



Full wwPDB EM Validation Report ⓘ

Oct 14, 2025 – 04:54 PM JST

PDB ID : 8Z5S / pdb_00008z5s
EMDB ID : EMD-39780
Title : Cryo-EM structure of the proximal rod-export apparatus of the polar flagellar motor
Authors : Zhang, L.; Tan, J.X.; Zhou, Y.; Zhu, Y.Q.
Deposited on : 2024-04-18
Resolution : 3.03 Å(reported)
Based on initial model : .

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.dev129
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

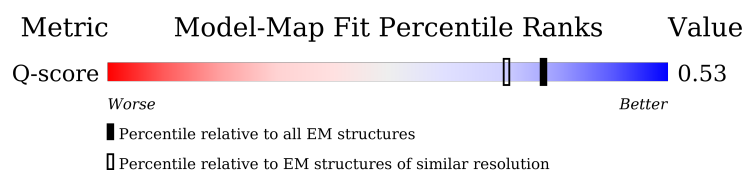
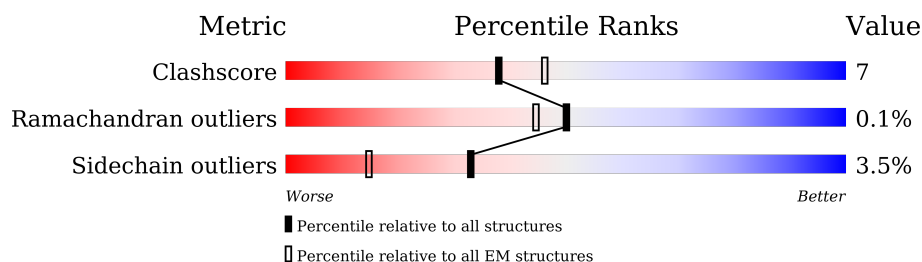
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.03 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.








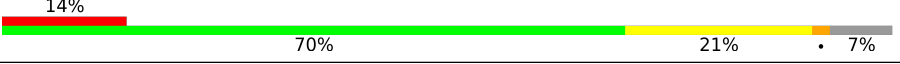
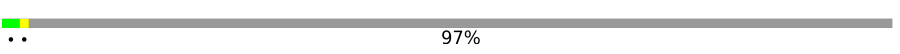
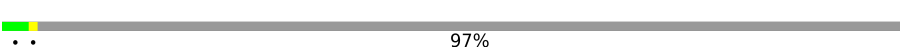
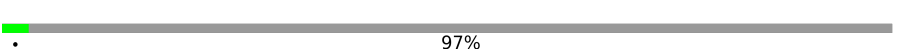

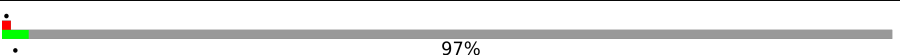
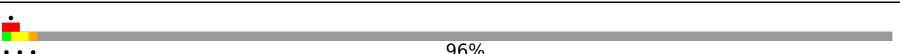
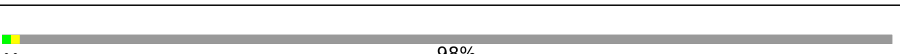
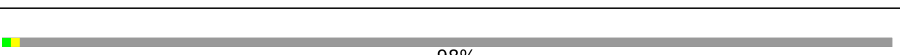
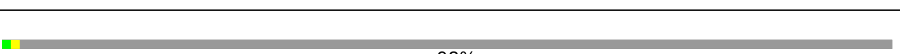
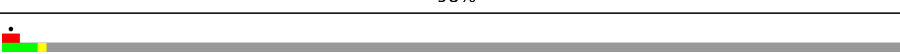
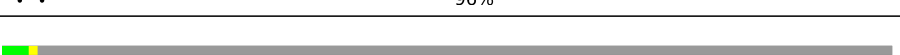
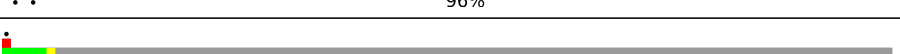
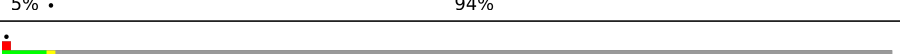
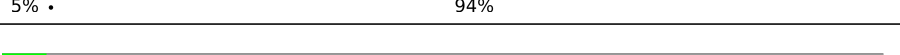
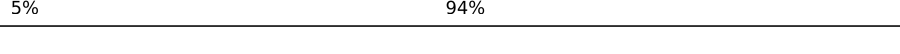
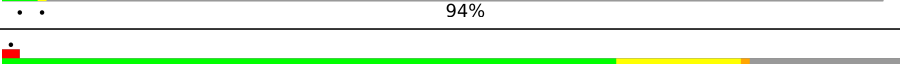
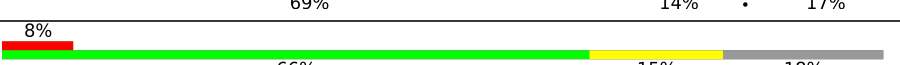
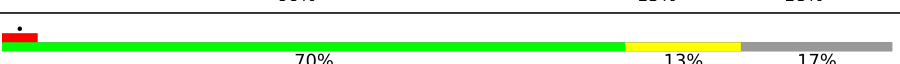
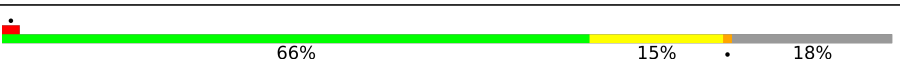
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	13929 (2.53 - 3.53)

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	1	289	
1	2	289	
1	3	289	
1	y	289	







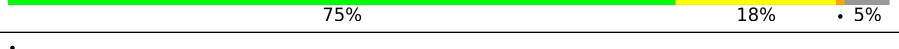
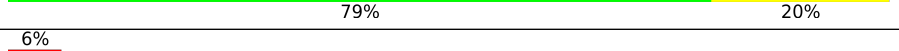
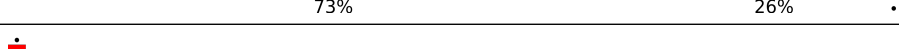
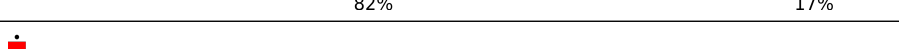
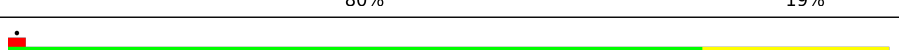

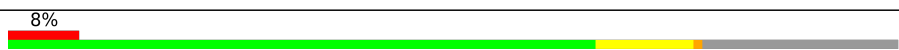

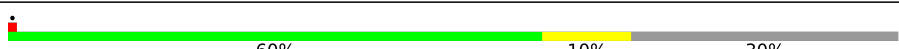




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Mol	Chain	Length	Quality of chain
1	z	289	
2	4	89	
2	5	89	
2	6	89	
2	7	89	
3	8	260	
4	AA	580	
4	AB	580	
4	AC	580	
4	AD	580	
4	AE	580	
4	AF	580	
4	AG	580	
4	AH	580	
4	AI	580	
4	AJ	580	
4	AK	580	
4	AL	580	
4	AM	580	
4	AN	580	
4	AO	580	
5	b	131	
5	c	131	
5	d	131	
5	e	131	

