



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 04:20 AM UTC

PDB ID : 9QGL / pdb_00009qgl
EMDB ID : EMD-53137
Title : Cryo-EM structure of the PIPVC1 baseplate, 6-fold symmetrized (C6), in extended state
Authors : Marin-Arraiza, L.; Taylor, N.M.I.
Deposited on : 2025-03-14
Resolution : 2.68 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:

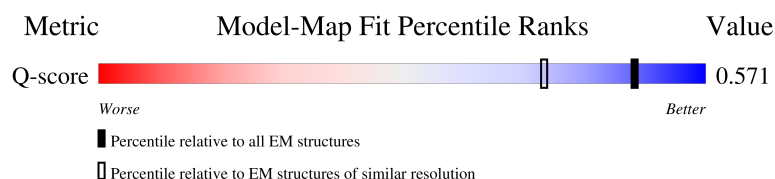
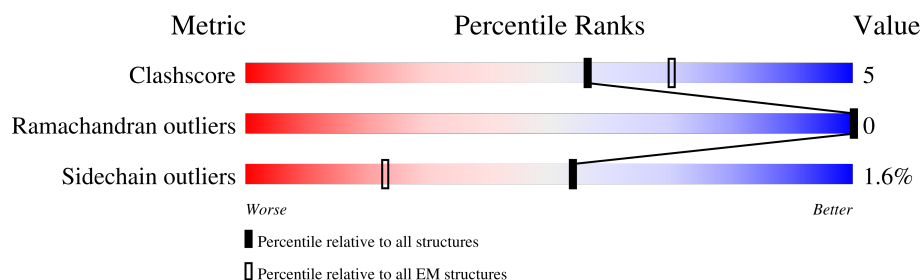
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 2.68 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.



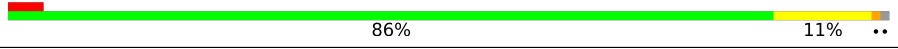
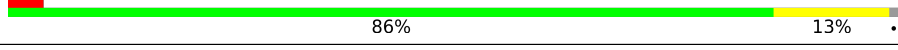
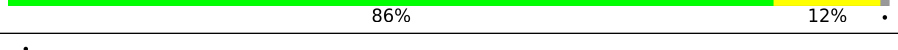
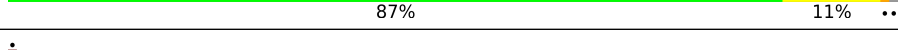
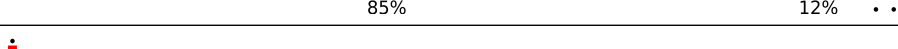
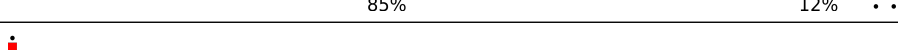
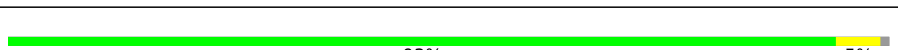
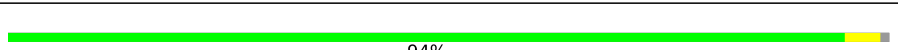
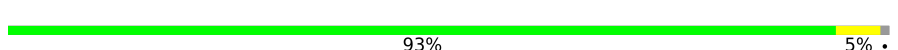
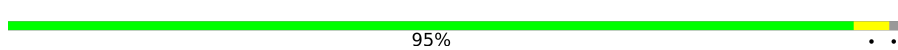
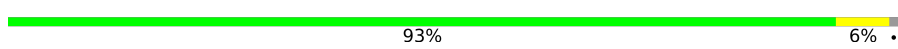
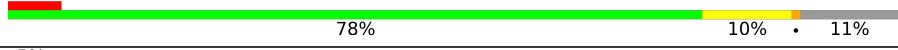
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	9255 (2.18 - 3.18)

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	1A	149	
1	1B	149	
1	1C	149	
1	1D	149	

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Mol	Chain	Length	Quality of chain
1	1E	149	
1	1F	149	
2	2A	354	
2	2B	354	
2	2C	354	
2	2D	354	
2	2E	354	
2	2F	354	
3	5A	152	
3	5B	152	
3	5C	152	
3	5D	152	
3	5E	152	
3	5F	152	
4	7A	227	
4	7B	227	
4	7C	227	
4	7D	227	
4	7E	227	
4	7F	227	
5	9A	239	
5	9B	239	
5	9C	239	
5	9D	239	
5	9E	239	

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Mol	Chain	Length	Quality of chain
5	9F	239	
6	A	905	
6	B	905	
6	C	905	
6	D	905	
6	E	905	
6	F	905	
7	a	966	
7	b	966	
7	c	966	
7	d	966	
7	e	966	
7	f	966	
8	3A	466	
8	3B	466	
8	3C	466	
8	3D	466	
8	3E	466	
8	3F	466	
9	4A	392	
9	4B	392	
9	4C	392	
9	4D	392	
9	4E	392	
9	4F	392	

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 171084 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 Phage tail protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1A	148	Total	C	N	O	S	0	0
			1160	741	188	229	2		
1	1B	148	Total	C	N	O	S	0	0
			1160	741	188	229	2		
1	1C	148	Total	C	N	O	S	0	0
			1160	741	188	229	2		
1	1D	148	Total	C	N	O	S	0	0
			1160	741	188	229	2		
1	1E	148	Total	C	N	O	S	0	0
			1160	741	188	229	2		
1	1F	148	Total	C	N	O	S	0	0
			1160	741	188	229	2		

- Molecule 2 is a protein called Phage tail sheath family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2A	349	Total	C	N	O	S	0	0
			2713	1736	444	525	8		
2	2B	349	Total	C	N	O	S	0	0
			2713	1736	444	525	8		
2	2C	349	Total	C	N	O	S	0	0
			2713	1736	444	525	8		
2	2D	349	Total	C	N	O	S	0	0
			2713	1736	444	525	8		
2	2E	349	Total	C	N	O	S	0	0
			2713	1736	444	525	8		
2	2F	349	Total	C	N	O	S	0	0
			2713	1736	444	525	8		

- Molecule 3 is a protein called Phage tail protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	5A	148	Total	C	N	O	S	0	0
			1175	748	207	216	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	5B	148	Total	C	N	O	S	0	0
			1175	748	207	216	4		
3	5C	148	Total	C	N	O	S	0	0
			1175	748	207	216	4		
3	5D	148	Total	C	N	O	S	0	0
			1175	748	207	216	4		
3	5E	148	Total	C	N	O	S	0	0
			1175	748	207	216	4		
3	5F	148	Total	C	N	O	S	0	0
			1175	748	207	216	4		

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5A	2	HIS	ASN	conflict	UNP A0A2S8PZE9
5A	35	GLY	SER	conflict	UNP A0A2S8PZE9
5A	45	TYR	LEU	conflict	UNP A0A2S8PZE9
5A	62	GLN	HIS	conflict	UNP A0A2S8PZE9
5A	65	SER	ARG	conflict	UNP A0A2S8PZE9
5B	2	HIS	ASN	conflict	UNP A0A2S8PZE9
5B	35	GLY	SER	conflict	UNP A0A2S8PZE9
5B	45	TYR	LEU	conflict	UNP A0A2S8PZE9
5B	62	GLN	HIS	conflict	UNP A0A2S8PZE9
5B	65	SER	ARG	conflict	UNP A0A2S8PZE9
5C	2	HIS	ASN	conflict	UNP A0A2S8PZE9
5C	35	GLY	SER	conflict	UNP A0A2S8PZE9
5C	45	TYR	LEU	conflict	UNP A0A2S8PZE9
5C	62	GLN	HIS	conflict	UNP A0A2S8PZE9
5C	65	SER	ARG	conflict	UNP A0A2S8PZE9
5D	2	HIS	ASN	conflict	UNP A0A2S8PZE9
5D	35	GLY	SER	conflict	UNP A0A2S8PZE9
5D	45	TYR	LEU	conflict	UNP A0A2S8PZE9
5D	62	GLN	HIS	conflict	UNP A0A2S8PZE9
5D	65	SER	ARG	conflict	UNP A0A2S8PZE9
5E	2	HIS	ASN	conflict	UNP A0A2S8PZE9
5E	35	GLY	SER	conflict	UNP A0A2S8PZE9
5E	45	TYR	LEU	conflict	UNP A0A2S8PZE9
5E	62	GLN	HIS	conflict	UNP A0A2S8PZE9
5E	65	SER	ARG	conflict	UNP A0A2S8PZE9
5F	2	HIS	ASN	conflict	UNP A0A2S8PZE9
5F	35	GLY	SER	conflict	UNP A0A2S8PZE9
5F	45	TYR	LEU	conflict	UNP A0A2S8PZE9
5F	62	GLN	HIS	conflict	UNP A0A2S8PZE9

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Chain	Residue	Modelled	Actual	Comment	Reference
5F	65	SER	ARG	conflict	UNP A0A2S8PZE9

- Molecule 4 is a protein called Contractile injection system tube protein N-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	7A	224	Total	C	N	O	S	0	0
			1724	1091	289	339	5		
4	7B	224	Total	C	N	O	S	0	0
			1724	1091	289	339	5		
4	7C	224	Total	C	N	O	S	0	0
			1724	1091	289	339	5		
4	7D	224	Total	C	N	O	S	0	0
			1724	1091	289	339	5		
4	7E	224	Total	C	N	O	S	0	0
			1724	1091	289	339	5		
4	7F	224	Total	C	N	O	S	0	0
			1724	1091	289	339	5		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
7A	64	PRO	GLN	conflict	UNP A0A2S8PZG1
7A	100	PRO	ALA	conflict	UNP A0A2S8PZG1
7A	121	SER	GLY	conflict	UNP A0A2S8PZG1
7A	174	THR	ALA	conflict	UNP A0A2S8PZG1
7B	64	PRO	GLN	conflict	UNP A0A2S8PZG1
7B	100	PRO	ALA	conflict	UNP A0A2S8PZG1
7B	121	SER	GLY	conflict	UNP A0A2S8PZG1
7B	174	THR	ALA	conflict	UNP A0A2S8PZG1
7C	64	PRO	GLN	conflict	UNP A0A2S8PZG1
7C	100	PRO	ALA	conflict	UNP A0A2S8PZG1
7C	121	SER	GLY	conflict	UNP A0A2S8PZG1
7C	174	THR	ALA	conflict	UNP A0A2S8PZG1
7D	64	PRO	GLN	conflict	UNP A0A2S8PZG1
7D	100	PRO	ALA	conflict	UNP A0A2S8PZG1
7D	121	SER	GLY	conflict	UNP A0A2S8PZG1
7D	174	THR	ALA	conflict	UNP A0A2S8PZG1
7E	64	PRO	GLN	conflict	UNP A0A2S8PZG1
7E	100	PRO	ALA	conflict	UNP A0A2S8PZG1
7E	121	SER	GLY	conflict	UNP A0A2S8PZG1
7E	174	THR	ALA	conflict	UNP A0A2S8PZG1

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Chain	Residue	Modelled	Actual	Comment	Reference
7F	64	PRO	GLN	conflict	UNP A0A2S8PZG1
7F	100	PRO	ALA	conflict	UNP A0A2S8PZG1
7F	121	SER	GLY	conflict	UNP A0A2S8PZG1
7F	174	THR	ALA	conflict	UNP A0A2S8PZG1

- Molecule 5 is a protein called Photorhabdus luminescens subsp. laumondii TTO1 complete genome segment 6/17.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	9A	212	Total	C	N	O	S	0	0
			1697	1073	287	331	6		
5	9B	212	Total	C	N	O	S	0	0
			1697	1073	287	331	6		
5	9C	212	Total	C	N	O	S	0	0
			1697	1073	287	331	6		
5	9D	212	Total	C	N	O	S	0	0
			1697	1073	287	331	6		
5	9E	212	Total	C	N	O	S	0	0
			1697	1073	287	331	6		
5	9F	212	Total	C	N	O	S	0	0
			1697	1073	287	331	6		

- Molecule 6 is a protein called Photorhabdus luminescens subsp. laumondii TTO1 complete genome segment 6/17.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	887	Total	C	N	O	S	0	0
			7040	4486	1166	1379	9		
6	B	887	Total	C	N	O	S	0	0
			7040	4486	1166	1379	9		
6	C	887	Total	C	N	O	S	0	0
			7040	4486	1166	1379	9		
6	D	887	Total	C	N	O	S	0	0
			7040	4486	1166	1379	9		
6	E	887	Total	C	N	O	S	0	0
			7040	4486	1166	1379	9		
6	F	887	Total	C	N	O	S	0	0
			7040	4486	1166	1379	9		

- Molecule 7 is a protein called Baseplate protein J-like domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	a	829	Total	C	N	O	S	0	0
			6720	4276	1115	1308	21		
7	b	829	Total	C	N	O	S	0	0
			6720	4276	1115	1308	21		
7	c	829	Total	C	N	O	S	0	0
			6720	4276	1115	1308	21		
7	d	829	Total	C	N	O	S	0	0
			6720	4276	1115	1308	21		
7	e	829	Total	C	N	O	S	0	0
			6720	4276	1115	1308	21		
7	f	829	Total	C	N	O	S	0	0
			6720	4276	1115	1308	21		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	?	-	GLN	deletion	UNP A0A6L9JN06
a	?	-	GLU	deletion	UNP A0A6L9JN06
b	?	-	GLN	deletion	UNP A0A6L9JN06
b	?	-	GLU	deletion	UNP A0A6L9JN06
c	?	-	GLN	deletion	UNP A0A6L9JN06
c	?	-	GLU	deletion	UNP A0A6L9JN06
d	?	-	GLN	deletion	UNP A0A6L9JN06
d	?	-	GLU	deletion	UNP A0A6L9JN06
e	?	-	GLN	deletion	UNP A0A6L9JN06
e	?	-	GLU	deletion	UNP A0A6L9JN06
f	?	-	GLN	deletion	UNP A0A6L9JN06
f	?	-	GLU	deletion	UNP A0A6L9JN06

- Molecule 8 is a protein called Phage tail sheath family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	3A	416	Total	C	N	O	S	0	0
			3241	2059	541	631	10		
8	3B	416	Total	C	N	O	S	0	0
			3241	2059	541	631	10		
8	3C	416	Total	C	N	O	S	0	0
			3241	2059	541	631	10		
8	3D	416	Total	C	N	O	S	0	0
			3241	2059	541	631	10		
8	3E	416	Total	C	N	O	S	0	0
			3241	2059	541	631	10		
8	3F	416	Total	C	N	O	S	0	0
			3241	2059	541	631	10		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3A	267	GLN	-	insertion	UNP A0A6L9JMV2
3A	268	LYS	-	insertion	UNP A0A6L9JMV2
3A	269	ILE	-	insertion	UNP A0A6L9JMV2
3A	309	ILE	VAL	conflict	UNP A0A6L9JMV2
3B	267	GLN	-	insertion	UNP A0A6L9JMV2
3B	268	LYS	-	insertion	UNP A0A6L9JMV2
3B	269	ILE	-	insertion	UNP A0A6L9JMV2
3B	309	ILE	VAL	conflict	UNP A0A6L9JMV2
3C	267	GLN	-	insertion	UNP A0A6L9JMV2
3C	268	LYS	-	insertion	UNP A0A6L9JMV2
3C	269	ILE	-	insertion	UNP A0A6L9JMV2
3C	309	ILE	VAL	conflict	UNP A0A6L9JMV2
3D	267	GLN	-	insertion	UNP A0A6L9JMV2
3D	268	LYS	-	insertion	UNP A0A6L9JMV2
3D	269	ILE	-	insertion	UNP A0A6L9JMV2
3D	309	ILE	VAL	conflict	UNP A0A6L9JMV2
3E	267	GLN	-	insertion	UNP A0A6L9JMV2
3E	268	LYS	-	insertion	UNP A0A6L9JMV2
3E	269	ILE	-	insertion	UNP A0A6L9JMV2
3E	309	ILE	VAL	conflict	UNP A0A6L9JMV2
3F	267	GLN	-	insertion	UNP A0A6L9JMV2
3F	268	LYS	-	insertion	UNP A0A6L9JMV2
3F	269	ILE	-	insertion	UNP A0A6L9JMV2
3F	309	ILE	VAL	conflict	UNP A0A6L9JMV2

- Molecule 9 is a protein called Phage tail sheath family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	4A	383	Total	C	N	O	S	0	0
			3044	1948	523	564	9		
9	4B	383	Total	C	N	O	S	0	0
			3044	1948	523	564	9		
9	4C	383	Total	C	N	O	S	0	0
			3044	1948	523	564	9		
9	4D	383	Total	C	N	O	S	0	0
			3044	1948	523	564	9		
9	4E	383	Total	C	N	O	S	0	0
			3044	1948	523	564	9		
9	4F	383	Total	C	N	O	S	0	0
			3044	1948	523	564	9		

3 Residue-property plots [i](#)

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

- Molecule 1: Phage tail protein

Chain 1A: 



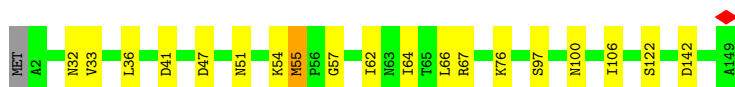
- Molecule 1: Phage tail protein

Chain 1B: 



- Molecule 1: Phage tail protein

Chain 1C: 



- Molecule 1: Phage tail protein

Chain 1D: 



- Molecule 1: Phage tail protein

Chain 1E: 



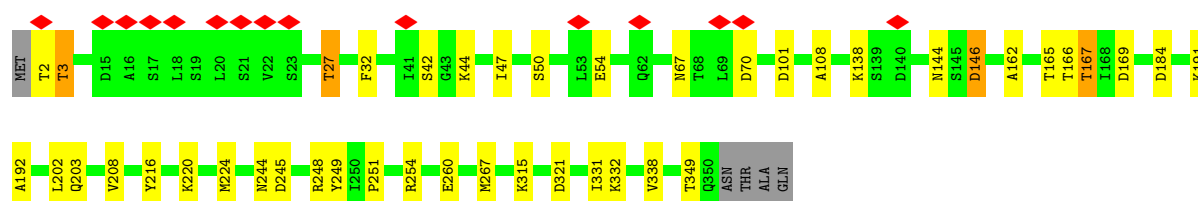
- Molecule 1: Phage tail protein

Chain 1F:  85% 14% ..



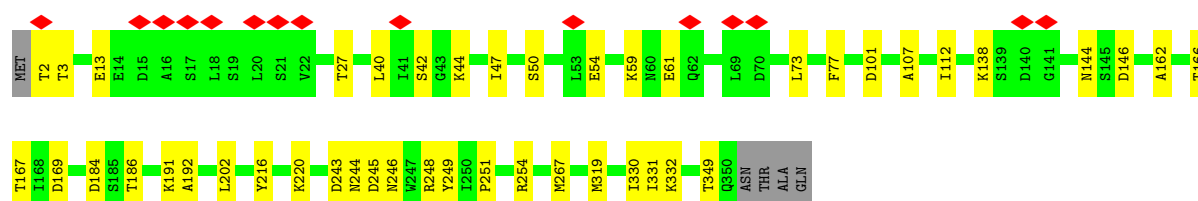
- Molecule 2: Phage tail sheath family protein

Chain 2A:  86% 11% ..



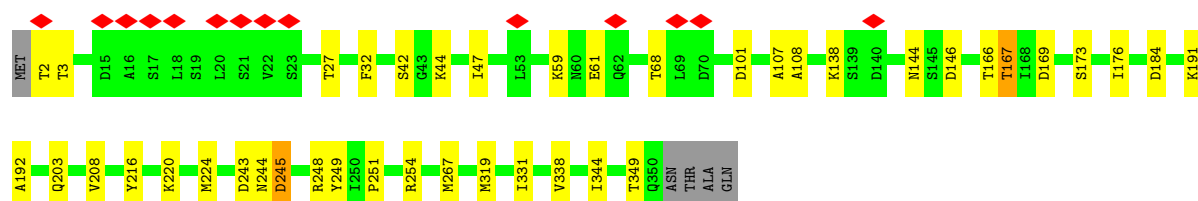
- Molecule 2: Phage tail sheath family protein

Chain 2B:  86% 13% ..



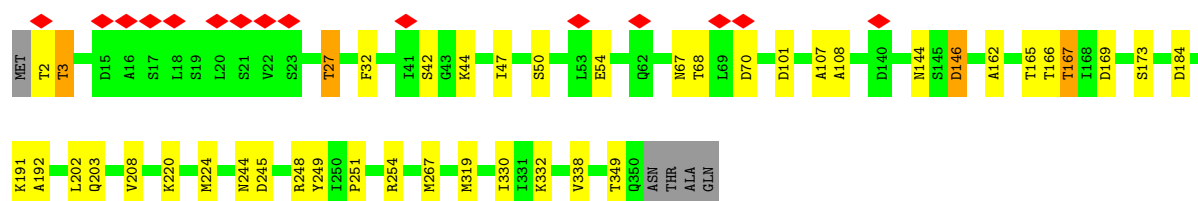
- Molecule 2: Phage tail sheath family protein

Chain 2C:  87% 11% ..

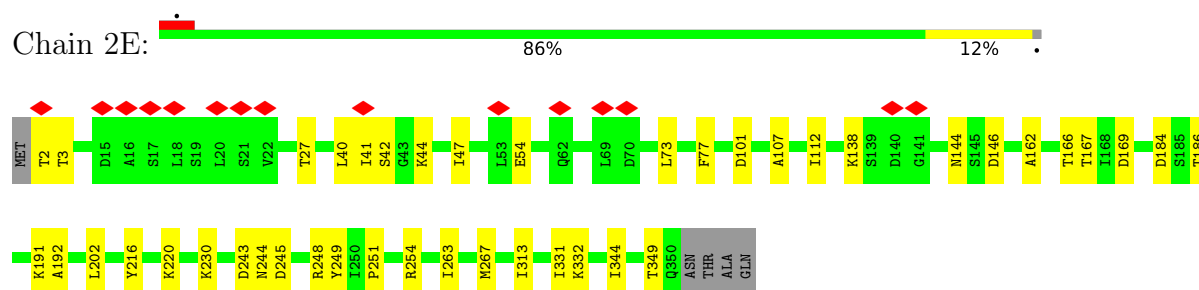


- Molecule 2: Phage tail sheath family protein

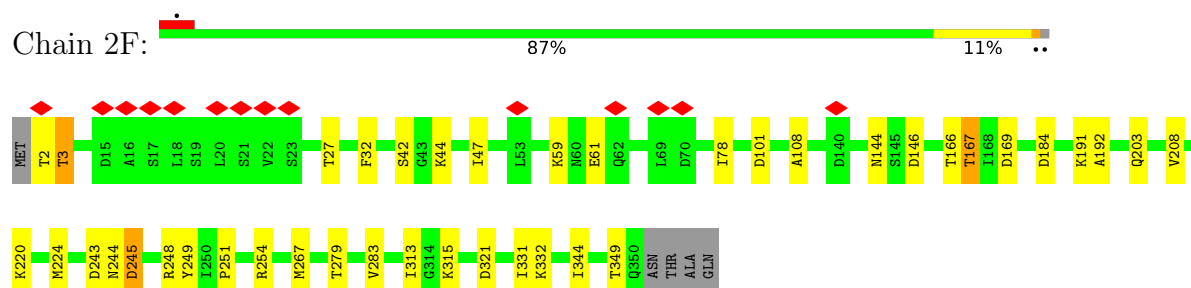
Chain 2D:  86% 11% ..



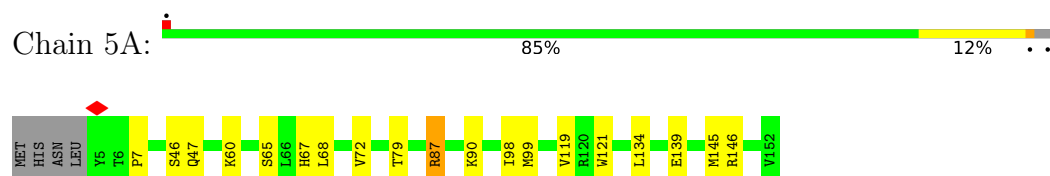
- Molecule 2: Phage tail sheath family protein



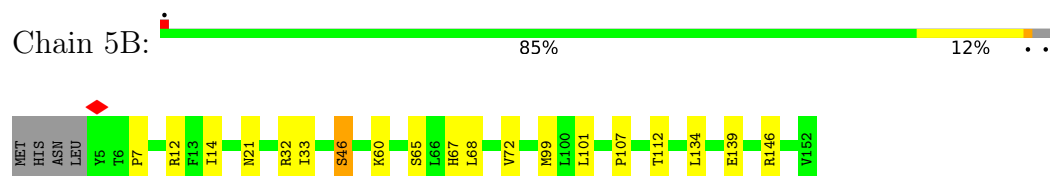
- Molecule 2: Phage tail sheath family protein



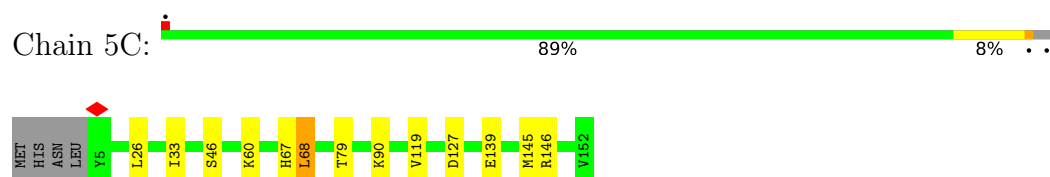
- Molecule 3: Phage tail protein



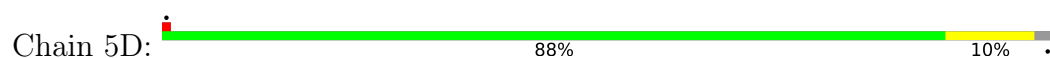
- Molecule 3: Phage tail protein

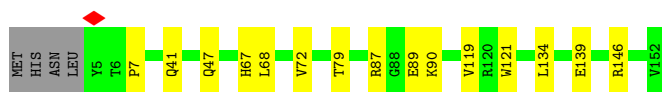


- Molecule 3: Phage tail protein

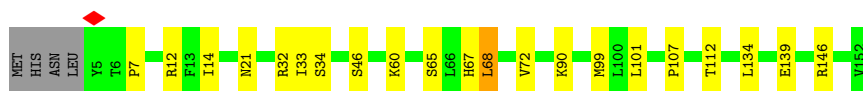
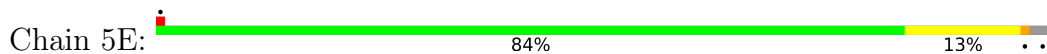


- Molecule 3: Phage tail protein

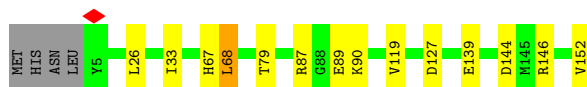
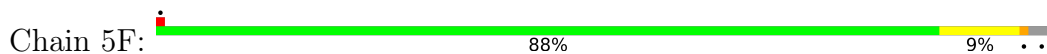




- Molecule 3: Phage tail protein



- Molecule 3: Phage tail protein



- Molecule 4: Contractile injection system tube protein N-terminal domain-containing protein



- Molecule 4: Contractile injection system tube protein N-terminal domain-containing protein



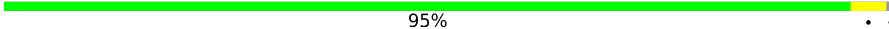
- Molecule 4: Contractile injection system tube protein N-terminal domain-containing protein



- Molecule 4: Contractile injection system tube protein N-terminal domain-containing protein



- Molecule 4: Contractile injection system tube protein N-terminal domain-containing protein

Chain 7E:  95% ..



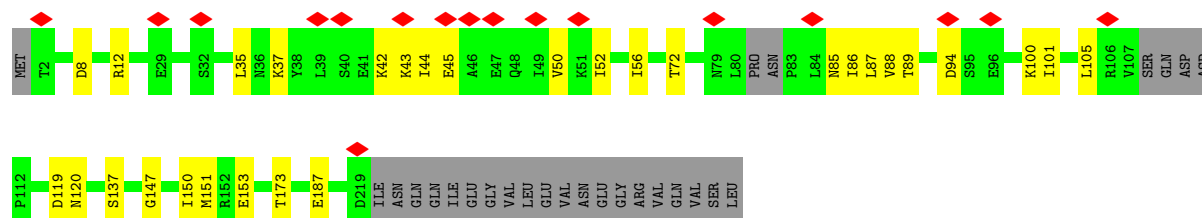
- Molecule 4: Contractile injection system tube protein N-terminal domain-containing protein

Chain 7F:  93% 6% .



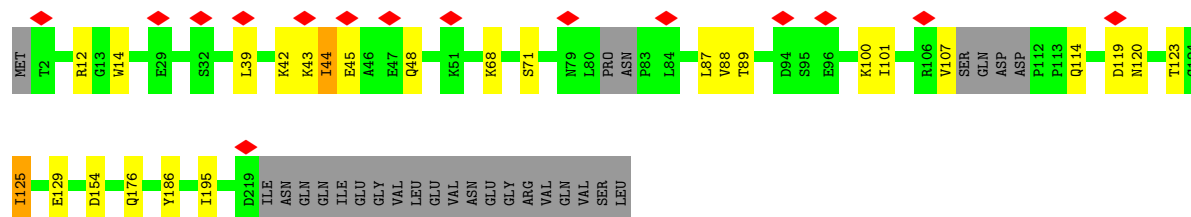
- Molecule 5: Photorhabdus luminescens subsp. laumondii TTO1 complete genome segment 6/17

Chain 9A:  76% 13% 11% 7%



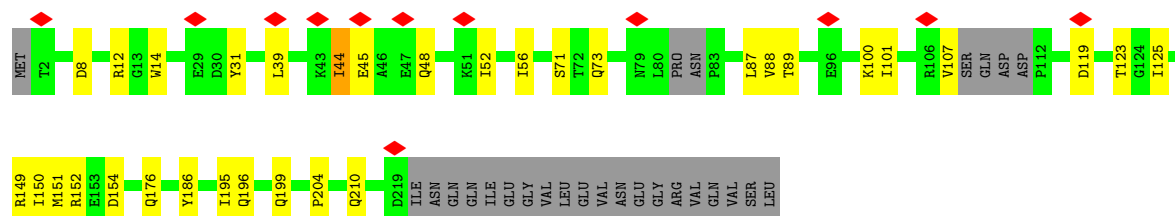
- Molecule 5: Photorhabdus luminescens subsp. laumondii TTO1 complete genome segment 6/17

Chain 9B:  78% 10% 11% 6%

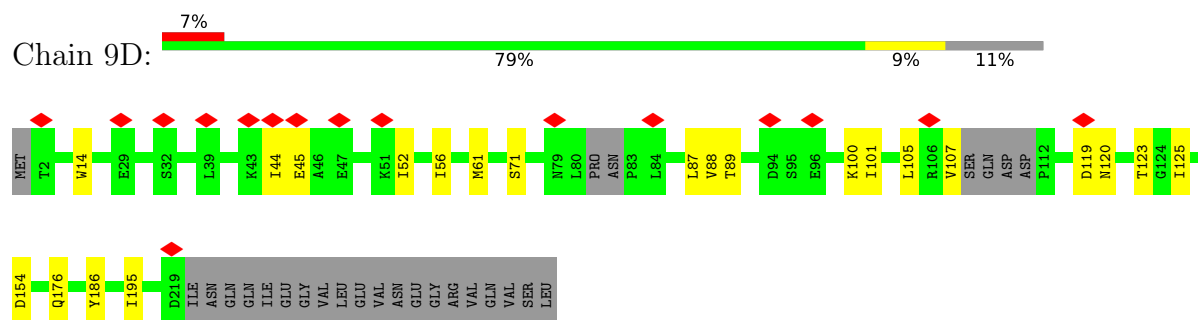


- Molecule 5: Photorhabdus luminescens subsp. laumondii TTO1 complete genome segment 6/17

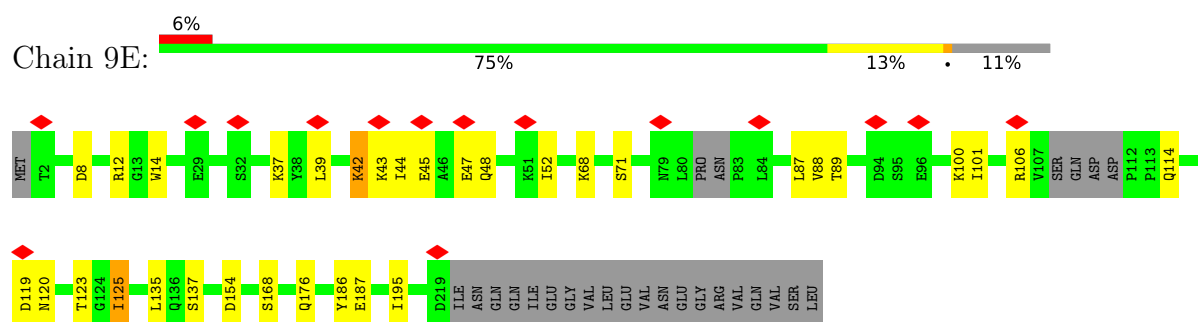
Chain 9C:  75% 13% 11% 5%



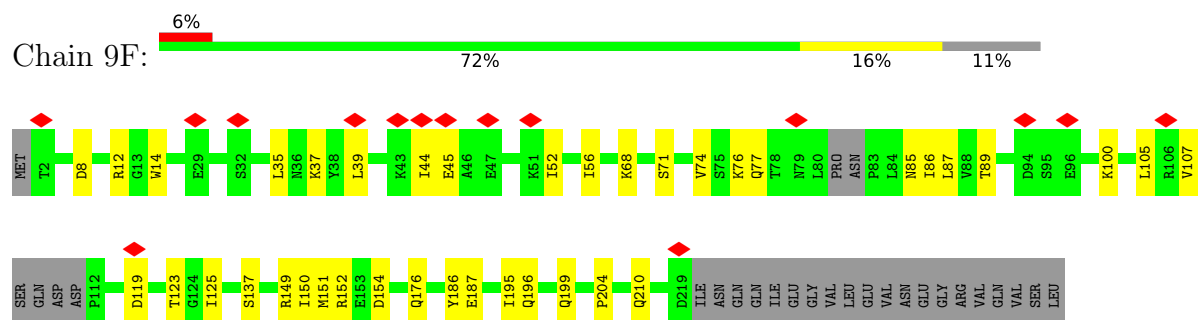
- Molecule 5: *Photorhabdus luminescens* subsp. *laumondii* TTO1 complete genome segment 6/17



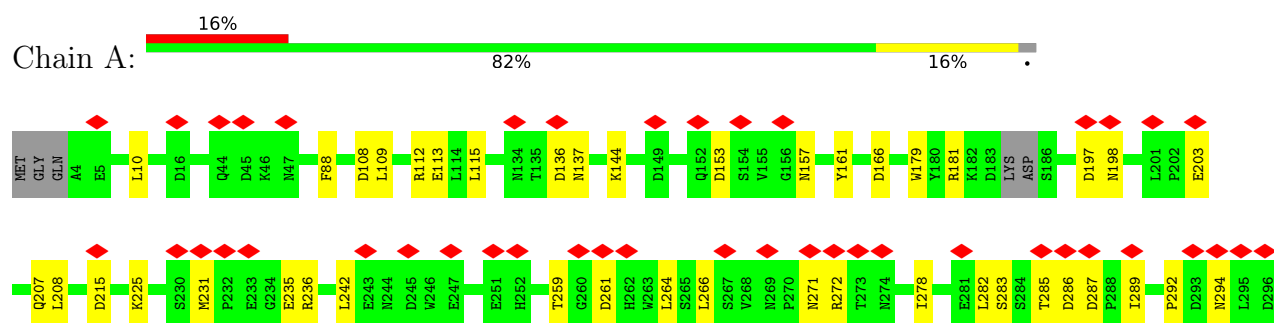
- Molecule 5: *Photorhabdus luminescens* subsp. *laumondii* TTO1 complete genome segment 6/17

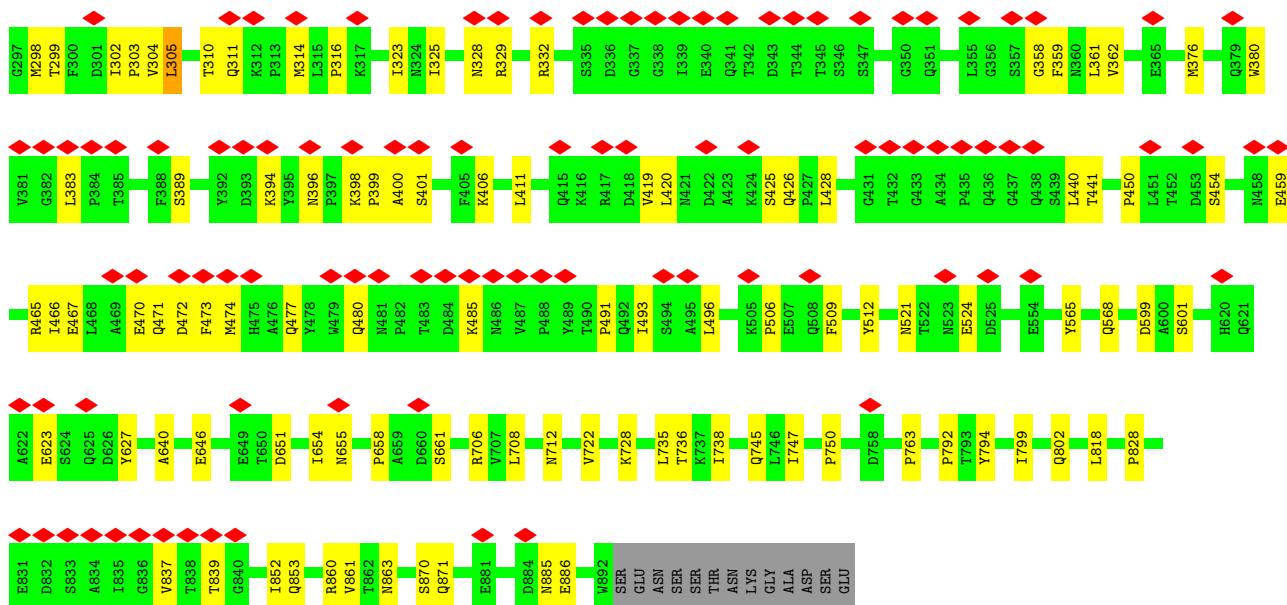


- Molecule 5: *Photorhabdus luminescens* subsp. *laumondii* TTO1 complete genome segment 6/17

