	0.23	0/2772	0.37	0/3791
6	P	0.26	0/2772	0.38	0/3791
6	Q	0.23	0/2772	0.36	0/3791
6	R	0.23	0/2668	0.37	0/3644
6	S	0.28	0/2668	0.39	0/3644
6	T	0.31	0/2668	0.44	0/3644
7	V	0.35	0/1506	0.54	1/2037 (0.0%)
7	W	0.37	0/1506	0.53	0/2037
7	X	0.33	0/1506	0.53	0/2037
8	a	0.23	0/1436	0.38	0/1952
8	b	0.14	0/1239	0.34	0/1681
8	c	0.23	0/1436	0.38	0/1952
8	d	0.40	0/1239	0.54	0/1681
8	e	0.24	0/1436	0.40	0/1952
8	f	0.28	0/1239	0.43	0/1681
9	g	0.13	0/133	0.33	0/180
9	h	0.14	0/133	0.28	0/180
9	i	0.14	0/133	0.32	0/180
10	j	0.26	0/849	0.42	0/1153
10	k	0.15	0/849	0.35	0/1153
10	l	0.33	0/849	0.44	0/1153
10	m	0.42	0/849	0.59	0/1153
10	n	0.14	0/849	0.32	0/1153
10	o	0.22	0/849	0.35	0/1153
10	p	0.21	0/849	0.36	0/1153
10	q	0.21	0/849	0.38	0/1153
10	r	0.23	0/849	0.41	1/1153 (0.1%)
All	All	0.27	1/116673 (0.0%)	0.43	6/158784 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	s	251	ASP	N-CA	5.08	1.49	1.46

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	s	290	GLU	N-CA-C	-7.65	104.55	114.04
10	r	5	ASP	N-CA-C	-6.17	105.59	112.57
1	t	272	ALA	N-CA-C	-5.50	106.57	113.28
7	V	105	GLY	CA-C-O	-5.33	116.38	121.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	217	GLY	N-CA-C	5.08	116.34	111.67
6	J	240	PRO	N-CA-C	5.06	118.56	111.33

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	3294	0	3260	61	0
1	s	3294	0	3260	67	0
1	t	3294	0	3260	66	0
1	u	3119	0	3108	48	0
1	v	3119	0	3108	46	0
1	w	3119	0	3108	51	0
2	1	3719	0	3646	51	0
2	2	3719	0	3646	55	0
2	3	3719	0	3646	54	0
2	x	3719	0	3646	72	0
2	y	3719	0	3646	59	0
2	z	3719	0	3646	55	0
3	4	880	0	861	13	0
3	5	880	0	861	17	0
3	6	880	0	861	16	0
3	7	880	0	861	15	0
3	8	880	0	861	20	0
3	9	880	0	861	19	0
4	A	1137	0	1094	18	0
4	B	1137	0	1094	7	0
4	C	1137	0	1094	14	0
4	D	1137	0	1094	14	0
4	E	1137	0	1094	17	0
4	F	1137	0	1094	14	0
5	G	2830	0	2815	60	0
5	N	2830	0	2815	55	0
5	U	2830	0	2815	60	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	H	2694	0	2665	48	0
6	I	2694	0	2665	54	0
6	J	2694	0	2665	53	0
6	K	2694	0	2665	67	0
6	L	2694	0	2665	44	0
6	M	2694	0	2665	52	0
6	O	2712	0	2683	35	0
6	P	2712	0	2683	30	0
6	Q	2712	0	2683	32	0
6	R	2609	0	2578	37	0
6	S	2609	0	2578	33	0
6	T	2609	0	2578	33	0
7	V	1486	0	1479	39	0
7	W	1486	0	1479	36	0
7	X	1486	0	1479	39	0
8	a	1401	0	1363	27	0
8	b	1208	0	1168	25	0
8	c	1401	0	1363	29	0
8	d	1208	0	1168	20	0
8	e	1401	0	1363	28	0
8	f	1208	0	1168	22	0
9	g	130	0	113	4	0
9	h	130	0	113	2	0
9	i	130	0	113	4	0
10	j	836	0	832	15	0
10	k	836	0	832	19	0
10	l	836	0	832	12	0
10	m	836	0	832	19	0
10	n	836	0	832	18	0
10	o	836	0	832	11	0
10	p	836	0	832	20	0
10	q	836	0	832	20	0
10	r	836	0	832	8	0
11	V	1	0	0	0	0
12	V	1	0	0	0	0
All	All	114473	0	112785	1661	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 7.