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Mol	Chain	Length	Quality of chain
5	f	131	
6	g	137	
6	h	137	
6	i	137	
6	j	137	
6	k	137	
6	l	137	
7	m	249	
7	n	249	
7	o	249	
7	p	249	
7	q	249	
8	r	103	
8	s	103	
8	t	103	
8	u	103	
8	v	103	
8	w	103	
9	x	376	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 38336 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 Flagellar biosynthetic protein FliP.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	207	Total	C	N	O	S	0	0
			1599	1055	243	282	19		
1	2	208	Total	C	N	O	S	0	0
			1608	1060	244	285	19		
1	3	208	Total	C	N	O	S	0	0
			1608	1060	244	285	19		
1	y	208	Total	C	N	O	S	0	0
			1608	1060	244	285	19		
1	z	208	Total	C	N	O	S	0	0
			1608	1060	244	285	19		

- Molecule 2 is a protein called Flagellar biosynthetic protein FliQ.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	4	89	Total	C	N	O	S	0	0
			722	489	107	117	9		
2	5	89	Total	C	N	O	S	0	0
			722	489	107	117	9		
2	6	89	Total	C	N	O	S	0	0
			722	489	107	117	9		
2	7	89	Total	C	N	O	S	0	0
			722	489	107	117	9		

- Molecule 3 is a protein called Flagellar biosynthetic protein FliR.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	8	242	Total	C	N	O	S	0	0
			1896	1265	295	315	21		

- Molecule 4 is a protein called Flagellar M-ring protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AA	19	Total	C	N	O	S	0	0
			135	82	23	29	1		
4	AB	19	Total	C	N	O	S	0	0
			135	82	23	29	1		
4	AC	20	Total	C	N	O	S	0	0
			139	84	24	30	1		
4	AD	19	Total	C	N	O	S	0	0
			135	82	23	29	1		
4	AE	19	Total	C	N	O	S	0	0
			135	82	23	29	1		
4	AF	23	Total	C	N	O	S	0	0
			158	97	27	33	1		
4	AG	11	Total	C	N	O		0	0
			73	46	13	14			
4	AH	11	Total	C	N	O		0	0
			73	46	13	14			
4	AI	11	Total	C	N	O		0	0
			73	46	13	14			
4	AJ	24	Total	C	N	O	S	0	0
			163	100	28	34	1		
4	AK	25	Total	C	N	O	S	0	0
			169	104	29	35	1		
4	AL	32	Total	C	N	O	S	0	0
			220	134	38	46	2		
4	AM	33	Total	C	N	O	S	0	0
			224	136	39	47	2		
4	AN	33	Total	C	N	O	S	0	0
			224	136	39	47	2		
4	AO	32	Total	C	N	O	S	0	0
			220	134	38	46	2		

- Molecule 5 is a protein called Flagellar basal body rod protein FlgB.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	b	109	Total	C	N	O	S	0	0
			845	523	155	166	1		
5	c	107	Total	C	N	O	S	0	0
			835	518	153	163	1		
5	d	109	Total	C	N	O	S	0	0
			845	523	155	166	1		
5	e	108	Total	C	N	O	S	0	0
			837	519	154	163	1		
5	f	108	Total	C	N	O	S	0	0
			837	519	154	163	1		

- Molecule 6 is a protein called Flagellar basal-body rod protein FlgC.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	g	130	Total	C	N	O	S	0	0
			983	605	168	203	7		
6	h	130	Total	C	N	O	S	0	0
			983	605	168	203	7		
6	i	130	Total	C	N	O	S	0	0
			983	605	168	203	7		
6	j	130	Total	C	N	O	S	0	0
			983	605	168	203	7		
6	k	130	Total	C	N	O	S	0	0
			983	605	168	203	7		
6	l	130	Total	C	N	O	S	0	0
			983	605	168	203	7		

- Molecule 7 is a protein called Flagellar basal-body rod protein FlgF.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	m	248	Total	C	N	O	S	0	0
			1879	1156	338	373	12		
7	n	248	Total	C	N	O	S	0	0
			1879	1156	338	373	12		
7	o	248	Total	C	N	O	S	0	0
			1879	1156	338	373	12		
7	p	248	Total	C	N	O	S	0	0
			1879	1156	338	373	12		
7	q	248	Total	C	N	O	S	0	0
			1879	1156	338	373	12		

- Molecule 8 is a protein called Flagellar hook-basal body complex protein FliE.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	r	72	Total	C	N	O	S	0	0
			560	345	99	113	3		
8	s	80	Total	C	N	O	S	0	0
			605	372	108	122	3		
8	t	80	Total	C	N	O	S	0	0
			605	372	108	122	3		
8	u	72	Total	C	N	O	S	0	0
			560	345	99	113	3		
8	v	72	Total	C	N	O	S	0	0
			560	345	99	113	3		
8	w	40	Total	C	N	O	S	0	0
			311	194	53	61	3		

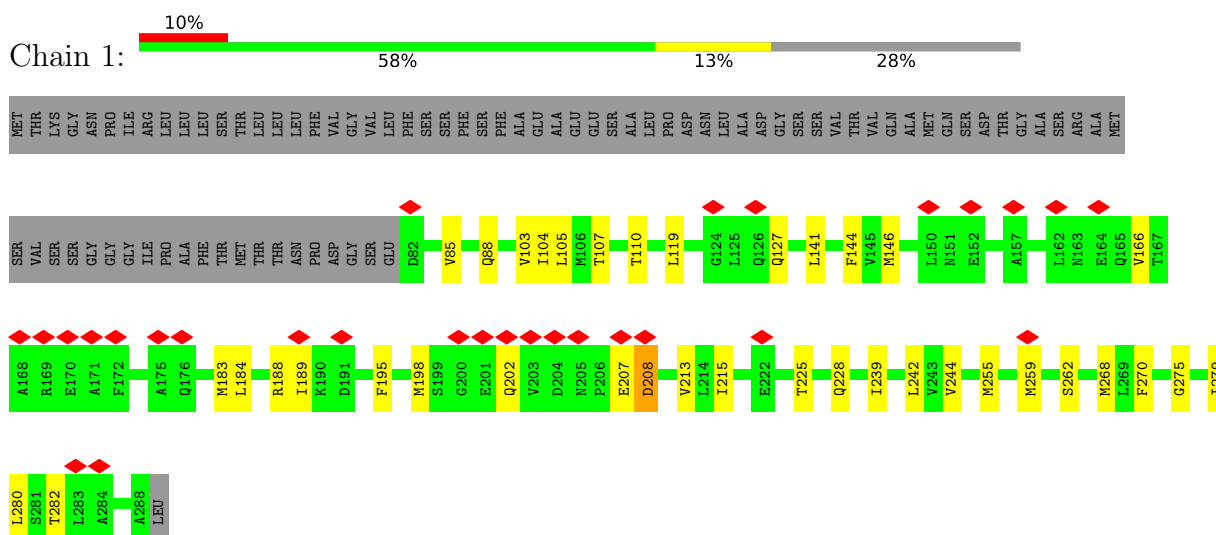
- Molecule 9 is a protein called Flagellar biosynthetic protein FlhB.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	x	71	Total	C	N	O	S	0	0
			552	370	83	95	4		

