



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 06:09 PM UTC

PDB ID : 3J9R / pdb_00003j9r
EMDB ID : EMD-6271
Title : Atomic structures of a bactericidal contractile nanotube in its pre- and post-contraction states
Authors : Ge, P.; Scholl, D.; Leiman, P.G.; Yu, X.; Miller, J.F.; Zhou, Z.H.
Deposited on : 2015-02-17
Resolution : 3.90 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

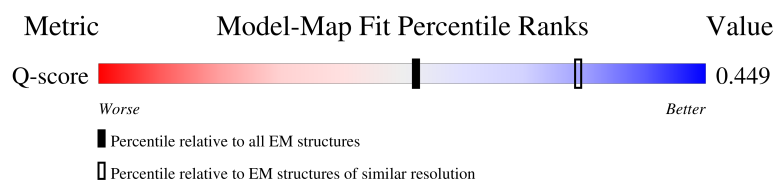
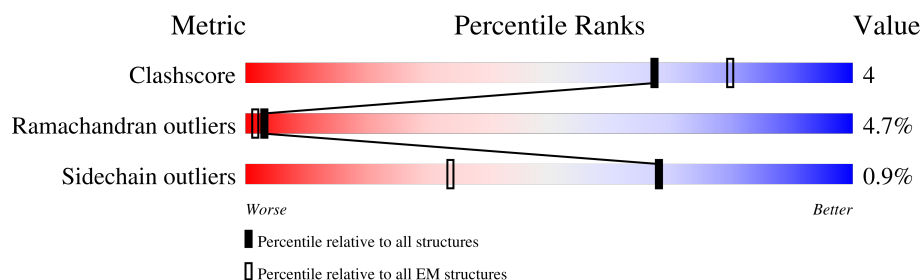
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.90 Å.

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



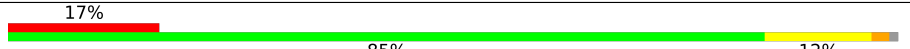
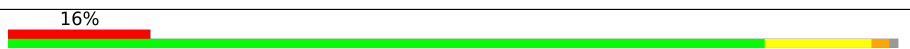
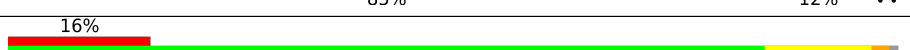
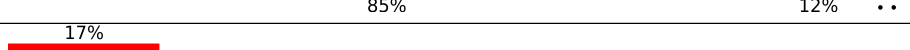
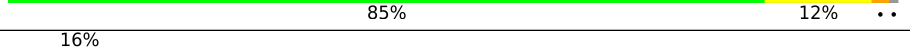
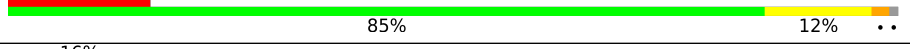
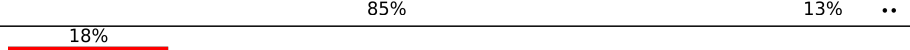
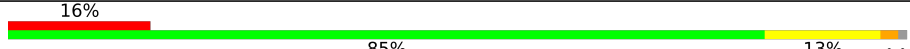
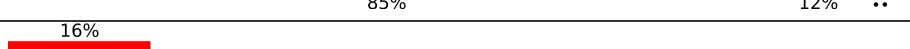
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8855 (3.40 - 4.40)

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

Mol	Chain	Length	Quality of chain
1	0	386	
1	1	386	
1	2	386	
1	3	386	

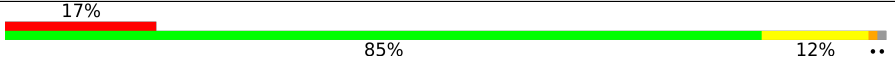
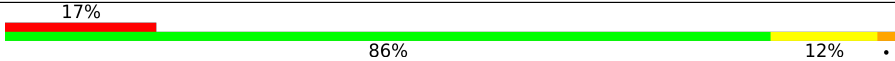
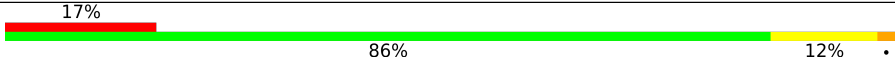
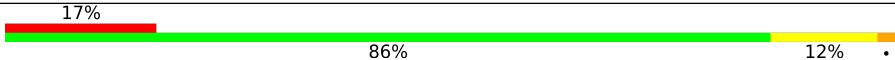
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Mol	Chain	Length	Quality of chain	
1	4	386	17% 	..
1	5	386	17% 	..
1	A	386	17% 	..
1	B	386	16% 	..
1	C	386	16% 	..
1	D	386	17% 	..
1	E	386	16% 	..
1	F	386	16% 	..
1	G	386	16% 	..
1	H	386	17% 	..
1	I	386	17% 	..
1	J	386	16% 	..
1	K	386	17% 	..
1	L	386	17% 	..
1	M	386	18% 	..
1	N	386	17% 	..
1	O	386	17% 	..
1	P	386	17% 	..
1	Q	386	17% 	..
1	R	386	16% 	..
1	a	386	17% 	..
1	b	386	17% 	..
1	c	386	16% 	..
1	d	386	16% 	..
1	e	386	17% 	..

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Mol	Chain	Length	Quality of chain
1	f	386	
1	g	386	
1	h	386	
1	i	386	
1	j	386	
1	k	386	
1	l	386	

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 103824 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 sheath.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	B	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	F	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	E	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	D	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	C	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	0	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	1	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	5	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	4	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	3	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	2	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	G	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	H	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	L	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	K	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	J	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		

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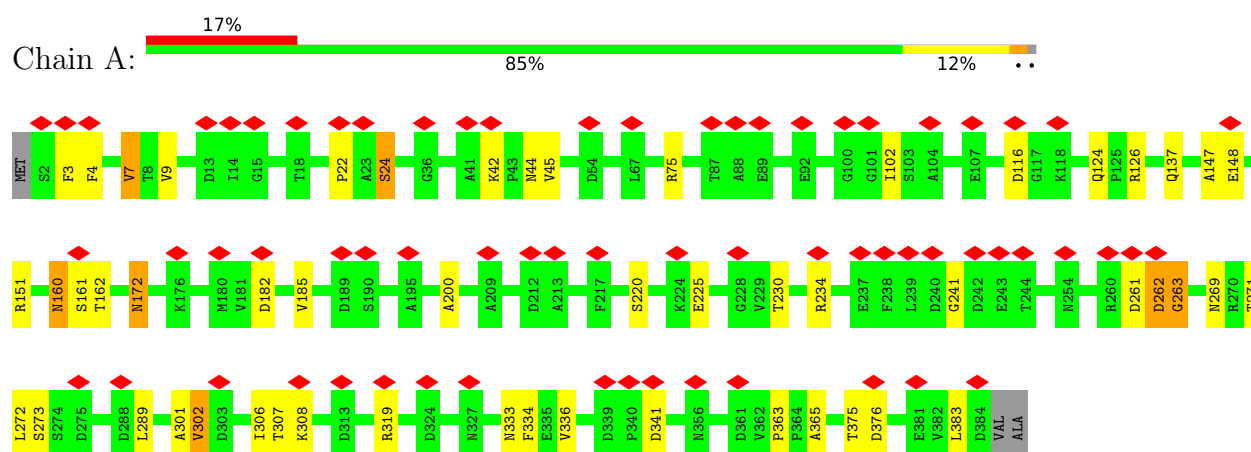
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Mol	Chain	Residues	Atoms					AltConf	Trace
1	I	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	M	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	N	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	R	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	Q	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	P	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	O	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	a	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	b	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	f	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	e	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	d	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	c	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	g	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	h	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	l	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	k	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	j	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		
1	i	383	Total	C	N	O	S	0	0
			2884	1817	504	555	8		

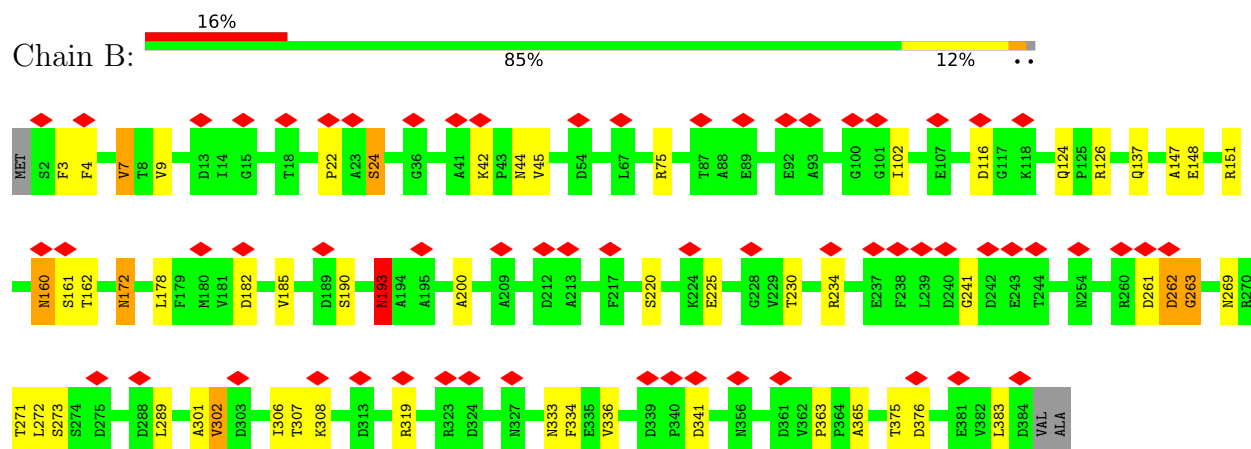
3 Residue-property plots [i](#)

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.

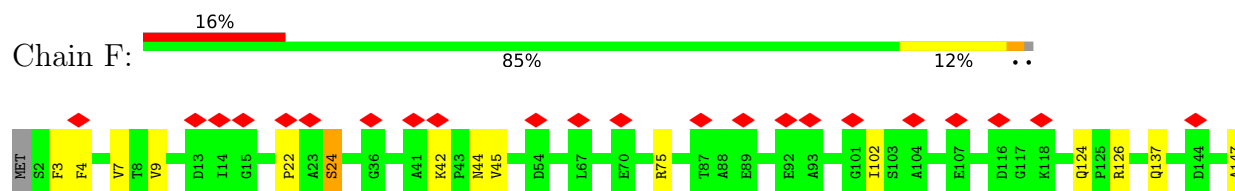
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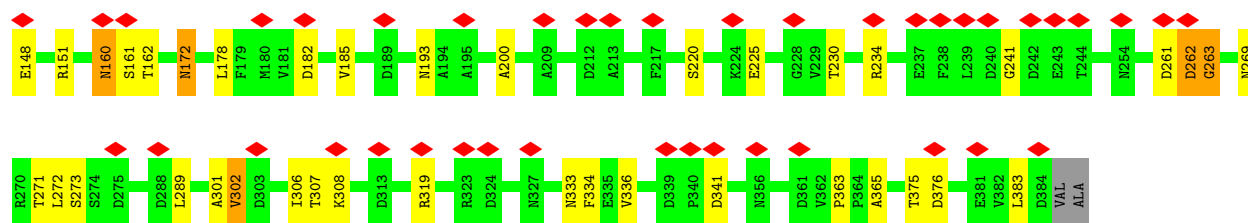


- Molecule 1: sheath

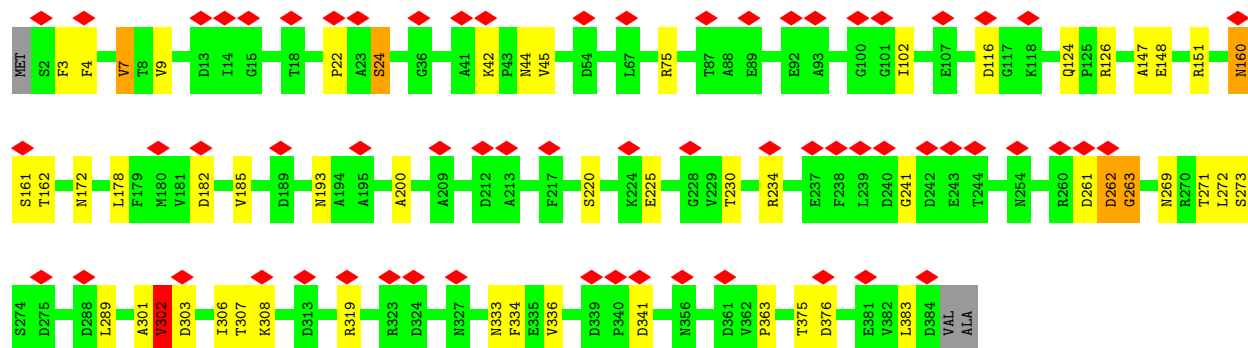
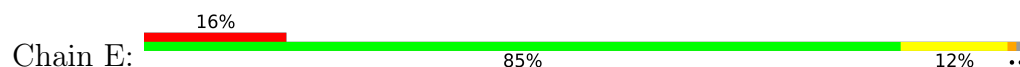


- Molecule 1: sheath

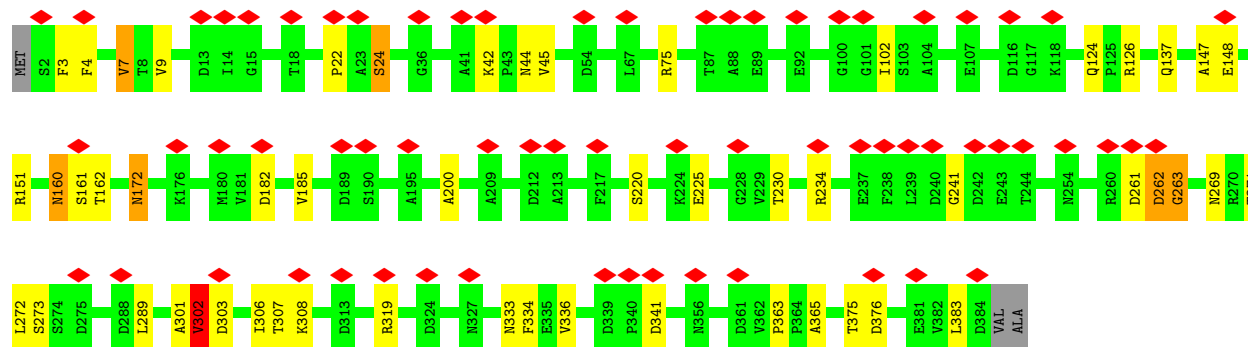
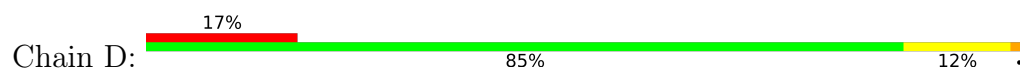




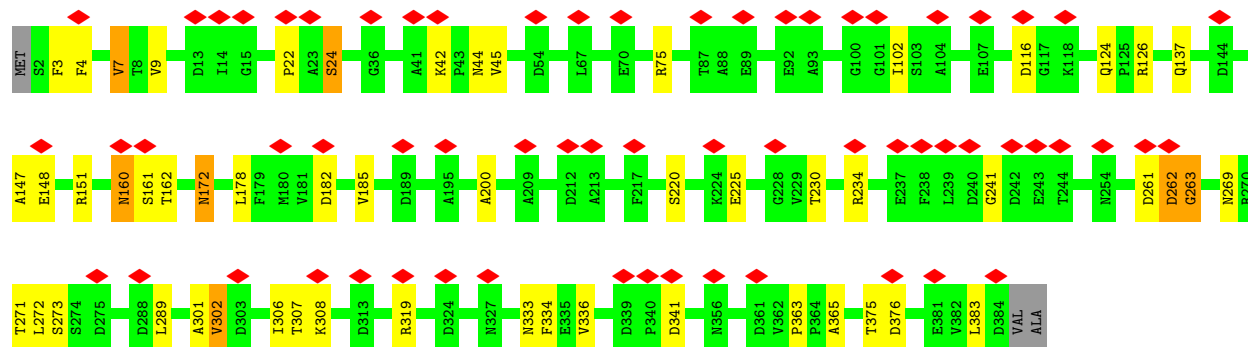
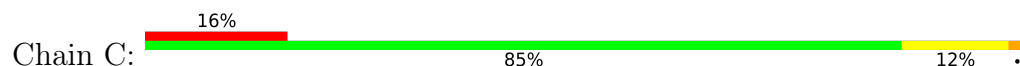
- Molecule 1: sheath



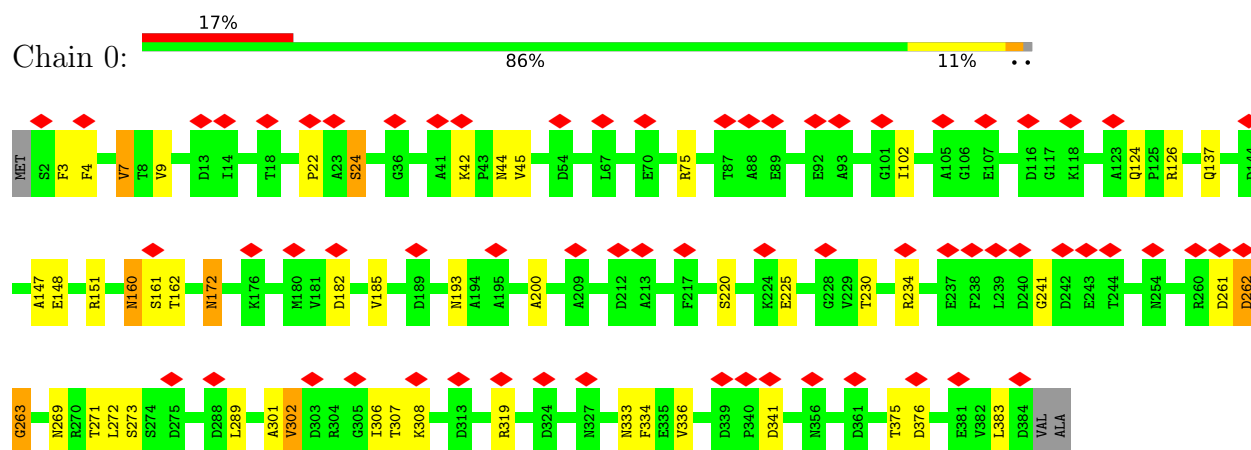
- Molecule 1: sheath



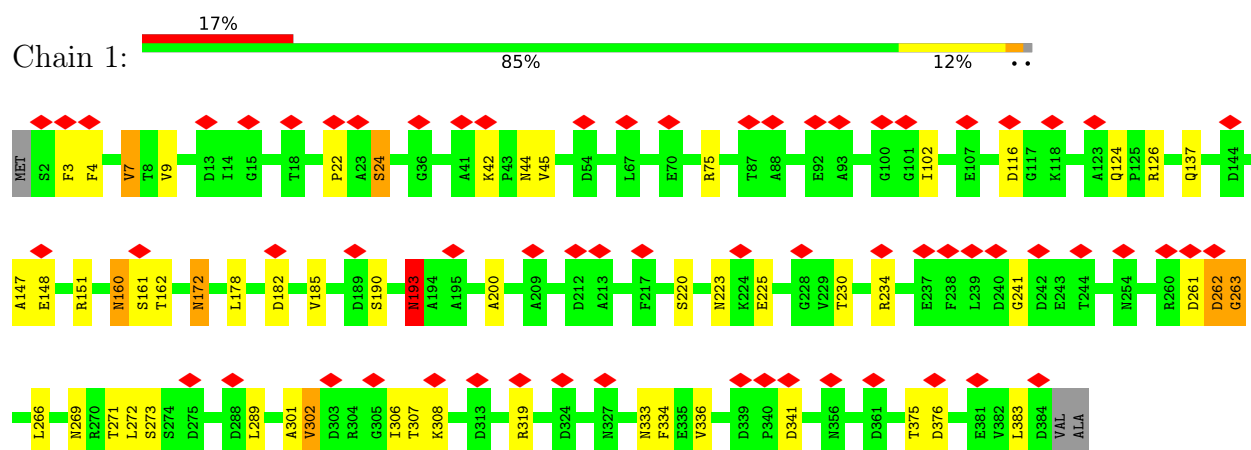
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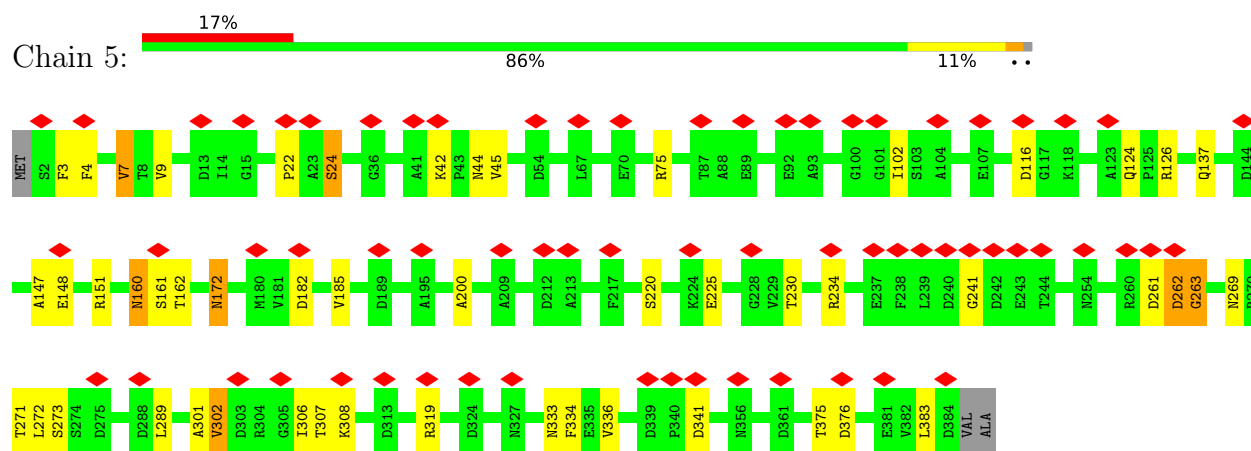
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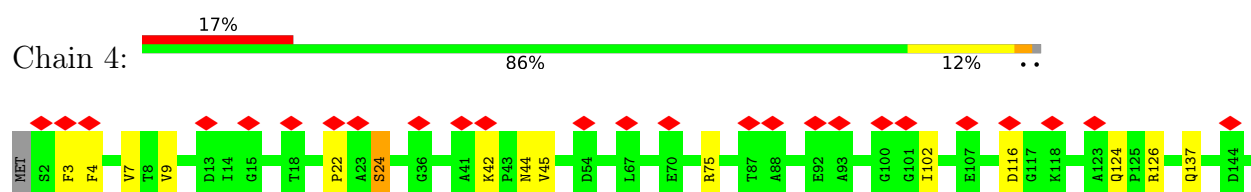
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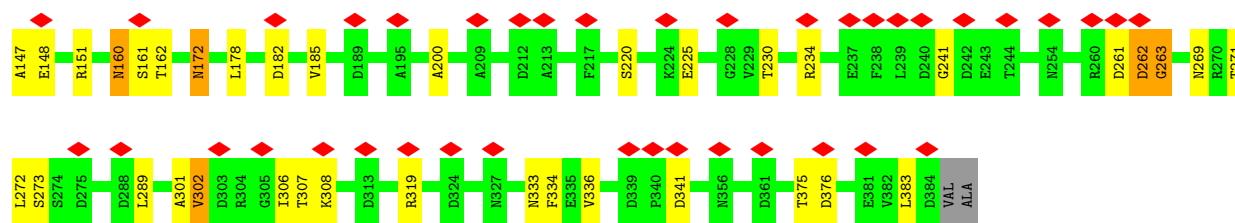


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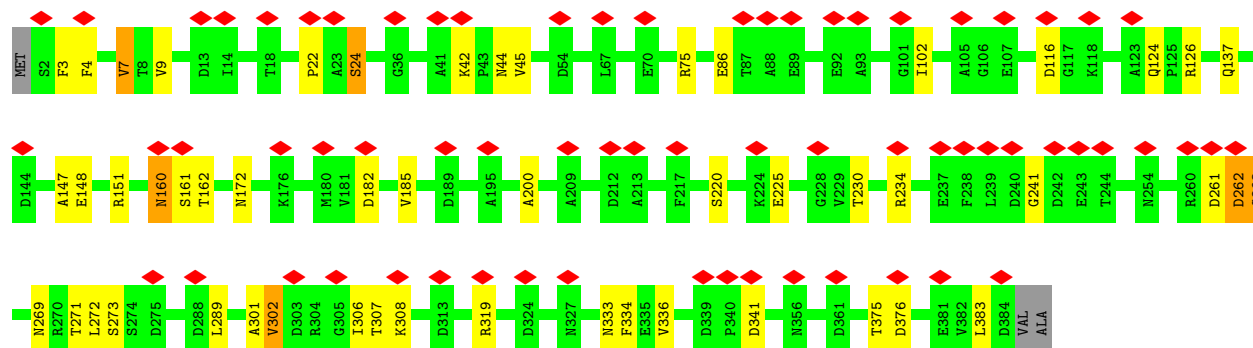
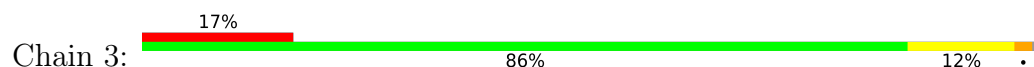