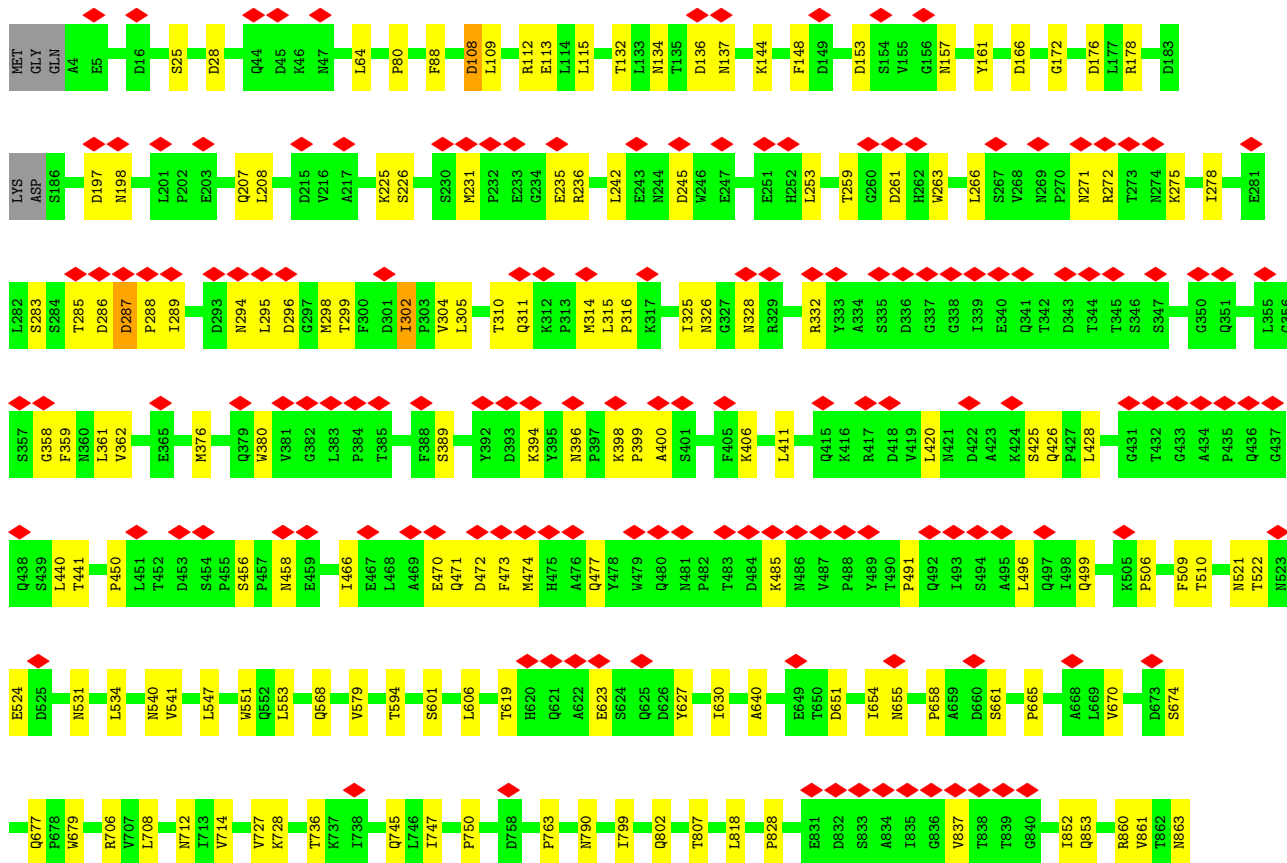
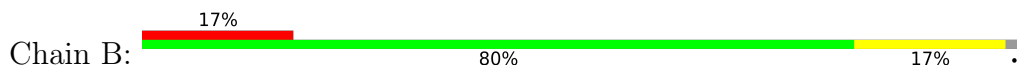


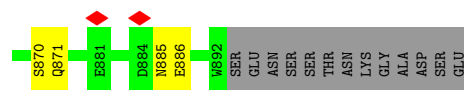
- Molecule 6: *Photorhabdus luminescens* subsp. *laumondii* TTO1 complete genome segment 6/17



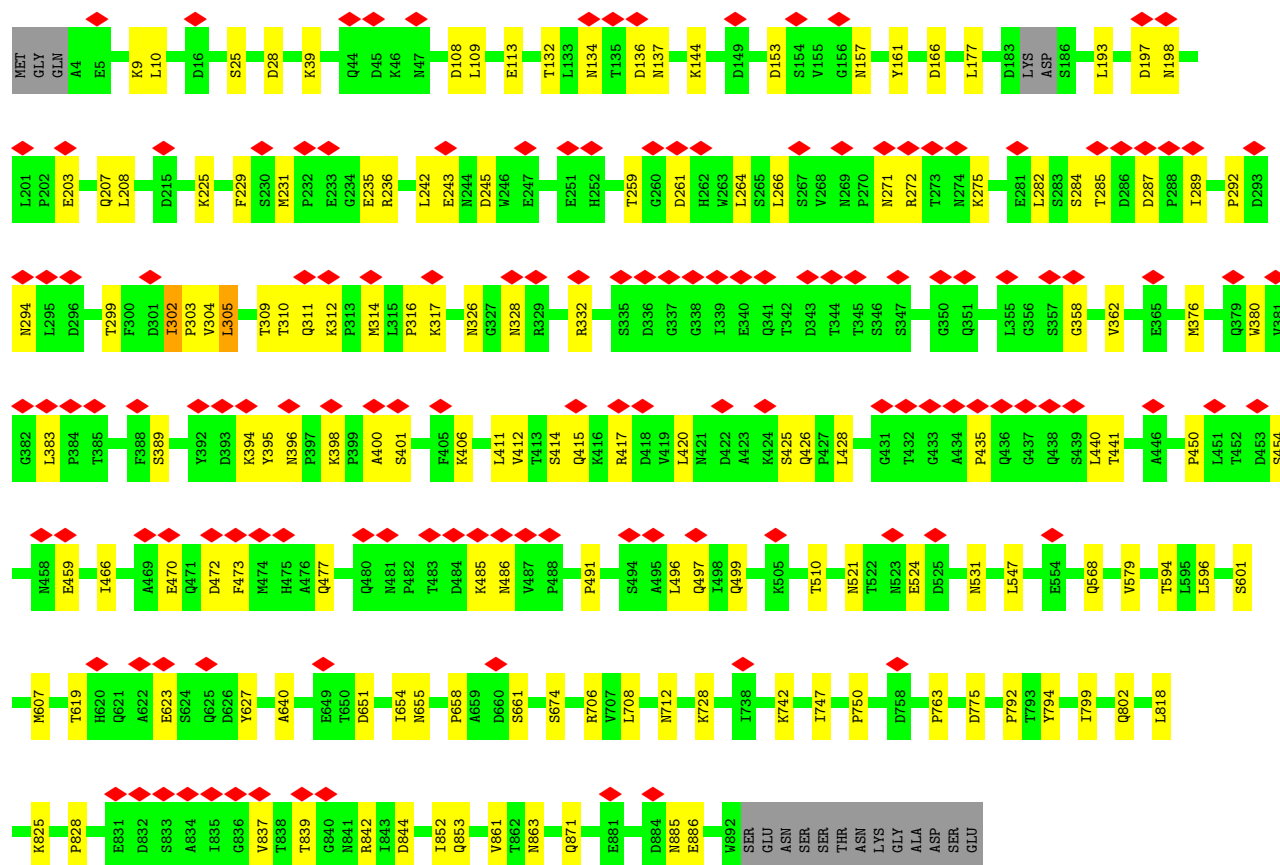
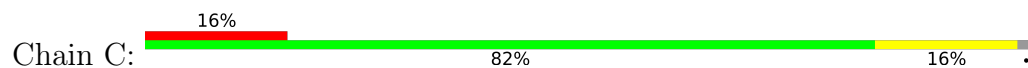


- Molecule 6: *Photorhabdus luminescens* subsp. *laumondii* TTO1 complete genome segment 6/17

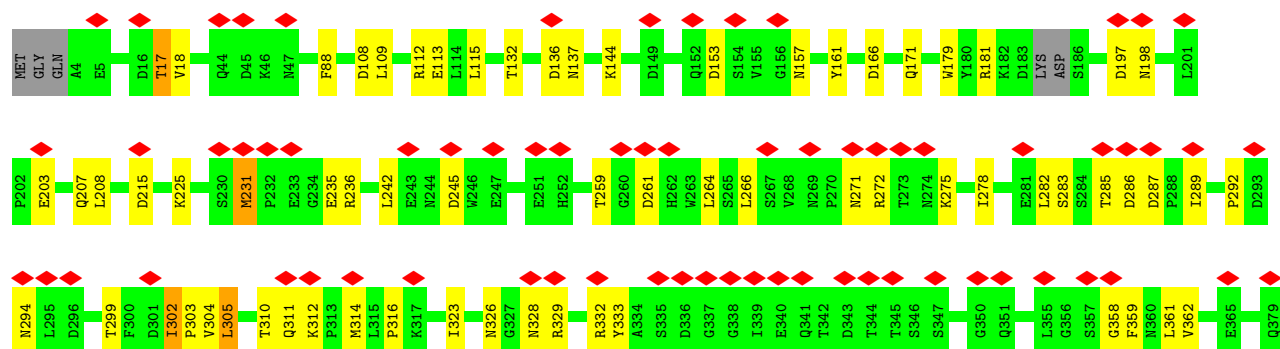
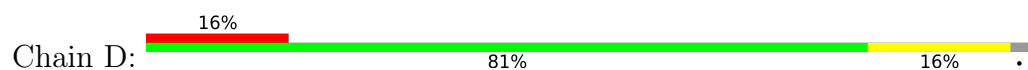


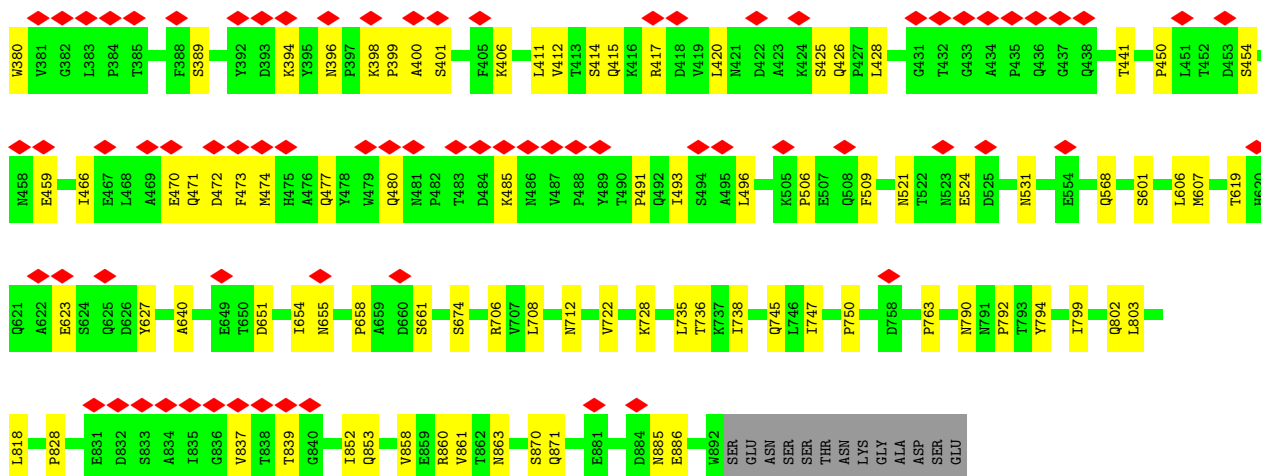


- Molecule 6: Photorhabdus luminescens subsp. laumondii TTO1 complete genome segment 6/17

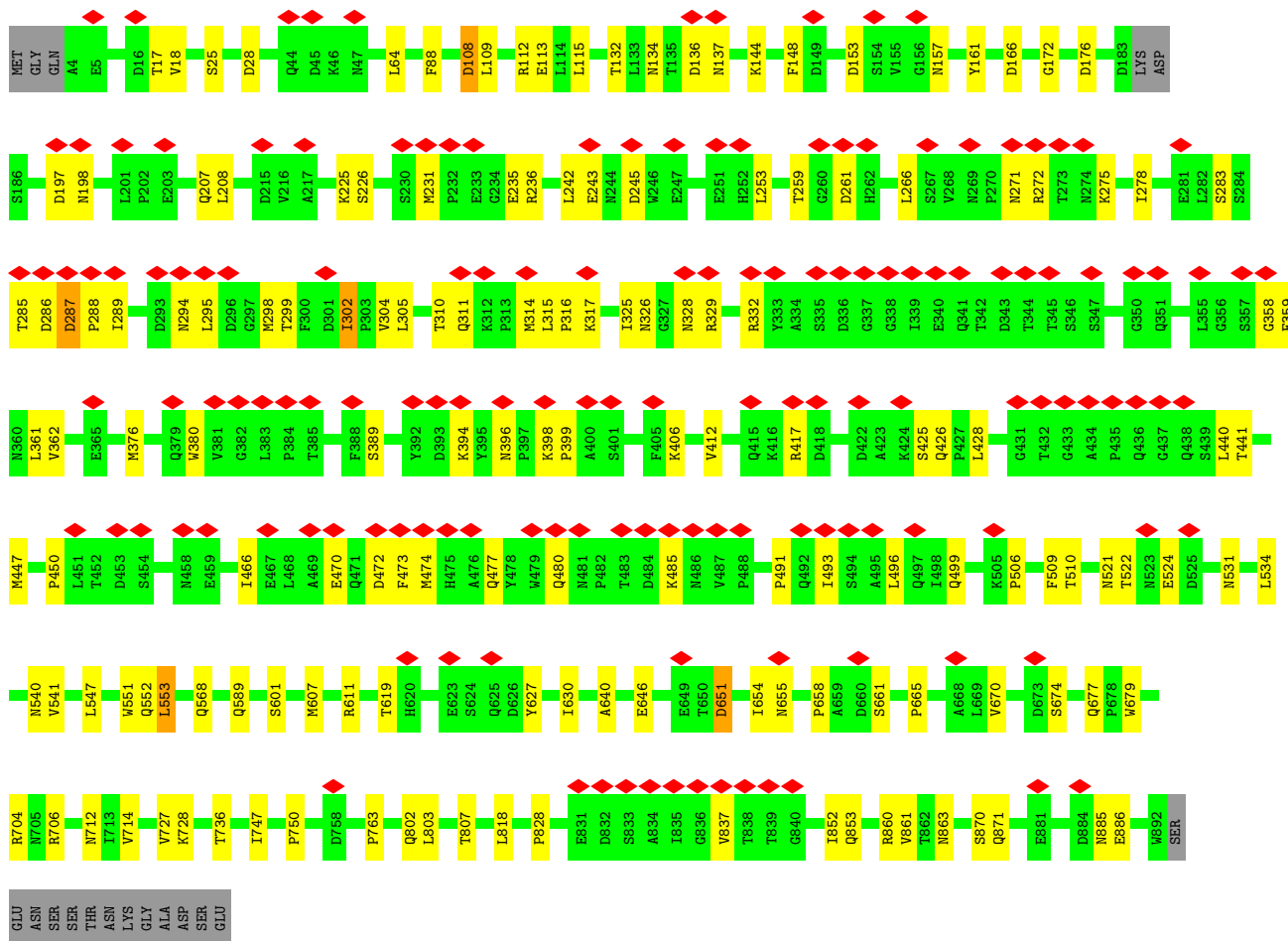
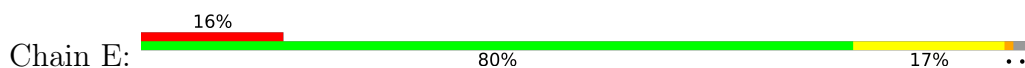


- Molecule 6: Photorhabdus luminescens subsp. laumondii TTO1 complete genome segment 6/17



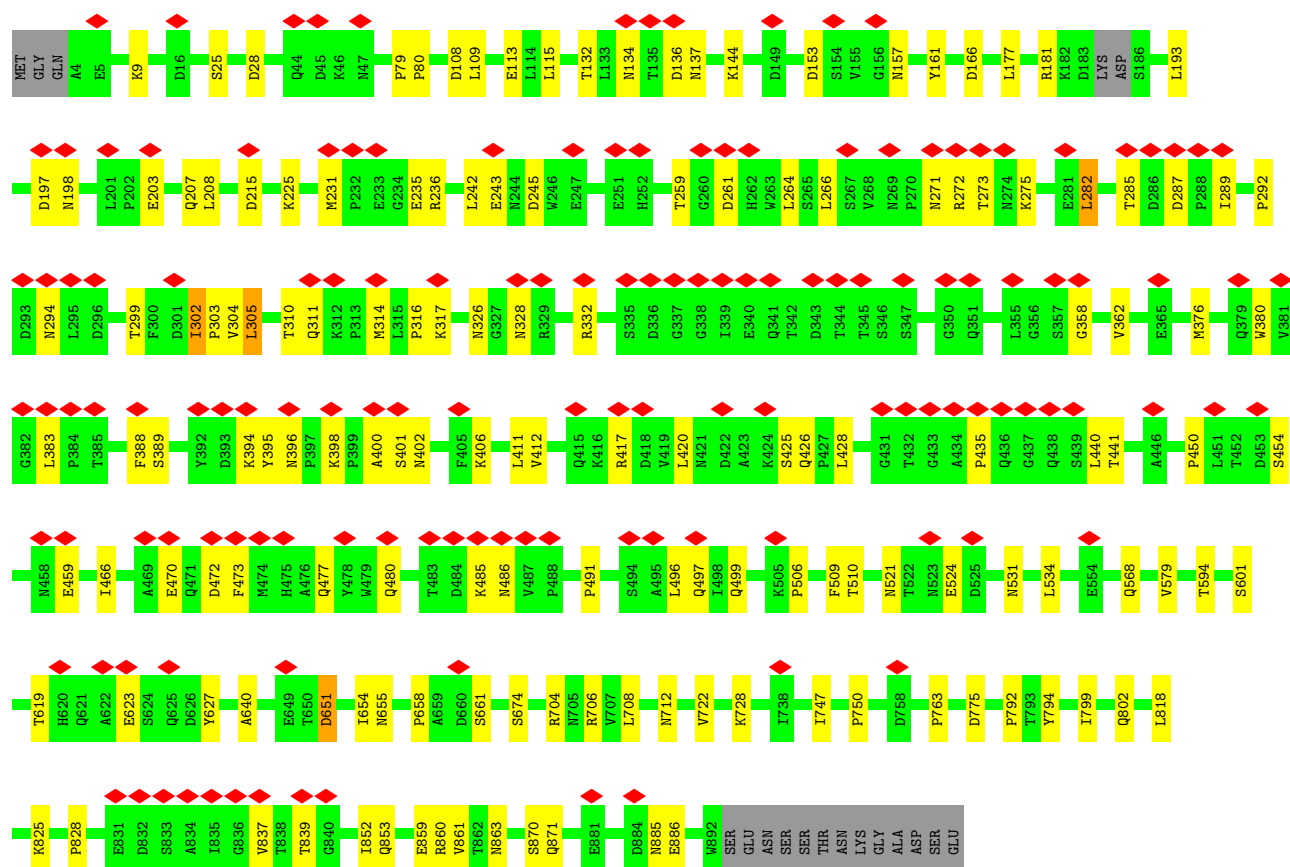


- Molecule 6: Photorhabdus luminescens subsp. laumondii TTO1 complete genome segment 6/17



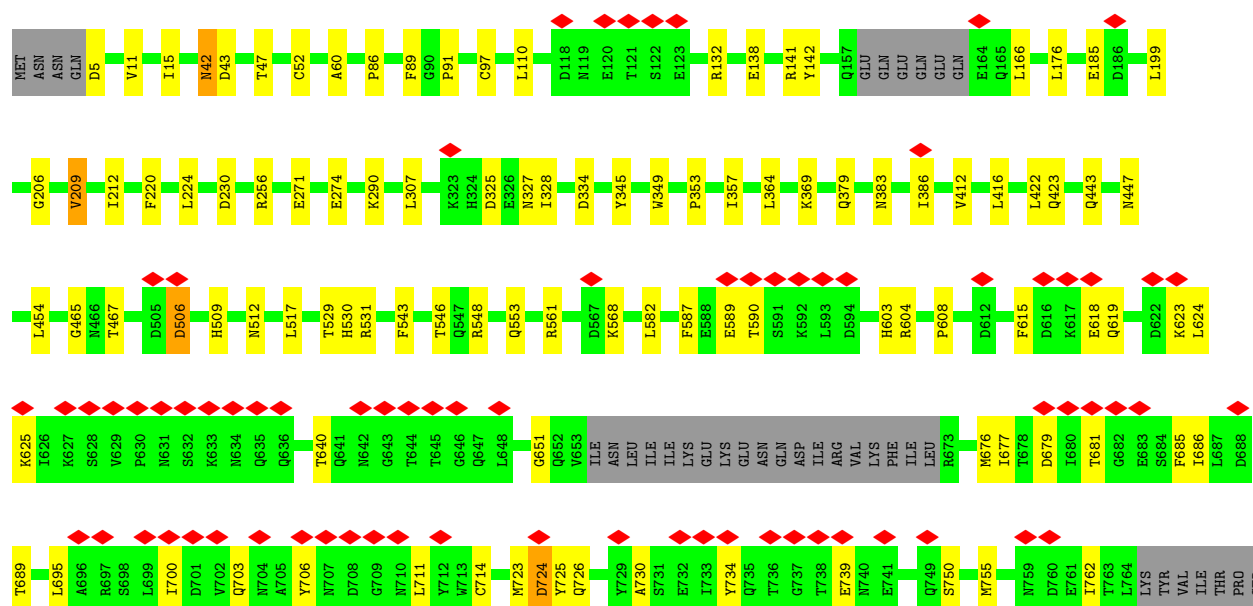
- Molecule 6: Photorhabdus luminescens subsp. laumondii TTO1 complete genome segment 6/17

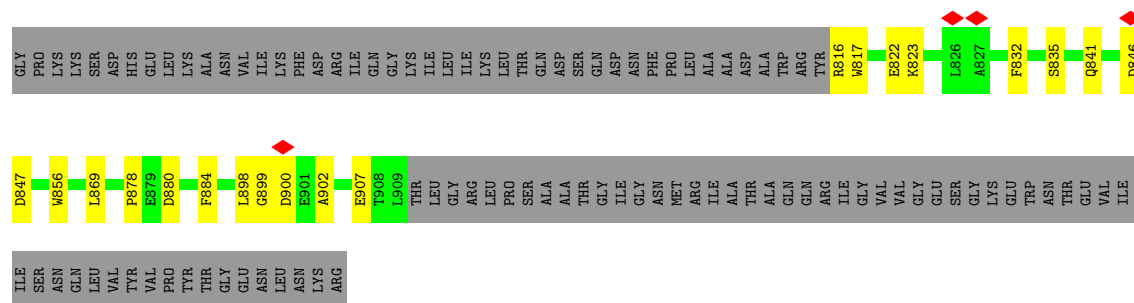
Chain F: 



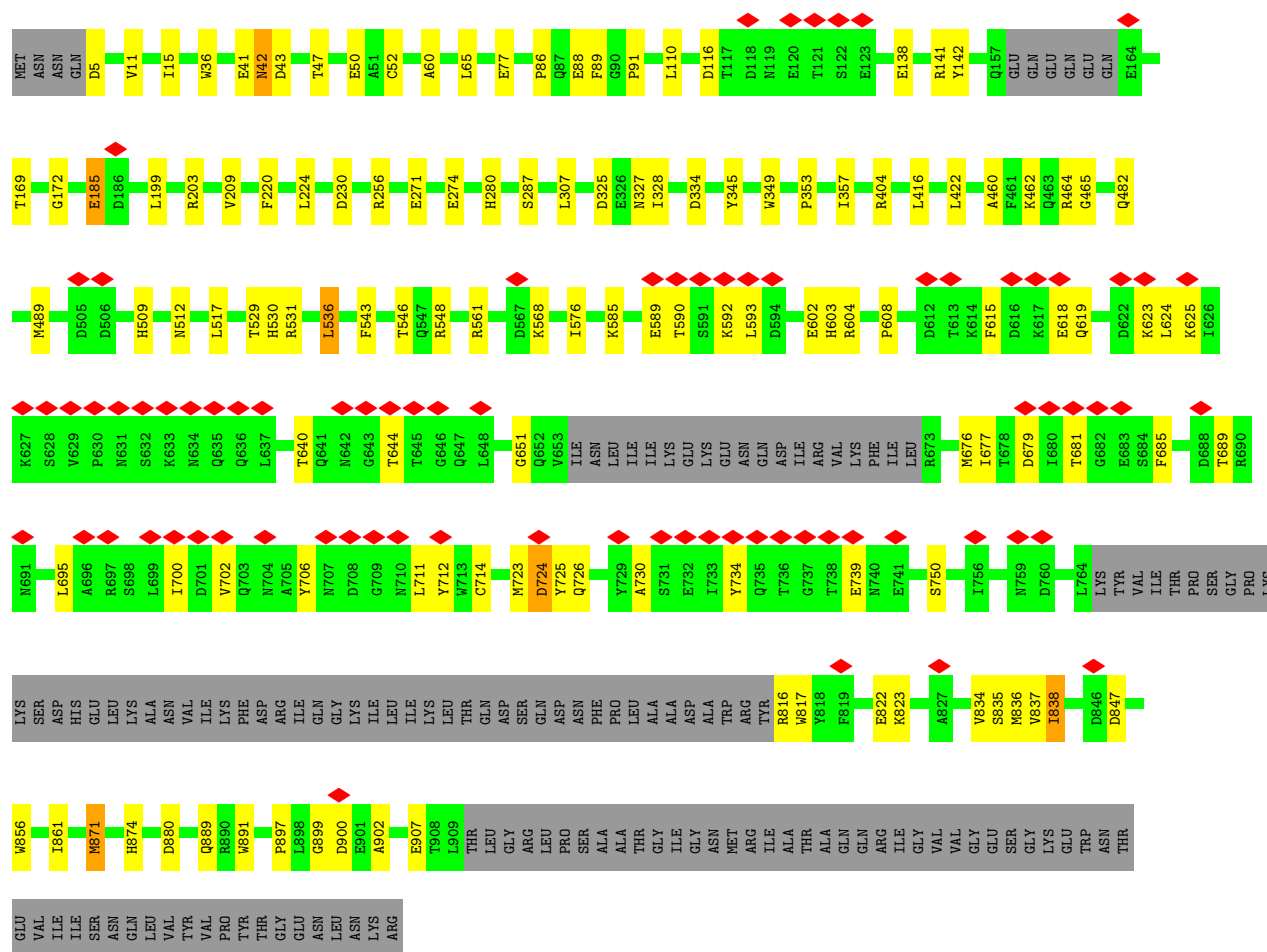
• Molecule 7: Baseplate protein J-like domain-containing protein

Chain a: 

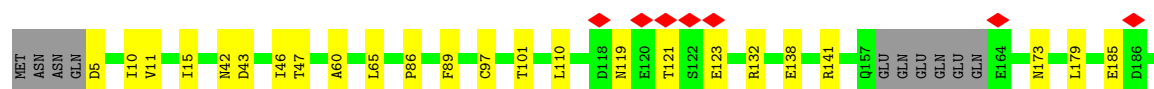
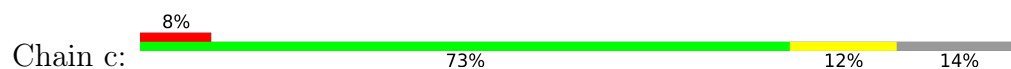


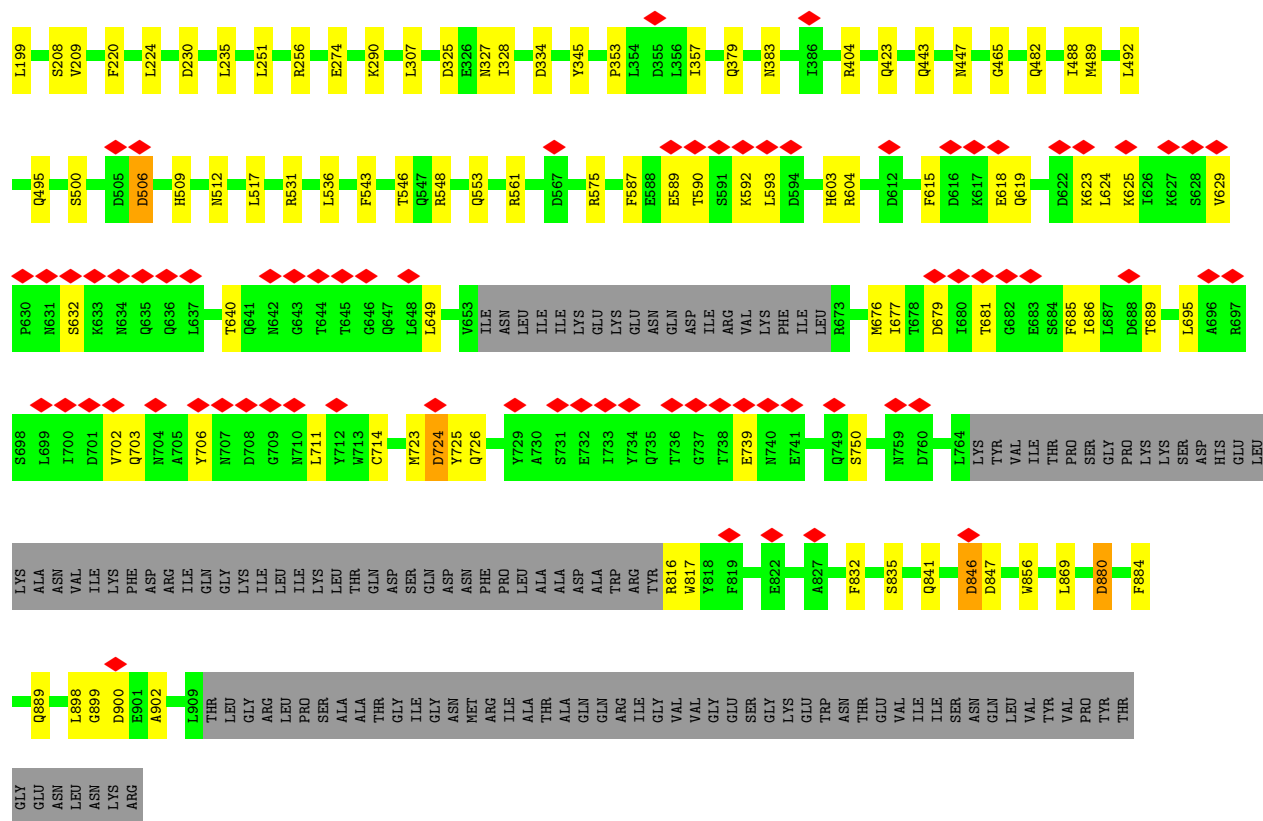


• Molecule 7: Baseplate protein J-like domain-containing protein

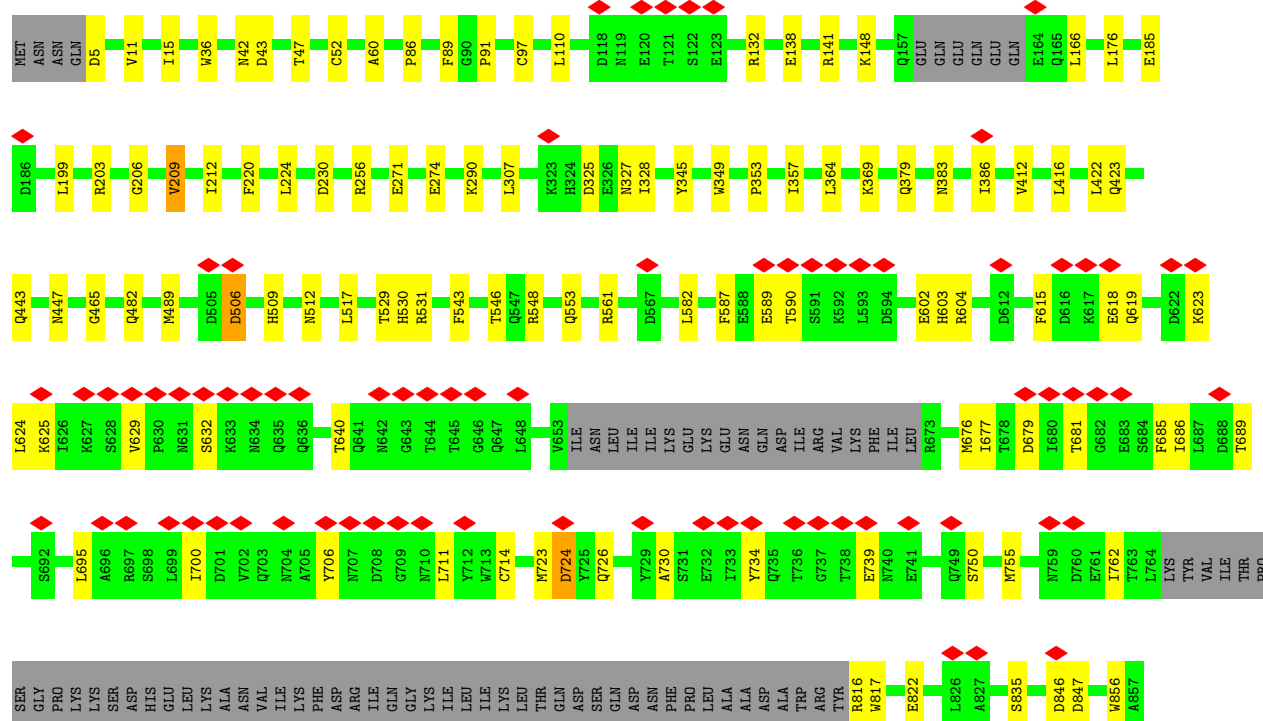
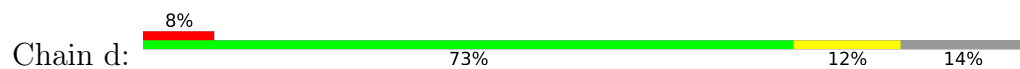


• Molecule 7: Baseplate protein J-like domain-containing protein

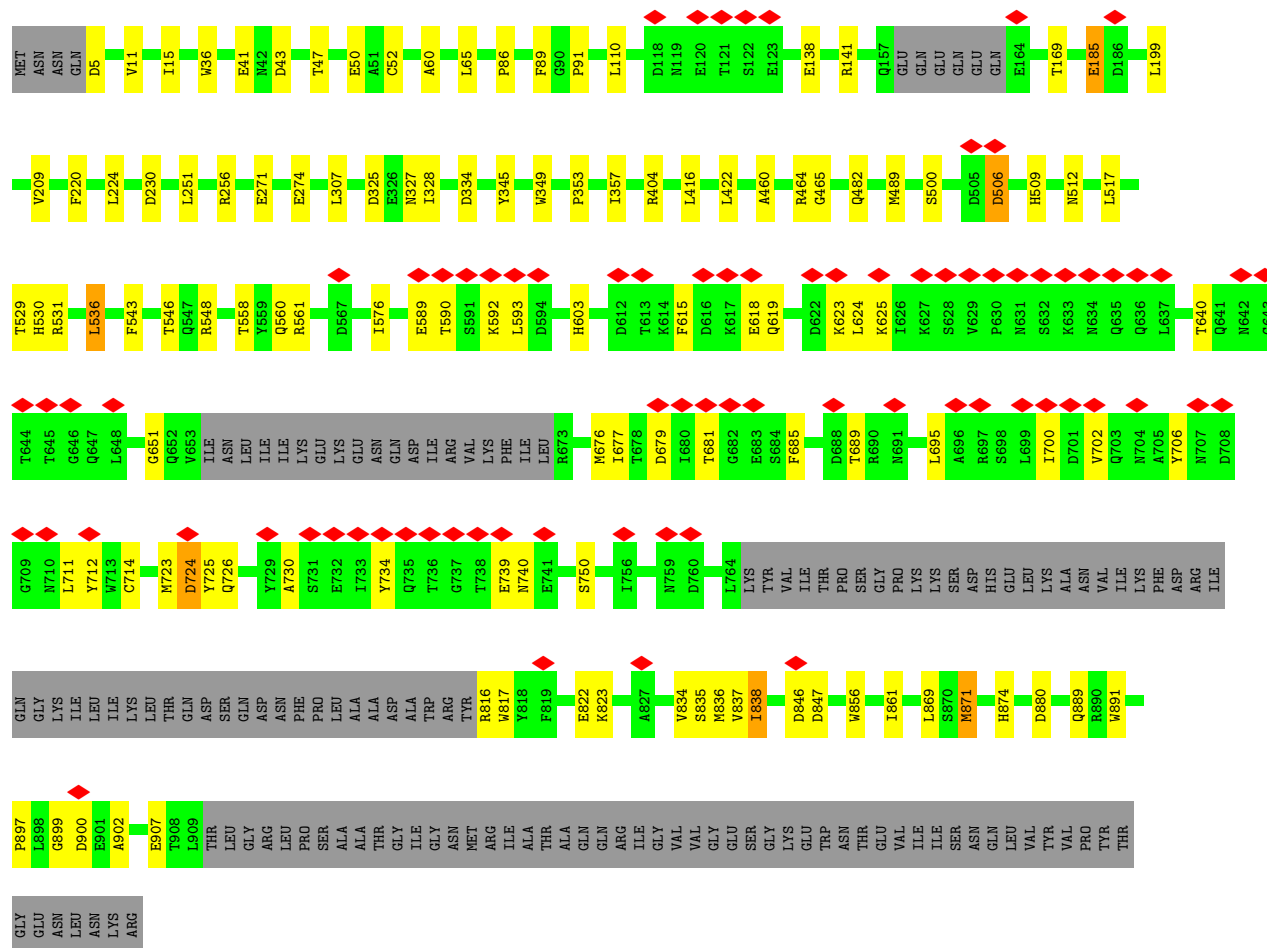
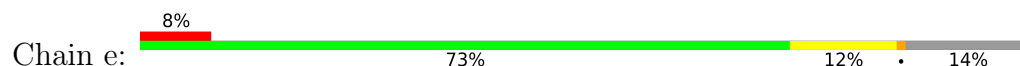