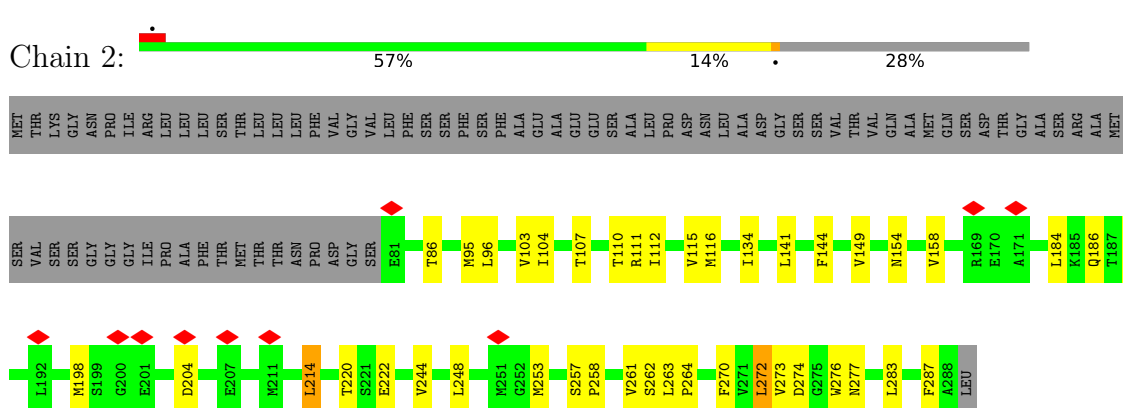
3 Residue-property plots

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

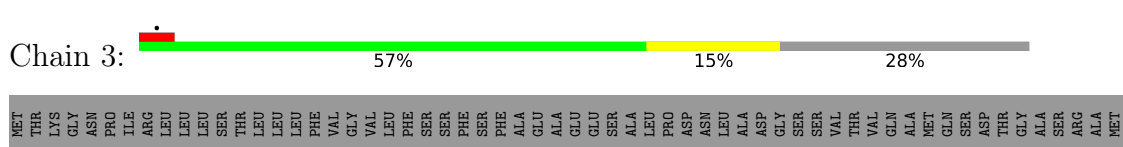
• Molecule 1: Flagellar biosynthetic protein FlpP

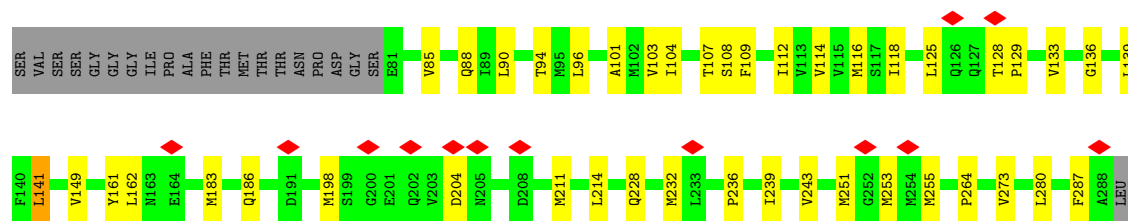


• Molecule 1: Flagellar biosynthetic protein FlpP



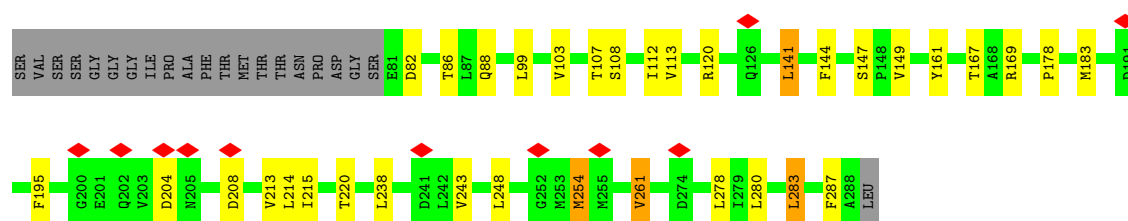
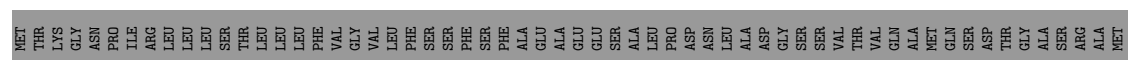
• Molecule 1: Flagellar biosynthetic protein FlpP





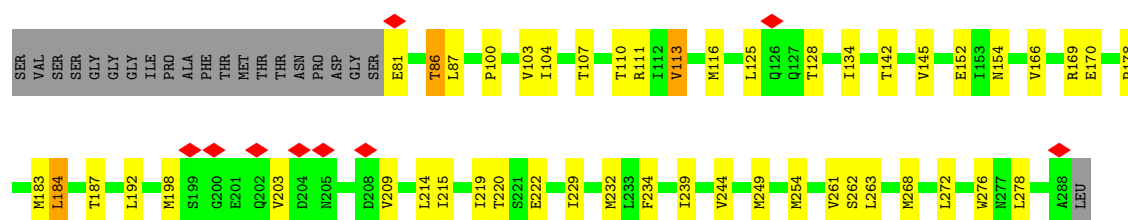
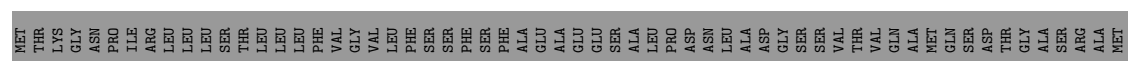
• Molecule 1: Flagellar biosynthetic protein FliP

Chain y: 60% 11% 28%



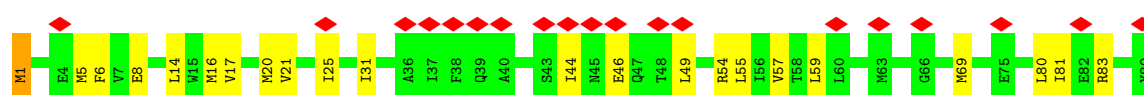
• Molecule 1: Flagellar biosynthetic protein FliP

Chain z: 55% 16% 28%



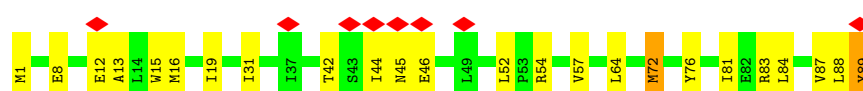
• Molecule 2: Flagellar biosynthetic protein FliQ

Chain 4: 21% 75% 24%



• Molecule 2: Flagellar biosynthetic protein FliQ

Chain 5: 9% 73% 25%



[illegible]