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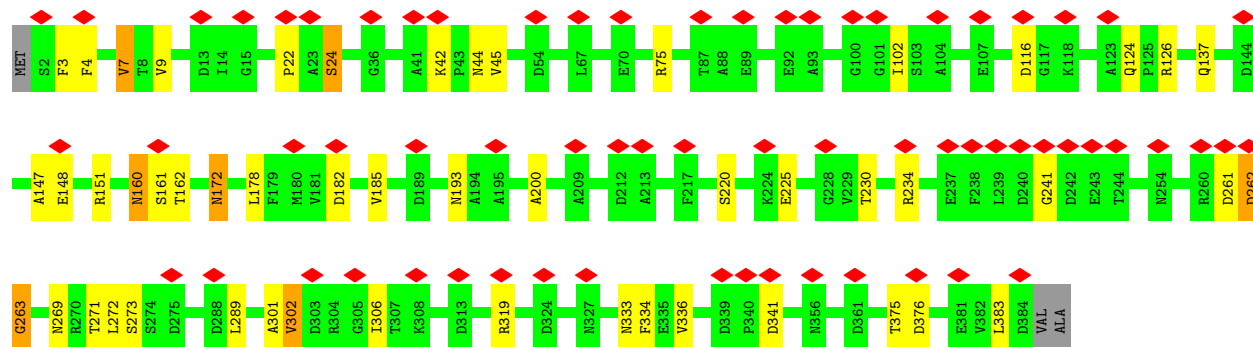
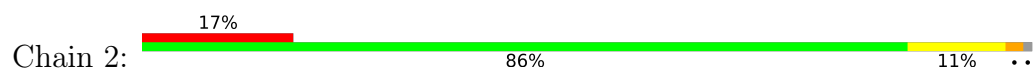




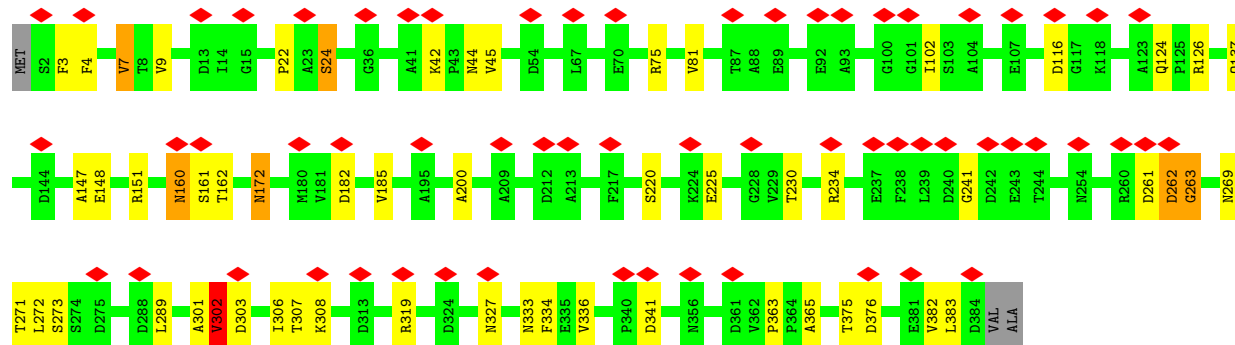
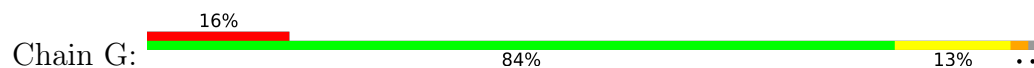
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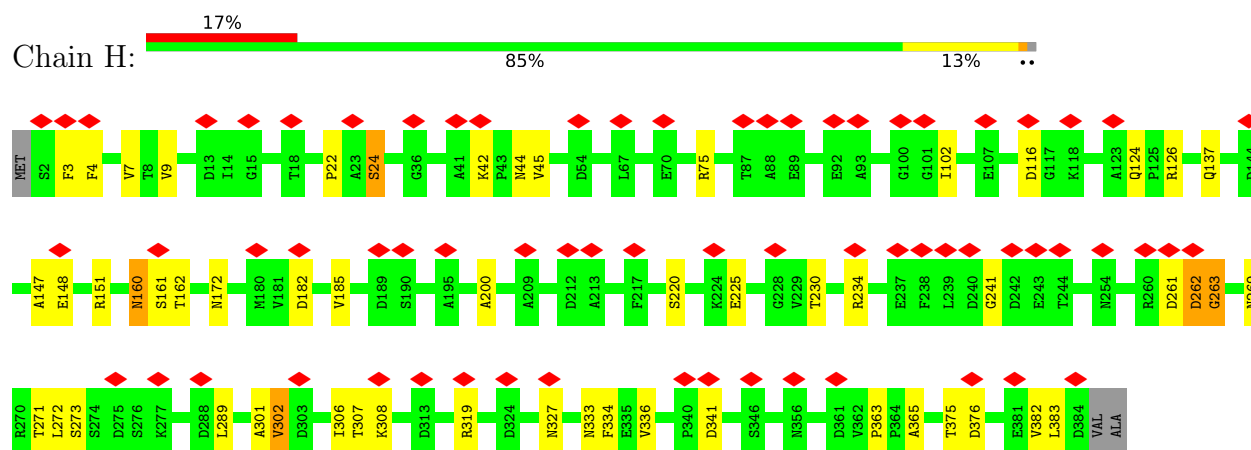
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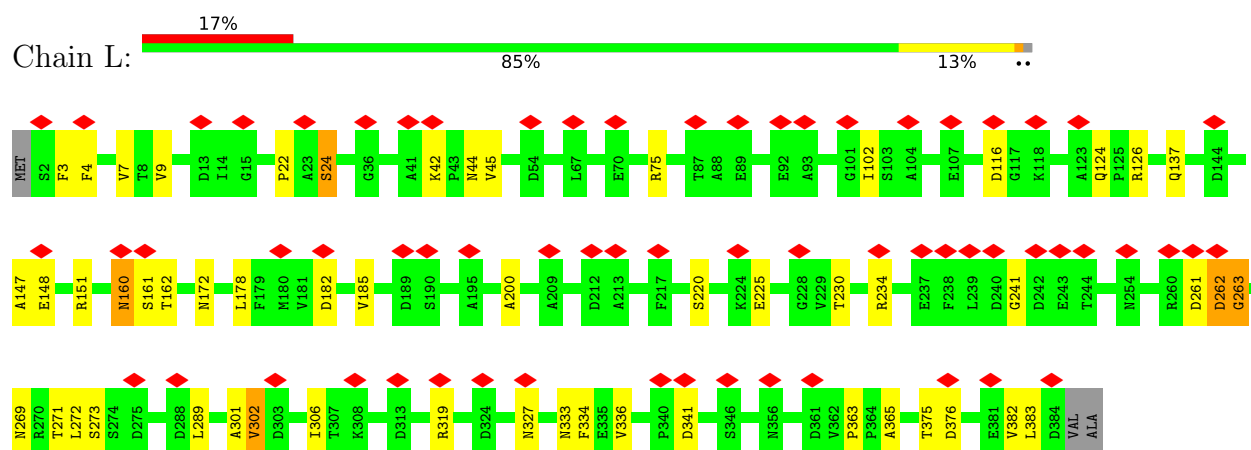
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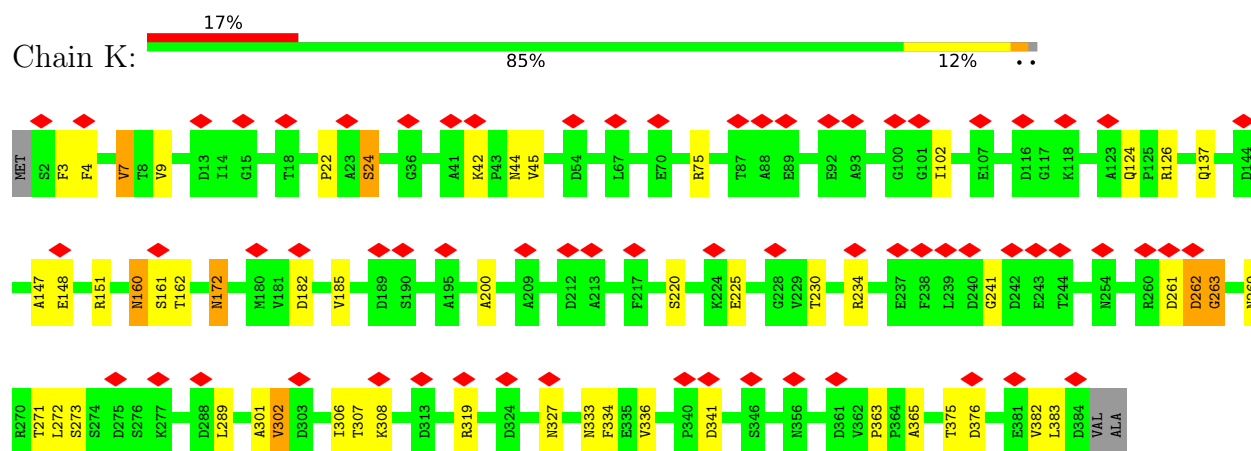
- Molecule 1: sheath



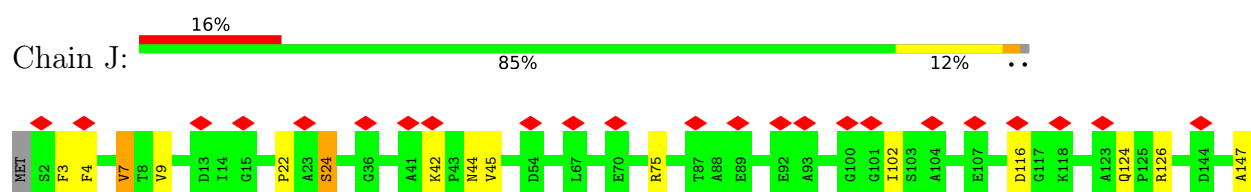
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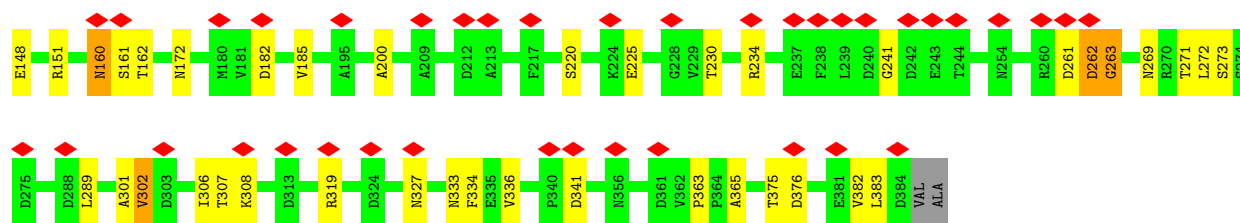


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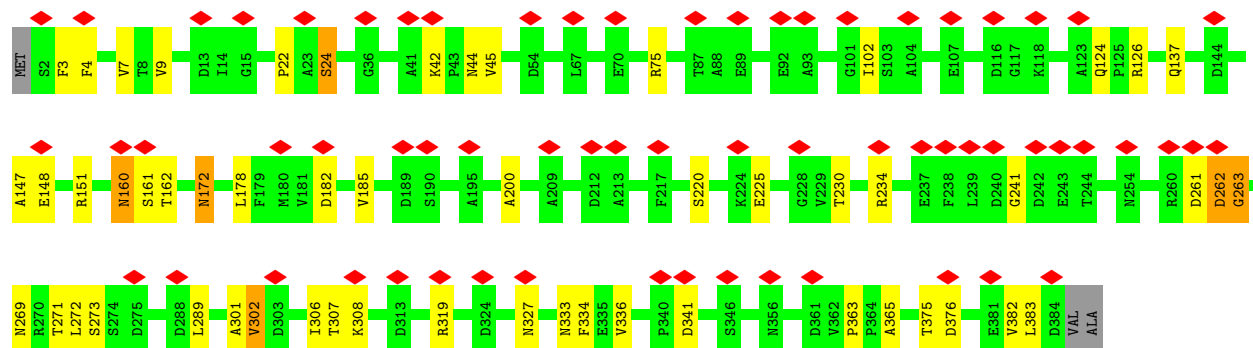
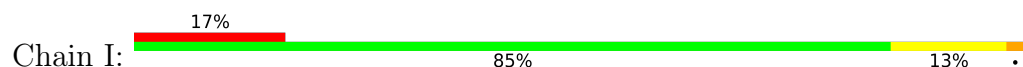


- Molecule 1: sheath

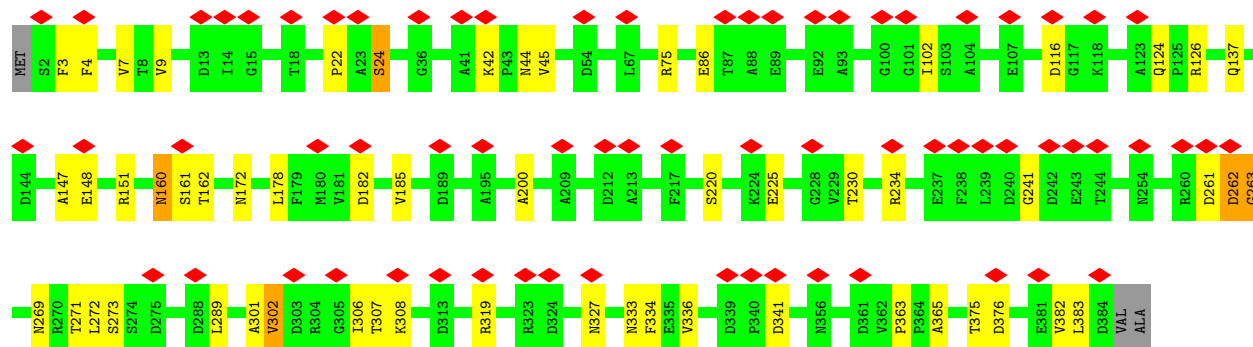
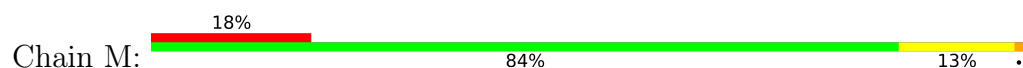




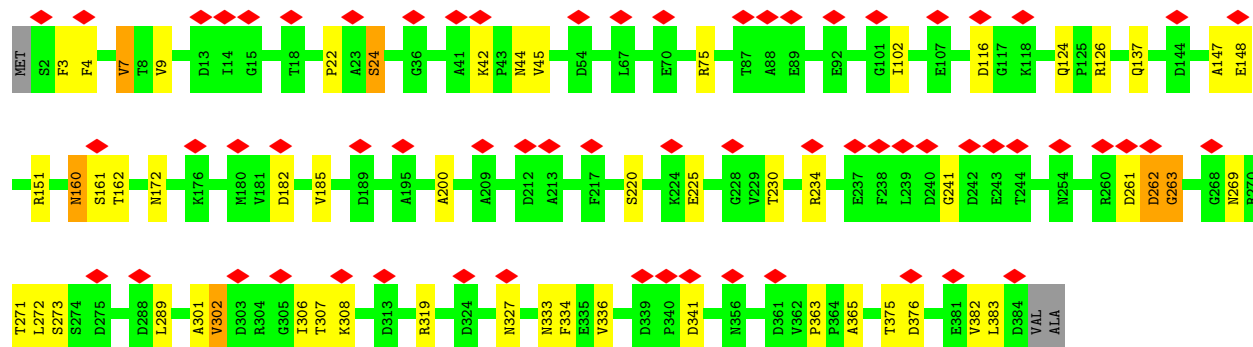
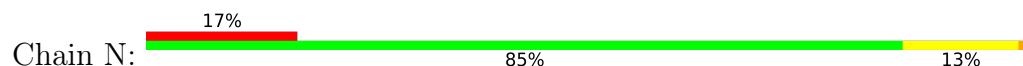
• Molecule 1: sheath



• Molecule 1: sheath

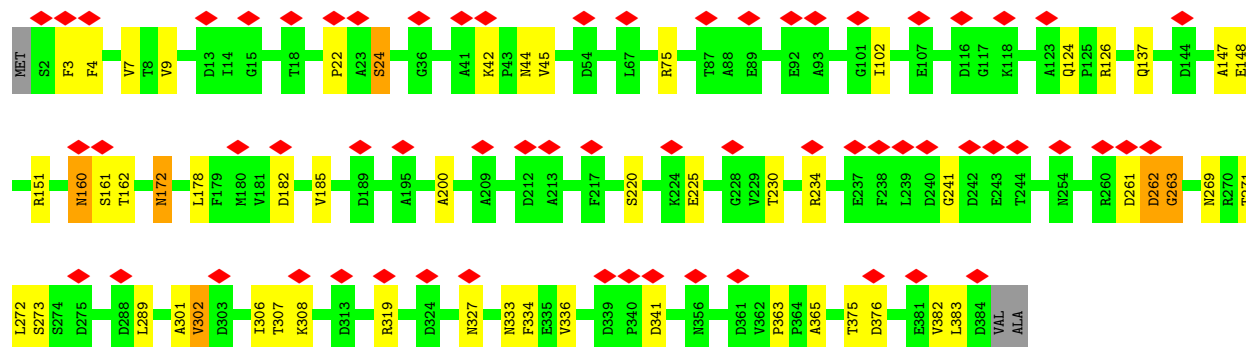


• Molecule 1: sheath



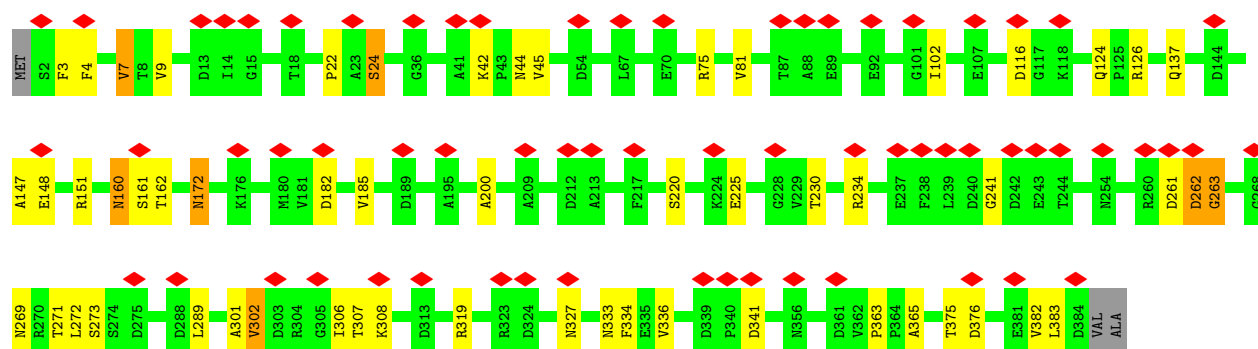
- Molecule 1: sheath

Chain R: 



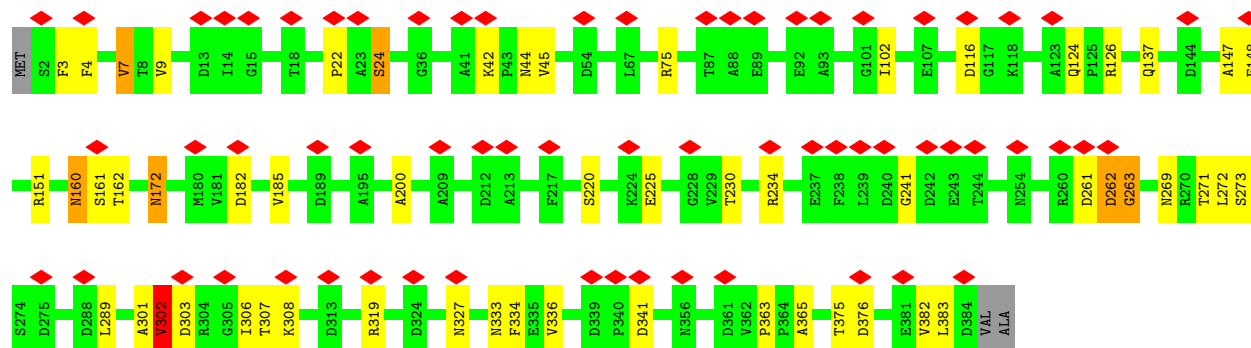
- Molecule 1: sheath

Chain Q: 



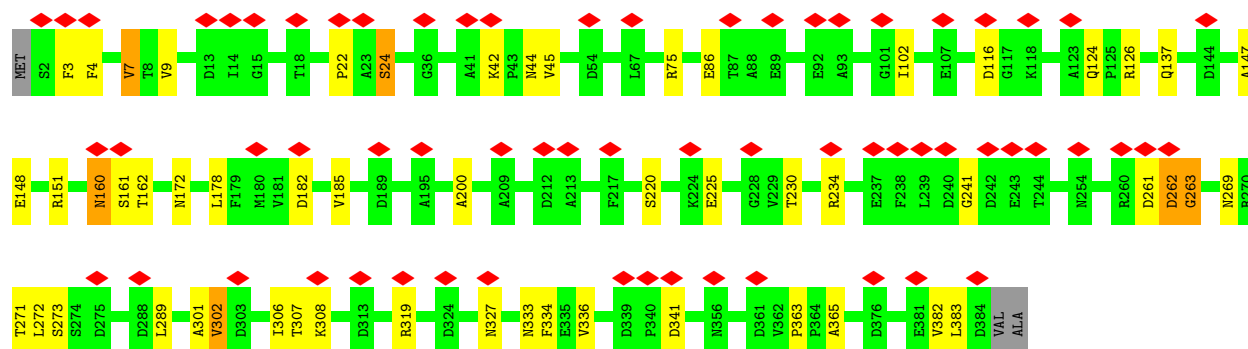
- Molecule 1: sheath

Chain P: 

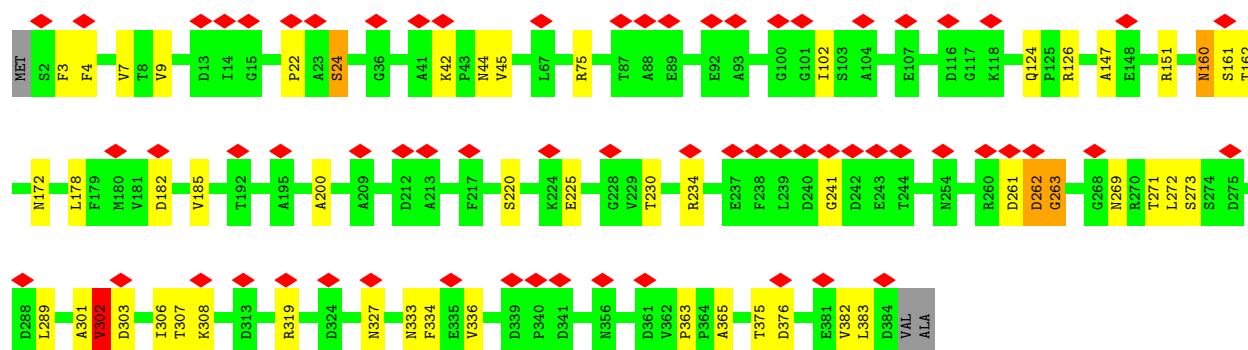
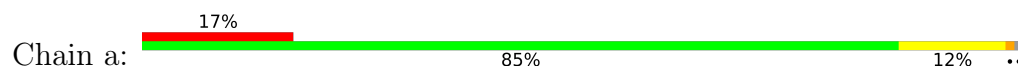