All (1661) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:286:ILE:HD13	6:K:359:TRP:HZ3	1.31	0.95
6:K:357:ILE:HG13	6:K:359:TRP:CE2	2.06	0.91
6:K:357:ILE:HG13	6:K:359:TRP:CZ2	2.08	0.88
1:0:182:ALA:HB2	6:S:309:ASN:HD21	1.38	0.86
6:T:309:ASN:HD21	1:s:182:ALA:HB2	1.41	0.85
3:8:95:ALA:HB3	3:8:108:VAL:HG13	1.60	0.83
3:6:95:ALA:HB3	3:6:108:VAL:HG13	1.60	0.83
3:4:95:ALA:HB3	3:4:108:VAL:HG13	1.60	0.83
1:0:319:ALA:HB2	1:0:383:THR:HG21	1.62	0.82
6:K:357:ILE:HG13	6:K:359:TRP:CH2	2.14	0.82
6:L:211:VAL:HA	6:L:232:MET:HG2	1.63	0.81
6:L:233:ASP:HA	6:L:238:ILE:HG23	1.62	0.81
3:5:95:ALA:HB3	3:5:108:VAL:HG13	1.62	0.81
6:R:309:ASN:HD21	1:t:182:ALA:HB2	1.44	0.80
5:G:186:VAL:HG12	5:G:301:ASP:HB3	1.60	0.80
6:J:232:MET:HE1	6:J:244:ASP:HB3	1.64	0.80
5:N:277:PHE:HB3	5:N:333:LEU:HB2	1.62	0.80
10:j:79:SER:HA	10:j:84:LEU:HD11	1.64	0.80
2:z:171:HIS:ND1	2:z:171:HIS:O	2.15	0.79
6:K:357:ILE:HG13	6:K:359:TRP:CD2	2.17	0.79
7:X:17:MET:HG2	9:g:690:TRP:HA	1.65	0.78
5:G:73:ARG:HH21	5:U:307:ILE:HG12	1.49	0.77
6:K:286:ILE:CD1	6:K:359:TRP:HZ3	1.98	0.77
10:p:79:SER:HA	10:p:84:LEU:HD21	1.67	0.77
3:9:95:ALA:HB3	3:9:108:VAL:HG13	1.66	0.76
1:w:328:ASN:HA	1:w:467:ARG:HG3	1.68	0.76
6:M:299:ILE:HD11	6:M:326:VAL:HG23	1.67	0.76
6:J:239:PHE:HE1	6:J:351:LEU:HD23	1.50	0.75
1:w:162:VAL:HG11	1:w:306:THR:HG21	1.67	0.75
4:D:82:PRO:HA	4:D:85:LEU:HD12	1.67	0.75
2:x:40:MET:HE1	2:x:77:MET:HB3	1.67	0.75
6:K:286:ILE:HD13	6:K:359:TRP:CZ3	2.21	0.75
5:G:5:VAL:HG12	5:G:58:ILE:HG12	1.67	0.74
6:T:265:GLY:H	8:a:97:ASN:HD22	1.36	0.74
1:t:269:ARG:O	1:t:271:ALA:N	2.21	0.74
6:K:357:ILE:HG13	6:K:359:TRP:CZ3	2.23	0.74
7:X:3:ARG:N	9:h:676:MET:SD	2.61	0.74
6:H:232:MET:HE1	6:H:244:ASP:HB3	1.67	0.74
6:L:332:LEU:HD11	6:L:335:PHE:HB3	1.69	0.74
4:A:82:PRO:HA	4:A:85:LEU:HD12	1.70	0.74
6:S:95:THR:HB	6:S:159:VAL:HG23	1.70	0.74
6:R:264:VAL:HB	8:c:97:ASN:HD22	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:V:3:ARG:N	9:i:676:MET:SD	2.61	0.73
6:Q:200:ASP:OD1	6:Q:203:ARG:NH2	2.22	0.73
1:0:181:THR:OG1	1:0:182:ALA:N	2.21	0.73
6:T:95:THR:HB	6:T:159:VAL:HG23	1.69	0.73
4:A:5:ALA:HB2	4:A:25:ASP:HB2	1.69	0.73
1:s:181:THR:OG1	1:s:182:ALA:N	2.21	0.73
4:F:82:PRO:HA	4:F:85:LEU:HD12	1.69	0.73
10:l:29:GLU:HA	10:l:36:ILE:HG23	1.71	0.73
5:N:5:VAL:HG12	5:N:58:ILE:HG12	1.72	0.72
6:O:200:ASP:OD1	6:O:203:ARG:NH2	2.22	0.72
7:W:17:MET:HG2	9:i:690:TRP:HA	1.71	0.72
6:P:200:ASP:OD1	6:P:203:ARG:NH2	2.22	0.72
8:b:94:MET:HE2	8:b:106:LEU:HD11	1.71	0.72
1:t:181:THR:OG1	1:t:182:ALA:N	2.21	0.72
1:t:195:ILE:HG21	1:t:222:LYS:HB2	1.71	0.72
5:N:186:VAL:HG12	5:N:301:ASP:HB3	1.69	0.72
2:1:123:ILE:HA	2:1:189:VAL:HG12	1.71	0.72
6:H:156:VAL:O	7:V:42:GLN:NE2	2.23	0.72
8:a:66:GLU:HG2	8:a:71:LEU:HD23	1.70	0.71
4:E:77:ARG:HG2	2:z:321:ARG:HE	1.55	0.71
5:N:73:ARG:HG2	5:N:82:ILE:HG23	1.72	0.71
1:0:195:ILE:HG21	1:0:222:LYS:HB2	1.71	0.71
6:K:357:ILE:HG13	6:K:359:TRP:CE3	2.26	0.71
5:U:5:VAL:HG12	5:U:58:ILE:HG12	1.72	0.71
6:J:156:VAL:O	7:X:42:GLN:NE2	2.23	0.71
6:O:91:LEU:HD22	6:O:163:ALA:HB1	1.71	0.71
3:7:95:ALA:HB3	3:7:108:VAL:HG13	1.71	0.71
8:e:94:MET:HE2	8:e:106:LEU:HD11	1.73	0.71
1:t:316:LEU:HD22	1:t:434:LEU:HD13	1.73	0.71
4:E:82:PRO:HA	4:E:85:LEU:HD12	1.73	0.70
2:2:40:MET:HE2	2:2:90:LEU:HD21	1.71	0.70
5:U:37:VAL:HG23	1:t:145:PRO:HD3	1.72	0.70
5:U:186:VAL:HG12	5:U:301:ASP:HB3	1.72	0.70
6:K:284:PRO:HD2	6:K:357:ILE:HA	1.73	0.70
6:M:332:LEU:HD11	6:M:335:PHE:HB3	1.74	0.70
1:s:362:LEU:O	1:s:363:THR:C	2.34	0.70
6:M:22:ARG:NH1	8:f:33:GLN:OE1	2.24	0.70
2:1:349:LEU:HD23	2:y:14:ARG:HB2	1.74	0.70
4:C:82:PRO:HA	4:C:85:LEU:HD12	1.73	0.69
7:V:55:GLU:OE2	7:W:26:ARG:NH2	2.24	0.69
7:W:3:ARG:N	9:g:676:MET:SD	2.65	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:195:ILE:HD11	1:0:221:MET:HE1	1.75	0.69
6:K:233:ASP:HA	6:K:238:ILE:HG22	1.74	0.69
7:W:117:THR:HG22	7:W:121:ARG:HB2	1.75	0.69
5:G:24:ARG:NH2	5:G:88:ASP:OD2	2.26	0.69
6:S:285:ARG:HG2	6:S:358:GLU:HB2	1.74	0.69
6:P:294:GLU:OE1	6:P:294:GLU:N	2.26	0.68
6:I:357:ILE:HG22	6:I:359:TRP:H	1.58	0.68
2:2:25:SER:OG	2:y:492:GLN:NE2	2.24	0.68
6:S:93:VAL:H	6:S:130:GLU:HG3	1.57	0.68
7:V:26:ARG:NH2	7:X:55:GLU:OE2	2.26	0.68
6:O:109:ARG:HH11	6:O:144:THR:HG22	1.57	0.68
6:S:265:GLY:H	8:e:97:ASN:HD22	1.42	0.68
1:0:317:THR:OG1	1:0:437:ARG:NH2	2.26	0.68
6:I:156:VAL:O	7:W:42:GLN:NE2	2.27	0.68
1:s:317:THR:OG1	1:s:437:ARG:NH2	2.27	0.68
2:3:123:ILE:HA	2:3:189:VAL:HG12	1.76	0.67
5:U:73:ARG:HG2	5:U:82:ILE:HG23	1.75	0.67
5:G:272:ALA:HB2	5:G:338:GLY:HA3	1.76	0.67
6:I:88:SER:HB2	6:I:134:THR:HG22	1.76	0.67
6:O:294:GLU:OE2	6:O:294:GLU:N	2.25	0.67
6:Q:109:ARG:HH11	6:Q:144:THR:HG22	1.59	0.67
6:R:95:THR:HB	6:R:159:VAL:HG23	1.74	0.67
2:3:251:LEU:HD23	2:3:287:LEU:HB3	1.76	0.67
6:S:86:ALA:HA	6:S:138:ALA:HA	1.77	0.67
1:w:152:SER:OG	1:w:437:ARG:NH2	2.28	0.67
2:2:14:ARG:O	2:y:368:ARG:NH1	2.28	0.67
10:r:29:GLU:HA	10:r:36:ILE:HG23	1.76	0.67
6:T:86:ALA:HA	6:T:138:ALA:HA	1.77	0.66
1:w:41:GLN:HG2	1:w:70:ARG:HB3	1.76	0.66
6:K:22:ARG:NH1	8:b:33:GLN:OE1	2.28	0.66
6:T:265:GLY:O	8:a:97:ASN:ND2	2.29	0.66
1:t:317:THR:OG1	1:t:437:ARG:NH2	2.28	0.66
6:O:91:LEU:HD21	6:O:150:LEU:HD12	1.78	0.66
8:b:100:ARG:O	8:b:104:GLU:HG3	1.96	0.66
6:I:153:ILE:HG22	6:I:154:THR:HG23	1.78	0.66
2:y:171:HIS:O	2:y:171:HIS:ND1	2.27	0.66
2:x:299:PRO:HG2	2:x:302:LEU:HD23	1.78	0.66
6:I:285:ARG:HD3	6:I:339:PHE:HB2	1.78	0.66
6:O:323:ILE:HG12	6:O:337:VAL:HG21	1.78	0.66
4:A:27:SER:HB3	4:A:135:PRO:HA	1.78	0.65
6:S:294:GLU:N	6:S:294:GLU:OE2	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:j:20:ARG:NH1	10:k:5:ASP:O	2.28	0.65
1:u:152:SER:OG	1:u:437:ARG:NH2	2.29	0.65
5:G:107:ASN:HB3	6:J:108:GLN:HE22	1.61	0.65
6:O:95:THR:HG22	6:O:159:VAL:HG22	1.79	0.65
6:P:95:THR:HG22	6:P:159:VAL:HG22	1.79	0.65
6:T:285:ARG:HG2	6:T:358:GLU:HB2	1.78	0.65
1:u:173:VAL:HG11	1:u:295:THR:HG21	1.78	0.65
6:L:22:ARG:NH1	8:d:33:GLN:OE1	2.30	0.64
10:p:20:ARG:NH1	10:q:5:ASP:O	2.29	0.64
1:u:253:ARG:HH22	1:u:322:PHE:HE2	1.44	0.64
1:v:253:ARG:HH22	1:v:322:PHE:HE2	1.44	0.64
2:3:39:LEU:HD11	2:3:93:ILE:HG13	1.80	0.64
6:J:153:ILE:HG22	6:J:154:THR:HG23	1.80	0.64
6:K:82:LYS:HZ1	6:K:184:ARG:HH22	1.45	0.64
2:z:139:ALA:HB2	2:z:170:THR:HG21	1.80	0.64
4:A:17:GLN:HA	4:A:22:MET:HA	1.78	0.64
5:G:72:ARG:NH2	5:U:195:ASP:OD2	2.30	0.64
10:q:57:GLU:OE2	10:r:75:LYS:NZ	2.30	0.64
6:S:75:ARG:NH2	2:z:116:ASN:OD1	2.30	0.64
5:U:24:ARG:NH2	5:U:88:ASP:OD2	2.31	0.64
10:k:63:ASP:OD1	10:k:64:LYS:N	2.31	0.64
1:v:331:ARG:H	1:v:467:ARG:HH21	1.46	0.64
6:P:91:LEU:HD22	6:P:163:ALA:HB1	1.80	0.64
1:t:390:VAL:HG22	1:t:475:ARG:HH21	1.62	0.64
6:K:319:PRO:HA	6:K:322:ILE:HD12	1.80	0.64
1:t:273:THR:OG1	1:t:274:ALA:N	2.31	0.64
5:G:277:PHE:HB3	5:G:333:LEU:HB2	1.79	0.64
7:V:151:GLU:OE1	7:W:143:ARG:NH1	2.31	0.64
1:u:162:VAL:HG11	1:u:306:THR:HG21	1.80	0.64
2:x:236:MET:HE2	2:x:247:LEU:HD22	1.79	0.64
5:U:296:LEU:H	5:U:314:VAL:HG22	1.63	0.63
6:H:153:ILE:HG22	6:H:154:THR:HG23	1.80	0.63
2:3:346:ASN:HD21	2:x:13:VAL:HA	1.64	0.63
5:N:27:GLU:OE1	5:N:269:ARG:NH2	2.32	0.63
5:U:147:GLU:OE2	7:W:19:ARG:NH2	2.31	0.63
2:2:240:ASP:HB3	2:2:243:ASN:HB2	1.79	0.63
5:N:195:ASP:OD2	5:U:72:ARG:NH2	2.32	0.63
8:c:144:ASN:OD1	8:c:145:VAL:N	2.31	0.63
1:s:121:ARG:NH2	1:s:133:THR:OG1	2.31	0.63
2:2:349:LEU:HD21	2:2:368:ARG:HD3	1.81	0.63
3:6:89:LEU:HD12	3:6:111:ALA:HB3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Q:95:THR:HG22	6:Q:159:VAL:HG22	1.80	0.63
1:w:478:ILE:HD13	1:w:484:VAL:HG22	1.81	0.63
2:1:490:GLN:NE2	2:y:21:GLU:OE2	2.32	0.63
10:p:108:ASP:OD2	10:q:104:ARG:NH1	2.32	0.63
3:5:53:LYS:HB2	3:5:110:MET:HG2	1.79	0.63
5:G:73:ARG:HG2	5:G:82:ILE:HG23	1.80	0.63
6:T:280:LYS:NZ	6:T:345:ARG:O	2.31	0.63
5:G:195:ASP:OD2	5:N:72:ARG:NH2	2.31	0.63
2:x:433:ILE:HD13	2:x:472:LEU:HD13	1.80	0.63
2:3:240:ASP:HB3	2:3:243:ASN:HB2	1.82	0.62
5:G:100:TYR:HE2	6:J:154:THR:HG21	1.64	0.62
5:G:147:GLU:OE2	7:X:19:ARG:NH2	2.32	0.62
1:v:152:SER:OG	1:v:437:ARG:NH2	2.32	0.62
2:1:14:ARG:O	2:x:368:ARG:NH1	2.33	0.62
2:1:240:ASP:HB3	2:1:243:ASN:HB2	1.79	0.62
6:M:232:MET:O	6:M:238:ILE:HA	1.99	0.62
1:s:316:LEU:HD22	1:s:434:LEU:HD23	1.82	0.62
6:I:81:ARG:HG3	6:I:181:LEU:HD11	1.82	0.62
2:3:266:VAL:HG21	2:3:308:CYS:HB2	1.82	0.62
8:d:52:GLU:OE2	8:d:60:TRP:N	2.26	0.62
6:R:75:ARG:NH2	2:y:116:ASN:OD1	2.32	0.62
2:2:39:LEU:HD11	2:2:93:ILE:HG13	1.81	0.62
6:M:319:PRO:HA	6:M:322:ILE:HD12	1.82	0.62
5:N:24:ARG:NH2	5:N:88:ASP:OD2	2.33	0.62
1:0:285:ASN:HD22	6:S:301:ASN:HB3	1.65	0.62
6:Q:91:LEU:HD22	6:Q:163:ALA:HB1	1.81	0.62
5:U:27:GLU:OE1	5:U:269:ARG:NH2	2.33	0.62
5:G:183:ASP:HB2	5:G:298:VAL:HG12	1.80	0.61
1:v:331:ARG:H	1:v:467:ARG:NH2	1.97	0.61
2:x:295:GLY:HA3	2:x:334:PRO:HB3	1.82	0.61
2:3:438:LEU:HD13	3:9:117:ILE:HD12	1.83	0.61
6:L:319:PRO:HA	6:L:322:ILE:HD12	1.81	0.61
1:v:162:VAL:HG11	1:v:306:THR:HG21	1.82	0.61
1:v:251:ASP:OD1	1:v:252:THR:N	2.30	0.61
2:2:438:LEU:HD13	3:7:117:ILE:HD12	1.82	0.61
6:O:212:THR:HG22	6:O:232:MET:HA	1.81	0.61
5:N:272:ALA:HB2	5:N:338:GLY:HA3	1.81	0.61
10:k:57:GLU:OE2	10:l:75:LYS:NZ	2.33	0.61
6:S:80:ARG:O	6:S:184:ARG:NH2	2.32	0.61
2:x:171:HIS:O	2:x:171:HIS:ND1	2.32	0.61
2:2:236:MET:HB3	2:2:267:THR:HG22	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:27:GLU:OE1	5:G:269:ARG:NH2	2.33	0.61
6:S:265:GLY:O	8:e:97:ASN:ND2	2.33	0.61
2:1:109:LEU:HG	2:1:205:THR:HG22	1.82	0.61
1:s:390:VAL:HG22	1:s:475:ARG:HH21	1.66	0.61
6:R:80:ARG:O	6:R:184:ARG:NH2	2.34	0.61
2:z:299:PRO:HG2	2:z:302:LEU:HD23	1.82	0.61
2:1:39:LEU:HD11	2:1:93:ILE:HG13	1.83	0.61
6:P:152:LEU:HD12	6:P:161:SER:HA	1.83	0.61
1:s:384:PRO:HG2	1:s:387:PHE:HB2	1.83	0.61
2:2:123:ILE:HA	2:2:189:VAL:HG12	1.82	0.60
2:3:23:ASP:OD2	2:z:490:GLN:NE2	2.32	0.60
6:J:22:ARG:NH1	8:e:33:GLN:OE1	2.34	0.60
6:L:194:PHE:HB2	6:L:197:ASN:HB2	1.83	0.60
5:U:203:ARG:NH2	5:U:237:ASP:OD2	2.33	0.60
2:1:266:VAL:HG21	2:1:308:CYS:HB2	1.83	0.60
4:C:27:SER:HB3	4:C:135:PRO:HA	1.83	0.60
6:M:194:PHE:HB2	6:M:197:ASN:HB2	1.84	0.60
8:c:175:TYR:O	8:c:176:HIS:ND1	2.31	0.60
10:q:63:ASP:OD1	10:q:64:LYS:N	2.34	0.60
2:y:286:HIS:HB3	2:y:373:TYR:HB2	1.83	0.60
5:U:76:THR:HG23	5:U:79:SER:H	1.67	0.60
1:t:188:MET:HE2	1:t:226:THR:HA	1.84	0.60
2:y:299:PRO:HG2	2:y:302:LEU:HD23	1.83	0.60
5:G:293:MET:HE3	5:G:294:PRO:HD2	1.83	0.60
6:K:194:PHE:HB2	6:K:197:ASN:HB2	1.83	0.60
8:c:98:LEU:HD23	8:c:166:PRO:HB3	1.84	0.60
10:q:50:GLU:O	10:q:54:THR:HG23	2.02	0.60
5:G:369:ARG:NH2	1:w:307:TYR:OH	2.34	0.60
6:K:357:ILE:CG1	6:K:359:TRP:CD2	2.85	0.60
6:Q:212:THR:HG22	6:Q:232:MET:HA	1.83	0.60
2:y:464:ARG:HA	2:y:472:LEU:HD23	1.83	0.60
4:E:27:SER:HB3	4:E:135:PRO:HA	1.83	0.59
6:J:101:ILE:HG22	6:J:105:THR:HG21	1.84	0.59
7:X:158:VAL:HG12	7:X:160:GLY:H	1.67	0.59
2:x:348:LEU:HD23	2:x:355:THR:HG22	1.84	0.59
6:H:22:ARG:NH1	8:a:33:GLN:OE1	2.34	0.59
1:t:269:ARG:C	1:t:271:ALA:H	2.10	0.59
2:z:295:GLY:HA3	2:z:334:PRO:HB3	1.84	0.59
6:H:154:THR:HG21	5:N:100:TYR:HE2	1.67	0.59
7:V:143:ARG:NH1	7:X:151:GLU:OE1	2.35	0.59
1:0:162:VAL:HG22	1:0:422:GLN:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:46:ARG:HH21	1:v:51:GLU:HB3	1.67	0.59
6:J:297:GLN:NE2	6:J:301:ASN:OD1	2.34	0.59
8:c:144:ASN:HB3	8:c:147:THR:HG23	1.84	0.59
8:c:94:MET:HE2	8:c:106:LEU:HD11	1.84	0.59
2:x:190:ARG:HD2	2:x:297:PRO:HB3	1.83	0.59
6:M:280:LYS:NZ	6:M:345:ARG:O	2.36	0.59
2:1:236:MET:HE2	2:1:247:LEU:HD22	1.85	0.59
4:C:76:SER:O	2:y:324:GLN:NE2	2.35	0.59
6:J:286:ILE:HD12	6:J:357:ILE:HG23	1.85	0.59
6:K:357:ILE:CG1	6:K:359:TRP:CE2	2.85	0.58
1:t:46:ARG:HH21	1:u:51:GLU:HB3	1.68	0.58
6:J:239:PHE:CE1	6:J:351:LEU:HD23	2.35	0.58
6:K:233:ASP:C	6:K:235:ARG:H	2.11	0.58
6:J:161:SER:OG	7:X:52:ASP:OD2	2.20	0.58
6:R:146:GLU:HG2	6:R:168:GLY:H	1.69	0.58
1:s:433:ASP:OD1	1:s:437:ARG:NH1	2.35	0.58
2:z:239:THR:HG21	2:z:269:LEU:HD13	1.85	0.58
6:H:239:PHE:CE1	6:H:351:LEU:HD23	2.39	0.58
5:N:296:LEU:H	5:N:314:VAL:HG22	1.68	0.58
6:O:296:LYS:HG2	6:O:360:LEU:HB2	1.85	0.58
6:P:269:GLY:HA2	8:d:169:GLN:HE21	1.68	0.58
1:w:187:VAL:HA	1:w:293:ILE:HD11	1.85	0.58
1:0:145:PRO:HB2	5:G:14:PHE:HD2	1.68	0.58
2:1:423:THR:HG23	3:5:63:PRO:HG2	1.86	0.58
5:G:296:LEU:H	5:G:314:VAL:HG22	1.68	0.58
6:K:232:MET:O	6:K:238:ILE:HA	2.04	0.58
6:Q:296:LYS:HG2	6:Q:360:LEU:HB2	1.85	0.58
6:T:75:ARG:NH2	2:x:116:ASN:OD1	2.36	0.58
10:m:20:ARG:NH1	10:n:5:ASP:O	2.31	0.58
3:4:69:ILE:HD13	3:4:107:LEU:HD11	1.85	0.58
5:G:26:ILE:HG23	5:G:294:PRO:HB2	1.86	0.58
5:U:272:ALA:HB2	5:U:338:GLY:HA3	1.84	0.58
1:0:118:TRP:NE1	1:v:43:GLY:O	2.37	0.58
6:J:288:ILE:HD11	6:J:359:TRP:CZ3	2.38	0.58
5:N:5:VAL:HG23	5:N:17:TRP:HD1	1.67	0.58
8:e:66:GLU:HG2	8:e:71:LEU:HD23	1.84	0.58
2:1:490:GLN:OE1	4:B:121:TYR:OH	2.20	0.58
6:L:280:LYS:NZ	6:L:345:ARG:O	2.37	0.58
3:8:117:ILE:HD12	2:z:438:LEU:HD13	1.86	0.57
5:G:5:VAL:HG23	5:G:17:TRP:HD1	1.68	0.57
1:u:123:LYS:O	1:u:125:ASP:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:e:144:ASN:HB3	8:e:147:THR:HG23	1.84	0.57
2:2:423:THR:HG23	3:7:63:PRO:HG2	1.85	0.57
6:L:285:ARG:HE	6:L:339:PHE:HD2	1.51	0.57
6:T:80:ARG:O	6:T:184:ARG:NH2	2.37	0.57
5:U:5:VAL:HG23	5:U:17:TRP:HD1	1.68	0.57
1:v:41:GLN:HG2	1:v:70:ARG:HB3	1.86	0.57
2:3:423:THR:HG23	3:9:63:PRO:HG2	1.86	0.57
4:E:2:THR:O	4:E:2:THR:OG1	2.23	0.57
6:P:296:LYS:HG2	6:P:360:LEU:HB2	1.85	0.57
6:R:208:VAL:HG21	6:R:248:VAL:HG22	1.86	0.57
5:U:38:ASN:HD22	1:u:50:ARG:HD2	1.69	0.57
3:6:69:ILE:HD13	3:6:107:LEU:HD11	1.84	0.57
2:1:40:MET:HG2	2:1:235:VAL:HB	1.86	0.57
3:5:22:MET:HE3	3:5:59:PRO:HB3	1.87	0.57
6:I:145:GLY:O	6:I:168:GLY:HA3	2.04	0.57
2:x:139:ALA:H	2:x:170:THR:HG21	1.70	0.57
6:H:156:VAL:HG12	6:H:157:ALA:H	1.68	0.57
10:l:89:LEU:O	10:l:93:LYS:HD2	2.05	0.57
6:I:156:VAL:HG12	6:I:157:ALA:H	1.70	0.57
6:Q:91:LEU:HD21	6:Q:150:LEU:HD12	1.87	0.57
6:T:301:ASN:HB3	1:s:285:ASN:HD21	1.68	0.57
7:W:55:GLU:OE2	7:X:26:ARG:NH2	2.38	0.57
10:m:79:SER:HA	10:m:84:LEU:HD21	1.85	0.57
1:t:331:ARG:HG2	1:t:332:ALA:H	1.69	0.57
5:U:39:VAL:HB	5:U:43:THR:HG21	1.85	0.57
6:K:228:VAL:HG13	6:K:274:VAL:HG13	1.87	0.57
1:0:285:ASN:ND2	6:S:301:ASN:HB3	2.20	0.56
4:F:26:ASP:OD1	4:F:26:ASP:N	2.38	0.56
6:H:152:LEU:HD21	6:H:156:VAL:HG23	1.87	0.56
6:L:288:ILE:HG22	6:L:290:PRO:HD2	1.85	0.56
6:M:289:SER:OG	6:M:290:PRO:HD3	2.04	0.56
7:V:158:VAL:HG12	7:V:160:GLY:H	1.70	0.56
1:s:162:VAL:HG22	1:s:422:GLN:HB3	1.87	0.56
2:x:9:ILE:HD12	2:x:17:LEU:HD23	1.85	0.56
2:1:23:ASP:OD2	2:x:490:GLN:NE2	2.36	0.56
2:3:291:MET:HE1	2:3:366:ILE:HG22	1.88	0.56
5:N:14:PHE:HD2	1:s:145:PRO:HB2	1.70	0.56
6:T:187:TYR:OH	1:s:265:ARG:NH1	2.38	0.56
10:o:29:GLU:HA	10:o:36:ILE:HG23	1.85	0.56
1:s:471:ARG:HH12	1:s:493:ILE:HG21	1.71	0.56
2:y:295:GLY:HA3	2:y:334:PRO:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:323:LEU:HD12	2:2:369:MET:HG3	1.88	0.56
6:P:213:ARG:HB2	6:P:231:VAL:HG12	1.88	0.56
6:R:166:VAL:HG23	6:R:167:LYS:HG3	1.88	0.56
2:x:43:GLN:H	2:x:73:MET:HE2	1.70	0.56
2:z:286:HIS:HB3	2:z:373:TYR:HB2	1.85	0.56
4:C:2:THR:O	4:C:2:THR:OG1	2.22	0.56
6:O:174:ASP:OD1	6:O:174:ASP:N	2.38	0.56
1:w:173:VAL:HG11	1:w:295:THR:HG21	1.88	0.56
2:z:74:LEU:HD21	2:z:92:CYS:HB3	1.88	0.56
4:C:123:TYR:OH	2:y:492:GLN:OE1	2.20	0.56
2:1:40:MET:HE1	2:1:78:ALA:HA	1.87	0.56
4:D:26:ASP:OD1	4:D:26:ASP:N	2.39	0.56
6:T:146:GLU:HG2	6:T:168:GLY:H	1.70	0.56
2:3:193:TYR:OH	2:3:333:PRO:O	2.24	0.56
4:A:107:ALA:N	4:A:127:THR:OG1	2.39	0.56
5:G:48:LEU:O	5:G:71:ARG:NH1	2.39	0.56
5:G:313:LEU:HD23	5:G:339:PHE:HD2	1.70	0.56
6:T:289:SER:OG	6:T:290:PRO:HD3	2.06	0.56
8:e:175:TYR:O	8:e:176:HIS:ND1	2.39	0.56
1:s:116:ASP:HB3	1:s:135:THR:HG23	1.87	0.56
1:s:118:TRP:NE1	1:w:43:GLY:O	2.39	0.56
2:z:399:TYR:O	2:z:403:THR:HG22	2.05	0.56
6:H:109:ARG:HE	6:H:111:ASP:HB3	1.71	0.56
6:I:22:ARG:HG3	8:c:34:ALA:HB2	1.86	0.56
6:J:306:MET:SD	6:J:321:ARG:HB3	2.46	0.56
3:8:69:ILE:HD13	3:8:107:LEU:HD11	1.88	0.55
6:P:91:LEU:HD21	6:P:150:LEU:HD12	1.88	0.55
7:V:71:GLU:OE2	7:V:92:ARG:NE	2.37	0.55
2:y:9:ILE:HD12	2:y:17:LEU:HD23	1.88	0.55
1:0:390:VAL:HG22	1:0:475:ARG:HH21	1.70	0.55
2:1:244:LEU:HB3	2:1:283:ARG:HH12	1.70	0.55
3:4:117:ILE:HD12	2:x:438:LEU:HD13	1.87	0.55
6:K:53:ILE:HG13	6:O:53:ILE:HD13	1.89	0.55
2:2:303:TYR:OH	2:2:332:MET:O	2.23	0.55
6:H:177:SER:OG	6:H:180:GLU:OE1	2.21	0.55
10:m:14:PRO:HB2	10:m:41:MET:HE1	1.88	0.55
1:v:459:LEU:HB2	1:v:472:LEU:HD13	1.88	0.55
6:K:288:ILE:HG22	6:K:290:PRO:HD2	1.86	0.55
1:v:116:ASP:HB3	1:v:135:THR:HG23	1.87	0.55
3:4:77:VAL:HB	3:4:89:LEU:HB2	1.89	0.55
2:1:371:THR:OG1	2:1:386:LEU:O	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:285:ARG:HE	6:K:339:PHE:HD2	1.54	0.55
8:d:66:GLU:HG2	8:d:71:LEU:HD23	1.88	0.55
2:y:40:MET:HE3	2:y:90:LEU:HD21	1.89	0.55
6:H:61:ILE:HD13	8:a:64:GLU:HB3	1.87	0.55
6:L:53:ILE:HG13	6:P:53:ILE:HD13	1.88	0.55
6:Q:329:VAL:HG12	6:Q:331:GLY:H	1.71	0.55
6:S:296:LYS:HG2	6:S:360:LEU:HB2	1.88	0.55
1:v:303:ALA:O	1:v:307:TYR:HD1	1.90	0.55
6:H:195:GLY:N	6:H:200:ASP:OD2	2.40	0.55
1:w:88:ALA:O	1:w:92:MET:HG2	2.06	0.55
6:H:101:ILE:HG22	6:H:105:THR:HG21	1.89	0.55
5:G:203:ARG:NH1	5:G:239:ASP:OD2	2.40	0.54
8:a:98:LEU:HD23	8:a:166:PRO:HB3	1.88	0.54
1:v:174:TRP:HB3	1:v:232:PRO:HB3	1.87	0.54
2:1:106:GLU:HG2	2:1:175:VAL:HG12	1.89	0.54
4:A:2:THR:O	4:A:2:THR:OG1	2.23	0.54
6:H:332:LEU:HD11	6:H:335:PHE:HB3	1.88	0.54
6:T:28:PRO:HD2	6:T:31:ARG:HG2	1.88	0.54
8:b:66:GLU:HG2	8:b:71:LEU:HD23	1.89	0.54
8:d:94:MET:HE1	8:d:106:LEU:HD11	1.89	0.54
1:u:432:ALA:O	1:u:436:LYS:HG2	2.07	0.54
1:w:331:ARG:HH12	1:w:467:ARG:CZ	2.20	0.54
2:x:366:ILE:HG12	2:x:366:ILE:O	2.08	0.54
2:y:139:ALA:H	2:y:170:THR:HG21	1.72	0.54
2:2:490:GLN:OE1	4:D:121:TYR:OH	2.24	0.54
3:8:22:MET:HG3	3:8:59:PRO:HD3	1.88	0.54
4:A:76:SER:O	2:x:324:GLN:NE2	2.40	0.54
4:D:52:SER:OG	4:D:53:ASP:N	2.40	0.54
6:J:195:GLY:N	6:J:200:ASP:OD2	2.40	0.54
6:M:233:ASP:HA	6:M:238:ILE:HG23	1.90	0.54
6:P:109:ARG:HH11	6:P:144:THR:HG22	1.72	0.54
5:U:15:THR:OG1	1:t:148:GLU:OE2	2.24	0.54
5:U:268:ARG:NH1	5:U:341:VAL:O	2.40	0.54
10:q:27:PHE:CZ	10:r:4:ILE:HD11	2.43	0.54
1:s:195:ILE:HG21	1:s:222:LYS:HB2	1.88	0.54
1:u:170:LEU:HD22	1:u:236:ALA:HB2	1.89	0.54
1:0:341:THR:HA	6:S:7:THR:HG23	1.90	0.54
6:K:286:ILE:CD1	6:K:359:TRP:CZ3	2.84	0.54
6:K:306:MET:HG3	6:K:325:ALA:HB2	1.90	0.54
1:u:41:GLN:HG2	1:u:70:ARG:HB3	1.88	0.54
2:x:106:GLU:HG2	2:x:175:VAL:HG22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:4:SER:O	6:J:4:SER:OG	2.26	0.54
6:L:322:ILE:O	6:L:326:VAL:HG12	2.08	0.54
2:y:239:THR:HG21	2:y:269:LEU:HD13	1.89	0.54
2:3:349:LEU:HD23	2:x:14:ARG:HB2	1.90	0.54
1:t:151:THR:HG22	1:t:433:ASP:HB2	1.90	0.54
6:O:269:GLY:HA2	8:b:169:GLN:HE21	1.72	0.54
5:U:223:ILE:HG12	5:U:228:ILE:HG13	1.90	0.54
1:v:320:LEU:HD12	1:v:437:ARG:HD2	1.90	0.54
2:z:46:SER:O	2:z:47:LYS:HG2	2.08	0.54
1:u:116:ASP:HB3	1:u:135:THR:HG23	1.90	0.54
2:x:41:PHE:HD1	2:x:95:GLN:HE22	1.56	0.54
6:H:288:ILE:HG22	6:H:290:PRO:HD2	1.88	0.54
6:I:267:PRO:HA	6:R:196:GLY:O	2.08	0.54
6:K:289:SER:OG	6:K:290:PRO:HD3	2.07	0.54
5:N:257:LYS:HA	5:N:260:GLN:HE21	1.72	0.54
2:x:46:SER:O	2:x:47:LYS:HG2	2.08	0.54
2:y:46:SER:O	2:y:47:LYS:HG2	2.08	0.54
2:3:490:GLN:OE1	4:F:121:TYR:OH	2.25	0.54
6:M:53:ILE:HG13	6:Q:53:ILE:HD13	1.89	0.54
1:t:162:VAL:HG22	1:t:422:GLN:HB3	1.90	0.54
2:2:285:ASP:OD1	2:2:288:ILE:HG22	2.08	0.53
2:2:366:ILE:HD11	2:2:369:MET:HG2	1.89	0.53
6:I:61:ILE:HD13	8:c:64:GLU:HB3	1.90	0.53
6:K:218:PRO:HA	6:K:226:VAL:HG12	1.89	0.53
7:V:72:ALA:HB2	7:V:89:VAL:HG12	1.90	0.53
2:z:9:ILE:HD12	2:z:17:LEU:HD23	1.89	0.53
10:p:78:MET:HA	10:q:78:MET:HE1	1.89	0.53
2:2:345:ARG:NH1	2:2:367:GLU:OE2	2.41	0.53
6:P:329:VAL:HG12	6:P:331:GLY:H	1.73	0.53
8:a:103:TYR:OH	8:a:164:TYR:O	2.22	0.53
1:w:459:LEU:HB2	1:w:472:LEU:HD13	1.91	0.53
6:T:296:LYS:HG2	6:T:360:LEU:HB2	1.90	0.53
8:c:66:GLU:HG2	8:c:71:LEU:HD23	1.90	0.53
8:c:142:LEU:HB2	10:q:36:ILE:HD11	1.91	0.53
2:3:401:LEU:HD23	2:3:440:LEU:HD23	1.91	0.53
5:N:268:ARG:NH1	5:N:341:VAL:O	2.41	0.53
6:Q:218:PRO:HA	6:Q:226:VAL:HG12	1.90	0.53
2:3:380:ASP:OD1	2:3:380:ASP:N	2.41	0.53
6:L:240:PRO:HB2	6:L:276:ALA:HB2	1.91	0.53
5:U:251:ASP:O	7:W:80:GLN:NE2	2.41	0.53
1:s:273:THR:OG1	1:s:274:ALA:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:t:384:PRO:HG3	1:t:387:PHE:HD2	1.73	0.53
4:F:52:SER:OG	4:F:53:ASP:N	2.42	0.53
6:P:19:ILE:HD12	6:P:39:ALA:HB2	1.91	0.53
6:Q:100:THR:HG22	6:Q:122:VAL:HG13	1.91	0.53
1:t:43:GLY:O	1:v:118:TRP:NE1	2.42	0.53
1:w:174:TRP:HB3	1:w:232:PRO:HB3	1.91	0.53
2:3:280:GLY:HA2	2:3:372:MET:HE3	1.90	0.53
7:V:193:THR:HG23	7:X:187:GLY:HA2	1.91	0.53
5:N:313:LEU:HD23	5:N:339:PHE:HD2	1.74	0.53
6:R:114:VAL:HG23	6:R:136:LEU:HB3	1.90	0.53
2:1:442:GLU:OE1	3:5:115:LYS:NZ	2.41	0.53
3:4:22:MET:HG3	3:4:59:PRO:HD3	1.91	0.53
6:H:42:GLN:NE2	8:a:35:ILE:O	2.42	0.53
6:P:144:THR:HB	6:P:148:THR:HG21	1.90	0.53
6:S:235:ARG:NH1	6:S:244:ASP:OD2	2.39	0.53
7:W:112:HIS:CE1	7:X:120:GLY:HA2	2.44	0.53
4:A:39:ASP:OD2	4:A:56:ARG:NH1	2.42	0.52
5:U:313:LEU:HD23	5:U:339:PHE:HD2	1.74	0.52
8:e:103:TYR:OH	8:e:164:TYR:O	2.26	0.52
1:w:116:ASP:HB3	1:w:135:THR:HG23	1.91	0.52
3:5:77:VAL:HB	3:5:89:LEU:HB2	1.91	0.52
6:H:22:ARG:HG3	8:a:34:ALA:HB2	1.90	0.52
6:J:196:GLY:HA3	8:e:98:LEU:HD21	1.91	0.52
6:J:285:ARG:HG2	6:J:358:GLU:HB3	1.90	0.52
5:N:187:LEU:HD13	5:N:194:LEU:HD23	1.90	0.52
7:W:168:ILE:HG22	7:X:162:SER:HB2	1.91	0.52
8:a:125:VAL:HG22	8:a:170:ILE:HG23	1.90	0.52
1:s:46:ARG:HH21	1:w:51:GLU:HB3	1.74	0.52
8:c:37:ASP:O	8:c:41:THR:HG23	2.09	0.52
8:e:98:LEU:HD23	8:e:166:PRO:HB3	1.90	0.52
1:t:267:GLU:O	1:t:268:ARG:C	2.51	0.52
3:7:14:VAL:HG12	3:7:77:VAL:HG22	1.90	0.52
5:U:26:ILE:HG23	5:U:294:PRO:HB2	1.91	0.52
7:V:56:ARG:NH2	7:V:58:GLN:OE1	2.42	0.52
7:W:71:GLU:OE2	7:W:92:ARG:NE	2.38	0.52
2:x:286:HIS:HB3	2:x:373:TYR:HB2	1.90	0.52
2:1:442:GLU:OE1	3:5:115:LYS:HG3	2.10	0.52
6:I:81:ARG:HD3	6:I:175:ILE:HD11	1.91	0.52
6:K:253:ALA:HA	6:K:266:GLN:HG2	1.92	0.52
2:x:107:ILE:O	2:x:173:ASP:HA	2.09	0.52
4:F:139:LYS:HG3	2:x:21:GLU:HG3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:P:100:THR:HG22	6:P:122:VAL:HG13	1.92	0.52
7:W:158:VAL:HG12	7:W:160:GLY:H	1.74	0.52
1:s:40:LYS:HB3	1:s:71:THR:HG23	1.92	0.52
2:y:109:LEU:HD23	2:y:205:THR:HG22	1.92	0.52
2:1:401:LEU:HD23	2:1:440:LEU:HD23	1.92	0.52
3:8:94:GLN:HE22	3:8:98:PRO:HG3	1.75	0.52
6:I:358:GLU:O	6:I:359:TRP:C	2.52	0.52
8:a:37:ASP:O	8:a:41:THR:HG23	2.10	0.52
4:E:26:ASP:N	4:E:26:ASP:OD1	2.42	0.52
6:H:81:ARG:HG3	6:H:181:LEU:HD11	1.91	0.52
6:L:83:GLN:HA	6:L:175:ILE:HG22	1.92	0.52
6:L:101:ILE:HB	6:L:121:ILE:HG22	1.92	0.52
6:R:130:GLU:OE2	6:R:130:GLU:N	2.43	0.52
7:W:72:ALA:HB2	7:W:89:VAL:HG12	1.92	0.52
8:e:96:GLY:HA3	8:e:102:PHE:CZ	2.45	0.52
8:f:98:LEU:HD23	8:f:166:PRO:HB3	1.92	0.52
10:m:25:ARG:HB3	10:n:9:GLY:HA3	1.92	0.52
1:s:309:ALA:HB1	1:s:430:VAL:HG21	1.92	0.52
1:u:195:ILE:HG21	1:u:222:LYS:HB2	1.90	0.52
2:3:14:ARG:O	2:z:368:ARG:NH1	2.42	0.52
3:4:90:ALA:HB1	2:x:442:GLU:OE2	2.10	0.52
6:H:256:THR:HG22	6:H:263:ILE:HG22	1.92	0.52
6:I:124:ASP:OD1	6:I:124:ASP:N	2.43	0.52
6:M:147:ASN:HA	6:M:165:THR:O	2.10	0.52
7:V:187:GLY:HA2	7:W:193:THR:HG23	1.91	0.52
8:a:96:GLY:HA3	8:a:102:PHE:CZ	2.45	0.52
5:U:187:LEU:HD13	5:U:194:LEU:HD23	1.92	0.52
8:b:71:LEU:HD22	8:b:88:ALA:HB2	1.91	0.52
10:k:78:MET:HA	10:l:78:MET:HE1	1.92	0.52
6:O:329:VAL:HG12	6:O:331:GLY:H	1.75	0.51
8:a:137:ARG:HB2	8:a:151:VAL:HG23	1.92	0.51
1:0:309:ALA:HB1	1:0:430:VAL:HG21	1.92	0.51
2:3:98:GLY:H	2:3:181:THR:HG23	1.74	0.51
6:S:289:SER:OG	6:S:290:PRO:HD3	2.10	0.51
5:U:87:ARG:NH1	9:g:681:TYR:O	2.43	0.51
2:1:39:LEU:HA	2:1:91:TRP:O	2.10	0.51
3:6:22:MET:HG3	3:6:59:PRO:HD3	1.92	0.51
6:H:81:ARG:HD3	6:H:175:ILE:HD11	1.91	0.51
6:O:19:ILE:HD12	6:O:39:ALA:HB2	1.93	0.51
7:W:52:ASP:OD1	7:W:53:GLU:N	2.43	0.51
10:m:78:MET:HA	10:n:78:MET:HE1	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:89:LEU:HD12	3:5:111:ALA:HB3	1.92	0.51
6:Q:19:ILE:HD12	6:Q:39:ALA:HB2	1.92	0.51
5:G:24:ARG:HD2	5:G:293:MET:HE1	1.93	0.51
6:I:231:VAL:HG13	6:I:238:ILE:HG23	1.92	0.51
6:M:82:LYS:HE2	6:M:184:ARG:HH12	1.76	0.51
1:v:187:VAL:HA	1:v:293:ILE:HD11	1.91	0.51
2:2:324:GLN:NE2	2:2:484:PHE:O	2.43	0.51
3:6:58:ILE:HD11	3:6:107:LEU:HD22	1.93	0.51
6:L:299:ILE:HD12	6:L:326:VAL:HG23	1.92	0.51
5:N:373:LYS:NZ	1:u:168:ASP:OD2	2.37	0.51
6:R:289:SER:OG	6:R:290:PRO:HD3	2.11	0.51
7:V:80:GLN:C	7:V:82:ASP:H	2.18	0.51
7:V:175:ILE:HG23	7:W:172:ASP:HA	1.92	0.51
7:X:27:ALA:HB1	7:X:43:VAL:HB	1.92	0.51
1:w:126:GLU:HG3	1:w:129:TYR:HB3	1.92	0.51
6:M:83:GLN:HA	6:M:175:ILE:HG22	1.93	0.51
6:Q:79:VAL:HG21	6:Q:185:LEU:HA	1.92	0.51
6:S:28:PRO:HD2	6:S:31:ARG:HG2	1.92	0.51
2:x:110:SER:OG	2:x:169:ASP:OD1	2.26	0.51
6:K:83:GLN:HA	6:K:175:ILE:HG22	1.92	0.51
6:M:288:ILE:HG22	6:M:290:PRO:HD2	1.91	0.51
6:O:100:THR:HG22	6:O:122:VAL:HG13	1.93	0.51
6:Q:144:THR:HB	6:Q:148:THR:HG21	1.92	0.51
5:U:373:LYS:NZ	1:v:168:ASP:OD2	2.39	0.51
10:q:54:THR:HG21	10:r:70:LEU:HD23	1.93	0.51
2:2:470:ASP:OD1	2:2:470:ASP:N	2.43	0.51
6:H:208:VAL:HG11	6:H:248:VAL:HG22	1.93	0.51
6:J:208:VAL:HG11	6:J:248:VAL:HG22	1.93	0.51
5:U:277:PHE:HB3	5:U:333:LEU:HB2	1.91	0.51
8:a:73:ASP:OD1	8:a:75:THR:HG22	2.11	0.51
1:s:485:PRO:HB2	1:s:488:VAL:HG22	1.91	0.51
1:w:438:GLY:O	1:w:475:ARG:NH2	2.44	0.51
2:y:167:ASP:N	2:y:167:ASP:OD1	2.44	0.51
2:y:251:LEU:HD23	2:y:287:LEU:HB3	1.93	0.51
2:z:107:ILE:O	2:z:173:ASP:HA	2.10	0.51
5:N:5:VAL:HG21	5:N:20:VAL:HG21	1.93	0.51
1:w:123:LYS:HB2	1:w:126:GLU:OE2	2.11	0.51
2:x:110:SER:OG	2:x:111:GLY:N	2.44	0.51
4:B:71:ARG:NH2	4:B:94:GLU:OE2	2.44	0.50
6:L:292:THR:O	6:L:296:LYS:HG2	2.11	0.50