- Molecule 4: Flagellar M-ring protein

Chain AB: 97%

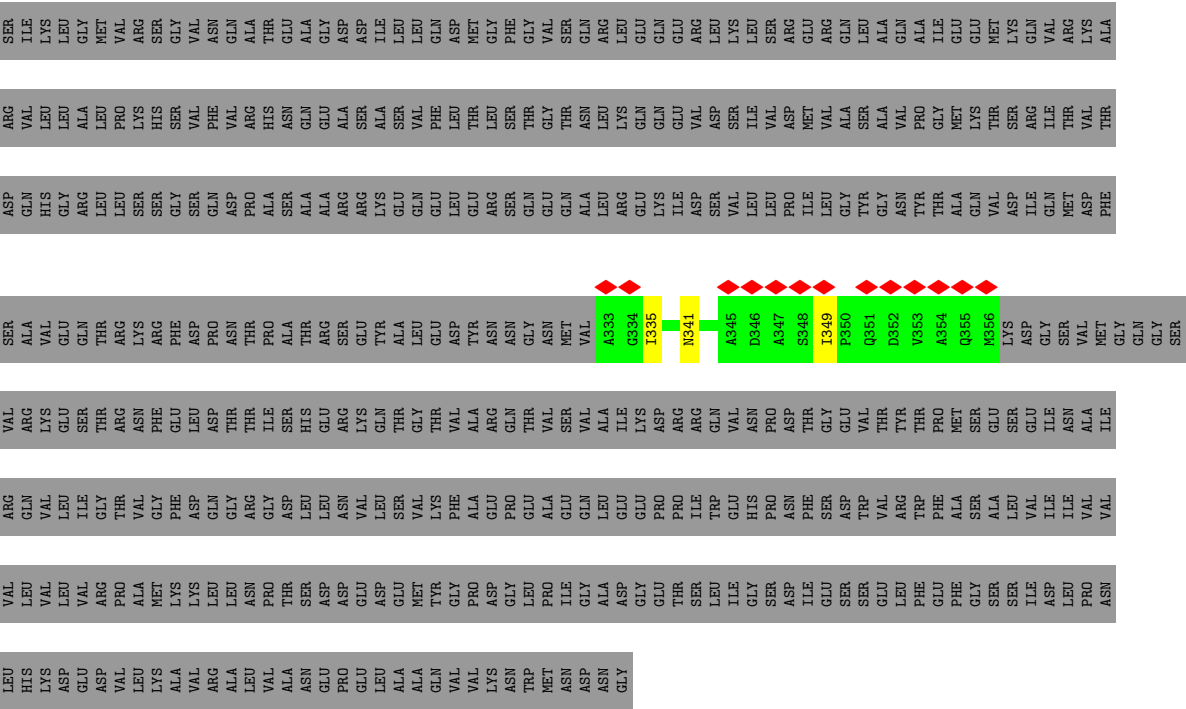
[illegible]

- Molecule 4: Flagellar M-ring protein

Chain AC: 97%

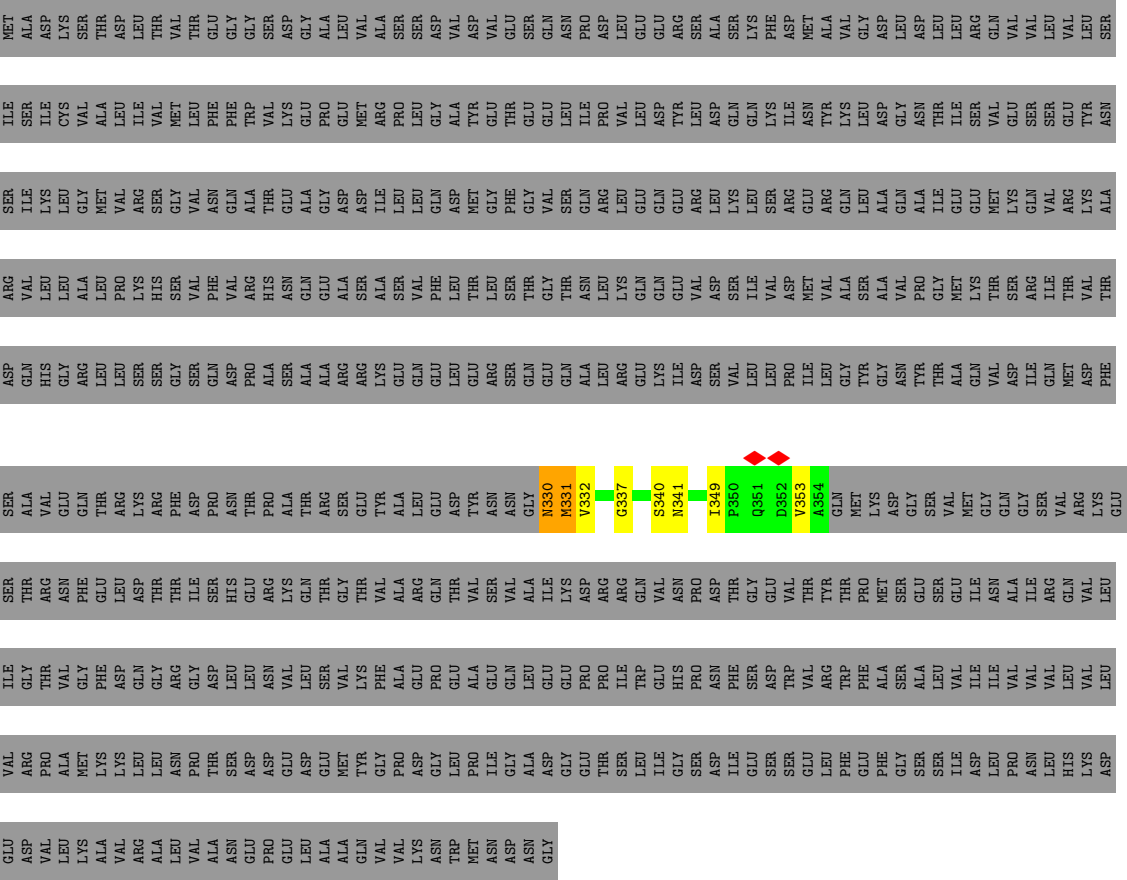
[illegible]





● Molecule 4: Flagellar M-ring protein

Chain AK: . . 96%



Chain AL: 5% 94%



[illegible]