- Molecule 1: sheath

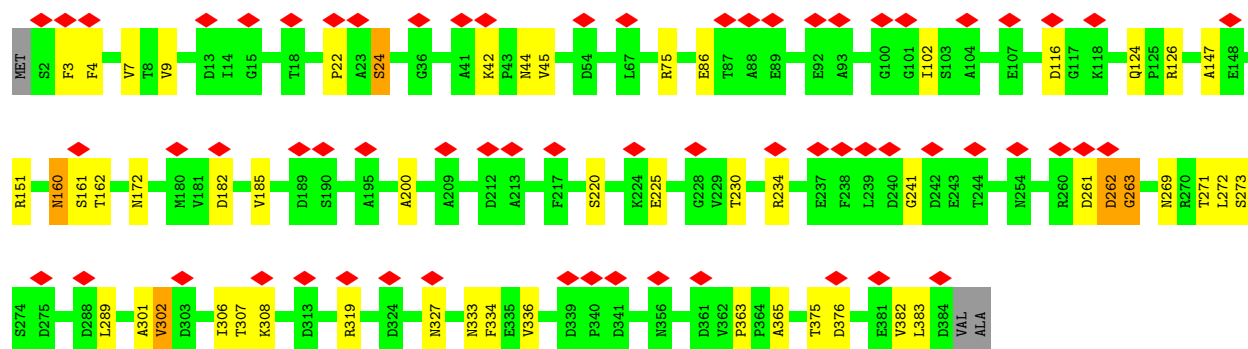
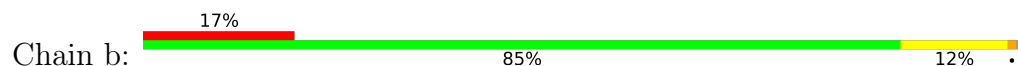
Chain O: 



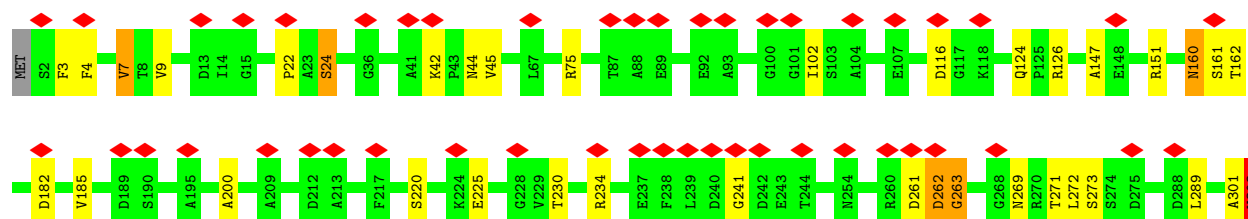
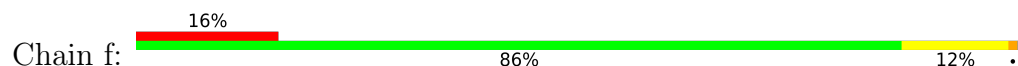
• Molecule 1: sheath

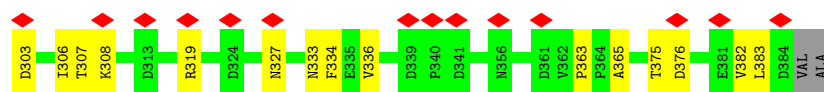


• Molecule 1: sheath

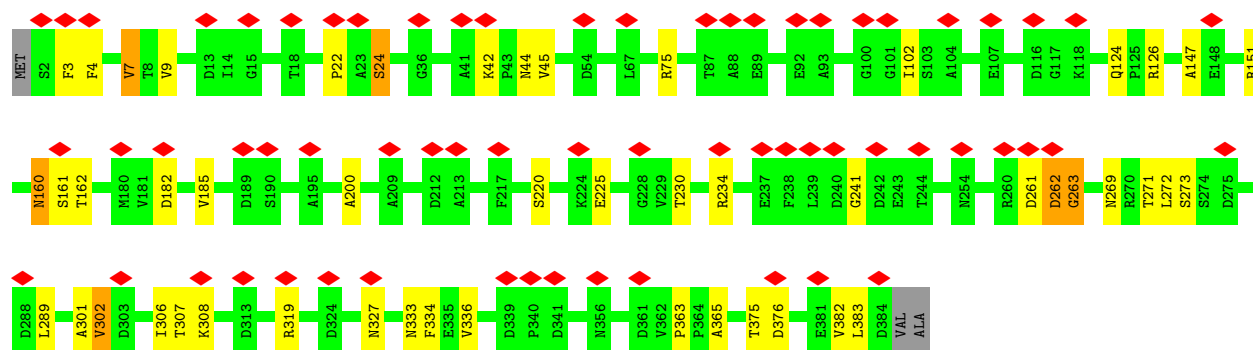
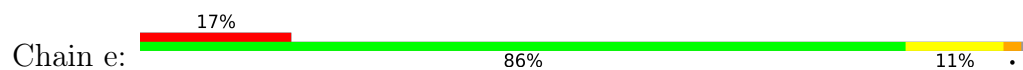


• Molecule 1: sheath

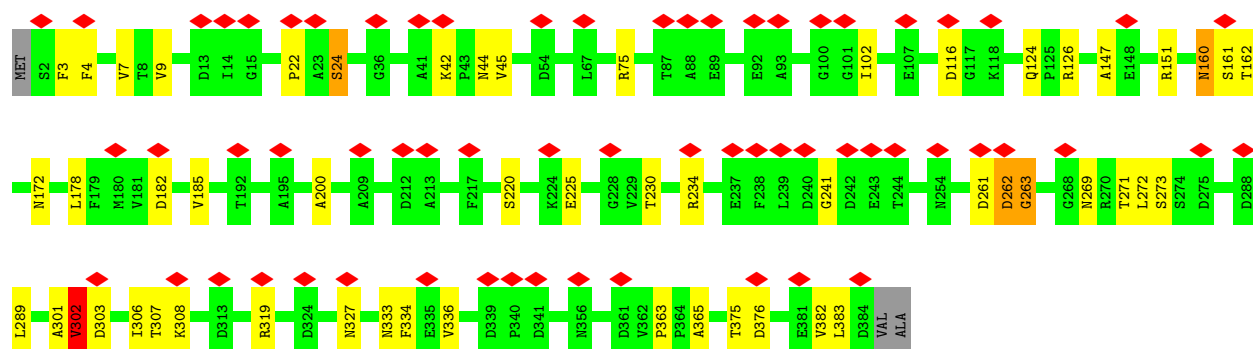
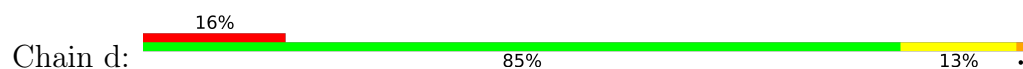




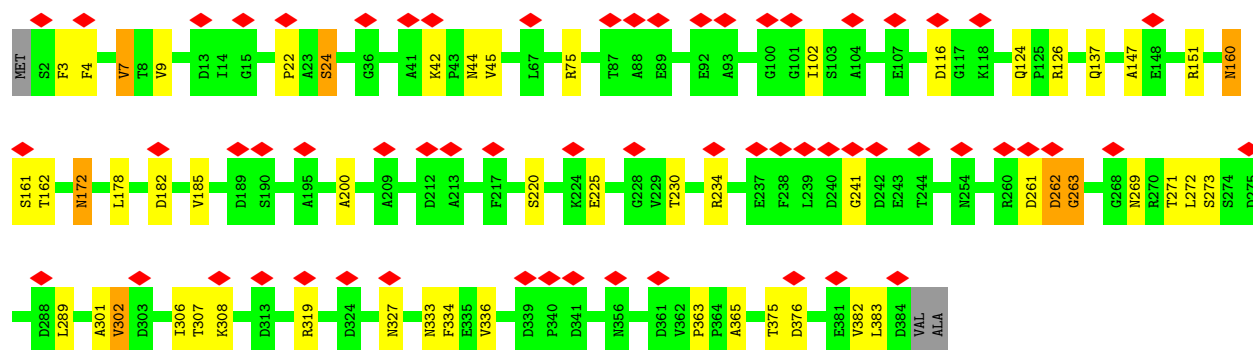
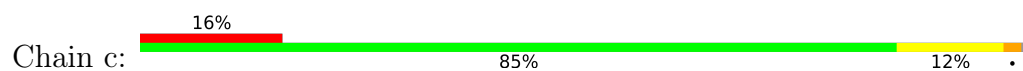
- Molecule 1: sheath



- Molecule 1: sheath

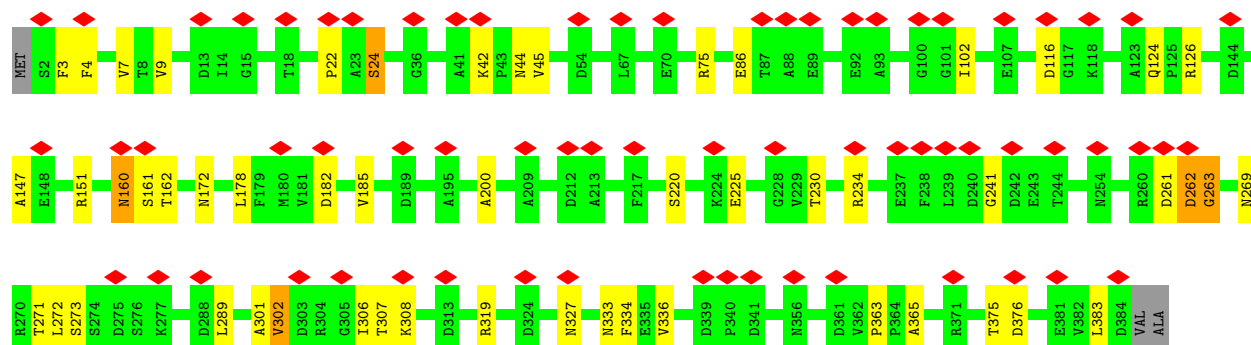


- Molecule 1: sheath



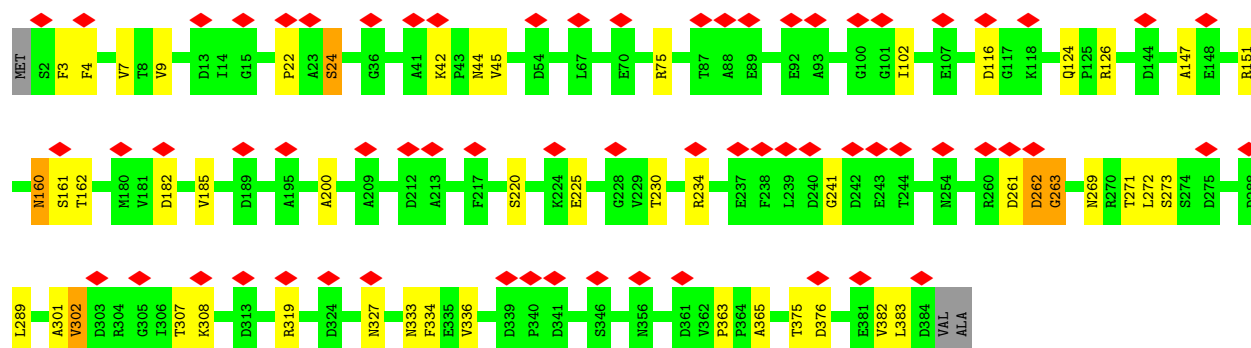
- Molecule 1: sheath

Chain g: 



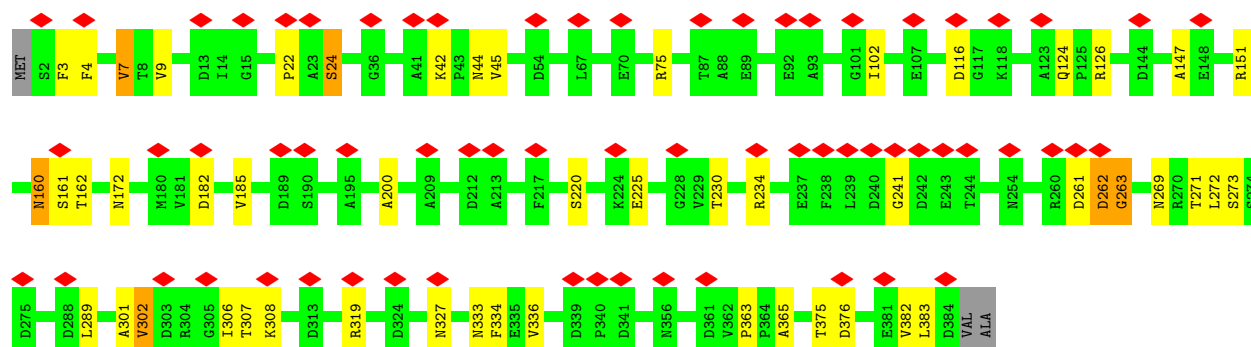
• Molecule 1: sheath

Chain h: 



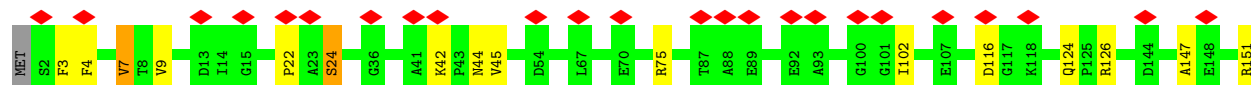
• Molecule 1: sheath

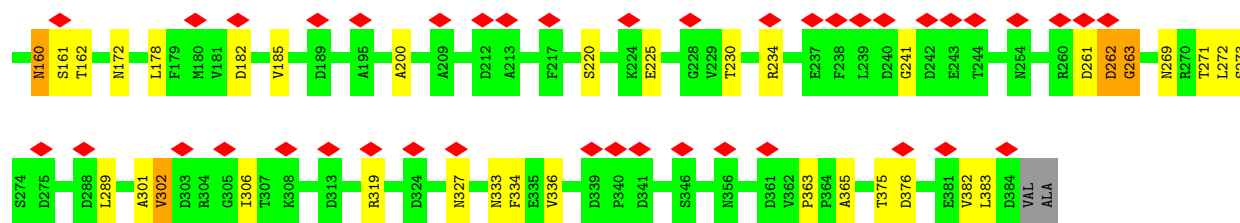
Chain i: 



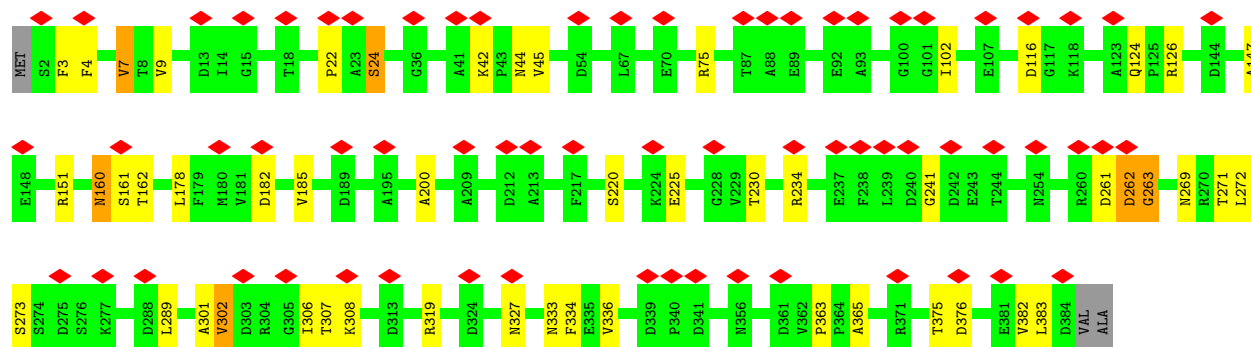
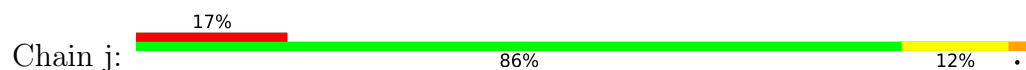
• Molecule 1: sheath

Chain k: 

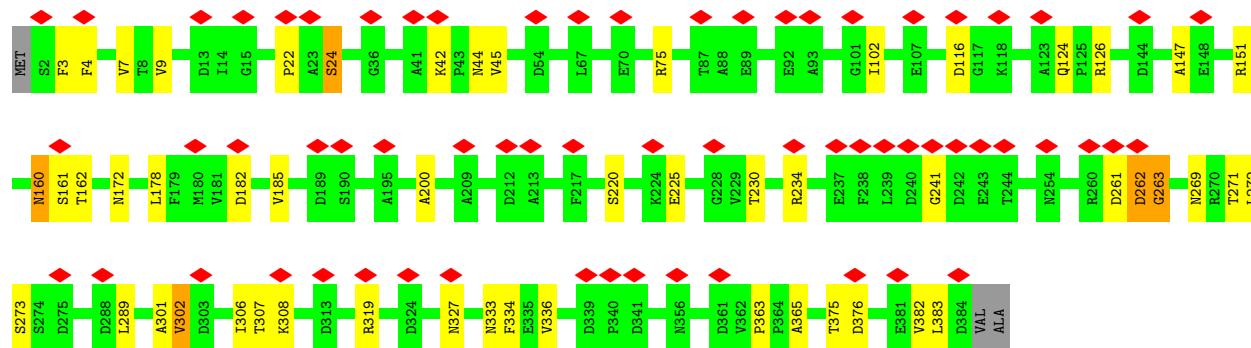
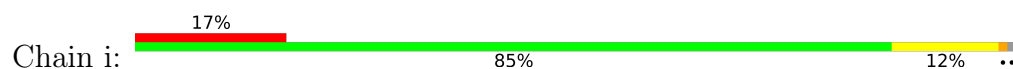




- Molecule 1: sheath



- Molecule 1: sheath



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=33.1°, rise=16.2 Å, axial sym=C6	Depositor
Number of segments used	Not provided	
Resolution determination method	OTHER	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	59000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	0.189	Depositor
Minimum map value	-0.136	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	331.19998, 331.19998, 331.19998	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.104, 1.104, 1.104	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	0	0.42	4/2942 (0.1%)	0.60	1/4010 (0.0%)
1	1	0.39	3/2942 (0.1%)	0.60	0/4010
1	2	0.44	4/2942 (0.1%)	0.60	1/4010 (0.0%)
1	3	0.38	3/2942 (0.1%)	0.60	0/4010
1	4	0.35	2/2942 (0.1%)	0.59	0/4010
1	5	0.35	2/2942 (0.1%)	0.59	0/4010
1	A	0.35	2/2942 (0.1%)	0.59	0/4010
1	B	0.39	3/2942 (0.1%)	0.60	0/4010
1	C	0.35	2/2942 (0.1%)	0.59	0/4010
1	D	0.36	2/2942 (0.1%)	0.59	0/4010
1	E	0.44	4/2942 (0.1%)	0.60	1/4010 (0.0%)
1	F	0.42	4/2942 (0.1%)	0.60	1/4010 (0.0%)
1	G	0.35	2/2942 (0.1%)	0.59	0/4010
1	H	0.37	3/2942 (0.1%)	0.59	0/4010
1	I	0.36	2/2942 (0.1%)	0.59	0/4010
1	J	0.35	2/2942 (0.1%)	0.59	0/4010
1	K	0.35	2/2942 (0.1%)	0.59	0/4010
1	L	0.36	3/2942 (0.1%)	0.60	0/4010
1	M	0.38	3/2942 (0.1%)	0.59	0/4010
1	N	0.37	3/2942 (0.1%)	0.59	0/4010
1	O	0.37	3/2942 (0.1%)	0.59	0/4010
1	P	0.35	2/2942 (0.1%)	0.59	0/4010
1	Q	0.36	2/2942 (0.1%)	0.59	0/4010
1	R	0.36	2/2942 (0.1%)	0.59	0/4010
1	a	0.35	2/2942 (0.1%)	0.59	0/4010
1	b	0.34	2/2942 (0.1%)	0.59	0/4010
1	c	0.35	2/2942 (0.1%)	0.59	0/4010
1	d	0.34	2/2942 (0.1%)	0.59	0/4010
1	e	0.34	0/2942	0.59	0/4010
1	f	0.34	0/2942	0.59	0/4010
1	g	0.35	2/2942 (0.1%)	0.59	0/4010
1	h	0.34	0/2942	0.59	0/4010
1	i	0.34	2/2942 (0.1%)	0.59	0/4010
1	j	0.33	0/2942	0.59	0/4010

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	k	0.34	2/2942 (0.1%)	0.59	0/4010
1	l	0.34	2/2942 (0.1%)	0.59	0/4010
All	All	0.36	80/105912 (0.1%)	0.59	4/144360 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	0	1
1	B	0	1
All	All	0	2

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	193	ASN	CG-ND2	-11.35	1.09	1.33
1	E	193	ASN	CG-ND2	-11.18	1.09	1.33
1	F	193	ASN	CG-ND2	-10.57	1.11	1.33
1	0	193	ASN	CG-ND2	-10.22	1.11	1.33
1	2	193	ASN	CG-OD1	-9.39	1.05	1.23
1	E	193	ASN	CG-OD1	-9.25	1.05	1.23
1	1	193	ASN	CG-ND2	-8.13	1.16	1.33
1	0	193	ASN	CG-OD1	-7.85	1.08	1.23
1	3	137	GLN	CD-NE2	-7.70	1.17	1.33
1	F	193	ASN	CG-OD1	-7.37	1.09	1.23
1	M	137	GLN	CD-NE2	-7.34	1.17	1.33
1	H	137	GLN	CD-NE2	-7.14	1.18	1.33
1	I	172	ASN	CG-ND2	-7.12	1.18	1.33
1	1	172	ASN	CG-ND2	-7.11	1.18	1.33
1	B	172	ASN	CG-ND2	-7.08	1.18	1.33
1	N	137	GLN	CD-NE2	-7.08	1.18	1.33
1	O	137	GLN	CD-NE2	-7.04	1.18	1.33
1	B	193	ASN	CG-ND2	-7.03	1.18	1.33
1	R	172	ASN	CG-ND2	-7.02	1.18	1.33
1	F	172	ASN	CG-ND2	-7.01	1.18	1.33
1	K	172	ASN	CG-ND2	-6.97	1.18	1.33
1	0	172	ASN	CG-ND2	-6.97	1.18	1.33
1	G	172	ASN	CG-ND2	-6.96	1.18	1.33
1	C	172	ASN	CG-ND2	-6.96	1.18	1.33
1	D	172	ASN	CG-ND2	-6.94	1.18	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	172	ASN	CG-ND2	-6.94	1.18	1.33
1	5	172	ASN	CG-ND2	-6.93	1.18	1.33
1	2	172	ASN	CG-ND2	-6.89	1.18	1.33
1	Q	172	ASN	CG-ND2	-6.88	1.18	1.33
1	A	172	ASN	CG-ND2	-6.86	1.18	1.33
1	4	172	ASN	CG-ND2	-6.86	1.18	1.33
1	c	172	ASN	CG-ND2	-6.79	1.19	1.33
1	L	137	GLN	CD-NE2	-6.24	1.20	1.33
1	B	172	ASN	CG-OD1	-5.75	1.12	1.23
1	1	172	ASN	CG-OD1	-5.67	1.12	1.23
1	I	172	ASN	CG-OD1	-5.67	1.12	1.23
1	M	172	ASN	CG-ND2	-5.67	1.21	1.33
1	g	172	ASN	CG-ND2	-5.67	1.21	1.33
1	l	172	ASN	CG-ND2	-5.67	1.21	1.33
1	a	172	ASN	CG-ND2	-5.64	1.21	1.33
1	N	172	ASN	CG-ND2	-5.62	1.21	1.33
1	d	172	ASN	CG-ND2	-5.62	1.21	1.33
1	i	172	ASN	CG-ND2	-5.62	1.21	1.33
1	g	172	ASN	CG-OD1	-5.61	1.12	1.23
1	M	172	ASN	CG-OD1	-5.59	1.12	1.23
1	O	172	ASN	CG-ND2	-5.59	1.21	1.33
1	H	172	ASN	CG-ND2	-5.59	1.21	1.33
1	b	172	ASN	CG-ND2	-5.59	1.21	1.33
1	R	172	ASN	CG-OD1	-5.58	1.12	1.23
1	2	172	ASN	CG-OD1	-5.58	1.12	1.23
1	d	172	ASN	CG-OD1	-5.58	1.12	1.23
1	J	172	ASN	CG-ND2	-5.57	1.21	1.33
1	L	172	ASN	CG-ND2	-5.57	1.21	1.33
1	E	172	ASN	CG-ND2	-5.56	1.21	1.33
1	P	172	ASN	CG-OD1	-5.54	1.13	1.23
1	3	172	ASN	CG-ND2	-5.53	1.21	1.33
1	l	172	ASN	CG-OD1	-5.53	1.13	1.23
1	F	172	ASN	CG-OD1	-5.53	1.13	1.23
1	K	172	ASN	CG-OD1	-5.53	1.13	1.23
1	D	172	ASN	CG-OD1	-5.53	1.13	1.23
1	k	172	ASN	CG-ND2	-5.52	1.21	1.33
1	a	172	ASN	CG-OD1	-5.52	1.13	1.23
1	0	172	ASN	CG-OD1	-5.52	1.13	1.23
1	i	172	ASN	CG-OD1	-5.52	1.13	1.23
1	J	172	ASN	CG-OD1	-5.51	1.13	1.23
1	C	172	ASN	CG-OD1	-5.50	1.13	1.23
1	G	172	ASN	CG-OD1	-5.49	1.13	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Q	172	ASN	CG-OD1	-5.49	1.13	1.23
1	L	172	ASN	CG-OD1	-5.49	1.13	1.23
1	N	172	ASN	CG-OD1	-5.48	1.13	1.23
1	A	172	ASN	CG-OD1	-5.48	1.13	1.23
1	5	172	ASN	CG-OD1	-5.45	1.13	1.23
1	H	172	ASN	CG-OD1	-5.44	1.13	1.23
1	4	172	ASN	CG-OD1	-5.43	1.13	1.23
1	k	172	ASN	CG-OD1	-5.41	1.13	1.23
1	E	172	ASN	CG-OD1	-5.37	1.13	1.23
1	3	172	ASN	CG-OD1	-5.36	1.13	1.23
1	c	172	ASN	CG-OD1	-5.35	1.13	1.23
1	b	172	ASN	CG-OD1	-5.34	1.13	1.23
1	O	172	ASN	CG-OD1	-5.29	1.13	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	193	ASN	OD1-CG-ND2	-5.58	117.02	122.60
1	2	193	ASN	OD1-CG-ND2	-5.54	117.06	122.60
1	F	193	ASN	OD1-CG-ND2	-5.33	117.27	122.60
1	0	193	ASN	OD1-CG-ND2	-5.25	117.35	122.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	193	ASN	Sidechain
1	B	193	ASN	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	2884	0	2841	22	0
1	1	2884	0	2841	26	0
1	2	2884	0	2841	23	0
1	3	2884	0	2841	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	4	2884	0	2841	24	0
1	5	2884	0	2841	23	0
1	A	2884	0	2841	24	0
1	B	2884	0	2841	26	0
1	C	2884	0	2841	26	0
1	D	2884	0	2841	25	0
1	E	2884	0	2841	25	0
1	F	2884	0	2841	24	0
1	G	2884	0	2841	29	0
1	H	2884	0	2841	26	0
1	I	2884	0	2841	27	0
1	J	2884	0	2841	26	0
1	K	2884	0	2841	26	0
1	L	2884	0	2841	26	0
1	M	2884	0	2841	27	0
1	N	2884	0	2841	26	0
1	O	2884	0	2841	28	0
1	P	2884	0	2841	29	0
1	Q	2884	0	2841	28	0
1	R	2884	0	2841	27	0
1	a	2884	0	2841	24	0
1	b	2884	0	2841	24	0
1	c	2884	0	2841	25	0
1	d	2884	0	2841	25	0
1	e	2884	0	2841	22	0
1	f	2884	0	2841	24	0
1	g	2884	0	2841	23	0
1	h	2884	0	2841	21	0
1	i	2884	0	2841	23	0
1	j	2884	0	2841	23	0
1	k	2884	0	2841	22	0
1	l	2884	0	2841	22	0
All	All	103824	0	102276	791	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 4.