5:U:183:ASP:HB2	5:U:298:VAL:HG12	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:W:23:MET:HE3	7:W:79:ALA:HB2	1.92	0.50
1:w:320:LEU:HD12	1:w:437:ARG:HD2	1.92	0.50
1:0:389:SER:HB2	1:0:392:ASP:OD1	2.11	0.50
6:J:156:VAL:HG12	6:J:157:ALA:H	1.76	0.50
6:K:257:ASP:OD2	6:O:192:PRO:HG3	2.11	0.50
6:L:45:LEU:HD13	6:P:46:ALA:HB2	1.93	0.50
6:L:257:ASP:OD2	6:P:192:PRO:HG3	2.11	0.50
5:N:26:ILE:HG23	5:N:294:PRO:HB2	1.93	0.50
10:p:78:MET:HA	10:q:78:MET:CE	2.41	0.50
2:3:236:MET:HB3	2:3:267:THR:HG22	1.92	0.50
5:G:248:ILE:HD11	5:G:266:GLU:HG2	1.93	0.50
6:I:230:PHE:HE2	6:I:232:MET:HE3	1.76	0.50
6:H:339:PHE:HB3	6:H:340:PRO:HD3	1.94	0.50
6:M:285:ARG:HE	6:M:339:PHE:HD2	1.58	0.50
1:t:162:VAL:HG11	1:t:306:THR:HG21	1.93	0.50
1:u:48:VAL:HG22	1:u:61:ASN:HB2	1.93	0.50
5:G:39:VAL:HB	5:G:43:THR:HG21	1.94	0.50
5:G:224:ASP:OD1	5:G:227:SER:OG	2.26	0.50
6:J:61:ILE:HD13	8:e:64:GLU:HB3	1.92	0.50
6:K:357:ILE:CG1	6:K:359:TRP:CE3	2.94	0.50
6:S:146:GLU:HG2	6:S:168:GLY:H	1.77	0.50
10:j:17:SER:OG	10:j:20:ARG:NH2	2.44	0.50
1:w:36:ILE:HG13	1:w:37:GLU:H	1.76	0.50
2:1:366:ILE:HD11	2:1:369:MET:HG2	1.92	0.50
2:3:322:PRO:HB2	2:3:324:GLN:HG3	1.93	0.50
6:H:196:GLY:HA3	8:a:98:LEU:HD21	1.93	0.50
6:R:213:ARG:HH12	6:R:308:PHE:HA	1.77	0.50
1:0:162:VAL:HG11	1:0:306:THR:HG21	1.93	0.50
3:8:54:VAL:HG23	3:8:89:LEU:HD11	1.94	0.50
4:E:107:ALA:N	4:E:127:THR:OG1	2.45	0.50
6:I:208:VAL:HG11	6:I:248:VAL:HG22	1.94	0.50
6:J:75:ARG:NH2	6:S:186:GLU:OE2	2.45	0.50
6:K:86:ALA:HA	6:K:138:ALA:HA	1.93	0.50
5:N:337:GLU:HG3	5:N:346:ASP:HB2	1.94	0.50
7:V:106:ILE:HD13	7:W:106:ILE:HG23	1.93	0.50
7:X:23:MET:HE3	7:X:79:ALA:HB2	1.93	0.50
10:p:107:LEU:HG	10:q:89:LEU:HD13	1.92	0.50
1:u:174:TRP:HB3	1:u:232:PRO:HB3	1.94	0.50
1:v:118:TRP:HA	1:v:133:THR:O	2.12	0.50
2:x:380:ASP:OD1	2:x:380:ASP:N	2.45	0.50
2:y:110:SER:OG	2:y:169:ASP:OD1	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:52:TYR:HD2	1:O:55:ARG:HD3	1.77	0.50
6:H:263:ILE:HD11	6:T:199:PHE:CE1	2.47	0.50
6:L:86:ALA:HA	6:L:138:ALA:HA	1.93	0.50
6:M:285:ARG:HG3	6:M:339:PHE:HB2	1.94	0.50
6:R:296:LYS:HG2	6:R:360:LEU:HB2	1.94	0.50
10:p:88:ASN:HD21	10:r:99:ALA:HB1	1.76	0.50
1:w:289:ALA:O	1:w:293:ILE:HG12	2.11	0.50
2:y:470:ASP:OD1	2:y:470:ASP:N	2.44	0.50
4:A:15:ILE:HG12	8:a:28:LEU:HD12	1.94	0.50
6:O:31:ARG:HG3	6:O:33:LYS:HE2	1.94	0.50
7:V:112:HIS:CE1	7:W:120:GLY:HA2	2.47	0.50
1:t:121:ARG:NH2	1:t:133:THR:OG1	2.44	0.50
1:v:162:VAL:HG22	1:v:422:GLN:HB3	1.94	0.50
2:z:470:ASP:OD1	2:z:470:ASP:N	2.45	0.50
6:K:45:LEU:HD13	6:O:46:ALA:HB2	1.93	0.49
5:N:39:VAL:HB	5:N:43:THR:HG21	1.94	0.49
5:N:224:ASP:OD1	5:N:224:ASP:N	2.41	0.49
7:V:120:GLY:HA2	7:X:112:HIS:CE1	2.47	0.49
8:e:158:GLU:O	8:e:162:GLU:HG2	2.10	0.49
2:x:35:ARG:HH12	2:x:37:ARG:NH1	2.10	0.49
6:I:154:THR:HG21	5:U:100:TYR:HE2	1.77	0.49
6:J:22:ARG:HG3	8:e:34:ALA:HB2	1.93	0.49
7:X:117:THR:HG22	7:X:118:LYS:H	1.77	0.49
8:b:69:LEU:HD21	8:b:92:MET:HB2	1.93	0.49
1:u:459:LEU:HB2	1:u:472:LEU:HD13	1.94	0.49
2:z:167:ASP:OD1	2:z:167:ASP:N	2.44	0.49
4:B:71:ARG:NH1	1:t:102:GLU:OE2	2.40	0.49
6:Q:17:GLN:HG3	1:w:335:LEU:HD11	1.93	0.49
6:T:72:GLU:OE2	6:T:75:ARG:NH1	2.46	0.49
1:v:289:ALA:O	1:v:293:ILE:HG12	2.12	0.49
2:x:239:THR:HG21	2:x:269:LEU:HD13	1.94	0.49
2:1:380:ASP:OD1	2:1:380:ASP:N	2.41	0.49
4:A:27:SER:CB	4:A:135:PRO:HA	2.42	0.49
5:G:107:ASN:HB3	6:J:108:GLN:NE2	2.28	0.49
8:e:37:ASP:O	8:e:41:THR:HG23	2.12	0.49
8:e:83:GLU:OE2	8:e:83:GLU:HA	2.12	0.49
1:s:269:ARG:O	1:s:271:ALA:N	2.46	0.49
2:x:77:MET:SD	2:x:301:TYR:HB2	2.53	0.49
3:6:117:ILE:HD12	2:y:438:LEU:HD13	1.94	0.49
6:I:288:ILE:HD11	6:I:359:TRP:CZ3	2.47	0.49
6:M:86:ALA:HA	6:M:138:ALA:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:U:14:PHE:HD2	1:t:145:PRO:HB2	1.78	0.49
8:d:118:ASP:OD1	8:d:119:SER:N	2.45	0.49
1:u:36:ILE:HG13	1:u:37:GLU:H	1.77	0.49
1:u:113:VAL:HB	1:u:136:VAL:HB	1.93	0.49
2:2:266:VAL:HG21	2:2:308:CYS:HB2	1.94	0.49
2:3:349:LEU:HD21	2:3:368:ARG:HD3	1.95	0.49
6:J:296:LYS:HG3	6:J:297:GLN:N	2.28	0.49
7:W:135:GLU:HB2	7:X:128:THR:HG22	1.95	0.49
2:x:167:ASP:OD1	2:x:167:ASP:N	2.45	0.49
3:6:14:VAL:HG12	3:6:77:VAL:HG22	1.94	0.49
3:6:88:MET:HE1	2:y:439:ALA:HB2	1.95	0.49
3:7:77:VAL:HB	3:7:89:LEU:HB2	1.93	0.49
4:E:77:ARG:HG3	2:z:322:PRO:O	2.13	0.49
6:H:286:ILE:HG21	6:H:326:VAL:HG21	1.94	0.49
5:N:203:ARG:NH1	5:N:239:ASP:OD2	2.46	0.49
8:a:144:ASN:HB3	8:a:147:THR:HG23	1.95	0.49
8:b:48:GLN:HE21	8:b:51:ARG:HH12	1.61	0.49
10:m:50:GLU:HA	10:m:50:GLU:OE1	2.12	0.49
1:t:52:TYR:HD2	1:t:55:ARG:HD3	1.76	0.49
2:x:82:LEU:HD13	2:x:90:LEU:HD12	1.94	0.49
2:3:219:ILE:HD13	2:3:236:MET:HE1	1.95	0.49
6:I:196:GLY:HA3	8:c:98:LEU:HD21	1.95	0.49
6:J:260:THR:HG23	6:J:262:LEU:H	1.77	0.49
5:N:183:ASP:HB2	5:N:298:VAL:HG12	1.94	0.49
6:S:213:ARG:HH12	6:S:308:PHE:HA	1.78	0.49
7:W:27:ALA:HB1	7:W:43:VAL:HB	1.94	0.49
1:t:250:CYS:SG	1:t:258:THR:HG21	2.53	0.49
2:x:121:THR:HG1	2:x:191:TRP:CD1	2.31	0.49
2:x:387:ASN:HB2	2:x:390:THR:HG23	1.94	0.49
2:y:74:LEU:HD21	2:y:92:CYS:HB3	1.94	0.49
2:3:74:LEU:HD21	2:3:92:CYS:HB3	1.94	0.49
3:9:88:MET:HE2	3:9:115:LYS:HB2	1.95	0.49
5:G:213:ALA:HB3	5:G:228:ILE:HA	1.93	0.49
6:P:289:SER:OG	6:P:290:PRO:HD3	2.13	0.49
10:j:78:MET:HA	10:k:78:MET:CE	2.43	0.49
1:t:76:ILE:HG22	1:t:130:TYR:HB2	1.95	0.49
1:0:182:ALA:HA	1:0:185:THR:HG22	1.95	0.49
5:G:5:VAL:HG21	5:G:20:VAL:HG21	1.95	0.49
6:I:237:ASN:O	6:I:238:ILE:HB	2.12	0.49
6:J:147:ASN:HA	6:J:165:THR:O	2.12	0.49
6:K:239:PHE:CE1	6:K:277:PRO:HG2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:320:SER:OG	6:T:334:ASP:OD1	2.23	0.49
10:j:78:MET:HA	10:k:78:MET:HE3	1.95	0.49
10:m:43:TRP:HE1	10:n:48:GLN:HG3	1.78	0.49
1:w:409:LEU:O	1:w:412:SER:OG	2.20	0.49
2:z:35:ARG:HH12	2:z:37:ARG:NH1	2.11	0.49
2:z:326:LEU:O	2:z:366:ILE:HG22	2.13	0.49
6:H:240:PRO:HD2	6:H:277:PRO:HD2	1.95	0.48
6:I:285:ARG:HG2	6:I:358:GLU:HB2	1.94	0.48
6:O:17:GLN:HG3	1:u:335:LEU:HD11	1.94	0.48
10:p:111:ASP:OD1	10:p:111:ASP:N	2.46	0.48
1:w:27:THR:HG22	1:w:32:PRO:HA	1.95	0.48
1:w:118:TRP:HA	1:w:133:THR:O	2.13	0.48
1:w:445:GLU:OE2	1:w:494:ASN:ND2	2.46	0.48
5:G:373:LYS:NZ	1:w:168:ASP:OD2	2.37	0.48
6:H:94:THR:HG23	6:H:160:VAL:HB	1.94	0.48
6:I:288:ILE:HG22	6:I:290:PRO:HD2	1.93	0.48
6:K:239:PHE:HE1	6:K:277:PRO:HG2	1.77	0.48
6:R:208:VAL:HG22	6:R:251:TYR:CD2	2.47	0.48
5:U:76:THR:OG1	5:U:77:ALA:N	2.46	0.48
8:a:142:LEU:HB2	10:k:36:ILE:HD11	1.94	0.48
10:p:25:ARG:HB3	10:q:9:GLY:HA3	1.95	0.48
1:s:37:GLU:HB2	1:s:73:SER:HB2	1.95	0.48
1:v:36:ILE:HG13	1:v:37:GLU:H	1.78	0.48
2:x:126:GLN:HB2	2:x:155:LEU:HD21	1.95	0.48
4:A:105:VAL:HG11	4:A:126:LEU:HD23	1.95	0.48
6:K:237:ASN:O	6:K:238:ILE:C	2.56	0.48
6:Q:323:ILE:HG12	6:Q:337:VAL:HG21	1.93	0.48
2:z:380:ASP:OD1	2:z:380:ASP:N	2.45	0.48
2:2:401:LEU:HD23	2:2:440:LEU:HD23	1.94	0.48
4:C:107:ALA:N	4:C:127:THR:OG1	2.46	0.48
6:I:156:VAL:HG12	6:I:157:ALA:N	2.29	0.48
6:J:286:ILE:HG21	6:J:326:VAL:HG21	1.94	0.48
6:J:288:ILE:HG22	6:J:290:PRO:HD2	1.95	0.48
6:L:147:ASN:HA	6:L:165:THR:O	2.13	0.48
6:P:79:VAL:HG21	6:P:185:LEU:HA	1.96	0.48
6:P:217:PHE:HZ	6:P:313:PRO:HB2	1.79	0.48
6:T:307:PHE:O	6:T:311:VAL:HB	2.13	0.48
5:U:224:ASP:OD1	5:U:224:ASP:N	2.46	0.48
7:V:106:ILE:HG22	7:V:107:TYR:H	1.77	0.48
8:b:96:GLY:HA3	8:b:102:PHE:CZ	2.49	0.48
10:n:106:ASN:HD21	10:o:90:SER:HA	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:z:387:ASN:HB2	2:z:390:THR:HG23	1.96	0.48
4:C:26:ASP:OD1	4:C:26:ASP:N	2.42	0.48
7:X:71:GLU:OE2	7:X:92:ARG:NE	2.46	0.48
10:m:78:MET:HA	10:n:78:MET:CE	2.43	0.48
1:u:254:THR:O	1:u:258:THR:HG22	2.13	0.48
1:w:113:VAL:HB	1:w:136:VAL:HB	1.95	0.48
2:1:18:THR:HG23	2:x:487:PHE:HB3	1.96	0.48
2:1:285:ASP:OD1	2:1:288:ILE:HG22	2.14	0.48
7:X:72:ALA:HB2	7:X:89:VAL:HG12	1.95	0.48
1:v:445:GLU:OE2	1:v:494:ASN:ND2	2.47	0.48
2:z:40:MET:HE2	2:z:92:CYS:SG	2.53	0.48
3:5:36:GLU:HB3	3:6:110:MET:HE1	1.95	0.48
5:G:75:MET:HE1	5:U:187:LEU:HD21	1.94	0.48
5:G:244:ARG:HA	5:N:96:CYS:SG	2.54	0.48
6:K:101:ILE:HB	6:K:121:ILE:HG22	1.96	0.48
6:M:119:ASP:N	6:M:119:ASP:OD1	2.47	0.48
5:U:10:ASP:HB2	5:U:52:LYS:HD2	1.95	0.48
1:t:56:ASP:HB3	1:v:65:LYS:HE2	1.95	0.48
2:x:470:ASP:OD1	2:x:470:ASP:N	2.44	0.48
4:F:143:ASN:OD1	4:F:143:ASN:N	2.44	0.48
6:I:155:PRO:HG2	7:W:50:GLU:HB2	1.94	0.48
6:L:82:LYS:HZ1	6:L:184:ARG:HH22	1.61	0.48
8:b:114:VAL:HG12	8:b:130:ILE:HG13	1.96	0.48
8:f:161:LEU:O	8:f:165:LYS:HB3	2.14	0.48
2:y:110:SER:OG	2:y:111:GLY:N	2.47	0.48
6:J:289:SER:HB3	6:J:290:PRO:HD3	1.95	0.48
6:M:45:LEU:HD13	6:Q:46:ALA:HB2	1.95	0.48
5:N:248:ILE:HD11	5:N:266:GLU:HG2	1.96	0.48
8:f:96:GLY:HA3	8:f:102:PHE:CZ	2.48	0.48
4:D:71:ARG:NH2	4:D:94:GLU:OE2	2.44	0.48
5:N:165:THR:HG22	5:N:166:SER:H	1.79	0.48
7:X:117:THR:HG22	7:X:118:LYS:N	2.29	0.48
8:b:66:GLU:OE1	8:b:84:ARG:NH1	2.47	0.48
1:s:48:VAL:HG23	1:s:61:ASN:HB2	1.96	0.48
1:t:267:GLU:C	1:t:269:ARG:N	2.71	0.48
1:w:49:LYS:H	1:w:49:LYS:HD2	1.79	0.48
6:Q:123:ILE:HD11	6:Q:129:THR:HG21	1.96	0.47
10:q:27:PHE:CE1	10:r:44:PHE:HB3	2.49	0.47
1:s:49:LYS:HA	1:s:60:VAL:HG12	1.96	0.47
1:s:52:TYR:HD2	1:s:55:ARG:HD3	1.79	0.47
2:y:464:ARG:HD2	2:y:472:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:146:VAL:HG21	2:1:161:VAL:HB	1.96	0.47
5:G:182:THR:OG1	5:G:183:ASP:OD1	2.29	0.47
6:J:91:LEU:HD12	6:J:165:THR:HG22	1.96	0.47
6:R:28:PRO:HD2	6:R:31:ARG:HG2	1.95	0.47
8:a:119:SER:OG	8:a:120:THR:N	2.47	0.47
8:e:142:LEU:HB2	10:n:36:ILE:HD11	1.94	0.47
1:u:195:ILE:HD11	1:u:221:MET:SD	2.54	0.47
2:x:251:LEU:HD23	2:x:287:LEU:HB3	1.96	0.47
2:3:36:GLN:N	2:3:36:GLN:OE1	2.46	0.47
3:5:42:VAL:HG21	3:6:51:ALA:HB2	1.95	0.47
6:I:239:PHE:HD1	6:I:239:PHE:H	1.61	0.47
6:J:238:ILE:HG22	6:J:238:ILE:O	2.14	0.47
6:L:240:PRO:HD2	6:L:276:ALA:HB1	1.96	0.47
8:e:144:ASN:OD1	8:e:145:VAL:N	2.46	0.47
1:u:243:LEU:HD11	1:u:300:MET:HE1	1.96	0.47
2:y:107:ILE:O	2:y:173:ASP:HA	2.14	0.47
2:y:306:THR:HG21	2:y:331:ARG:HH11	1.79	0.47
6:I:233:ASP:HA	6:I:238:ILE:HG12	1.96	0.47
6:R:294:GLU:HG2	6:R:295:LEU:N	2.29	0.47
2:2:36:GLN:OE1	2:2:36:GLN:N	2.46	0.47
6:K:240:PRO:HD2	6:K:276:ALA:HB1	1.96	0.47
5:N:186:VAL:HG23	5:N:189:GLU:H	1.79	0.47
6:Q:269:GLY:HA2	8:f:169:GLN:HE21	1.79	0.47
1:s:162:VAL:HG11	1:s:306:THR:HG21	1.96	0.47
1:v:123:LYS:C	1:v:125:ASP:H	2.22	0.47
2:2:42:GLY:O	2:2:94:PRO:HA	2.15	0.47
2:3:462:VAL:HG22	2:3:474:VAL:HG22	1.96	0.47
6:J:346:SER:HB2	6:J:350:GLU:HB2	1.97	0.47
6:K:329:VAL:HB	6:K:332:LEU:HD23	1.95	0.47
6:L:253:ALA:HA	6:L:266:GLN:HG2	1.97	0.47
5:N:223:ILE:HG12	5:N:228:ILE:HG13	1.97	0.47
10:j:78:MET:HE3	10:j:78:MET:HB2	1.63	0.47
10:l:5:ASP:OD2	10:l:64:LYS:NZ	2.43	0.47
1:s:174:TRP:HB3	1:s:232:PRO:HB3	1.97	0.47
3:9:113:GLN:HE21	3:9:115:LYS:HE3	1.80	0.47
6:I:321:ARG:HG3	6:I:321:ARG:HH11	1.80	0.47
6:J:176:GLU:OE1	6:J:184:ARG:NH1	2.46	0.47
6:K:233:ASP:C	6:K:235:ARG:N	2.72	0.47
6:M:94:THR:HG23	6:M:160:VAL:HB	1.97	0.47
6:M:236:SER:O	6:M:238:ILE:HG13	2.15	0.47
6:O:212:THR:HG21	6:O:233:ASP:OD1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:O:213:ARG:HB2	6:O:231:VAL:HG12	1.96	0.47
6:O:289:SER:OG	6:O:290:PRO:HD3	2.15	0.47
6:P:17:GLN:HG3	1:v:335:LEU:HD11	1.96	0.47
8:b:108:ALA:HA	8:b:112:PHE:O	2.15	0.47
8:c:119:SER:OG	8:c:120:THR:N	2.46	0.47
1:t:384:PRO:HG2	1:t:387:PHE:HB2	1.96	0.47
1:u:92:MET:CE	1:u:120:CYS:HB2	2.44	0.47
2:2:18:THR:HG23	2:y:487:PHE:HB3	1.96	0.47
2:3:164:ASP:N	2:3:164:ASP:OD1	2.46	0.47
6:H:232:MET:O	6:H:238:ILE:HA	2.15	0.47
6:O:289:SER:HG	6:O:290:PRO:HD3	1.78	0.47
8:c:96:GLY:HA3	8:c:102:PHE:CZ	2.50	0.47
10:o:93:LYS:HG2	10:o:100:GLN:NE2	2.29	0.47
1:s:441:LEU:HD23	1:s:441:LEU:HA	1.80	0.47
1:t:262:LEU:HD23	1:t:262:LEU:HA	1.80	0.47
1:v:46:ARG:HG3	1:v:66:LYS:HG3	1.96	0.47
1:v:215:MET:HE3	1:v:215:MET:HA	1.95	0.47
1:v:468:ASN:HB3	1:v:471:ARG:HD2	1.97	0.47
2:2:349:LEU:HD23	2:z:14:ARG:HG3	1.97	0.47
3:7:30:SER:HB3	3:7:52:ALA:HB2	1.97	0.47
6:I:263:ILE:HD11	6:R:199:PHE:CE1	2.50	0.47
6:K:18:ASN:HB3	8:b:34:ALA:HB1	1.96	0.47
6:Q:289:SER:HG	6:Q:334:ASP:H	1.63	0.47
6:T:130:GLU:N	6:T:130:GLU:OE1	2.48	0.47
7:V:124:ILE:HG22	7:V:126:CYS:SG	2.55	0.47
7:W:175:ILE:HG23	7:X:172:ASP:HA	1.97	0.47
2:2:40:MET:HG2	2:2:235:VAL:HB	1.97	0.47
2:2:113:ALA:HB2	2:2:203:ILE:HD11	1.96	0.47
2:2:219:ILE:HD13	2:2:236:MET:HE1	1.97	0.47
2:3:285:ASP:OD2	2:3:287:LEU:HB2	2.15	0.47
3:5:29:PRO:HG3	3:6:66:LEU:HD13	1.97	0.47
3:6:69:ILE:HG21	3:6:107:LEU:HD11	1.96	0.47
4:A:105:VAL:HG21	4:A:108:ILE:HD11	1.95	0.47
6:H:285:ARG:HG2	6:H:358:GLU:HB2	1.97	0.47
6:I:195:GLY:N	6:I:200:ASP:OD2	2.46	0.47
6:I:239:PHE:CE2	6:I:351:LEU:HD23	2.50	0.47
7:V:172:ASP:HA	7:X:175:ILE:HG23	1.96	0.47
8:a:77:GLU:HG3	8:a:83:GLU:HG3	1.97	0.47
10:k:98:SER:O	10:k:102:THR:OG1	2.31	0.47
1:w:243:LEU:HD11	1:w:300:MET:HE1	1.96	0.47
4:F:62:SER:O	1:w:467:ARG:NH2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:313:PRO:HG3	6:L:351:LEU:HB2	1.97	0.46
6:M:144:THR:HB	6:M:148:THR:HG21	1.96	0.46
7:V:128:THR:O	7:V:128:THR:OG1	2.34	0.46
10:j:66:LYS:HE2	10:j:69:GLN:HE21	1.80	0.46
10:p:66:LYS:HE2	10:p:69:GLN:HE21	1.80	0.46
2:y:236:MET:HG3	2:y:236:MET:O	2.15	0.46
6:H:240:PRO:HB2	6:H:276:ALA:HB2	1.97	0.46
6:J:155:PRO:HB3	7:X:52:ASP:HB2	1.97	0.46
6:J:339:PHE:HB3	6:J:340:PRO:HD3	1.95	0.46
6:P:323:ILE:HG12	6:P:337:VAL:HG21	1.97	0.46
10:m:17:SER:OG	10:m:20:ARG:NH2	2.48	0.46
1:v:326:MET:HE2	1:v:326:MET:HB2	1.83	0.46
1:v:418:THR:O	1:v:419:ASP:C	2.59	0.46
1:w:302:ALA:O	1:w:306:THR:HG23	2.15	0.46
1:0:46:ARG:NH2	1:v:51:GLU:HB3	2.30	0.46
3:5:27:PHE:HD1	3:5:54:VAL:HG22	1.80	0.46
3:6:78:GLU:CD	2:y:435:THR:HG21	2.40	0.46
3:8:14:VAL:HG12	3:8:77:VAL:HG22	1.97	0.46
6:I:95:THR:OG1	6:I:96:SER:N	2.48	0.46
6:M:240:PRO:HD2	6:M:276:ALA:HB1	1.97	0.46
5:N:244:ARG:HA	5:U:96:CYS:SG	2.55	0.46
6:T:284:PRO:HA	6:T:340:PRO:HG3	1.98	0.46
8:f:71:LEU:HD22	8:f:88:ALA:HB2	1.98	0.46
1:t:228:LEU:O	1:t:230:ASN:N	2.48	0.46
1:u:193:GLY:HA3	1:u:269:ARG:HH12	1.81	0.46
4:F:15:ILE:HD12	4:F:22:MET:HE2	1.96	0.46
6:K:147:ASN:HA	6:K:165:THR:O	2.16	0.46
6:P:295:LEU:HD22	6:P:332:LEU:HD12	1.97	0.46
5:U:167:ASN:OD1	5:U:168:ALA:N	2.46	0.46
1:s:46:ARG:NH2	1:w:51:GLU:HB3	2.30	0.46
1:t:273:THR:O	1:t:274:ALA:HB3	2.15	0.46
6:H:230:PHE:HE2	6:H:232:MET:HE3	1.81	0.46
6:J:124:ASP:N	6:J:124:ASP:OD1	2.45	0.46
6:R:235:ARG:NH1	6:R:244:ASP:OD2	2.45	0.46
8:b:161:LEU:O	8:b:165:LYS:HB3	2.16	0.46
1:u:215:MET:HE3	1:u:215:MET:HB3	1.81	0.46
1:v:113:VAL:HB	1:v:136:VAL:HB	1.97	0.46
2:z:251:LEU:HD23	2:z:287:LEU:HB3	1.97	0.46
2:2:322:PRO:HB2	2:2:324:GLN:HG3	1.98	0.46
6:H:92:THR:OG1	6:H:164:ILE:O	2.33	0.46
6:I:107:TRP:HZ3	6:I:117:LEU:HB2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:V:129:VAL:HG12	7:X:133:ALA:HB2	1.96	0.46
8:f:66:GLU:HG2	8:f:71:LEU:HD23	1.97	0.46
1:t:126:GLU:OE1	1:t:129:TYR:HB3	2.16	0.46
1:u:36:ILE:HD12	1:u:36:ILE:HA	1.86	0.46
3:7:42:VAL:HG21	3:8:51:ALA:HB2	1.96	0.46
6:H:262:LEU:HD22	6:T:203:ARG:HH21	1.81	0.46
6:I:91:LEU:HD12	6:I:165:THR:HG22	1.98	0.46
6:K:233:ASP:O	6:K:235:ARG:N	2.48	0.46
6:Q:289:SER:OG	6:Q:290:PRO:HD3	2.16	0.46
6:R:194:PHE:O	8:c:97:ASN:ND2	2.48	0.46
10:m:44:PHE:HB3	10:o:27:PHE:CD2	2.50	0.46
10:r:12:VAL:HG22	2:y:204:ILE:HG12	1.98	0.46
1:t:174:TRP:HB3	1:t:232:PRO:HB3	1.98	0.46
1:t:205:LEU:HD11	1:t:250:CYS:SG	2.55	0.46
3:5:30:SER:HB3	3:5:52:ALA:HB2	1.98	0.46
5:N:213:ALA:HB3	5:N:228:ILE:HA	1.97	0.46
8:d:161:LEU:O	8:d:165:LYS:HB3	2.16	0.46
10:m:83:LEU:HB2	10:o:83:LEU:HD13	1.98	0.46
1:s:148:GLU:HG2	1:s:149:THR:H	1.80	0.46
1:v:27:THR:HG22	1:v:32:PRO:HA	1.97	0.46
1:w:169:THR:HG21	1:w:419:ASP:OD2	2.16	0.46
2:z:421:PHE:HD2	2:z:427:VAL:HG21	1.81	0.46
3:8:42:VAL:HB	3:9:112:LYS:HG3	1.98	0.46
4:F:15:ILE:HG12	8:f:28:LEU:HD12	1.98	0.46
6:L:284:PRO:HD2	6:L:357:ILE:HA	1.98	0.46
6:Q:295:LEU:HD22	6:Q:332:LEU:HD12	1.96	0.46
8:c:78:ASN:HB2	8:c:153:GLU:OE1	2.16	0.46
10:k:27:PHE:CZ	10:l:4:ILE:HD11	2.50	0.46
1:s:36:ILE:HG12	1:s:75:CYS:HB3	1.98	0.46
2:x:38:VAL:HG12	2:x:233:TYR:HB2	1.96	0.46
2:y:41:PHE:HD2	2:y:236:MET:HB2	1.81	0.46
2:y:193:TYR:CE2	2:y:332:MET:HE3	2.50	0.46
1:0:205:LEU:HD11	1:0:250:CYS:SG	2.56	0.46
3:5:14:VAL:HG12	3:5:77:VAL:HG22	1.97	0.46
5:G:307:ILE:HG12	5:N:73:ARG:HH21	1.81	0.46
6:I:75:ARG:NH2	6:R:186:GLU:OE2	2.48	0.46
6:J:209:SER:O	6:J:247:ARG:NH2	2.48	0.46
8:e:27:LYS:HA	8:e:27:LYS:HD3	1.69	0.46
10:m:66:LYS:HE2	10:m:69:GLN:HE21	1.81	0.46
10:p:29:GLU:HG3	10:q:41:MET:SD	2.56	0.46
2:z:349:LEU:HD21	2:z:368:ARG:HD3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:433:ASP:OD1	1:0:437:ARG:NH1	2.49	0.45
2:1:387:ASN:O	2:1:390:THR:OG1	2.33	0.45
3:8:85:GLU:HG3	3:8:116:ARG:NH2	2.31	0.45
3:9:69:ILE:HD13	3:9:107:LEU:HD11	1.98	0.45
4:C:12:ARG:NH2	8:c:20:TRP:O	2.48	0.45
4:D:58:TRP:CE2	8:d:15:PRO:HG3	2.51	0.45
6:S:257:ASP:HB3	6:S:260:THR:O	2.16	0.45
8:f:118:ASP:OD1	8:f:119:SER:N	2.48	0.45
1:u:158:GLN:HE21	1:u:162:VAL:HG23	1.81	0.45
2:y:380:ASP:N	2:y:380:ASP:OD1	2.47	0.45
2:3:35:ARG:NH2	2:3:89:GLU:OE2	2.46	0.45
2:3:295:GLY:HA3	2:3:334:PRO:HB3	1.97	0.45
5:G:337:GLU:HG3	5:G:346:ASP:HB2	1.98	0.45
6:J:296:LYS:NZ	6:J:359:TRP:HE1	2.14	0.45
6:K:226:VAL:HG11	8:b:167:ALA:HB1	1.98	0.45
6:S:284:PRO:HA	6:S:340:PRO:HG3	1.97	0.45
10:k:46:ILE:O	10:k:50:GLU:HG3	2.16	0.45
10:k:107:LEU:N	10:l:93:LYS:HE2	2.32	0.45
10:n:14:PRO:HB2	10:n:41:MET:HE1	1.97	0.45
2:z:122:TYR:O	2:z:189:VAL:HA	2.15	0.45
1:0:43:GLY:O	1:w:118:TRP:NE1	2.49	0.45
3:8:27:PHE:HD1	3:8:54:VAL:HG22	1.81	0.45
6:H:124:ASP:OD1	6:H:124:ASP:N	2.46	0.45
6:I:209:SER:O	6:I:247:ARG:NH2	2.49	0.45
6:M:101:ILE:HB	6:M:121:ILE:HG22	1.97	0.45
6:M:292:THR:HG22	6:M:294:GLU:H	1.81	0.45
5:N:217:GLY:HA3	7:V:53:GLU:OE1	2.16	0.45
6:S:346:SER:HB3	6:S:350:GLU:HB2	1.98	0.45
7:V:151:GLU:HB3	7:W:145:THR:HG22	1.98	0.45
10:p:17:SER:OG	10:p:20:ARG:NH2	2.50	0.45
1:w:76:ILE:HD11	1:w:91:LEU:HD22	1.97	0.45
1:0:185:THR:O	1:0:189:GLU:HG2	2.16	0.45
2:2:70:GLN:O	2:2:179:LYS:NZ	2.40	0.45
2:2:251:LEU:HD23	2:2:287:LEU:HB3	1.98	0.45
6:K:233:ASP:OD1	6:K:233:ASP:N	2.48	0.45
6:M:239:PHE:HE1	6:M:277:PRO:HG2	1.82	0.45
6:O:286:ILE:HB	6:O:360:LEU:HD21	1.98	0.45
6:P:289:SER:HG	6:P:334:ASP:H	1.62	0.45
10:n:19:GLN:NE2	10:n:21:SER:O	2.50	0.45
1:t:37:GLU:HB2	1:t:73:SER:HB2	1.99	0.45
1:t:46:ARG:NH1	1:t:63:LEU:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:u:27:THR:HG22	1:u:32:PRO:HA	1.99	0.45
2:x:35:ARG:HH12	2:x:37:ARG:CZ	2.29	0.45
2:1:229:LEU:HD12	2:1:229:LEU:HA	1.84	0.45
2:2:355:THR:OG1	2:2:367:GLU:OE1	2.31	0.45
2:3:346:ASN:ND2	2:x:13:VAL:HA	2.31	0.45
3:9:30:SER:HB3	3:9:52:ALA:HB2	1.99	0.45
5:G:96:CYS:SG	5:U:244:ARG:HA	2.57	0.45
6:I:239:PHE:N	6:I:239:PHE:CD1	2.85	0.45
6:M:323:ILE:O	6:M:326:VAL:HG12	2.17	0.45
6:O:91:LEU:HD12	6:O:133:VAL:HG21	1.99	0.45
6:R:284:PRO:HA	6:R:340:PRO:HG3	1.99	0.45
2:y:456:PHE:HE1	2:y:476:CYS:HB3	1.82	0.45
3:9:53:LYS:HB2	3:9:110:MET:HG2	1.98	0.45
7:X:128:THR:O	7:X:128:THR:OG1	2.34	0.45
10:q:89:LEU:HD22	10:q:92:ILE:HD11	1.99	0.45
2:y:35:ARG:HH12	2:y:37:ARG:NH1	2.15	0.45
2:z:38:VAL:HG22	2:z:233:TYR:HB2	1.99	0.45
2:2:39:LEU:HA	2:2:91:TRP:O	2.16	0.45
2:3:58:ILE:HG22	2:3:63:GLN:HG2	1.99	0.45
2:3:112:THR:O	2:3:112:THR:HG22	2.17	0.45
2:3:324:GLN:NE2	2:3:484:PHE:O	2.49	0.45
3:7:27:PHE:HD1	3:7:54:VAL:HG22	1.81	0.45
3:8:78:GLU:CD	2:z:435:THR:HG21	2.42	0.45
6:H:230:PHE:CE2	6:H:232:MET:HE3	2.52	0.45
6:J:286:ILE:HD12	6:J:357:ILE:CG2	2.45	0.45
6:T:200:ASP:OD1	6:T:203:ARG:NH1	2.42	0.45
5:U:226:LYS:HA	7:X:28:VAL:HG11	1.99	0.45
8:d:69:LEU:HD21	8:d:92:MET:HB2	1.99	0.45
10:j:25:ARG:HB3	10:k:9:GLY:HA3	1.97	0.45
10:n:89:LEU:HD13	10:n:92:ILE:HD11	1.97	0.45
1:u:478:ILE:HD13	1:u:484:VAL:HG22	1.99	0.45
2:1:323:LEU:HD12	2:1:369:MET:HG3	1.99	0.45
3:7:7:GLN:HG2	3:8:103:GLY:HA2	1.99	0.45
6:I:149:LEU:C	6:I:150:LEU:HD12	2.42	0.45
6:L:91:LEU:CD1	6:L:150:LEU:HD11	2.46	0.45
8:f:69:LEU:HD21	8:f:92:MET:HB2	1.97	0.45
1:0:151:THR:HG22	1:0:433:ASP:HB2	1.98	0.45
4:D:2:THR:O	4:D:2:THR:OG1	2.32	0.45
4:F:61:ASP:OD1	4:F:67:PRO:HA	2.16	0.45
6:K:193:PRO:HD2	8:b:95:THR:HG22	1.99	0.45
10:k:27:PHE:CE1	10:l:44:PHE:HB3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:x:110:SER:HB3	2:x:204:ILE:HB	1.97	0.45
2:y:387:ASN:HB2	2:y:390:THR:HG23	1.99	0.45
2:2:93:ILE:HG21	2:2:222:SER:OG	2.17	0.45
5:G:264:LEU:HA	5:G:264:LEU:HD23	1.84	0.45
6:P:51:GLU:HB3	1:v:481:PRO:HG3	1.98	0.45
6:R:67:GLU:OE2	6:R:81:ARG:NH2	2.50	0.45
1:s:301:LEU:HD23	1:s:301:LEU:HA	1.85	0.45
1:v:302:ALA:O	1:v:306:THR:HG23	2.17	0.45
2:y:110:SER:HB3	2:y:204:ILE:HB	1.98	0.45
2:2:146:VAL:HG21	2:2:161:VAL:HB	1.99	0.44
4:D:89:ARG:HD2	4:D:111:ARG:HA	1.97	0.44
6:H:257:ASP:OD1	6:H:258:PRO:HD2	2.17	0.44
6:I:295:LEU:HD13	6:I:332:LEU:HB3	1.99	0.44
6:M:240:PRO:HB2	6:M:276:ALA:HB2	1.98	0.44
6:Q:286:ILE:HB	6:Q:360:LEU:HD21	1.99	0.44
6:R:73:HIS:NE2	8:c:53:ARG:HD2	2.31	0.44
6:R:286:ILE:HD13	6:R:326:VAL:HG21	1.99	0.44
6:T:301:ASN:HB3	1:s:285:ASN:ND2	2.31	0.44
5:U:144:ASP:HB2	5:U:147:GLU:HG3	1.99	0.44
5:U:213:ALA:HB3	5:U:228:ILE:HA	1.98	0.44
10:q:19:GLN:NE2	10:q:21:SER:O	2.50	0.44
1:t:49:LYS:HA	1:t:60:VAL:HG12	1.99	0.44
1:u:438:GLY:O	1:u:475:ARG:NH2	2.50	0.44
2:x:40:MET:HE2	2:x:40:MET:HB3	1.68	0.44
2:y:326:LEU:H	2:y:366:ILE:HG22	1.82	0.44
2:z:77:MET:SD	2:z:237:PRO:HG3	2.58	0.44
2:z:348:LEU:HD23	2:z:355:THR:HG22	1.98	0.44
1:0:69:SER:O	1:0:69:SER:OG	2.35	0.44
1:0:318:ALA:HB3	1:0:383:THR:OG1	2.17	0.44
2:1:18:THR:HG21	4:A:37:PHE:CE1	2.52	0.44
2:1:112:THR:HG22	2:1:112:THR:O	2.17	0.44
2:3:146:VAL:HG21	2:3:161:VAL:HB	1.99	0.44
2:3:411:ASN:OD1	2:3:411:ASN:N	2.50	0.44
4:C:100:LYS:HB3	4:C:100:LYS:HE3	1.82	0.44
5:G:160:ARG:HA	5:G:160:ARG:HD3	1.55	0.44
6:K:197:ASN:H	6:K:200:ASP:HB2	1.83	0.44
6:L:144:THR:HB	6:L:148:THR:HG21	1.98	0.44
6:O:91:LEU:O	6:O:130:GLU:HA	2.17	0.44
6:Q:92:THR:HG21	10:m:12:VAL:HG21	1.98	0.44
6:Q:145:GLY:H	6:Q:148:THR:HG21	1.82	0.44
6:Q:212:THR:HG21	6:Q:233:ASP:OD1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:b:118:ASP:OD1	8:b:119:SER:N	2.47	0.44
1:s:123:LYS:HE3	1:s:123:LYS:HB3	1.84	0.44
1:t:36:ILE:HG13	1:t:37:GLU:H	1.82	0.44
1:t:309:ALA:HB1	1:t:430:VAL:HG21	1.99	0.44
2:2:373:TYR:CD2	2:2:385:TYR:HB2	2.52	0.44
2:3:371:THR:OG1	2:3:385:TYR:O	2.32	0.44
3:9:89:LEU:HD12	3:9:111:ALA:HB3	1.98	0.44
4:F:17:GLN:HG3	8:f:27:LYS:HE3	1.99	0.44
7:X:52:ASP:OD1	7:X:53:GLU:N	2.50	0.44
8:a:27:LYS:HA	8:a:27:LYS:HD3	1.71	0.44
8:e:116:LEU:HD22	8:e:128:VAL:HG22	2.00	0.44
1:s:331:ARG:HG2	1:s:332:ALA:H	1.82	0.44
1:s:355:VAL:HG12	1:s:360:LEU:HD12	1.99	0.44
1:t:472:LEU:HD11	1:t:492:VAL:HG22	1.99	0.44
1:v:243:LEU:HD11	1:v:300:MET:HE1	1.99	0.44
2:1:322:PRO:HB2	2:1:324:GLN:HG3	2.00	0.44
3:9:65:GLY:O	3:9:69:ILE:HG13	2.17	0.44
6:H:88:SER:HB3	6:H:134:THR:HG22	1.99	0.44
6:R:205:ALA:O	6:R:211:VAL:HG21	2.16	0.44
6:S:220:TRP:O	6:S:225:THR:HB	2.17	0.44
6:T:213:ARG:HH12	6:T:308:PHE:HA	1.81	0.44
1:s:88:ALA:O	1:s:92:MET:HG3	2.17	0.44
1:s:155:VAL:HB	1:s:156:PRO:HD3	2.00	0.44
1:t:273:THR:HG21	1:t:297:ASN:ND2	2.31	0.44
1:0:56:ASP:HB3	1:w:65:LYS:HE2	2.00	0.44
1:0:355:VAL:HG11	5:G:169:ALA:HB2	1.99	0.44
2:1:113:ALA:HB2	2:1:203:ILE:HD11	1.99	0.44
2:2:35:ARG:NH2	2:2:89:GLU:OE2	2.51	0.44
3:6:88:MET:HE3	3:6:88:MET:HB2	1.83	0.44
3:7:76:THR:O	3:7:76:THR:OG1	2.36	0.44
4:C:30:THR:HA	4:C:33:THR:HG22	2.00	0.44
5:G:268:ARG:NH1	5:G:341:VAL:O	2.51	0.44
6:K:346:SER:HB2	6:K:350:GLU:HG3	1.99	0.44
2:1:42:GLY:O	2:1:94:PRO:HA	2.17	0.44
2:1:405:ILE:HD13	2:1:405:ILE:HA	1.88	0.44
4:A:65:ASP:HB2	1:s:332:ALA:HB2	2.00	0.44
6:J:95:THR:OG1	6:J:96:SER:N	2.51	0.44
5:N:144:ASP:O	5:N:147:GLU:HB2	2.17	0.44
5:U:5:VAL:HG21	5:U:20:VAL:HG21	2.00	0.44
10:p:101:ARG:O	10:p:105:GLU:HG2	2.17	0.44
1:w:158:GLN:HE21	1:w:162:VAL:HG23	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:316:LEU:HD22	1:0:434:LEU:HD23	1.98	0.44
2:1:293:ILE:HD12	2:1:293:ILE:HA	1.93	0.44
3:4:85:GLU:HG3	3:4:116:ARG:NH2	2.33	0.44
4:F:58:TRP:CE2	8:f:15:PRO:HG3	2.53	0.44
6:J:235:ARG:NH2	6:J:244:ASP:OD2	2.50	0.44
6:M:287:TYR:HD2	6:M:336:GLU:HG2	1.82	0.44
6:P:285:ARG:HG2	6:P:358:GLU:HB2	1.99	0.44
5:U:191:LEU:O	1:t:53:PRO:HD2	2.18	0.44
2:z:269:LEU:HD23	2:z:276:ILE:HG12	2.00	0.44
2:2:286:HIS:HB3	2:2:373:TYR:HB2	2.00	0.44
3:4:51:ALA:HB2	3:9:42:VAL:HG21	2.00	0.44
6:I:101:ILE:HG22	6:I:105:THR:HG21	2.00	0.44
6:I:238:ILE:O	6:I:239:PHE:C	2.61	0.44
6:K:94:THR:HG23	6:K:160:VAL:HB	1.99	0.44
6:K:280:LYS:NZ	6:K:345:ARG:O	2.45	0.44
7:W:114:ILE:HG12	7:W:124:ILE:HG23	2.00	0.44
7:W:187:GLY:HA2	7:X:193:THR:HG23	1.99	0.44
10:k:106:ASN:CG	10:l:93:LYS:HD3	2.43	0.44
10:m:2:PHE:CE2	10:m:55:LEU:HD11	2.53	0.44
1:v:198:ILE:O	1:v:202:VAL:HG23	2.17	0.44
2:y:349:LEU:HD21	2:y:368:ARG:HD3	2.00	0.44
1:0:49:LYS:HA	1:0:60:VAL:HG12	2.00	0.44
2:1:470:ASP:OD1	2:1:470:ASP:N	2.43	0.44
3:8:42:VAL:HG21	3:9:51:ALA:HB2	2.00	0.44
6:L:70:LEU:HD23	6:L:178:ALA:HB1	1.98	0.44
6:S:306:MET:HE3	6:S:306:MET:HB3	1.81	0.44
6:T:235:ARG:HH22	6:T:241:GLN:HG2	1.82	0.44
8:f:7:GLN:HG3	8:f:8:THR:N	2.33	0.44
10:m:26:TRP:CE2	10:n:13:MET:HB2	2.53	0.44
1:u:85:ARG:HA	1:u:85:ARG:HD2	1.73	0.44
2:x:166:GLY:O	2:x:170:THR:HA	2.17	0.44
2:x:285:ASP:OD2	2:x:288:ILE:HD12	2.18	0.44
2:2:109:LEU:HD23	2:2:205:THR:HG22	2.00	0.43
2:2:462:VAL:HG22	2:2:474:VAL:HG22	2.00	0.43
3:8:36:GLU:HB3	3:9:110:MET:HE1	2.00	0.43
5:G:45:LEU:HD23	5:G:45:LEU:HA	1.84	0.43
6:M:346:SER:HB2	6:M:350:GLU:HG3	2.00	0.43
5:N:294:PRO:HA	5:N:314:VAL:HG23	1.99	0.43
7:X:124:ILE:HG22	7:X:126:CYS:SG	2.58	0.43
1:w:409:LEU:HD23	1:w:409:LEU:HA	1.87	0.43
2:x:74:LEU:HD21	2:x:92:CYS:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:49:SER:O	2:1:49:SER:OG	2.35	0.43
2:1:283:ARG:HB2	2:1:372:MET:HE2	1.99	0.43