- Molecule 4: Flagellar M-ring protein

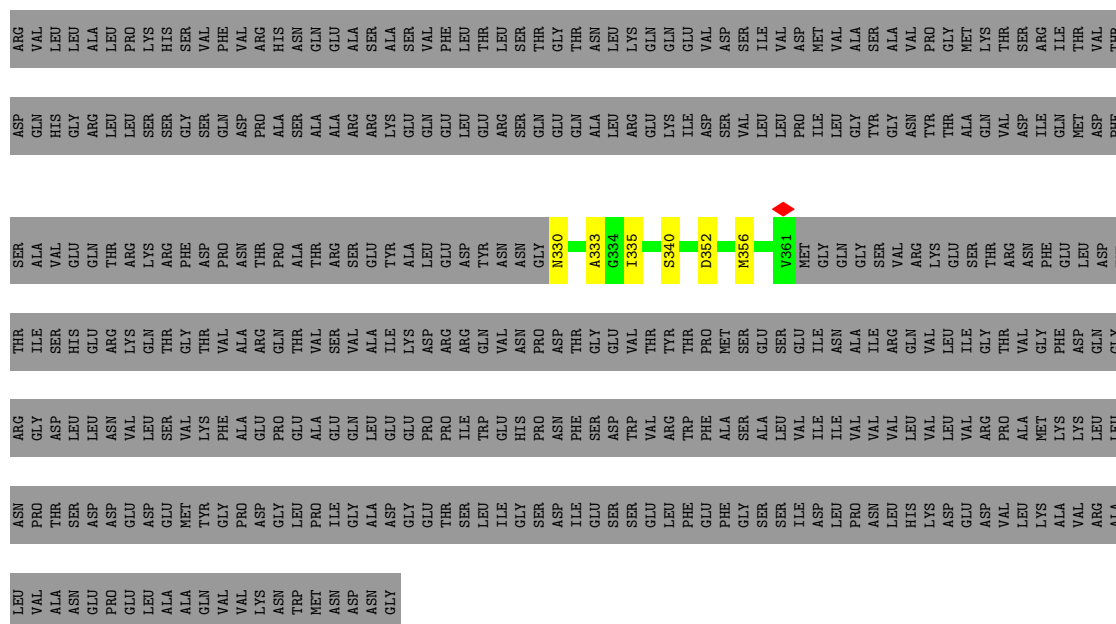
Chain AN:  5% 94%

GLU	ASP	LEU	GLU	SER	ASP	ASP	GLN	ARG	SER	ILE	MET
PRO	ASP	ASN	ARG	ALA	ALA	VAL	GLN	VAL	LYS	SER	ALA
GLU	GLU	VAL	LYS	VAL	VAL	GLU	HIS	HIS	LYS	ILE	SER
LEU	ASP	LEU	GLN	GLU	GLU	THR	ARG	GLY	LEU	CYS	LYS
ALA	GLU	SER	THR	GLN	THR	THR	LEU	ALA	MET	VAL	THR
GLN	TYR	LYS	THR	ARG	ARG	ARG	LEU	PRO	VAL	ALA	ASP
VAL	GLY	PHE	VAL	LYS	LYS	VAL	SER	LYS	ARG	ILE	THR
VAL	PRO	ALA	ALA	ARG	PRO	ALA	HIS	HIS	GLY	MET	THR
LYS	ASP	GLU	ARG	PHE	GLY	GLY	SER	ASN	VAL	VAL	THR
ASN	GLY	PRO	GLN	ASP	SER	SER	GLN	PHE	ASN	GLU	THR
LEU	LEU	GLU	THR	PRO	ASN	VAL	GLN	VAL	GLN	PHE	GLY
PRO	PRO	ALA	VAL	ASN	THR	THR	ASP	VAL	GLN	PHE	ASN
ASN	ILE	GLU	SER	THR	THR	THR	PRO	ARG	ALA	GLY	LEU
ASP	GLY	GLU	ILE	THR	THR	ALA	ALA	GLN	ALA	GLY	GLY
GLY	GLY	GLU	LYS	ARG	SER	ARG	ALA	GLU	GLY	PRO	LEU
GLU	GLU	PRO	ASP	SER	ARG	ARG	ARG	ALA	ASP	GLU	LEU
THR	THR	PRO	ARG	GLU	GLU	GLU	LYS	ALA	ASP	MET	VAL
SER	SER	ILE	ARG	TYR	TYR	ALA	ALA	ALA	ASP	ALA	VAL
LEU	LEU	TRP	GLN	ALA	ALA	GLN	GLN	GLN	LEU	THR	ASN
ILE	ILE	GLU	VAL	LEU	LEU	GLU	GLU	THR	GLY	GLY	SER
GLY	GLY	HIS	ASN	GLU	ASP	GLU	GLN	THR	GLN	THR	ASN
SER	SER	PRO	PRO	ASP	ASP	TYR	ARG	LEU	VAL	ALA	VAL
ASP	ASP	ASN	THR	ASN	ASN	ASN	GLU	GLU	GLU	GLY	GLY
ILE	ILE	PHE	THR	GLY	GLY	GLY	GLN	SER	GLY	THR	THR
SER	SER	SER	GLU	ASN	SER	SER	GLN	THR	GLY	GLY	GLN
GLU	GLU	TRP	VAL	L329	L329	GLU	GLN	GLY	VAL	GLU	ASN
LEU	LEU	ARG	THR	L399	L399	THR	ALA	THR	SER	ILE	ASN
THR	PHE	TRP	THR	D352	D352	PRO	LEU	LEU	ARG	PRO	ASN
GLU	GLU	PHE	PRO	K356	K356	GLU	ARG	LYS	VAL	VAL	THR
PHE	PHE	ALA	MET			MET	GLN	GLN	GLN	LEU	GLY
GLY	GLY	SER	SER			SER	LYS	GLN	LYS	ASP	GLU
SER	SER	ALA	GLU	\$360	\$360	GLU	ILE	GLN	GLY	TYR	ASN
ILE	ILE	LEU	SER	V361	V361	LEU	ASP	VAL	ASP	LEU	GLY
SER	SER	VAL	GLU	MET	MET	GLU	SER	SER	LYS	GLY	GLY
ILE	ILE	ILE	ILE	GLY	GLY	ILE	VAL	ILE	GLN	GLN	GLY
LEU	LEU	ILE	ASN	GLN	GLN	GLN	LEU	ILE	SER	LYS	PHE
VAL	PRO	VAL	ALA	GLY	GLY	LEU	LEU	VAL	SER	THR	THR
ASN	ASN	VAL	ILE	SER	SER	ILE	PRO	ASP	ARG	ILE	ASN
LEU	LEU	VAL	ARG	VAL	VAL	ARG	ILE	MET	GLU	THR	ASN
HIS	HIS	LEU	GLN	ARG	ARG	VAL	GLY	VAL	ARG	LYS	VAL
LYS	LYS	VAL	VAL	LYS	LYS	VAL	GLY	ALA	GLM	THR	GLY
ASP	ASP	LEU	LEU	GLU	GLU	LEU	TYR	SER	LEU	LEU	ASP
GLU	GLU	VAL	ILE	SER	SER	VAL	GLY	ALA	ALA	ASP	GLY
ASP	ASP	ARG	GLY	THR	THR	ASN	ASN	VAL	GLM	GLY	LEU
VAL	VAL	PRO	THR	ASN	ASN	PRO	PRO	VAL	ALA	ASN	ASN
LEU	LEU	ALA	VAL	ASN	ASN	THR	THR	GLY	ILE	THR	THR
LYS	LYS	MET	PHE	PHE	PHE	ALA	ALA	MET	GLY	ILE	ARG
ALA	ALA	LYS	ASP	GLU	GLU	VAL	GLN	LYS	GLY	SER	GLN
VAL	VAL	LYS	ASP	LEU	LEU	THR	VAL	THR	MET	VAL	VAL
ARG	ARG	LEU	GLN	ASP	ASP	ARG	ASP	SER	LYS	GLY	VAL
ALA	ALA	LEU	GLY	THR	THR	ILE	ILE	THR	VAL	GLY	VAL
LEU	LEU	ASN	ARG	THR	THR	GLY	GLN	THR	ARG	GLY	THR
ASN	ASN	THR	PHE	SER	SER	THR	THR	THR	LYS	ASN	SER
ALA	ALA	SER	THR	ILE	ILE	ASN	ASN	THR	THR	THR	THR
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR

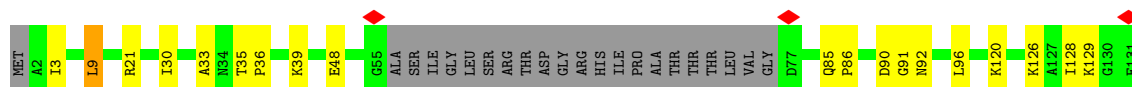
- Molecule 4: Flagellar M-ring protein

Chain AO: 94%

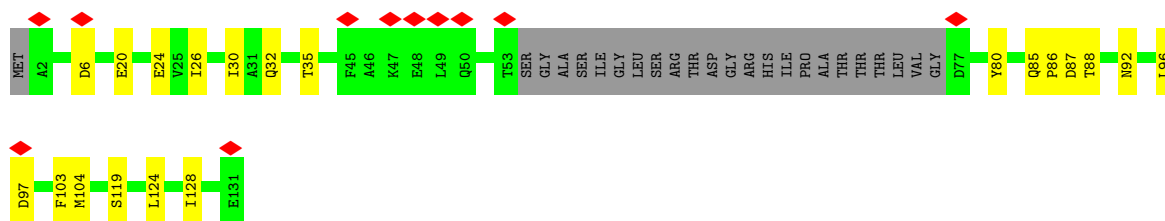
[illegible]



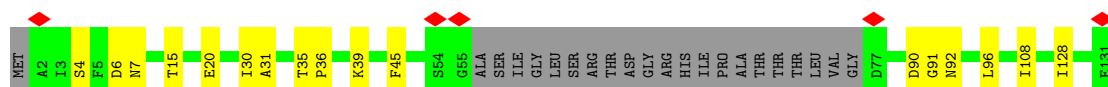
• Molecule 5: Flagellar basal body rod protein FlgB



• Molecule 5: Flagellar basal body rod protein FlgB

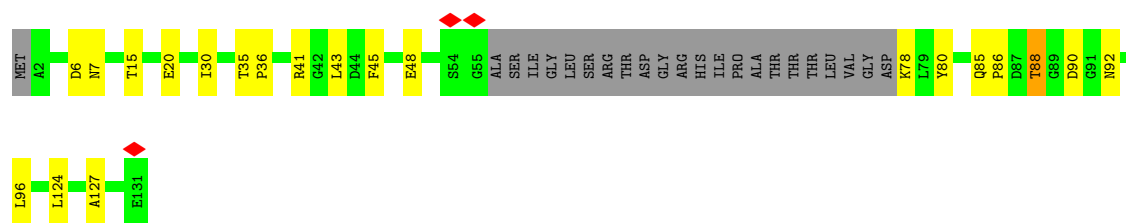


• Molecule 5: Flagellar basal body rod protein FlgB

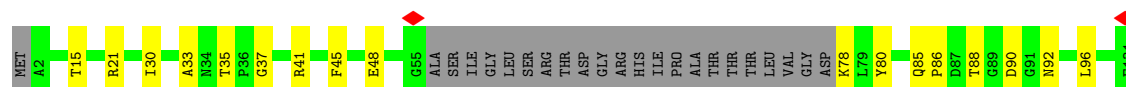


• Molecule 5: Flagellar basal body rod protein FlgB

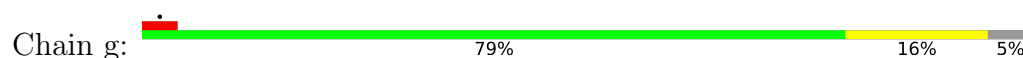




- Molecule 5: Flagellar basal body rod protein FlgB



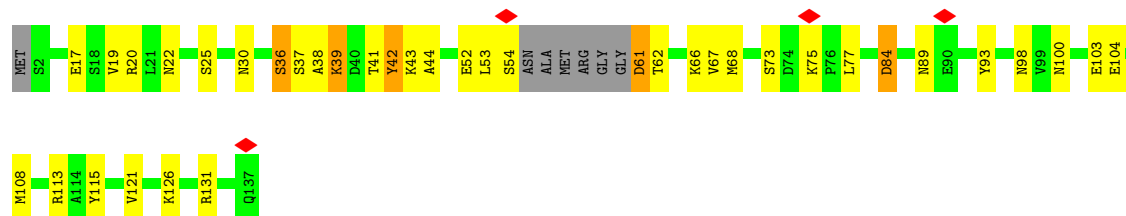
- Molecule 6: Flagellar basal-body rod protein FlgC



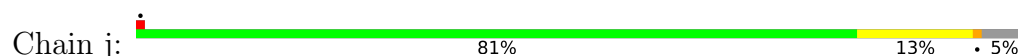
- Molecule 6: Flagellar basal-body rod protein FlgC

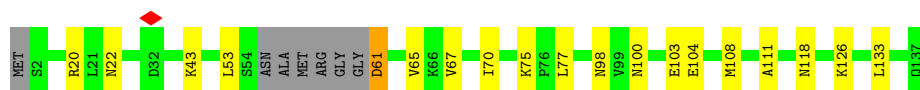


- Molecule 6: Flagellar basal-body rod protein FlgC

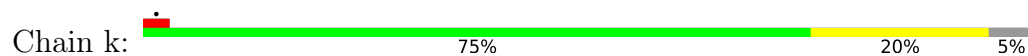


- Molecule 6: Flagellar basal-body rod protein FlgC

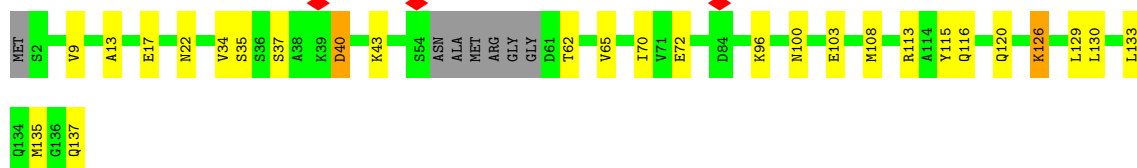
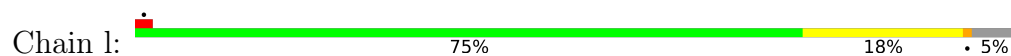




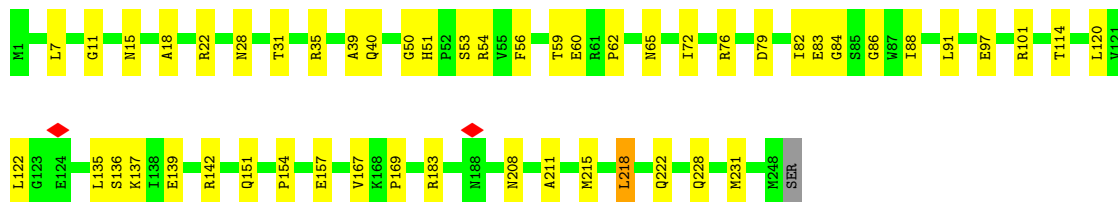
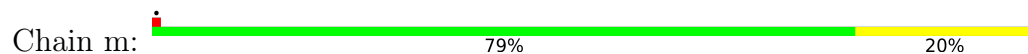
- Molecule 6: Flagellar basal-body rod protein FlgC