All (791) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:220:SER:OG	1:L:269:ASN:OD1	2.11	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:220:SER:OG	1:4:269:ASN:OD1	2.11	0.69
1:5:220:SER:OG	1:5:269:ASN:OD1	2.11	0.68
1:D:148:GLU:OE2	1:O:75:ARG:NH2	2.27	0.68
1:O:220:SER:OG	1:O:269:ASN:OD1	2.12	0.68
1:E:220:SER:OG	1:E:269:ASN:OD1	2.12	0.68
1:1:220:SER:OG	1:1:269:ASN:OD1	2.11	0.68
1:N:220:SER:OG	1:N:269:ASN:OD1	2.12	0.68
1:R:220:SER:OG	1:R:269:ASN:OD1	2.12	0.68
1:F:220:SER:OG	1:F:269:ASN:OD1	2.12	0.68
1:i:220:SER:OG	1:i:269:ASN:OD1	2.12	0.68
1:G:220:SER:OG	1:G:269:ASN:OD1	2.12	0.68
1:I:220:SER:OG	1:I:269:ASN:OD1	2.12	0.68
1:b:220:SER:OG	1:b:269:ASN:OD1	2.12	0.67
1:h:220:SER:OG	1:h:269:ASN:OD1	2.12	0.67
1:l:220:SER:OG	1:l:269:ASN:OD1	2.11	0.67
1:K:220:SER:OG	1:K:269:ASN:OD1	2.12	0.67
1:j:220:SER:OG	1:j:269:ASN:OD1	2.11	0.67
1:a:220:SER:OG	1:a:269:ASN:OD1	2.12	0.67
1:c:220:SER:OG	1:c:269:ASN:OD1	2.13	0.67
1:A:220:SER:OG	1:A:269:ASN:OD1	2.12	0.67
1:3:220:SER:OG	1:3:269:ASN:OD1	2.12	0.67
1:Q:220:SER:OG	1:Q:269:ASN:OD1	2.12	0.67
1:M:220:SER:OG	1:M:269:ASN:OD1	2.12	0.67
1:f:220:SER:OG	1:f:269:ASN:OD1	2.13	0.67
1:2:220:SER:OG	1:2:269:ASN:OD1	2.12	0.67
1:e:220:SER:OG	1:e:269:ASN:OD1	2.12	0.67
1:O:220:SER:OG	1:O:269:ASN:OD1	2.12	0.67
1:4:148:GLU:OE2	1:J:75:ARG:NH2	2.28	0.67
1:d:220:SER:OG	1:d:269:ASN:OD1	2.12	0.67
1:H:220:SER:OG	1:H:269:ASN:OD1	2.12	0.67
1:g:220:SER:OG	1:g:269:ASN:OD1	2.12	0.67
1:D:220:SER:OG	1:D:269:ASN:OD1	2.12	0.67
1:k:220:SER:OG	1:k:269:ASN:OD1	2.12	0.67
1:L:148:GLU:OE2	1:e:75:ARG:NH2	2.28	0.67
1:P:220:SER:OG	1:P:269:ASN:OD1	2.12	0.67
1:J:220:SER:OG	1:J:269:ASN:OD1	2.12	0.66
1:N:148:GLU:OE2	1:g:75:ARG:NH2	2.28	0.66
1:R:148:GLU:OE2	1:k:75:ARG:NH2	2.28	0.66
1:C:148:GLU:OE2	1:N:75:ARG:NH2	2.28	0.66
1:E:148:GLU:OE2	1:P:75:ARG:NH2	2.29	0.66
1:A:148:GLU:OE2	1:R:75:ARG:NH2	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:SER:OG	1:B:269:ASN:OD1	2.12	0.66
1:M:148:GLU:OE2	1:l:75:ARG:NH2	2.29	0.66
1:C:220:SER:OG	1:C:269:ASN:OD1	2.12	0.66
1:F:148:GLU:OE2	1:Q:75:ARG:NH2	2.28	0.66
1:O:124:GLN:OE1	1:O:126:ARG:NH2	2.29	0.66
1:Q:148:GLU:OE2	1:j:75:ARG:NH2	2.29	0.65
1:O:148:GLU:OE2	1:h:75:ARG:NH2	2.30	0.65
1:G:148:GLU:OE2	1:f:75:ARG:NH2	2.29	0.65
1:H:148:GLU:OE2	1:a:75:ARG:NH2	2.29	0.65
1:d:124:GLN:OE1	1:d:126:ARG:NH2	2.29	0.65
1:J:124:GLN:OE1	1:J:126:ARG:NH2	2.29	0.65
1:M:124:GLN:OE1	1:M:126:ARG:NH2	2.30	0.65
1:1:148:GLU:OE2	1:G:75:ARG:NH2	2.29	0.65
1:5:148:GLU:OE2	1:K:75:ARG:NH2	2.29	0.65
1:2:124:GLN:OE1	1:2:126:ARG:NH2	2.30	0.65
1:L:124:GLN:OE1	1:L:126:ARG:NH2	2.30	0.65
1:J:148:GLU:OE2	1:c:75:ARG:NH2	2.30	0.65
1:j:124:GLN:OE1	1:j:126:ARG:NH2	2.30	0.65
1:A:124:GLN:OE1	1:A:126:ARG:NH2	2.30	0.65
1:E:124:GLN:OE1	1:E:126:ARG:NH2	2.30	0.65
1:a:124:GLN:OE1	1:a:126:ARG:NH2	2.30	0.65
1:e:124:GLN:OE1	1:e:126:ARG:NH2	2.29	0.65
1:B:148:GLU:OE2	1:M:75:ARG:NH2	2.29	0.65
1:F:124:GLN:OE1	1:F:126:ARG:NH2	2.30	0.65
1:R:124:GLN:OE1	1:R:126:ARG:NH2	2.30	0.65
1:i:124:GLN:OE1	1:i:126:ARG:NH2	2.30	0.65
1:C:124:GLN:OE1	1:C:126:ARG:NH2	2.30	0.65
1:K:124:GLN:OE1	1:K:126:ARG:NH2	2.30	0.65
1:B:124:GLN:OE1	1:B:126:ARG:NH2	2.29	0.65
1:5:124:GLN:OE1	1:5:126:ARG:NH2	2.30	0.65
1:3:148:GLU:OE2	1:I:75:ARG:NH2	2.30	0.65
1:G:124:GLN:OE1	1:G:126:ARG:NH2	2.30	0.65
1:K:148:GLU:OE2	1:d:75:ARG:NH2	2.30	0.65
1:I:124:GLN:OE1	1:I:126:ARG:NH2	2.30	0.65
1:f:124:GLN:OE1	1:f:126:ARG:NH2	2.30	0.65
1:c:124:GLN:OE1	1:c:126:ARG:NH2	2.29	0.65
1:2:148:GLU:OE2	1:H:75:ARG:NH2	2.29	0.65
1:I:148:GLU:OE2	1:b:75:ARG:NH2	2.30	0.65
1:P:124:GLN:OE1	1:P:126:ARG:NH2	2.29	0.65
1:l:124:GLN:OE1	1:l:126:ARG:NH2	2.30	0.65
1:D:124:GLN:OE1	1:D:126:ARG:NH2	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:124:GLN:OE1	1:1:126:ARG:NH2	2.30	0.64
1:4:124:GLN:OE1	1:4:126:ARG:NH2	2.30	0.64
1:N:124:GLN:OE1	1:N:126:ARG:NH2	2.30	0.64
1:b:124:GLN:OE1	1:b:126:ARG:NH2	2.30	0.64
1:k:124:GLN:OE1	1:k:126:ARG:NH2	2.30	0.64
1:0:124:GLN:OE1	1:0:126:ARG:NH2	2.30	0.64
1:Q:124:GLN:OE1	1:Q:126:ARG:NH2	2.30	0.64
1:g:124:GLN:OE1	1:g:126:ARG:NH2	2.30	0.64
1:h:124:GLN:OE1	1:h:126:ARG:NH2	2.30	0.64
1:3:124:GLN:OE1	1:3:126:ARG:NH2	2.30	0.64
1:P:148:GLU:OE2	1:i:75:ARG:NH2	2.31	0.64
1:H:124:GLN:OE1	1:H:126:ARG:NH2	2.30	0.64
1:0:148:GLU:OE2	1:L:75:ARG:NH2	2.30	0.63
1:E:182:ASP:OD2	1:E:234:ARG:NH1	2.34	0.61
1:j:182:ASP:OD2	1:j:234:ARG:NH1	2.34	0.61
1:Q:182:ASP:OD2	1:Q:234:ARG:NH1	2.34	0.61
1:F:182:ASP:OD2	1:F:234:ARG:NH1	2.34	0.61
1:4:182:ASP:OD2	1:4:234:ARG:NH1	2.34	0.61
1:L:182:ASP:OD2	1:L:234:ARG:NH1	2.34	0.61
1:i:182:ASP:OD2	1:i:234:ARG:NH1	2.34	0.61
1:d:182:ASP:OD2	1:d:234:ARG:NH1	2.34	0.60
1:R:182:ASP:OD2	1:R:234:ARG:NH1	2.34	0.60
1:P:182:ASP:OD2	1:P:234:ARG:NH1	2.34	0.60
1:c:182:ASP:OD2	1:c:234:ARG:NH1	2.34	0.60
1:K:182:ASP:OD2	1:K:234:ARG:NH1	2.34	0.60
1:e:182:ASP:OD2	1:e:234:ARG:NH1	2.34	0.60
1:J:182:ASP:OD2	1:J:234:ARG:NH1	2.34	0.60
1:O:182:ASP:OD2	1:O:234:ARG:NH1	2.34	0.60
1:0:182:ASP:OD2	1:0:234:ARG:NH1	2.34	0.60
1:5:182:ASP:OD2	1:5:234:ARG:NH1	2.35	0.60
1:I:182:ASP:OD2	1:I:234:ARG:NH1	2.34	0.60
1:f:182:ASP:OD2	1:f:234:ARG:NH1	2.34	0.60
1:1:182:ASP:OD2	1:1:234:ARG:NH1	2.34	0.60
1:g:182:ASP:OD2	1:g:234:ARG:NH1	2.34	0.60
1:k:182:ASP:OD2	1:k:234:ARG:NH1	2.34	0.60
1:B:182:ASP:OD2	1:B:234:ARG:NH1	2.34	0.60
1:h:182:ASP:OD2	1:h:234:ARG:NH1	2.34	0.60
1:C:182:ASP:OD2	1:C:234:ARG:NH1	2.34	0.59
1:G:182:ASP:OD2	1:G:234:ARG:NH1	2.34	0.59
1:a:182:ASP:OD2	1:a:234:ARG:NH1	2.34	0.59
1:A:182:ASP:OD2	1:A:234:ARG:NH1	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:160:ASN:O	1:H:162:THR:N	2.36	0.59
1:H:182:ASP:OD2	1:H:234:ARG:NH1	2.34	0.59
1:M:182:ASP:OD2	1:M:234:ARG:NH1	2.34	0.59
1:3:182:ASP:OD2	1:3:234:ARG:NH1	2.34	0.59
1:g:160:ASN:O	1:g:162:THR:N	2.36	0.59
1:l:160:ASN:O	1:l:162:THR:N	2.36	0.59
1:l:182:ASP:OD2	1:l:234:ARG:NH1	2.34	0.59
1:D:182:ASP:OD2	1:D:234:ARG:NH1	2.34	0.59
1:I:160:ASN:O	1:I:162:THR:N	2.36	0.59
1:2:182:ASP:OD2	1:2:234:ARG:NH1	2.34	0.59
1:b:182:ASP:OD2	1:b:234:ARG:NH1	2.34	0.59
1:C:160:ASN:O	1:C:162:THR:N	2.36	0.58
1:N:160:ASN:O	1:N:162:THR:N	2.36	0.58
1:3:160:ASN:O	1:3:162:THR:N	2.36	0.58
1:N:182:ASP:OD2	1:N:234:ARG:NH1	2.34	0.58
1:h:160:ASN:O	1:h:162:THR:N	2.36	0.58
1:B:160:ASN:O	1:B:162:THR:N	2.36	0.58
1:G:160:ASN:O	1:G:162:THR:N	2.36	0.58
1:L:75:ARG:NH1	1:L:225:GLU:O	2.36	0.58
1:I:75:ARG:NH1	1:I:225:GLU:O	2.37	0.58
1:M:160:ASN:O	1:M:162:THR:N	2.36	0.58
1:a:160:ASN:O	1:a:162:THR:N	2.36	0.58
1:b:160:ASN:O	1:b:162:THR:N	2.36	0.58
1:d:160:ASN:O	1:d:162:THR:N	2.36	0.58
1:l:75:ARG:NH1	1:l:225:GLU:O	2.37	0.58
1:2:75:ARG:NH1	1:2:225:GLU:O	2.37	0.58
1:i:75:ARG:NH1	1:i:225:GLU:O	2.36	0.58
1:D:160:ASN:O	1:D:162:THR:N	2.36	0.58
1:F:160:ASN:O	1:F:162:THR:N	2.36	0.58
1:5:160:ASN:O	1:5:162:THR:N	2.36	0.58
1:K:75:ARG:NH1	1:K:225:GLU:O	2.37	0.58
1:O:75:ARG:NH1	1:O:225:GLU:O	2.37	0.58
1:f:160:ASN:O	1:f:162:THR:N	2.36	0.58
1:g:75:ARG:NH1	1:g:225:GLU:O	2.37	0.58
1:i:160:ASN:O	1:i:162:THR:N	2.36	0.58
1:B:75:ARG:NH1	1:B:225:GLU:O	2.37	0.58
1:C:75:ARG:NH1	1:C:225:GLU:O	2.37	0.58
1:L:160:ASN:O	1:L:162:THR:N	2.36	0.58
1:J:160:ASN:O	1:J:162:THR:N	2.36	0.58
1:a:75:ARG:NH1	1:a:225:GLU:O	2.37	0.58
1:f:75:ARG:NH1	1:f:225:GLU:O	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:j:160:ASN:O	1:j:162:THR:N	2.36	0.58
1:M:75:ARG:NH1	1:M:225:GLU:O	2.37	0.58
1:P:160:ASN:O	1:P:162:THR:N	2.36	0.58
1:j:75:ARG:NH1	1:j:225:GLU:O	2.37	0.58
1:E:75:ARG:NH1	1:E:225:GLU:O	2.37	0.58
1:2:160:ASN:O	1:2:162:THR:N	2.36	0.58
1:O:160:ASN:O	1:O:162:THR:N	2.36	0.58
1:e:160:ASN:O	1:e:162:THR:N	2.36	0.58
1:c:137:GLN:OE1	1:c:172:ASN:ND2	2.33	0.58
1:g:261:ASP:OD2	1:g:262:ASP:N	2.37	0.58
1:A:75:ARG:NH1	1:A:225:GLU:O	2.37	0.57
1:F:75:ARG:NH1	1:F:225:GLU:O	2.37	0.57
1:H:75:ARG:NH1	1:H:225:GLU:O	2.37	0.57
1:d:75:ARG:NH1	1:d:225:GLU:O	2.37	0.57
1:k:160:ASN:O	1:k:162:THR:N	2.37	0.57
1:0:160:ASN:O	1:0:162:THR:N	2.36	0.57
1:R:160:ASN:O	1:R:162:THR:N	2.36	0.57
1:0:75:ARG:NH1	1:0:225:GLU:O	2.37	0.57
1:5:75:ARG:NH1	1:5:225:GLU:O	2.37	0.57
1:Q:160:ASN:O	1:Q:162:THR:N	2.37	0.57
1:c:75:ARG:NH1	1:c:225:GLU:O	2.37	0.57
1:c:160:ASN:O	1:c:162:THR:N	2.36	0.57
1:h:261:ASP:OD2	1:h:262:ASP:N	2.38	0.57
1:A:137:GLN:OE1	1:A:172:ASN:ND2	2.37	0.57
1:1:75:ARG:NH1	1:1:225:GLU:O	2.37	0.57
1:K:160:ASN:O	1:K:162:THR:N	2.36	0.57
1:J:75:ARG:NH1	1:J:225:GLU:O	2.37	0.57
1:N:75:ARG:NH1	1:N:225:GLU:O	2.37	0.57
1:R:75:ARG:NH1	1:R:225:GLU:O	2.37	0.57
1:Q:75:ARG:NH1	1:Q:225:GLU:O	2.37	0.57
1:P:75:ARG:NH1	1:P:225:GLU:O	2.37	0.57
1:i:261:ASP:OD2	1:i:262:ASP:N	2.38	0.57
1:E:160:ASN:O	1:E:162:THR:N	2.36	0.57
1:E:261:ASP:OD2	1:E:262:ASP:N	2.38	0.57
1:D:75:ARG:NH1	1:D:225:GLU:O	2.37	0.57
1:1:261:ASP:OD2	1:1:262:ASP:N	2.38	0.57
1:3:261:ASP:OD2	1:3:262:ASP:N	2.38	0.57
1:R:261:ASP:OD2	1:R:262:ASP:N	2.38	0.57
1:Q:261:ASP:OD2	1:Q:262:ASP:N	2.38	0.57
1:k:75:ARG:NH1	1:k:225:GLU:O	2.37	0.57
1:1:160:ASN:O	1:1:162:THR:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:261:ASP:OD2	1:L:262:ASP:N	2.38	0.57
1:e:75:ARG:NH1	1:e:225:GLU:O	2.37	0.57
1:e:261:ASP:OD2	1:e:262:ASP:N	2.38	0.57
1:A:160:ASN:O	1:A:162:THR:N	2.37	0.57
1:B:261:ASP:OD2	1:B:262:ASP:N	2.38	0.57
1:3:75:ARG:NH1	1:3:225:GLU:O	2.37	0.57
1:G:75:ARG:NH1	1:G:225:GLU:O	2.37	0.57
1:N:261:ASP:OD2	1:N:262:ASP:N	2.38	0.57
1:h:75:ARG:NH1	1:h:225:GLU:O	2.37	0.57
1:l:261:ASP:OD2	1:l:262:ASP:N	2.38	0.57
1:4:261:ASP:OD2	1:4:262:ASP:N	2.38	0.57
1:M:261:ASP:OD2	1:M:262:ASP:N	2.38	0.57
1:Q:137:GLN:OE1	1:Q:172:ASN:ND2	2.38	0.57
1:a:261:ASP:OD2	1:a:262:ASP:N	2.38	0.57
1:b:75:ARG:NH1	1:b:225:GLU:O	2.37	0.57
1:b:261:ASP:OD2	1:b:262:ASP:N	2.38	0.57
1:f:261:ASP:OD2	1:f:262:ASP:N	2.38	0.57
1:c:261:ASP:OD2	1:c:262:ASP:N	2.38	0.57
1:C:261:ASP:OD2	1:C:262:ASP:N	2.38	0.57
1:4:75:ARG:NH1	1:4:225:GLU:O	2.37	0.57
1:H:261:ASP:OD2	1:H:262:ASP:N	2.38	0.57
1:J:261:ASP:OD2	1:J:262:ASP:N	2.38	0.57
1:j:261:ASP:OD2	1:j:262:ASP:N	2.37	0.57
1:D:261:ASP:OD2	1:D:262:ASP:N	2.38	0.56
1:4:160:ASN:O	1:4:162:THR:N	2.36	0.56
1:K:261:ASP:OD2	1:K:262:ASP:N	2.38	0.56
1:F:261:ASP:OD2	1:F:262:ASP:N	2.38	0.56
1:O:261:ASP:OD2	1:O:262:ASP:N	2.38	0.56
1:5:261:ASP:OD2	1:5:262:ASP:N	2.38	0.56
1:2:261:ASP:OD2	1:2:262:ASP:N	2.38	0.56
1:G:261:ASP:OD2	1:G:262:ASP:N	2.38	0.56
1:P:261:ASP:OD2	1:P:262:ASP:N	2.38	0.56
1:k:261:ASP:OD2	1:k:262:ASP:N	2.38	0.56
1:B:190:SER:O	1:B:193:ASN:OD1	2.24	0.56
1:0:261:ASP:OD2	1:0:262:ASP:N	2.38	0.56
1:O:341:ASP:O	1:h:327:ASN:ND2	2.39	0.56
1:A:261:ASP:OD2	1:A:262:ASP:N	2.38	0.56
1:N:341:ASP:O	1:g:327:ASN:ND2	2.39	0.56
1:d:261:ASP:OD2	1:d:262:ASP:N	2.38	0.56
1:I:261:ASP:OD2	1:I:262:ASP:N	2.38	0.56
1:A:341:ASP:O	1:R:327:ASN:ND2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:341:ASP:O	1:c:327:ASN:ND2	2.40	0.55
1:O:137:GLN:OE1	1:O:172:ASN:ND2	2.39	0.55
1:1:190:SER:O	1:1:193:ASN:OD1	2.23	0.55
1:K:137:GLN:OE1	1:K:172:ASN:ND2	2.40	0.55
1:E:341:ASP:O	1:P:327:ASN:ND2	2.40	0.55
1:L:341:ASP:O	1:e:327:ASN:ND2	2.40	0.55
1:5:137:GLN:OE1	1:5:172:ASN:ND2	2.38	0.55
1:R:341:ASP:O	1:k:327:ASN:ND2	2.39	0.55
1:A:185:VAL:HG12	1:A:200:ALA:HB2	1.89	0.55
1:R:185:VAL:HG12	1:R:200:ALA:HB2	1.89	0.55
1:N:185:VAL:HG12	1:N:200:ALA:HB2	1.89	0.54
1:C:341:ASP:O	1:N:327:ASN:ND2	2.40	0.54
1:G:137:GLN:OE1	1:G:172:ASN:ND2	2.40	0.54
1:l:185:VAL:HG12	1:l:200:ALA:HB2	1.90	0.54
1:k:185:VAL:HG12	1:k:200:ALA:HB2	1.89	0.54
1:H:185:VAL:HG12	1:H:200:ALA:HB2	1.89	0.54
1:e:185:VAL:HG12	1:e:200:ALA:HB2	1.90	0.54
1:3:185:VAL:HG12	1:3:200:ALA:HB2	1.89	0.54
1:Q:341:ASP:O	1:j:327:ASN:ND2	2.41	0.54
1:O:185:VAL:HG12	1:O:200:ALA:HB2	1.89	0.54
1:1:185:VAL:HG12	1:1:200:ALA:HB2	1.89	0.54
1:5:185:VAL:HG12	1:5:200:ALA:HB2	1.89	0.54
1:H:261:ASP:O	1:H:263:GLY:N	2.41	0.54
1:I:341:ASP:O	1:b:327:ASN:ND2	2.41	0.54
1:5:341:ASP:O	1:K:327:ASN:ND2	2.41	0.53
1:2:341:ASP:O	1:H:327:ASN:ND2	2.40	0.53
1:N:261:ASP:O	1:N:263:GLY:N	2.41	0.53
1:b:261:ASP:O	1:b:263:GLY:N	2.41	0.53
1:l:261:ASP:O	1:l:263:GLY:N	2.41	0.53
1:D:341:ASP:O	1:O:327:ASN:ND2	2.41	0.53
1:P:137:GLN:OE1	1:P:172:ASN:ND2	2.41	0.53
1:D:261:ASP:O	1:D:263:GLY:N	2.42	0.53
1:J:261:ASP:O	1:J:263:GLY:N	2.41	0.53
1:I:185:VAL:HG12	1:I:200:ALA:HB2	1.90	0.53
1:3:261:ASP:O	1:3:263:GLY:N	2.42	0.53
1:j:261:ASP:O	1:j:263:GLY:N	2.41	0.53
1:c:261:ASP:O	1:c:263:GLY:N	2.41	0.53
1:O:261:ASP:O	1:O:263:GLY:N	2.41	0.53
1:f:261:ASP:O	1:f:263:GLY:N	2.41	0.53
1:4:341:ASP:O	1:J:327:ASN:ND2	2.41	0.53
1:K:185:VAL:HG12	1:K:200:ALA:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:261:ASP:O	1:d:263:GLY:N	2.41	0.53
1:4:185:VAL:HG12	1:4:200:ALA:HB2	1.90	0.53
1:H:341:ASP:O	1:a:327:ASN:ND2	2.42	0.53
1:i:261:ASP:O	1:i:263:GLY:N	2.41	0.53
1:F:341:ASP:O	1:Q:327:ASN:ND2	2.41	0.53
1:G:261:ASP:O	1:G:263:GLY:N	2.41	0.53
1:g:261:ASP:O	1:g:263:GLY:N	2.41	0.53
1:B:341:ASP:O	1:M:327:ASN:ND2	2.41	0.52
1:F:185:VAL:HG12	1:F:200:ALA:HB2	1.91	0.52
1:1:341:ASP:O	1:G:327:ASN:ND2	2.42	0.52
1:G:185:VAL:HG12	1:G:200:ALA:HB2	1.90	0.52
1:J:185:VAL:HG12	1:J:200:ALA:HB2	1.89	0.52
1:h:261:ASP:O	1:h:263:GLY:N	2.42	0.52
1:i:185:VAL:HG12	1:i:200:ALA:HB2	1.90	0.52
1:B:261:ASP:O	1:B:263:GLY:N	2.42	0.52
1:L:261:ASP:O	1:L:263:GLY:N	2.42	0.52
1:R:261:ASP:O	1:R:263:GLY:N	2.41	0.52
1:a:261:ASP:O	1:a:263:GLY:N	2.41	0.52
1:G:341:ASP:O	1:f:327:ASN:ND2	2.41	0.52
1:M:341:ASP:O	1:l:327:ASN:ND2	2.42	0.52
1:F:137:GLN:OE1	1:F:172:ASN:ND2	2.41	0.52
1:0:261:ASP:O	1:0:263:GLY:N	2.42	0.52
1:0:341:ASP:O	1:L:327:ASN:ND2	2.42	0.52
1:K:261:ASP:O	1:K:263:GLY:N	2.41	0.52
1:M:261:ASP:O	1:M:263:GLY:N	2.41	0.52
1:Q:261:ASP:O	1:Q:263:GLY:N	2.41	0.52
1:2:261:ASP:O	1:2:263:GLY:N	2.42	0.52
1:R:137:GLN:OE1	1:R:172:ASN:ND2	2.42	0.52
1:F:261:ASP:O	1:F:263:GLY:N	2.42	0.52
1:D:306:ILE:O	1:P:382:VAL:HG11	2.10	0.52
1:4:137:GLN:OE1	1:4:172:ASN:ND2	2.38	0.52
1:A:261:ASP:O	1:A:263:GLY:N	2.42	0.52
1:P:261:ASP:O	1:P:263:GLY:N	2.42	0.52
1:e:261:ASP:O	1:e:263:GLY:N	2.42	0.52
1:E:261:ASP:O	1:E:263:GLY:N	2.42	0.52
1:C:261:ASP:O	1:C:263:GLY:N	2.42	0.52
1:H:306:ILE:HG23	1:H:306:ILE:O	2.10	0.52
1:I:261:ASP:O	1:I:263:GLY:N	2.42	0.52
1:k:261:ASP:O	1:k:263:GLY:N	2.41	0.52
1:3:341:ASP:O	1:I:327:ASN:ND2	2.43	0.51
1:1:261:ASP:O	1:1:263:GLY:N	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:261:ASP:O	1:5:263:GLY:N	2.42	0.51
1:1:306:ILE:HG23	1:1:306:ILE:O	2.10	0.51
1:C:185:VAL:HG12	1:C:200:ALA:HB2	1.92	0.51
1:2:185:VAL:HG12	1:2:200:ALA:HB2	1.92	0.51
1:D:137:GLN:OE1	1:D:172:ASN:ND2	2.40	0.51
1:K:341:ASP:O	1:d:327:ASN:ND2	2.43	0.51
1:P:341:ASP:O	1:i:327:ASN:ND2	2.43	0.51
1:4:261:ASP:O	1:4:263:GLY:N	2.42	0.51
1:4:306:ILE:HG23	1:4:306:ILE:O	2.11	0.51
1:D:185:VAL:HG12	1:D:200:ALA:HB2	1.93	0.50
1:C:306:ILE:HG23	1:C:306:ILE:O	2.10	0.50
1:2:137:GLN:OE1	1:2:172:ASN:ND2	2.39	0.50
1:M:306:ILE:HG23	1:M:306:ILE:O	2.11	0.50
1:I:306:ILE:O	1:c:382:VAL:HG11	2.11	0.50
1:O:185:VAL:HG12	1:O:200:ALA:HB2	1.93	0.50
1:B:306:ILE:O	1:N:382:VAL:HG11	2.12	0.50
1:j:185:VAL:HG12	1:j:200:ALA:HB2	1.93	0.50
1:O:306:ILE:HG23	1:O:306:ILE:O	2.11	0.50
1:g:185:VAL:HG12	1:g:200:ALA:HB2	1.94	0.50
1:Q:306:ILE:HG23	1:Q:306:ILE:O	2.11	0.50
1:d:185:VAL:HG12	1:d:200:ALA:HB2	1.94	0.50
1:E:185:VAL:HG12	1:E:200:ALA:HB2	1.94	0.50
1:G:306:ILE:O	1:a:382:VAL:HG11	2.11	0.50
1:a:185:VAL:HG12	1:a:200:ALA:HB2	1.93	0.50
1:K:306:ILE:HG23	1:K:306:ILE:O	2.11	0.49
1:I:137:GLN:OE1	1:I:172:ASN:ND2	2.45	0.49
1:M:185:VAL:HG12	1:M:200:ALA:HB2	1.95	0.49
1:Q:185:VAL:HG12	1:Q:200:ALA:HB2	1.94	0.49
1:P:306:ILE:HG23	1:P:306:ILE:O	2.11	0.49
1:h:185:VAL:HG12	1:h:200:ALA:HB2	1.94	0.49
1:5:306:ILE:O	1:L:382:VAL:HG11	2.12	0.49
1:f:185:VAL:HG12	1:f:200:ALA:HB2	1.94	0.49
1:a:22:PRO:O	1:a:24:SER:N	2.46	0.49
1:f:22:PRO:O	1:f:24:SER:N	2.46	0.49
1:c:185:VAL:HG12	1:c:200:ALA:HB2	1.94	0.49
1:B:137:GLN:OE1	1:B:172:ASN:ND2	2.46	0.49
1:B:185:VAL:HG12	1:B:200:ALA:HB2	1.95	0.49
1:C:137:GLN:OE1	1:C:172:ASN:ND2	2.41	0.49
1:1:22:PRO:O	1:1:24:SER:N	2.46	0.49
1:2:22:PRO:O	1:2:24:SER:N	2.46	0.49
1:E:306:ILE:O	1:Q:382:VAL:HG11	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:306:ILE:O	1:f:382:VAL:HG11	2.12	0.48
1:C:22:PRO:O	1:C:24:SER:N	2.45	0.48
1:0:306:ILE:O	1:G:382:VAL:HG11	2.12	0.48
1:P:185:VAL:HG12	1:P:200:ALA:HB2	1.95	0.48
1:3:306:ILE:O	1:J:382:VAL:HG11	2.14	0.48
1:e:22:PRO:O	1:e:24:SER:N	2.46	0.48
1:B:22:PRO:O	1:B:24:SER:N	2.45	0.48
1:0:22:PRO:O	1:0:24:SER:N	2.45	0.48
1:1:137:GLN:OE1	1:1:172:ASN:ND2	2.46	0.48
1:k:178:LEU:O	1:k:271:THR:OG1	2.26	0.48
1:g:22:PRO:O	1:g:24:SER:N	2.46	0.48
1:D:375:THR:OG1	1:D:376:ASP:N	2.47	0.48
1:3:375:THR:OG1	1:3:376:ASP:N	2.47	0.48
1:2:375:THR:OG1	1:2:376:ASP:N	2.47	0.48
1:J:375:THR:OG1	1:J:376:ASP:N	2.47	0.48
1:M:375:THR:OG1	1:M:376:ASP:N	2.47	0.48
1:l:22:PRO:O	1:l:24:SER:N	2.46	0.48
1:G:375:THR:OG1	1:G:376:ASP:N	2.47	0.48
1:J:306:ILE:O	1:d:382:VAL:HG11	2.14	0.48
1:C:375:THR:OG1	1:C:376:ASP:N	2.47	0.47
1:2:271:THR:O	1:2:273:SER:N	2.47	0.47
1:L:185:VAL:HG12	1:L:200:ALA:HB2	1.96	0.47
1:k:271:THR:O	1:k:273:SER:N	2.47	0.47
1:B:271:THR:O	1:B:273:SER:N	2.48	0.47
1:5:271:THR:O	1:5:273:SER:N	2.47	0.47
1:H:271:THR:O	1:H:273:SER:N	2.47	0.47
1:I:271:THR:O	1:I:273:SER:N	2.47	0.47
1:M:271:THR:O	1:M:273:SER:N	2.48	0.47
1:N:271:THR:O	1:N:273:SER:N	2.47	0.47
1:A:271:THR:O	1:A:273:SER:N	2.47	0.47
1:1:271:THR:O	1:1:273:SER:N	2.47	0.47
1:L:306:ILE:HG22	1:R:363:PRO:O	2.14	0.47
1:Q:271:THR:O	1:Q:273:SER:N	2.47	0.47
1:h:271:THR:O	1:h:273:SER:N	2.47	0.47
1:k:22:PRO:O	1:k:24:SER:N	2.46	0.47
1:i:271:THR:O	1:i:273:SER:N	2.48	0.47
1:A:22:PRO:O	1:A:24:SER:N	2.45	0.47
1:G:271:THR:O	1:G:273:SER:N	2.48	0.47
1:C:271:THR:O	1:C:273:SER:N	2.47	0.47
1:R:271:THR:O	1:R:273:SER:N	2.48	0.47
1:b:271:THR:O	1:b:273:SER:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:271:THR:O	1:e:273:SER:N	2.48	0.47
1:g:375:THR:OG1	1:g:376:ASP:N	2.48	0.47
1:j:271:THR:O	1:j:273:SER:N	2.48	0.47
1:A:306:ILE:O	1:M:382:VAL:HG11	2.13	0.47
1:2:178:LEU:O	1:2:271:THR:OG1	2.26	0.47