3:6:77:VAL:HB	3:6:89:LEU:HB2	2.00	0.43
3:9:77:VAL:HB	3:9:89:LEU:HB2	2.00	0.43
6:H:239:PHE:HE1	6:H:351:LEU:HD23	1.81	0.43
6:M:70:LEU:HD23	6:M:178:ALA:HB1	2.00	0.43
6:O:99:THR:OG1	6:O:100:THR:N	2.51	0.43
8:d:71:LEU:HD22	8:d:88:ALA:HB2	1.98	0.43
8:e:7:GLN:HG3	8:e:8:THR:N	2.34	0.43
1:u:46:ARG:HG3	1:u:66:LYS:HG3	2.00	0.43
2:2:276:ILE:HG22	2:2:348:LEU:HD11	2.00	0.43
4:F:60:GLY:O	4:F:64:ARG:HG2	2.18	0.43
6:L:306:MET:HG3	6:L:325:ALA:HB2	2.00	0.43
6:M:192:PRO:HA	6:M:193:PRO:HD3	1.84	0.43
6:M:233:ASP:C	6:M:235:ARG:H	2.25	0.43
6:O:150:LEU:HB2	6:O:163:ALA:HB3	2.00	0.43
7:V:161:LYS:HD3	7:X:166:SER:HB3	2.00	0.43
8:e:161:LEU:HD23	8:e:161:LEU:HA	1.90	0.43
10:m:75:LYS:NZ	10:o:57:GLU:OE2	2.30	0.43
1:t:182:ALA:HA	1:t:185:THR:HG22	2.00	0.43
2:y:184:LEU:HD13	2:y:301:TYR:HD1	1.82	0.43
2:y:368:ARG:HE	2:y:370:ILE:HD11	1.83	0.43
2:2:288:ILE:HG23	2:2:372:MET:HE3	2.00	0.43
2:3:58:ILE:HD12	2:3:64:ALA:HB2	1.99	0.43
2:3:387:ASN:O	2:3:390:THR:OG1	2.32	0.43
4:A:4:LEU:HD22	4:A:22:MET:HB2	2.00	0.43
4:E:44:ASP:HA	4:E:55:ARG:CZ	2.49	0.43
4:F:7:ILE:HD12	4:F:16:ALA:HB3	1.99	0.43
5:N:87:ARG:NH1	9:i:681:TYR:O	2.51	0.43
7:V:106:ILE:O	7:X:63:PHE:HE1	2.01	0.43
8:e:117:THR:HG22	8:e:118:ASP:H	1.83	0.43
10:q:98:SER:O	10:q:102:THR:OG1	2.34	0.43
1:s:185:THR:O	1:s:189:GLU:HG2	2.18	0.43
1:s:273:THR:O	1:s:274:ALA:HB3	2.17	0.43
1:w:198:ILE:O	1:w:202:VAL:HG23	2.17	0.43
2:x:126:GLN:OE1	2:x:152:GLN:NE2	2.47	0.43
2:x:236:MET:HE3	2:x:236:MET:HB3	1.92	0.43
2:y:122:TYR:O	2:y:189:VAL:HA	2.18	0.43
2:1:23:ASP:OD1	2:1:23:ASP:N	2.51	0.43
2:1:107:ILE:HG22	2:1:174:VAL:HB	1.99	0.43
6:K:70:LEU:HD23	6:K:178:ALA:HB1	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:240:PRO:HB2	6:K:276:ALA:HB2	2.00	0.43
6:K:288:ILE:HA	6:K:334:ASP:O	2.19	0.43
6:K:337:VAL:HG22	6:K:340:PRO:HD2	2.00	0.43
5:U:219:GLU:O	5:U:223:ILE:HG22	2.18	0.43
5:U:224:ASP:OD1	5:U:227:SER:OG	2.31	0.43
5:U:286:ARG:N	5:U:290:GLN:O	2.46	0.43
7:W:153:GLN:HB2	7:X:147:THR:HA	2.01	0.43
8:c:7:GLN:HG3	8:c:8:THR:N	2.33	0.43
8:d:18:LEU:HD21	2:z:18:THR:OG1	2.19	0.43
10:n:78:MET:HE2	10:n:78:MET:HB2	1.94	0.43
10:p:78:MET:HE3	10:p:78:MET:HB2	1.66	0.43
1:t:137:TYR:CE2	1:u:49:LYS:HD3	2.53	0.43
2:x:326:LEU:HB2	2:x:366:ILE:HG21	2.00	0.43
2:x:386:LEU:HD23	2:x:386:LEU:HA	1.91	0.43
1:0:459:LEU:O	1:0:463:THR:HG22	2.18	0.43
4:B:3:ASP:OD1	4:B:3:ASP:C	2.62	0.43
6:J:92:THR:OG1	6:J:164:ILE:O	2.37	0.43
6:L:192:PRO:HA	6:L:193:PRO:HD3	1.83	0.43
6:P:306:MET:HE2	6:P:321:ARG:HB3	1.99	0.43
5:U:248:ILE:HD11	5:U:266:GLU:HG2	2.00	0.43
1:s:123:LYS:C	1:s:125:ASP:H	2.25	0.43
1:s:349:SER:OG	1:s:350:SER:N	2.52	0.43
1:t:40:LYS:HD2	1:v:119:GLU:CD	2.44	0.43
1:u:162:VAL:HG22	1:u:422:GLN:HB3	2.00	0.43
1:0:424:THR:O	1:0:428:LEU:HG	2.18	0.43
4:E:60:GLY:O	4:E:64:ARG:HG2	2.17	0.43
5:G:186:VAL:HG23	5:G:189:GLU:H	1.83	0.43
6:K:42:GLN:NE2	6:O:42:GLN:HG2	2.34	0.43
6:M:42:GLN:OE1	8:f:39:ILE:HD11	2.19	0.43
6:P:92:THR:HG21	10:p:12:VAL:HG21	2.01	0.43
8:a:7:GLN:HG3	8:a:8:THR:N	2.34	0.43
1:s:450:PRO:HB2	2:x:362:GLY:HA3	2.00	0.43
1:u:302:ALA:O	1:u:306:THR:HG23	2.19	0.43
2:x:33:ALA:O	2:x:35:ARG:HG3	2.19	0.43
2:x:86:ARG:HE	2:x:86:ARG:HB3	1.57	0.43
2:z:122:TYR:CE2	2:z:127:ARG:HB3	2.53	0.43
2:2:386:LEU:HD21	2:z:14:ARG:NH1	2.34	0.43
2:3:42:GLY:O	2:3:94:PRO:HA	2.19	0.43
5:G:364:GLU:OE2	5:G:364:GLU:HA	2.17	0.43
6:H:243:ALA:O	6:H:246:GLU:HG3	2.19	0.43
5:N:91:ALA:HA	5:N:94:ILE:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:23:LEU:HD23	6:R:23:LEU:HA	1.87	0.43
5:U:38:ASN:OD1	1:u:52:TYR:OH	2.34	0.43
7:V:9:LEU:HD23	7:V:9:LEU:HA	1.92	0.43
7:V:133:ALA:HB3	7:X:141:THR:HG23	2.00	0.43
7:V:147:THR:HA	7:X:153:GLN:HB2	2.00	0.43
8:d:7:GLN:HG3	8:d:8:THR:N	2.33	0.43
8:e:14:LEU:HD23	8:e:14:LEU:HA	1.90	0.43
10:n:27:PHE:CE1	10:o:44:PHE:HB3	2.53	0.43
1:s:256:PHE:CE1	1:s:312:ALA:HB2	2.54	0.43
1:t:123:LYS:HE3	1:t:123:LYS:HB3	1.88	0.43
1:0:33:PHE:HB3	1:0:91:LEU:HD11	2.00	0.43
2:2:240:ASP:OD1	2:2:242:PRO:HD2	2.19	0.43
2:3:433:ILE:CD1	2:3:472:LEU:HD13	2.48	0.43
5:N:160:ARG:HA	5:N:160:ARG:HD3	1.53	0.43
5:N:191:LEU:O	1:s:53:PRO:HD2	2.18	0.43
7:V:17:MET:HG2	7:X:16:LEU:HD22	2.00	0.43
8:b:20:TRP:H	8:b:20:TRP:CD1	2.36	0.43
1:u:198:ILE:O	1:u:202:VAL:HG23	2.18	0.43
2:z:376:ASN:OD1	2:z:377:LYS:N	2.45	0.43
2:z:405:ILE:HD13	2:z:405:ILE:HA	1.85	0.43
2:2:491:VAL:HG22	4:D:124:ILE:HD12	2.00	0.43
3:4:29:PRO:HG3	3:5:66:LEU:HD13	2.01	0.43
5:G:144:ASP:HB2	5:G:147:GLU:HG3	2.00	0.43
6:J:240:PRO:HD2	6:J:277:PRO:HD2	2.00	0.43
5:N:212:TYR:HE1	5:N:229:VAL:HG23	1.84	0.43
6:T:294:GLU:OE1	6:T:294:GLU:N	2.50	0.43
7:V:17:MET:HG3	9:h:690:TRP:HA	2.00	0.43
10:l:12:VAL:HG22	2:x:204:ILE:HG12	2.01	0.43
1:s:459:LEU:O	1:s:463:THR:HG22	2.19	0.43
1:t:424:THR:O	1:t:428:LEU:HG	2.18	0.43
1:0:270:HIS:HA	1:0:273:THR:HG22	2.00	0.42
2:1:160:GLU:OE2	2:1:160:GLU:HA	2.19	0.42
2:2:411:ASN:OD1	2:2:411:ASN:N	2.51	0.42
4:B:58:TRP:CE2	8:b:15:PRO:HG3	2.54	0.42
5:G:165:THR:HG22	5:G:166:SER:H	1.84	0.42
6:H:95:THR:OG1	6:H:96:SER:N	2.52	0.42
6:K:115:TYR:HA	6:K:135:ALA:HA	2.00	0.42
6:K:232:MET:SD	6:K:235:ARG:NH2	2.92	0.42
6:L:239:PHE:CE1	6:L:277:PRO:HG2	2.54	0.42
6:L:239:PHE:HE1	6:L:277:PRO:HG2	1.84	0.42
5:N:10:ASP:HB2	5:N:52:LYS:HD2	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:U:294:PRO:HA	5:U:314:VAL:HG23	2.01	0.42
7:V:153:GLN:HB2	7:W:147:THR:HA	2.01	0.42
8:c:133:ILE:HD12	8:c:133:ILE:HA	1.93	0.42
1:0:123:LYS:C	1:0:125:ASP:H	2.26	0.42
2:1:93:ILE:HG21	2:1:222:SER:OG	2.19	0.42
2:1:306:THR:O	2:1:310:VAL:HG22	2.20	0.42
4:C:60:GLY:O	4:C:64:ARG:HG2	2.18	0.42
5:G:269:ARG:HD2	5:G:269:ARG:HA	1.79	0.42
6:H:238:ILE:HG22	6:H:238:ILE:O	2.19	0.42
7:V:106:ILE:CD1	7:W:106:ILE:HG23	2.48	0.42
7:W:196:MET:HB2	7:W:196:MET:HE3	1.80	0.42
10:k:77:ILE:HG22	10:l:78:MET:HE2	2.01	0.42
10:n:77:ILE:HG22	10:o:78:MET:SD	2.60	0.42
1:v:92:MET:HG2	1:v:118:TRP:CH2	2.54	0.42
1:v:193:GLY:HA3	1:v:269:ARG:HH12	1.83	0.42
1:w:201:ALA:HB2	1:w:262:LEU:HD21	2.00	0.42
2:y:184:LEU:HD11	2:y:237:PRO:O	2.20	0.42
1:0:148:GLU:HG2	1:0:149:THR:H	1.84	0.42
1:0:485:PRO:HB2	1:0:488:VAL:HG22	2.01	0.42
2:2:288:ILE:CG2	2:2:372:MET:HE3	2.49	0.42
2:3:40:MET:HE3	2:3:235:VAL:HG21	2.02	0.42
2:3:42:GLY:HA3	2:3:74:LEU:HD13	2.00	0.42
3:7:88:MET:HE2	3:7:88:MET:HB3	1.93	0.42
3:9:69:ILE:HG21	3:9:107:LEU:HD11	2.00	0.42
4:D:60:GLY:O	4:D:64:ARG:HG2	2.19	0.42
6:L:42:GLN:HE21	8:d:35:ILE:HG23	1.84	0.42
6:L:237:ASN:O	6:L:238:ILE:C	2.61	0.42
6:R:220:TRP:O	6:R:225:THR:HB	2.18	0.42
8:a:161:LEU:O	8:a:165:LYS:HB3	2.19	0.42
8:e:129:ASN:HB3	8:e:131:TYR:HE1	1.84	0.42
1:s:151:THR:HG22	1:s:433:ASP:HB2	2.00	0.42
1:s:424:THR:O	1:s:428:LEU:HG	2.19	0.42
1:t:170:LEU:HB2	1:t:299:VAL:HG21	2.00	0.42
2:x:230:GLN:HG3	2:x:262:ASP:H	1.84	0.42
2:z:411:ASN:OD1	2:z:411:ASN:N	2.52	0.42
5:G:29:VAL:O	5:G:29:VAL:HG12	2.18	0.42
6:J:156:VAL:HG12	6:J:157:ALA:N	2.34	0.42
6:J:306:MET:HE3	6:J:306:MET:HB3	1.90	0.42
6:L:335:PHE:CE1	6:S:320:SER:HB3	2.54	0.42
6:M:320:SER:O	6:M:323:ILE:HG22	2.19	0.42
5:N:264:LEU:O	5:N:265:ARG:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:228:VAL:HG23	6:R:274:VAL:HG13	2.01	0.42
5:U:29:VAL:HG23	9:g:683:GLY:HA3	2.01	0.42
5:U:150:TYR:CE1	5:U:154:VAL:HG21	2.54	0.42
5:U:214:ARG:HD2	5:U:253:LYS:HD3	2.00	0.42
10:k:55:LEU:HD21	10:k:69:GLN:OE1	2.20	0.42
1:w:123:LYS:C	1:w:125:ASP:H	2.26	0.42
2:3:303:TYR:OH	2:3:332:MET:O	2.34	0.42
2:3:435:THR:HG21	3:9:78:GLU:HG2	2.01	0.42
4:D:20:ILE:HD13	4:D:20:ILE:HA	1.91	0.42
5:G:254:ILE:HD11	5:G:259:ALA:HB2	2.02	0.42
6:M:239:PHE:CE1	6:M:277:PRO:HG2	2.54	0.42
6:S:5:PRO:HA	6:S:6:PRO:HD3	1.94	0.42
6:T:115:TYR:OH	6:T:142:GLY:O	2.37	0.42
5:U:313:LEU:HD23	5:U:339:PHE:CD2	2.55	0.42
8:b:7:GLN:HG3	8:b:8:THR:N	2.33	0.42
8:f:62:LEU:HD23	8:f:62:LEU:HA	1.88	0.42
1:s:269:ARG:C	1:s:271:ALA:N	2.77	0.42
1:s:449:LEU:HD23	1:s:449:LEU:HA	1.87	0.42
2:x:456:PHE:HE1	2:x:476:CYS:HB3	1.84	0.42
1:0:48:VAL:HG23	1:0:61:ASN:HB2	2.01	0.42
2:2:107:ILE:HG23	2:2:174:VAL:HB	2.01	0.42
2:2:306:THR:O	2:2:310:VAL:HG22	2.20	0.42
5:G:144:ASP:O	5:G:147:GLU:HB2	2.20	0.42
6:H:209:SER:O	6:H:247:ARG:NH2	2.53	0.42
6:K:359:TRP:CE3	6:K:359:TRP:HA	2.55	0.42
6:L:205:ALA:O	6:L:211:VAL:HG11	2.19	0.42
6:R:200:ASP:OD1	6:R:203:ARG:NH1	2.43	0.42
7:V:165:ASP:HB3	7:W:159:LYS:HA	2.01	0.42
10:p:81:ASN:HB2	10:q:78:MET:SD	2.59	0.42
1:t:256:PHE:CE1	1:t:312:ALA:HB2	2.54	0.42
1:v:158:GLN:HE21	1:v:162:VAL:HG23	1.84	0.42
2:z:236:MET:HE2	2:z:247:LEU:HD22	2.02	0.42
2:z:433:ILE:HD12	2:z:472:LEU:HD22	2.01	0.42
1:0:44:GLY:H	1:0:66:LYS:HG2	1.84	0.42
2:1:411:ASN:OD1	2:1:411:ASN:N	2.52	0.42
2:2:295:GLY:HA3	2:2:334:PRO:HB3	2.02	0.42
2:2:368:ARG:NH1	2:z:14:ARG:O	2.52	0.42
2:2:387:ASN:O	2:2:390:THR:OG1	2.37	0.42
3:8:58:ILE:HD11	3:8:107:LEU:HD22	2.01	0.42
6:O:79:VAL:HG21	6:O:185:LEU:HA	2.01	0.42
6:S:84:ALA:HB1	6:S:138:ALA:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:V:127:LYS:HB3	7:W:120:GLY:O	2.20	0.42
8:c:62:LEU:HA	8:c:62:LEU:HD23	1.79	0.42
10:o:12:VAL:HG22	2:z:204:ILE:HG12	2.00	0.42
1:s:472:LEU:HD11	1:s:492:VAL:HG22	2.01	0.42
1:u:320:LEU:HD12	1:u:437:ARG:HD2	2.02	0.42
1:v:280:ILE:HD12	1:v:280:ILE:HA	1.89	0.42
2:y:77:MET:SD	2:y:237:PRO:HG3	2.60	0.42
1:0:174:TRP:HB3	1:0:232:PRO:HB3	2.02	0.42
2:3:240:ASP:OD1	2:3:242:PRO:HD2	2.19	0.42
5:G:293:MET:HB3	5:G:294:PRO:HD2	2.01	0.42
6:I:238:ILE:HG22	6:I:239:PHE:N	2.34	0.42
6:L:228:VAL:HG13	6:L:274:VAL:HG13	2.01	0.42
6:M:42:GLN:HE21	8:f:35:ILE:HG23	1.85	0.42
5:N:214:ARG:HH11	5:N:253:LYS:HD2	1.84	0.42
6:O:145:GLY:H	6:O:148:THR:HG21	1.83	0.42
8:b:48:GLN:HE21	8:b:51:ARG:NH1	2.17	0.42
8:c:4:THR:HA	8:c:5:PRO:HD3	1.89	0.42
10:p:50:GLU:HA	10:p:50:GLU:OE1	2.19	0.42
1:0:332:ALA:HB2	4:E:65:ASP:HB2	2.01	0.42
1:0:472:LEU:HD11	1:0:492:VAL:HG22	2.01	0.42
6:K:287:TYR:HD2	6:K:336:GLU:HB3	1.84	0.42
6:M:149:LEU:HD12	6:M:164:ILE:HB	2.02	0.42
6:M:313:PRO:HG3	6:M:351:LEU:HB2	2.02	0.42
5:N:264:LEU:HD23	5:N:264:LEU:HA	1.86	0.42
6:Q:161:SER:O	6:Q:161:SER:OG	2.34	0.42
7:V:117:THR:HG22	7:V:118:LYS:N	2.35	0.42
8:e:163:LYS:HB3	8:e:163:LYS:HE3	1.81	0.42
8:f:66:GLU:OE2	8:f:84:ARG:NH1	2.53	0.42
10:k:108:ASP:HA	10:k:110:TYR:CE2	2.55	0.42
1:w:46:ARG:HG3	1:w:66:LYS:HG3	2.02	0.42
2:x:411:ASN:N	2:x:411:ASN:OD1	2.53	0.42
2:y:234:ILE:O	2:y:265:ALA:HA	2.20	0.42
1:0:256:PHE:CE1	1:0:312:ALA:HB2	2.54	0.42
3:4:78:GLU:CD	2:x:435:THR:HG21	2.44	0.42
4:A:58:TRP:CE2	8:a:15:PRO:HG3	2.55	0.42
6:K:212:THR:HG22	6:K:213:ARG:HG3	2.01	0.42
6:K:278:LYS:HB3	6:K:278:LYS:HE2	1.96	0.42
6:K:283:ASN:ND2	6:K:356:THR:O	2.47	0.42
6:L:200:ASP:HA	6:L:203:ARG:HG2	2.01	0.42
6:R:307:PHE:O	6:R:311:VAL:HB	2.20	0.42
6:T:84:ALA:HB1	6:T:138:ALA:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:W:52:ASP:O	7:W:53:GLU:HB2	2.20	0.42
10:l:89:LEU:O	10:l:92:ILE:HG12	2.20	0.42
2:y:166:GLY:O	2:y:170:THR:HA	2.20	0.42
2:y:368:ARG:NE	2:y:370:ILE:HD11	2.35	0.42
2:z:126:GLN:OE1	2:z:152:GLN:NE2	2.50	0.42
2:3:229:LEU:HD23	2:3:229:LEU:HA	1.94	0.41
3:7:13:ARG:NH1	3:7:18:GLU:OE2	2.53	0.41
5:N:80:MET:HB3	5:N:80:MET:HE3	1.85	0.41
5:N:313:LEU:HD23	5:N:339:PHE:CD2	2.55	0.41
8:c:27:LYS:HD3	8:c:27:LYS:HA	1.68	0.41
8:c:103:TYR:OH	8:c:164:TYR:O	2.26	0.41
8:e:149:LEU:HD23	8:e:149:LEU:HA	1.94	0.41
8:f:108:ALA:HA	8:f:112:PHE:O	2.20	0.41
10:m:29:GLU:OE2	10:n:41:MET:HG2	2.20	0.41
10:n:78:MET:SD	10:o:78:MET:HE2	2.60	0.41
1:t:450:PRO:HB2	2:y:362:GLY:HA3	2.01	0.41
2:x:306:THR:HG21	2:x:331:ARG:HH11	1.85	0.41
2:y:86:ARG:HE	2:y:86:ARG:HB3	1.56	0.41
2:z:307:LEU:HD11	2:z:366:ILE:HD12	2.02	0.41
1:0:228:LEU:HD23	1:0:228:LEU:HA	1.78	0.41
3:4:69:ILE:HG21	3:4:107:LEU:HD11	2.01	0.41
4:A:28:LEU:HD13	4:A:28:LEU:HA	1.92	0.41
4:E:100:LYS:HB3	4:E:100:LYS:HE3	1.80	0.41
6:I:286:ILE:HD12	6:I:357:ILE:CG2	2.50	0.41
6:I:289:SER:HB3	6:I:290:PRO:HD3	2.02	0.41
6:L:31:ARG:HH21	6:S:141:ALA:HA	1.85	0.41
6:M:237:ASN:O	6:M:238:ILE:C	2.63	0.41
5:U:146:SER:O	5:U:146:SER:OG	2.30	0.41
5:U:160:ARG:HD3	5:U:160:ARG:HA	1.58	0.41
10:j:73:SER:O	10:j:77:ILE:HG13	2.20	0.41
10:j:91:GLU:H	10:j:91:GLU:CD	2.28	0.41
10:k:19:GLN:NE2	10:k:21:SER:O	2.52	0.41
1:s:126:GLU:H	1:s:126:GLU:HG2	1.62	0.41
1:t:123:LYS:C	1:t:125:ASP:H	2.28	0.41
1:t:126:GLU:OE1	1:t:129:TYR:HD2	2.03	0.41
1:v:438:GLY:O	1:v:475:ARG:NH2	2.54	0.41
2:x:341:THR:OG1	2:x:342:TRP:N	2.53	0.41
2:y:466:LYS:HE3	2:y:466:LYS:HB3	1.84	0.41
1:0:265:ARG:HA	1:0:268:ARG:HD2	2.01	0.41
2:2:285:ASP:OD1	2:2:285:ASP:C	2.63	0.41
2:3:93:ILE:HG21	2:3:222:SER:OG	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:8:69:ILE:HG21	3:8:107:LEU:HD11	2.01	0.41
4:E:14:ASP:OD1	4:E:14:ASP:C	2.63	0.41
6:I:91:LEU:HD22	6:I:133:VAL:HG11	2.02	0.41
6:R:257:ASP:HB3	6:R:260:THR:O	2.19	0.41
6:S:278:LYS:HD2	6:S:350:GLU:HG2	2.02	0.41
5:U:314:VAL:HG12	5:U:333:LEU:CD2	2.50	0.41
8:d:108:ALA:HA	8:d:112:PHE:O	2.21	0.41
10:m:14:PRO:HA	10:m:15:PRO:HD3	1.95	0.41
1:s:211:VAL:HG12	1:s:249:LEU:HD13	2.03	0.41
1:t:52:TYR:CD2	1:t:55:ARG:HD3	2.54	0.41
1:u:262:LEU:HA	1:u:262:LEU:HD23	1.82	0.41
1:w:331:ARG:HH22	1:w:467:ARG:NH1	2.18	0.41
2:y:244:LEU:HD12	2:y:288:ILE:HD13	2.02	0.41
2:z:236:MET:HE1	2:z:244:LEU:CD2	2.51	0.41
4:E:50:ASP:OD1	2:z:325:THR:HG22	2.20	0.41
6:I:107:TRP:CD1	6:I:152:LEU:HD13	2.55	0.41
6:J:267:PRO:HA	6:S:196:GLY:O	2.20	0.41
6:K:339:PHE:HB3	6:K:340:PRO:HD3	2.03	0.41
6:L:42:GLN:OE1	8:d:39:ILE:HD11	2.19	0.41
6:L:197:ASN:H	6:L:200:ASP:HB2	1.85	0.41
5:N:62:ILE:HD12	1:s:360:LEU:HD13	2.01	0.41
6:O:81:ARG:HG3	6:O:181:LEU:HD22	2.03	0.41
6:Q:27:TRP:HE3	6:Q:31:ARG:HH21	1.68	0.41
5:U:78:ASP:OD1	5:U:78:ASP:C	2.64	0.41
8:a:35:ILE:HD13	8:a:35:ILE:HA	1.80	0.41
10:n:27:PHE:CZ	10:o:4:ILE:HD11	2.56	0.41
10:p:46:ILE:O	10:p:50:GLU:HG2	2.20	0.41
1:s:122:THR:OG1	1:s:123:LYS:N	2.53	0.41
1:t:46:ARG:NH2	1:u:51:GLU:HB3	2.35	0.41
1:t:459:LEU:O	1:t:463:THR:HG22	2.20	0.41
1:w:36:ILE:HD12	1:w:36:ILE:HA	1.88	0.41
2:x:469:LYS:HA	2:x:469:LYS:HD3	1.77	0.41
1:0:155:VAL:HB	1:0:156:PRO:HD3	2.02	0.41
4:D:63:TYR:O	1:v:333:PRO:HD3	2.21	0.41
4:D:139:LYS:HG2	2:z:21:GLU:HG3	2.03	0.41
5:G:93:LEU:HB3	5:G:149:VAL:HB	2.03	0.41
5:G:100:TYR:CE2	6:J:154:THR:HG21	2.51	0.41
5:G:129:LEU:HD11	5:G:162:VAL:HG13	2.03	0.41
6:I:286:ILE:HD12	6:I:357:ILE:HG23	2.01	0.41
10:j:55:LEU:HD23	10:j:73:SER:HB2	2.03	0.41
1:t:69:SER:O	1:t:69:SER:OG	2.31	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:t:185:THR:O	1:t:189:GLU:HG2	2.20	0.41
1:u:183:ALA:HB1	1:u:289:ALA:HB2	2.02	0.41
2:x:288:ILE:O	2:x:372:MET:HG3	2.20	0.41
6:H:260:THR:HG23	6:H:262:LEU:H	1.86	0.41
8:c:77:GLU:HG3	8:c:83:GLU:HG3	2.02	0.41
10:j:1:MET:O	10:j:64:LYS:NZ	2.45	0.41
1:t:228:LEU:O	1:t:229:ILE:C	2.61	0.41
1:u:462:PHE:HD2	1:u:492:VAL:HG21	1.86	0.41
1:w:178:LYS:HB3	1:w:178:LYS:HE2	1.87	0.41
2:y:35:ARG:HH12	2:y:37:ARG:CZ	2.34	0.41
2:2:469:LYS:HA	2:2:469:LYS:HD3	1.93	0.41
3:7:29:PRO:HG3	3:8:66:LEU:HD13	2.02	0.41
4:C:121:TYR:HE1	4:C:123:TYR:HB2	1.86	0.41
4:E:42:ALA:HB2	4:E:73:TRP:CZ2	2.56	0.41
4:E:110:VAL:HA	4:E:123:TYR:O	2.21	0.41
5:G:10:ASP:HB2	5:G:52:LYS:HD2	2.02	0.41
5:G:224:ASP:OD1	5:G:224:ASP:N	2.46	0.41
6:H:107:TRP:HZ3	6:H:117:LEU:HB2	1.85	0.41
6:H:147:ASN:HA	6:H:165:THR:O	2.21	0.41
6:K:42:GLN:HE21	8:b:35:ILE:HG23	1.85	0.41
6:M:18:ASN:HB3	8:f:34:ALA:HB1	2.02	0.41
5:N:146:SER:O	7:V:18:ARG:NE	2.53	0.41
5:U:211:GLY:HA3	5:U:254:ILE:HG21	2.02	0.41
7:X:80:GLN:C	7:X:82:ASP:H	2.29	0.41
8:f:20:TRP:CD1	8:f:20:TRP:H	2.38	0.41
1:0:120:CYS:HA	1:0:131:ALA:O	2.20	0.41
2:3:281:VAL:HG13	2:3:374:ARG:NH1	2.36	0.41
3:4:115:LYS:HE3	2:x:453:PHE:CZ	2.55	0.41
3:5:112:LYS:HE3	3:5:112:LYS:HB2	1.91	0.41
3:7:65:GLY:O	3:7:69:ILE:HG13	2.21	0.41
3:8:29:PRO:HG3	3:9:66:LEU:HD13	2.02	0.41
6:I:81:ARG:HD2	1:t:207:VAL:O	2.21	0.41
6:I:194:PHE:HE1	8:c:102:PHE:HE2	1.68	0.41
6:K:192:PRO:HA	6:K:193:PRO:HD3	1.84	0.41
6:M:212:THR:HG22	6:M:213:ARG:HG3	2.02	0.41
8:c:69:LEU:HD23	8:c:91:LYS:HG2	2.01	0.41
8:d:131:TYR:CZ	8:d:176:HIS:HD2	2.39	0.41
10:j:29:GLU:CD	10:k:41:MET:HG2	2.45	0.41
10:m:105:GLU:HG2	10:m:110:TYR:HE1	1.86	0.41
1:s:69:SER:O	1:s:69:SER:OG	2.35	0.41
1:s:142:ASP:OD2	1:w:57:THR:HG21	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:u:118:TRP:HB3	1:u:134:VAL:HG22	2.03	0.41
1:u:166:LEU:O	1:u:169:THR:HG22	2.21	0.41
1:0:60:VAL:HG22	1:w:138:PRO:O	2.20	0.41
1:0:198:ILE:HG22	1:0:218:LEU:HD21	2.03	0.41
1:0:433:ASP:OD1	1:0:433:ASP:C	2.64	0.41
2:1:355:THR:OG1	2:1:367:GLU:OE1	2.28	0.41
2:2:408:LYS:NZ	2:2:436:GLU:OE1	2.53	0.41
2:3:82:LEU:HD23	2:3:82:LEU:HA	1.92	0.41
2:3:487:PHE:HB3	2:x:18:THR:HG22	2.03	0.41
6:I:232:MET:O	6:I:238:ILE:HA	2.21	0.41
6:J:177:SER:OG	6:J:180:GLU:HG3	2.20	0.41
6:K:310:GLU:OE1	6:K:321:ARG:NH1	2.54	0.41
6:M:57:GLY:C	6:M:59:GLN:H	2.29	0.41
6:M:85:THR:OG1	6:M:171:GLY:O	2.37	0.41
6:M:94:THR:HA	6:M:128:THR:HA	2.03	0.41
6:M:193:PRO:HD2	8:f:95:THR:HG22	2.03	0.41
6:M:335:PHE:CE1	6:T:320:SER:HB3	2.55	0.41
6:O:144:THR:HB	6:O:148:THR:HG21	2.02	0.41
6:R:93:VAL:H	6:R:130:GLU:HG2	1.86	0.41
5:U:186:VAL:HG23	5:U:189:GLU:H	1.86	0.41
7:V:105:GLY:O	7:X:63:PHE:CD1	2.74	0.41
8:b:4:THR:HA	8:b:5:PRO:HD3	1.94	0.41
8:c:158:GLU:O	8:c:162:GLU:HG2	2.21	0.41
10:j:14:PRO:HA	10:j:15:PRO:HD3	1.97	0.41
10:n:55:LEU:HD21	10:n:69:GLN:OE1	2.20	0.41
10:p:13:MET:HB2	10:r:26:TRP:CG	2.55	0.41
10:p:55:LEU:HD23	10:p:55:LEU:HA	1.84	0.41
1:s:56:ASP:HB3	1:u:65:LYS:HE2	2.01	0.41
1:s:262:LEU:HD23	1:s:262:LEU:HA	1.83	0.41
1:s:284:TYR:CD1	1:s:284:TYR:N	2.89	0.41
2:z:106:GLU:HG2	2:z:175:VAL:HG22	2.01	0.41
2:z:469:LYS:HD3	2:z:469:LYS:HA	1.79	0.41
1:0:142:ASP:OD2	1:v:57:THR:HG21	2.20	0.41
2:3:270:SER:HA	2:3:293:ILE:HG22	2.03	0.41
3:5:7:GLN:HG2	3:6:103:GLY:HA2	2.03	0.41
4:A:60:GLY:O	4:A:64:ARG:HG2	2.21	0.41
6:H:289:SER:HB3	6:H:290:PRO:HD3	2.02	0.41
6:M:278:LYS:HB2	6:M:278:LYS:HE3	1.82	0.41
6:O:123:ILE:HD13	6:O:123:ILE:HA	1.93	0.41
6:Q:51:GLU:HB3	1:w:481:PRO:HG3	2.03	0.41
6:Q:60:ILE:HG13	6:Q:61:ILE:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:136:LEU:HD23	6:R:136:LEU:O	2.22	0.41
6:S:334:ASP:OD1	6:S:335:PHE:N	2.54	0.41
10:q:55:LEU:HD21	10:q:69:GLN:OE1	2.21	0.41
2:x:101:ASN:OD1	2:x:101:ASN:N	2.50	0.41
1:0:326:MET:SD	5:G:61:GLN:NE2	2.93	0.40
2:3:18:THR:HG21	4:E:37:PHE:CE1	2.56	0.40
4:E:30:THR:HA	4:E:33:THR:HG22	2.03	0.40
6:I:319:PRO:HB3	6:I:340:PRO:O	2.21	0.40
6:M:35:LEU:HD23	6:M:35:LEU:HA	1.94	0.40
5:N:22:VAL:HG11	5:N:63:VAL:HG11	2.03	0.40
5:N:29:VAL:HG23	9:i:683:GLY:HA3	2.04	0.40
6:Q:174:ASP:OD1	6:Q:174:ASP:N	2.39	0.40
6:Q:196:GLY:HA3	6:Q:267:PRO:HD3	2.03	0.40
6:R:7:THR:HG23	1:t:341:THR:HA	2.03	0.40
7:V:141:THR:HG23	7:W:133:ALA:HB3	2.04	0.40
8:a:116:LEU:HD22	8:a:128:VAL:HG22	2.02	0.40
8:b:116:LEU:HD22	8:b:128:VAL:HG13	2.03	0.40
8:c:172:LYS:HD3	8:c:172:LYS:HA	1.93	0.40
8:f:131:TYR:CZ	8:f:176:HIS:HD2	2.39	0.40
1:s:384:PRO:HG3	1:s:387:PHE:HD2	1.87	0.40
1:w:100:SER:HB3	1:w:114:MET:HG3	2.02	0.40
2:x:17:LEU:HD12	2:x:17:LEU:HA	1.94	0.40
2:y:348:LEU:HD23	2:y:355:THR:HG22	2.02	0.40
2:y:411:ASN:OD1	2:y:411:ASN:N	2.52	0.40
2:z:101:ASN:OD1	2:z:101:ASN:N	2.49	0.40
2:1:85:ASN:HB2	2:1:309:ALA:HB1	2.03	0.40
6:I:230:PHE:CE2	6:I:232:MET:HE3	2.54	0.40
6:I:260:THR:HG23	6:I:262:LEU:H	1.86	0.40
6:J:321:ARG:HG3	6:J:321:ARG:HH11	1.86	0.40
6:K:269:GLY:HA3	6:O:270:VAL:HG11	2.03	0.40
6:L:320:SER:O	6:L:323:ILE:HG22	2.21	0.40
5:N:323:ASP:OD1	5:N:323:ASP:C	2.64	0.40
6:T:317:LEU:HD23	6:T:317:LEU:HA	1.93	0.40
5:U:172:LEU:HD23	5:U:172:LEU:HA	1.90	0.40
8:d:20:TRP:CD1	8:d:20:TRP:H	2.37	0.40
8:e:161:LEU:O	8:e:165:LYS:HB3	2.21	0.40
10:j:107:LEU:HD23	10:j:107:LEU:HA	1.85	0.40
1:s:118:TRP:HA	1:s:133:THR:O	2.21	0.40
1:t:433:ASP:OD1	1:t:433:ASP:C	2.64	0.40
1:u:211:VAL:HG12	1:u:249:LEU:HD13	2.03	0.40
1:w:262:LEU:HD23	1:w:262:LEU:HA	1.81	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:x:3:ASP:HB3	2:x:4:ILE:H	1.66	0.40
2:x:90:LEU:HD23	2:x:90:LEU:HA	1.90	0.40
2:x:464:ARG:HE	2:x:464:ARG:HB3	1.75	0.40
2:z:35:ARG:HH12	2:z:37:ARG:CZ	2.34	0.40
2:z:291:MET:SD	2:z:356:PHE:HB3	2.62	0.40
1:0:461:ARG:HE	1:0:461:ARG:HB3	1.61	0.40
2:3:254:ARG:HB3	2:3:261:ALA:O	2.20	0.40
2:3:470:ASP:OD1	2:3:470:ASP:N	2.45	0.40
3:4:66:LEU:HD13	3:9:29:PRO:HG3	2.04	0.40
3:8:41:ARG:CZ	1:s:23:THR:HA	2.52	0.40
4:C:65:ASP:HB2	1:t:332:ALA:HB2	2.02	0.40
5:G:150:TYR:CE1	5:G:154:VAL:HG21	2.56	0.40
6:H:100:THR:HG22	6:H:122:VAL:HG23	2.03	0.40
6:I:192:PRO:HA	6:I:193:PRO:HD3	1.89	0.40
6:M:197:ASN:H	6:M:200:ASP:HB2	1.87	0.40
5:N:52:LYS:HD3	5:N:52:LYS:HA	1.96	0.40
5:N:58:ILE:HG21	5:N:291:LEU:HD21	2.04	0.40
6:P:91:LEU:HD23	6:P:91:LEU:HA	1.86	0.40
6:S:106:ARG:HG3	6:S:153:ILE:HD11	2.03	0.40
7:W:127:LYS:HB3	7:X:120:GLY:O	2.21	0.40
8:b:53:ARG:HE	8:b:53:ARG:HB2	1.69	0.40
10:q:14:PRO:HA	10:q:15:PRO:HD3	1.96	0.40
1:s:269:ARG:C	1:s:271:ALA:H	2.29	0.40
2:y:122:TYR:CE2	2:y:127:ARG:HB3	2.56	0.40
2:z:3:ASP:HB3	2:z:4:ILE:H	1.63	0.40
1:0:52:TYR:CD2	1:0:55:ARG:HD3	2.56	0.40
1:0:102:GLU:OE2	4:D:71:ARG:NH1	2.50	0.40
1:0:208:THR:HG22	6:J:71:LEU:HD13	2.03	0.40
2:1:22:PHE:CD2	2:x:491:VAL:HB	2.56	0.40
4:B:63:TYR:O	1:u:333:PRO:HD3	2.22	0.40
5:G:80:MET:O	1:v:50:ARG:NH1	2.54	0.40
5:G:185:LEU:HD23	5:G:191:LEU:HD21	2.03	0.40
6:J:256:THR:HG22	6:J:263:ILE:HG22	2.03	0.40
6:J:322:ILE:H	6:J:322:ILE:HG12	1.74	0.40
6:P:227:GLY:HA2	6:P:273:THR:HG22	2.04	0.40
1:0:116:ASP:HB3	1:0:135:THR:HG23	2.04	0.40
1:0:225:VAL:HA	1:0:228:LEU:HB2	2.03	0.40
1:0:243:LEU:HD23	1:0:243:LEU:HA	1.95	0.40
1:0:463:THR:HG23	1:0:465:ASN:H	1.86	0.40
2:1:236:MET:O	2:1:267:THR:HG22	2.22	0.40
2:1:487:PHE:HB3	2:y:18:THR:HG22	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:491:VAL:HG22	4:B:124:ILE:HD12	2.03	0.40
2:2:49:SER:O	2:2:49:SER:OG	2.35	0.40
3:7:89:LEU:HD12	3:7:111:ALA:HB3	2.03	0.40
4:C:41:ARG:HA	4:C:56:ARG:O	2.20	0.40
6:H:194:PHE:HE1	8:a:102:PHE:HE2	1.70	0.40
6:L:61:ILE:CD1	8:d:64:GLU:HB3	2.52	0.40
6:L:306:MET:HE2	6:L:321:ARG:C	2.47	0.40
6:M:288:ILE:HG23	6:M:332:LEU:HB2	2.02	0.40
5:N:224:ASP:OD1	5:N:227:SER:OG	2.22	0.40
6:R:35:LEU:HD23	6:R:35:LEU:HA	1.98	0.40
6:R:188:ARG:HA	6:R:260:THR:HG22	2.03	0.40
6:T:92:THR:HB	6:T:164:ILE:HG23	2.03	0.40
6:T:93:VAL:HG22	6:T:159:VAL:HG21	2.04	0.40
5:U:144:ASP:O	5:U:147:GLU:HB2	2.20	0.40
7:X:117:THR:CG2	7:X:118:LYS:H	2.35	0.40
8:d:94:MET:HB2	8:d:94:MET:HE2	1.80	0.40
8:d:130:ILE:HD12	8:d:130:ILE:N	2.37	0.40
1:t:36:ILE:HG23	1:t:37:GLU:HG2	2.04	0.40
1:t:142:ASP:OD2	1:u:57:THR:HG21	2.21	0.40
1:t:263:ALA:O	1:t:264:GLN:C	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	440/495 (89%)	417 (95%)	23 (5%)	0	100	100
1	s	440/495 (89%)	414 (94%)	26 (6%)	0	100	100
1	t	440/495 (89%)	406 (92%)	33 (8%)	1 (0%)	43	71
1	u	413/495 (83%)	397 (96%)	16 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	v	413/495 (83%)	395 (96%)	18 (4%)	0	100	100
1	w	413/495 (83%)	395 (96%)	18 (4%)	0	100	100
2	1	491/495 (99%)	469 (96%)	22 (4%)	0	100	100
2	2	491/495 (99%)	470 (96%)	21 (4%)	0	100	100
2	3	491/495 (99%)	469 (96%)	22 (4%)	0	100	100
2	x	491/495 (99%)	459 (94%)	32 (6%)	0	100	100
2	y	491/495 (99%)	455 (93%)	36 (7%)	0	100	100
2	z	491/495 (99%)	458 (93%)	33 (7%)	0	100	100
3	4	113/118 (96%)	104 (92%)	9 (8%)	0	100	100
3	5	113/118 (96%)	106 (94%)	7 (6%)	0	100	100
3	6	113/118 (96%)	105 (93%)	8 (7%)	0	100	100
3	7	113/118 (96%)	106 (94%)	7 (6%)	0	100	100
3	8	113/118 (96%)	102 (90%)	11 (10%)	0	100	100
3	9	113/118 (96%)	107 (95%)	6 (5%)	0	100	100
4	A	141/145 (97%)	133 (94%)	8 (6%)	0	100	100
4	B	141/145 (97%)	136 (96%)	5 (4%)	0	100	100
4	C	141/145 (97%)	136 (96%)	5 (4%)	0	100	100
4	D	141/145 (97%)	136 (96%)	5 (4%)	0	100	100
4	E	141/145 (97%)	135 (96%)	6 (4%)	0	100	100
4	F	141/145 (97%)	135 (96%)	6 (4%)	0	100	100
5	G	362/379 (96%)	349 (96%)	13 (4%)	0	100	100
5	N	362/379 (96%)	350 (97%)	12 (3%)	0	100	100
5	U	362/379 (96%)	350 (97%)	12 (3%)	0	100	100
6	H	354/360 (98%)	343 (97%)	10 (3%)	1 (0%)	36	65
6	I	354/360 (98%)	341 (96%)	13 (4%)	0	100	100
6	J	354/360 (98%)	344 (97%)	9 (2%)	1 (0%)	36	65
6	K	354/360 (98%)	340 (96%)	13 (4%)	1 (0%)	36	65
6	L	354/360 (98%)	341 (96%)	13 (4%)	0	100	100
6	M	354/360 (98%)	341 (96%)	13 (4%)	0	100	100
6	O	357/360 (99%)	339 (95%)	18 (5%)	0	100	100
6	P	357/360 (99%)	342 (96%)	15 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	Q	357/360 (99%)	342 (96%)	15 (4%)	0	100	100
6	R	337/360 (94%)	323 (96%)	14 (4%)	0	100	100
6	S	337/360 (94%)	327 (97%)	10 (3%)	0	100	100
6	T	337/360 (94%)	327 (97%)	10 (3%)	0	100	100
7	V	192/197 (98%)	170 (88%)	22 (12%)	0	100	100
7	W	192/197 (98%)	172 (90%)	20 (10%)	0	100	100
7	X	192/197 (98%)	174 (91%)	18 (9%)	0	100	100
8	a	172/180 (96%)	161 (94%)	11 (6%)	0	100	100
8	b	146/180 (81%)	140 (96%)	6 (4%)	0	100	100
8	c	172/180 (96%)	164 (95%)	8 (5%)	0	100	100
8	d	146/180 (81%)	138 (94%)	8 (6%)	0	100	100
8	e	172/180 (96%)	165 (96%)	7 (4%)	0	100	100
8	f	146/180 (81%)	139 (95%)	7 (5%)	0	100	100
9	g	15/690 (2%)	15 (100%)	0	0	100	100
9	h	15/690 (2%)	15 (100%)	0	0	100	100
9	i	15/690 (2%)	14 (93%)	1 (7%)	0	100	100
10	j	104/504 (21%)	102 (98%)	2 (2%)	0	100	100
10	k	104/504 (21%)	100 (96%)	4 (4%)	0	100	100
10	l	104/504 (21%)	102 (98%)	2 (2%)	0	100	100
10	m	104/504 (21%)	102 (98%)	2 (2%)	0	100	100
10	n	104/504 (21%)	99 (95%)	5 (5%)	0	100	100
10	o	104/504 (21%)	102 (98%)	2 (2%)	0	100	100
10	p	104/504 (21%)	101 (97%)	3 (3%)	0	100	100
10	q	104/504 (21%)	99 (95%)	5 (5%)	0	100	100
10	r	104/504 (21%)	102 (98%)	2 (2%)	0	100	100
All	All	14832/21252 (70%)	14120 (95%)	708 (5%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	t	270	HIS
6	K	234	ASN
6	J	238	ILE