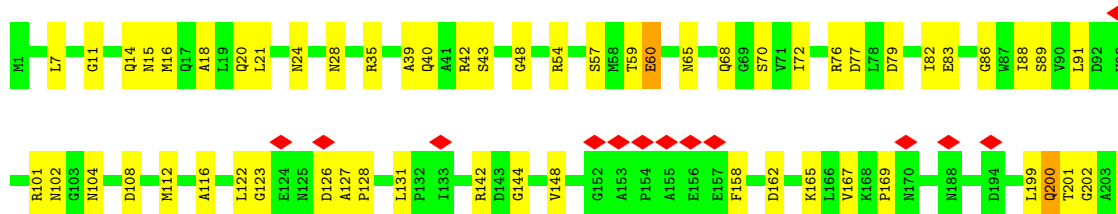
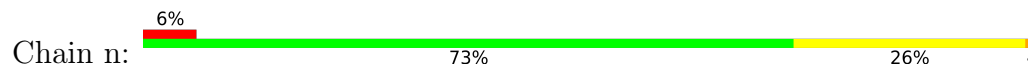
- Molecule 6: Flagellar basal-body rod protein FlgC



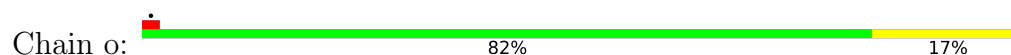
- Molecule 7: Flagellar basal-body rod protein FlgF

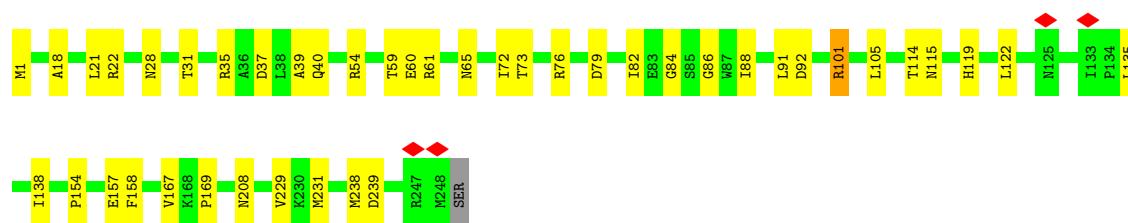


- Molecule 7: Flagellar basal-body rod protein FlgF

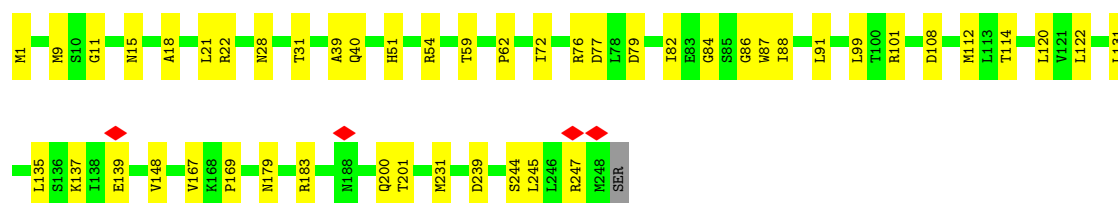
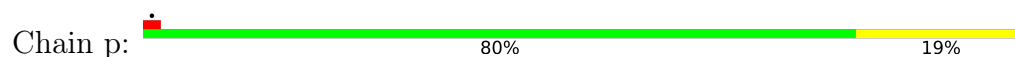


- Molecule 7: Flagellar basal-body rod protein FlgF

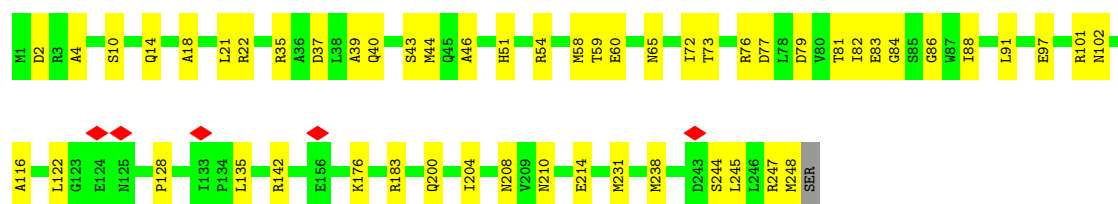
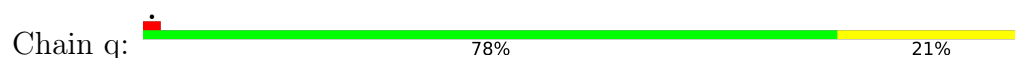




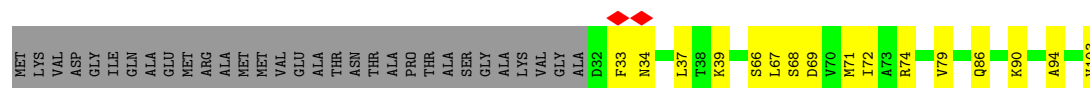
- Molecule 7: Flagellar basal-body rod protein FlgF



- Molecule 7: Flagellar basal-body rod protein FlgF



- Molecule 8: Flagellar hook-basal body complex protein FliE

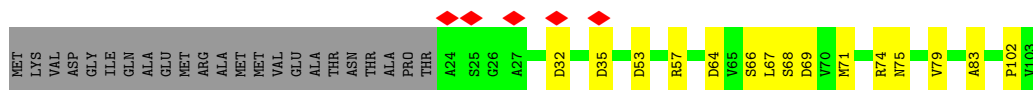


- Molecule 8: Flagellar hook-basal body complex protein FliE

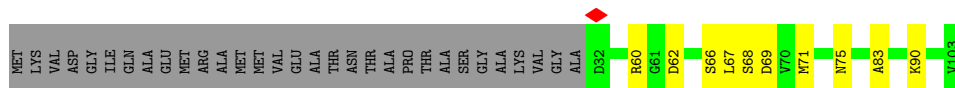


- Molecule 8: Flagellar hook-basal body complex protein FliE

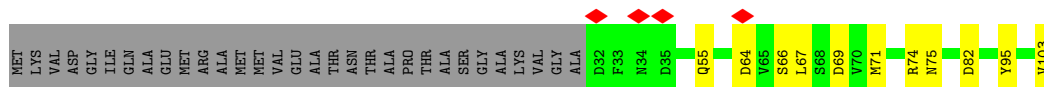




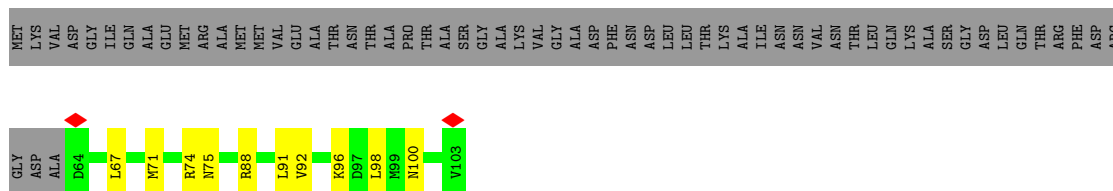
- Molecule 8: Flagellar hook-basal body complex protein FliE