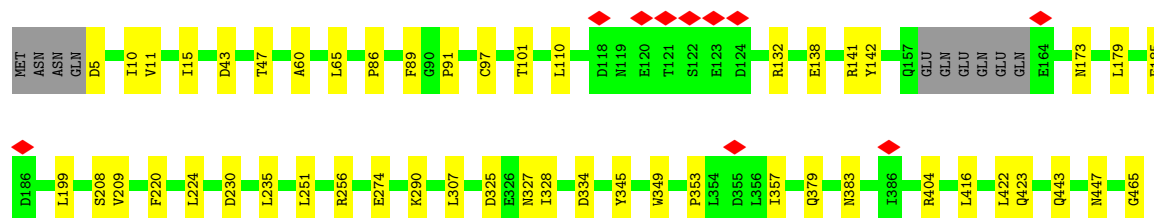
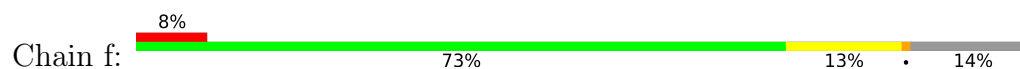
• Molecule 7: Baseplate protein J-like domain-containing protein

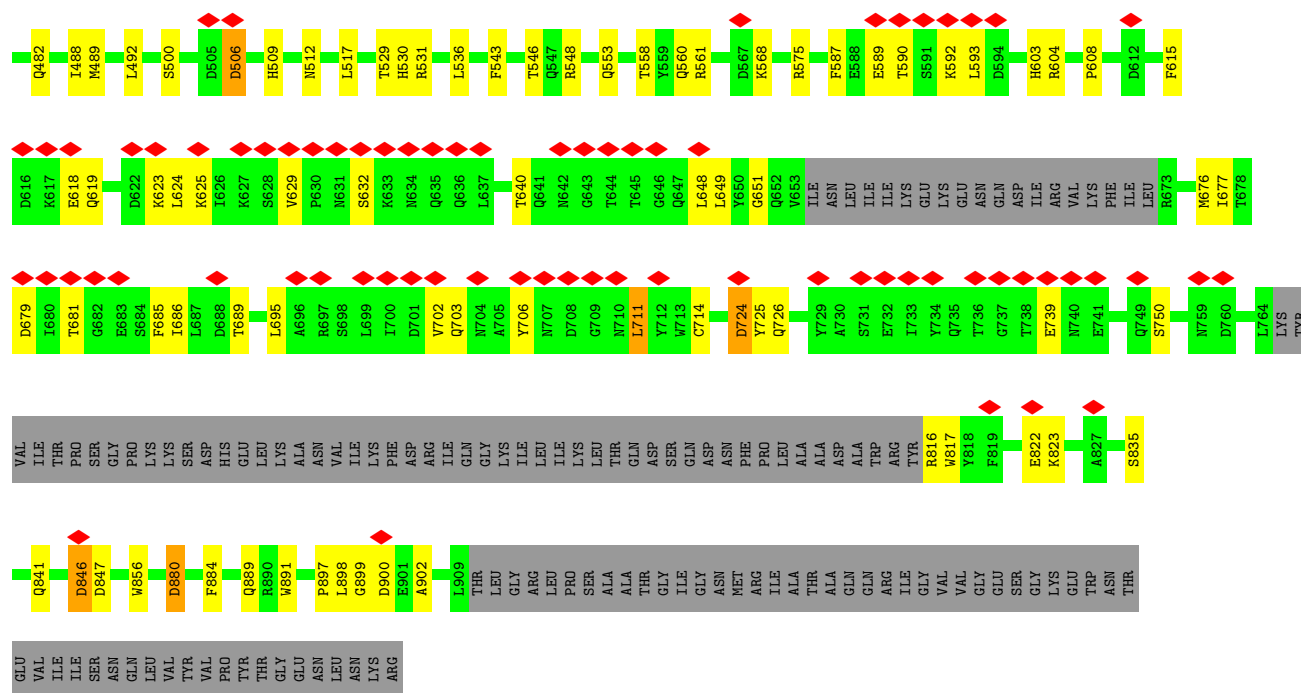


- Molecule 7: Baseplate protein J-like domain-containing protein

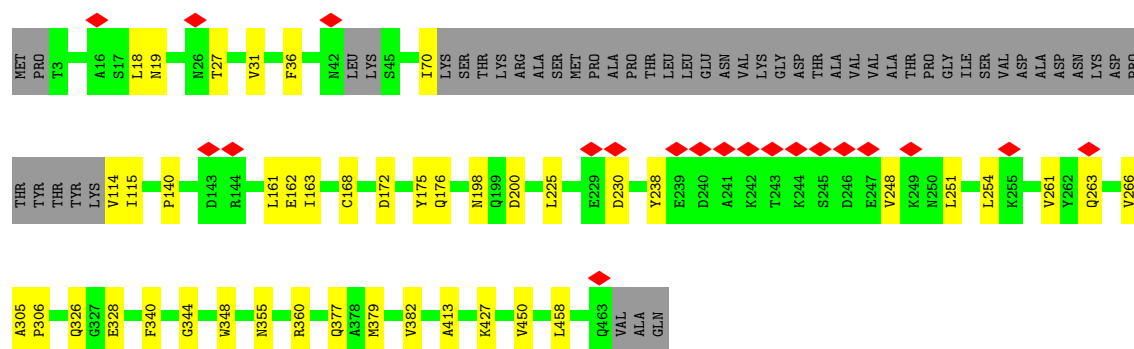
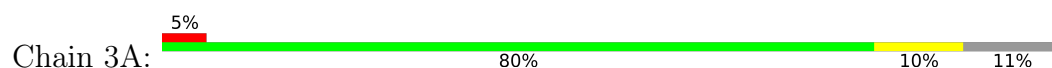


- Molecule 7: Baseplate protein J-like domain-containing protein

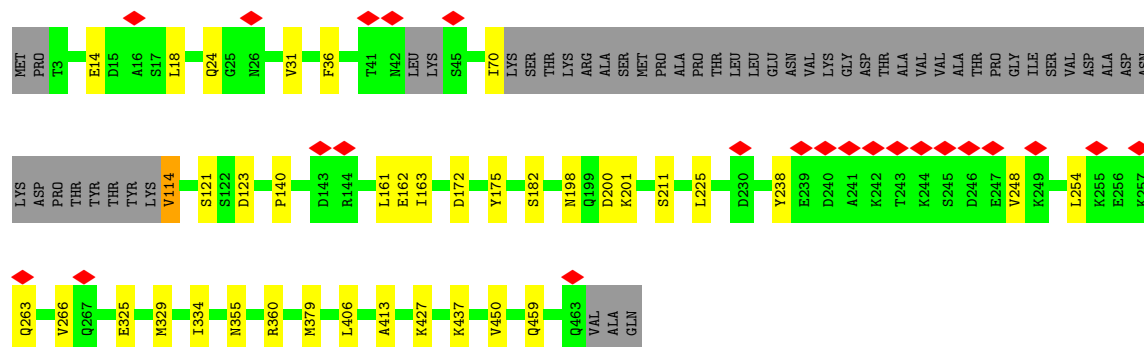
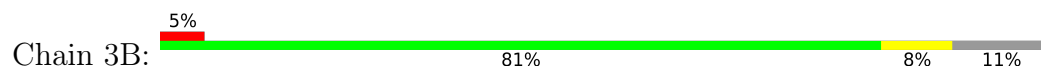




• Molecule 8: Phage tail sheath family protein

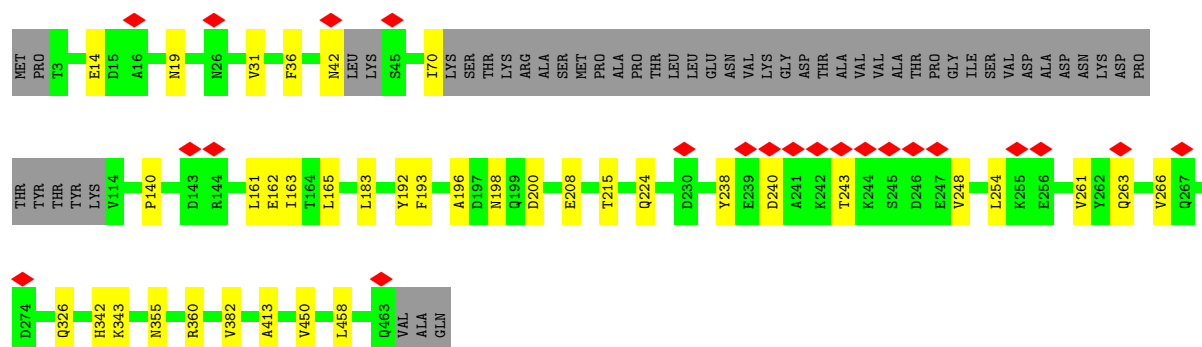


• Molecule 8: Phage tail sheath family protein



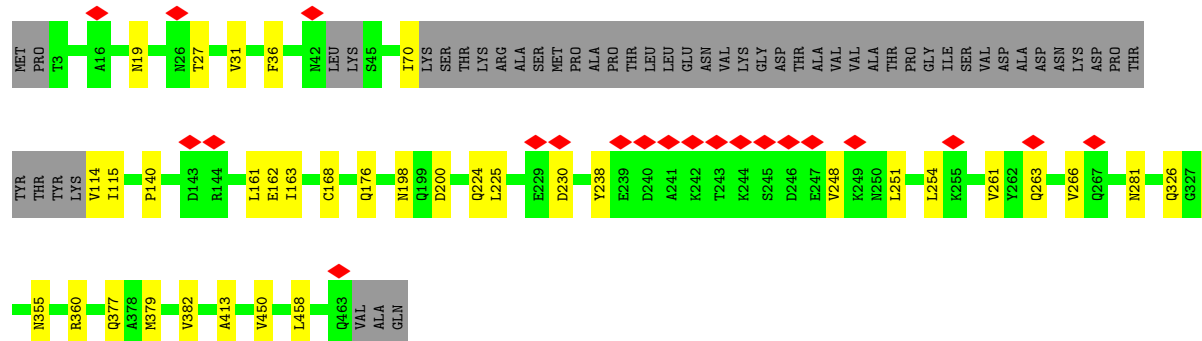
- Molecule 8: Phage tail sheath family protein

Chain 3C: 



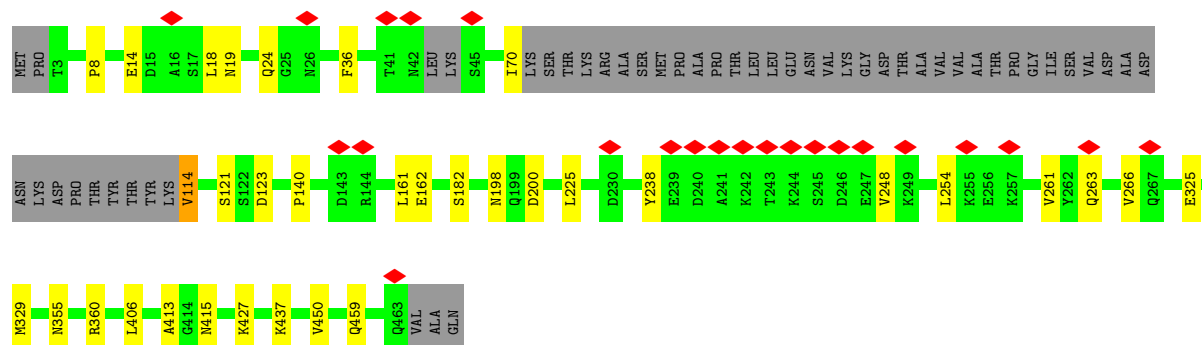
- Molecule 8: Phage tail sheath family protein

Chain 3D: 



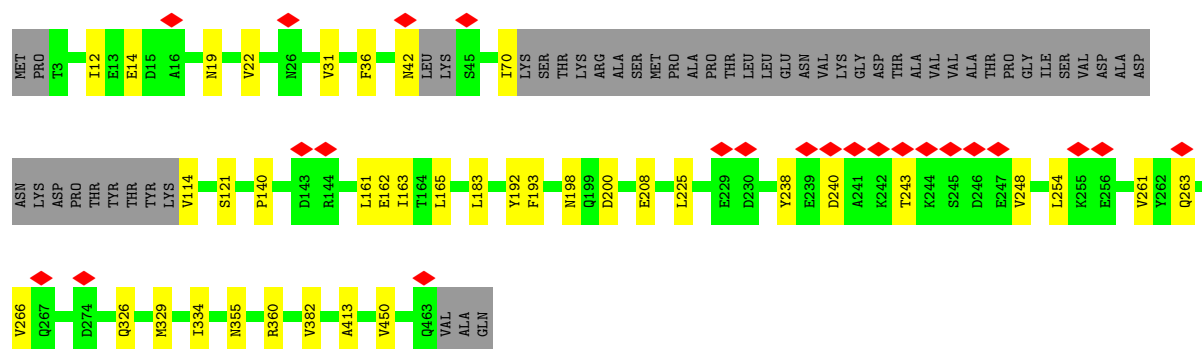
- Molecule 8: Phage tail sheath family protein

Chain 3E: 



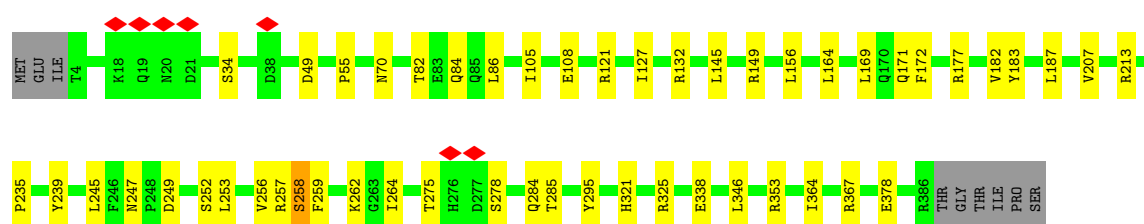
- Molecule 8: Phage tail sheath family protein

Chain 3F: 



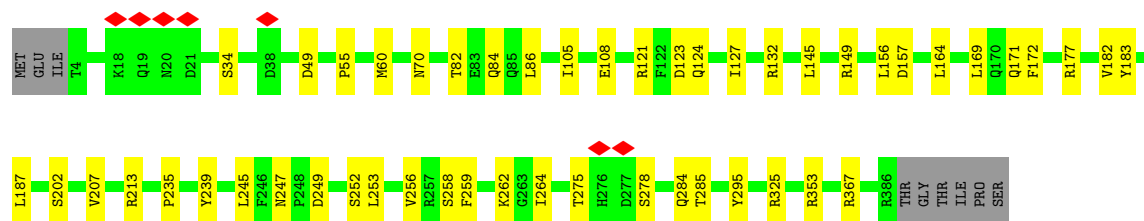
- Molecule 9: Phage tail sheath family protein

Chain 4A: 85% 13% .



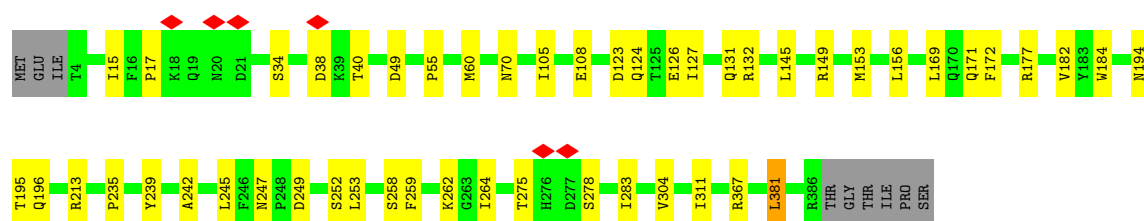
- Molecule 9: Phage tail sheath family protein

Chain 4B: 85% 13% .



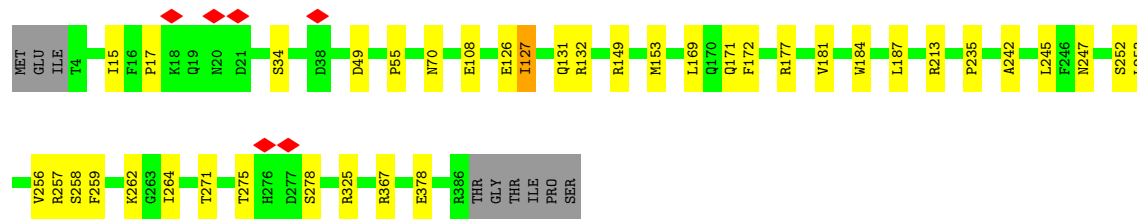
- Molecule 9: Phage tail sheath family protein

Chain 4C: 85% 12% .

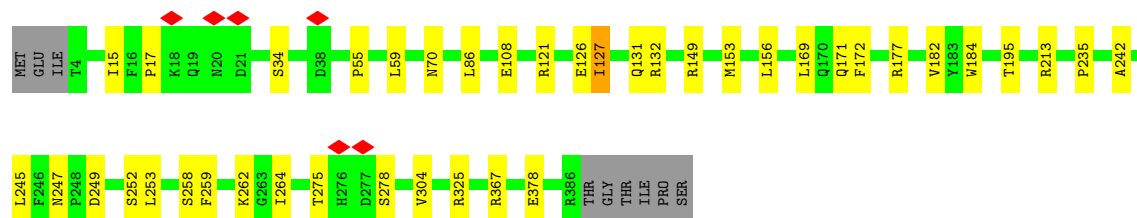


- Molecule 9: Phage tail sheath family protein

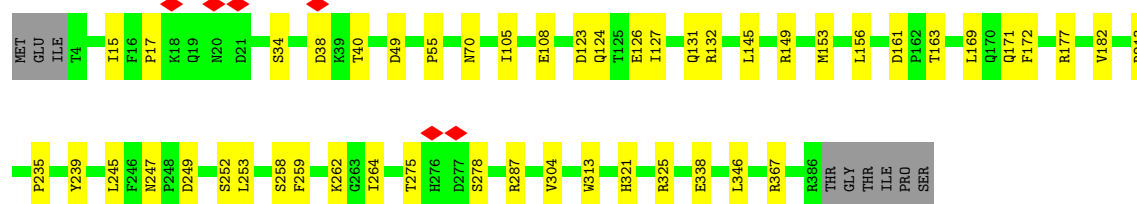
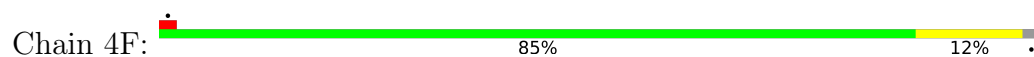
Chain 4D: 88% 10% .



• Molecule 9: Phage tail sheath family protein



• Molecule 9: Phage tail sheath family protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	53537	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; Patch CTF Estimation in cryoSPARC, fit local CTF to micrograph, including tilted, bent, deformed samples	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	41	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.689	Depositor
Minimum map value	-0.810	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.044	Depositor
Recommended contour level	0.35	Depositor
Map size ($\text{\AA}$)	840.00006, 840.00006, 840.00006	wwPDB
Map dimensions	700, 700, 700	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.2, 1.2, 1.2	Depositor

5 Model quality

5.1 Standard geometry

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	1A	0.12	0/1185	0.30	0/1618
1	1B	0.13	0/1185	0.32	0/1618
1	1C	0.12	0/1185	0.29	0/1618
1	1D	0.12	0/1185	0.30	0/1618
1	1E	0.13	0/1185	0.32	0/1618
1	1F	0.12	0/1185	0.29	0/1618
2	2A	0.10	0/2781	0.26	0/3802
2	2B	0.10	0/2781	0.25	0/3802
2	2C	0.10	0/2781	0.22	0/3802
2	2D	0.10	0/2781	0.26	0/3802
2	2E	0.10	0/2781	0.23	0/3802
2	2F	0.10	0/2781	0.23	0/3802
3	5A	0.12	0/1201	0.24	0/1635
3	5B	0.11	0/1201	0.24	0/1635
3	5C	0.11	0/1201	0.24	0/1635
3	5D	0.12	0/1201	0.25	0/1635
3	5E	0.11	0/1201	0.23	0/1635
3	5F	0.12	0/1201	0.27	0/1635
4	7A	0.12	0/1760	0.27	0/2399
4	7B	0.11	0/1760	0.24	0/2399
4	7C	0.12	0/1760	0.26	0/2399
4	7D	0.11	0/1760	0.24	0/2399
4	7E	0.11	0/1760	0.24	0/2399
4	7F	0.12	0/1760	0.26	0/2399
5	9A	0.12	0/1725	0.29	0/2333
5	9B	0.12	0/1725	0.31	0/2333
5	9C	0.11	0/1725	0.27	0/2333
5	9D	0.10	0/1725	0.24	0/2333
5	9E	0.11	0/1725	0.29	0/2333
5	9F	0.12	0/1725	0.28	0/2333
6	A	0.09	0/7225	0.25	0/9886
6	B	0.09	0/7225	0.26	0/9886
6	C	0.09	0/7225	0.25	0/9886
6	D	0.09	0/7225	0.25	0/9886

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	E	0.09	0/7225	0.25	0/9886
6	F	0.09	0/7225	0.25	0/9886
7	a	0.09	0/6876	0.24	0/9347
7	b	0.10	0/6876	0.25	0/9347
7	c	0.09	0/6876	0.24	0/9347
7	d	0.09	0/6876	0.25	0/9347
7	e	0.10	0/6876	0.25	0/9347
7	f	0.10	0/6876	0.25	0/9347
8	3A	0.10	0/3303	0.26	1/4493 (0.0%)
8	3B	0.11	0/3303	0.25	0/4493
8	3C	0.10	0/3303	0.26	1/4493 (0.0%)
8	3D	0.10	0/3303	0.26	1/4493 (0.0%)
8	3E	0.10	0/3303	0.25	0/4493
8	3F	0.10	0/3303	0.26	1/4493 (0.0%)
9	4A	0.10	0/3115	0.24	0/4242
9	4B	0.10	0/3115	0.24	0/4242
9	4C	0.10	0/3115	0.25	0/4242
9	4D	0.10	0/3115	0.25	0/4242
9	4E	0.10	0/3115	0.26	0/4242
9	4F	0.10	0/3115	0.26	0/4242
All	All	0.10	0/175026	0.25	4/238530 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	3C	382	VAL	N-CA-C	-5.55	107.87	113.20
8	3F	382	VAL	N-CA-C	-5.40	108.02	113.20
8	3D	382	VAL	N-CA-C	-5.18	108.23	113.20
8	3A	382	VAL	N-CA-C	-5.14	108.27	113.20

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	1A	1160	0	1135	12	0
1	1B	1160	0	1135	12	0
1	1C	1160	0	1135	12	0
1	1D	1160	0	1135	11	0
1	1E	1160	0	1135	10	0
1	1F	1160	0	1135	13	0
2	2A	2713	0	2661	26	0
2	2B	2713	0	2661	27	0
2	2C	2713	0	2661	26	0
2	2D	2713	0	2661	25	0
2	2E	2713	0	2661	31	0
2	2F	2713	0	2661	28	0
3	5A	1175	0	1170	13	0
3	5B	1175	0	1170	13	0
3	5C	1175	0	1170	11	0
3	5D	1175	0	1170	12	0
3	5E	1175	0	1170	16	0
3	5F	1175	0	1170	13	0
4	7A	1724	0	1712	5	0
4	7B	1724	0	1712	6	0
4	7C	1724	0	1712	7	0
4	7D	1724	0	1712	6	0
4	7E	1724	0	1712	7	0
4	7F	1724	0	1712	5	0
5	9A	1697	0	1692	18	0
5	9B	1697	0	1692	16	0
5	9C	1697	0	1692	20	0
5	9D	1697	0	1692	11	0
5	9E	1697	0	1692	21	0
5	9F	1697	0	1692	24	0
6	A	7040	0	6829	84	0
6	B	7040	0	6829	97	0
6	C	7040	0	6829	95	0
6	D	7040	0	6829	95	0
6	E	7040	0	6829	94	0
6	F	7040	0	6829	95	0
7	a	6720	0	6538	80	0
7	b	6720	0	6538	81	0
7	c	6720	0	6538	77	0
7	d	6720	0	6538	71	0
7	e	6720	0	6538	72	0
7	f	6720	0	6538	80	0
8	3A	3241	0	3207	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	3B	3241	0	3207	21	0
8	3C	3241	0	3207	20	0
8	3D	3241	0	3207	19	0
8	3E	3241	0	3207	22	0
8	3F	3241	0	3207	20	0
9	4A	3044	0	3027	31	0
9	4B	3044	0	3027	29	0
9	4C	3044	0	3027	33	0
9	4D	3044	0	3027	26	0
9	4E	3044	0	3027	29	0
9	4F	3044	0	3027	32	0
All	All	171084	0	167826	1647	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 5.