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Mol	Chain	Res	Type
6	H	238	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	353/391 (90%)	353 (100%)	0	100	100
1	s	353/391 (90%)	344 (98%)	9 (2%)	42	64
1	t	353/391 (90%)	348 (99%)	5 (1%)	59	73
1	u	333/391 (85%)	332 (100%)	1 (0%)	86	86
1	v	333/391 (85%)	332 (100%)	1 (0%)	86	86
1	w	333/391 (85%)	331 (99%)	2 (1%)	78	81
2	1	391/394 (99%)	391 (100%)	0	100	100
2	2	391/394 (99%)	391 (100%)	0	100	100
2	3	391/394 (99%)	390 (100%)	1 (0%)	86	86
2	x	391/394 (99%)	391 (100%)	0	100	100
2	y	391/394 (99%)	391 (100%)	0	100	100
2	z	391/394 (99%)	391 (100%)	0	100	100
3	4	91/92 (99%)	91 (100%)	0	100	100
3	5	91/92 (99%)	91 (100%)	0	100	100
3	6	91/92 (99%)	90 (99%)	1 (1%)	65	76
3	7	91/92 (99%)	91 (100%)	0	100	100
3	8	91/92 (99%)	91 (100%)	0	100	100
3	9	91/92 (99%)	91 (100%)	0	100	100
4	A	118/120 (98%)	117 (99%)	1 (1%)	73	79
4	B	118/120 (98%)	115 (98%)	3 (2%)	42	64
4	C	118/120 (98%)	118 (100%)	0	100	100
4	D	118/120 (98%)	117 (99%)	1 (1%)	73	79
4	E	118/120 (98%)	118 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
4	F	118/120 (98%)	116 (98%)	2 (2%)	53	71	
5	G	300/313 (96%)	300 (100%)	0	100	100	
5	N	300/313 (96%)	300 (100%)	0	100	100	
5	U	300/313 (96%)	296 (99%)	4 (1%)	61	74	
6	H	283/286 (99%)	280 (99%)	3 (1%)	65	76	
6	I	283/286 (99%)	282 (100%)	1 (0%)	84	84	
6	J	283/286 (99%)	280 (99%)	3 (1%)	65	76	
6	K	283/286 (99%)	280 (99%)	3 (1%)	65	76	
6	L	283/286 (99%)	279 (99%)	4 (1%)	59	73	
6	M	283/286 (99%)	280 (99%)	3 (1%)	65	76	
6	O	284/286 (99%)	284 (100%)	0	100	100	
6	P	284/286 (99%)	283 (100%)	1 (0%)	84	84	
6	Q	284/286 (99%)	284 (100%)	0	100	100	
6	R	273/286 (96%)	272 (100%)	1 (0%)	84	84	
6	S	273/286 (96%)	271 (99%)	2 (1%)	76	80	
6	T	273/286 (96%)	271 (99%)	2 (1%)	76	80	
7	V	162/166 (98%)	160 (99%)	2 (1%)	63	75	
7	W	162/166 (98%)	161 (99%)	1 (1%)	78	81	
7	X	162/166 (98%)	160 (99%)	2 (1%)	63	75	
8	a	147/152 (97%)	147 (100%)	0	100	100	
8	b	125/152 (82%)	125 (100%)	0	100	100	
8	c	147/152 (97%)	146 (99%)	1 (1%)	76	80	
8	d	125/152 (82%)	125 (100%)	0	100	100	
8	e	147/152 (97%)	147 (100%)	0	100	100	
8	f	125/152 (82%)	125 (100%)	0	100	100	
9	g	12/520 (2%)	12 (100%)	0	100	100	
9	h	12/520 (2%)	12 (100%)	0	100	100	
9	i	12/520 (2%)	12 (100%)	0	100	100	
10	j	90/412 (22%)	89 (99%)	1 (1%)	65	76	
10	k	90/412 (22%)	90 (100%)	0	100	100	
10	l	90/412 (22%)	90 (100%)	0	100	100	