1:2:306:ILE:O	1:I:382:VAL:HG11	2.15	0.47
1:I:319:ARG:NH1	1:I:336:VAL:O	2.48	0.47
1:P:22:PRO:O	1:P:24:SER:N	2.46	0.47
1:a:271:THR:O	1:a:273:SER:N	2.48	0.47
1:A:363:PRO:O	1:0:306:ILE:HG22	2.15	0.47
1:A:375:THR:OG1	1:A:376:ASP:N	2.47	0.47
1:E:22:PRO:O	1:E:24:SER:N	2.45	0.47
1:E:375:THR:OG1	1:E:376:ASP:N	2.47	0.47
1:G:319:ARG:NH1	1:G:336:VAL:O	2.48	0.47
1:K:319:ARG:NH1	1:K:336:VAL:O	2.48	0.47
1:N:319:ARG:NH1	1:N:336:VAL:O	2.48	0.47
1:O:271:THR:O	1:O:273:SER:N	2.48	0.47
1:O:319:ARG:NH1	1:O:336:VAL:O	2.48	0.47
1:a:306:ILE:HG22	1:g:363:PRO:O	2.15	0.47
1:f:271:THR:O	1:f:273:SER:N	2.48	0.47
1:d:271:THR:O	1:d:273:SER:N	2.48	0.47
1:l:271:THR:O	1:l:273:SER:N	2.48	0.47
1:j:319:ARG:NH1	1:j:336:VAL:O	2.48	0.47
1:F:306:ILE:O	1:R:382:VAL:HG11	2.14	0.47
1:F:375:THR:OG1	1:F:376:ASP:N	2.47	0.47
1:0:319:ARG:NH1	1:0:336:VAL:O	2.48	0.47
1:5:22:PRO:O	1:5:24:SER:N	2.45	0.47
1:L:271:THR:O	1:L:273:SER:N	2.48	0.47
1:J:271:THR:O	1:J:273:SER:N	2.47	0.47
1:M:319:ARG:NH1	1:M:336:VAL:O	2.48	0.47
1:R:306:ILE:O	1:l:382:VAL:HG11	2.14	0.47
1:b:185:VAL:HG12	1:b:200:ALA:HB2	1.96	0.47
1:b:375:THR:OG1	1:b:376:ASP:N	2.47	0.47
1:c:271:THR:O	1:c:273:SER:N	2.48	0.47
1:g:42:LYS:HB2	1:g:45:VAL:HG22	1.97	0.47
1:h:375:THR:OG1	1:h:376:ASP:N	2.47	0.47
1:F:271:THR:O	1:F:273:SER:N	2.47	0.47
1:E:306:ILE:HG22	1:K:363:PRO:O	2.15	0.47
1:4:375:THR:OG1	1:4:376:ASP:N	2.47	0.47
1:H:319:ARG:NH1	1:H:336:VAL:O	2.48	0.47
1:K:42:LYS:HB2	1:K:45:VAL:HG22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:22:PRO:O	1:I:24:SER:N	2.46	0.47
1:R:42:LYS:HB2	1:R:45:VAL:HG22	1.97	0.47
1:P:271:THR:O	1:P:273:SER:N	2.48	0.47
1:a:375:THR:OG1	1:a:376:ASP:N	2.48	0.47
1:e:42:LYS:HB2	1:e:45:VAL:HG22	1.97	0.47
1:c:319:ARG:NH1	1:c:336:VAL:O	2.48	0.47
1:F:319:ARG:NH1	1:F:336:VAL:O	2.48	0.47
1:D:271:THR:O	1:D:273:SER:N	2.47	0.47
1:R:306:ILE:HG22	1:f:363:PRO:O	2.15	0.47
1:b:319:ARG:NH1	1:b:336:VAL:O	2.48	0.47
1:d:22:PRO:O	1:d:24:SER:N	2.46	0.47
1:c:42:LYS:HB2	1:c:45:VAL:HG22	1.97	0.47
1:i:22:PRO:O	1:i:24:SER:N	2.46	0.47
1:E:271:THR:O	1:E:273:SER:N	2.47	0.46
1:K:271:THR:O	1:K:273:SER:N	2.48	0.46
1:j:22:PRO:O	1:j:24:SER:N	2.45	0.46
1:B:319:ARG:NH1	1:B:336:VAL:O	2.48	0.46
1:I:375:THR:OG1	1:I:376:ASP:N	2.48	0.46
1:Q:22:PRO:O	1:Q:24:SER:N	2.45	0.46
1:P:319:ARG:NH1	1:P:336:VAL:O	2.49	0.46
1:f:319:ARG:NH1	1:f:336:VAL:O	2.48	0.46
1:g:271:THR:O	1:g:273:SER:N	2.48	0.46
1:h:319:ARG:NH1	1:h:336:VAL:O	2.48	0.46
1:A:42:LYS:HB2	1:A:45:VAL:HG22	1.97	0.46
1:H:375:THR:OG1	1:H:376:ASP:N	2.47	0.46
1:L:375:THR:OG1	1:L:376:ASP:N	2.48	0.46
1:a:42:LYS:HB2	1:a:45:VAL:HG22	1.97	0.46
1:a:319:ARG:NH1	1:a:336:VAL:O	2.48	0.46
1:E:319:ARG:NH1	1:E:336:VAL:O	2.47	0.46
1:O:375:THR:OG1	1:O:376:ASP:N	2.47	0.46
1:5:42:LYS:HB2	1:5:45:VAL:HG22	1.98	0.46
1:4:271:THR:O	1:4:273:SER:N	2.48	0.46
1:2:42:LYS:HB2	1:2:45:VAL:HG22	1.98	0.46
1:N:42:LYS:HB2	1:N:45:VAL:HG22	1.98	0.46
1:N:375:THR:OG1	1:N:376:ASP:N	2.47	0.46
1:R:319:ARG:NH1	1:R:336:VAL:O	2.49	0.46
1:Q:319:ARG:NH1	1:Q:336:VAL:O	2.48	0.46
1:k:42:LYS:HB2	1:k:45:VAL:HG22	1.97	0.46
1:i:375:THR:OG1	1:i:376:ASP:N	2.47	0.46
1:B:375:THR:OG1	1:B:376:ASP:N	2.47	0.46
1:O:271:THR:O	1:O:273:SER:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:271:THR:O	1:3:273:SER:N	2.48	0.46
1:J:22:PRO:O	1:J:24:SER:N	2.46	0.46
1:M:178:LEU:O	1:M:271:THR:OG1	2.27	0.46
1:Q:42:LYS:HB2	1:Q:45:VAL:HG22	1.98	0.46
1:j:42:LYS:HB2	1:j:45:VAL:HG22	1.98	0.46
1:C:319:ARG:NH1	1:C:336:VAL:O	2.49	0.46
1:H:42:LYS:HB2	1:H:45:VAL:HG22	1.98	0.46
1:L:319:ARG:NH1	1:L:336:VAL:O	2.49	0.46
1:h:42:LYS:HB2	1:h:45:VAL:HG22	1.98	0.46
1:l:319:ARG:NH1	1:l:336:VAL:O	2.48	0.46
1:k:375:THR:OG1	1:k:376:ASP:N	2.47	0.46
1:A:319:ARG:NH1	1:A:336:VAL:O	2.49	0.46
1:E:42:LYS:HB2	1:E:45:VAL:HG22	1.98	0.46
1:4:319:ARG:NH1	1:4:336:VAL:O	2.49	0.46
1:L:42:LYS:HB2	1:L:45:VAL:HG22	1.98	0.46
1:N:306:ILE:HG22	1:b:363:PRO:O	2.15	0.46
1:O:22:PRO:O	1:O:24:SER:N	2.45	0.46
1:d:319:ARG:NH1	1:d:336:VAL:O	2.48	0.46
1:g:319:ARG:NH1	1:g:336:VAL:O	2.48	0.46
1:k:319:ARG:NH1	1:k:336:VAL:O	2.48	0.46
1:B:42:LYS:HB2	1:B:45:VAL:HG22	1.98	0.46
1:D:42:LYS:HB2	1:D:45:VAL:HG22	1.98	0.46
1:3:319:ARG:NH1	1:3:336:VAL:O	2.48	0.46
1:G:22:PRO:O	1:G:24:SER:N	2.45	0.46
1:J:319:ARG:NH1	1:J:336:VAL:O	2.48	0.46
1:d:42:LYS:HB2	1:d:45:VAL:HG22	1.98	0.46
1:i:319:ARG:NH1	1:i:336:VAL:O	2.48	0.46
1:F:22:PRO:O	1:F:24:SER:N	2.45	0.46
1:F:42:LYS:HB2	1:F:45:VAL:HG22	1.98	0.46
1:D:319:ARG:NH1	1:D:336:VAL:O	2.49	0.46
1:H:22:PRO:O	1:H:24:SER:N	2.46	0.46
1:O:42:LYS:HB2	1:O:45:VAL:HG22	1.98	0.46
1:e:319:ARG:NH1	1:e:336:VAL:O	2.48	0.46
1:j:375:THR:OG1	1:j:376:ASP:N	2.47	0.46
1:P:42:LYS:HB2	1:P:45:VAL:HG22	1.98	0.46
1:d:178:LEU:O	1:d:271:THR:OG1	2.27	0.46
1:B:363:PRO:O	1:1:306:ILE:HG22	2.17	0.45
1:C:42:LYS:HB2	1:C:45:VAL:HG22	1.99	0.45
1:C:178:LEU:O	1:C:271:THR:OG1	2.27	0.45
1:1:319:ARG:NH1	1:1:336:VAL:O	2.48	0.45
1:5:375:THR:OG1	1:5:376:ASP:N	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:42:LYS:HB2	1:I:45:VAL:HG22	1.98	0.45
1:N:306:ILE:O	1:h:382:VAL:HG11	2.17	0.45
1:l:42:LYS:HB2	1:l:45:VAL:HG22	1.98	0.45
1:E:363:PRO:O	1:4:306:ILE:HG22	2.16	0.45
1:5:319:ARG:NH1	1:5:336:VAL:O	2.49	0.45
1:2:319:ARG:NH1	1:2:336:VAL:O	2.49	0.45
1:K:22:PRO:O	1:K:24:SER:N	2.46	0.45
1:J:42:LYS:HB2	1:J:45:VAL:HG22	1.99	0.45
1:M:42:LYS:HB2	1:M:45:VAL:HG22	1.98	0.45
1:1:42:LYS:HB2	1:1:45:VAL:HG22	1.98	0.45
1:5:306:ILE:O	1:5:306:ILE:HG23	2.17	0.45
1:4:42:LYS:HB2	1:4:45:VAL:HG22	1.99	0.45
1:3:42:LYS:HB2	1:3:45:VAL:HG22	1.99	0.45
1:L:22:PRO:O	1:L:24:SER:N	2.46	0.45
1:I:306:ILE:HG22	1:O:363:PRO:O	2.16	0.45
1:1:333:ASN:OD1	1:1:334:PHE:N	2.50	0.45
1:G:306:ILE:O	1:G:306:ILE:HG23	2.17	0.45
1:N:22:PRO:O	1:N:24:SER:N	2.45	0.45
1:c:22:PRO:O	1:c:24:SER:N	2.46	0.45
1:k:147:ALA:O	1:k:151:ARG:N	2.50	0.45
1:i:42:LYS:HB2	1:i:45:VAL:HG22	1.99	0.45
1:A:306:ILE:HG22	1:G:363:PRO:O	2.17	0.45
1:B:333:ASN:OD1	1:B:334:PHE:N	2.50	0.45
1:C:363:PRO:O	1:2:306:ILE:HG22	2.17	0.45
1:N:147:ALA:O	1:N:151:ARG:N	2.50	0.45
1:A:306:ILE:O	1:A:306:ILE:HG23	2.17	0.45
1:C:306:ILE:HG22	1:I:363:PRO:O	2.17	0.45
1:O:306:ILE:O	1:O:306:ILE:HG23	2.17	0.45
1:O:333:ASN:OD1	1:O:334:PHE:N	2.50	0.45
1:G:147:ALA:O	1:G:151:ARG:N	2.50	0.45
1:G:306:ILE:HG22	1:M:363:PRO:O	2.17	0.45
1:L:178:LEU:O	1:L:271:THR:OG1	2.26	0.45
1:I:178:LEU:O	1:I:271:THR:OG1	2.27	0.45
1:a:178:LEU:O	1:a:271:THR:OG1	2.28	0.45
1:E:306:ILE:O	1:E:306:ILE:HG23	2.17	0.45
1:D:306:ILE:O	1:D:306:ILE:HG23	2.17	0.45
1:4:22:PRO:O	1:4:24:SER:N	2.46	0.45
1:L:306:ILE:O	1:L:306:ILE:HG23	2.17	0.45
1:M:147:ALA:O	1:M:151:ARG:N	2.51	0.45
1:Q:375:THR:OG1	1:Q:376:ASP:N	2.47	0.45
1:l:147:ALA:O	1:l:151:ARG:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:333:ASN:OD1	1:E:334:PHE:N	2.50	0.44
1:2:306:ILE:O	1:2:306:ILE:HG23	2.17	0.44
1:I:306:ILE:O	1:I:306:ILE:HG23	2.17	0.44
1:R:306:ILE:O	1:R:306:ILE:HG23	2.17	0.44
1:f:147:ALA:O	1:f:151:ARG:N	2.50	0.44
1:g:147:ALA:O	1:g:151:ARG:N	2.50	0.44
1:B:306:ILE:O	1:B:306:ILE:HG23	2.17	0.44
1:F:178:LEU:O	1:F:271:THR:OG1	2.28	0.44
1:C:147:ALA:O	1:C:151:ARG:N	2.50	0.44
1:G:42:LYS:HB2	1:G:45:VAL:HG22	1.99	0.44
1:P:306:ILE:HG22	1:d:363:PRO:O	2.17	0.44
1:b:42:LYS:HB2	1:b:45:VAL:HG22	1.99	0.44
1:b:147:ALA:O	1:b:151:ARG:N	2.51	0.44
1:f:333:ASN:OD1	1:f:334:PHE:N	2.50	0.44
1:e:333:ASN:OD1	1:e:334:PHE:N	2.50	0.44
1:d:375:THR:OG1	1:d:376:ASP:N	2.47	0.44
1:g:178:LEU:O	1:g:271:THR:OG1	2.27	0.44
1:B:147:ALA:O	1:B:151:ARG:N	2.50	0.44
1:D:147:ALA:O	1:D:151:ARG:N	2.51	0.44
1:0:42:LYS:HB2	1:0:45:VAL:HG22	1.99	0.44
1:4:333:ASN:OD1	1:4:334:PHE:N	2.50	0.44
1:2:147:ALA:O	1:2:151:ARG:N	2.51	0.44
1:K:375:THR:OG1	1:K:376:ASP:N	2.48	0.44
1:a:147:ALA:O	1:a:151:ARG:N	2.51	0.44
1:h:147:ALA:O	1:h:151:ARG:N	2.50	0.44
1:j:147:ALA:O	1:j:151:ARG:N	2.50	0.44
1:F:147:ALA:O	1:F:151:ARG:N	2.50	0.44
1:4:178:LEU:O	1:4:271:THR:OG1	2.27	0.44
1:J:306:ILE:HG22	1:P:363:PRO:O	2.16	0.44
1:f:42:LYS:HB2	1:f:45:VAL:HG22	1.99	0.44
1:h:22:PRO:O	1:h:24:SER:N	2.46	0.44
1:l:333:ASN:OD1	1:l:334:PHE:N	2.50	0.44
1:L:147:ALA:O	1:L:151:ARG:N	2.50	0.44
1:I:333:ASN:OD1	1:I:334:PHE:N	2.50	0.44
1:R:333:ASN:OD1	1:R:334:PHE:N	2.50	0.44
1:c:333:ASN:OD1	1:c:334:PHE:N	2.50	0.44
1:E:178:LEU:O	1:E:271:THR:OG1	2.27	0.44
1:3:147:ALA:O	1:3:151:ARG:N	2.51	0.44
1:H:147:ALA:O	1:H:151:ARG:N	2.51	0.44
1:H:333:ASN:OD1	1:H:334:PHE:N	2.50	0.44
1:J:306:ILE:O	1:J:306:ILE:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:306:ILE:HG22	1:e:363:PRO:O	2.18	0.44
1:O:333:ASN:OD1	1:O:334:PHE:N	2.50	0.44
1:b:22:PRO:O	1:b:24:SER:N	2.46	0.44
1:c:147:ALA:O	1:c:151:ARG:N	2.50	0.44
1:i:147:ALA:O	1:i:151:ARG:N	2.50	0.44
1:I:147:ALA:O	1:I:151:ARG:N	2.51	0.44
1:e:147:ALA:O	1:e:151:ARG:N	2.51	0.44
1:e:306:ILE:HG22	1:k:363:PRO:O	2.18	0.44
1:j:178:LEU:O	1:j:271:THR:OG1	2.27	0.44
1:i:333:ASN:OD1	1:i:334:PHE:N	2.50	0.44
1:E:147:ALA:O	1:E:151:ARG:N	2.50	0.44
1:3:22:PRO:O	1:3:24:SER:N	2.45	0.44
1:L:333:ASN:OD1	1:L:334:PHE:N	2.50	0.44
1:R:147:ALA:O	1:R:151:ARG:N	2.51	0.44
1:A:147:ALA:O	1:A:151:ARG:N	2.51	0.44
1:D:22:PRO:O	1:D:24:SER:N	2.45	0.44
1:1:147:ALA:O	1:1:151:ARG:N	2.51	0.44
1:5:147:ALA:O	1:5:151:ARG:N	2.51	0.44
1:O:306:ILE:HG22	1:c:363:PRO:O	2.18	0.44
1:e:375:THR:OG1	1:e:376:ASP:N	2.47	0.44
1:i:178:LEU:O	1:i:271:THR:OG1	2.26	0.44
1:4:147:ALA:O	1:4:151:ARG:N	2.50	0.43
1:3:306:ILE:O	1:3:306:ILE:HG23	2.17	0.43
1:K:147:ALA:O	1:K:151:ARG:N	2.51	0.43
1:M:22:PRO:O	1:M:24:SER:N	2.45	0.43
1:Q:333:ASN:OD1	1:Q:334:PHE:N	2.50	0.43
1:b:306:ILE:HG22	1:h:363:PRO:O	2.17	0.43
1:d:147:ALA:O	1:d:151:ARG:N	2.50	0.43
1:g:333:ASN:OD1	1:g:334:PHE:N	2.50	0.43
1:J:147:ALA:O	1:J:151:ARG:N	2.51	0.43
1:Q:147:ALA:O	1:Q:151:ARG:N	2.50	0.43
1:1:375:THR:OG1	1:1:376:ASP:N	2.47	0.43
1:2:333:ASN:OD1	1:2:334:PHE:N	2.50	0.43
1:R:22:PRO:O	1:R:24:SER:N	2.46	0.43
1:O:147:ALA:O	1:O:151:ARG:N	2.50	0.43
1:F:306:ILE:O	1:F:306:ILE:HG23	2.17	0.43
1:C:333:ASN:OD1	1:C:334:PHE:N	2.50	0.43
1:f:306:ILE:HG22	1:l:363:PRO:O	2.19	0.43
1:H:306:ILE:HG22	1:N:363:PRO:O	2.18	0.43
1:K:306:ILE:HG22	1:Q:363:PRO:O	2.19	0.43
1:R:375:THR:OG1	1:R:376:ASP:N	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:333:ASN:OD1	1:a:334:PHE:N	2.50	0.43
1:K:333:ASN:OD1	1:K:334:PHE:N	2.50	0.43
1:N:306:ILE:O	1:N:306:ILE:HG23	2.18	0.43
1:P:147:ALA:O	1:P:151:ARG:N	2.51	0.43
1:O:178:LEU:O	1:O:271:THR:OG1	2.27	0.43
1:a:306:ILE:HG23	1:a:306:ILE:O	2.18	0.43
1:b:306:ILE:HG23	1:b:306:ILE:O	2.18	0.43
1:d:306:ILE:HG22	1:j:363:PRO:O	2.17	0.43
1:N:333:ASN:OD1	1:N:334:PHE:N	2.50	0.43
1:O:147:ALA:O	1:O:151:ARG:N	2.51	0.43
1:H:306:ILE:O	1:b:382:VAL:HG11	2.19	0.42
1:M:333:ASN:OD1	1:M:334:PHE:N	2.50	0.42
1:P:333:ASN:OD1	1:P:334:PHE:N	2.50	0.42
1:f:306:ILE:HG23	1:f:306:ILE:O	2.19	0.42
1:D:306:ILE:HG22	1:J:363:PRO:O	2.18	0.42
1:c:375:THR:OG1	1:c:376:ASP:N	2.48	0.42
1:F:333:ASN:OD1	1:F:334:PHE:N	2.50	0.42
1:K:307:THR:HG22	1:K:308:LYS:N	2.35	0.42
1:M:306:ILE:HG22	1:a:363:PRO:O	2.20	0.42
1:c:306:ILE:HG23	1:c:306:ILE:O	2.19	0.42
1:j:333:ASN:OD1	1:j:334:PHE:N	2.50	0.42
1:D:363:PRO:O	1:3:306:ILE:HG22	2.18	0.42
1:G:333:ASN:OD1	1:G:334:PHE:N	2.50	0.42
1:J:333:ASN:OD1	1:J:334:PHE:N	2.50	0.42
1:e:306:ILE:HG23	1:e:306:ILE:O	2.19	0.42
1:R:178:LEU:O	1:R:271:THR:OG1	2.27	0.42
1:c:306:ILE:HG22	1:i:363:PRO:O	2.20	0.42
1:D:333:ASN:OD1	1:D:334:PHE:N	2.50	0.42
1:C:306:ILE:O	1:O:382:VAL:HG11	2.20	0.42
1:1:116:ASP:OD2	1:1:116:ASP:N	2.53	0.42
1:5:333:ASN:OD1	1:5:334:PHE:N	2.50	0.42
1:A:333:ASN:OD1	1:A:334:PHE:N	2.50	0.42
1:F:363:PRO:O	1:5:306:ILE:HG22	2.19	0.42
1:M:116:ASP:OD2	1:M:116:ASP:N	2.53	0.42
1:d:306:ILE:O	1:d:306:ILE:HG23	2.19	0.42
1:k:333:ASN:OD1	1:k:334:PHE:N	2.50	0.42
1:4:307:THR:HG22	1:4:308:LYS:N	2.35	0.42
1:3:333:ASN:OD1	1:3:334:PHE:N	2.50	0.42
1:c:116:ASP:N	1:c:116:ASP:OD2	2.53	0.42
1:h:333:ASN:OD1	1:h:334:PHE:N	2.50	0.42
1:1:178:LEU:O	1:1:271:THR:OG1	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:86:GLU:OE1	1:3:86:GLU:N	2.50	0.41
1:P:307:THR:HG22	1:P:308:LYS:N	2.35	0.41
1:P:375:THR:OG1	1:P:376:ASP:N	2.48	0.41
1:g:307:THR:HG22	1:g:308:LYS:N	2.35	0.41
1:j:307:THR:HG22	1:j:308:LYS:N	2.35	0.41
1:B:307:THR:HG22	1:B:308:LYS:N	2.35	0.41
1:4:116:ASP:N	1:4:116:ASP:OD2	2.53	0.41
1:3:116:ASP:OD2	1:3:116:ASP:N	2.53	0.41
1:H:307:THR:HG22	1:H:308:LYS:N	2.35	0.41
1:L:116:ASP:OD2	1:L:116:ASP:N	2.54	0.41
1:O:307:THR:HG22	1:O:308:LYS:N	2.35	0.41
1:F:307:THR:HG22	1:F:308:LYS:N	2.36	0.41
1:I:307:THR:HG22	1:I:308:LYS:N	2.35	0.41
1:R:307:THR:HG22	1:R:308:LYS:N	2.36	0.41
1:d:333:ASN:OD1	1:d:334:PHE:N	2.50	0.41
1:g:86:GLU:OE1	1:g:86:GLU:N	2.51	0.41
1:h:116:ASP:N	1:h:116:ASP:OD2	2.54	0.41
1:f:116:ASP:OD2	1:f:116:ASP:N	2.54	0.41
1:e:307:THR:HG22	1:e:308:LYS:N	2.36	0.41
1:j:116:ASP:OD2	1:j:116:ASP:N	2.53	0.41
1:F:306:ILE:HG22	1:L:363:PRO:O	2.21	0.41
1:l:307:THR:HG22	1:l:308:LYS:N	2.35	0.41
1:P:302:VAL:HG12	1:P:303:ASP:H	1.85	0.41
1:P:306:ILE:O	1:j:382:VAL:HG11	2.20	0.41
1:O:307:THR:HG22	1:O:308:LYS:N	2.36	0.41
1:H:116:ASP:OD2	1:H:116:ASP:N	2.54	0.41
1:K:306:ILE:O	1:e:382:VAL:HG11	2.20	0.41
1:Q:116:ASP:OD2	1:Q:116:ASP:N	2.54	0.41
1:l:307:THR:HG22	1:l:308:LYS:N	2.36	0.41
1:k:116:ASP:OD2	1:k:116:ASP:N	2.54	0.41
1:A:116:ASP:OD2	1:A:116:ASP:N	2.54	0.41
1:a:307:THR:HG22	1:a:308:LYS:N	2.35	0.41
1:f:307:THR:HG22	1:f:308:LYS:N	2.36	0.41
1:c:178:LEU:O	1:c:271:THR:OG1	2.28	0.41
1:c:307:THR:HG22	1:c:308:LYS:N	2.36	0.41
1:l:306:ILE:HG23	1:l:306:ILE:O	2.21	0.41
1:j:306:ILE:HG23	1:j:306:ILE:O	2.21	0.41
1:E:116:ASP:OD2	1:E:116:ASP:N	2.53	0.41
1:D:307:THR:HG22	1:D:308:LYS:N	2.35	0.41
1:5:116:ASP:N	1:5:116:ASP:OD2	2.54	0.41
1:G:307:THR:HG22	1:G:308:LYS:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:307:THR:HG22	1:Q:308:LYS:N	2.35	0.41
1:g:306:ILE:HG23	1:g:306:ILE:O	2.21	0.41
1:i:307:THR:HG22	1:i:308:LYS:N	2.36	0.41
1:B:178:LEU:O	1:B:271:THR:OG1	2.27	0.41
1:B:306:ILE:HG22	1:H:363:PRO:O	2.20	0.41
1:E:302:VAL:HG12	1:E:303:ASP:H	1.85	0.41
1:D:308:LYS:N	1:P:382:VAL:HG13	2.36	0.41
1:C:116:ASP:OD2	1:C:116:ASP:N	2.54	0.41
1:C:307:THR:HG22	1:C:308:LYS:N	2.36	0.41
1:3:307:THR:HG22	1:3:308:LYS:N	2.36	0.41
1:2:116:ASP:OD2	1:2:116:ASP:N	2.53	0.41
1:G:302:VAL:HG12	1:G:303:ASP:H	1.86	0.41
1:J:307:THR:HG22	1:J:308:LYS:N	2.36	0.41
1:N:307:THR:HG22	1:N:308:LYS:N	2.36	0.41
1:a:302:VAL:HG12	1:a:303:ASP:H	1.86	0.41
1:b:86:GLU:OE1	1:b:86:GLU:N	2.51	0.41
1:b:333:ASN:OD1	1:b:334:PHE:N	2.50	0.41
1:g:116:ASP:OD2	1:g:116:ASP:N	2.54	0.41
1:l:375:THR:OG1	1:l:376:ASP:N	2.48	0.41
1:1:306:ILE:O	1:H:382:VAL:HG11	2.20	0.41
1:5:307:THR:HG22	1:5:308:LYS:N	2.36	0.41
1:M:86:GLU:OE1	1:M:86:GLU:N	2.51	0.41
1:M:307:THR:HG22	1:M:308:LYS:N	2.35	0.41
1:P:116:ASP:N	1:P:116:ASP:OD2	2.53	0.41
1:b:116:ASP:N	1:b:116:ASP:OD2	2.54	0.41
1:d:116:ASP:OD2	1:d:116:ASP:N	2.54	0.41
1:i:116:ASP:OD2	1:i:116:ASP:N	2.54	0.41
1:B:116:ASP:OD2	1:B:116:ASP:N	2.54	0.40
1:E:307:THR:HG22	1:E:308:LYS:N	2.36	0.40
1:D:302:VAL:HG12	1:D:303:ASP:H	1.85	0.40
1:C:308:LYS:N	1:O:382:VAL:HG13	2.36	0.40
1:N:116:ASP:N	1:N:116:ASP:OD2	2.54	0.40
1:Q:81:VAL:HG13	1:Q:81:VAL:O	2.21	0.40
1:b:307:THR:HG22	1:b:308:LYS:N	2.36	0.40
1:f:375:THR:OG1	1:f:376:ASP:N	2.48	0.40
1:d:302:VAL:HG12	1:d:303:ASP:H	1.86	0.40
1:d:307:THR:HG22	1:d:308:LYS:N	2.36	0.40
1:h:307:THR:HG22	1:h:308:LYS:N	2.36	0.40
1:k:306:ILE:HG23	1:k:306:ILE:O	2.21	0.40
1:O:86:GLU:OE1	1:O:86:GLU:N	2.50	0.40
1:O:306:ILE:O	1:i:382:VAL:HG11	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:302:VAL:HG12	1:f:303:ASP:H	1.85	0.40
1:l:116:ASP:OD2	1:l:116:ASP:N	2.53	0.40
1:A:307:THR:HG22	1:A:308:LYS:N	2.36	0.40
1:G:116:ASP:OD2	1:G:116:ASP:N	2.54	0.40
1:J:116:ASP:OD2	1:J:116:ASP:N	2.54	0.40
1:Q:306:ILE:O	1:k:382:VAL:HG11	2.21	0.40
1:i:306:ILE:O	1:i:306:ILE:HG23	2.21	0.40
1:1:223:ASN:N	1:1:266:LEU:O	2.54	0.40
1:4:306:ILE:O	1:K:382:VAL:HG11	2.22	0.40
1:O:116:ASP:OD2	1:O:116:ASP:N	2.54	0.40
1:G:81:VAL:O	1:G:81:VAL:HG13	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	381/386 (99%)	307 (81%)	57 (15%)	17 (4%)	2	19
1	1	381/386 (99%)	307 (81%)	57 (15%)	17 (4%)	2	19
1	2	381/386 (99%)	307 (81%)	57 (15%)	17 (4%)	2	19
1	3	381/386 (99%)	307 (81%)	57 (15%)	17 (4%)	2	19
1	4	381/386 (99%)	308 (81%)	56 (15%)	17 (4%)	2	19
1	5	381/386 (99%)	309 (81%)	55 (14%)	17 (4%)	2	19
1	A	381/386 (99%)	309 (81%)	54 (14%)	18 (5%)	2	19
1	B	381/386 (99%)	307 (81%)	56 (15%)	18 (5%)	2	19
1	C	381/386 (99%)	307 (81%)	56 (15%)	18 (5%)	2	19
1	D	381/386 (99%)	308 (81%)	55 (14%)	18 (5%)	2	19
1	E	381/386 (99%)	308 (81%)	56 (15%)	17 (4%)	2	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	381/386 (99%)	306 (80%)	57 (15%)	18 (5%)	2	19
1	G	381/386 (99%)	308 (81%)	55 (14%)	18 (5%)	2	19
1	H	381/386 (99%)	309 (81%)	54 (14%)	18 (5%)	2	19
1	I	381/386 (99%)	307 (81%)	56 (15%)	18 (5%)	2	19
1	J	381/386 (99%)	308 (81%)	55 (14%)	18 (5%)	2	19
1	K	381/386 (99%)	309 (81%)	54 (14%)	18 (5%)	2	19
1	L	381/386 (99%)	308 (81%)	55 (14%)	18 (5%)	2	19
1	M	381/386 (99%)	309 (81%)	54 (14%)	18 (5%)	2	19
1	N	381/386 (99%)	307 (81%)	56 (15%)	18 (5%)	2	19
1	O	381/386 (99%)	309 (81%)	54 (14%)	18 (5%)	2	19
1	P	381/386 (99%)	309 (81%)	54 (14%)	18 (5%)	2	19
1	Q	381/386 (99%)	308 (81%)	55 (14%)	18 (5%)	2	19
1	R	381/386 (99%)	307 (81%)	56 (15%)	18 (5%)	2	19
1	a	381/386 (99%)	308 (81%)	55 (14%)	18 (5%)	2	19
1	b	381/386 (99%)	309 (81%)	54 (14%)	18 (5%)	2	19
1	c	381/386 (99%)	307 (81%)	56 (15%)	18 (5%)	2	19
1	d	381/386 (99%)	307 (81%)	56 (15%)	18 (5%)	2	19
1	e	381/386 (99%)	308 (81%)	55 (14%)	18 (5%)	2	19
1	f	381/386 (99%)	308 (81%)	55 (14%)	18 (5%)	2	19
1	g	381/386 (99%)	308 (81%)	55 (14%)	18 (5%)	2	19
1	h	381/386 (99%)	308 (81%)	55 (14%)	18 (5%)	2	19
1	i	381/386 (99%)	308 (81%)	55 (14%)	18 (5%)	2	19
1	j	381/386 (99%)	308 (81%)	55 (14%)	18 (5%)	2	19
1	k	381/386 (99%)	308 (81%)	55 (14%)	18 (5%)	2	19
1	l	381/386 (99%)	307 (81%)	56 (15%)	18 (5%)	2	19
All	All	13716/13896 (99%)	11082 (81%)	1993 (14%)	641 (5%)	3	19