All (1647) 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)
3:5F:146:ARG:HH11	9:4E:325:ARG:HD2	1.34	0.92
7:e:603:HIS:HE2	7:e:835:SER:HG	1.22	0.81
5:9F:45:GLU:OE2	5:9F:45:GLU:N	2.18	0.76
7:c:199:LEU:HD13	7:c:209:VAL:HG21	1.69	0.75
5:9E:45:GLU:OE2	5:9E:45:GLU:N	2.21	0.73
5:9D:45:GLU:N	5:9D:45:GLU:OE1	2.21	0.73
7:f:199:LEU:HD13	7:f:209:VAL:HG21	1.69	0.72
8:3E:162:GLU:OE1	8:3E:162:GLU:N	2.22	0.71
9:4D:15:ILE:HG23	9:4D:17:PRO:HD3	1.72	0.71
5:9C:45:GLU:OE1	5:9C:45:GLU:N	2.20	0.71
8:3D:162:GLU:N	8:3D:162:GLU:OE2	2.24	0.71
5:9B:45:GLU:OE2	5:9B:45:GLU:N	2.20	0.70
7:e:199:LEU:HD13	7:e:209:VAL:HG21	1.73	0.70
2:2E:192:ALA:HA	2:2E:251:PRO:HG3	1.74	0.70
6:F:231:MET:HB3	6:F:236:ARG:HG2	1.74	0.70
4:7C:118:GLU:HG3	4:7D:93:LYS:HG2	1.73	0.70
7:b:199:LEU:HD13	7:b:209:VAL:HG21	1.73	0.70
8:3A:162:GLU:N	8:3A:162:GLU:OE2	2.24	0.70
2:2B:192:ALA:HA	2:2B:251:PRO:HG3	1.73	0.69
2:2C:192:ALA:HA	2:2C:251:PRO:HG3	1.74	0.69
5:9A:45:GLU:OE2	5:9A:45:GLU:N	2.22	0.69
9:4E:15:ILE:HG23	9:4E:17:PRO:HD3	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:623:GLU:N	6:A:623:GLU:OE2	2.27	0.68
6:E:712:ASN:OD1	7:e:561:ARG:NH2	2.21	0.68
8:3B:162:GLU:OE2	8:3B:162:GLU:N	2.26	0.68
9:4F:258:SER:HB3	9:4F:264:ILE:HG13	1.75	0.68
6:C:231:MET:HG2	6:C:236:ARG:HG2	1.76	0.68
6:D:225:LYS:HG3	6:D:304:VAL:HG12	1.76	0.68
9:4C:126:GLU:OE2	9:4C:126:GLU:N	2.27	0.68
2:2F:192:ALA:HA	2:2F:251:PRO:HG3	1.74	0.67
7:d:623:LYS:HB3	7:d:640:THR:HB	1.76	0.67
2:2A:192:ALA:HA	2:2A:251:PRO:HG3	1.75	0.67
2:2D:192:ALA:HA	2:2D:251:PRO:HG3	1.75	0.67
9:4F:15:ILE:HG23	9:4F:17:PRO:HD3	1.76	0.67
9:4C:15:ILE:HG23	9:4C:17:PRO:HD3	1.76	0.67
1:1C:54:LYS:NZ	1:1D:142:ASP:OD1	2.27	0.67
9:4F:172:PHE:O	9:4F:177:ARG:NH2	2.28	0.67
1:1B:47:ASP:OD2	1:1B:51:ASN:ND2	2.26	0.67
6:D:623:GLU:N	6:D:623:GLU:OE2	2.27	0.67
6:F:109:LEU:HD12	6:F:113:GLU:HG3	1.77	0.67
8:3F:162:GLU:OE2	8:3F:162:GLU:N	2.28	0.67
6:B:623:GLU:N	6:B:623:GLU:OE2	2.26	0.67
9:4C:258:SER:HB3	9:4C:264:ILE:HG13	1.76	0.67
1:1A:142:ASP:OD1	1:1F:54:LYS:NZ	2.28	0.67
6:E:225:LYS:HG3	6:E:304:VAL:HG12	1.77	0.67
9:4F:126:GLU:OE2	9:4F:126:GLU:N	2.27	0.67
6:A:225:LYS:HG3	6:A:304:VAL:HG12	1.76	0.67
1:1C:47:ASP:OD1	1:1C:51:ASN:ND2	2.26	0.67
5:9F:154:ASP:OD1	5:9F:186:TYR:OH	2.11	0.67
8:3A:355:ASN:OD1	8:3A:360:ARG:NH1	2.28	0.66
8:3C:224:GLN:OE1	8:3C:224:GLN:N	2.28	0.66
9:4E:258:SER:HB3	9:4E:264:ILE:HG13	1.77	0.66
8:3D:355:ASN:OD1	8:3D:360:ARG:NH1	2.29	0.66
8:3C:70:ILE:HD12	8:3C:238:TYR:HB2	1.76	0.66
6:D:109:LEU:HD12	6:D:113:GLU:HG3	1.77	0.66
6:E:109:LEU:HD12	6:E:113:GLU:HG3	1.78	0.66
7:e:110:LEU:O	7:e:256:ARG:NH2	2.29	0.66
5:9C:154:ASP:OD1	5:9C:186:TYR:OH	2.11	0.66
7:a:623:LYS:HB3	7:a:640:THR:HB	1.76	0.66
7:a:199:LEU:HD13	7:a:209:VAL:HG21	1.77	0.66
7:b:110:LEU:O	7:b:256:ARG:NH2	2.29	0.66
8:3C:162:GLU:OE2	8:3C:162:GLU:N	2.28	0.66
9:4C:172:PHE:O	9:4C:177:ARG:NH2	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:4D:34:SER:HB2	9:4D:55:PRO:HD2	1.78	0.66
6:F:389:SER:HG	6:F:398:LYS:HZ3	1.41	0.65
2:2E:313:ILE:HB	2:2E:331:ILE:HG23	1.76	0.65
9:4B:34:SER:HB2	9:4B:55:PRO:HD2	1.79	0.65
9:4C:153:MET:HE1	9:4C:283:ILE:HG13	1.78	0.65
6:A:294:ASN:H	6:A:299:THR:HG22	1.62	0.65
6:E:389:SER:OG	6:E:398:LYS:NZ	2.29	0.65
7:c:603:HIS:NE2	7:c:835:SER:OG	2.28	0.65
8:3B:355:ASN:OD1	8:3B:360:ARG:NH1	2.29	0.65
9:4A:34:SER:HB2	9:4A:55:PRO:HD2	1.78	0.65
7:b:603:HIS:NE2	7:b:835:SER:OG	2.28	0.65
8:3F:70:ILE:HD12	8:3F:238:TYR:HB2	1.78	0.65
6:C:109:LEU:HD12	6:C:113:GLU:HG3	1.77	0.65
7:b:172:GLY:O	7:b:604:ARG:NH2	2.30	0.65
7:d:199:LEU:HD13	7:d:209:VAL:HG21	1.77	0.65
6:B:225:LYS:HG3	6:B:304:VAL:HG12	1.77	0.65
7:c:110:LEU:O	7:c:256:ARG:NH2	2.30	0.65
7:f:110:LEU:O	7:f:256:ARG:NH2	2.30	0.65
8:3F:355:ASN:OD1	8:3F:360:ARG:NH1	2.30	0.65
6:A:109:LEU:HD12	6:A:113:GLU:HG3	1.77	0.65
1:1E:47:ASP:OD2	1:1E:51:ASN:ND2	2.26	0.64
6:B:109:LEU:HD12	6:B:113:GLU:HG3	1.78	0.64
7:d:615:PHE:HA	7:d:619:GLN:HE22	1.62	0.64
7:d:762:ILE:HD11	7:d:817:TRP:HB2	1.77	0.64
7:c:623:LYS:HB3	7:c:640:THR:HB	1.79	0.64
8:3C:355:ASN:OD1	8:3C:360:ARG:NH1	2.31	0.64
6:F:225:LYS:HG3	6:F:304:VAL:HG12	1.79	0.64
1:1F:47:ASP:OD2	1:1F:51:ASN:ND2	2.28	0.64
7:f:603:HIS:NE2	7:f:835:SER:OG	2.27	0.64
7:a:110:LEU:O	7:a:256:ARG:NH2	2.31	0.64
9:4E:172:PHE:O	9:4E:177:ARG:NH2	2.30	0.64
3:5F:144:ASP:OD2	9:4E:325:ARG:NH1	2.29	0.64
8:3D:70:ILE:HD12	8:3D:238:TYR:HB2	1.79	0.64
1:1A:47:ASP:OD1	1:1A:51:ASN:ND2	2.27	0.64
6:C:225:LYS:HG3	6:C:304:VAL:HG12	1.78	0.64
7:f:880:ASP:OD1	7:f:880:ASP:N	2.31	0.64
8:3E:355:ASN:OD1	8:3E:360:ARG:NH1	2.29	0.64
9:4D:169:LEU:HD11	9:4D:253:LEU:HG	1.80	0.64
6:B:225:LYS:HG2	6:B:302:ILE:HD11	1.80	0.64
6:E:225:LYS:HG2	6:E:302:ILE:HD11	1.80	0.64
6:D:294:ASN:H	6:D:299:THR:HG22	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:f:623:LYS:HB3	7:f:640:THR:HB	1.79	0.63
9:4E:34:SER:HB2	9:4E:55:PRO:HD2	1.79	0.63
6:E:294:ASN:H	6:E:299:THR:HG22	1.63	0.63
7:a:615:PHE:HA	7:a:619:GLN:HE22	1.62	0.63
9:4D:172:PHE:O	9:4D:177:ARG:NH2	2.32	0.63
2:2D:184:ASP:OD2	2:2D:254:ARG:NH2	2.32	0.63
6:A:328:ASN:ND2	6:A:496:LEU:O	2.31	0.63
7:c:880:ASP:OD1	7:c:880:ASP:N	2.31	0.63
2:2C:184:ASP:OD2	2:2C:254:ARG:NH2	2.32	0.63
6:F:294:ASN:H	6:F:299:THR:HG22	1.63	0.63
2:2D:191:LYS:NZ	2:2D:192:ALA:O	2.32	0.63
7:d:110:LEU:O	7:d:256:ARG:NH2	2.31	0.63
9:4E:169:LEU:HD11	9:4E:253:LEU:HG	1.79	0.63
6:B:376:MET:HG3	6:B:440:LEU:HB2	1.81	0.63
6:B:398:LYS:HZ1	6:B:400:ALA:HB2	1.63	0.63
6:F:568:GLN:HG3	6:F:601:SER:HB2	1.81	0.63
7:c:615:PHE:HA	7:c:619:GLN:HE22	1.64	0.63
6:D:136:ASP:OD2	6:D:137:ASN:ND2	2.32	0.63
6:D:328:ASN:ND2	6:D:496:LEU:O	2.31	0.63
9:4F:34:SER:HB2	9:4F:55:PRO:HD2	1.81	0.63
3:5F:146:ARG:NH1	9:4E:325:ARG:HD2	2.11	0.63
6:B:328:ASN:ND2	6:B:496:LEU:O	2.32	0.63
6:C:568:GLN:HG3	6:C:601:SER:HB2	1.81	0.62
9:4B:258:SER:HB3	9:4B:264:ILE:HG13	1.79	0.62
2:2D:144:ASN:ND2	2:2D:220:LYS:O	2.30	0.62
6:E:376:MET:HG3	6:E:440:LEU:HB2	1.81	0.62
8:3B:70:ILE:HD12	8:3B:238:TYR:HB2	1.79	0.62
9:4F:153:MET:HE1	9:4F:287:ARG:HG2	1.80	0.62
6:C:328:ASN:ND2	6:C:496:LEU:O	2.32	0.62
6:C:294:ASN:H	6:C:299:THR:HG22	1.63	0.62
7:b:724:ASP:O	7:b:816:ARG:NH1	2.32	0.62
8:3E:70:ILE:HD12	8:3E:238:TYR:HB2	1.80	0.62
9:4C:34:SER:HB2	9:4C:55:PRO:HD2	1.81	0.62
1:1B:54:LYS:NZ	1:1C:142:ASP:OD2	2.32	0.62
2:2F:184:ASP:OD2	2:2F:254:ARG:NH2	2.32	0.62
4:7D:77:SER:OG	4:7D:145:ARG:NH2	2.33	0.62
6:B:294:ASN:H	6:B:299:THR:HG22	1.64	0.62
9:4F:275:THR:HB	9:4F:278:SER:HB2	1.82	0.62
2:2A:191:LYS:NZ	2:2A:192:ALA:O	2.32	0.62
6:F:136:ASP:OD2	6:F:137:ASN:ND2	2.32	0.62
6:A:136:ASP:OD2	6:A:137:ASN:ND2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:e:724:ASP:O	7:e:816:ARG:NH1	2.33	0.62
1:1D:47:ASP:OD1	1:1D:51:ASN:ND2	2.27	0.61
6:A:651:ASP:O	6:A:655:ASN:ND2	2.33	0.61
6:C:136:ASP:OD2	6:C:137:ASN:ND2	2.33	0.61
6:D:651:ASP:O	6:D:655:ASN:ND2	2.33	0.61
7:d:739:GLU:OE2	7:d:739:GLU:N	2.33	0.61
9:4C:275:THR:HB	9:4C:278:SER:HB2	1.81	0.61
2:2A:184:ASP:OD2	2:2A:254:ARG:NH2	2.32	0.61
6:E:328:ASN:ND2	6:E:496:LEU:O	2.32	0.61
7:f:615:PHE:HA	7:f:619:GLN:HE22	1.63	0.61
6:E:231:MET:HB2	6:E:289:ILE:HD12	1.82	0.61
6:F:264:LEU:HD11	6:F:287:ASP:HB3	1.83	0.61
6:B:651:ASP:O	6:B:655:ASN:ND2	2.33	0.61
6:F:328:ASN:ND2	6:F:496:LEU:O	2.33	0.61
6:C:651:ASP:O	6:C:655:ASN:ND2	2.33	0.61
6:D:398:LYS:HZ1	6:D:400:ALA:HB2	1.65	0.61
6:E:651:ASP:OD1	6:E:651:ASP:N	2.31	0.61
6:F:398:LYS:HZ1	6:F:400:ALA:HB2	1.65	0.61
7:d:603:HIS:NE2	7:d:835:SER:OG	2.27	0.61
9:4A:169:LEU:HD11	9:4A:253:LEU:HG	1.81	0.61
4:7A:77:SER:OG	4:7A:145:ARG:NH2	2.33	0.61
6:A:651:ASP:N	6:A:651:ASP:OD1	2.33	0.61
6:D:389:SER:OG	6:D:398:LYS:NZ	2.29	0.61
6:F:651:ASP:O	6:F:655:ASN:ND2	2.33	0.61
7:b:739:GLU:OE2	7:b:739:GLU:N	2.34	0.61
2:2F:191:LYS:NZ	2:2F:192:ALA:O	2.33	0.61
6:A:398:LYS:HZ1	6:A:400:ALA:HB2	1.65	0.61
6:D:651:ASP:OD1	6:D:651:ASP:N	2.33	0.61
6:D:712:ASN:OD1	7:d:561:ARG:NH1	2.34	0.61
3:5E:21:ASN:ND2	9:4A:295:TYR:OH	2.33	0.60
6:E:651:ASP:O	6:E:655:ASN:ND2	2.34	0.60
2:2B:191:LYS:NZ	2:2B:192:ALA:O	2.30	0.60
6:B:136:ASP:OD2	6:B:137:ASN:ND2	2.35	0.60
6:C:264:LEU:HD11	6:C:287:ASP:HB3	1.83	0.60
2:2C:44:LYS:HD2	2:2C:47:ILE:HD11	1.83	0.60
8:3A:70:ILE:HG23	8:3A:114:VAL:HG12	1.84	0.60
2:2E:191:LYS:NZ	2:2E:192:ALA:O	2.30	0.60
2:2E:267:MET:HE3	8:3C:458:LEU:HD21	1.84	0.60
6:A:376:MET:HG3	6:A:440:LEU:HB2	1.83	0.60
6:E:853:GLN:HG3	6:E:861:VAL:HG23	1.84	0.60
8:3F:198:ASN:ND2	8:3F:200:ASP:O	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:f:677:ILE:HG23	7:f:685:PHE:HB2	1.84	0.60
9:4C:169:LEU:HD11	9:4C:253:LEU:HG	1.84	0.60
7:c:15:ILE:HD12	7:c:60:ALA:HB1	1.83	0.60
7:e:880:ASP:OD1	7:e:880:ASP:N	2.35	0.60
2:2E:166:THR:HG22	2:2E:167:THR:H	1.67	0.60
6:E:259:THR:HG22	6:E:289:ILE:HA	1.84	0.60
9:4D:258:SER:HB3	9:4D:264:ILE:HG13	1.84	0.60
6:B:750:PRO:HG2	6:B:763:PRO:HB2	1.83	0.59
6:E:750:PRO:HG2	6:E:763:PRO:HB2	1.83	0.59
9:4B:169:LEU:HD11	9:4B:253:LEU:HG	1.82	0.59
6:B:706:ARG:NH1	7:b:274:GLU:OE2	2.30	0.59
8:3D:70:ILE:HG23	8:3D:114:VAL:HG12	1.84	0.59
6:B:853:GLN:HG3	6:B:861:VAL:HG23	1.83	0.59
6:D:658:PRO:O	6:D:661:SER:OG	2.21	0.59
7:f:15:ILE:HD12	7:f:60:ALA:HB1	1.84	0.59
6:C:398:LYS:HZ1	6:C:400:ALA:HB2	1.66	0.59
2:2F:44:LYS:HD2	2:2F:47:ILE:HD11	1.83	0.59
6:A:712:ASN:OD1	7:a:561:ARG:NH1	2.34	0.59
6:C:259:THR:HG22	6:C:289:ILE:HA	1.84	0.59
6:E:136:ASP:OD2	6:E:137:ASN:ND2	2.35	0.59
7:a:723:MET:HE1	7:a:907:GLU:HG3	1.82	0.59
9:4C:38:ASP:OD1	9:4C:40:THR:OG1	2.21	0.59
9:4F:169:LEU:HD11	9:4F:253:LEU:HG	1.83	0.59
2:2D:166:THR:HG22	2:2D:167:THR:H	1.68	0.59
6:D:396:ASN:O	6:D:477:GLN:NE2	2.32	0.59
7:f:423:GLN:OE1	9:4F:239:TYR:OH	2.20	0.59
8:3A:70:ILE:HD12	8:3A:238:TYR:HB2	1.84	0.59
8:3E:198:ASN:ND2	8:3E:200:ASP:O	2.35	0.59
6:C:285:THR:HG23	6:D:450:PRO:HD3	1.85	0.59
6:E:396:ASN:O	6:E:477:GLN:NE2	2.33	0.59
7:b:623:LYS:HB3	7:b:640:THR:HB	1.83	0.59
2:2C:144:ASN:ND2	2:2C:220:LYS:O	2.31	0.59
6:C:651:ASP:OD1	6:C:651:ASP:N	2.35	0.59
6:F:259:THR:HG22	6:F:289:ILE:HA	1.85	0.59
7:b:679:ASP:HB3	7:b:681:THR:HG23	1.85	0.59
7:e:623:LYS:HB3	7:e:640:THR:HB	1.83	0.59
3:5E:32:ARG:NH1	3:5F:127:ASP:OD1	2.36	0.59
7:a:724:ASP:O	7:a:816:ARG:NH1	2.36	0.59
2:2B:101:ASP:OD1	2:2B:101:ASP:N	2.34	0.58
6:A:266:LEU:HD11	6:A:305:LEU:HD21	1.84	0.58
6:C:396:ASN:O	6:C:477:GLN:NE2	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:9A:52:ILE:HD12	5:9A:105:LEU:HD21	1.85	0.58
6:B:207:GLN:NE2	6:B:627:TYR:O	2.36	0.58
6:D:266:LEU:HD11	6:D:305:LEU:HD21	1.84	0.58
6:D:706:ARG:NH1	7:d:274:GLU:OE2	2.35	0.58
3:5D:146:ARG:HH21	9:4F:325:ARG:CZ	2.16	0.58
5:9E:154:ASP:OD2	5:9E:186:TYR:OH	2.18	0.58
6:D:231:MET:HB2	6:D:289:ILE:HD12	1.84	0.58
6:E:231:MET:HB3	6:E:236:ARG:HG2	1.85	0.58
7:e:679:ASP:HB3	7:e:681:THR:HG23	1.85	0.58
8:3A:248:VAL:HG11	8:3A:254:LEU:HD23	1.84	0.58
2:2A:144:ASN:ND2	2:2A:220:LYS:O	2.29	0.58
5:9E:47:GLU:OE1	5:9E:48:GLN:NE2	2.36	0.58
6:F:326:ASN:HB2	6:F:499:GLN:HG2	1.85	0.58
3:5E:33:ILE:HG12	3:5E:68:LEU:HD23	1.85	0.58
6:A:389:SER:OG	6:A:398:LYS:NZ	2.29	0.58
7:c:423:GLN:OE1	9:4C:239:TYR:OH	2.21	0.58
7:d:880:ASP:OD1	7:d:880:ASP:N	2.34	0.58
7:f:589:GLU:HG2	7:f:590:THR:HG23	1.85	0.58
2:2A:315:LYS:NZ	2:2A:321:ASP:OD1	2.31	0.58
6:A:207:GLN:NE2	6:A:627:TYR:O	2.37	0.58
7:d:679:ASP:HB2	7:d:686:ILE:HD13	1.85	0.58
2:2D:2:THR:OG1	2:2D:3:THR:N	2.36	0.58
7:c:589:GLU:HG2	7:c:590:THR:HG23	1.85	0.58
2:2B:44:LYS:HD2	2:2B:47:ILE:HD11	1.85	0.58
6:B:389:SER:OG	6:B:398:LYS:NZ	2.29	0.58
6:F:231:MET:HB2	6:F:289:ILE:HD12	1.86	0.58
6:F:750:PRO:HG2	6:F:763:PRO:HB2	1.85	0.58
6:F:853:GLN:HG3	6:F:861:VAL:HG23	1.86	0.58
7:a:880:ASP:OD1	7:a:880:ASP:N	2.34	0.58
7:e:702:VAL:HG12	7:e:711:LEU:HD21	1.85	0.58
8:3C:198:ASN:ND2	8:3C:200:ASP:O	2.34	0.58
9:4A:258:SER:HB3	9:4A:264:ILE:HG13	1.83	0.58
9:4F:259:PHE:HB2	9:4F:262:LYS:HB2	1.86	0.58
3:5B:32:ARG:NH1	3:5C:127:ASP:OD1	2.37	0.58
6:B:259:THR:HG22	6:B:289:ILE:HA	1.84	0.58
6:D:207:GLN:NE2	6:D:627:TYR:O	2.37	0.58
6:D:259:THR:HG22	6:D:289:ILE:HA	1.84	0.58
6:E:207:GLN:NE2	6:E:627:TYR:O	2.36	0.58
7:a:739:GLU:N	7:a:739:GLU:OE2	2.37	0.58
7:b:615:PHE:HA	7:b:619:GLN:HE22	1.69	0.58
7:c:677:ILE:HG23	7:c:685:PHE:HB2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2D:44:LYS:HD2	2:2D:47:ILE:HD11	1.85	0.58
5:9C:149:ARG:NH2	7:e:50:GLU:OE1	2.36	0.58
6:A:658:PRO:O	6:A:661:SER:OG	2.21	0.57
6:A:853:GLN:HG3	6:A:861:VAL:HG23	1.86	0.57
7:b:702:VAL:HG12	7:b:711:LEU:HD21	1.85	0.57
2:2C:191:LYS:NZ	2:2C:192:ALA:O	2.33	0.57
6:C:39:LYS:NZ	7:c:495:GLN:OE1	2.35	0.57
6:D:750:PRO:HG2	6:D:763:PRO:HB2	1.86	0.57
8:3E:70:ILE:HG23	8:3E:114:VAL:HG12	1.87	0.57
2:2B:249:TYR:HB3	2:2B:251:PRO:HD2	1.86	0.57
2:2E:44:LYS:HD2	2:2E:47:ILE:HD11	1.84	0.57
6:A:259:THR:HG22	6:A:289:ILE:HA	1.85	0.57
6:A:750:PRO:HG2	6:A:763:PRO:HB2	1.85	0.57
7:a:679:ASP:HB3	7:a:681:THR:HG23	1.86	0.57
9:4F:38:ASP:OD1	9:4F:40:THR:OG1	2.21	0.57
2:2B:166:THR:HG22	2:2B:167:THR:H	1.69	0.57
2:2E:249:TYR:HB3	2:2E:251:PRO:HD2	1.86	0.57
3:5B:21:ASN:ND2	9:4B:295:TYR:OH	2.37	0.57
6:C:207:GLN:NE2	6:C:627:TYR:O	2.38	0.57
6:D:853:GLN:HG3	6:D:861:VAL:HG23	1.86	0.57
7:e:739:GLU:N	7:e:739:GLU:OE2	2.38	0.57
8:3B:70:ILE:HG23	8:3B:114:VAL:HG12	1.86	0.57
6:C:750:PRO:HG2	6:C:763:PRO:HB2	1.85	0.57
7:a:603:HIS:NE2	7:a:835:SER:OG	2.27	0.57
7:e:615:PHE:HA	7:e:619:GLN:HE22	1.70	0.57
8:3D:198:ASN:ND2	8:3D:200:ASP:O	2.36	0.57
2:2C:208:VAL:HG11	2:2C:224:MET:HG2	1.86	0.57
2:2F:208:VAL:HG11	2:2F:224:MET:HG2	1.87	0.57
3:5D:67:HIS:NE2	3:5D:139:GLU:OE2	2.37	0.57
8:3D:248:VAL:HG11	8:3D:254:LEU:HD23	1.86	0.57
2:2A:249:TYR:HB3	2:2A:251:PRO:HD2	1.87	0.57
6:C:242:LEU:HD22	6:C:316:PRO:HD2	1.87	0.57
7:b:15:ILE:HD12	7:b:60:ALA:HB1	1.86	0.57
1:1B:32:ASN:HB3	1:1B:67:ARG:HB2	1.86	0.57
2:2A:44:LYS:HD2	2:2A:47:ILE:HD11	1.85	0.57
2:2B:184:ASP:OD2	2:2B:254:ARG:NH2	2.38	0.57
6:A:818:LEU:HD21	6:A:852:ILE:HG23	1.86	0.57
7:d:724:ASP:O	7:d:816:ARG:NH1	2.38	0.57
8:3B:198:ASN:ND2	8:3B:200:ASP:O	2.37	0.57
2:2D:249:TYR:HB3	2:2D:251:PRO:HD2	1.86	0.57
3:5A:145:MET:O	3:5A:146:ARG:NH1	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:207:GLN:NE2	6:F:627:TYR:O	2.38	0.57
7:b:36:TRP:NE1	7:b:43:ASP:OD2	2.37	0.57
2:2A:166:THR:HG22	2:2A:167:THR:H	1.70	0.56
5:9A:87:LEU:HD11	5:9A:100:LYS:HB3	1.87	0.56
6:B:712:ASN:OD1	7:b:561:ARG:NH1	2.37	0.56
1:1E:110:TRP:NE1	1:1F:122:SER:OG	2.38	0.56
6:A:450:PRO:HD3	6:F:285:THR:HG23	1.86	0.56
6:D:329:ARG:HA	6:D:329:ARG:HH11	1.69	0.56
9:4C:259:PHE:HB2	9:4C:262:LYS:HB2	1.86	0.56
9:4E:70:ASN:O	9:4E:213:ARG:NH1	2.38	0.56
1:1D:112:VAL:HG22	1:1D:144:VAL:HG22	1.88	0.56
7:c:679:ASP:HB2	7:c:686:ILE:HD13	1.87	0.56
6:B:231:MET:HB2	6:B:289:ILE:HD12	1.86	0.56
6:C:853:GLN:HG3	6:C:861:VAL:HG23	1.86	0.56
6:F:242:LEU:HD22	6:F:316:PRO:HD2	1.87	0.56
7:c:517:LEU:HD22	7:c:531:ARG:HD2	1.88	0.56
2:2F:144:ASN:ND2	2:2F:220:LYS:O	2.31	0.56
3:5B:33:ILE:HG12	3:5B:68:LEU:HD23	1.88	0.56
3:5F:33:ILE:HG12	3:5F:68:LEU:HD23	1.87	0.56
5:9B:45:GLU:HB2	5:9B:48:GLN:HG2	1.87	0.56
6:E:266:LEU:HD11	6:E:305:LEU:HD21	1.88	0.56
2:2F:166:THR:HG22	2:2F:167:THR:H	1.71	0.56
6:A:706:ARG:NH1	7:a:274:GLU:OE1	2.34	0.56
7:a:423:GLN:OE1	9:4A:239:TYR:OH	2.24	0.56
7:f:724:ASP:O	7:f:816:ARG:NH1	2.39	0.56
9:4D:70:ASN:O	9:4D:213:ARG:NH1	2.38	0.56
2:2F:332:LYS:HD3	8:3E:19:ASN:OD1	2.06	0.56
5:9B:154:ASP:OD2	5:9B:186:TYR:OH	2.24	0.56
6:E:144:LYS:N	6:E:166:ASP:OD1	2.38	0.56
9:4B:127:ILE:HG23	9:4B:164:LEU:HB2	1.86	0.56
7:c:726:GLN:HB3	7:c:750:SER:HB2	1.87	0.56
7:d:15:ILE:HD12	7:d:60:ALA:HB1	1.88	0.56
9:4A:132:ARG:NH1	9:4A:171:GLN:OE1	2.39	0.56
6:D:818:LEU:HD21	6:D:852:ILE:HG23	1.87	0.56
7:d:517:LEU:HD22	7:d:531:ARG:HD2	1.89	0.56
7:f:517:LEU:HD22	7:f:531:ARG:HD2	1.88	0.56
2:2C:59:LYS:HE3	2:2C:61:GLU:HB2	1.88	0.55
2:2E:184:ASP:OD2	2:2E:254:ARG:NH2	2.38	0.55
7:b:677:ILE:HG23	7:b:685:PHE:HB2	1.88	0.55
7:d:423:GLN:OE1	9:4B:239:TYR:OH	2.24	0.55
7:e:15:ILE:HD12	7:e:60:ALA:HB1	1.86	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1B:110:TRP:NE1	1:1C:122:SER:OG	2.39	0.55
6:C:708:LEU:HD23	7:c:561:ARG:HG2	1.88	0.55
6:D:828:PRO:HG3	6:D:837:VAL:HB	1.87	0.55
7:f:173:ASN:OD1	7:f:604:ARG:NH2	2.39	0.55
9:4D:132:ARG:NH1	9:4D:171:GLN:OE1	2.39	0.55
6:B:231:MET:HE3	6:B:236:ARG:HB3	1.88	0.55
6:B:326:ASN:HB2	6:B:499:GLN:HG2	1.87	0.55
7:d:679:ASP:HB3	7:d:681:THR:HG23	1.88	0.55
7:e:677:ILE:HG23	7:e:685:PHE:HB2	1.88	0.55
9:4E:132:ARG:NH1	9:4E:171:GLN:OE1	2.39	0.55
2:2F:59:LYS:HE3	2:2F:61:GLU:HB2	1.88	0.55
7:a:15:ILE:HD12	7:a:60:ALA:HB1	1.88	0.55
2:2C:101:ASP:OD1	2:2C:101:ASP:N	2.35	0.55
6:A:828:PRO:HG3	6:A:837:VAL:HB	1.87	0.55
6:C:818:LEU:HD21	6:C:852:ILE:HG23	1.88	0.55
6:F:144:LYS:N	6:F:166:ASP:OD1	2.40	0.55
7:a:517:LEU:HD22	7:a:531:ARG:HD2	1.89	0.55
6:B:266:LEU:HD11	6:B:305:LEU:HD21	1.88	0.55
6:C:389:SER:OG	6:C:398:LYS:NZ	2.30	0.55
7:f:726:GLN:HB3	7:f:750:SER:HB2	1.87	0.55
1:1E:32:ASN:HB3	1:1E:67:ARG:HB2	1.87	0.55
2:2B:169:ASP:OD1	2:2B:169:ASP:N	2.40	0.55
3:5C:33:ILE:HG12	3:5C:68:LEU:HD23	1.87	0.55
6:B:242:LEU:HD22	6:B:316:PRO:HD2	1.89	0.55
7:b:86:PRO:HG2	7:b:89:PHE:CD1	2.42	0.55
7:e:509:HIS:HB3	7:e:512:ASN:HB2	1.87	0.55
7:f:185:GLU:OE1	7:f:345:TYR:OH	2.24	0.55
7:f:847:ASP:OD1	7:f:847:ASP:N	2.39	0.55
9:4C:70:ASN:O	9:4C:213:ARG:NH1	2.40	0.55
6:B:651:ASP:OD1	6:B:651:ASP:N	2.33	0.55
6:C:742:LYS:HE3	6:C:742:LYS:HA	1.89	0.55
7:f:86:PRO:HG2	7:f:89:PHE:CD1	2.42	0.55
7:f:679:ASP:HB3	7:f:681:THR:HG23	1.87	0.55
2:2C:2:THR:OG1	2:2C:3:THR:N	2.40	0.55
2:2D:42:SER:O	2:2D:44:LYS:NZ	2.40	0.55
6:B:144:LYS:N	6:B:166:ASP:OD1	2.38	0.55
6:C:326:ASN:HB2	6:C:499:GLN:HG2	1.87	0.55
6:E:242:LEU:HD22	6:E:316:PRO:HD2	1.89	0.55
7:d:86:PRO:HG2	7:d:89:PHE:CD1	2.42	0.55
7:e:86:PRO:HG2	7:e:89:PHE:CD1	2.42	0.55
9:4D:259:PHE:HB2	9:4D:262:LYS:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:394:LYS:HB2	6:C:485:LYS:HD3	1.90	0.54
7:c:679:ASP:HB3	7:c:681:THR:HG23	1.88	0.54
2:2C:166:THR:HG22	2:2C:167:THR:H	1.71	0.54
2:2C:169:ASP:OD1	2:2C:169:ASP:N	2.40	0.54
5:9F:149:ARG:NH2	7:b:50:GLU:OE1	2.36	0.54
6:C:144:LYS:N	6:C:166:ASP:OD1	2.40	0.54
8:3D:379:MET:HA	8:3D:379:MET:HE2	1.90	0.54
9:4B:132:ARG:NH1	9:4B:171:GLN:OE1	2.40	0.54
2:2F:249:TYR:HB3	2:2F:251:PRO:HD2	1.89	0.54
5:9D:87:LEU:HD11	5:9D:100:LYS:HB3	1.89	0.54
6:E:326:ASN:HB2	6:E:499:GLN:HG2	1.89	0.54
9:4E:247:ASN:H	9:4E:252:SER:HB3	1.72	0.54
3:5A:87:ARG:HG2	3:5F:146:ARG:HE	1.73	0.54
6:C:208:LEU:HB3	6:C:627:TYR:HB3	1.90	0.54
6:F:818:LEU:HD21	6:F:852:ILE:HG23	1.87	0.54
7:e:517:LEU:HD22	7:e:531:ARG:HD2	1.90	0.54
9:4B:156:LEU:HB2	9:4B:182:VAL:HG22	1.89	0.54
1:1A:112:VAL:HG22	1:1A:144:VAL:HG22	1.88	0.54
2:2A:42:SER:O	2:2A:44:LYS:NZ	2.40	0.54
6:B:231:MET:HB3	6:B:236:ARG:HG2	1.90	0.54
6:B:396:ASN:O	6:B:477:GLN:NE2	2.33	0.54
6:E:802:GLN:HB2	6:E:863:ASN:HB3	1.90	0.54
6:F:651:ASP:OD1	6:F:651:ASP:N	2.32	0.54
7:b:517:LEU:HD22	7:b:531:ARG:HD2	1.90	0.54
7:c:185:GLU:OE1	7:c:345:TYR:OH	2.24	0.54
2:2C:249:TYR:HB3	2:2C:251:PRO:HD2	1.89	0.54
6:B:818:LEU:HD21	6:B:852:ILE:HG23	1.89	0.54
6:E:818:LEU:HD21	6:E:852:ILE:HG23	1.89	0.54
6:F:266:LEU:HD11	6:F:305:LEU:HD21	1.90	0.54
7:b:185:GLU:OE1	7:b:345:TYR:OH	2.24	0.54
7:c:724:ASP:O	7:c:816:ARG:NH1	2.39	0.54
6:A:144:LYS:N	6:A:166:ASP:OD1	2.41	0.54
6:B:747:ILE:HG13	6:B:885:ASN:HA	1.90	0.54
6:F:394:LYS:HB2	6:F:485:LYS:HD3	1.89	0.54
7:a:86:PRO:HG2	7:a:89:PHE:CD1	2.42	0.54
7:d:589:GLU:HG2	7:d:590:THR:HG23	1.89	0.54
2:2B:144:ASN:ND2	2:2B:220:LYS:O	2.34	0.54
6:A:708:LEU:HD23	7:a:561:ARG:HG2	1.89	0.54
6:B:802:GLN:HB2	6:B:863:ASN:HB3	1.90	0.54
7:b:726:GLN:HB3	7:b:750:SER:HB2	1.90	0.54
7:c:86:PRO:HG2	7:c:89:PHE:CD1	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:d:185:GLU:OE1	7:d:345:TYR:OH	2.25	0.54
6:D:242:LEU:HD22	6:D:316:PRO:HD2	1.90	0.54
6:E:658:PRO:O	6:E:661:SER:OG	2.25	0.54
6:F:208:LEU:HB3	6:F:627:TYR:HB3	1.89	0.54
6:F:708:LEU:HD23	7:f:561:ARG:HG2	1.88	0.54
7:a:185:GLU:OE1	7:a:345:TYR:OH	2.25	0.54
7:d:132:ARG:NH1	7:d:290:LYS:O	2.41	0.54
9:4A:127:ILE:HG23	9:4A:164:LEU:HB2	1.88	0.54
6:D:708:LEU:HD23	7:d:561:ARG:HG2	1.88	0.54
7:b:509:HIS:HB3	7:b:512:ASN:HB2	1.89	0.54
7:e:726:GLN:HB3	7:e:750:SER:HB2	1.90	0.54
2:2E:313:ILE:HD12	2:2E:331:ILE:HG12	1.89	0.53
6:D:394:LYS:HB2	6:D:485:LYS:HD3	1.90	0.53
6:E:706:ARG:NH1	7:e:274:GLU:OE1	2.34	0.53
7:d:726:GLN:HB3	7:d:750:SER:HB2	1.89	0.53
9:4F:70:ASN:O	9:4F:213:ARG:NH1	2.41	0.53
2:2A:349:THR:HG23	9:4B:367:ARG:HG3	1.90	0.53
5:9E:8:ASP:OD1	5:9E:12:ARG:NH2	2.41	0.53
6:C:261:ASP:OD1	6:C:261:ASP:N	2.39	0.53
6:E:747:ILE:HG13	6:E:885:ASN:HA	1.90	0.53
5:9A:37:LYS:HD2	5:9A:37:LYS:C	2.33	0.53
6:E:568:GLN:HG3	6:E:601:SER:HB2	1.90	0.53
7:f:553:GLN:NE2	7:f:587:PHE:O	2.42	0.53
6:A:242:LEU:HD22	6:A:316:PRO:HD2	1.90	0.53
7:a:132:ARG:NH1	7:a:290:LYS:O	2.41	0.53
8:3C:254:LEU:HD11	8:3C:261:VAL:HG23	1.91	0.53
2:2B:146:ASP:OD1	2:2B:146:ASP:N	2.35	0.53
9:4A:105:ILE:HD12	9:4A:145:LEU:HD22	1.91	0.53
9:4B:172:PHE:O	9:4B:177:ARG:NH2	2.41	0.53
9:4B:259:PHE:HB2	9:4B:262:LYS:HB2	1.90	0.53
2:2A:101:ASP:OD1	2:2A:101:ASP:N	2.34	0.53
2:2E:144:ASN:ND2	2:2E:220:LYS:O	2.34	0.53
6:D:208:LEU:HB3	6:D:627:TYR:HB3	1.91	0.53
7:a:589:GLU:HG2	7:a:590:THR:HG23	1.90	0.53
7:d:723:MET:HE1	7:d:907:GLU:HG3	1.89	0.53
8:3C:36:PHE:HB2	8:3C:140:PRO:HB3	1.91	0.53
3:5A:67:HIS:NE2	3:5A:139:GLU:OE2	2.40	0.53
5:9C:152:ARG:HG2	7:e:41:GLU:OE1	2.09	0.53
5:9F:76:LYS:HG3	5:9F:77:GLN:OE1	2.09	0.53
6:A:208:LEU:HB3	6:A:627:TYR:HB3	1.91	0.53
6:F:261:ASP:OD1	6:F:261:ASP:N	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:d:677:ILE:HG23	7:d:685:PHE:HB2	1.90	0.53
7:e:592:LYS:O	7:e:889:GLN:NE2	2.42	0.53
9:4A:259:PHE:HB2	9:4A:262:LYS:HB2	1.89	0.53
2:2A:146:ASP:OD1	2:2A:146:ASP:N	2.34	0.53
5:9C:39:LEU:HB3	5:9C:44:ILE:HG21	1.91	0.53
5:9D:88:VAL:HB	5:9D:101:ILE:HG23	1.91	0.53
6:D:144:LYS:N	6:D:166:ASP:OD1	2.41	0.53
7:e:618:GLU:HA	7:e:714:CYS:HB3	1.90	0.53
8:3F:36:PHE:HB2	8:3F:140:PRO:HB3	1.91	0.53
2:2A:2:THR:OG1	2:2A:3:THR:N	2.36	0.53
4:7A:93:LYS:NZ	4:7F:118:GLU:OE2	2.41	0.53
5:9F:152:ARG:HG2	7:b:41:GLU:OE1	2.09	0.53
7:a:726:GLN:HB3	7:a:750:SER:HB2	1.89	0.53
7:b:592:LYS:O	7:b:889:GLN:NE2	2.42	0.53
7:e:185:GLU:OE1	7:e:345:TYR:OH	2.24	0.53
2:2F:349:THR:HG23	9:4C:367:ARG:HG3	1.90	0.53
5:9C:45:GLU:HB2	5:9C:48:GLN:HG2	1.89	0.53
7:c:553:GLN:NE2	7:c:587:PHE:O	2.42	0.53
1:1A:32:ASN:HB3	1:1A:67:ARG:HB2	1.91	0.52
7:d:856:TRP:NE1	7:e:230:ASP:OD2	2.38	0.52
8:3D:36:PHE:HB2	8:3D:140:PRO:HB3	1.91	0.52
9:4B:105:ILE:HD12	9:4B:145:LEU:HD22	1.91	0.52
3:5D:87:ARG:NH1	3:5D:89:GLU:OE2	2.40	0.52
5:9A:119:ASP:OD1	5:9A:120:ASN:N	2.42	0.52
7:a:847:ASP:OD1	7:a:847:ASP:N	2.34	0.52
8:3F:254:LEU:HD11	8:3F:261:VAL:HG23	1.90	0.52
5:9F:35:LEU:HD23	5:9F:74:VAL:HG22	1.92	0.52
6:E:646:GLU:H	6:E:646:GLU:CD	2.17	0.52
7:d:618:GLU:HA	7:d:714:CYS:HB3	1.91	0.52
7:f:208:SER:HB2	7:f:604:ARG:HH21	1.74	0.52
8:3A:36:PHE:HB2	8:3A:140:PRO:HB3	1.92	0.52
1:1E:76:LYS:NZ	1:1E:76:LYS:HB3	2.25	0.52
2:2D:319:MET:HB3	2:2D:330:ILE:HD12	1.92	0.52
5:9B:68:LYS:HB2	5:9B:68:LYS:NZ	2.24	0.52
7:a:224:LEU:HD21	7:a:307:LEU:HD11	1.92	0.52
7:b:880:ASP:OD1	7:b:880:ASP:N	2.35	0.52
7:f:224:LEU:HD21	7:f:307:LEU:HD11	1.92	0.52
9:4C:127:ILE:O	9:4C:127:ILE:HG22	2.10	0.52
2:2D:208:VAL:HG11	2:2D:224:MET:HG2	1.91	0.52
2:2D:349:THR:HG23	9:4A:367:ARG:HG3	1.90	0.52
2:2E:349:THR:HG23	9:4E:367:ARG:HG3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:406:LYS:HB2	6:B:470:GLU:HG3	1.92	0.52
6:F:314:MET:HE3	6:F:314:MET:HA	1.91	0.52
7:b:618:GLU:HA	7:b:714:CYS:HB3	1.91	0.52
7:f:353:PRO:O	7:f:357:ILE:HG12	2.10	0.52
1:1B:76:LYS:NZ	1:1B:76:LYS:HB3	2.25	0.52
6:C:266:LEU:HD11	6:C:305:LEU:HD21	1.91	0.52
6:F:396:ASN:O	6:F:477:GLN:NE2	2.34	0.52
7:a:676:MET:HE3	7:a:898:LEU:HB2	1.92	0.52
2:2A:332:LYS:HG2	8:3E:459:GLN:HB2	1.92	0.52
2:2C:349:THR:HG23	9:4F:367:ARG:HG3	1.90	0.52
3:5D:47:GLN:O	3:5E:60:LYS:NZ	2.42	0.52
6:B:394:LYS:HB2	6:B:485:LYS:HD3	1.92	0.52
6:B:399:PRO:HD3	6:B:474:MET:HE1	1.92	0.52
6:F:706:ARG:NH1	7:f:274:GLU:OE2	2.35	0.52
8:3A:168:CYS:O	8:3A:176:GLN:NE2	2.40	0.52
3:5A:47:GLN:O	3:5B:60:LYS:NZ	2.42	0.52
6:B:568:GLN:HG3	6:B:601:SER:HB2	1.90	0.52
6:C:229:PHE:HA	6:C:231:MET:HE3	1.92	0.52
6:C:406:LYS:HB3	6:C:425:SER:HB2	1.91	0.52
7:a:325:ASP:OD2	7:a:327:ASN:ND2	2.43	0.52
7:c:224:LEU:HD21	7:c:307:LEU:HD11	1.92	0.52
7:d:325:ASP:OD2	7:d:327:ASN:ND2	2.43	0.52
7:e:353:PRO:O	7:e:357:ILE:HG12	2.10	0.52
8:3F:413:ALA:HB2	8:3F:450:VAL:HG22	1.91	0.52
9:4A:172:PHE:O	9:4A:177:ARG:NH2	2.43	0.52
9:4E:259:PHE:HB2	9:4E:262:LYS:HB2	1.91	0.52
5:9A:8:ASP:OD1	5:9A:12:ARG:NH2	2.43	0.52
6:A:406:LYS:HB2	6:A:470:GLU:HG3	1.92	0.52
6:B:658:PRO:O	6:B:661:SER:OG	2.26	0.52
6:E:406:LYS:HB3	6:E:425:SER:HB2	1.92	0.52
7:a:677:ILE:HG23	7:a:685:PHE:HB2	1.90	0.52
7:b:65:LEU:HD13	7:b:404:ARG:HD3	1.91	0.52
6:D:406:LYS:HB3	6:D:425:SER:HB2	1.92	0.51
6:E:406:LYS:HB2	6:E:470:GLU:HG3	1.92	0.51
9:4F:245:LEU:HD13	9:4F:253:LEU:HD12	1.91	0.51
1:1D:32:ASN:HB3	1:1D:67:ARG:HB2	1.91	0.51
6:A:565:TYR:OH	6:A:599:ASP:OD2	2.27	0.51
7:b:353:PRO:O	7:b:357:ILE:HG12	2.10	0.51
7:c:353:PRO:O	7:c:357:ILE:HG12	2.10	0.51
7:d:899:GLY:H	7:d:902:ALA:HB3	1.74	0.51
2:2A:208:VAL:HG11	2:2A:224:MET:HG2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:9E:135:LEU:HD12	9:4C:381:LEU:HD13	1.92	0.51
6:A:399:PRO:HD3	6:A:474:MET:HE1	1.91	0.51
7:a:856:TRP:NE1	7:b:230:ASP:OD2	2.39	0.51
7:a:899:GLY:H	7:a:902:ALA:HB3	1.75	0.51
9:4C:108:GLU:O	9:4C:149:ARG:NH2	2.44	0.51
5:9A:147:GLY:HA2	5:9A:153:GLU:HG3	1.91	0.51
7:c:208:SER:HB2	7:c:604:ARG:HH21	1.75	0.51
6:F:658:PRO:O	6:F:661:SER:OG	2.26	0.51
7:a:618:GLU:HA	7:a:714:CYS:HB3	1.92	0.51
9:4F:132:ARG:NH1	9:4F:171:GLN:OE1	2.44	0.51
5:9E:68:LYS:HB2	5:9E:68:LYS:NZ	2.25	0.51
6:A:394:LYS:HB2	6:A:485:LYS:HD3	1.92	0.51
6:C:380:TRP:HZ3	6:C:491:PRO:HB3	1.76	0.51
2:2B:349:THR:HG23	9:4D:367:ARG:HG3	1.91	0.51
6:E:394:LYS:HB2	6:E:485:LYS:HD3	1.92	0.51
6:E:704:ARG:NH1	7:e:558:THR:OG1	2.44	0.51
6:F:406:LYS:HB3	6:F:425:SER:HB2	1.92	0.51
7:b:856:TRP:NE1	7:c:230:ASP:OD2	2.42	0.51
8:3E:248:VAL:HG11	8:3E:254:LEU:HD23	1.93	0.51
3:5C:146:ARG:HH11	3:5C:146:ARG:HA	1.75	0.51
6:A:329:ARG:HA	6:A:329:ARG:HH11	1.75	0.51
6:D:380:TRP:HZ3	6:D:491:PRO:HB3	1.75	0.51
7:e:65:LEU:HD13	7:e:404:ARG:HD3	1.91	0.51
7:e:623:LYS:HZ1	7:e:625:LYS:HB3	1.76	0.51
7:e:730:ALA:HB1	7:e:734:TYR:HD2	1.75	0.51
8:3C:413:ALA:HB2	8:3C:450:VAL:HG22	1.91	0.51
9:4A:239:TYR:HB3	9:4A:257:ARG:HG3	1.93	0.51
6:C:332:ARG:HB2	6:C:362:VAL:HG12	1.93	0.51
6:C:706:ARG:NH1	7:c:274:GLU:OE2	2.35	0.51
6:E:380:TRP:HZ2	6:E:428:LEU:HD22	1.76	0.51
6:F:332:ARG:HB2	6:F:362:VAL:HG12	1.93	0.51
7:d:224:LEU:HD21	7:d:307:LEU:HD11	1.92	0.51
8:3A:328:GLU:OE2	8:3A:328:GLU:HA	2.11	0.51
8:3B:36:PHE:HB2	8:3B:140:PRO:HB3	1.93	0.51
9:4F:127:ILE:O	9:4F:127:ILE:HG22	2.10	0.51
2:2E:101:ASP:OD1	2:2E:101:ASP:N	2.34	0.51
6:B:406:LYS:HB3	6:B:425:SER:HB2	1.91	0.51
7:b:623:LYS:HZ1	7:b:625:LYS:HB3	1.76	0.51
7:b:836:MET:HE2	7:b:871:MET:SD	2.51	0.51
7:e:36:TRP:NE1	7:e:43:ASP:OD2	2.38	0.51
7:e:836:MET:HE2	7:e:871:MET:SD	2.51	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:704:ARG:NH1	7:f:558:THR:OG1	2.44	0.50
7:a:369:LYS:HG3	7:f:536:LEU:HD12	1.92	0.50
1:1A:76:LYS:HB3	1:1A:76:LYS:NZ	2.26	0.50
6:A:153:ASP:OD1	6:A:157:ASN:N	2.44	0.50
6:B:115:LEU:HA	7:b:91:PRO:HG3	1.93	0.50
6:D:231:MET:HB3	6:D:236:ARG:HG2	1.94	0.50
6:E:115:LEU:HA	7:e:91:PRO:HG3	1.94	0.50
6:F:231:MET:HE3	6:F:236:ARG:HB3	1.92	0.50
9:4B:247:ASN:H	9:4B:252:SER:HB3	1.76	0.50
9:4D:247:ASN:H	9:4D:252:SER:HB3	1.76	0.50
3:5E:146:ARG:HA	3:5E:146:ARG:HH11	1.76	0.50
5:9F:14:TRP:CE2	5:9F:125:ILE:HD13	2.47	0.50
6:A:380:TRP:HZ3	6:A:491:PRO:HB3	1.74	0.50
6:B:380:TRP:HZ2	6:B:428:LEU:HD22	1.75	0.50
6:C:414:SER:OG	6:C:415:GLN:OE1	2.30	0.50
6:F:623:GLU:OE1	6:F:623:GLU:N	2.44	0.50
7:b:543:PHE:O	7:b:546:THR:OG1	2.28	0.50
7:b:730:ALA:HB1	7:b:734:TYR:HD2	1.76	0.50
7:c:618:GLU:HA	7:c:714:CYS:HB3	1.92	0.50
7:d:847:ASP:OD1	7:d:847:ASP:N	2.34	0.50
9:4D:257:ARG:NH1	9:4D:258:SER:O	2.45	0.50
2:2E:169:ASP:OD1	2:2E:169:ASP:N	2.40	0.50
2:2F:42:SER:O	2:2F:44:LYS:NZ	2.42	0.50
2:2F:169:ASP:OD1	2:2F:169:ASP:N	2.40	0.50
6:C:406:LYS:HB2	6:C:470:GLU:HG3	1.94	0.50
7:c:676:MET:CE	7:c:898:LEU:H	2.24	0.50
9:4B:70:ASN:O	9:4B:213:ARG:NH1	2.44	0.50
6:B:261:ASP:OD1	6:B:261:ASP:N	2.41	0.50
6:C:579:VAL:HA	6:C:594:THR:HG22	1.94	0.50
6:D:285:THR:HG23	6:E:450:PRO:HD3	1.94	0.50
6:D:406:LYS:HB2	6:D:470:GLU:HG3	1.93	0.50
6:D:568:GLN:HG3	6:D:601:SER:HB2	1.94	0.50
7:c:536:LEU:HD12	7:d:369:LYS:HG3	1.93	0.50
9:4F:108:GLU:O	9:4F:149:ARG:NH2	2.45	0.50
5:9E:39:LEU:HB3	5:9E:44:ILE:HG21	1.94	0.50
6:C:623:GLU:N	6:C:623:GLU:OE1	2.44	0.50
7:c:11:VAL:O	7:c:15:ILE:HG12	2.12	0.50
7:c:482:GLN:NE2	7:c:489:MET:SD	2.78	0.50
7:d:553:GLN:NE2	7:d:587:PHE:O	2.45	0.50
7:e:589:GLU:HG2	7:e:590:THR:HG23	1.93	0.50
7:f:679:ASP:HB2	7:f:686:ILE:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:4A:70:ASN:O	9:4A:213:ARG:NH1	2.44	0.50
9:4D:127:ILE:HG22	9:4D:127:ILE:O	2.12	0.50
2:2B:243:ASP:OD1	2:2B:248:ARG:NH1	2.43	0.50
2:2C:42:SER:O	2:2C:44:LYS:NZ	2.42	0.50
2:2D:146:ASP:OD1	2:2D:146:ASP:N	2.34	0.50
7:e:847:ASP:OD1	7:e:847:ASP:N	2.34	0.50
7:f:65:LEU:HD13	7:f:404:ARG:HD3	1.93	0.50
9:4D:245:LEU:HD13	9:4D:253:LEU:HD12	1.94	0.50
5:9B:39:LEU:HB3	5:9B:44:ILE:HG21	1.94	0.50
6:A:380:TRP:HZ2	6:A:428:LEU:HD22	1.76	0.50
6:A:396:ASN:O	6:A:477:GLN:NE2	2.33	0.50
6:B:208:LEU:HB3	6:B:627:TYR:HB3	1.94	0.50
6:F:380:TRP:HZ3	6:F:491:PRO:HB3	1.76	0.50
6:F:406:LYS:HB2	6:F:470:GLU:HG3	1.94	0.50
7:b:589:GLU:HG2	7:b:590:THR:HG23	1.93	0.50
7:c:900:ASP:N	7:c:900:ASP:OD1	2.45	0.50
8:3D:224:GLN:N	8:3D:224:GLN:OE1	2.45	0.50
9:4E:127:ILE:HG22	9:4E:127:ILE:O	2.12	0.50
5:9B:71:SER:HB2	5:9B:89:THR:HB	1.93	0.50
5:9C:14:TRP:CE2	5:9C:125:ILE:HD13	2.47	0.50
6:A:406:LYS:HB3	6:A:425:SER:HB2	1.93	0.50
6:C:658:PRO:O	6:C:661:SER:OG	2.26	0.50
6:E:153:ASP:OD1	6:E:157:ASN:N	2.45	0.50
6:E:208:LEU:HB3	6:E:627:TYR:HB3	1.94	0.50
6:F:153:ASP:OD1	6:F:157:ASN:N	2.45	0.50
7:f:618:GLU:HA	7:f:714:CYS:HB3	1.93	0.50
7:f:702:VAL:HG23	7:f:711:LEU:HG	1.94	0.50
7:f:891:TRP:CD1	7:f:897:PRO:HD2	2.47	0.50
6:A:471:GLN:NE2	6:A:472:ASP:O	2.44	0.49
6:B:828:PRO:HG3	6:B:837:VAL:HB	1.94	0.49
6:F:9:LYS:HD3	7:f:10:ILE:HG22	1.93	0.49
7:a:623:LYS:HZ1	7:a:625:LYS:HB3	1.77	0.49
8:3A:198:ASN:ND2	8:3A:200:ASP:O	2.44	0.49
8:3E:18:LEU:HD22	8:3E:19:ASN:H	1.76	0.49
2:2B:42:SER:O	2:2B:44:LYS:NZ	2.44	0.49
3:5F:67:HIS:NE2	3:5F:139:GLU:OE1	2.45	0.49
7:c:847:ASP:OD1	7:c:847:ASP:N	2.39	0.49
7:f:11:VAL:O	7:f:15:ILE:HG12	2.12	0.49
8:3D:328:GLU:HA	8:3D:328:GLU:OE2	2.11	0.49
9:4C:132:ARG:NH1	9:4C:171:GLN:OE1	2.45	0.49
6:A:568:GLN:HG3	6:A:601:SER:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:828:PRO:HG3	6:F:837:VAL:HB	1.93	0.49
7:c:65:LEU:HD13	7:c:404:ARG:HD3	1.93	0.49
7:c:592:LYS:O	7:c:889:GLN:NE2	2.45	0.49
7:f:592:LYS:O	7:f:889:GLN:NE2	2.45	0.49
8:3E:24:GLN:OE1	8:3E:24:GLN:N	2.45	0.49
6:B:132:THR:OG1	6:B:674:SER:O	2.31	0.49
6:C:203:GLU:N	6:C:203:GLU:OE2	2.46	0.49
6:D:153:ASP:OD1	6:D:157:ASN:N	2.45	0.49
7:b:847:ASP:OD1	7:b:847:ASP:N	2.36	0.49
7:d:623:LYS:HZ1	7:d:625:LYS:HB3	1.77	0.49
8:3E:36:PHE:HB2	8:3E:140:PRO:HB3	1.94	0.49
9:4A:247:ASN:H	9:4A:252:SER:HB3	1.77	0.49
1:1C:33:VAL:HG22	1:1C:66:LEU:HD22	1.93	0.49
1:1D:76:LYS:NZ	1:1D:76:LYS:HB3	2.26	0.49
6:A:285:THR:HG23	6:B:450:PRO:HD3	1.93	0.49
6:B:153:ASP:OD1	6:B:157:ASN:N	2.45	0.49
7:a:553:GLN:NE2	7:a:587:PHE:O	2.45	0.49
3:5C:145:MET:O	3:5C:146:ARG:NH1	2.46	0.49
6:C:9:LYS:HD3	7:c:10:ILE:HG22	1.93	0.49
6:C:153:ASP:OD1	6:C:157:ASN:N	2.45	0.49
6:C:472:ASP:OD1	6:C:473:PHE:N	2.46	0.49
7:f:900:ASP:OD1	7:f:900:ASP:N	2.45	0.49
2:2B:59:LYS:HE3	2:2B:61:GLU:HB2	1.94	0.49
6:B:285:THR:HG23	6:C:450:PRO:HD3	1.94	0.49
6:C:161:TYR:HB3	6:C:640:ALA:HB1	1.95	0.49
6:C:426:GLN:NE2	6:C:441:THR:O	2.41	0.49
6:D:426:GLN:NE2	6:D:441:THR:O	2.38	0.49
7:b:624:LEU:HD13	7:b:706:TYR:HB2	1.94	0.49
7:e:899:GLY:H	7:e:902:ALA:HB3	1.77	0.49
8:3D:168:CYS:O	8:3D:176:GLN:NE2	2.40	0.49
1:1F:33:VAL:HG22	1:1F:66:LEU:HD22	1.94	0.49
5:9C:71:SER:HB2	5:9C:89:THR:HB	1.95	0.49
5:9D:154:ASP:OD2	5:9D:186:TYR:OH	2.30	0.49
6:A:203:GLU:N	6:A:203:GLU:OE2	2.46	0.49
6:D:203:GLU:OE2	6:D:203:GLU:N	2.45	0.49
6:D:332:ARG:HB2	6:D:362:VAL:HG12	1.95	0.49
7:d:730:ALA:HB1	7:d:734:TYR:HD1	1.78	0.49
9:4F:249:ASP:OD1	9:4F:249:ASP:N	2.46	0.49
2:2E:243:ASP:OD1	2:2E:248:ARG:NH1	2.42	0.49
4:7C:5:GLU:OE2	4:7C:7:GLY:N	2.31	0.49
5:9D:52:ILE:O	5:9D:56:ILE:HG12	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:9D:71:SER:HB2	5:9D:89:THR:HB	1.95	0.49
5:9E:71:SER:HB2	5:9E:89:THR:HB	1.93	0.49
5:9F:39:LEU:HB3	5:9F:44:ILE:HG21	1.95	0.49
6:D:380:TRP:HZ2	6:D:428:LEU:HD22	1.76	0.49
6:E:285:THR:HG23	6:F:450:PRO:HD3	1.95	0.49
6:F:579:VAL:HA	6:F:594:THR:HG22	1.94	0.49
7:c:443:GLN:NE2	7:c:447:ASN:OD1	2.42	0.49
3:5B:46:SER:HB2	3:5C:60:LYS:HE2	1.94	0.49
6:C:380:TRP:HZ2	6:C:428:LEU:HD22	1.77	0.49
6:E:728:LYS:NZ	6:E:886:GLU:O	2.46	0.49
7:f:624:LEU:HD13	7:f:706:TYR:HB2	1.95	0.49
8:3B:24:GLN:N	8:3B:24:GLN:OE1	2.46	0.49
3:5D:79:THR:HG23	3:5D:121:TRP:HH2	1.77	0.48
5:9C:52:ILE:O	5:9C:56:ILE:HG12	2.12	0.48
5:9F:71:SER:HB2	5:9F:89:THR:HB	1.95	0.48
8:3A:254:LEU:HD11	8:3A:261:VAL:HG13	1.94	0.48
5:9F:176:GLN:HG3	5:9F:195:ILE:HB	1.95	0.48
6:A:426:GLN:NE2	6:A:441:THR:O	2.38	0.48
6:D:471:GLN:NE2	6:D:472:ASP:O	2.45	0.48
6:E:134:ASN:OD1	6:E:137:ASN:ND2	2.45	0.48
6:F:380:TRP:HZ2	6:F:428:LEU:HD22	1.77	0.48
8:3E:325:GLU:O	8:3E:329:MET:HG3	2.13	0.48
6:A:472:ASP:OD1	6:A:473:PHE:N	2.45	0.48
6:E:132:THR:OG1	6:E:674:SER:O	2.31	0.48
7:e:11:VAL:O	7:e:15:ILE:HG12	2.13	0.48
7:f:623:LYS:HZ1	7:f:625:LYS:HB3	1.78	0.48
9:4C:245:LEU:HD13	9:4C:253:LEU:HD12	1.95	0.48
2:2D:27:THR:OG1	2:2D:184:ASP:OD2	2.31	0.48
4:7E:77:SER:OG	4:7E:145:ARG:NH2	2.46	0.48
6:C:828:PRO:HG3	6:C:837:VAL:HB	1.94	0.48
6:D:264:LEU:HD11	6:D:287:ASP:HB3	1.96	0.48
6:E:399:PRO:HD3	6:E:474:MET:HE1	1.93	0.48
7:a:5:ASP:N	7:a:5:ASP:OD1	2.46	0.48
7:a:11:VAL:O	7:a:15:ILE:HG12	2.14	0.48
7:e:856:TRP:NE1	7:f:230:ASP:OD2	2.43	0.48
8:3D:225:LEU:HD21	8:3D:281:ASN:HB3	1.95	0.48
8:3D:254:LEU:HD11	8:3D:261:VAL:HG13	1.94	0.48
6:A:264:LEU:HD11	6:A:287:ASP:HB3	1.96	0.48
6:E:261:ASP:OD1	6:E:261:ASP:N	2.41	0.48
7:e:723:MET:HE1	7:e:907:GLU:HA	1.94	0.48
8:3A:326:GLN:HE21	8:3A:348:TRP:HD1	1.59	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:3B:325:GLU:O	8:3B:329:MET:HG3	2.14	0.48
6:F:25:SER:OG	6:F:28:ASP:OD1	2.26	0.48
6:F:161:TYR:HB3	6:F:640:ALA:HB1	1.95	0.48
8:3B:413:ALA:HB2	8:3B:450:VAL:HG22	1.95	0.48
2:2B:2:THR:OG1	2:2B:3:THR:N	2.45	0.48
6:F:651:ASP:HA	6:F:654:ILE:HD12	1.96	0.48
6:B:472:ASP:OD1	6:B:473:PHE:N	2.46	0.48
6:E:287:ASP:OD1	6:E:288:PRO:HD2	2.14	0.48
6:F:426:GLN:NE2	6:F:441:THR:O	2.40	0.48
6:F:747:ILE:HG13	6:F:885:ASN:HA	1.96	0.48
7:c:624:LEU:HD13	7:c:706:TYR:HB2	1.94	0.48
9:4D:126:GLU:HG2	9:4D:131:GLN:HG3	1.95	0.48
9:4F:126:GLU:HG2	9:4F:131:GLN:HG3	1.96	0.48
1:1B:97:SER:HB3	1:1B:106:ILE:HG23	1.95	0.48
3:5E:14:ILE:HG22	3:5E:99:MET:HB2	1.94	0.48
4:7B:77:SER:OG	4:7B:145:ARG:NH2	2.46	0.48
6:A:261:ASP:OD1	6:A:261:ASP:N	2.41	0.48
6:A:860:ARG:NH1	7:b:334:ASP:OD2	2.47	0.48
6:B:287:ASP:OD1	6:B:288:PRO:HD2	2.13	0.48
6:E:828:PRO:HG3	6:E:837:VAL:HB	1.95	0.48
7:b:899:GLY:H	7:b:902:ALA:HB3	1.78	0.48
7:c:724:ASP:OD2	7:c:816:ARG:NH1	2.47	0.48
7:d:11:VAL:O	7:d:15:ILE:HG12	2.14	0.48
7:e:624:LEU:HD13	7:e:706:TYR:HB2	1.94	0.48
6:D:399:PRO:HD3	6:D:474:MET:HE1	1.96	0.48
6:D:472:ASP:OD1	6:D:473:PHE:N	2.46	0.48
3:5B:14:ILE:HG22	3:5B:99:MET:HB2	1.95	0.47
4:7D:118:GLU:HG3	4:7E:93:LYS:HG2	1.96	0.47
6:E:472:ASP:OD1	6:E:473:PHE:N	2.46	0.47
7:a:730:ALA:HB1	7:a:734:TYR:HD2	1.79	0.47
7:c:623:LYS:HZ1	7:c:625:LYS:HB3	1.78	0.47
9:4C:126:GLU:HG2	9:4C:131:GLN:HG3	1.96	0.47
2:2A:27:THR:OG1	2:2A:184:ASP:OD2	2.32	0.47
3:5E:146:ARG:HH21	9:4A:325:ARG:NH2	2.12	0.47
5:9B:119:ASP:OD1	5:9B:120:ASN:N	2.47	0.47
6:B:295:LEU:O	6:B:298:MET:HG2	2.14	0.47
6:C:292:PRO:HD3	6:C:303:PRO:HA	1.96	0.47
6:E:295:LEU:O	6:E:298:MET:HG2	2.14	0.47
9:4A:156:LEU:HB2	9:4A:182:VAL:HG22	1.96	0.47
9:4D:181:VAL:HG22	9:4D:271:THR:HG22	1.97	0.47
9:4E:126:GLU:HG2	9:4E:131:GLN:HG3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2F:243:ASP:OD1	2:2F:248:ARG:NH1	2.45	0.47
2:2F:315:LYS:NZ	2:2F:321:ASP:OD1	2.37	0.47
5:9F:52:ILE:O	5:9F:56:ILE:HG12	2.14	0.47
6:B:651:ASP:HA	6:B:654:ILE:HD12	1.95	0.47
6:C:747:ILE:HG13	6:C:885:ASN:HA	1.96	0.47
7:a:224:LEU:HB3	7:a:364:LEU:HD12	1.97	0.47
7:c:629:VAL:HG23	7:c:632:SER:HB3	1.97	0.47
8:3B:248:VAL:HG11	8:3B:254:LEU:HD23	1.95	0.47
5:9B:176:GLN:HG3	5:9B:195:ILE:HB	1.96	0.47
7:b:723:MET:HE1	7:b:907:GLU:HA	1.94	0.47
7:c:899:GLY:H	7:c:902:ALA:HB3	1.78	0.47
7:d:900:ASP:OD1	7:d:900:ASP:N	2.48	0.47
7:e:900:ASP:N	7:e:900:ASP:OD1	2.48	0.47
7:f:724:ASP:OD2	7:f:816:ARG:NH1	2.47	0.47
9:4C:249:ASP:OD1	9:4C:249:ASP:N	2.46	0.47
6:D:728:LYS:NZ	6:D:886:GLU:O	2.47	0.47
9:4A:108:GLU:O	9:4A:149:ARG:NH2	2.48	0.47
9:4A:245:LEU:HD13	9:4A:253:LEU:HD12	1.94	0.47
6:A:197:ASP:OD1	6:A:198:ASN:N	2.48	0.47
6:A:728:LYS:NZ	6:A:886:GLU:O	2.46	0.47
6:B:134:ASN:OD1	6:B:137:ASN:ND2	2.46	0.47
6:B:426:GLN:NE2	6:B:441:THR:O	2.44	0.47
8:3E:413:ALA:HB2	8:3E:450:VAL:HG22	1.95	0.47
9:4B:157:ASP:OD1	9:4B:202:SER:OG	2.24	0.47
2:2D:101:ASP:OD1	2:2D:101:ASP:N	2.34	0.47
5:9B:114:GLN:N	5:9B:114:GLN:OE1	2.47	0.47
5:9D:52:ILE:HD12	5:9D:105:LEU:HD21	1.97	0.47
6:A:231:MET:HE1	6:A:323:ILE:HG23	1.95	0.47
6:C:651:ASP:HA	6:C:654:ILE:HD12	1.96	0.47
6:E:485:LYS:O	6:F:480:GLN:NE2	2.47	0.47
7:a:230:ASP:OD2	7:f:856:TRP:NE1	2.41	0.47
7:c:841:GLN:O	7:c:841:GLN:NE2	2.48	0.47
7:c:856:TRP:NE1	7:d:230:ASP:OD2	2.42	0.47
7:d:5:ASP:OD1	7:d:5:ASP:N	2.46	0.47
7:f:629:VAL:HG23	7:f:632:SER:HB3	1.97	0.47
1:1E:97:SER:HB3	1:1E:106:ILE:HG23	1.95	0.47
4:7C:77:SER:OG	4:7C:145:ARG:NH2	2.48	0.47
5:9B:44:ILE:HD12	5:9B:44:ILE:HA	1.81	0.47
6:A:359:PHE:HE2	6:A:361:LEU:HD11	1.80	0.47
6:D:414:SER:OG	6:D:415:GLN:OE1	2.27	0.47
6:F:472:ASP:OD1	6:F:473:PHE:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:b:203:ARG:NH2	7:b:602:GLU:OE1	2.35	0.47
7:d:624:LEU:HD13	7:d:706:TYR:HB2	1.97	0.47
7:f:543:PHE:O	7:f:546:THR:OG1	2.29	0.47
2:2E:244:ASN:O	2:2E:248:ARG:HB2	2.15	0.47
5:9A:137:SER:OG	5:9A:187:GLU:OE2	2.31	0.47
6:B:708:LEU:HD23	7:b:561:ARG:HG2	1.95	0.47
6:E:553:LEU:HD22	6:E:630:ILE:HG12	1.97	0.47
7:a:841:GLN:O	7:a:841:GLN:NE2	2.47	0.47
7:b:11:VAL:O	7:b:15:ILE:HG12	2.13	0.47
5:9C:44:ILE:HD12	5:9C:44:ILE:HA	1.81	0.47
5:9C:176:GLN:HG3	5:9C:195:ILE:HB	1.95	0.47
2:2C:107:ALA:O	2:2C:173:SER:OG	2.30	0.46
3:5B:12:ARG:HG3	3:5B:101:LEU:HB2	1.96	0.46
4:7E:114:LYS:HG2	5:9A:173:THR:HG21	1.96	0.46
5:9A:52:ILE:O	5:9A:56:ILE:HG12	2.15	0.46
6:B:745:GLN:HE22	6:B:790:ASN:HB2	1.78	0.46
2:2E:146:ASP:OD1	2:2E:146:ASP:N	2.34	0.46
6:D:197:ASP:OD1	6:D:198:ASN:N	2.48	0.46
6:D:261:ASP:OD1	6:D:261:ASP:N	2.40	0.46
7:b:460:ALA:O	7:b:464:ARG:NH1	2.48	0.46
8:3C:196:ALA:HB3	8:3C:215:THR:HG22	1.97	0.46
1:1A:55:MET:HE1	3:5B:7:PRO:HG2	1.98	0.46
1:1F:47:ASP:C	1:1F:47:ASP:OD1	2.59	0.46
6:B:176:ASP:OD2	6:B:178:ARG:NH1	2.48	0.46
9:4B:245:LEU:HD13	9:4B:253:LEU:HD12	1.96	0.46
9:4C:49:ASP:OD1	9:4C:49:ASP:N	2.48	0.46
9:4F:321:HIS:NE2	9:4F:338:GLU:OE2	2.48	0.46
2:2B:2:THR:HB	2:2B:13:GLU:OE2	2.14	0.46
3:5A:99:MET:HE1	9:4C:311:ILE:HG23	1.97	0.46
7:e:224:LEU:HD21	7:e:307:LEU:HD11	1.98	0.46
7:f:482:GLN:NE2	7:f:489:MET:SD	2.79	0.46
8:3C:342:HIS:CE1	8:3C:343:LYS:HG3	2.50	0.46
5:9B:43:LYS:HB2	5:9B:43:LYS:HE2	1.73	0.46
5:9E:176:GLN:HG3	5:9E:195:ILE:HB	1.98	0.46
6:B:172:GLY:HA2	6:B:540:ASN:HB2	1.96	0.46
7:d:224:LEU:HB3	7:d:364:LEU:HD12	1.97	0.46
7:d:724:ASP:OD2	7:d:816:ARG:NH1	2.48	0.46
7:e:43:ASP:O	7:e:47:THR:HG23	2.16	0.46