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	m	90/412 (22%)	90 (100%)	0	100	100
10	n	90/412 (22%)	90 (100%)	0	100	100
10	o	90/412 (22%)	90 (100%)	0	100	100
10	p	90/412 (22%)	89 (99%)	1 (1%)	65	76
10	q	90/412 (22%)	90 (100%)	0	100	100
10	r	90/412 (22%)	90 (100%)	0	100	100
All	All	12075/17031 (71%)	12013 (100%)	62 (0%)	78	83

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	3	287	LEU
3	6	14	VAL
4	A	28	LEU
4	B	54	ASP
4	B	68	ILE
4	B	84	THR
4	D	68	ILE
4	F	31	ASP
4	F	133	VAL
6	H	147	ASN
6	H	236	SER
6	H	238	ILE
6	I	232	MET
6	J	147	ASN
6	J	296	LYS
6	J	332	LEU
6	K	150	LEU
6	K	357	ILE
6	K	359	TRP
6	L	149	LEU
6	L	150	LEU
6	L	233	ASP
6	L	235	ARG
6	M	150	LEU
6	M	151	THR
6	M	358	GLU
6	P	231	VAL
6	R	232	MET
6	S	8	LEU

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Mol	Chain	Res	Type
6	S	232	MET
6	T	232	MET
6	T	278	LYS
5	U	29	VAL
5	U	37	VAL
5	U	264	LEU
5	U	276	THR
7	V	126	CYS
7	V	167	ASN
7	W	196	MET
7	X	106	ILE
7	X	144	THR
8	c	48	GLN
10	j	78	MET
10	p	78	MET
1	s	36	ILE
1	s	221	MET
1	s	273	THR
1	s	284	TYR
1	s	288	VAL
1	s	300	MET
1	s	301	LEU
1	s	360	LEU
1	s	362	LEU
1	t	264	GLN
1	t	284	TYR
1	t	288	VAL
1	t	362	LEU
1	t	383	THR
1	u	418	THR
1	v	170	LEU
1	w	48	VAL
1	w	170	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (110) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	204	ASN
1	0	231	GLN
1	0	448	HIS
2	1	365	GLN
2	1	482	ASN