All (641) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	VAL
1	B	9	VAL
1	F	9	VAL

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Mol	Chain	Res	Type
1	E	9	VAL
1	D	9	VAL
1	C	9	VAL
1	0	9	VAL
1	1	9	VAL
1	5	9	VAL
1	4	9	VAL
1	3	9	VAL
1	2	9	VAL
1	G	9	VAL
1	H	9	VAL
1	L	9	VAL
1	K	9	VAL
1	J	9	VAL
1	I	9	VAL
1	M	9	VAL
1	N	9	VAL
1	R	9	VAL
1	Q	9	VAL
1	P	9	VAL
1	O	9	VAL
1	a	9	VAL
1	b	9	VAL
1	f	9	VAL
1	e	9	VAL
1	d	9	VAL
1	c	9	VAL
1	g	9	VAL
1	h	9	VAL
1	l	9	VAL
1	k	9	VAL
1	j	9	VAL
1	i	9	VAL
1	A	7	VAL
1	A	102	ILE
1	A	160	ASN
1	A	161	SER
1	A	263	GLY
1	A	301	ALA
1	A	302	VAL
1	B	7	VAL
1	B	102	ILE

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Mol	Chain	Res	Type
1	B	160	ASN
1	B	161	SER
1	B	263	GLY
1	B	301	ALA
1	B	302	VAL
1	F	7	VAL
1	F	102	ILE
1	F	160	ASN
1	F	161	SER
1	F	263	GLY
1	F	301	ALA
1	F	302	VAL
1	E	7	VAL
1	E	102	ILE
1	E	160	ASN
1	E	161	SER
1	E	263	GLY
1	E	301	ALA
1	E	302	VAL
1	D	7	VAL
1	D	102	ILE
1	D	160	ASN
1	D	161	SER
1	D	263	GLY
1	D	301	ALA
1	D	302	VAL
1	C	7	VAL
1	C	102	ILE
1	C	160	ASN
1	C	161	SER
1	C	263	GLY
1	C	301	ALA
1	C	302	VAL
1	0	7	VAL
1	0	102	ILE
1	0	160	ASN
1	0	161	SER
1	0	263	GLY
1	0	301	ALA
1	0	302	VAL
1	1	7	VAL
1	1	102	ILE

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Mol	Chain	Res	Type
1	1	160	ASN
1	1	161	SER
1	1	263	GLY
1	1	301	ALA
1	1	302	VAL
1	5	7	VAL
1	5	102	ILE
1	5	160	ASN
1	5	161	SER
1	5	263	GLY
1	5	301	ALA
1	5	302	VAL
1	4	7	VAL
1	4	102	ILE
1	4	160	ASN
1	4	161	SER
1	4	263	GLY
1	4	301	ALA
1	4	302	VAL
1	3	7	VAL
1	3	102	ILE
1	3	160	ASN
1	3	161	SER
1	3	263	GLY
1	3	301	ALA
1	3	302	VAL
1	2	7	VAL
1	2	102	ILE
1	2	160	ASN
1	2	161	SER
1	2	263	GLY
1	2	301	ALA
1	2	302	VAL
1	G	7	VAL
1	G	102	ILE
1	G	160	ASN
1	G	161	SER
1	G	263	GLY
1	G	301	ALA
1	G	302	VAL
1	H	7	VAL
1	H	102	ILE