7:e:543:PHE:O	7:e:546:THR:OG1	2.29	0.46
9:4D:187:LEU:HD21	9:4D:256:VAL:HG11	1.97	0.46
2:2D:332:LYS:HG2	8:3B:459:GLN:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2E:2:THR:OG1	2:2E:3:THR:N	2.38	0.46
2:2E:27:THR:OG1	2:2E:184:ASP:OD2	2.34	0.46
3:5A:79:THR:HG23	3:5A:121:TRP:HH2	1.81	0.46
4:7F:77:SER:OG	4:7F:145:ARG:NH2	2.48	0.46
7:a:379:GLN:O	7:a:383:ASN:ND2	2.46	0.46
7:b:43:ASP:O	7:b:47:THR:HG23	2.16	0.46
7:b:142:TYR:OH	7:b:608:PRO:O	2.31	0.46
7:c:119:ASN:ND2	7:c:121:THR:O	2.48	0.46
7:c:132:ARG:NH1	7:c:290:LYS:O	2.46	0.46
7:e:836:MET:HG2	7:e:838:ILE:HD11	1.97	0.46
7:f:841:GLN:NE2	7:f:841:GLN:O	2.48	0.46
7:f:899:GLY:H	7:f:902:ALA:HB3	1.80	0.46
8:3F:263:GLN:HA	8:3F:266:VAL:HG22	1.98	0.46
9:4E:245:LEU:HD13	9:4E:253:LEU:HD12	1.96	0.46
9:4F:247:ASN:H	9:4F:252:SER:HB3	1.81	0.46
2:2C:32:PHE:HD1	2:2C:108:ALA:HB2	1.81	0.46
5:9A:42:LYS:O	5:9A:43:LYS:HG2	2.15	0.46
6:A:411:LEU:HB2	6:A:420:LEU:HD21	1.97	0.46
6:A:747:ILE:HG13	6:A:885:ASN:HA	1.98	0.46
6:B:728:LYS:NZ	6:B:886:GLU:O	2.48	0.46
6:D:747:ILE:HG13	6:D:885:ASN:HA	1.98	0.46
7:f:443:GLN:NE2	7:f:447:ASN:OD1	2.42	0.46
9:4B:108:GLU:O	9:4B:149:ARG:NH2	2.49	0.46
9:4D:235:PRO:HD3	9:4D:264:ILE:HG12	1.97	0.46
9:4F:49:ASP:OD1	9:4F:49:ASP:N	2.48	0.46
1:1D:55:MET:HE1	3:5E:7:PRO:HG2	1.97	0.46
3:5C:67:HIS:CD2	3:5C:139:GLU:HB2	2.50	0.46
6:E:651:ASP:HA	6:E:654:ILE:HD12	1.97	0.46
7:b:224:LEU:HD21	7:b:307:LEU:HD11	1.98	0.46
2:2D:67:ASN:HB3	2:2D:70:ASP:HB2	1.98	0.46
5:9D:176:GLN:HG3	5:9D:195:ILE:HB	1.97	0.46
6:D:411:LEU:HB2	6:D:420:LEU:HD21	1.98	0.46
7:e:891:TRP:CD1	7:e:897:PRO:HD2	2.51	0.46
9:4E:153:MET:HE2	9:4E:153:MET:HB3	1.74	0.46
1:1F:55:MET:HE1	3:5A:7:PRO:HG2	1.97	0.46
2:2B:27:THR:OG1	2:2B:184:ASP:OD2	2.33	0.46
2:2D:32:PHE:HD1	2:2D:108:ALA:HB2	1.81	0.46
3:5A:119:VAL:HG23	3:5A:139:GLU:HG2	1.98	0.46
3:5D:119:VAL:HG23	3:5D:139:GLU:HG2	1.98	0.46
5:9D:14:TRP:CE2	5:9D:125:ILE:HD13	2.51	0.46
6:A:283:SER:N	6:A:286:ASP:OD2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:359:PHE:HE2	6:E:361:LEU:HD11	1.81	0.46
7:a:624:LEU:HD13	7:a:706:TYR:HB2	1.97	0.46
7:e:138:GLU:OE2	7:e:141:ARG:NH2	2.49	0.46
7:e:325:ASP:OD2	7:e:327:ASN:ND2	2.49	0.46
7:e:651:GLY:HA2	7:e:676:MET:SD	2.57	0.46
8:3E:123:ASP:OD2	8:3E:123:ASP:N	2.49	0.46
8:3F:31:VAL:HB	8:3F:163:ILE:HD12	1.98	0.46
9:4A:321:HIS:NE2	9:4A:338:GLU:OE2	2.49	0.46
1:1C:55:MET:HE1	3:5D:7:PRO:HG2	1.97	0.45
2:2B:244:ASN:O	2:2B:248:ARG:HB2	2.16	0.45
5:9F:87:LEU:HD11	5:9F:100:LYS:HB3	1.99	0.45
6:E:176:ASP:OD2	6:E:611:ARG:NH2	2.49	0.45
6:E:677:GLN:NE2	6:E:679:TRP:O	2.41	0.45
7:a:15:ILE:HG23	7:a:60:ALA:HB3	1.98	0.45
7:b:116:ASP:OD1	7:b:280:HIS:NE2	2.35	0.45
7:c:506:ASP:OD1	7:c:506:ASP:N	2.49	0.45
7:d:543:PHE:O	7:d:546:THR:OG1	2.30	0.45
8:3F:248:VAL:HG11	8:3F:254:LEU:HD23	1.98	0.45
9:4B:249:ASP:OD1	9:4B:249:ASP:N	2.50	0.45
2:2C:267:MET:SD	8:3A:458:LEU:HD21	2.57	0.45
2:2F:267:MET:HB2	2:2F:283:VAL:HG13	1.99	0.45
6:D:292:PRO:HD3	6:D:303:PRO:HA	1.98	0.45
6:D:870:SER:OG	6:D:871:GLN:OE1	2.33	0.45
7:a:42:ASN:OD1	7:a:42:ASN:N	2.46	0.45
7:b:325:ASP:OD2	7:b:327:ASN:ND2	2.49	0.45
7:f:325:ASP:OD2	7:f:327:ASN:ND2	2.49	0.45
9:4B:49:ASP:OD1	9:4B:49:ASP:N	2.50	0.45
9:4E:249:ASP:OD1	9:4E:249:ASP:N	2.49	0.45
2:2A:67:ASN:HB3	2:2A:70:ASP:HB2	1.98	0.45
2:2F:2:THR:OG1	2:2F:3:THR:N	2.46	0.45
5:9A:150:ILE:HG13	5:9A:151:MET:HG2	1.97	0.45
7:a:506:ASP:N	7:a:506:ASP:OD1	2.50	0.45
7:b:837:VAL:HG22	7:b:874:HIS:HB2	1.99	0.45
7:d:15:ILE:HG23	7:d:60:ALA:HB3	1.98	0.45
8:3F:70:ILE:HG23	8:3F:114:VAL:HG12	1.98	0.45
2:2D:244:ASN:O	2:2D:248:ARG:HB2	2.16	0.45
4:7A:168:LYS:HE2	4:7A:168:LYS:HB2	1.62	0.45
6:A:88:PHE:CE1	7:a:52:CYS:HB3	2.51	0.45
7:b:138:GLU:OE2	7:b:141:ARG:NH2	2.49	0.45
7:f:506:ASP:N	7:f:506:ASP:OD1	2.49	0.45
9:4E:126:GLU:N	9:4E:126:GLU:OE1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1C:97:SER:HB3	1:1C:106:ILE:HG23	1.98	0.45
1:1E:100:ASN:HB2	1:1E:105:GLU:HB3	1.99	0.45
2:2C:243:ASP:OD1	2:2C:248:ARG:NH1	2.45	0.45
3:5D:72:VAL:HG21	3:5D:134:LEU:HD23	1.98	0.45
5:9E:87:LEU:HD21	5:9E:100:LYS:HE3	1.99	0.45
5:9F:137:SER:OG	5:9F:187:GLU:OE2	2.26	0.45
6:B:553:LEU:HD22	6:B:630:ILE:HG12	1.97	0.45
6:D:108:ASP:OD1	6:D:112:ARG:NH1	2.49	0.45
6:E:314:MET:SD	6:E:314:MET:N	2.90	0.45
8:3C:31:VAL:HB	8:3C:163:ILE:HD12	1.97	0.45
8:3E:263:GLN:HA	8:3E:266:VAL:HG22	1.98	0.45
9:4C:247:ASN:H	9:4C:252:SER:HB3	1.81	0.45
2:2A:32:PHE:HD1	2:2A:108:ALA:HB2	1.82	0.45
2:2C:138:LYS:O	2:2C:216:TYR:OH	2.28	0.45
6:B:380:TRP:HZ3	6:B:491:PRO:HB3	1.82	0.45
6:E:172:GLY:HA2	6:E:540:ASN:HB2	1.98	0.45
7:f:132:ARG:NH1	7:f:290:LYS:O	2.46	0.45
8:3C:263:GLN:HA	8:3C:266:VAL:HG22	1.98	0.45
9:4A:82:THR:HG22	9:4A:84:GLN:HG2	1.99	0.45
9:4D:275:THR:HB	9:4D:278:SER:HB2	1.99	0.45
1:1B:47:ASP:OD1	1:1B:47:ASP:C	2.60	0.45
3:5C:146:ARG:HH21	9:4D:325:ARG:CZ	2.30	0.45
5:9F:125:ILE:HD11	6:B:80:PRO:HB2	1.97	0.45
6:A:108:ASP:OD1	6:A:112:ARG:NH1	2.49	0.45
6:B:359:PHE:HE2	6:B:361:LEU:HD11	1.81	0.45
7:c:325:ASP:OD2	7:c:327:ASN:ND2	2.49	0.45
7:d:443:GLN:NE2	7:d:447:ASN:OD1	2.46	0.45
7:e:5:ASP:OD1	7:e:5:ASP:N	2.50	0.45
7:e:460:ALA:O	7:e:464:ARG:NH1	2.48	0.45
8:3C:248:VAL:HG11	8:3C:254:LEU:HD23	1.99	0.45
1:1C:41:ASP:O	1:1C:57:GLY:N	2.48	0.45
2:2C:344:ILE:HD13	9:4F:304:VAL:HG22	1.98	0.45
2:2E:162:ALA:HB2	2:2E:202:LEU:HD23	1.99	0.45
4:7C:31:MET:HE3	4:7C:31:MET:HB2	1.84	0.45
5:9B:14:TRP:CE2	5:9B:125:ILE:HD13	2.52	0.45
6:B:358:GLY:HA3	6:B:466:ILE:O	2.17	0.45
6:C:314:MET:HA	6:C:314:MET:HE3	1.98	0.45
6:C:328:ASN:HD22	6:C:497:GLN:HA	1.82	0.45
6:D:88:PHE:CE1	7:d:52:CYS:HB3	2.51	0.45
7:a:651:GLY:HA2	7:a:676:MET:HE2	1.99	0.45
7:c:689:THR:HG22	7:c:695:LEU:HG	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:3C:240:ASP:OD2	8:3C:243:THR:OG1	2.33	0.45
9:4A:249:ASP:OD1	9:4A:249:ASP:N	2.50	0.45
1:1E:47:ASP:C	1:1E:47:ASP:OD1	2.60	0.45
1:1F:76:LYS:HB2	1:1F:76:LYS:HE2	1.73	0.45
1:1F:97:SER:HB3	1:1F:106:ILE:HG23	1.99	0.45
6:F:531:ASN:HD22	6:F:619:THR:HA	1.82	0.45
7:a:762:ILE:HD11	7:a:817:TRP:HB2	1.98	0.45
7:b:482:GLN:NE2	7:b:489:MET:SD	2.86	0.45
7:b:836:MET:HG2	7:b:838:ILE:HD11	1.97	0.45
8:3E:427:LYS:O	8:3E:427:LYS:HG3	2.16	0.45
9:4D:126:GLU:C	9:4D:127:ILE:HD12	2.42	0.45
5:9A:89:THR:OG1	5:9A:100:LYS:NZ	2.48	0.45
5:9F:196:GLN:HB2	5:9F:210:GLN:HB3	1.99	0.45
6:A:271:ASN:OD1	6:A:272:ARG:N	2.50	0.45
6:B:471:GLN:NE2	6:B:472:ASP:O	2.50	0.45
6:E:88:PHE:CE1	7:e:52:CYS:HB3	2.52	0.45
6:F:728:LYS:NZ	6:F:886:GLU:O	2.49	0.45
7:b:822:GLU:OE2	7:b:823:LYS:NZ	2.39	0.45
7:c:543:PHE:O	7:c:546:THR:OG1	2.29	0.45
1:1E:62:ILE:HG12	1:1E:144:VAL:HG23	1.99	0.44
2:2A:244:ASN:O	2:2A:248:ARG:HB2	2.16	0.44
2:2F:32:PHE:HD1	2:2F:108:ALA:HB2	1.82	0.44
5:9B:12:ARG:HB2	5:9B:129:GLU:HG2	1.98	0.44
5:9C:196:GLN:HB2	5:9C:210:GLN:HB3	1.99	0.44
6:A:738:ILE:HD13	7:a:755:MET:HG2	1.99	0.44
6:F:292:PRO:HD3	6:F:303:PRO:HA	1.97	0.44
7:a:679:ASP:HB2	7:a:686:ILE:HD13	1.99	0.44
7:b:42:ASN:OD1	7:b:42:ASN:N	2.49	0.44
7:d:203:ARG:NH2	7:d:602:GLU:OE1	2.37	0.44
7:e:506:ASP:OD1	7:e:506:ASP:N	2.50	0.44
9:4A:49:ASP:N	9:4A:49:ASP:OD1	2.50	0.44
1:1C:32:ASN:HB3	1:1C:67:ARG:HB2	1.99	0.44
4:7B:181:LEU:HD23	4:7B:181:LEU:HA	1.88	0.44
6:C:871:GLN:OE1	6:C:871:GLN:N	2.49	0.44
6:F:197:ASP:OD1	6:F:198:ASN:N	2.50	0.44
7:b:891:TRP:CD1	7:b:897:PRO:HD2	2.52	0.44
7:b:900:ASP:OD1	7:b:900:ASP:N	2.48	0.44
7:e:592:LYS:C	7:e:593:LEU:HD23	2.42	0.44
7:e:837:VAL:HG22	7:e:874:HIS:HB2	1.99	0.44
2:2F:344:ILE:HD13	9:4C:304:VAL:HG22	1.98	0.44
4:7B:31:MET:HE3	4:7B:31:MET:HB2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:7B:183:LEU:HD21	4:7B:204:ALA:HB2	1.99	0.44
4:7D:186:ILE:HG22	4:7D:203:LEU:HD21	1.98	0.44
6:B:88:PHE:CE1	7:b:52:CYS:HB3	2.52	0.44
6:C:177:LEU:HB3	6:C:193:LEU:HB3	2.00	0.44
6:E:552:GLN:NE2	6:E:589:GLN:OE1	2.51	0.44
6:F:243:GLU:OE2	6:F:317:LYS:NZ	2.41	0.44
7:f:379:GLN:O	7:f:383:ASN:ND2	2.47	0.44
1:1C:47:ASP:OD2	1:1C:47:ASP:C	2.60	0.44
3:5F:67:HIS:CD2	3:5F:139:GLU:HB2	2.53	0.44
6:B:283:SER:N	6:B:286:ASP:OD2	2.51	0.44
6:C:706:ARG:HG3	7:c:97:CYS:SG	2.58	0.44
6:E:329:ARG:HH11	6:E:329:ARG:HA	1.81	0.44
6:E:358:GLY:HA3	6:E:466:ILE:O	2.17	0.44
7:c:702:VAL:HG23	7:c:711:LEU:HG	1.98	0.44
7:f:846:ASP:OD1	7:f:846:ASP:N	2.50	0.44
1:1B:62:ILE:HG12	1:1B:144:VAL:HG23	1.99	0.44
1:1D:41:ASP:O	1:1D:57:GLY:N	2.46	0.44
1:1D:47:ASP:C	1:1D:47:ASP:OD2	2.60	0.44
1:1F:32:ASN:HB3	1:1F:67:ARG:HB2	1.98	0.44
2:2D:107:ALA:O	2:2D:173:SER:OG	2.26	0.44
3:5D:79:THR:HG23	3:5D:121:TRP:CH2	2.52	0.44
6:A:454:SER:OG	6:A:459:GLU:OE1	2.36	0.44
6:E:380:TRP:HZ3	6:E:491:PRO:HB3	1.82	0.44
6:E:447:MET:HE3	6:E:447:MET:HB3	1.85	0.44
6:F:712:ASN:OD1	7:f:561:ARG:NH1	2.50	0.44
7:b:592:LYS:C	7:b:593:LEU:HD23	2.42	0.44
8:3B:123:ASP:OD2	8:3B:123:ASP:N	2.50	0.44
8:3B:172:ASP:OD1	8:3B:175:TYR:N	2.37	0.44
8:3E:406:LEU:HD12	8:3E:406:LEU:HA	1.88	0.44
9:4E:235:PRO:HD3	9:4E:264:ILE:HG12	1.99	0.44
2:2F:27:THR:OG1	2:2F:184:ASP:OD2	2.35	0.44
2:2F:101:ASP:OD1	2:2F:101:ASP:N	2.35	0.44
3:5A:72:VAL:HG21	3:5A:134:LEU:HD23	1.99	0.44
5:9A:85:ASN:C	5:9A:86:ILE:HD12	2.43	0.44
5:9A:88:VAL:HB	5:9A:101:ILE:HG23	1.98	0.44
6:A:870:SER:OG	6:A:871:GLN:OE1	2.33	0.44
6:B:314:MET:SD	6:B:314:MET:N	2.90	0.44
6:D:231:MET:HE1	6:D:323:ILE:HG23	1.98	0.44
6:D:282:LEU:HD23	6:D:282:LEU:HA	1.81	0.44
7:c:179:LEU:HD21	7:c:251:LEU:HD11	1.99	0.44
7:d:676:MET:CE	7:d:898:LEU:H	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:e:739:GLU:OE1	7:e:740:ASN:ND2	2.50	0.44
9:4F:161:ASP:OD2	9:4F:163:THR:OG1	2.33	0.44
1:1A:47:ASP:OD2	1:1A:47:ASP:C	2.60	0.44
2:2B:162:ALA:HB2	2:2B:202:LEU:HD23	1.98	0.44
2:2C:244:ASN:O	2:2C:248:ARG:HB2	2.18	0.44
2:2F:244:ASN:O	2:2F:248:ARG:HB2	2.17	0.44
3:5A:90:LYS:HB3	3:5A:90:LYS:HE3	1.76	0.44
4:7D:168:LYS:HB2	4:7D:168:LYS:HE2	1.62	0.44
5:9E:119:ASP:OD1	5:9E:120:ASN:N	2.47	0.44
6:A:802:GLN:HB2	6:A:863:ASN:HB3	2.00	0.44
6:D:802:GLN:HB2	6:D:863:ASN:HB3	2.00	0.44
6:E:25:SER:OG	6:E:28:ASP:OD1	2.27	0.44
6:E:860:ARG:NH1	7:f:334:ASP:OD2	2.50	0.44
6:F:358:GLY:HA3	6:F:466:ILE:O	2.18	0.44
7:b:651:GLY:HA2	7:b:676:MET:SD	2.58	0.44
7:f:220:PHE:HD1	7:f:328:ILE:HD13	1.83	0.44
7:f:568:LYS:HE2	7:f:568:LYS:HB3	1.77	0.44
7:f:822:GLU:OE2	7:f:823:LYS:NZ	2.41	0.44
9:4F:105:ILE:HD12	9:4F:145:LEU:HD22	2.00	0.44
2:2E:138:LYS:O	2:2E:216:TYR:OH	2.28	0.44
4:7E:183:LEU:HD21	4:7E:204:ALA:HB2	2.00	0.44
5:9B:87:LEU:HD21	5:9B:100:LYS:HE3	1.99	0.44
5:9D:119:ASP:OD1	5:9D:120:ASN:N	2.50	0.44
5:9E:14:TRP:CE2	5:9E:125:ILE:HD13	2.52	0.44
5:9F:8:ASP:OD1	5:9F:12:ARG:NH2	2.50	0.44
6:A:401:SER:O	6:A:401:SER:OG	2.33	0.44
6:C:197:ASP:OD1	6:C:198:ASN:N	2.50	0.44
6:C:531:ASN:HD22	6:C:619:THR:HA	1.83	0.44
6:E:332:ARG:HB2	6:E:362:VAL:HG12	2.00	0.44
6:F:328:ASN:HD22	6:F:497:GLN:HA	1.83	0.44
7:b:349:TRP:CE3	7:b:357:ILE:HD11	2.53	0.44
7:f:465:GLY:O	7:f:548:ARG:NH2	2.50	0.44
7:f:689:THR:HG22	7:f:695:LEU:HG	1.99	0.44
9:4C:156:LEU:HB2	9:4C:182:VAL:HG22	1.99	0.44
9:4E:126:GLU:C	9:4E:127:ILE:HD12	2.42	0.44
1:1D:97:SER:HB3	1:1D:106:ILE:HG23	1.99	0.44
1:1F:80:TRP:CZ2	1:1F:92:LYS:HG3	2.53	0.44
2:2F:313:ILE:HD12	2:2F:331:ILE:HG12	1.99	0.44
6:B:736:THR:HA	7:b:871:MET:O	2.17	0.44
6:C:728:LYS:NZ	6:C:886:GLU:O	2.49	0.44
6:D:738:ILE:HD13	7:d:755:MET:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:a:349:TRP:CE3	7:a:357:ILE:HD11	2.53	0.44
7:b:5:ASP:OD1	7:b:5:ASP:N	2.50	0.44
7:c:884:PHE:CD1	7:c:884:PHE:C	2.96	0.44
7:d:349:TRP:CE3	7:d:357:ILE:HD11	2.53	0.44
7:d:379:GLN:O	7:d:383:ASN:ND2	2.47	0.44
7:e:689:THR:HG22	7:e:695:LEU:HG	2.00	0.44
7:f:739:GLU:N	7:f:739:GLU:OE2	2.51	0.44
8:3A:230:ASP:HB3	8:3A:251:LEU:HB3	2.00	0.44
8:3B:263:GLN:HA	8:3B:266:VAL:HG22	1.99	0.44
9:4B:275:THR:HB	9:4B:278:SER:HB2	2.00	0.44
9:4D:126:GLU:N	9:4D:126:GLU:OE2	2.51	0.44
9:4E:275:THR:HB	9:4E:278:SER:HB2	1.99	0.44
1:1B:100:ASN:OD1	1:1B:101:GLU:N	2.51	0.43
3:5B:67:HIS:NE2	3:5B:139:GLU:HG3	2.33	0.43
3:5E:12:ARG:HG3	3:5E:101:LEU:HB2	2.00	0.43
6:D:271:ASN:OD1	6:D:272:ARG:N	2.50	0.43
6:E:271:ASN:OD1	6:E:272:ARG:N	2.51	0.43
6:F:177:LEU:HB3	6:F:193:LEU:HB3	2.00	0.43
7:b:576:ILE:HG12	7:b:861:ILE:HD12	2.00	0.43
7:c:43:ASP:O	7:c:47:THR:HG23	2.18	0.43
7:c:465:GLY:O	7:c:548:ARG:NH2	2.50	0.43
7:d:689:THR:HG22	7:d:695:LEU:HG	2.00	0.43
7:e:349:TRP:CE3	7:e:357:ILE:HD11	2.53	0.43
9:4A:187:LEU:HD21	9:4A:256:VAL:HG11	2.00	0.43
9:4C:105:ILE:HD12	9:4C:145:LEU:HD22	2.00	0.43
2:2A:332:LYS:HD3	8:3F:19:ASN:OD1	2.17	0.43
2:2B:138:LYS:O	2:2B:216:TYR:OH	2.28	0.43
2:2C:146:ASP:OD1	2:2C:146:ASP:N	2.34	0.43
2:2D:162:ALA:HB2	2:2D:202:LEU:HD23	2.00	0.43
2:2F:78:ILE:HD12	2:2F:78:ILE:HA	1.85	0.43
6:C:547:LEU:HD11	6:C:596:LEU:HD13	2.00	0.43
6:C:712:ASN:OD1	7:c:561:ARG:NH1	2.51	0.43
6:D:485:LYS:O	6:E:480:GLN:NE2	2.47	0.43
6:F:271:ASN:OD1	6:F:272:ARG:N	2.51	0.43
6:F:282:LEU:HD23	6:F:282:LEU:HA	1.80	0.43
7:a:224:LEU:HD12	7:a:224:LEU:HA	1.88	0.43
7:f:43:ASP:O	7:f:47:THR:HG23	2.18	0.43
1:1C:36:LEU:O	1:1D:122:SER:HB2	2.18	0.43
1:1E:4:THR:HB	1:1E:7:GLN:HG3	2.00	0.43
3:5A:79:THR:HG21	3:5F:152:VAL:HG11	1.99	0.43
4:7F:186:ILE:HG21	4:7F:221:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:298:MET:HE2	6:A:298:MET:HB3	1.80	0.43
6:A:358:GLY:HA3	6:A:466:ILE:O	2.18	0.43
6:C:775:ASP:OD2	6:C:775:ASP:C	2.62	0.43
6:E:243:GLU:OE2	6:E:317:LYS:NZ	2.44	0.43
6:F:395:TYR:OH	6:F:486:ASN:O	2.34	0.43
7:a:465:GLY:O	7:a:548:ARG:NH2	2.51	0.43
7:c:220:PHE:HD1	7:c:328:ILE:HD13	1.83	0.43
7:c:846:ASP:N	7:c:846:ASP:OD1	2.51	0.43
7:d:465:GLY:O	7:d:548:ARG:NH2	2.51	0.43
7:e:576:ILE:HG12	7:e:861:ILE:HD12	2.00	0.43
8:3B:254:LEU:HD11	8:3B:261:VAL:HG23	2.00	0.43
2:2E:230:LYS:HE2	2:2E:230:LYS:HB2	1.92	0.43
3:5A:79:THR:HG23	3:5A:121:TRP:CH2	2.54	0.43
5:9F:68:LYS:HB2	5:9F:68:LYS:NZ	2.33	0.43
6:C:132:THR:OG1	6:C:674:SER:O	2.37	0.43
6:F:376:MET:HG3	6:F:440:LEU:HB2	2.00	0.43
6:F:860:ARG:NH1	7:a:334:ASP:OD2	2.52	0.43
8:3A:340:PHE:O	8:3A:344:GLY:N	2.50	0.43
8:3B:427:LYS:O	8:3B:427:LYS:HG3	2.18	0.43
9:4A:275:THR:HB	9:4A:278:SER:HB2	2.00	0.43
2:2C:27:THR:OG1	2:2C:184:ASP:OD2	2.35	0.43
5:9C:87:LEU:HD11	5:9C:100:LYS:HB3	2.00	0.43
6:A:310:THR:C	6:A:311:GLN:HG3	2.43	0.43
6:B:226:SER:C	6:B:302:ILE:HD13	2.44	0.43
6:B:271:ASN:OD1	6:B:272:ARG:N	2.51	0.43
7:a:353:PRO:O	7:a:357:ILE:HG12	2.19	0.43
7:a:900:ASP:OD1	7:a:900:ASP:N	2.48	0.43
7:b:220:PHE:HD1	7:b:328:ILE:HD13	1.83	0.43
7:f:179:LEU:HD21	7:f:251:LEU:HD11	2.00	0.43
9:4D:108:GLU:O	9:4D:149:ARG:NH2	2.52	0.43
1:1C:76:LYS:HE2	1:1C:76:LYS:HB2	1.73	0.43
2:2D:332:LYS:HD3	8:3C:19:ASN:OD1	2.19	0.43
2:2F:267:MET:SD	8:3D:458:LEU:HD21	2.58	0.43
3:5C:67:HIS:NE2	3:5C:139:GLU:OE1	2.52	0.43
6:B:310:THR:C	6:B:311:GLN:HG3	2.44	0.43
6:D:310:THR:C	6:D:311:GLN:HG3	2.43	0.43
6:F:132:THR:OG1	6:F:674:SER:O	2.36	0.43
8:3A:31:VAL:HB	8:3A:163:ILE:HD12	2.00	0.43
1:1E:100:ASN:OD1	1:1E:101:GLU:N	2.51	0.43
2:2A:50:SER:N	2:2A:54:GLU:OE1	2.43	0.43
2:2A:162:ALA:HB2	2:2A:202:LEU:HD23	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2D:244:ASN:OD1	2:2D:245:ASP:N	2.52	0.43
3:5C:90:LYS:HE3	3:5C:90:LYS:HB3	1.76	0.43
3:5E:67:HIS:NE2	3:5E:139:GLU:HG3	2.34	0.43
4:7A:186:ILE:HG22	4:7A:203:LEU:HD21	1.99	0.43
6:A:292:PRO:HD3	6:A:303:PRO:HA	1.99	0.43
6:B:108:ASP:OD1	6:B:112:ARG:NH1	2.52	0.43
6:C:358:GLY:HA3	6:C:466:ILE:O	2.18	0.43
6:E:870:SER:OG	6:E:871:GLN:OE1	2.36	0.43
6:F:454:SER:OG	6:F:459:GLU:OE1	2.37	0.43
7:a:443:GLN:NE2	7:a:447:ASN:OD1	2.47	0.43
7:d:353:PRO:O	7:d:357:ILE:HG12	2.18	0.43
7:d:416:LEU:HD12	7:d:422:LEU:HD12	2.01	0.43
7:d:506:ASP:N	7:d:506:ASP:OD1	2.50	0.43
7:e:725:TYR:HB2	7:e:817:TRP:CE2	2.54	0.43
8:3A:225:LEU:HD21	8:3A:281:ASN:HB3	2.01	0.43
8:3D:31:VAL:HB	8:3D:163:ILE:HD12	2.00	0.43
8:3D:413:ALA:HB2	8:3D:450:VAL:HG22	2.00	0.43
4:7E:46:GLN:HB3	4:7E:59:HIS:CE1	2.54	0.43
6:B:714:VAL:HG22	6:B:727:VAL:HB	2.01	0.43
6:C:271:ASN:OD1	6:C:272:ARG:N	2.51	0.43
6:C:310:THR:C	6:C:311:GLN:HG3	2.43	0.43
6:D:358:GLY:HA3	6:D:466:ILE:O	2.18	0.43
6:E:310:THR:C	6:E:311:GLN:HG3	2.44	0.43
7:a:138:GLU:OE2	7:a:141:ARG:NH2	2.52	0.43
7:c:739:GLU:N	7:c:739:GLU:OE2	2.51	0.43
7:d:138:GLU:OE2	7:d:141:ARG:NH2	2.52	0.43
7:d:220:PHE:HD1	7:d:328:ILE:HD13	1.84	0.43
7:d:482:GLN:NE2	7:d:489:MET:SD	2.87	0.43
7:f:648:LEU:HD13	7:f:677:ILE:HD13	2.00	0.43
1:1F:41:ASP:O	1:1F:57:GLY:N	2.48	0.43
2:2C:176:ILE:HD13	2:2C:176:ILE:HA	1.87	0.43
3:5D:146:ARG:NH2	9:4F:325:ARG:CZ	2.81	0.43
5:9E:137:SER:OG	5:9E:187:GLU:OE2	2.34	0.43
6:B:551:TRP:HB3	6:B:553:LEU:HD21	2.01	0.43
6:C:395:TYR:OH	6:C:486:ASN:O	2.35	0.43
6:C:398:LYS:HE3	6:C:398:LYS:HB3	1.87	0.43
6:D:115:LEU:HA	7:d:91:PRO:HG3	2.01	0.43
6:D:454:SER:OG	6:D:459:GLU:OE1	2.36	0.43
7:c:5:ASP:N	7:c:5:ASP:OD1	2.51	0.43
7:e:536:LEU:HD12	7:e:536:LEU:HA	1.85	0.43
7:f:5:ASP:OD1	7:f:5:ASP:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:f:676:MET:HE1	7:f:898:LEU:H	1.84	0.43
7:f:725:TYR:HB2	7:f:817:TRP:CE2	2.54	0.43
5:9E:106:ARG:CZ	5:9E:106:ARG:HB2	2.49	0.43
6:A:332:ARG:HB2	6:A:362:VAL:HG12	2.00	0.43
6:B:677:GLN:NE2	6:B:679:TRP:O	2.41	0.43
6:E:226:SER:C	6:E:302:ILE:HD13	2.44	0.43
6:E:283:SER:N	6:E:286:ASP:OD2	2.51	0.43
7:b:77:GLU:OE2	7:b:77:GLU:C	2.62	0.43
7:c:561:ARG:HG3	7:c:575:ARG:NH1	2.34	0.43
8:3B:31:VAL:HB	8:3B:163:ILE:HD12	2.01	0.43
2:2D:169:ASP:OD1	2:2D:169:ASP:N	2.40	0.42
3:5A:121:TRP:CD1	3:5A:121:TRP:C	2.97	0.42
3:5F:87:ARG:NH1	3:5F:89:GLU:OE2	2.44	0.42
6:B:25:SER:OG	6:B:28:ASP:OD1	2.27	0.42
6:B:242:LEU:HD11	6:B:278:ILE:HG12	2.01	0.42
6:D:161:TYR:HB3	6:D:640:ALA:HB1	2.01	0.42
6:D:401:SER:O	6:D:401:SER:OG	2.33	0.42
6:F:203:GLU:OE2	6:F:203:GLU:N	2.52	0.42
6:F:706:ARG:HG3	7:f:97:CYS:SG	2.58	0.42
6:F:775:ASP:OD2	6:F:775:ASP:C	2.62	0.42
7:f:884:PHE:C	7:f:884:PHE:CD1	2.96	0.42
9:4B:82:THR:HG22	9:4B:84:GLN:HG2	2.00	0.42
3:5B:67:HIS:CD2	3:5B:139:GLU:HG3	2.54	0.42
5:9C:87:LEU:HD21	5:9C:100:LYS:HE2	2.00	0.42
6:A:282:LEU:HD23	6:A:282:LEU:HA	1.82	0.42
6:C:235:GLU:OE1	6:C:284:SER:N	2.51	0.42
6:F:225:LYS:HG2	6:F:302:ILE:HD11	2.01	0.42
6:F:802:GLN:HB2	6:F:863:ASN:HB3	2.02	0.42
7:a:529:THR:OG1	7:a:530:HIS:N	2.52	0.42
7:d:529:THR:OG1	7:d:530:HIS:N	2.52	0.42
8:3C:163:ILE:HB	8:3C:192:TYR:HE2	1.85	0.42
9:4B:235:PRO:HD3	9:4B:264:ILE:HG12	2.01	0.42
2:2A:138:LYS:O	2:2A:216:TYR:OH	2.32	0.42
5:9A:44:ILE:HD12	5:9A:44:ILE:HA	1.87	0.42
5:9B:88:VAL:HB	5:9B:101:ILE:HG23	2.01	0.42
6:D:792:PRO:HG2	6:D:794:TYR:CZ	2.54	0.42
6:F:310:THR:C	6:F:311:GLN:HG3	2.43	0.42
7:a:884:PHE:C	7:a:884:PHE:CD1	2.98	0.42
7:b:689:THR:HG22	7:b:695:LEU:HG	1.99	0.42
7:c:725:TYR:HB2	7:c:817:TRP:CE2	2.54	0.42
7:f:142:TYR:OH	7:f:608:PRO:O	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:f:509:HIS:HB3	7:f:512:ASN:HB2	2.00	0.42
9:4A:183:TYR:CZ	9:4A:207:VAL:HG11	2.54	0.42
9:4B:183:TYR:CZ	9:4B:207:VAL:HG11	2.54	0.42
1:1A:41:ASP:O	1:1A:57:GLY:N	2.46	0.42
1:1A:97:SER:HB3	1:1A:106:ILE:HG23	2.00	0.42
2:2F:146:ASP:OD1	2:2F:146:ASP:N	2.34	0.42
4:7C:181:LEU:HD23	4:7C:181:LEU:HA	1.88	0.42
5:9C:88:VAL:HB	5:9C:101:ILE:HG23	2.01	0.42
6:B:332:ARG:HB2	6:B:362:VAL:HG12	2.01	0.42
6:D:412:VAL:HG22	6:D:417:ARG:HG2	2.01	0.42
7:f:561:ARG:HG3	7:f:575:ARG:NH1	2.34	0.42
8:3A:413:ALA:HB2	8:3A:450:VAL:HG22	2.00	0.42
8:3F:165:LEU:HD23	8:3F:193:PHE:HB3	2.01	0.42
9:4D:49:ASP:N	9:4D:49:ASP:OD1	2.53	0.42
1:1A:122:SER:HB2	1:1F:36:LEU:O	2.18	0.42
2:2A:244:ASN:OD1	2:2A:245:ASP:N	2.52	0.42
2:2B:73:LEU:HD12	2:2B:77:PHE:CE2	2.54	0.42
3:5F:90:LYS:HB3	3:5F:90:LYS:HE3	1.76	0.42
5:9F:87:LEU:HD21	5:9F:100:LYS:HE2	2.00	0.42
6:A:792:PRO:HG2	6:A:794:TYR:CZ	2.54	0.42
6:B:161:TYR:HB3	6:B:640:ALA:HB1	2.01	0.42
6:B:606:LEU:HD23	6:B:606:LEU:HA	1.90	0.42
6:C:411:LEU:HB2	6:C:420:LEU:HD21	2.01	0.42
6:E:531:ASN:HD22	6:E:619:THR:HA	1.85	0.42
6:E:551:TRP:HB3	6:E:553:LEU:HD21	2.01	0.42
7:a:416:LEU:HD12	7:a:422:LEU:HD12	2.01	0.42
7:a:841:GLN:HB2	7:a:878:PRO:HG3	2.01	0.42
7:c:509:HIS:HB3	7:c:512:ASN:HB2	2.00	0.42
8:3B:36:PHE:CZ	8:3B:121:SER:HB2	2.55	0.42
4:7B:118:GLU:OE2	4:7C:93:LYS:HD2	2.19	0.42
6:A:480:GLN:NE2	6:F:485:LYS:O	2.51	0.42
6:D:860:ARG:NH1	7:e:334:ASP:OD2	2.53	0.42
6:E:506:PRO:HA	6:E:509:PHE:HE1	1.85	0.42
7:a:220:PHE:HD1	7:a:328:ILE:HD13	1.84	0.42
7:c:121:THR:OG1	7:c:123:GLU:OE1	2.29	0.42
7:e:220:PHE:HD1	7:e:328:ILE:HD13	1.84	0.42
7:e:822:GLU:OE2	7:e:823:LYS:NZ	2.39	0.42
8:3E:254:LEU:HD11	8:3E:261:VAL:HG23	2.02	0.42
8:3F:163:ILE:HB	8:3F:192:TYR:HE2	1.85	0.42
9:4D:257:ARG:HD3	9:4D:259:PHE:CZ	2.54	0.42
2:2A:169:ASP:OD1	2:2A:169:ASP:N	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5B:99:MET:HB3	3:5B:107:PRO:HB3	2.02	0.42
4:7B:46:GLN:HB3	4:7B:59:HIS:CE1	2.54	0.42
5:9B:87:LEU:HD11	5:9B:100:LYS:HB3	2.02	0.42
5:9E:43:LYS:HB2	5:9E:43:LYS:HE2	1.73	0.42
6:C:25:SER:OG	6:C:28:ASP:OD1	2.26	0.42
6:C:376:MET:HG3	6:C:440:LEU:HB2	2.00	0.42
6:D:242:LEU:HD11	6:D:278:ILE:HG12	2.01	0.42
6:E:242:LEU:HD11	6:E:278:ILE:HG12	2.01	0.42
7:a:176:LEU:HB3	7:a:212:ILE:HD13	2.01	0.42
7:a:689:THR:HG22	7:a:695:LEU:HG	2.00	0.42
7:b:536:LEU:HD12	7:b:536:LEU:HA	1.84	0.42
7:e:869:LEU:HD23	7:e:869:LEU:HA	1.93	0.42
7:f:138:GLU:OE2	7:f:141:ARG:NH2	2.53	0.42
8:3D:326:GLN:OE1	8:3E:8:PRO:HD2	2.20	0.42
9:4D:184:TRP:CZ3	9:4D:242:ALA:HB2	2.55	0.42
2:2D:50:SER:N	2:2D:54:GLU:OE1	2.43	0.42
3:5E:99:MET:HB3	3:5E:107:PRO:HB3	2.02	0.42
4:7C:186:ILE:HG21	4:7C:221:LEU:HD12	2.00	0.42
5:9E:87:LEU:HD11	5:9E:100:LYS:HB3	2.01	0.42
6:A:161:TYR:HB3	6:A:640:ALA:HB1	2.01	0.42
6:B:263:TRP:NE1	6:B:296:ASP:OD1	2.46	0.42
6:B:521:ASN:HB2	6:B:524:GLU:CD	2.45	0.42
6:E:521:ASN:HB2	6:E:524:GLU:CD	2.45	0.42
6:F:401:SER:O	6:F:401:SER:OG	2.33	0.42
7:a:624:LEU:HD23	7:a:625:LYS:N	2.35	0.42
7:a:724:ASP:OD2	7:a:816:ARG:NH1	2.53	0.42
7:a:725:TYR:HB2	7:a:817:TRP:CE2	2.55	0.42
7:c:251:LEU:HD12	7:c:251:LEU:HA	1.90	0.42
7:e:465:GLY:O	7:e:548:ARG:NH2	2.53	0.42
9:4B:86:LEU:HD22	9:4B:121:ARG:HD2	2.02	0.42
1:1D:62:ILE:HG12	1:1D:144:VAL:HG23	2.01	0.42
3:5D:121:TRP:CD1	3:5D:121:TRP:C	2.98	0.42
5:9A:35:LEU:HB3	5:9A:72:THR:HG23	2.01	0.42
5:9F:119:ASP:OD1	5:9F:119:ASP:N	2.53	0.42
6:B:326:ASN:OD1	6:C:415:GLN:NE2	2.52	0.42
6:C:282:LEU:HD12	6:C:289:ILE:HD11	2.01	0.42
6:C:383:LEU:HD13	6:C:435:PRO:HG2	2.02	0.42
6:F:245:ASP:OD1	6:F:275:LYS:HB3	2.20	0.42
9:4E:108:GLU:O	9:4E:149:ARG:NH2	2.52	0.42
2:2E:73:LEU:HD12	2:2E:77:PHE:CE2	2.54	0.42
5:9E:44:ILE:HD12	5:9E:44:ILE:HA	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:9F:52:ILE:HD12	5:9F:105:LEU:HD21	2.01	0.42
5:9F:150:ILE:HG13	5:9F:151:MET:HG2	2.02	0.42
6:B:860:ARG:NH1	7:c:334:ASP:OD2	2.53	0.42
6:C:10:LEU:HD23	6:C:10:LEU:HA	1.90	0.42
7:a:43:ASP:O	7:a:47:THR:HG23	2.20	0.42
7:d:884:PHE:CD1	7:d:884:PHE:C	2.98	0.42
7:f:488:ILE:HG22	7:f:492:LEU:HG	2.01	0.42
8:3D:230:ASP:HB3	8:3D:251:LEU:HB3	2.01	0.42
4:7E:118:GLU:OE2	4:7F:93:LYS:HD2	2.20	0.41
5:9C:8:ASP:OD1	5:9C:12:ARG:NH2	2.53	0.41
6:B:456:SER:OG	6:B:458:ASN:ND2	2.47	0.41
6:B:818:LEU:HD12	6:B:818:LEU:HA	1.95	0.41
6:E:541:VAL:HG21	6:E:547:LEU:HD11	2.02	0.41
6:E:551:TRP:HE3	6:E:553:LEU:HD21	1.85	0.41
7:b:711:LEU:C	7:b:712:TYR:HD2	2.28	0.41
7:c:379:GLN:O	7:c:383:ASN:ND2	2.46	0.41
7:d:176:LEU:HB3	7:d:212:ILE:HD13	2.01	0.41
7:e:846:ASP:OD1	7:e:846:ASP:N	2.53	0.41
8:3A:172:ASP:OD1	8:3A:175:TYR:N	2.37	0.41
8:3E:36:PHE:CZ	8:3E:121:SER:HB2	2.55	0.41
9:4D:153:MET:HB3	9:4D:153:MET:HE2	1.74	0.41
2:2E:107:ALA:HB2	2:2E:112:ILE:HG12	2.02	0.41
5:9C:31:TYR:O	5:9C:73:GLN:NE2	2.53	0.41
5:9E:37:LYS:HD2	5:9E:37:LYS:C	2.45	0.41
5:9E:88:VAL:HB	5:9E:101:ILE:HG23	2.02	0.41
6:A:231:MET:SD	6:A:236:ARG:HG2	2.60	0.41
6:A:242:LEU:HD11	6:A:278:ILE:HG12	2.03	0.41
6:C:454:SER:OG	6:C:459:GLU:OE1	2.37	0.41
6:E:728:LYS:HB2	6:E:747:ILE:HB	2.02	0.41
6:F:389:SER:OG	6:F:398:LYS:NZ	2.30	0.41
7:b:834:VAL:O	7:b:871:MET:HA	2.20	0.41
7:c:46:ILE:HD13	7:c:46:ILE:HA	1.92	0.41
7:d:509:HIS:HB3	7:d:512:ASN:HB2	2.02	0.41
7:f:592:LYS:O	7:f:593:LEU:HD13	2.20	0.41
8:3F:42:ASN:OD1	8:3F:42:ASN:N	2.53	0.41
9:4F:235:PRO:HD3	9:4F:264:ILE:HG12	2.02	0.41
2:2B:244:ASN:OD1	2:2B:245:ASP:N	2.53	0.41
2:2F:279:THR:O	2:2F:283:VAL:HG23	2.21	0.41
3:5B:72:VAL:HG21	3:5B:134:LEU:HD23	2.01	0.41
3:5E:146:ARG:HH21	9:4A:325:ARG:CZ	2.34	0.41
6:A:10:LEU:HD23	6:A:10:LEU:HA	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:197:ASP:OD1	6:B:198:ASN:N	2.53	0.41
6:B:551:TRP:HE3	6:B:553:LEU:HD21	1.85	0.41
6:C:231:MET:CG	6:C:236:ARG:HG2	2.48	0.41
6:C:412:VAL:HG22	6:C:417:ARG:HG2	2.01	0.41
6:C:521:ASN:HB2	6:C:524:GLU:CD	2.46	0.41
6:E:714:VAL:HG22	6:E:727:VAL:HB	2.02	0.41
6:F:388:PHE:H	6:F:402:ASN:HD21	1.68	0.41
7:b:725:TYR:HB2	7:b:817:TRP:CE2	2.54	0.41
8:3B:379:MET:HE2	8:3B:379:MET:HA	2.02	0.41
8:3E:18:LEU:HD22	8:3E:19:ASN:N	2.35	0.41
8:3F:240:ASP:OD2	8:3F:243:THR:OG1	2.33	0.41
9:4A:284:GLN:HG2	9:4A:285:THR:N	2.35	0.41
9:4E:195:THR:O	9:4E:195:THR:OG1	2.34	0.41
2:2E:244:ASN:OD1	2:2E:245:ASP:N	2.54	0.41
2:2F:244:ASN:OD1	2:2F:245:ASP:N	2.54	0.41
6:A:383:LEU:HD23	6:A:383:LEU:HA	1.91	0.41
6:D:314:MET:SD	6:D:314:MET:N	2.94	0.41
6:D:706:ARG:HG3	7:d:97:CYS:SG	2.60	0.41
6:E:161:TYR:HB3	6:E:640:ALA:HB1	2.01	0.41
7:a:832:PHE:HB3	7:a:869:LEU:HD23	2.02	0.41
7:b:465:GLY:O	7:b:548:ARG:NH2	2.52	0.41
7:c:488:ILE:HG22	7:c:492:LEU:HG	2.01	0.41
7:d:43:ASP:O	7:d:47:THR:HG23	2.20	0.41
7:d:624:LEU:HD23	7:d:625:LYS:N	2.36	0.41
9:4A:346:LEU:HD13	9:4A:364:ILE:HG13	2.02	0.41
9:4F:126:GLU:C	9:4F:127:ILE:HD12	2.46	0.41
1:1B:100:ASN:HB2	1:1B:105:GLU:HB3	2.03	0.41
2:2C:267:MET:HE2	2:2C:267:MET:HB3	1.81	0.41
6:B:411:LEU:HB2	6:B:420:LEU:HD21	2.02	0.41
6:B:506:PRO:HA	6:B:509:PHE:HE1	1.85	0.41
6:C:245:ASP:OD1	6:C:275:LYS:HB3	2.20	0.41
6:D:181:ARG:NH2	6:D:215:ASP:OD2	2.54	0.41
6:D:329:ARG:HA	6:D:329:ARG:NH1	2.36	0.41
6:D:359:PHE:HE2	6:D:361:LEU:HD11	1.85	0.41
6:F:208:LEU:HD11	6:F:534:LEU:HD13	2.02	0.41
6:F:870:SER:OG	6:F:871:GLN:OE1	2.35	0.41
7:a:543:PHE:O	7:a:546:THR:OG1	2.30	0.41
7:a:703:GLN:O	7:a:703:GLN:NE2	2.53	0.41
7:b:416:LEU:HD12	7:b:422:LEU:HD12	2.01	0.41
7:b:568:LYS:HE2	7:b:568:LYS:HB3	1.79	0.41
8:3D:263:GLN:HA	8:3D:266:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:4B:187:LEU:HD21	9:4B:256:VAL:HG11	2.02	0.41
9:4C:184:TRP:CZ3	9:4C:242:ALA:HB2	2.55	0.41
9:4E:86:LEU:HD22	9:4E:121:ARG:HD2	2.01	0.41
9:4F:123:ASP:OD1	9:4F:124:GLN:N	2.53	0.41
2:2B:319:MET:HB3	2:2B:330:ILE:HD12	2.01	0.41
2:2E:267:MET:H	2:2E:267:MET:HG3	1.78	0.41
6:A:115:LEU:HA	7:a:91:PRO:HG3	2.01	0.41
6:C:282:LEU:HD23	6:C:282:LEU:HA	1.83	0.41
6:C:802:GLN:HB2	6:C:863:ASN:HB3	2.02	0.41
6:F:411:LEU:HB2	6:F:420:LEU:HD21	2.01	0.41
7:e:416:LEU:HD12	7:e:422:LEU:HD12	2.01	0.41
7:e:482:GLN:NE2	7:e:489:MET:SD	2.85	0.41
7:f:15:ILE:HG23	7:f:60:ALA:HB3	2.03	0.41
8:3A:263:GLN:HA	8:3A:266:VAL:HG22	2.02	0.41
8:3B:406:LEU:HD12	8:3B:406:LEU:HA	1.88	0.41
8:3F:183:LEU:O	8:3F:208:GLU:HG3	2.20	0.41
1:1A:104:THR:OG1	8:3E:415:ASN:OD1	2.37	0.41
2:2B:107:ALA:HB2	2:2B:112:ILE:HG12	2.02	0.41
3:5B:146:ARG:HH21	9:4B:325:ARG:HD2	1.86	0.41
5:9A:87:LEU:HD21	5:9A:100:LYS:HD3	2.03	0.41
6:B:88:PHE:HE1	7:b:52:CYS:HB3	1.86	0.41
6:B:531:ASN:HD22	6:B:619:THR:HA	1.86	0.41
6:B:541:VAL:HG21	6:B:547:LEU:HD11	2.03	0.41
6:E:412:VAL:HG22	6:E:417:ARG:HG2	2.03	0.41
7:a:615:PHE:CD1	7:a:615:PHE:N	2.87	0.41
7:b:529:THR:OG1	7:b:530:HIS:N	2.53	0.41
7:c:592:LYS:O	7:c:593:LEU:HD13	2.20	0.41
7:d:36:TRP:NE1	7:d:43:ASP:OD2	2.53	0.41
7:d:615:PHE:CD1	7:d:615:PHE:N	2.88	0.41
7:e:711:LEU:C	7:e:712:TYR:HD2	2.28	0.41
7:f:703:GLN:O	7:f:703:GLN:NE2	2.52	0.41
8:3B:329:MET:HB3	8:3B:334:ILE:HB	2.03	0.41
9:4C:235:PRO:HD3	9:4C:264:ILE:HG12	2.03	0.41
9:4E:59:LEU:HD12	9:4E:59:LEU:HA	1.92	0.41
9:4F:156:LEU:HB2	9:4F:182:VAL:HG22	2.01	0.41
1:1B:4:THR:HB	1:1B:7:GLN:HG3	2.03	0.41
2:2E:54:GLU:HG3	9:4A:353:ARG:NH2	2.35	0.41
5:9C:199:GLN:NE2	5:9C:204:PRO:O	2.37	0.41
5:9F:85:ASN:C	5:9F:86:ILE:HD12	2.46	0.41
6:A:506:PRO:HA	6:A:509:PHE:HE1	1.86	0.41
6:A:706:ARG:HG3	7:a:97:CYS:SG	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:792:PRO:HG2	6:C:794:TYR:CZ	2.56	0.41
6:E:803:LEU:HD12	6:E:803:LEU:HA	1.87	0.41
6:F:506:PRO:HA	6:F:509:PHE:HE1	1.86	0.41
7:a:142:TYR:OH	7:a:608:PRO:O	2.31	0.41
1:1A:62:ILE:HG12	1:1A:144:VAL:HG23	2.02	0.41
2:2B:186:THR:HG23	3:5C:26:LEU:HD11	2.02	0.41
2:2E:42:SER:O	2:2E:44:LYS:NZ	2.44	0.41
2:2E:186:THR:HG23	3:5F:26:LEU:HD11	2.02	0.41
2:2E:263:ILE:O	2:2E:267:MET:HG3	2.21	0.41
3:5D:90:LYS:HB3	3:5D:90:LYS:HE3	1.76	0.41
3:5E:34:SER:HB3	3:5E:67:HIS:HB2	2.02	0.41
3:5E:72:VAL:HG21	3:5E:134:LEU:HD23	2.02	0.41
3:5E:90:LYS:HB3	3:5E:90:LYS:HE3	1.77	0.41
3:5F:119:VAL:HG23	3:5F:139:GLU:HG2	2.03	0.41
5:9C:119:ASP:OD1	5:9C:119:ASP:N	2.54	0.41
5:9D:52:ILE:HD13	5:9D:52:ILE:HA	1.97	0.41
5:9F:37:LYS:HZ2	5:9F:37:LYS:C	2.29	0.41
6:A:181:ARG:NH2	6:A:215:ASP:OD2	2.54	0.41
6:B:272:ARG:HH22	6:B:275:LYS:HA	1.85	0.41
6:C:134:ASN:OD1	6:C:137:ASN:ND2	2.54	0.41
6:C:485:LYS:O	6:D:480:GLN:NE2	2.50	0.41
6:C:825:LYS:O	6:C:837:VAL:HG11	2.21	0.41
6:D:179:TRP:CD1	6:D:179:TRP:C	2.99	0.41
6:D:225:LYS:HG2	6:D:302:ILE:HD11	2.03	0.41
6:D:531:ASN:HD22	6:D:619:THR:HA	1.86	0.41
6:D:651:ASP:HA	6:D:654:ILE:HD12	2.02	0.41
6:D:803:LEU:HD21	6:D:858:VAL:HG22	2.03	0.41
6:E:197:ASP:OD1	6:E:198:ASN:N	2.53	0.41
6:E:245:ASP:OD1	6:E:275:LYS:HB3	2.21	0.41
6:E:426:GLN:NE2	6:E:441:THR:O	2.44	0.41
6:F:181:ARG:NH2	6:F:215:ASP:OD2	2.48	0.41
6:F:412:VAL:HG22	6:F:417:ARG:HG2	2.02	0.41
6:F:792:PRO:HG2	6:F:794:TYR:CZ	2.56	0.41
7:a:509:HIS:HB3	7:a:512:ASN:HB2	2.02	0.41
7:b:88:GLU:OE2	7:b:462:LYS:NZ	2.31	0.41
7:b:585:LYS:HA	7:b:585:LYS:HD3	1.92	0.41
7:b:624:LEU:HD23	7:b:625:LYS:N	2.36	0.41
7:c:173:ASN:OD1	7:c:604:ARG:NH2	2.52	0.41
7:d:206:GLY:HA2	7:d:604:ARG:HD2	2.03	0.41
7:e:251:LEU:HD12	7:e:251:LEU:HA	1.93	0.41
7:e:529:THR:OG1	7:e:530:HIS:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:f:416:LEU:HD12	7:f:422:LEU:HD12	2.03	0.41
8:3A:305:ALA:HA	8:3A:306:PRO:HD3	1.94	0.41
8:3C:42:ASN:OD1	8:3C:42:ASN:N	2.53	0.41
8:3C:165:LEU:HD23	8:3C:193:PHE:HB3	2.02	0.41
8:3F:329:MET:HB3	8:3F:334:ILE:HB	2.02	0.41
9:4B:123:ASP:OD1	9:4B:124:GLN:N	2.54	0.41
9:4B:284:GLN:HG2	9:4B:285:THR:N	2.35	0.41
9:4C:60:MET:HE2	9:4C:60:MET:HB2	1.85	0.41
9:4C:126:GLU:C	9:4C:127:ILE:HD12	2.46	0.41
9:4C:195:THR:O	9:4C:195:THR:OG1	2.37	0.41
2:2E:344:ILE:HD13	9:4E:304:VAL:HG22	2.03	0.41
4:7F:167:LEU:HD23	4:7F:167:LEU:HA	1.91	0.41
6:A:136:ASP:OD2	6:A:136:ASP:C	2.64	0.41
6:A:314:MET:N	6:A:314:MET:SD	2.94	0.41
6:B:245:ASP:OD1	6:B:275:LYS:HB3	2.21	0.41
6:C:136:ASP:OD2	6:C:136:ASP:C	2.64	0.41
6:C:243:GLU:OE2	6:C:317:LYS:NZ	2.42	0.41
6:D:132:THR:OG1	6:D:674:SER:O	2.36	0.41
6:D:245:ASP:OD1	6:D:275:LYS:HB3	2.21	0.41
6:D:745:GLN:HE22	6:D:790:ASN:HB2	1.86	0.41
6:E:148:PHE:HA	6:E:665:PRO:HA	2.03	0.41
6:E:607:MET:HE3	6:E:607:MET:HB3	1.88	0.41
6:F:136:ASP:OD2	6:F:136:ASP:C	2.64	0.41
6:F:282:LEU:HD12	6:F:289:ILE:HD11	2.03	0.41
6:F:728:LYS:HB2	6:F:747:ILE:HB	2.02	0.41
7:a:568:LYS:HE2	7:a:568:LYS:HB3	1.80	0.41
7:b:711:LEU:HD22	7:b:711:LEU:HA	1.95	0.41
7:c:15:ILE:HG23	7:c:60:ALA:HB3	2.03	0.41
7:c:42:ASN:OD1	7:c:42:ASN:N	2.50	0.41
7:c:703:GLN:O	7:c:703:GLN:NE2	2.52	0.41
7:f:651:GLY:HA2	7:f:676:MET:SD	2.60	0.41
8:3C:183:LEU:O	8:3C:208:GLU:HG3	2.21	0.41
9:4A:86:LEU:HD22	9:4A:121:ARG:HD2	2.02	0.41
1:1B:117:PRO:HA	1:1B:139:LEU:HD23	2.03	0.40
2:2B:54:GLU:HG3	9:4B:353:ARG:NH2	2.35	0.40
5:9F:199:GLN:NE2	5:9F:204:PRO:O	2.37	0.40
6:A:521:ASN:HB2	6:A:524:GLU:CD	2.45	0.40
6:A:651:ASP:HA	6:A:654:ILE:HD12	2.03	0.40
6:B:579:VAL:HA	6:B:594:THR:HG22	2.03	0.40
6:C:309:THR:OG1	6:C:310:THR:N	2.54	0.40
6:E:253:LEU:HD21	6:E:315:LEU:HD21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:272:ARG:HH22	6:E:275:LYS:HA	1.85	0.40
6:F:383:LEU:HD13	6:F:435:PRO:HG2	2.02	0.40
7:a:454:LEU:HD21	7:a:467:THR:HG23	2.03	0.40
7:c:138:GLU:OE2	7:c:141:ARG:NH2	2.54	0.40
7:d:629:VAL:HG23	7:d:632:SER:HB3	2.02	0.40
7:e:834:VAL:O	7:e:871:MET:HA	2.21	0.40
8:3A:379:MET:HE2	8:3A:379:MET:HA	2.03	0.40
9:4A:235:PRO:HD3	9:4A:264:ILE:HG12	2.03	0.40
9:4C:194:ASN:O	9:4C:196:GLN:NE2	2.53	0.40
9:4E:156:LEU:HB2	9:4E:182:VAL:HG22	2.03	0.40
9:4E:184:TRP:CZ3	9:4E:242:ALA:HB2	2.55	0.40
1:1F:117:PRO:HA	1:1F:139:LEU:HD23	2.03	0.40
2:2B:50:SER:N	2:2B:54:GLU:OE1	2.40	0.40
5:9E:42:LYS:HD2	5:9E:42:LYS:HA	1.95	0.40
6:A:465:ARG:NE	6:A:467:GLU:OE2	2.49	0.40
6:B:870:SER:OG	6:B:871:GLN:OE1	2.36	0.40
6:C:312:LYS:HE2	6:C:312:LYS:HB2	1.86	0.40
6:C:842:ARG:NH2	6:C:844:ASP:OD1	2.55	0.40
6:D:283:SER:N	6:D:286:ASP:OD2	2.50	0.40
6:D:521:ASN:HB2	6:D:524:GLU:CD	2.45	0.40
6:D:607:MET:HE3	6:D:607:MET:HB3	1.89	0.40
6:E:493:ILE:HD13	6:E:493:ILE:HA	1.82	0.40
6:F:825:LYS:O	6:F:837:VAL:HG11	2.22	0.40
7:a:676:MET:CE	7:a:898:LEU:H	2.34	0.40
7:b:615:PHE:HZ	7:b:644:THR:HG22	1.87	0.40
7:c:723:MET:HE2	7:c:723:MET:HB2	1.88	0.40
7:f:529:THR:OG1	7:f:530:HIS:N	2.55	0.40
8:3A:115:ILE:HD12	8:3A:115:ILE:O	2.21	0.40
8:3F:36:PHE:CZ	8:3F:121:SER:HB2	2.56	0.40
9:4F:313:TRP:HB3	9:4F:346:LEU:HG	2.04	0.40
2:2A:260:GLU:HB3	8:3F:12:ILE:HD13	2.03	0.40
2:2E:41:ILE:HD12	2:2E:41:ILE:HA	1.94	0.40
3:5C:119:VAL:HG23	3:5C:139:GLU:HG2	2.04	0.40
3:5E:67:HIS:CD2	3:5E:139:GLU:HG3	2.56	0.40
4:7A:5:GLU:OE2	5:9E:168:SER:HB2	2.21	0.40
4:7D:118:GLU:CG	4:7E:93:LYS:HG2	2.51	0.40
6:A:179:TRP:CD1	6:A:179:TRP:C	2.99	0.40
6:B:136:ASP:OD2	6:B:136:ASP:C	2.63	0.40
6:B:148:PHE:HA	6:B:665:PRO:HA	2.03	0.40
6:B:253:LEU:HD21	6:B:315:LEU:HD21	2.03	0.40
6:D:17:THR:OG1	6:D:18:VAL:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:136:ASP:OD2	6:D:136:ASP:C	2.64	0.40
6:D:312:LYS:HE2	6:D:312:LYS:HB2	1.87	0.40
6:D:326:ASN:N	6:D:326:ASN:OD1	2.54	0.40
6:E:108:ASP:OD1	6:E:112:ARG:NH1	2.53	0.40
6:F:521:ASN:HB2	6:F:524:GLU:CD	2.46	0.40
7:f:349:TRP:CE3	7:f:357:ILE:HD11	2.57	0.40
2:2C:244:ASN:OD1	2:2C:245:ASP:N	2.54	0.40
6:A:225:LYS:HE2	6:A:512:TYR:HE2	1.87	0.40
6:C:401:SER:O	6:C:401:SER:OG	2.33	0.40
6:C:607:MET:HE3	6:C:607:MET:HB3	1.90	0.40
6:D:506:PRO:HA	6:D:509:PHE:HE1	1.86	0.40
6:E:17:THR:OG1	6:E:18:VAL:N	2.55	0.40
6:F:79:PRO:HA	6:F:80:PRO:HD3	1.95	0.40
6:F:115:LEU:HA	7:f:91:PRO:HG3	2.03	0.40
7:d:148:LYS:HE2	7:d:822:GLU:CD	2.47	0.40
5:9C:150:ILE:HG13	5:9C:151:MET:HG2	2.02	0.40
6:C:225:LYS:HG2	6:C:302:ILE:HD11	2.04	0.40
6:D:137:ASN:O	6:D:171:GLN:NE2	2.31	0.40
6:D:333:TYR:HB2	6:D:361:LEU:HD23	2.04	0.40
6:D:606:LEU:HD23	6:D:606:LEU:HA	1.91	0.40
6:F:134:ASN:OD1	6:F:137:ASN:ND2	2.54	0.40
6:F:271:ASN:HB2	6:F:273:THR:HG23	2.03	0.40
7:a:206:GLY:HA2	7:a:604:ARG:HD2	2.03	0.40
7:a:822:GLU:OE2	7:a:823:LYS:NZ	2.43	0.40
7:c:832:PHE:HB3	7:c:869:LEU:HD23	2.04	0.40
9:4C:123:ASP:OD1	9:4C:124:GLN:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1A	146/149 (98%)	143 (98%)	3 (2%)	0	100	100
1	1B	146/149 (98%)	143 (98%)	3 (2%)	0	100	100
1	1C	146/149 (98%)	143 (98%)	3 (2%)	0	100	100
1	1D	146/149 (98%)	143 (98%)	3 (2%)	0	100	100
1	1E	146/149 (98%)	143 (98%)	3 (2%)	0	100	100
1	1F	146/149 (98%)	143 (98%)	3 (2%)	0	100	100
2	2A	347/354 (98%)	342 (99%)	5 (1%)	0	100	100
2	2B	347/354 (98%)	342 (99%)	5 (1%)	0	100	100
2	2C	347/354 (98%)	341 (98%)	6 (2%)	0	100	100
2	2D	347/354 (98%)	342 (99%)	5 (1%)	0	100	100
2	2E	347/354 (98%)	342 (99%)	5 (1%)	0	100	100
2	2F	347/354 (98%)	341 (98%)	6 (2%)	0	100	100
3	5A	146/152 (96%)	141 (97%)	5 (3%)	0	100	100
3	5B	146/152 (96%)	142 (97%)	4 (3%)	0	100	100
3	5C	146/152 (96%)	140 (96%)	6 (4%)	0	100	100
3	5D	146/152 (96%)	141 (97%)	5 (3%)	0	100	100
3	5E	146/152 (96%)	141 (97%)	5 (3%)	0	100	100
3	5F	146/152 (96%)	140 (96%)	6 (4%)	0	100	100
4	7A	222/227 (98%)	220 (99%)	2 (1%)	0	100	100
4	7B	222/227 (98%)	219 (99%)	3 (1%)	0	100	100
4	7C	222/227 (98%)	220 (99%)	2 (1%)	0	100	100
4	7D	222/227 (98%)	220 (99%)	2 (1%)	0	100	100
4	7E	222/227 (98%)	220 (99%)	2 (1%)	0	100	100
4	7F	222/227 (98%)	220 (99%)	2 (1%)	0	100	100
5	9A	206/239 (86%)	204 (99%)	2 (1%)	0	100	100
5	9B	206/239 (86%)	203 (98%)	3 (2%)	0	100	100
5	9C	206/239 (86%)	203 (98%)	3 (2%)	0	100	100
5	9D	206/239 (86%)	204 (99%)	2 (1%)	0	100	100
5	9E	206/239 (86%)	203 (98%)	3 (2%)	0	100	100
5	9F	206/239 (86%)	203 (98%)	3 (2%)	0	100	100
6	A	883/905 (98%)	856 (97%)	27 (3%)	0	100	100
6	B	883/905 (98%)	853 (97%)	30 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	C	883/905 (98%)	855 (97%)	28 (3%)	0	100	100
6	D	883/905 (98%)	856 (97%)	27 (3%)	0	100	100
6	E	883/905 (98%)	853 (97%)	30 (3%)	0	100	100
6	F	883/905 (98%)	855 (97%)	28 (3%)	0	100	100
7	a	821/966 (85%)	806 (98%)	15 (2%)	0	100	100
7	b	821/966 (85%)	804 (98%)	17 (2%)	0	100	100
7	c	821/966 (85%)	806 (98%)	15 (2%)	0	100	100
7	d	821/966 (85%)	806 (98%)	15 (2%)	0	100	100
7	e	821/966 (85%)	805 (98%)	16 (2%)	0	100	100
7	f	821/966 (85%)	806 (98%)	15 (2%)	0	100	100
8	3A	43/466 (9%)	43 (100%)	0	0	100	100
8	3B	372/466 (80%)	370 (100%)	2 (0%)	0	100	100
8	3C	410/466 (88%)	405 (99%)	5 (1%)	0	100	100
8	3D	410/466 (88%)	406 (99%)	4 (1%)	0	100	100
8	3E	410/466 (88%)	406 (99%)	4 (1%)	0	100	100
8	3F	410/466 (88%)	405 (99%)	5 (1%)	0	100	100
9	4A	381/392 (97%)	377 (99%)	4 (1%)	0	100	100
9	4B	381/392 (97%)	377 (99%)	4 (1%)	0	100	100
9	4C	381/392 (97%)	376 (99%)	5 (1%)	0	100	100
9	4D	381/392 (97%)	377 (99%)	4 (1%)	0	100	100
9	4E	381/392 (97%)	376 (99%)	5 (1%)	0	100	100
9	4F	381/392 (97%)	375 (98%)	6 (2%)	0	100	100
All	All	20967/23100 (91%)	20546 (98%)	421 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	1A	128/129 (99%)	124 (97%)	4 (3%)	35	62
1	1B	128/129 (99%)	125 (98%)	3 (2%)	44	71
1	1C	128/129 (99%)	124 (97%)	4 (3%)	35	62
1	1D	128/129 (99%)	124 (97%)	4 (3%)	35	62
1	1E	128/129 (99%)	126 (98%)	2 (2%)	55	78
1	1F	128/129 (99%)	124 (97%)	4 (3%)	35	62
2	2A	294/298 (99%)	285 (97%)	9 (3%)	35	62
2	2B	294/298 (99%)	289 (98%)	5 (2%)	53	77
2	2C	294/298 (99%)	287 (98%)	7 (2%)	43	70
2	2D	294/298 (99%)	285 (97%)	9 (3%)	35	62
2	2E	294/298 (99%)	292 (99%)	2 (1%)	76	89
2	2F	294/298 (99%)	290 (99%)	4 (1%)	59	80
3	5A	130/134 (97%)	124 (95%)	6 (5%)	24	48
3	5B	130/134 (97%)	127 (98%)	3 (2%)	44	71
3	5C	130/134 (97%)	127 (98%)	3 (2%)	44	71
3	5D	130/134 (97%)	128 (98%)	2 (2%)	57	79
3	5E	130/134 (97%)	126 (97%)	4 (3%)	35	62
3	5F	130/134 (97%)	128 (98%)	2 (2%)	57	79
4	7A	192/194 (99%)	186 (97%)	6 (3%)	35	62
4	7B	192/194 (99%)	191 (100%)	1 (0%)	81	91
4	7C	192/194 (99%)	185 (96%)	7 (4%)	31	57
4	7D	192/194 (99%)	185 (96%)	7 (4%)	31	57
4	7E	192/194 (99%)	192 (100%)	0	100	100
4	7F	192/194 (99%)	185 (96%)	7 (4%)	31	57
5	9A	191/216 (88%)	189 (99%)	2 (1%)	68	84
5	9B	191/216 (88%)	186 (97%)	5 (3%)	40	68
5	9C	191/216 (88%)	188 (98%)	3 (2%)	55	78
5	9D	191/216 (88%)	187 (98%)	4 (2%)	47	73
5	9E	191/216 (88%)	186 (97%)	5 (3%)	40	68
5	9F	191/216 (88%)	189 (99%)	2 (1%)	68	84
6	A	782/797 (98%)	769 (98%)	13 (2%)	53	77
6	B	782/797 (98%)	770 (98%)	12 (2%)	57	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	C	782/797 (98%)	776 (99%)	6 (1%)	73	87
6	D	782/797 (98%)	771 (99%)	11 (1%)	59	80
6	E	782/797 (98%)	768 (98%)	14 (2%)	51	76
6	F	782/797 (98%)	771 (99%)	11 (1%)	59	80
7	a	744/864 (86%)	732 (98%)	12 (2%)	55	78
7	b	744/864 (86%)	734 (99%)	10 (1%)	61	81
7	c	744/864 (86%)	736 (99%)	8 (1%)	65	83
7	d	744/864 (86%)	731 (98%)	13 (2%)	53	77
7	e	744/864 (86%)	733 (98%)	11 (2%)	57	79
7	f	744/864 (86%)	734 (99%)	10 (1%)	61	81
8	3A	353/395 (89%)	346 (98%)	7 (2%)	48	74
8	3B	353/395 (89%)	344 (98%)	9 (2%)	42	69
8	3C	353/395 (89%)	350 (99%)	3 (1%)	73	87
8	3D	353/395 (89%)	348 (99%)	5 (1%)	59	80
8	3E	353/395 (89%)	347 (98%)	6 (2%)	53	77
8	3F	353/395 (89%)	348 (99%)	5 (1%)	59	80
9	4A	329/337 (98%)	327 (99%)	2 (1%)	78	90
9	4B	329/337 (98%)	328 (100%)	1 (0%)	86	94
9	4C	329/337 (98%)	328 (100%)	1 (0%)	86	94
9	4D	329/337 (98%)	327 (99%)	2 (1%)	78	90
9	4E	329/337 (98%)	327 (99%)	2 (1%)	78	90
9	4F	329/337 (98%)	329 (100%)	0	100	100
All	All	18858/20184 (93%)	18558 (98%)	300 (2%)	54	78