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Mol	Chain	Res	Type
2	2	24	ASN
2	2	70	GLN
2	2	482	ASN
2	3	24	ASN
2	3	26	ASN
2	3	70	GLN
2	3	346	ASN
2	3	387	ASN
2	3	482	ASN
3	7	113	GLN
3	9	113	GLN
4	A	17	GLN
4	B	10	ASN
4	B	116	HIS
4	D	10	ASN
4	D	17	GLN
6	H	147	ASN
6	I	59	GLN
6	I	237	ASN
6	I	297	GLN
6	J	59	GLN
6	J	143	ASN
6	J	147	ASN
6	K	42	GLN
6	K	241	GLN
6	L	42	GLN
6	M	42	GLN
6	M	234	ASN
6	M	241	GLN
6	M	266	GLN
6	M	283	ASN
5	N	260	GLN
6	O	73	HIS
6	O	241	GLN
6	Q	17	GLN
6	Q	21	GLN
6	Q	237	ASN
6	R	29	GLN
6	R	283	ASN
6	R	309	ASN
6	S	29	GLN
6	S	283	ASN

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Mol	Chain	Res	Type
6	S	309	ASN
6	T	29	GLN
6	T	283	ASN
6	T	309	ASN
7	V	39	GLN
7	V	59	ASN
7	V	98	ASN
7	V	112	HIS
7	W	59	ASN
7	W	98	ASN
7	W	109	HIS
7	W	112	HIS
7	X	59	ASN
7	X	98	ASN
7	X	108	HIS
7	X	109	HIS
7	X	112	HIS
8	b	48	GLN
8	b	129	ASN
8	c	90	ASN
8	c	135	ASN
8	d	85	GLN
8	d	127	GLN
8	d	129	ASN
8	f	12	GLN
8	f	127	GLN
8	f	129	ASN
9	h	679	ASN
9	i	679	ASN
10	j	87	ASN
10	k	88	ASN
10	m	6	ASN
10	m	53	ASN
10	m	80	ASN
10	m	81	ASN
10	m	88	ASN
10	n	48	GLN
10	n	88	ASN
10	o	6	ASN
10	p	88	ASN
10	r	106	ASN
1	s	78	ASN

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Mol	Chain	Res	Type
1	s	204	ASN
1	s	231	GLN
1	s	270	HIS
1	s	297	ASN
1	s	448	HIS
1	t	158	GLN
1	t	297	ASN
1	t	422	GLN
1	u	414	GLN
1	v	175	GLN
1	w	61	ASN
1	w	175	GLN
1	w	285	ASN
2	x	26	ASN
2	x	43	GLN
2	x	482	ASN
2	y	26	ASN
2	y	387	ASN
2	y	482	ASN
2	z	365	GLN
2	z	482	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

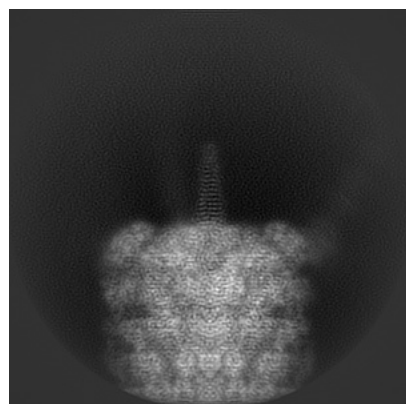
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62362. These allow visual inspection of the internal detail of the map and identification of artifacts.

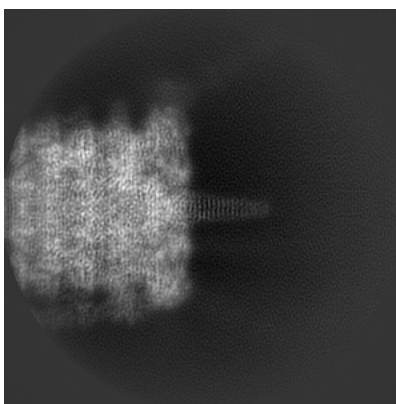
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

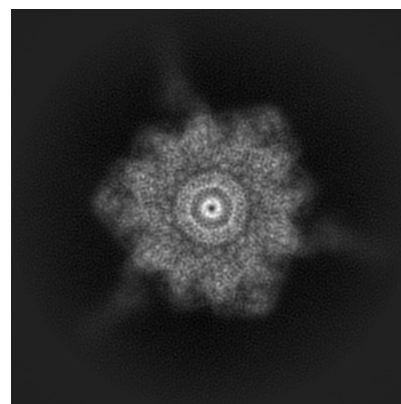
6.1.1 Primary map



X

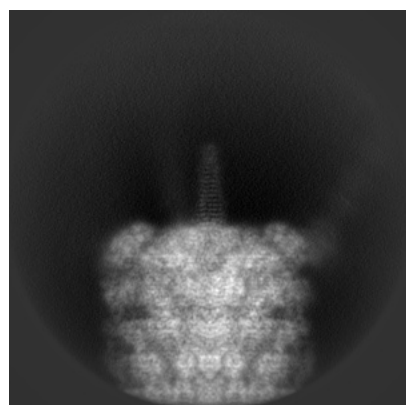


Y

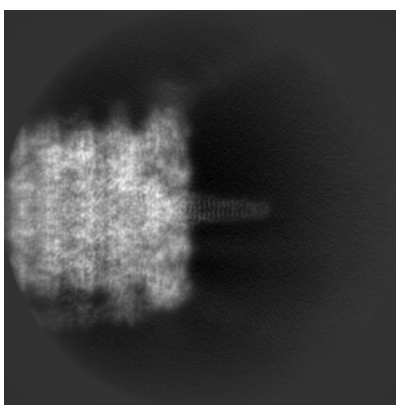


Z

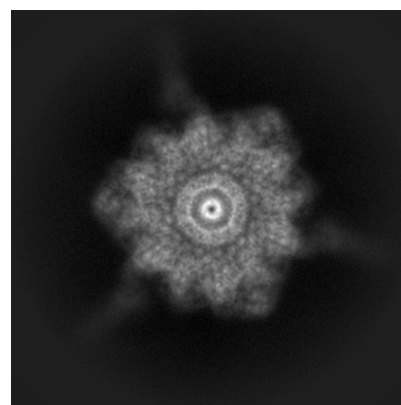
6.1.2 Raw map



X



Y

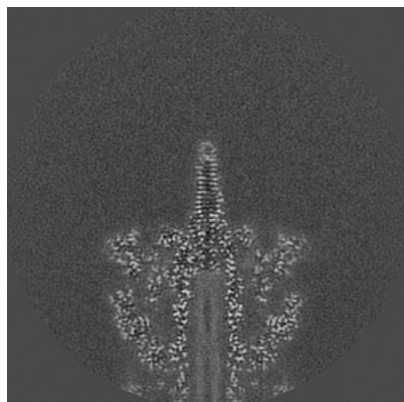


Z

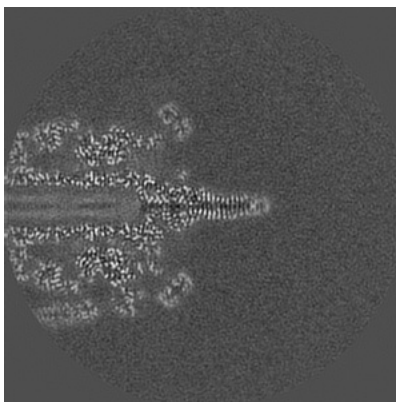
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

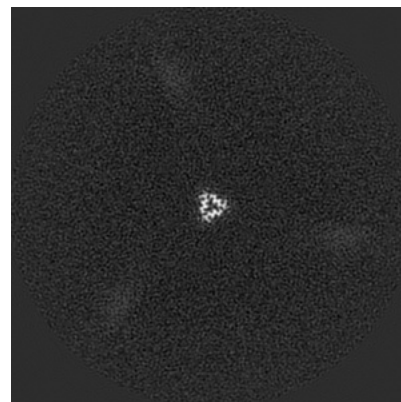
6.2.1 Primary map



X Index: 150

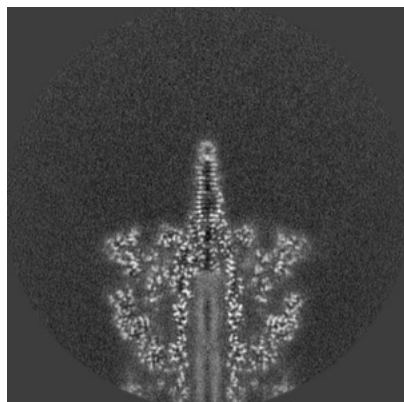


Y Index: 150

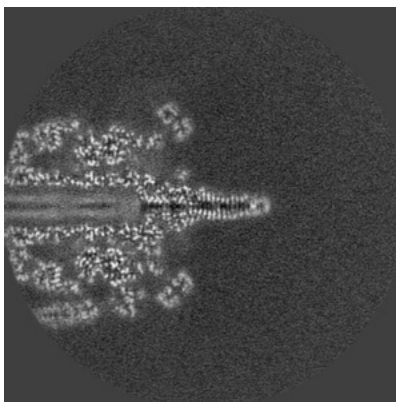


Z Index: 150

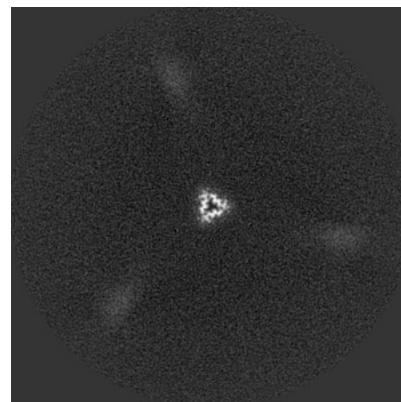
6.2.2 Raw map



X Index: 150



Y Index: 150

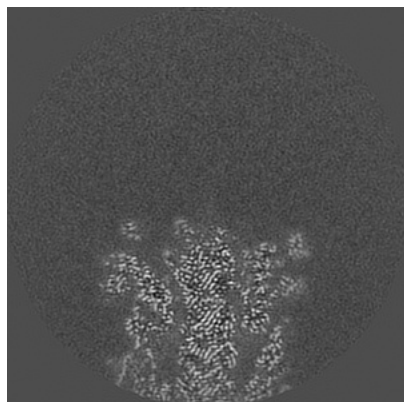


Z Index: 150

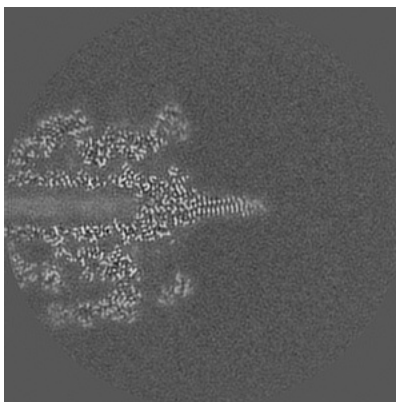
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

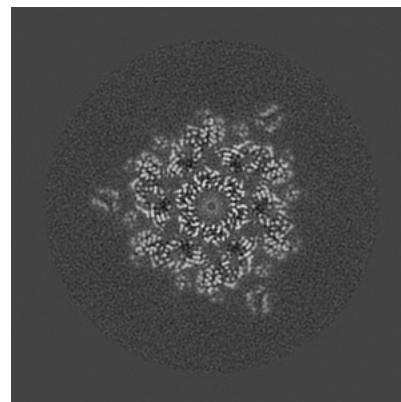
6.3.1 Primary map



X Index: 167

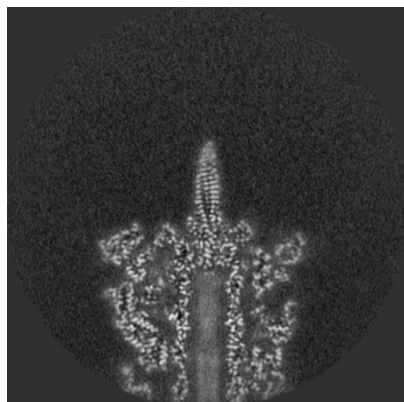


Y Index: 155

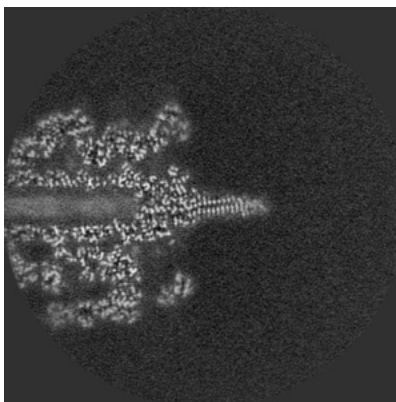


Z Index: 65

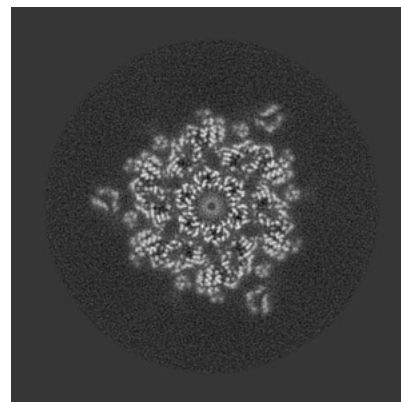
6.3.2 Raw map



X Index: 154



Y Index: 155

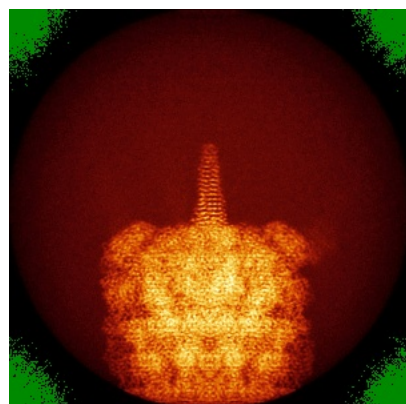


Z Index: 65

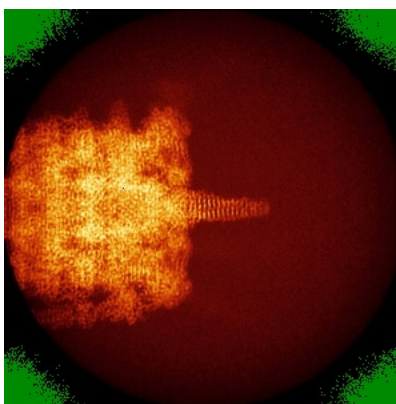
The images above show the largest variance slices of the map in three orthogonal directions.

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

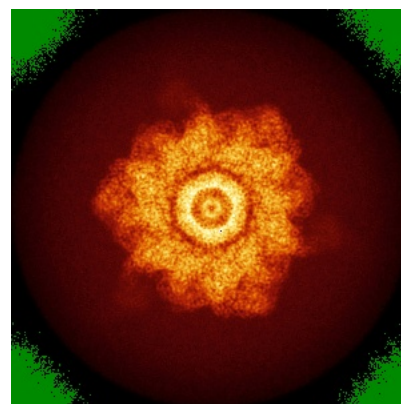
6.4.1 Primary map



X

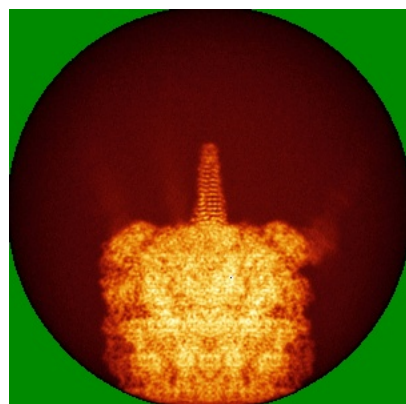


Y

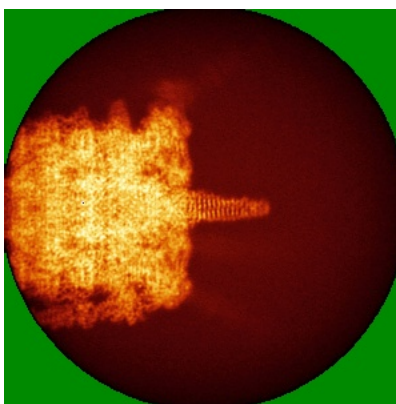


Z

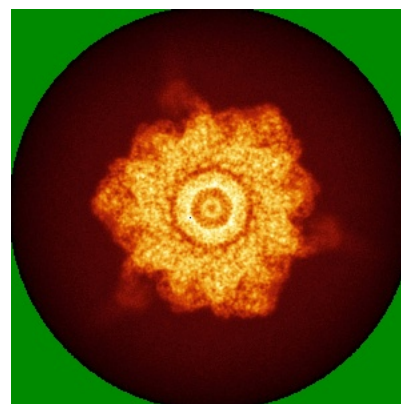
6.4.2 Raw map



X



Y

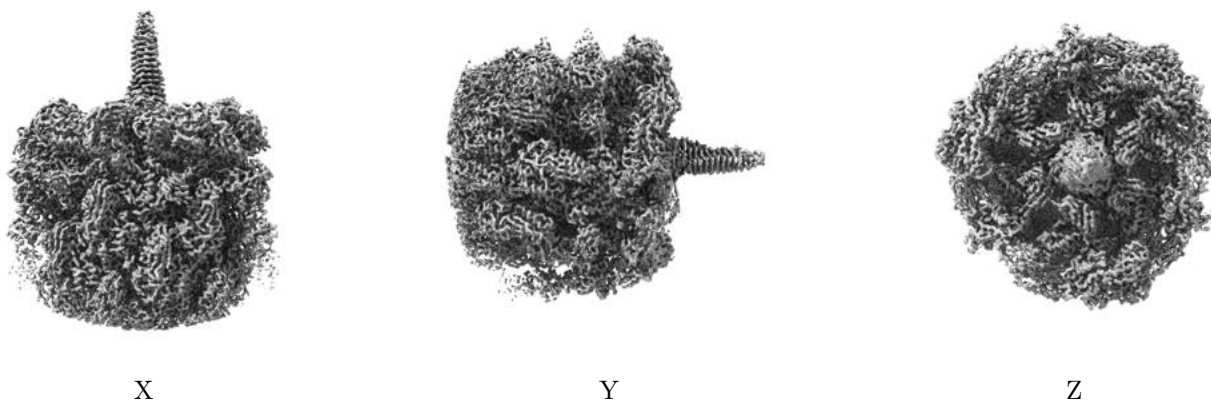


Z

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

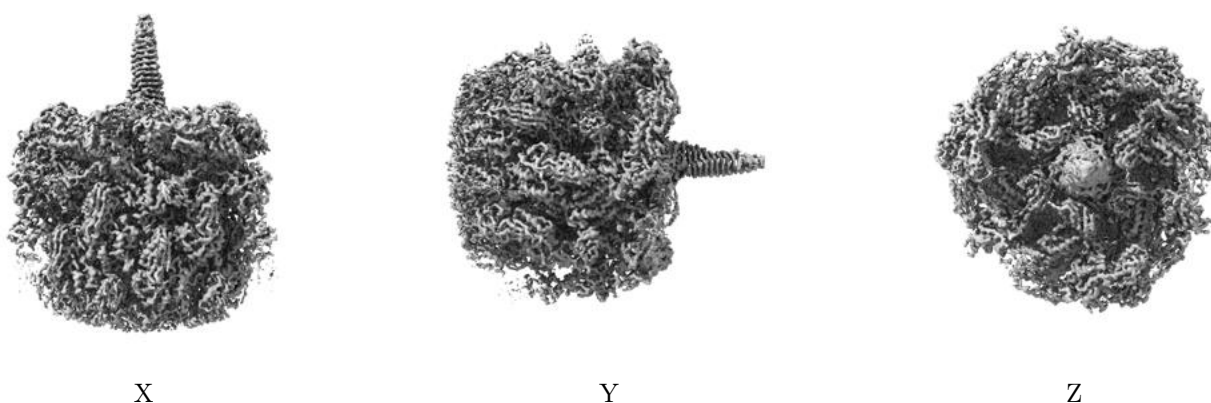
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

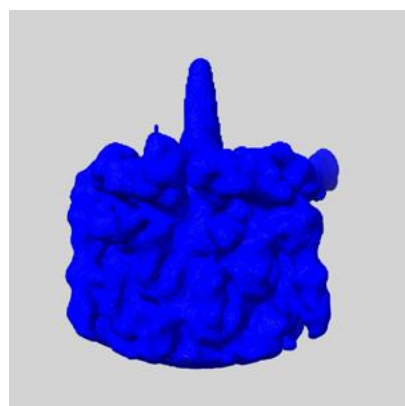
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

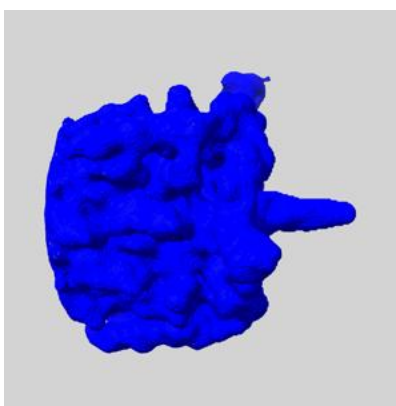
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

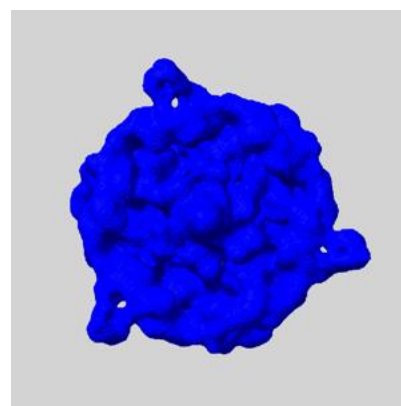
6.6.1 emd_62362_msk_1.map [i](#)