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Mol	Chain	Res	Type
1	H	160	ASN
1	H	161	SER
1	H	263	GLY
1	H	301	ALA
1	H	302	VAL
1	L	7	VAL
1	L	102	ILE
1	L	160	ASN
1	L	161	SER
1	L	263	GLY
1	L	301	ALA
1	L	302	VAL
1	K	7	VAL
1	K	102	ILE
1	K	160	ASN
1	K	161	SER
1	K	230	THR
1	K	263	GLY
1	K	301	ALA
1	K	302	VAL
1	J	7	VAL
1	J	102	ILE
1	J	160	ASN
1	J	161	SER
1	J	263	GLY
1	J	301	ALA
1	J	302	VAL
1	I	7	VAL
1	I	102	ILE
1	I	160	ASN
1	I	161	SER
1	I	263	GLY
1	I	301	ALA
1	I	302	VAL
1	M	7	VAL
1	M	102	ILE
1	M	160	ASN
1	M	161	SER
1	M	263	GLY
1	M	301	ALA
1	M	302	VAL
1	N	7	VAL

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Mol	Chain	Res	Type
1	N	102	ILE
1	N	160	ASN
1	N	161	SER
1	N	263	GLY
1	N	301	ALA
1	N	302	VAL
1	R	7	VAL
1	R	102	ILE
1	R	160	ASN
1	R	161	SER
1	R	263	GLY
1	R	302	VAL
1	Q	7	VAL
1	Q	102	ILE
1	Q	160	ASN
1	Q	161	SER
1	Q	263	GLY
1	Q	301	ALA
1	Q	302	VAL
1	P	7	VAL
1	P	102	ILE
1	P	160	ASN
1	P	161	SER
1	P	263	GLY
1	P	301	ALA
1	P	302	VAL
1	O	7	VAL
1	O	102	ILE
1	O	160	ASN
1	O	161	SER
1	O	263	GLY
1	O	301	ALA
1	O	302	VAL
1	a	7	VAL
1	a	102	ILE
1	a	160	ASN
1	a	161	SER
1	a	230	THR
1	a	263	GLY
1	a	301	ALA
1	a	302	VAL
1	b	7	VAL

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Mol	Chain	Res	Type
1	b	102	ILE
1	b	160	ASN
1	b	161	SER
1	b	263	GLY
1	b	301	ALA
1	b	302	VAL
1	f	7	VAL
1	f	102	ILE
1	f	160	ASN
1	f	161	SER
1	f	263	GLY
1	f	301	ALA
1	f	302	VAL
1	e	7	VAL
1	e	102	ILE
1	e	160	ASN
1	e	161	SER
1	e	263	GLY
1	e	301	ALA
1	e	302	VAL
1	d	7	VAL
1	d	102	ILE
1	d	160	ASN
1	d	161	SER
1	d	230	THR
1	d	263	GLY
1	d	301	ALA
1	d	302	VAL
1	c	7	VAL
1	c	102	ILE
1	c	160	ASN
1	c	161	SER
1	c	263	GLY
1	c	301	ALA
1	c	302	VAL
1	g	7	VAL
1	g	102	ILE
1	g	160	ASN
1	g	161	SER
1	g	263	GLY
1	g	301	ALA
1	g	302	VAL

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Mol	Chain	Res	Type
1	h	7	VAL
1	h	102	ILE
1	h	160	ASN
1	h	161	SER
1	h	263	GLY
1	h	301	ALA
1	h	302	VAL
1	l	7	VAL
1	l	102	ILE
1	l	160	ASN
1	l	161	SER
1	l	263	GLY
1	l	301	ALA
1	l	302	VAL
1	k	7	VAL
1	k	102	ILE
1	k	160	ASN
1	k	161	SER
1	k	263	GLY
1	k	301	ALA
1	k	302	VAL
1	j	7	VAL
1	j	102	ILE
1	j	160	ASN
1	j	161	SER
1	j	263	GLY
1	j	301	ALA
1	j	302	VAL
1	i	7	VAL
1	i	102	ILE
1	i	160	ASN
1	i	161	SER
1	i	263	GLY
1	i	301	ALA
1	i	302	VAL
1	A	230	THR
1	A	272	LEU
1	A	383	LEU
1	B	230	THR
1	B	262	ASP
1	B	272	LEU
1	B	383	LEU

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Mol	Chain	Res	Type
1	F	230	THR
1	F	262	ASP
1	F	272	LEU
1	F	383	LEU
1	E	230	THR
1	E	262	ASP
1	E	272	LEU
1	E	383	LEU
1	D	230	THR
1	D	262	ASP
1	D	272	LEU
1	D	383	LEU
1	C	230	THR
1	C	262	ASP
1	C	272	LEU
1	C	383	LEU
1	0	230	THR
1	0	262	ASP
1	0	272	LEU
1	0	383	LEU
1	1	230	THR
1	1	262	ASP
1	1	272	LEU
1	1	383	LEU
1	5	230	THR
1	5	262	ASP
1	5	272	LEU
1	5	383	LEU
1	4	230	THR
1	4	262	ASP
1	4	272	LEU
1	4	383	LEU
1	3	230	THR
1	3	262	ASP
1	3	272	LEU
1	3	383	LEU
1	2	230	THR
1	2	262	ASP
1	2	272	LEU
1	2	383	LEU
1	G	230	THR
1	G	262	ASP

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Mol	Chain	Res	Type
1	G	272	LEU
1	G	383	LEU
1	H	230	THR
1	H	272	LEU
1	H	383	LEU
1	L	230	THR
1	L	262	ASP
1	L	272	LEU
1	L	383	LEU
1	K	262	ASP
1	K	272	LEU
1	K	383	LEU
1	J	230	THR
1	J	272	LEU
1	J	383	LEU
1	I	230	THR
1	I	272	LEU
1	I	383	LEU
1	M	230	THR
1	M	272	LEU
1	M	383	LEU
1	N	230	THR
1	N	262	ASP
1	N	272	LEU
1	N	383	LEU
1	R	230	THR
1	R	262	ASP
1	R	272	LEU
1	R	301	ALA
1	R	383	LEU
1	Q	230	THR
1	Q	262	ASP
1	Q	272	LEU
1	Q	383	LEU
1	P	230	THR
1	P	272	LEU
1	P	383	LEU
1	O	230	THR
1	O	272	LEU
1	O	383	LEU
1	a	272	LEU
1	a	383	LEU

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Mol	Chain	Res	Type
1	b	230	THR
1	b	272	LEU
1	b	383	LEU
1	f	230	THR
1	f	272	LEU
1	f	383	LEU
1	e	230	THR
1	e	272	LEU
1	e	383	LEU
1	d	272	LEU
1	d	383	LEU
1	c	230	THR
1	c	272	LEU
1	c	383	LEU
1	g	230	THR
1	g	272	LEU
1	g	383	LEU
1	h	230	THR
1	h	272	LEU
1	h	383	LEU
1	l	230	THR
1	l	272	LEU
1	l	383	LEU
1	k	230	THR
1	k	272	LEU
1	k	383	LEU
1	j	230	THR
1	j	272	LEU
1	j	383	LEU
1	i	230	THR
1	i	262	ASP
1	i	272	LEU
1	i	383	LEU
1	A	262	ASP
1	H	262	ASP
1	J	262	ASP
1	I	262	ASP
1	M	262	ASP
1	P	262	ASP
1	O	262	ASP
1	a	262	ASP
1	b	262	ASP

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Mol	Chain	Res	Type
1	f	262	ASP
1	e	262	ASP
1	d	262	ASP
1	c	262	ASP
1	g	262	ASP
1	h	262	ASP
1	l	262	ASP
1	k	262	ASP
1	j	262	ASP
1	A	4	PHE
1	A	365	ALA
1	B	4	PHE
1	F	4	PHE
1	E	4	PHE
1	D	4	PHE
1	D	24	SER
1	D	365	ALA
1	C	4	PHE
1	C	365	ALA
1	0	4	PHE
1	1	4	PHE
1	5	4	PHE
1	4	4	PHE
1	3	4	PHE
1	2	4	PHE
1	G	4	PHE
1	G	365	ALA
1	H	4	PHE
1	H	365	ALA
1	L	4	PHE
1	K	4	PHE
1	K	365	ALA
1	J	4	PHE
1	J	365	ALA
1	I	4	PHE
1	I	365	ALA
1	M	4	PHE
1	M	365	ALA
1	N	4	PHE
1	R	3	PHE
1	R	4	PHE
1	R	365	ALA

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Mol	Chain	Res	Type
1	Q	4	PHE
1	Q	365	ALA
1	P	4	PHE
1	P	365	ALA
1	O	4	PHE
1	O	365	ALA
1	a	4	PHE
1	a	365	ALA
1	b	4	PHE
1	f	4	PHE
1	e	4	PHE
1	e	365	ALA
1	d	4	PHE
1	d	365	ALA
1	c	4	PHE
1	g	4	PHE
1	h	4	PHE
1	h	365	ALA
1	l	4	PHE
1	l	365	ALA
1	k	4	PHE
1	k	365	ALA
1	j	4	PHE
1	i	4	PHE
1	i	365	ALA
1	A	3	PHE
1	A	24	SER
1	A	44	ASN
1	B	3	PHE
1	B	24	SER
1	B	44	ASN
1	B	365	ALA
1	F	3	PHE
1	F	24	SER
1	F	44	ASN
1	F	365	ALA
1	E	3	PHE
1	E	24	SER
1	E	44	ASN
1	D	3	PHE
1	D	44	ASN
1	C	3	PHE

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Mol	Chain	Res	Type
1	C	24	SER
1	C	44	ASN
1	0	3	PHE
1	0	24	SER
1	0	44	ASN
1	1	3	PHE
1	1	24	SER
1	1	44	ASN
1	5	3	PHE
1	5	24	SER
1	5	44	ASN
1	4	3	PHE
1	4	24	SER
1	4	44	ASN
1	3	3	PHE
1	3	24	SER
1	3	44	ASN
1	2	3	PHE
1	2	24	SER
1	2	44	ASN
1	G	3	PHE
1	G	24	SER
1	G	44	ASN
1	H	3	PHE
1	H	24	SER
1	H	44	ASN
1	L	3	PHE
1	L	24	SER
1	L	44	ASN
1	L	365	ALA
1	K	3	PHE
1	K	24	SER
1	K	44	ASN
1	J	3	PHE
1	J	24	SER
1	J	44	ASN
1	I	3	PHE
1	I	24	SER
1	I	44	ASN
1	M	3	PHE
1	M	24	SER
1	M	44	ASN

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Mol	Chain	Res	Type
1	N	3	PHE
1	N	24	SER
1	N	44	ASN
1	N	365	ALA
1	R	24	SER
1	R	44	ASN
1	Q	3	PHE
1	Q	24	SER
1	Q	44	ASN
1	P	3	PHE
1	P	24	SER
1	P	44	ASN
1	O	3	PHE
1	O	24	SER
1	O	44	ASN
1	a	3	PHE
1	a	24	SER
1	a	44	ASN
1	b	3	PHE
1	b	24	SER
1	b	44	ASN
1	b	365	ALA
1	f	3	PHE
1	f	24	SER
1	f	44	ASN
1	f	365	ALA
1	e	3	PHE
1	e	24	SER
1	e	44	ASN
1	d	3	PHE
1	d	24	SER
1	d	44	ASN
1	c	3	PHE
1	c	24	SER
1	c	44	ASN
1	c	365	ALA
1	g	3	PHE
1	g	24	SER
1	g	44	ASN
1	g	365	ALA
1	h	3	PHE
1	h	24	SER

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Mol	Chain	Res	Type
1	h	44	ASN
1	l	3	PHE
1	l	24	SER
1	l	44	ASN
1	k	3	PHE
1	k	24	SER
1	k	44	ASN
1	j	3	PHE
1	j	24	SER
1	j	44	ASN
1	j	365	ALA
1	i	3	PHE
1	i	24	SER
1	i	44	ASN
1	A	241	GLY
1	B	241	GLY
1	F	241	GLY
1	E	241	GLY
1	D	241	GLY
1	C	241	GLY
1	0	241	GLY
1	1	241	GLY
1	5	241	GLY
1	4	241	GLY
1	3	241	GLY
1	2	241	GLY
1	G	241	GLY
1	H	241	GLY
1	L	241	GLY
1	K	241	GLY
1	J	241	GLY
1	I	241	GLY
1	M	241	GLY
1	N	241	GLY
1	R	241	GLY
1	Q	241	GLY
1	P	241	GLY
1	O	241	GLY
1	a	241	GLY
1	b	241	GLY
1	f	241	GLY
1	e	241	GLY

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Mol	Chain	Res	Type
1	d	241	GLY
1	c	241	GLY
1	g	241	GLY
1	h	241	GLY
1	l	241	GLY
1	k	241	GLY
1	j	241	GLY
1	i	241	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	296/298 (99%)	293 (99%)	3 (1%)	68	75
1	1	296/298 (99%)	293 (99%)	3 (1%)	68	75
1	2	296/298 (99%)	293 (99%)	3 (1%)	68	75
1	3	296/298 (99%)	293 (99%)	3 (1%)	68	75
1	4	296/298 (99%)	294 (99%)	2 (1%)	76	78
1	5	296/298 (99%)	293 (99%)	3 (1%)	68	75
1	A	296/298 (99%)	293 (99%)	3 (1%)	68	75
1	B	296/298 (99%)	293 (99%)	3 (1%)	68	75
1	C	296/298 (99%)	293 (99%)	3 (1%)	68	75
1	D	296/298 (99%)	293 (99%)	3 (1%)	68	75
1	E	296/298 (99%)	293 (99%)	3 (1%)	68	75
1	F	296/298 (99%)	294 (99%)	2 (1%)	76	78
1	G	296/298 (99%)	293 (99%)	3 (1%)	68	75
1	H	296/298 (99%)	294 (99%)	2 (1%)	76	78
1	I	296/298 (99%)	294 (99%)	2 (1%)	76	78
1	J	296/298 (99%)	293 (99%)	3 (1%)	68	75
1	K	296/298 (99%)	293 (99%)	3 (1%)	68	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	296/298 (99%)	294 (99%)	2 (1%)	76	78
1	M	296/298 (99%)	294 (99%)	2 (1%)	76	78
1	N	296/298 (99%)	293 (99%)	3 (1%)	68	75
1	O	296/298 (99%)	293 (99%)	3 (1%)	68	75
1	P	296/298 (99%)	293 (99%)	3 (1%)	68	75
1	Q	296/298 (99%)	293 (99%)	3 (1%)	68	75
1	R	296/298 (99%)	294 (99%)	2 (1%)	76	78
1	a	296/298 (99%)	294 (99%)	2 (1%)	76	78
1	b	296/298 (99%)	294 (99%)	2 (1%)	76	78
1	c	296/298 (99%)	293 (99%)	3 (1%)	68	75
1	d	296/298 (99%)	294 (99%)	2 (1%)	76	78
1	e	296/298 (99%)	293 (99%)	3 (1%)	68	75
1	f	296/298 (99%)	293 (99%)	3 (1%)	68	75
1	g	296/298 (99%)	294 (99%)	2 (1%)	76	78
1	h	296/298 (99%)	294 (99%)	2 (1%)	76	78
1	i	296/298 (99%)	294 (99%)	2 (1%)	76	78
1	j	296/298 (99%)	293 (99%)	3 (1%)	68	75
1	k	296/298 (99%)	293 (99%)	3 (1%)	68	75
1	l	296/298 (99%)	293 (99%)	3 (1%)	68	75
All	All	10656/10728 (99%)	10561 (99%)	95 (1%)	68	75

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	289	LEU
1	A	302	VAL
1	B	7	VAL
1	B	289	LEU
1	B	302	VAL
1	F	289	LEU
1	F	302	VAL
1	E	7	VAL
1	E	289	LEU
1	E	302	VAL

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Mol	Chain	Res	Type
1	D	7	VAL
1	D	289	LEU
1	D	302	VAL
1	C	7	VAL
1	C	289	LEU
1	C	302	VAL
1	0	7	VAL
1	0	289	LEU
1	0	302	VAL
1	1	7	VAL
1	1	289	LEU
1	1	302	VAL
1	5	7	VAL
1	5	289	LEU
1	5	302	VAL
1	4	289	LEU
1	4	302	VAL
1	3	7	VAL
1	3	289	LEU
1	3	302	VAL
1	2	7	VAL
1	2	289	LEU
1	2	302	VAL
1	G	7	VAL
1	G	289	LEU
1	G	302	VAL
1	H	289	LEU
1	H	302	VAL
1	L	289	LEU
1	L	302	VAL
1	K	7	VAL
1	K	289	LEU
1	K	302	VAL
1	J	7	VAL
1	J	289	LEU
1	J	302	VAL
1	I	289	LEU
1	I	302	VAL
1	M	289	LEU
1	M	302	VAL
1	N	7	VAL
1	N	289	LEU

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Mol	Chain	Res	Type
1	N	302	VAL
1	R	289	LEU
1	R	302	VAL
1	Q	7	VAL
1	Q	289	LEU
1	Q	302	VAL
1	P	7	VAL
1	P	289	LEU
1	P	302	VAL
1	O	7	VAL
1	O	289	LEU
1	O	302	VAL
1	a	289	LEU
1	a	302	VAL
1	b	289	LEU
1	b	302	VAL
1	f	7	VAL
1	f	289	LEU
1	f	302	VAL
1	e	7	VAL
1	e	289	LEU
1	e	302	VAL
1	d	289	LEU
1	d	302	VAL
1	c	7	VAL
1	c	289	LEU
1	c	302	VAL
1	g	289	LEU
1	g	302	VAL
1	h	289	LEU
1	h	302	VAL
1	l	7	VAL
1	l	289	LEU
1	l	302	VAL
1	k	7	VAL
1	k	289	LEU
1	k	302	VAL
1	j	7	VAL
1	j	289	LEU
1	j	302	VAL
1	i	289	LEU
1	i	302	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	347	GLN
1	E	347	GLN
1	D	347	GLN
1	C	347	GLN
1	0	193	ASN
1	5	347	GLN
1	4	347	GLN
1	H	172	ASN
1	H	347	GLN
1	L	172	ASN
1	M	172	ASN
1	M	347	GLN
1	N	172	ASN
1	a	172	ASN
1	b	172	ASN
1	f	172	ASN
1	e	172	ASN
1	d	172	ASN
1	d	347	GLN
1	g	172	ASN
1	h	172	ASN
1	l	172	ASN
1	k	172	ASN
1	j	172	ASN
1	i	172	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

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.

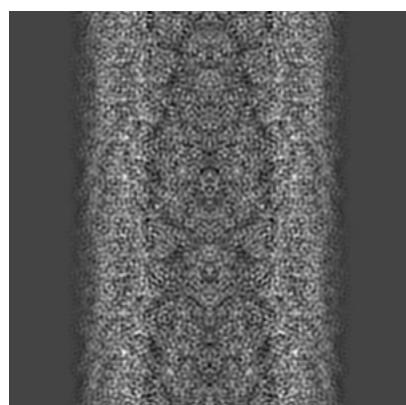
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6271. These allow visual inspection of the internal detail of the map and identification of artifacts.

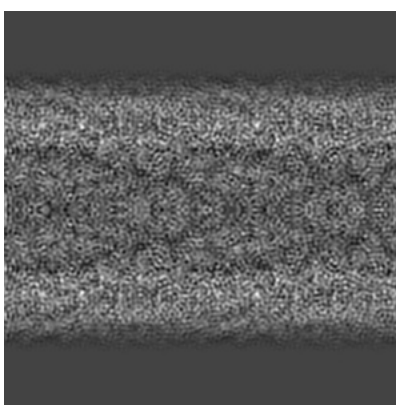
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

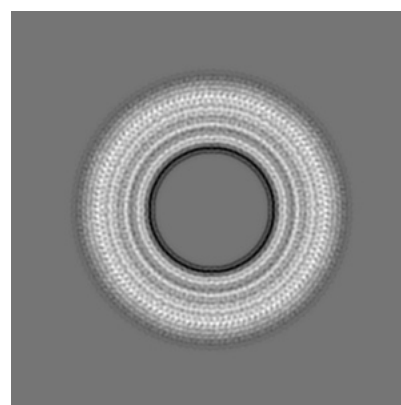
6.1.1 Primary map



X



Y

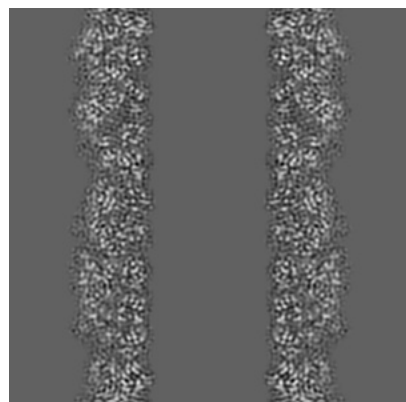


Z

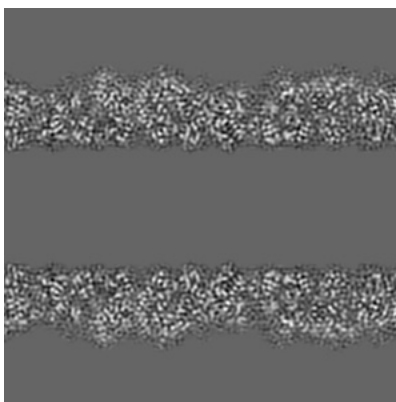
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

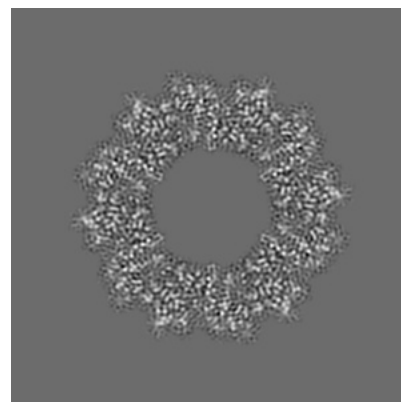
6.2.1 Primary map



X Index: 150



Y Index: 150

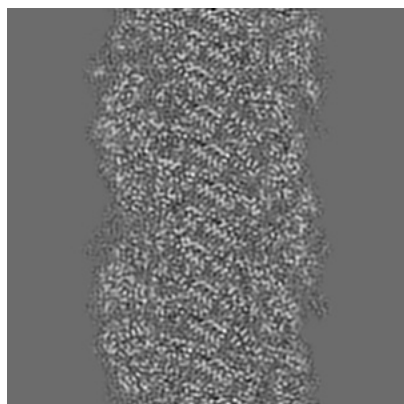


Z Index: 150

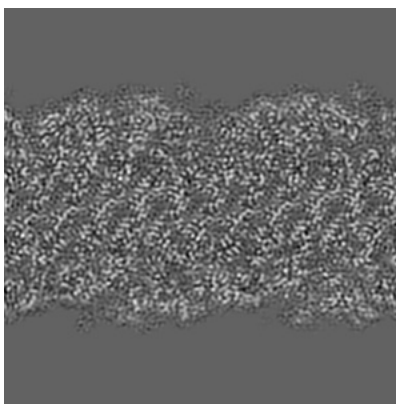
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

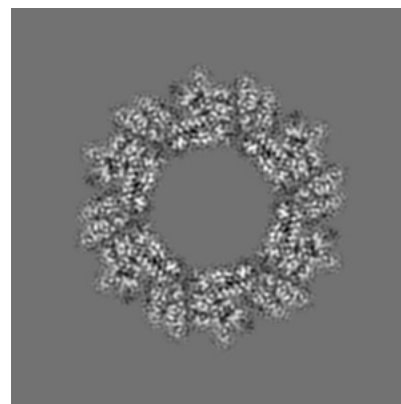
6.3.1 Primary map



X Index: 96



Y Index: 99

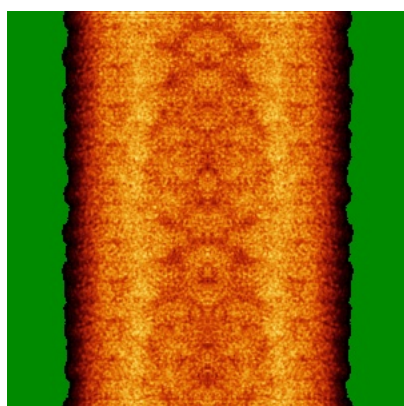


Z Index: 1

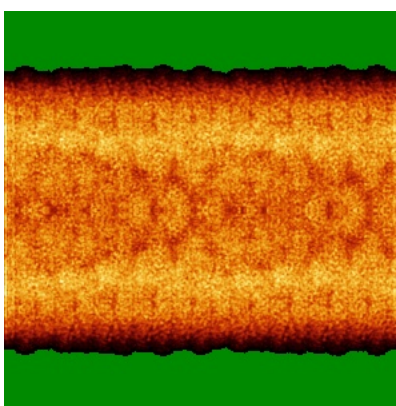
The images above show the largest variance slices of the map in three orthogonal directions.