All (300) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1A	55	MET
1	1A	90	GLU
1	1A	99	THR
1	1A	119	SER
1	1B	64	ILE
1	1B	105	GLU
1	1B	124	SER

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Mol	Chain	Res	Type
1	1C	55	MET
1	1C	62	ILE
1	1C	64	ILE
1	1C	100	ASN
1	1D	55	MET
1	1D	62	ILE
1	1D	90	GLU
1	1D	119	SER
1	1E	64	ILE
1	1E	124	SER
1	1F	55	MET
1	1F	62	ILE
1	1F	64	ILE
1	1F	105	GLU
2	2A	3	THR
2	2A	27	THR
2	2A	146	ASP
2	2A	165	THR
2	2A	167	THR
2	2A	203	GLN
2	2A	267	MET
2	2A	331	ILE
2	2A	338	VAL
2	2B	40	LEU
2	2B	246	ASN
2	2B	267	MET
2	2B	331	ILE
2	2B	332	LYS
2	2C	68	THR
2	2C	167	THR
2	2C	203	GLN
2	2C	245	ASP
2	2C	319	MET
2	2C	331	ILE
2	2C	338	VAL
2	2D	3	THR
2	2D	27	THR
2	2D	68	THR
2	2D	146	ASP
2	2D	165	THR
2	2D	167	THR
2	2D	203	GLN