X



Y

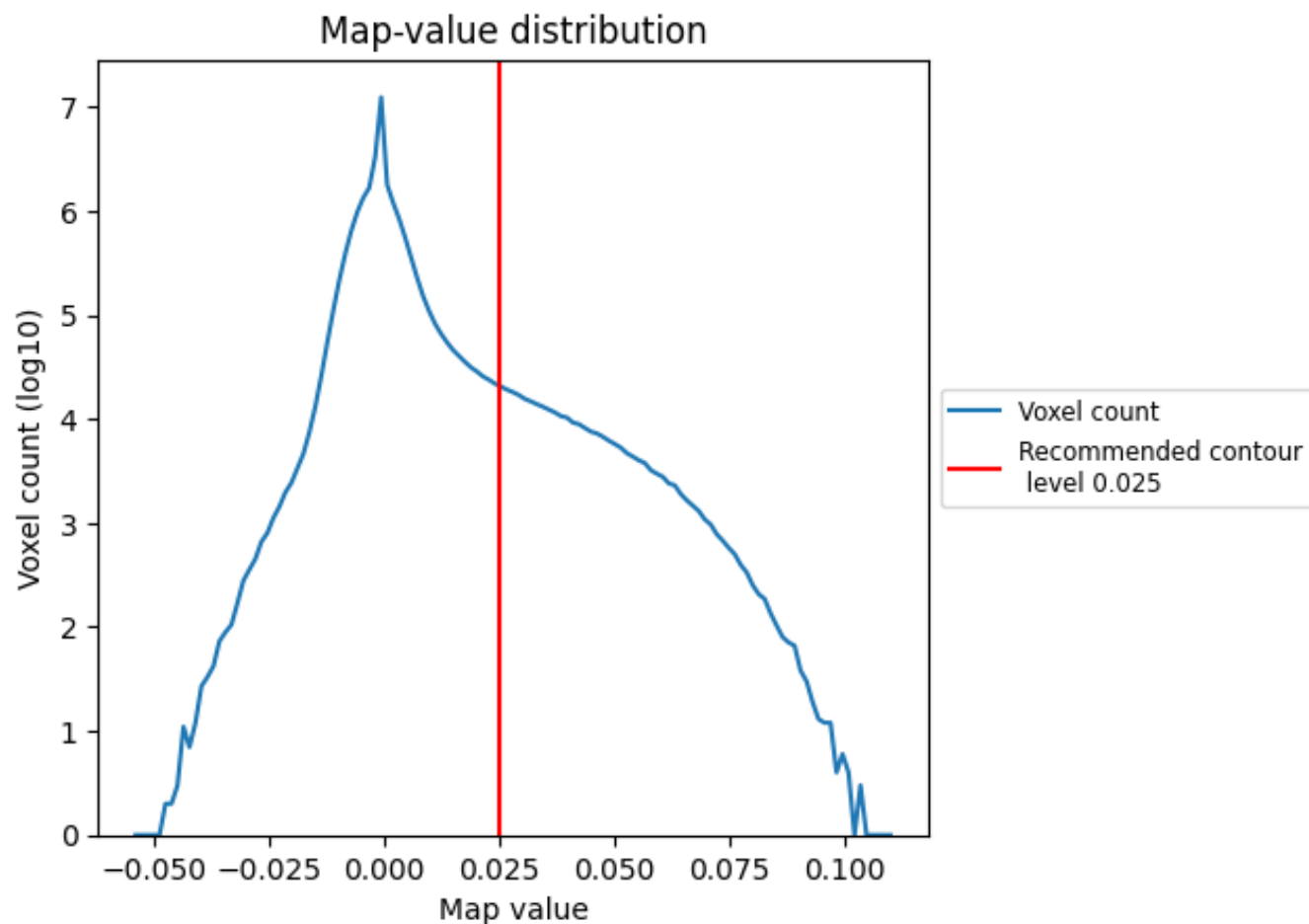


Z

7 Map analysis [i](#)

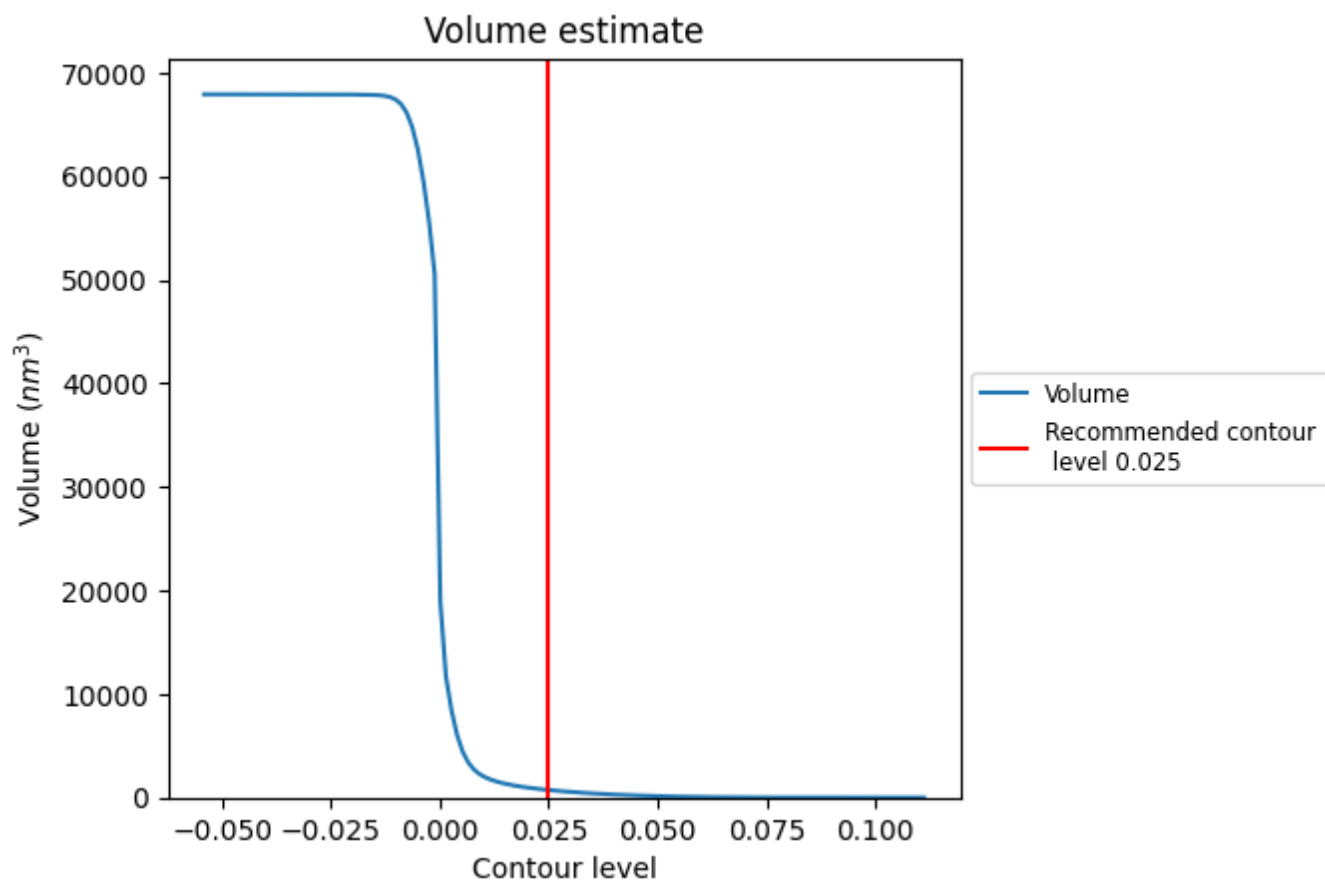
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

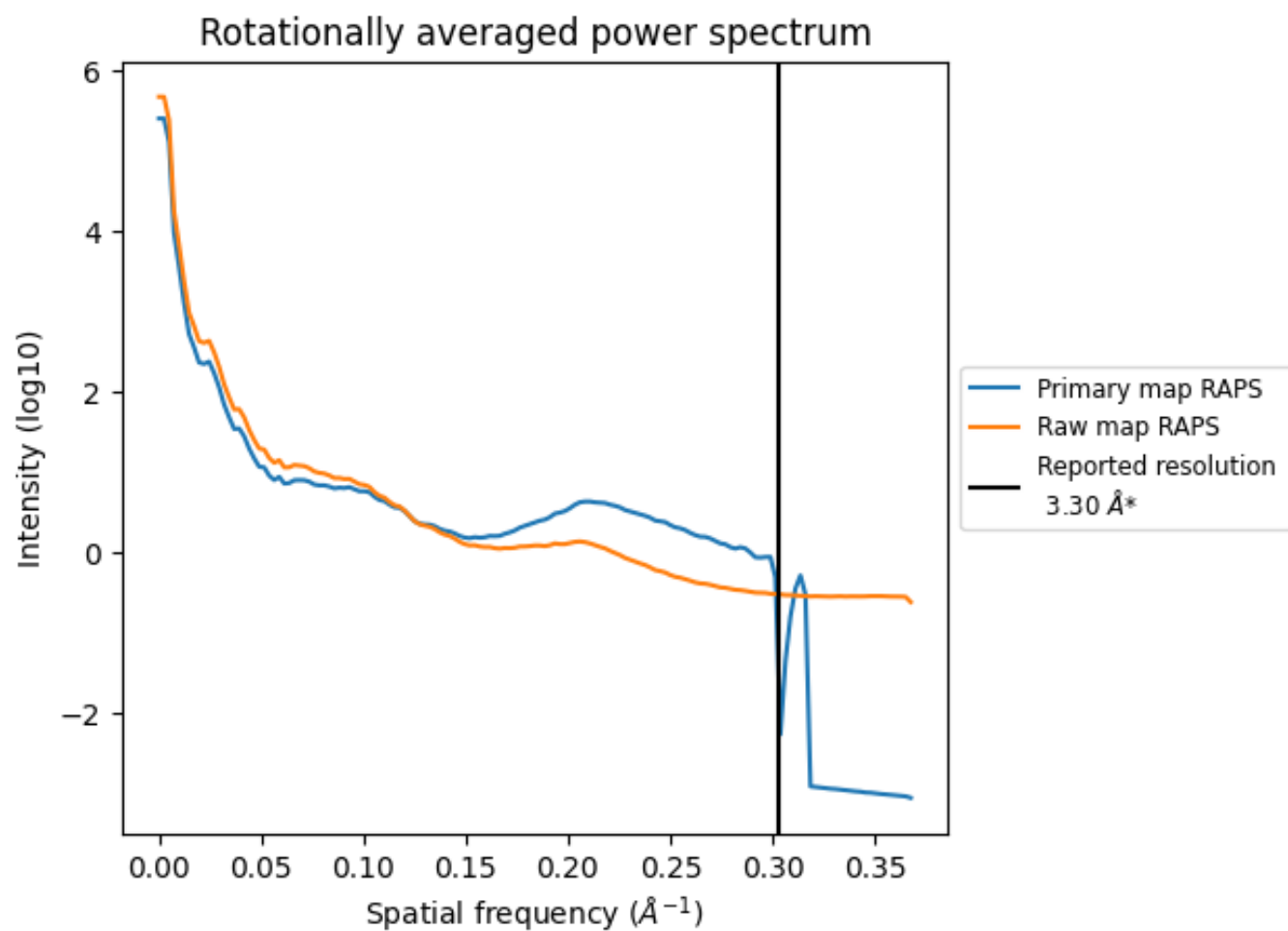
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 727 nm³; this corresponds to an approximate mass of 657 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

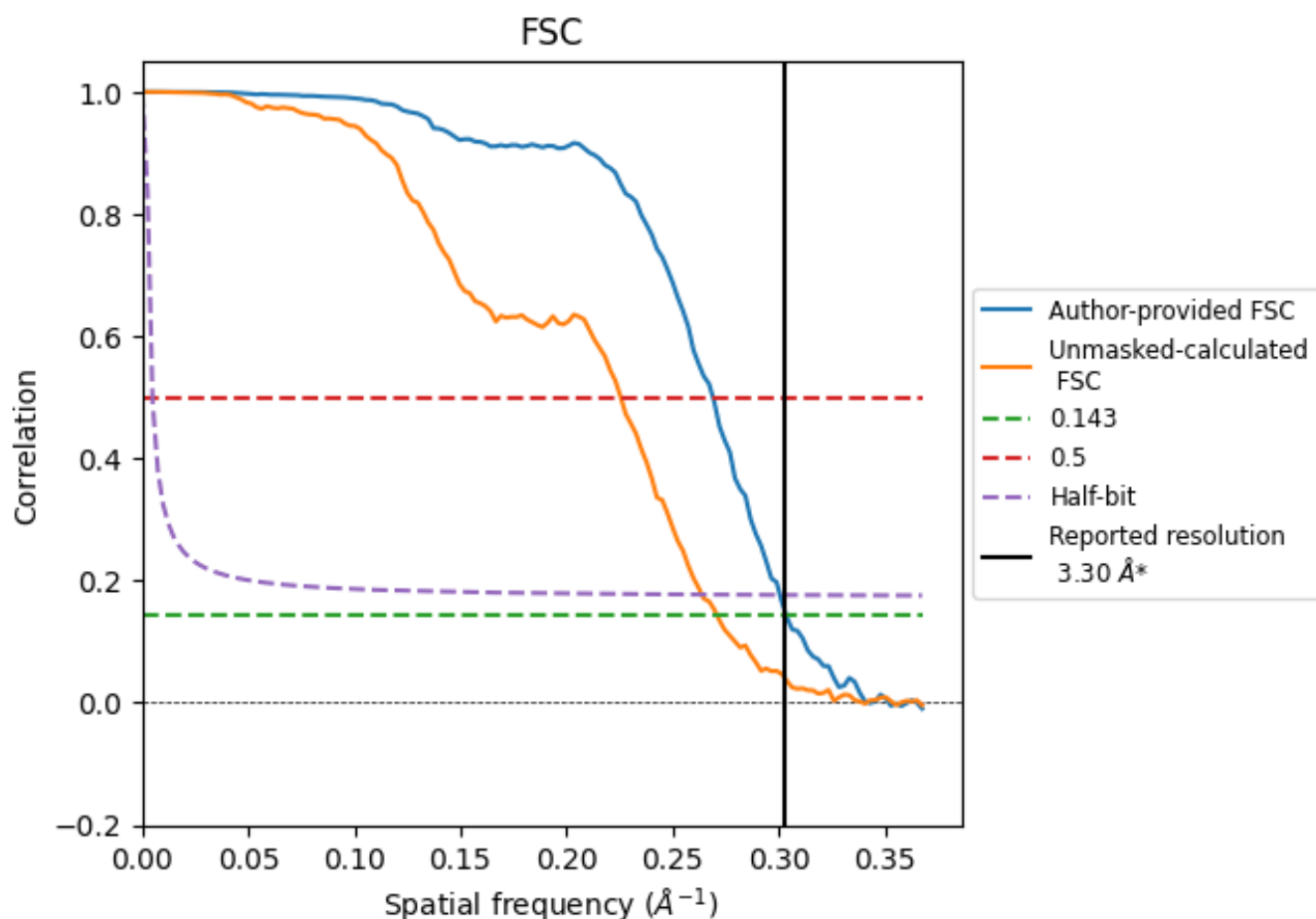


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

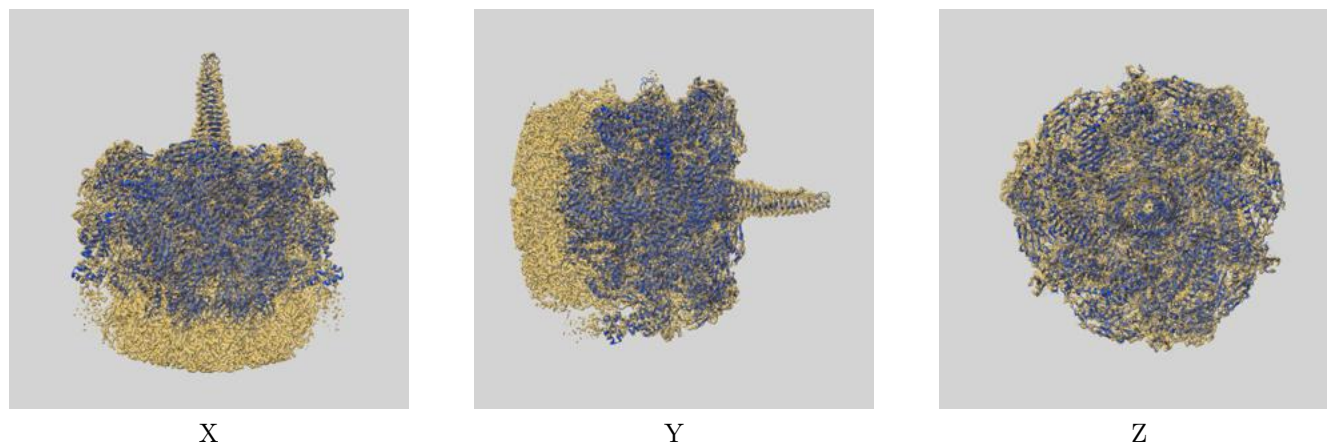
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.29	3.72	3.33
Unmasked-calculated*	3.69	4.43	3.79

*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 3.69 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

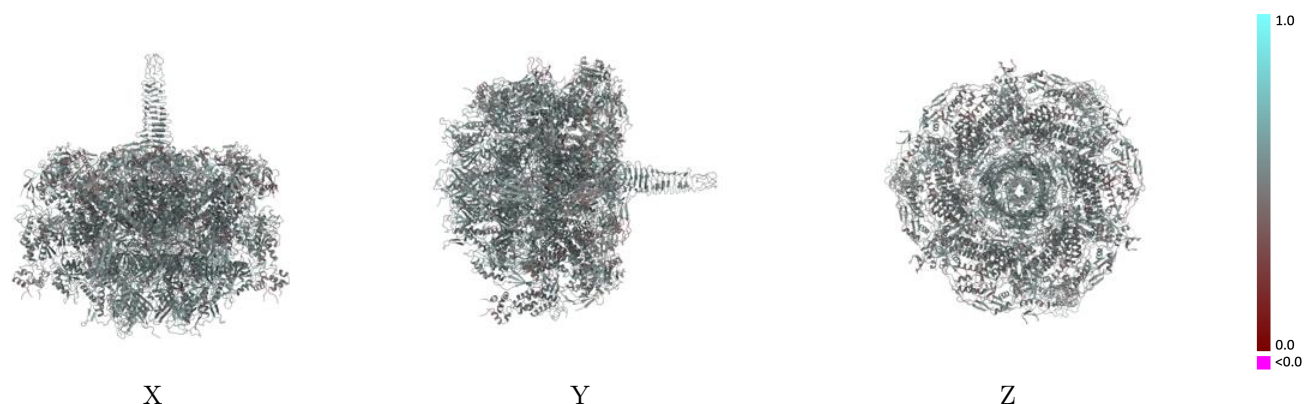
This section contains information regarding the fit between EMDB map EMD-62362 and PDB model 9KI1. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



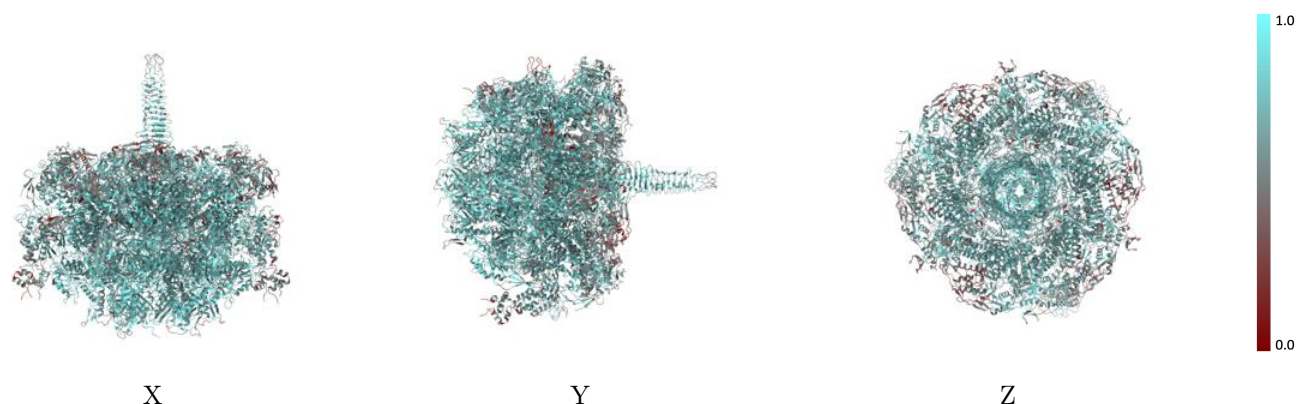
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



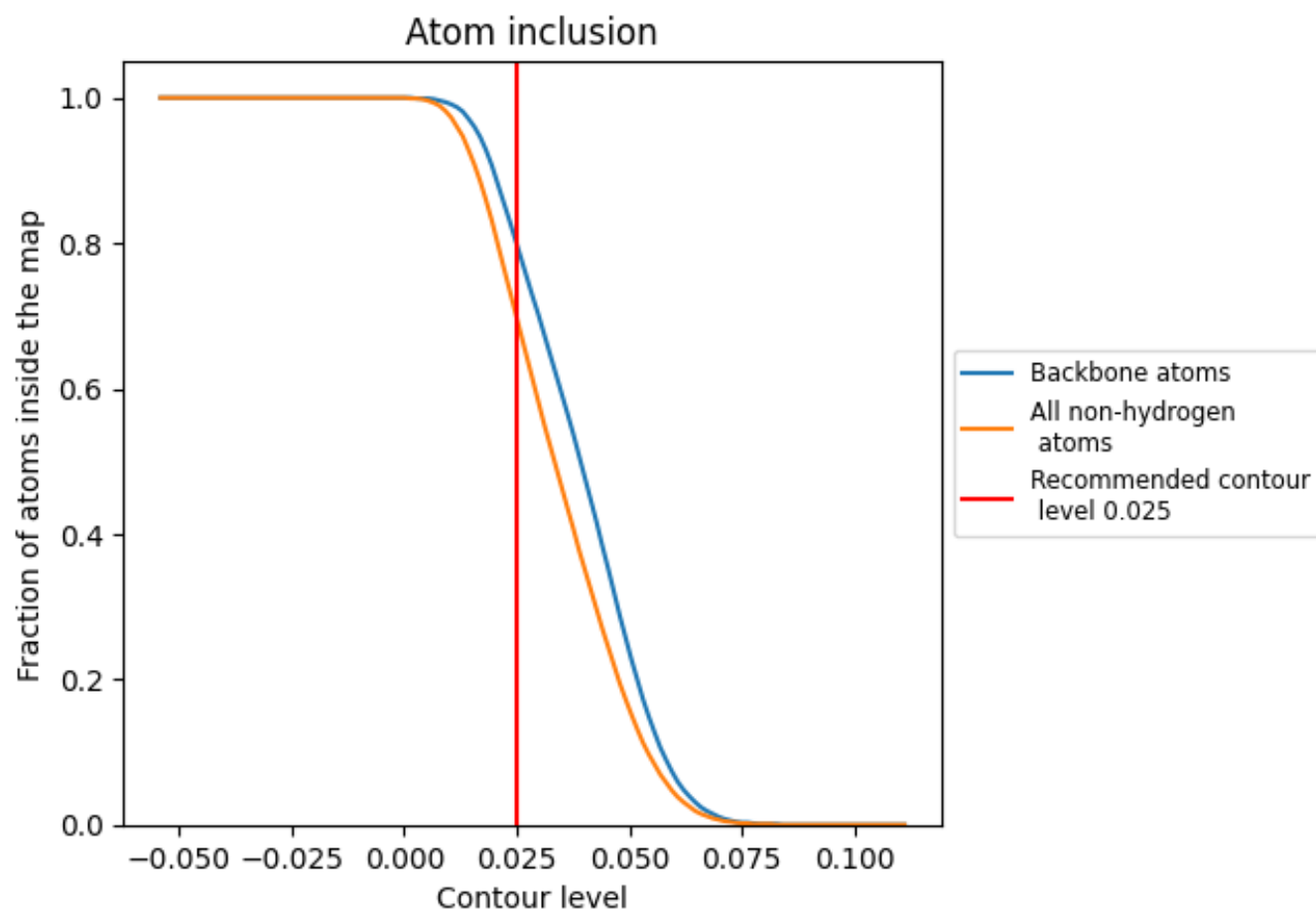
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 70% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6980	 0.5170
0	 0.7320	 0.5190
1	 0.7230	 0.5230
2	 0.7190	 0.5230
3	 0.7220	 0.5230
4	 0.7750	 0.5420
5	 0.7620	 0.5340
6	 0.7670	 0.5430
7	 0.7600	 0.5380
8	 0.7720	 0.5450
9	 0.7760	 0.5320
A	 0.7950	 0.5350
B	 0.7820	 0.5360
C	 0.8010	 0.5400
D	 0.7900	 0.5420
E	 0.8020	 0.5360
F	 0.7900	 0.5410
G	 0.7940	 0.5460
H	 0.6920	 0.5120
I	 0.6960	 0.5150
J	 0.6890	 0.5150
K	 0.5920	 0.4920
L	 0.5890	 0.4910
M	 0.5910	 0.4910
N	 0.7940	 0.5470
O	 0.5790	 0.4970
P	 0.5790	 0.4980
Q	 0.5840	 0.4980
R	 0.6160	 0.4990
S	 0.6100	 0.4980
T	 0.6100	 0.4980
U	 0.7890	 0.5490
V	 0.7330	 0.5320
W	 0.7320	 0.5290
X	 0.7340	 0.5280



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Chain	Atom inclusion	Q-score
a	 0.7200	 0.5200
b	 0.6290	 0.4940
c	 0.7360	 0.5200
d	 0.6320	 0.4870
e	 0.7300	 0.5180
f	 0.6340	 0.4870
g	 0.7010	 0.4910
h	 0.6770	 0.4930
i	 0.6690	 0.4710
j	 0.6200	 0.5070
k	 0.5820	 0.4980
l	 0.6170	 0.5020
m	 0.6250	 0.5060
n	 0.5880	 0.4980
o	 0.6150	 0.5020
p	 0.6120	 0.5130
q	 0.5840	 0.4970
r	 0.6270	 0.5080
s	 0.7360	 0.5210
t	 0.7300	 0.5220
u	 0.7260	 0.5170
v	 0.7340	 0.5180
w	 0.7270	 0.5150
x	 0.7350	 0.5220
y	 0.7430	 0.5220
z	 0.7410	 0.5220