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

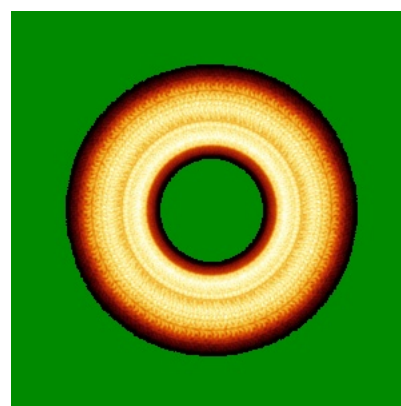
6.4.1 Primary map



X



Y

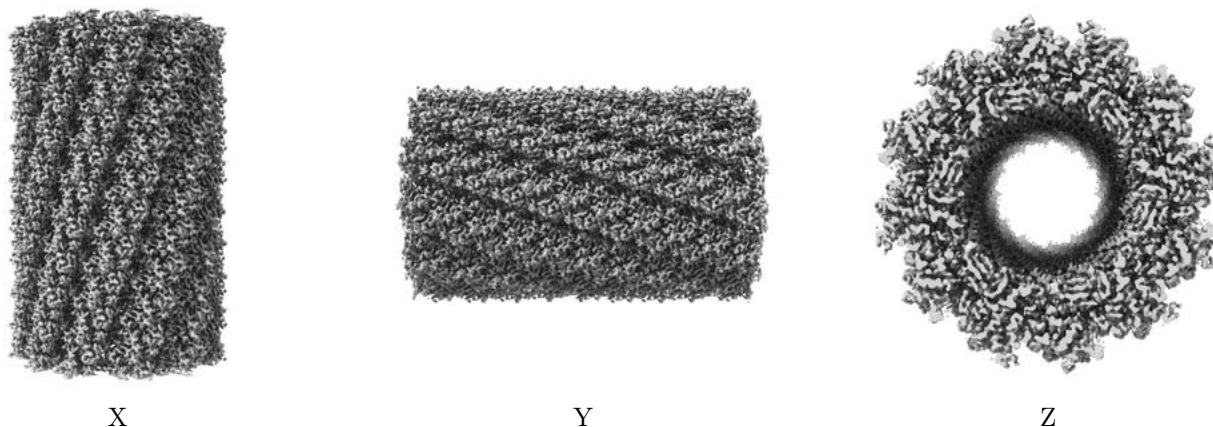


Z

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 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

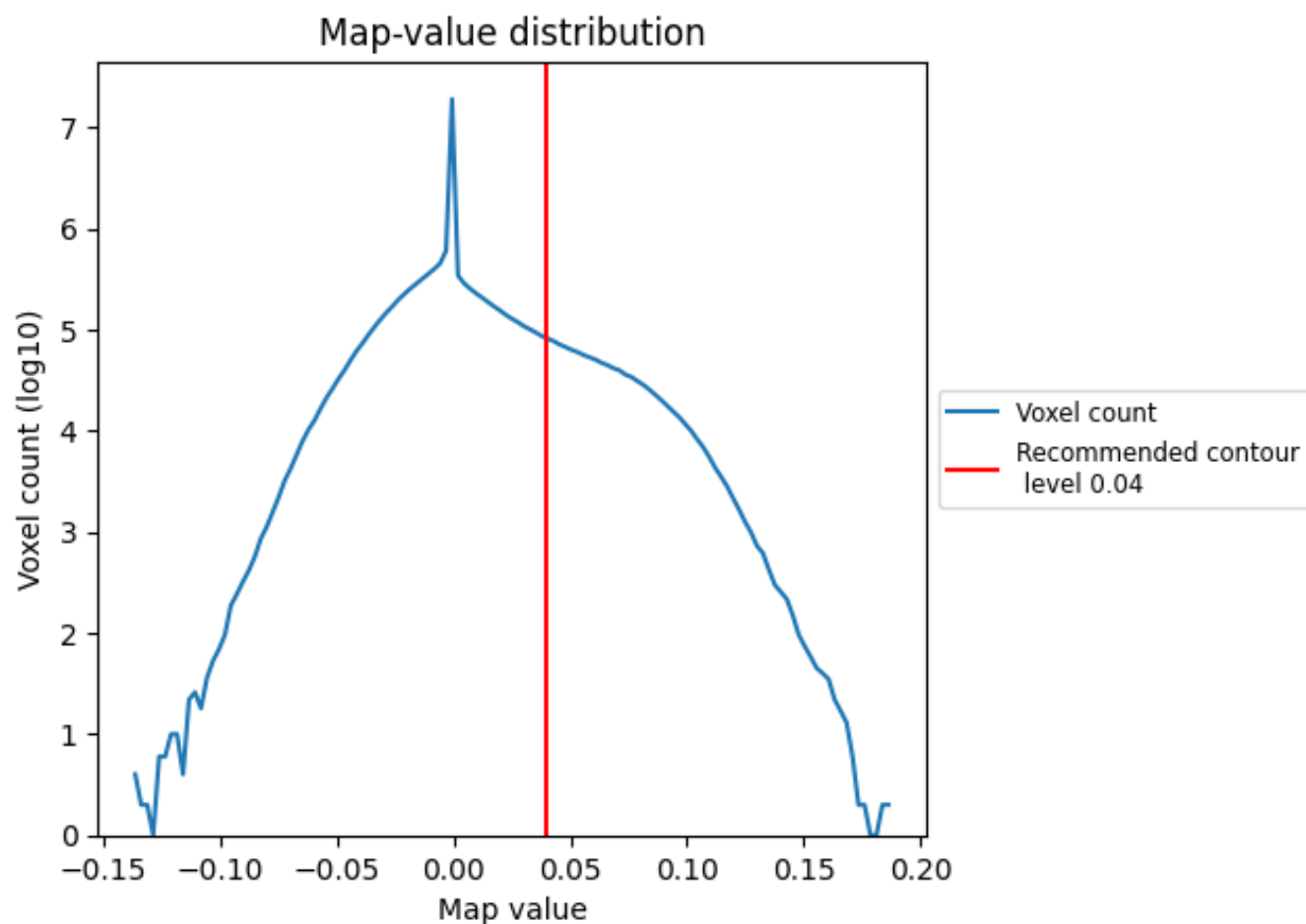
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

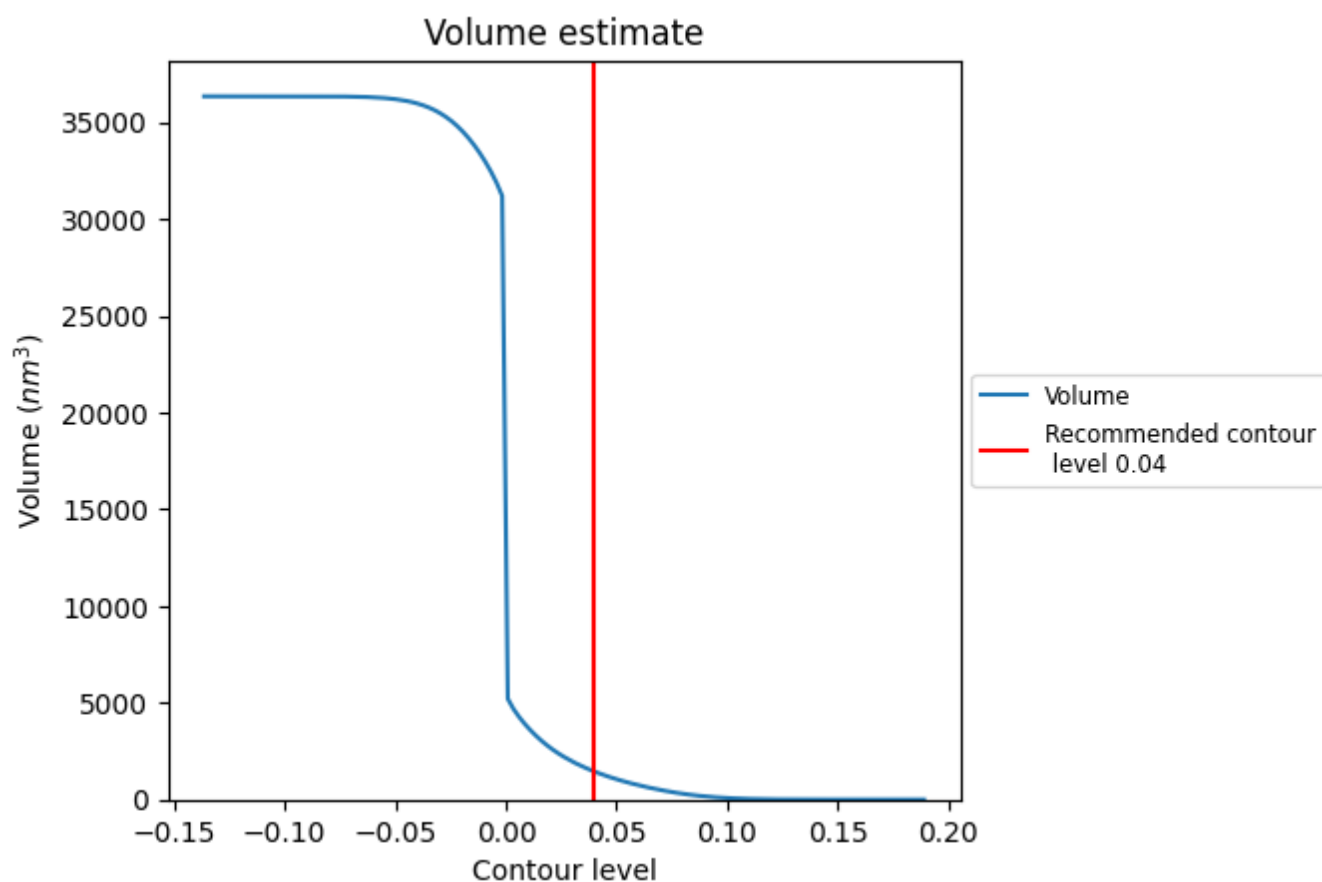
This section contains the results of statistical analysis of the map.

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.

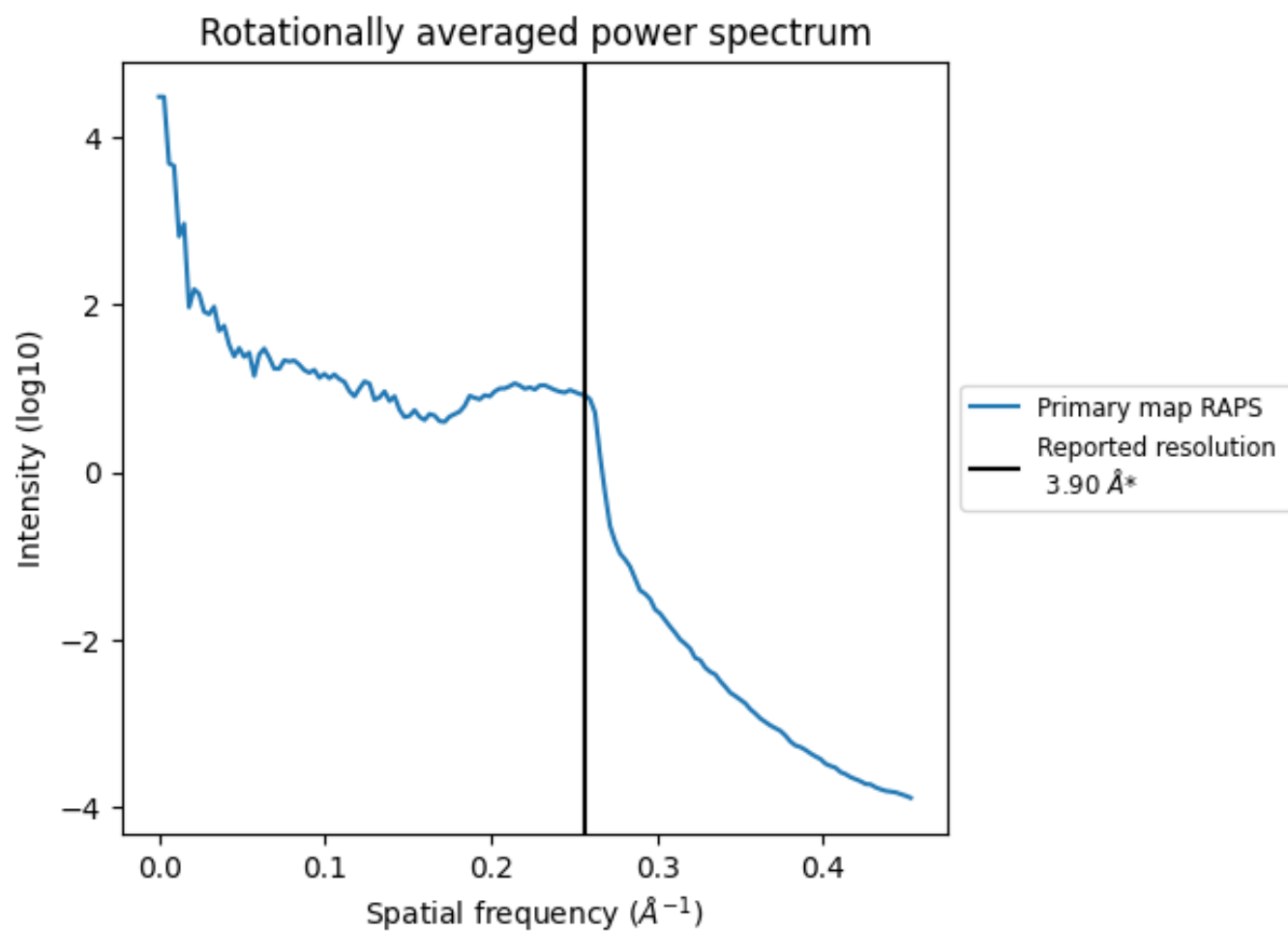
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1448 nm³; this corresponds to an approximate mass of 1308 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

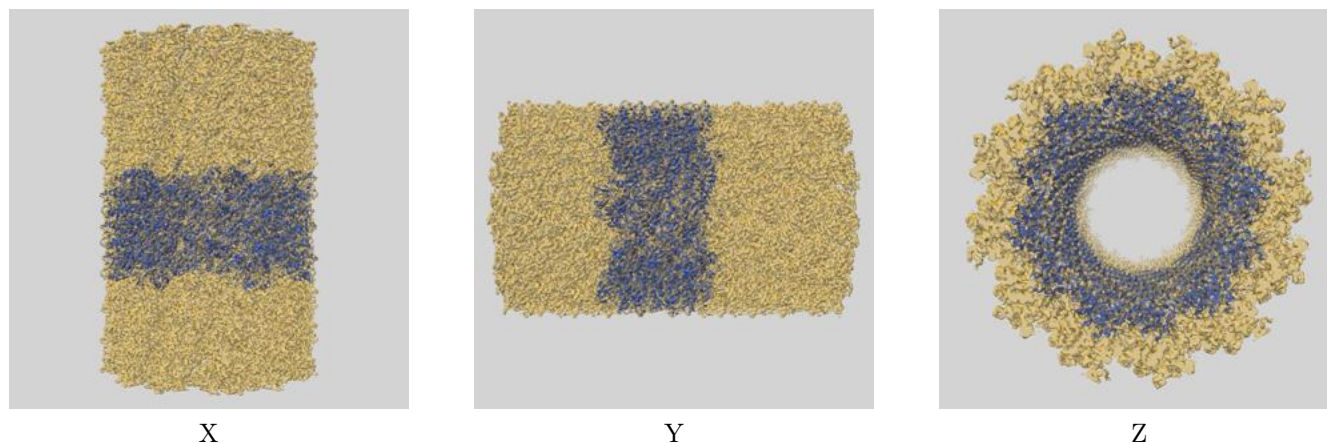
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

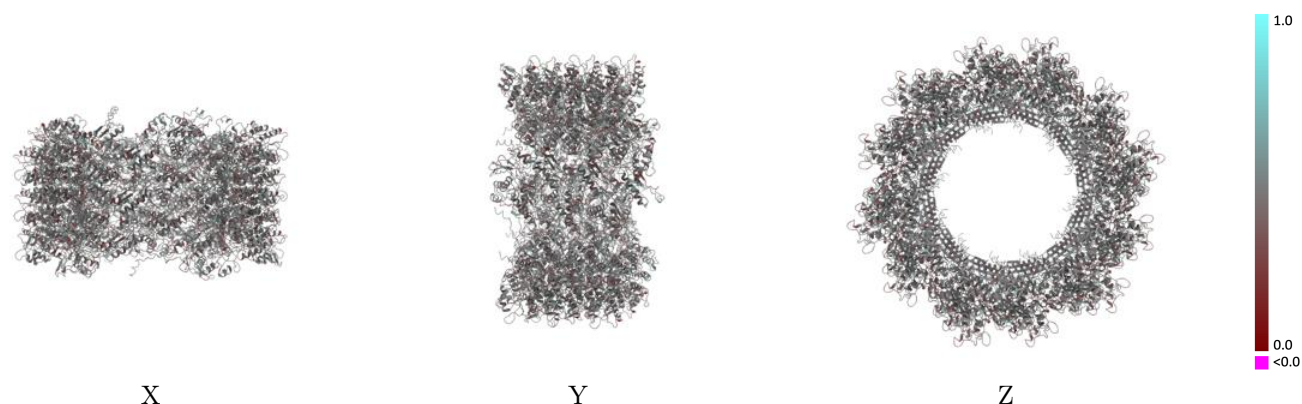
This section contains information regarding the fit between EMDB map EMD-6271 and PDB model 3J9R. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



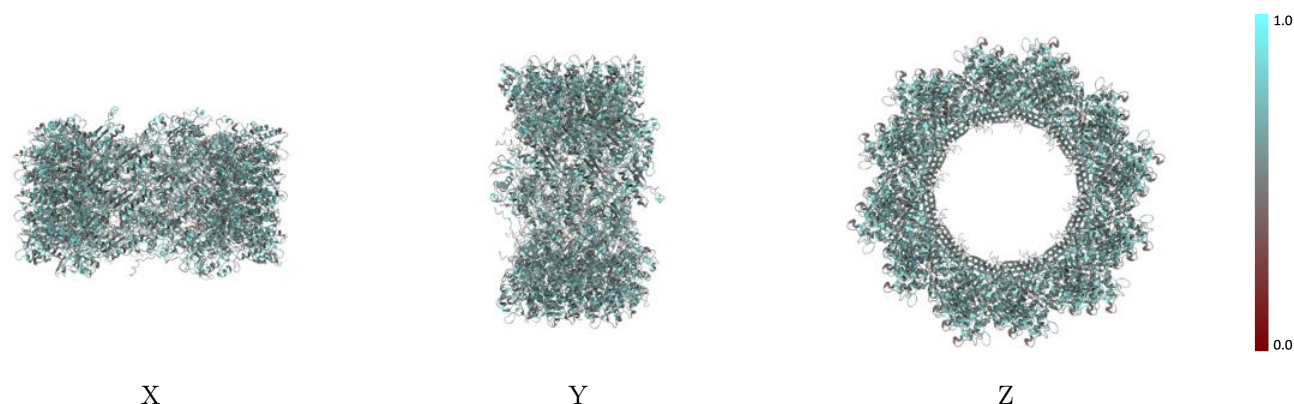
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



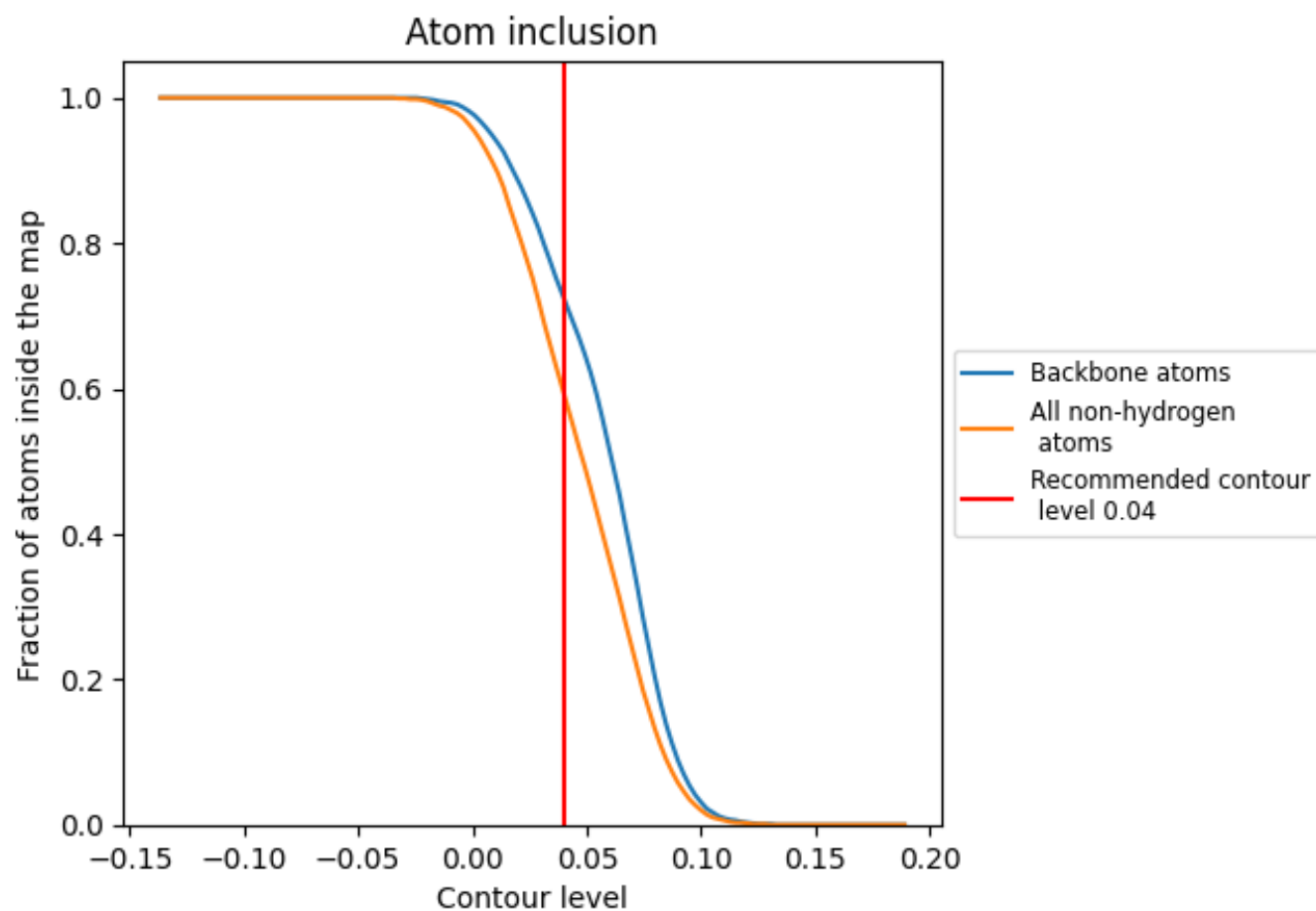
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 59% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5930	 0.4490
0	 0.5900	 0.4480
1	 0.5910	 0.4470
2	 0.5900	 0.4480
3	 0.5870	 0.4470
4	 0.5920	 0.4480
5	 0.5930	 0.4490
A	 0.5940	 0.4480
B	 0.5950	 0.4490
C	 0.5920	 0.4470
D	 0.5950	 0.4490
E	 0.5940	 0.4490
F	 0.5930	 0.4480
G	 0.5950	 0.4490
H	 0.5940	 0.4490
I	 0.5940	 0.4500
J	 0.5960	 0.4500
K	 0.5970	 0.4490
L	 0.5930	 0.4490
M	 0.5920	 0.4490
N	 0.5910	 0.4480
O	 0.5970	 0.4490
P	 0.5920	 0.4500
Q	 0.5910	 0.4490
R	 0.5980	 0.4490
a	 0.5950	 0.4490
b	 0.5930	 0.4500
c	 0.5940	 0.4490
d	 0.5940	 0.4490
e	 0.5900	 0.4490
f	 0.5940	 0.4480
g	 0.5920	 0.4500
h	 0.5910	 0.4500
i	 0.5950	 0.4500
j	 0.5910	 0.4510



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Chain	Atom inclusion	Q-score
k	 0.5920	 0.4490
l	 0.5940	 0.4490