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Mol	Chain	Res	Type
2	2D	267	MET
2	2D	338	VAL
2	2E	40	LEU
2	2E	332	LYS
2	2F	3	THR
2	2F	167	THR
2	2F	203	GLN
2	2F	245	ASP
3	5A	46	SER
3	5A	60	LYS
3	5A	65	SER
3	5A	68	LEU
3	5A	87	ARG
3	5A	98	ILE
3	5B	46	SER
3	5B	65	SER
3	5B	112	THR
3	5C	46	SER
3	5C	68	LEU
3	5C	79	THR
3	5D	41	GLN
3	5D	68	LEU
3	5E	46	SER
3	5E	65	SER
3	5E	68	LEU
3	5E	112	THR
3	5F	68	LEU
3	5F	79	THR
4	7A	14	THR
4	7A	86	GLU
4	7A	101	SER
4	7A	126	ARG
4	7A	155	ASP
4	7A	168	LYS
4	7B	14	THR
4	7C	55	ARG
4	7C	86	GLU
4	7C	101	SER
4	7C	155	ASP
4	7C	180	MET
4	7C	193	SER
4	7C	220	THR

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Mol	Chain	Res	Type
4	7D	5	GLU
4	7D	14	THR
4	7D	86	GLU
4	7D	101	SER
4	7D	126	ARG
4	7D	155	ASP
4	7D	168	LYS
4	7F	5	GLU
4	7F	86	GLU
4	7F	101	SER
4	7F	155	ASP
4	7F	180	MET
4	7F	193	SER
4	7F	196	SER
5	9A	50	VAL
5	9A	94	ASP
5	9B	42	LYS
5	9B	44	ILE
5	9B	107	VAL
5	9B	123	THR
5	9B	125	ILE
5	9C	44	ILE
5	9C	107	VAL
5	9C	123	THR
5	9D	44	ILE
5	9D	61	MET
5	9D	107	VAL
5	9D	123	THR
5	9E	42	LYS
5	9E	52	ILE
5	9E	114	GLN
5	9E	123	THR
5	9E	125	ILE
5	9F	107	VAL
5	9F	123	THR
6	A	235	GLU
6	A	302	ILE
6	A	305	LEU
6	A	325	ILE
6	A	419	VAL
6	A	493	ILE
6	A	646	GLU

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Mol	Chain	Res	Type
6	A	722	VAL
6	A	735	LEU
6	A	736	THR
6	A	745	GLN
6	A	799	ILE
6	A	839	THR
6	B	64	LEU
6	B	108	ASP
6	B	235	GLU
6	B	287	ASP
6	B	302	ILE
6	B	325	ILE
6	B	510	THR
6	B	522	THR
6	B	534	LEU
6	B	670	VAL
6	B	799	ILE
6	B	807	THR
6	C	108	ASP
6	C	302	ILE
6	C	305	LEU
6	C	510	THR
6	C	799	ILE
6	C	839	THR
6	D	17	THR
6	D	231	MET
6	D	235	GLU
6	D	302	ILE
6	D	305	LEU
6	D	493	ILE
6	D	722	VAL
6	D	735	LEU
6	D	736	THR
6	D	799	ILE
6	D	839	THR
6	E	64	LEU
6	E	108	ASP
6	E	235	GLU
6	E	287	ASP
6	E	302	ILE
6	E	325	ILE
6	E	510	THR

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Mol	Chain	Res	Type
6	E	522	THR
6	E	534	LEU
6	E	553	LEU
6	E	651	ASP
6	E	670	VAL
6	E	736	THR
6	E	807	THR
6	F	108	ASP
6	F	235	GLU
6	F	282	LEU
6	F	302	ILE
6	F	305	LEU
6	F	510	THR
6	F	651	ASP
6	F	722	VAL
6	F	799	ILE
6	F	839	THR
6	F	859	GLU
7	a	42	ASN
7	a	166	LEU
7	a	209	VAL
7	a	271	GLU
7	a	386	ILE
7	a	412	VAL
7	a	506	ASP
7	a	582	LEU
7	a	700	ILE
7	a	711	LEU
7	a	724	ASP
7	a	846	ASP
7	b	42	ASN
7	b	169	THR
7	b	185	GLU
7	b	271	GLU
7	b	287	SER
7	b	536	LEU
7	b	700	ILE
7	b	724	ASP
7	b	838	ILE
7	b	871	MET
7	c	101	THR
7	c	235	LEU

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Mol	Chain	Res	Type
7	c	500	SER
7	c	506	ASP
7	c	649	LEU
7	c	724	ASP
7	c	846	ASP
7	c	880	ASP
7	d	42	ASN
7	d	166	LEU
7	d	209	VAL
7	d	271	GLU
7	d	386	ILE
7	d	412	VAL
7	d	506	ASP
7	d	582	LEU
7	d	700	ILE
7	d	711	LEU
7	d	724	ASP
7	d	846	ASP
7	d	858	LYS
7	e	169	THR
7	e	185	GLU
7	e	271	GLU
7	e	500	SER
7	e	506	ASP
7	e	536	LEU
7	e	560	GLN
7	e	700	ILE
7	e	724	ASP
7	e	838	ILE
7	e	871	MET
7	f	101	THR
7	f	235	LEU
7	f	500	SER
7	f	506	ASP
7	f	560	GLN
7	f	649	LEU
7	f	711	LEU
7	f	724	ASP
7	f	846	ASP
7	f	880	ASP
8	3A	18	LEU
8	3A	19	ASN

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Mol	Chain	Res	Type
8	3A	27	THR
8	3A	161	LEU
8	3A	267	GLN
8	3A	377	GLN
8	3A	427	LYS
8	3B	14	GLU
8	3B	18	LEU
8	3B	114	VAL
8	3B	161	LEU
8	3B	182	SER
8	3B	201	LYS
8	3B	211	SER
8	3B	225	LEU
8	3B	437	LYS
8	3C	14	GLU
8	3C	161	LEU
8	3C	326	GLN
8	3D	19	ASN
8	3D	27	THR
8	3D	115	ILE
8	3D	161	LEU
8	3D	377	GLN
8	3E	14	GLU
8	3E	114	VAL
8	3E	161	LEU
8	3E	182	SER
8	3E	225	LEU
8	3E	437	LYS
8	3F	14	GLU
8	3F	22	VAL
8	3F	161	LEU
8	3F	225	LEU
8	3F	326	GLN
9	4A	258	SER
9	4A	378	GLU
9	4B	60	MET
9	4C	381	LEU
9	4D	127	ILE
9	4D	378	GLU
9	4E	127	ILE
9	4E	378	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (208)

such sidechains are listed below:

Mol	Chain	Res	Type
1	1B	7	GLN
1	1B	39	HIS
1	1C	39	HIS
1	1D	39	HIS
1	1D	114	ASN
1	1E	7	GLN
1	1E	39	HIS
1	1E	85	GLN
1	1F	39	HIS
2	2A	215	GLN
2	2A	303	ASN
2	2A	312	GLN
2	2B	312	GLN
2	2C	312	GLN
2	2D	312	GLN
2	2E	312	GLN
2	2F	312	GLN
3	5A	44	GLN
3	5A	129	ASN
3	5B	21	ASN
3	5B	51	ASN
3	5B	62	GLN
3	5B	136	ASN
3	5C	129	ASN
3	5D	129	ASN
3	5E	21	ASN
3	5E	51	ASN
3	5F	129	ASN
4	7A	53	HIS
4	7A	88	GLN
4	7B	38	GLN
4	7B	59	HIS
4	7B	88	GLN
4	7C	53	HIS
4	7C	59	HIS
4	7C	133	ASN
4	7D	53	HIS
4	7E	59	HIS
4	7E	88	GLN
4	7F	53	HIS
4	7F	59	HIS
5	9A	3	ASN

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Mol	Chain	Res	Type
5	9B	66	HIS
5	9E	48	GLN
5	9E	66	HIS
5	9F	48	GLN
6	A	48	GLN
6	A	137	ASN
6	A	311	GLN
6	A	402	ASN
6	A	523	ASN
6	A	585	ASN
6	A	603	GLN
6	A	620	HIS
6	A	720	GLN
6	A	853	GLN
6	B	96	ASN
6	B	134	ASN
6	B	137	ASN
6	B	396	ASN
6	B	402	ASN
6	B	523	ASN
6	B	585	ASN
6	B	603	GLN
6	B	620	HIS
6	B	720	GLN
6	B	816	HIS
6	B	853	GLN
6	C	48	GLN
6	C	96	ASN
6	C	137	ASN
6	C	396	ASN
6	C	402	ASN
6	C	523	ASN
6	C	585	ASN
6	C	720	GLN
6	C	745	GLN
6	C	816	HIS
6	C	853	GLN
6	D	48	GLN
6	D	137	ASN
6	D	252	HIS
6	D	396	ASN
6	D	402	ASN

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Mol	Chain	Res	Type
6	D	523	ASN
6	D	585	ASN
6	D	603	GLN
6	D	720	GLN
6	D	745	GLN
6	D	853	GLN
6	E	96	ASN
6	E	134	ASN
6	E	137	ASN
6	E	396	ASN
6	E	402	ASN
6	E	523	ASN
6	E	585	ASN
6	E	603	GLN
6	E	720	GLN
6	E	745	GLN
6	E	816	HIS
6	E	853	GLN
6	F	48	GLN
6	F	96	ASN
6	F	137	ASN
6	F	396	ASN
6	F	402	ASN
6	F	523	ASN
6	F	552	GLN
6	F	585	ASN
6	F	720	GLN
6	F	745	GLN
6	F	853	GLN
7	a	314	GLN
7	a	327	ASN
7	a	435	HIS
7	a	619	GLN
7	a	642	ASN
7	a	647	GLN
7	b	23	GLN
7	b	314	GLN
7	b	327	ASN
7	b	435	HIS
7	b	619	GLN
7	b	635	GLN
7	b	642	ASN

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Mol	Chain	Res	Type
7	b	647	GLN
7	c	314	GLN
7	c	327	ASN
7	c	433	HIS
7	c	619	GLN
7	c	634	ASN
7	c	642	ASN
7	c	647	GLN
7	d	223	GLN
7	d	241	GLN
7	d	314	GLN
7	d	327	ASN
7	d	435	HIS
7	d	619	GLN
7	d	642	ASN
7	d	740	ASN
7	e	23	GLN
7	e	314	GLN
7	e	327	ASN
7	e	435	HIS
7	e	619	GLN
7	e	635	GLN
7	e	642	ASN
7	e	647	GLN
7	e	889	GLN
7	f	314	GLN
7	f	327	ASN
7	f	433	HIS
7	f	619	GLN
7	f	642	ASN
7	f	647	GLN
7	f	889	GLN
8	3A	23	ASN
8	3A	51	ASN
8	3A	61	ASN
8	3A	273	GLN
8	3A	438	GLN
8	3A	459	GLN
8	3B	23	ASN
8	3B	51	ASN
8	3B	61	ASN
8	3B	227	GLN

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Mol	Chain	Res	Type
8	3B	273	GLN
8	3B	438	GLN
8	3C	23	ASN
8	3C	51	ASN
8	3C	61	ASN
8	3C	232	GLN
8	3C	330	ASN
8	3C	342	HIS
8	3C	459	GLN
8	3C	462	GLN
8	3D	23	ASN
8	3D	51	ASN
8	3D	61	ASN
8	3D	273	GLN
8	3D	438	GLN
8	3E	23	ASN
8	3E	51	ASN
8	3E	61	ASN
8	3E	438	GLN
8	3F	23	ASN
8	3F	51	ASN
8	3F	61	ASN
8	3F	342	HIS
8	3F	438	GLN
8	3F	459	GLN
8	3F	462	GLN
9	4A	19	GLN
9	4B	19	GLN
9	4B	144	ASN
9	4B	276	HIS
9	4C	19	GLN
9	4C	274	ASN
9	4D	19	GLN
9	4D	45	HIS
9	4D	197	ASN
9	4E	19	GLN
9	4E	45	HIS
9	4F	19	GLN
9	4F	45	HIS
9	4F	274	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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

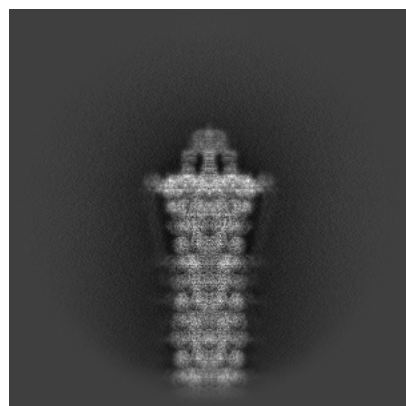
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53137. These allow visual inspection of the internal detail of the map and identification of artifacts.

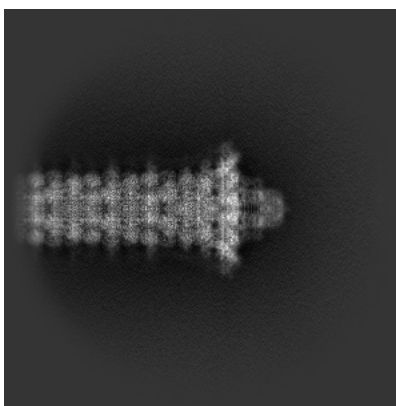
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

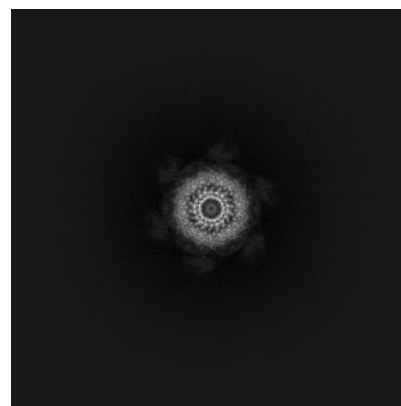
6.1.1 Primary map



X

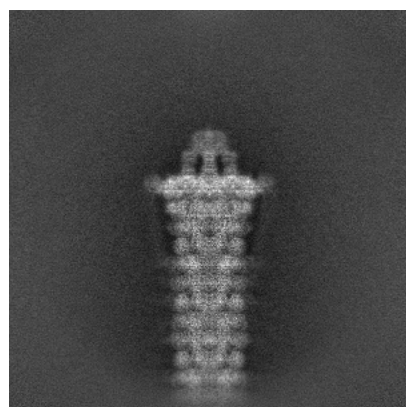


Y

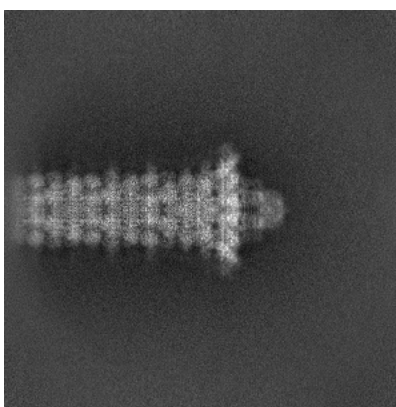


Z

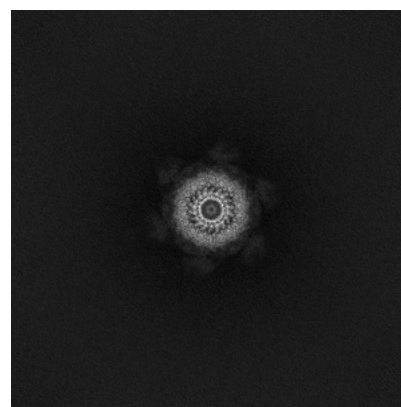
6.1.2 Raw map



X



Y

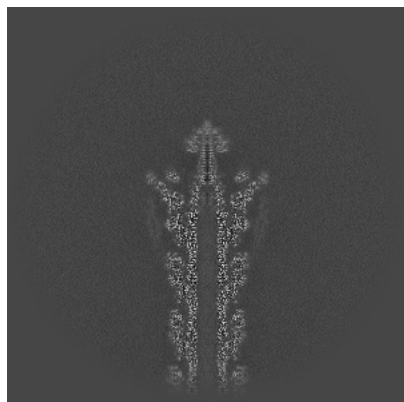


Z

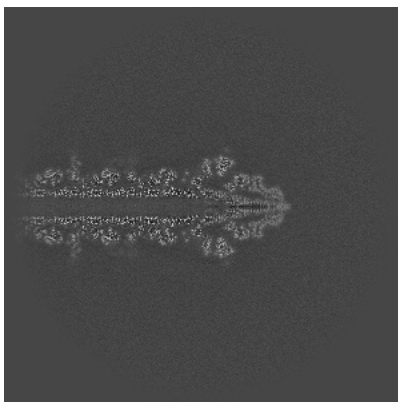
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

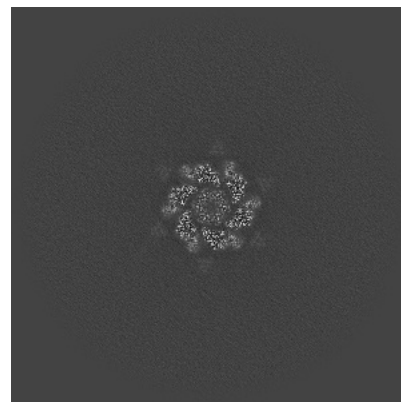
6.2.1 Primary map



X Index: 350

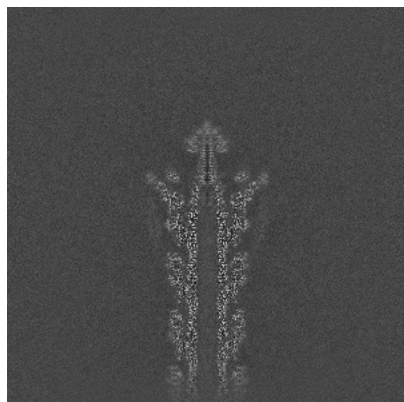


Y Index: 350

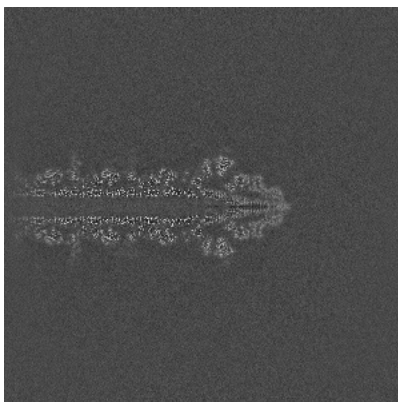


Z Index: 350

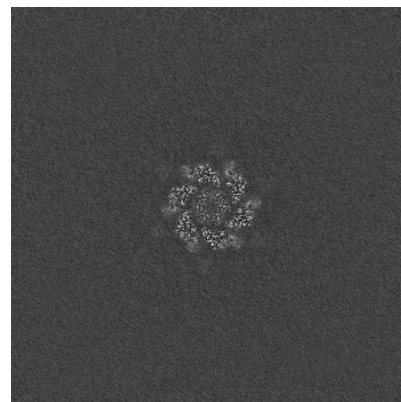
6.2.2 Raw map



X Index: 350



Y Index: 350

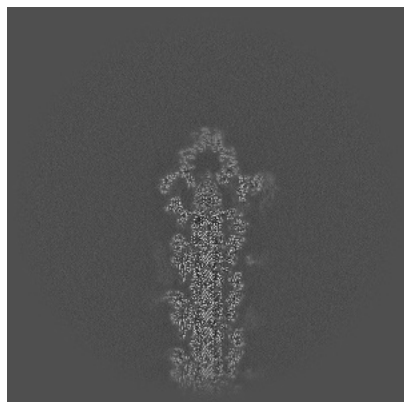


Z Index: 350

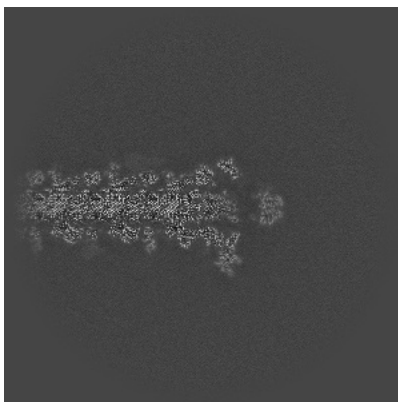
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

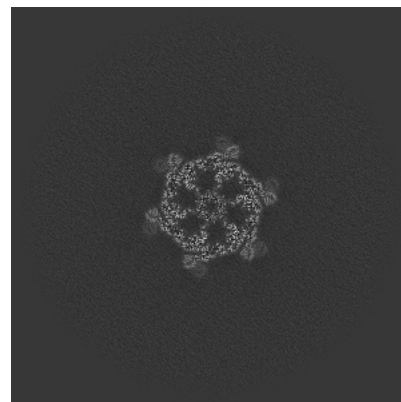
6.3.1 Primary map



X Index: 370

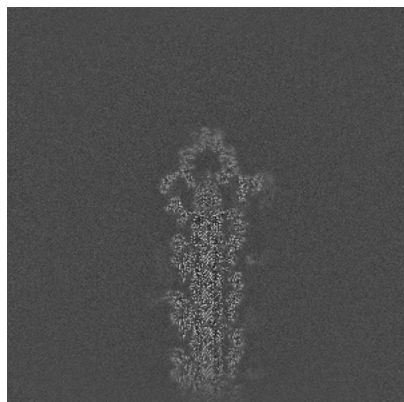


Y Index: 330

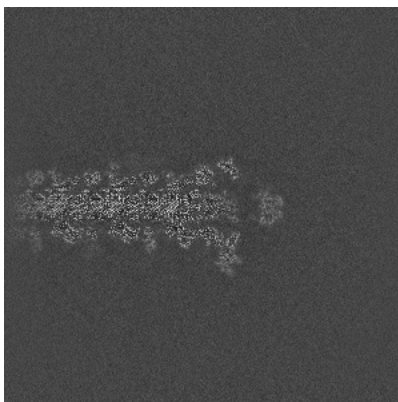


Z Index: 383

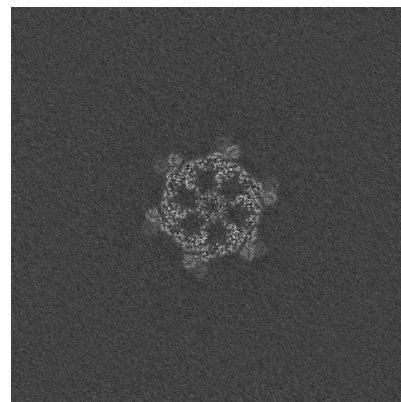
6.3.2 Raw map



X Index: 370



Y Index: 330

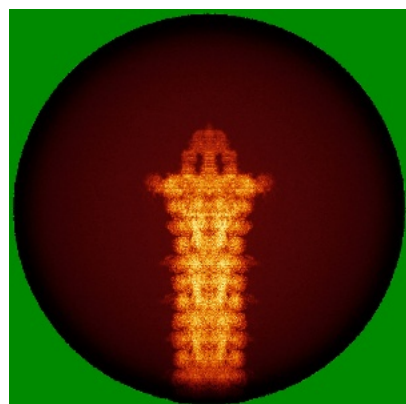


Z Index: 383

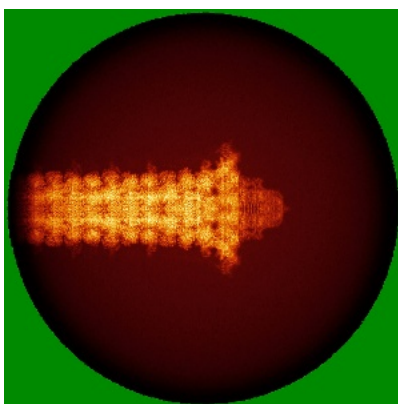
The images above show the largest variance slices of the map in three orthogonal directions.

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

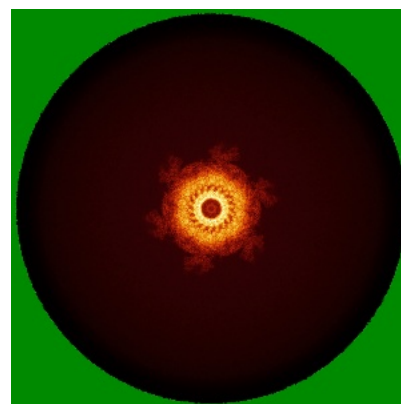
6.4.1 Primary map



X

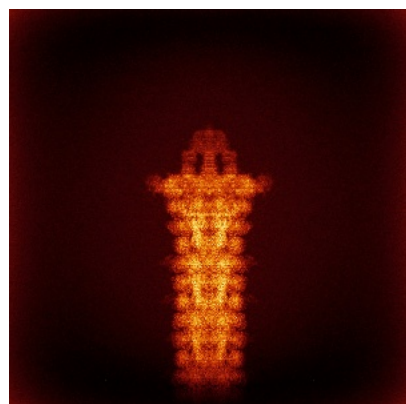


Y

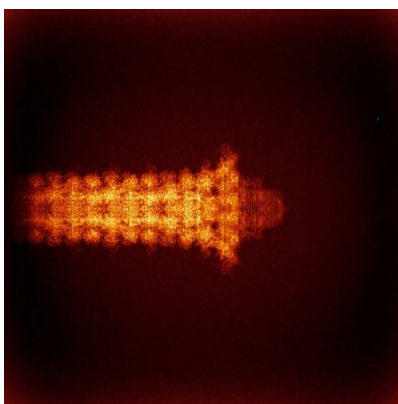


Z

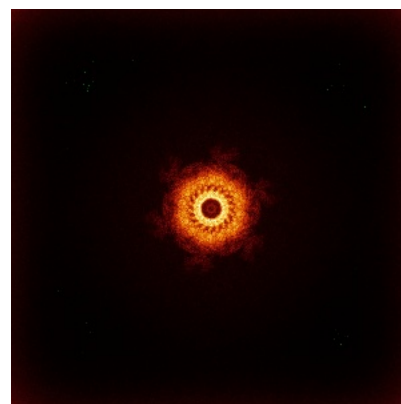
6.4.2 Raw map



X



Y

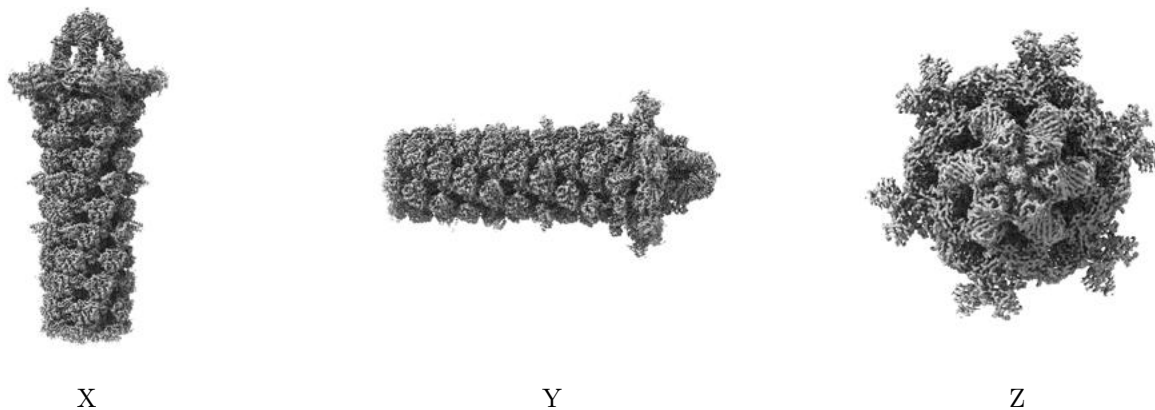


Z

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.

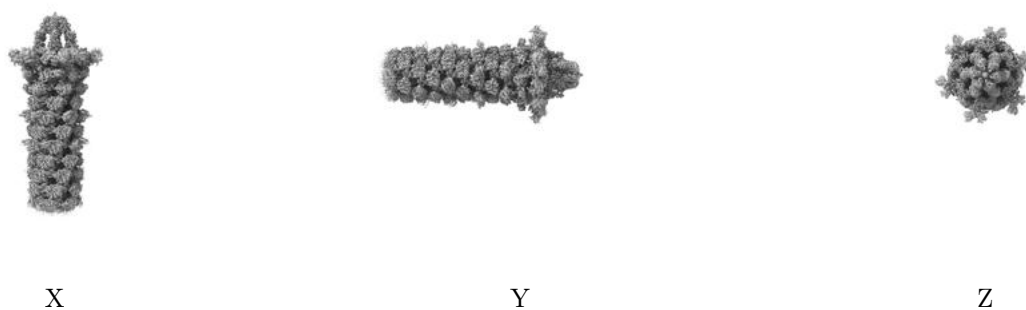
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.35. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

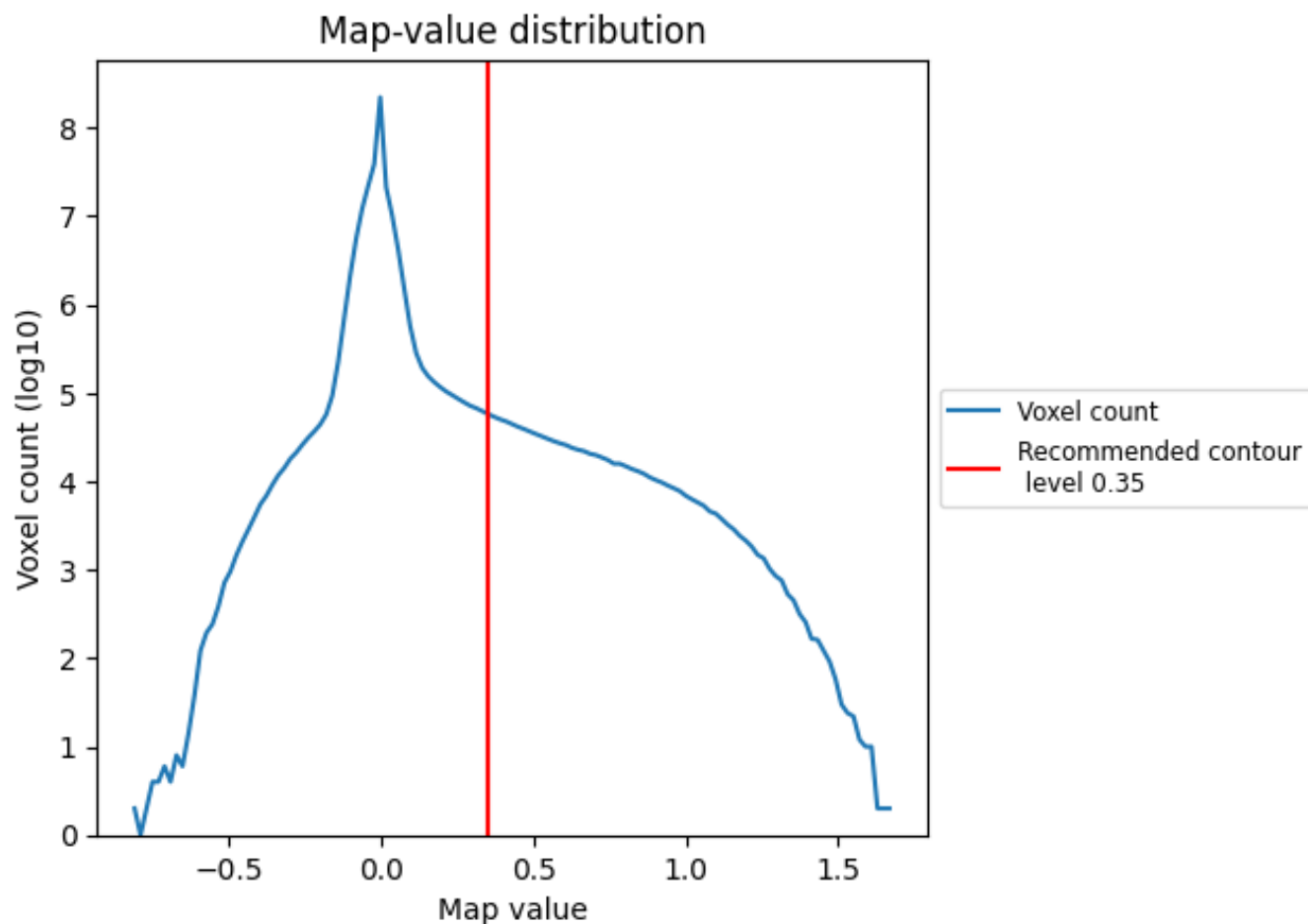
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

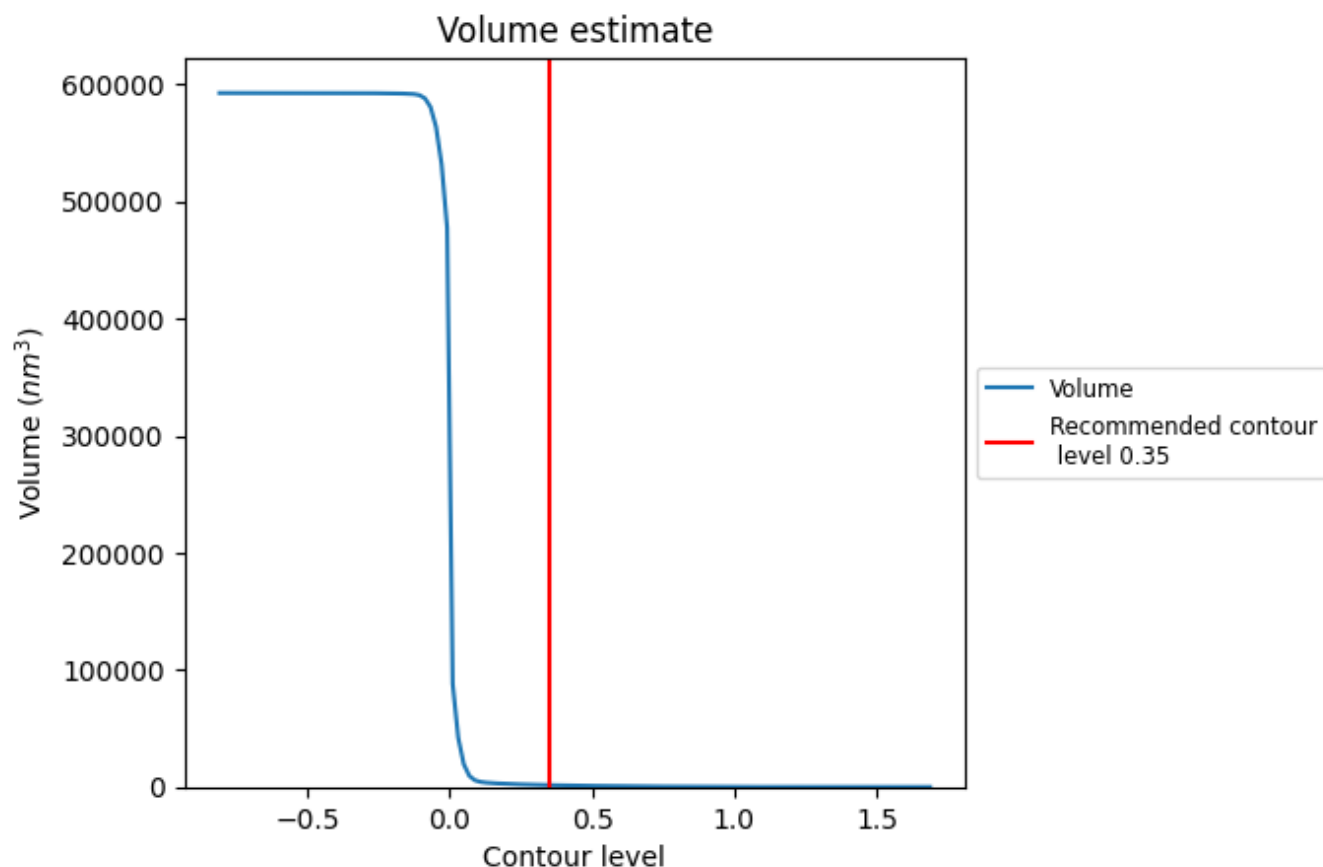
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

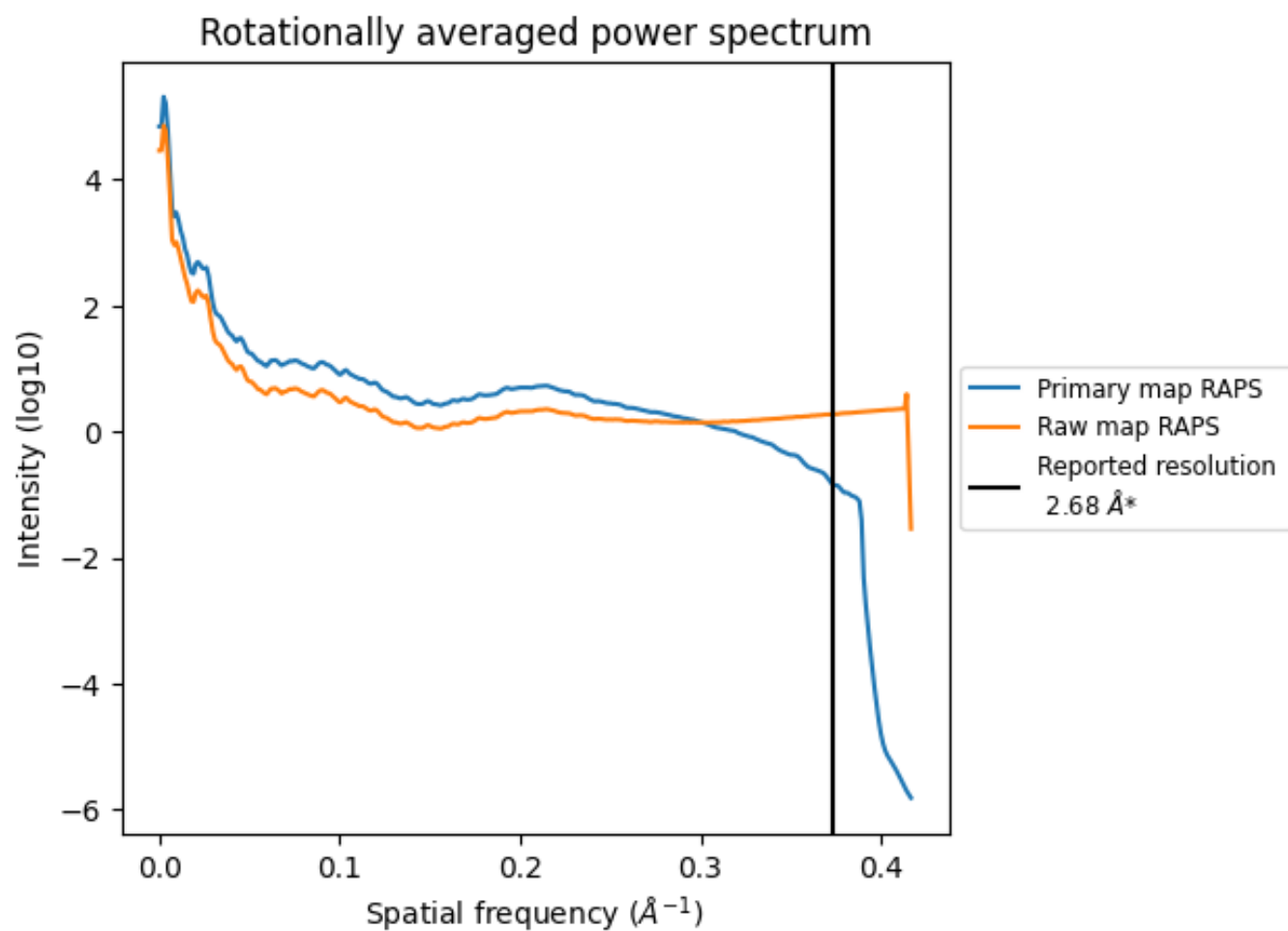
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1549 nm³; this corresponds to an approximate mass of 1399 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 ⓘ

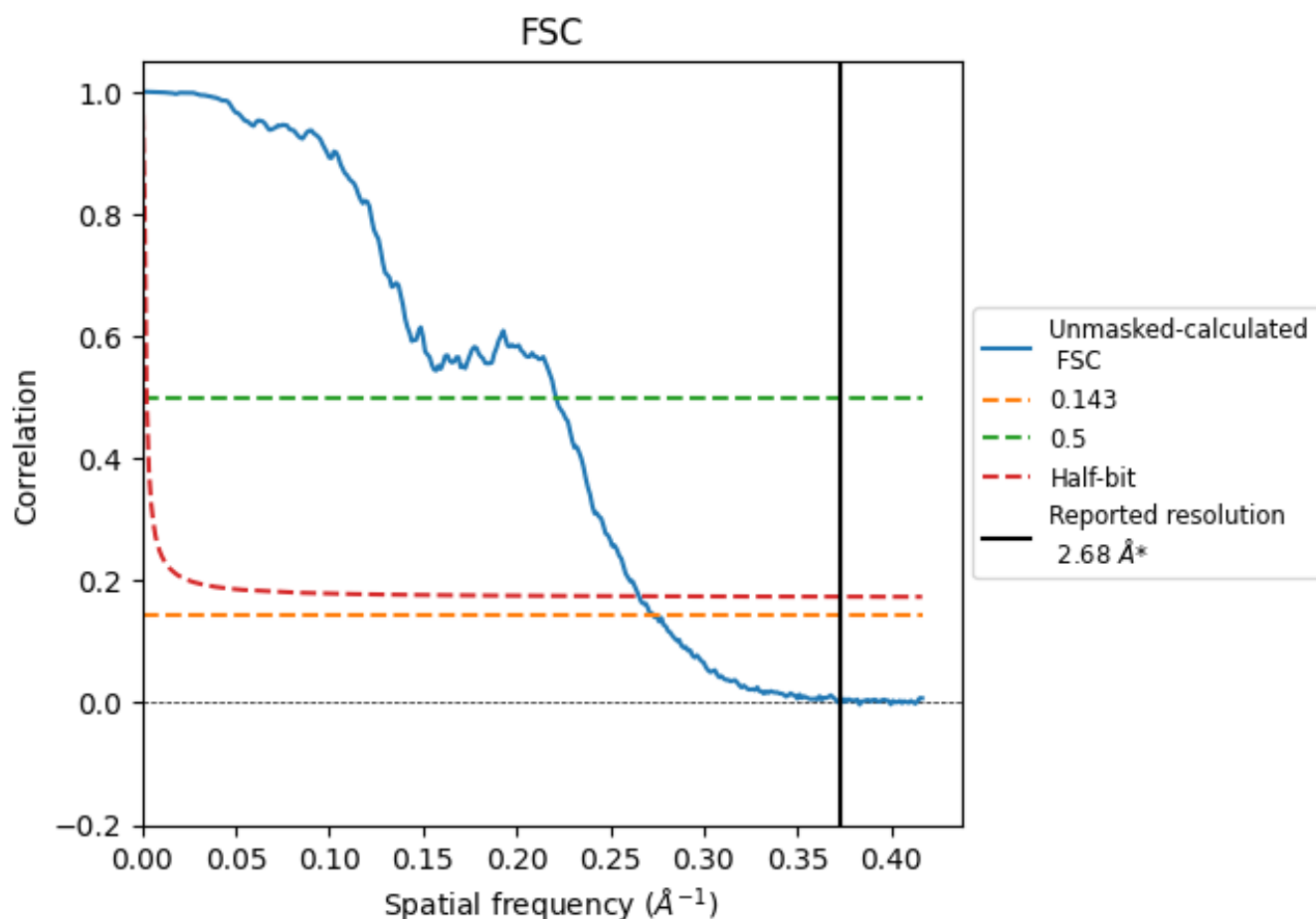


*Reported resolution corresponds to spatial frequency of 0.373 Å⁻¹

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 0.373 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

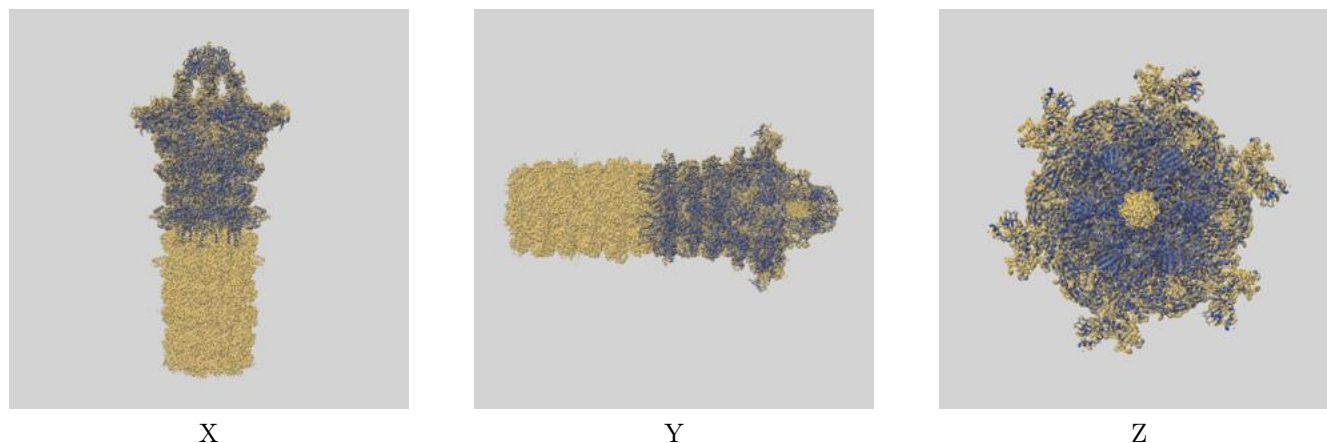
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.68	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.66	4.52	3.77

*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 3.66 differs from the reported value 2.68 by more than 10 %

9 Map-model fit [i](#)

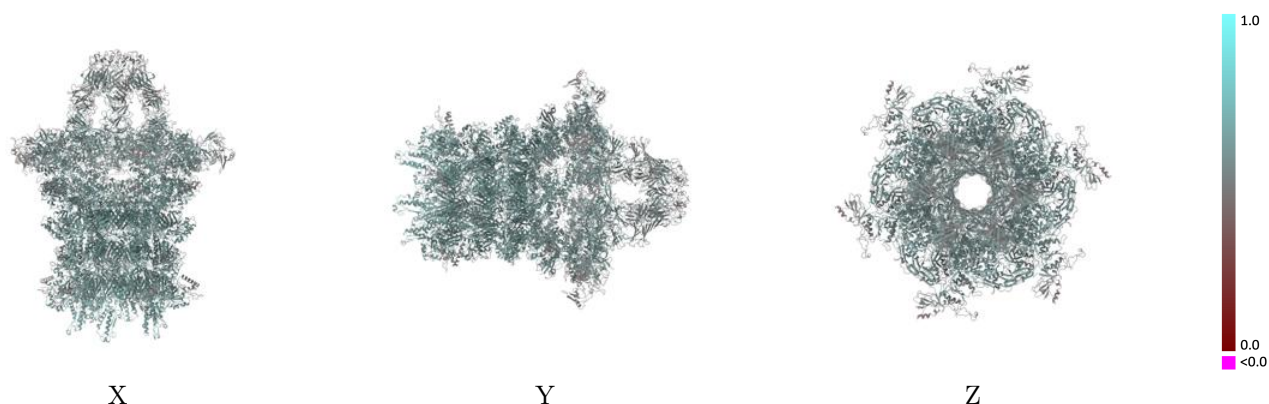
This section contains information regarding the fit between EMDB map EMD-53137 and PDB model 9QGL. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



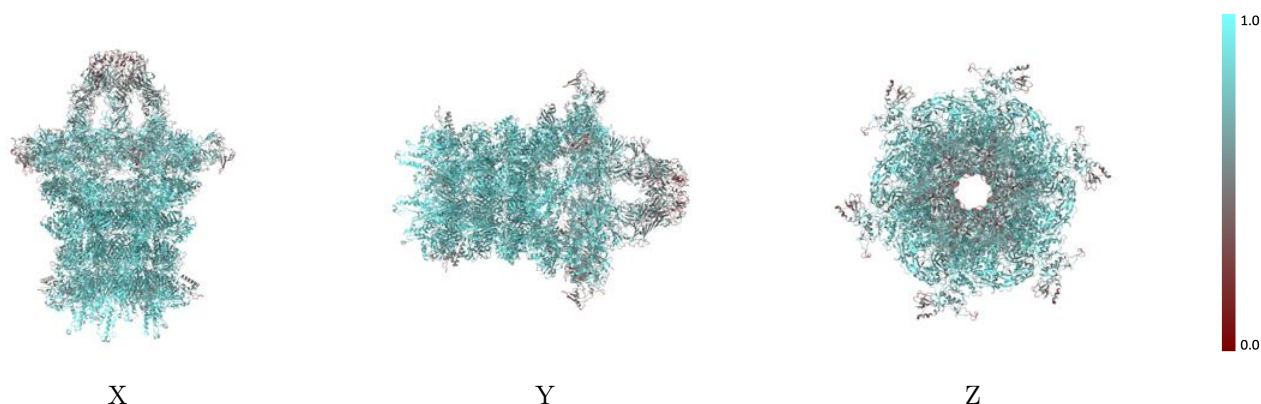
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



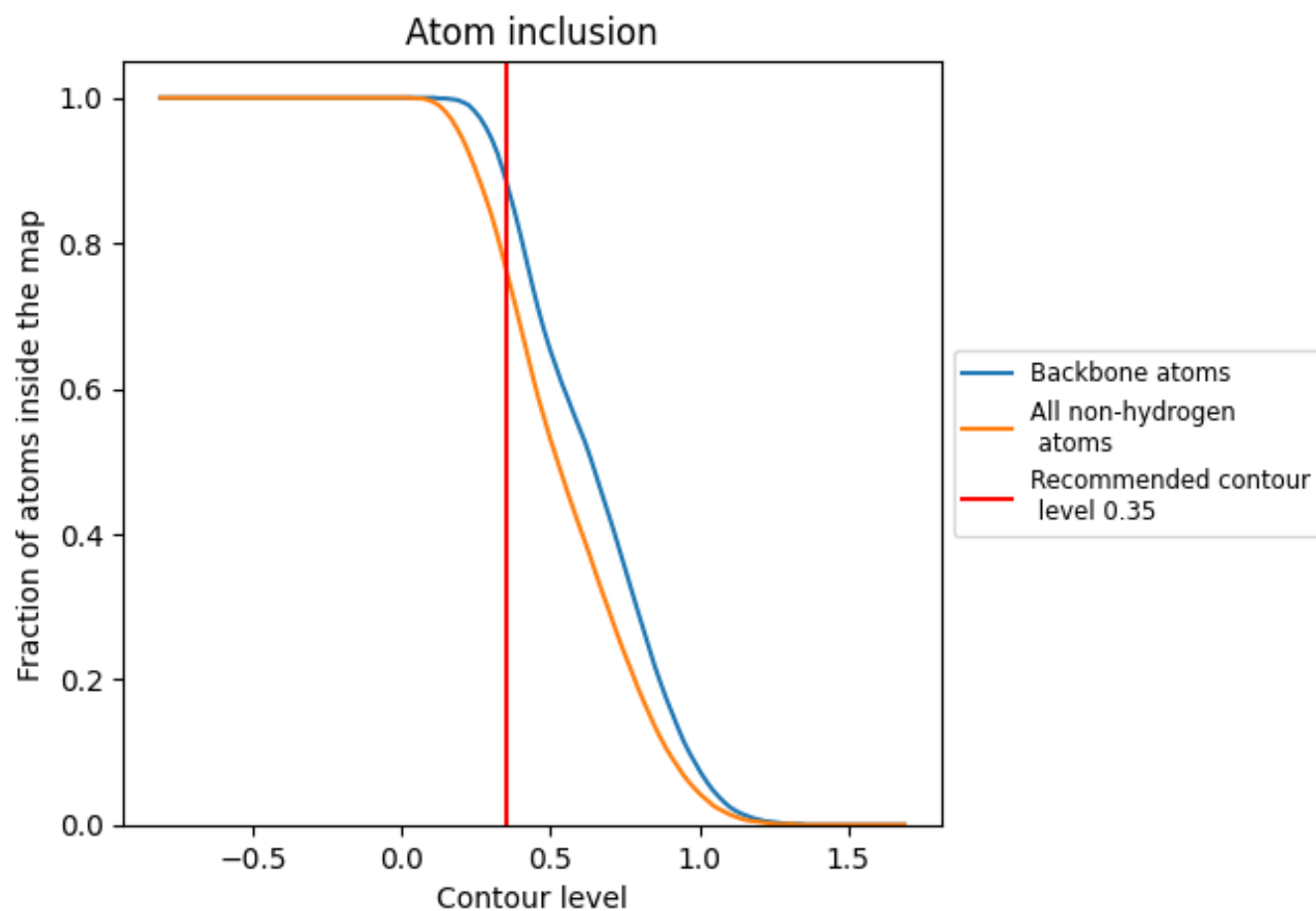
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.35).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 76% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7650	 0.5710
1A	 0.9030	 0.6260
1B	 0.8990	 0.6210
1C	 0.9040	 0.6230
1D	 0.9030	 0.6230
1E	 0.8970	 0.6250
1F	 0.9040	 0.6260
2A	 0.8130	 0.5850
2B	 0.8080	 0.5840
2C	 0.8100	 0.5840
2D	 0.8130	 0.5850
2E	 0.8110	 0.5840
2F	 0.8100	 0.5850
3A	 0.7790	 0.5820
3B	 0.7790	 0.5820
3C	 0.7770	 0.5810
3D	 0.7790	 0.5820
3E	 0.7780	 0.5810
3F	 0.7770	 0.5810
4A	 0.8500	 0.6000
4B	 0.8480	 0.6010
4C	 0.8430	 0.6000
4D	 0.8500	 0.6000
4E	 0.8490	 0.5990
4F	 0.8430	 0.6000
5A	 0.9170	 0.6280
5B	 0.9150	 0.6280
5C	 0.9110	 0.6290
5D	 0.9200	 0.6280
5E	 0.9100	 0.6260
5F	 0.9080	 0.6290
7A	 0.8950	 0.6200
7B	 0.8900	 0.6190
7C	 0.8910	 0.6200
7D	 0.8950	 0.6190



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Chain	Atom inclusion	Q-score
7E	 0.8900	 0.6190
7F	 0.8920	 0.6200
9A	 0.7690	 0.5650
9B	 0.7690	 0.5640
9C	 0.7760	 0.5640
9D	 0.7710	 0.5670
9E	 0.7720	 0.5660
9F	 0.7730	 0.5660
A	 0.6560	 0.5380
B	 0.6530	 0.5380
C	 0.6570	 0.5380
D	 0.6560	 0.5390
E	 0.6540	 0.5380
F	 0.6560	 0.5370
a	 0.7390	 0.5530
b	 0.7350	 0.5500
c	 0.7330	 0.5510
d	 0.7390	 0.5520
e	 0.7340	 0.5500
f	 0.7330	 0.5510