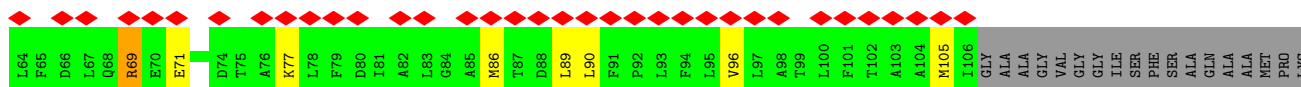
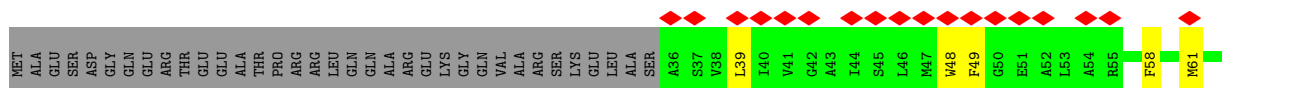
- Molecule 8: Flagellar hook-basal body complex protein FliE



- Molecule 8: Flagellar hook-basal body complex protein FliE



- Molecule 9: Flagellar biosynthetic protein FlhB



ASP
TYR
ASP
LEU
PRO
ILE
PRO
PRO
GLU
HIS
ARG
HIS

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	58418	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	105000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.875	Depositor
Minimum map value	-2.095	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.103	Depositor
Recommended contour level	0.42	Depositor
Map size (Å)	744.0, 744.0, 744.0	wwPDB
Map dimensions	620, 620, 620	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2, 1.2, 1.2	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	1	0.14	0/1628	0.30	0/2209
1	2	0.16	0/1637	0.33	0/2221
1	3	0.10	0/1637	0.26	0/2221
1	y	0.10	0/1637	0.27	0/2221
1	z	0.11	0/1637	0.28	0/2221
2	4	0.12	0/739	0.31	0/1005
2	5	0.16	0/739	0.34	0/1005
2	6	0.28	0/739	0.49	0/1005
2	7	0.16	0/739	0.33	0/1005
3	8	0.09	0/1941	0.25	0/2631
4	AA	0.35	0/137	0.45	0/188
4	AB	0.29	0/137	0.43	0/188
4	AC	0.14	0/141	0.31	0/193
4	AD	0.30	0/137	0.46	0/188
4	AE	0.12	0/137	0.28	0/188
4	AF	0.92	0/161	1.23	0/221
4	AG	0.16	0/75	0.32	0/103
4	AH	0.20	0/75	0.42	0/103
4	AI	0.94	0/75	1.34	0/103
4	AJ	0.37	0/166	0.57	0/228
4	AK	0.31	0/172	0.70	0/237
4	AL	0.39	0/223	0.62	0/304
4	AM	0.20	0/227	0.44	0/309
4	AN	0.23	0/227	0.49	0/309
4	AO	0.16	0/223	0.40	0/304
5	b	0.22	0/856	0.36	0/1151
5	c	0.22	0/846	0.30	0/1138
5	d	0.23	0/856	0.31	0/1151
5	e	0.19	0/848	0.31	0/1140
5	f	0.22	0/848	0.35	0/1140
6	g	0.11	0/996	0.26	0/1348
6	h	0.10	0/996	0.26	0/1348
6	i	0.30	0/996	0.46	0/1348
6	j	0.10	0/996	0.24	0/1348

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	k	0.11	0/996	0.28	0/1348
6	l	0.13	0/996	0.30	0/1348
7	m	0.11	0/1905	0.26	0/2572
7	n	0.13	0/1905	0.26	0/2572
7	o	0.10	0/1905	0.26	0/2572
7	p	0.11	0/1905	0.26	0/2572
7	q	0.10	0/1905	0.25	0/2572
8	r	0.32	0/564	0.43	0/759
8	s	0.08	0/609	0.20	0/819
8	t	0.07	0/609	0.17	0/819
8	u	0.07	0/564	0.16	0/759
8	v	0.07	0/564	0.18	0/759
8	w	0.09	0/313	0.19	0/420
9	x	0.08	0/562	0.19	0/760
All	All	0.17	0/38926	0.32	0/52673

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	2	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	2	188	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1599	0	1685	23	0
1	2	1608	0	1691	27	0
1	3	1608	0	1691	33	0
1	y	1608	0	1691	24	0
1	z	1608	0	1691	34	0
2	4	722	0	768	16	0
2	5	722	0	768	19	0
2	6	722	0	768	15	0
2	7	722	0	768	10	0
3	8	1896	0	1968	44	0
4	AA	135	0	128	3	0
4	AB	135	0	128	2	0
4	AC	139	0	131	0	0
4	AD	135	0	128	2	0
4	AE	135	0	128	2	0
4	AF	158	0	152	13	0
4	AG	73	0	72	4	0
4	AH	73	0	72	4	0
4	AI	73	0	72	8	0
4	AJ	163	0	157	4	0
4	AK	169	0	164	5	0
4	AL	220	0	215	3	0
4	AM	224	0	218	4	0
4	AN	224	0	218	2	0
4	AO	220	0	215	3	0
5	b	845	0	833	12	0
5	c	835	0	825	18	0
5	d	845	0	833	10	0
5	e	837	0	829	14	0
5	f	837	0	829	11	0
6	g	983	0	958	12	0
6	h	983	0	958	23	0
6	i	983	0	958	30	0
6	j	983	0	958	12	0
6	k	983	0	958	20	0
6	l	983	0	958	23	0
7	m	1879	0	1864	31	0
7	n	1879	0	1864	46	0
7	o	1879	0	1864	24	0
7	p	1879	0	1864	30	0
7	q	1879	0	1864	37	0
8	r	560	0	561	11	0
8	s	605	0	609	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	t	605	0	609	10	0
8	u	560	0	561	7	0
8	v	560	0	561	10	0
8	w	311	0	320	8	0
9	x	552	0	577	13	0
All	All	38336	0	38702	558	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (558) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:i:52:GLU:HG3	6:i:52:GLU:O	1.47	1.06
6:i:52:GLU:O	6:i:52:GLU:CG	2.15	0.94
1:y:82:ASP:HB3	1:y:167:THR:HG23	1.62	0.80
7:n:102:ASN:HD21	7:n:116:ALA:HB3	1.55	0.72
5:c:86:PRO:O	7:n:54:ARG:NH1	2.24	0.71
2:4:25:ILE:HG13	2:5:52:LEU:HD12	1.73	0.71
3:8:47:LEU:HD21	8:s:98:LEU:HD21	1.72	0.69
8:v:103:VAL:O	1:y:120:ARG:NH2	2.25	0.69
7:m:22:ARG:HE	7:m:39:ALA:HB3	1.58	0.69
4:AL:341:ASN:ND2	5:c:88:THR:OG1	2.26	0.68
6:l:40:ASP:N	6:l:40:ASP:OD1	2.26	0.68
8:r:103:VAL:HG23	1:z:113:VAL:HG13	1.76	0.68
4:AF:335:ILE:HG13	4:AF:338:ALA:HB2	1.74	0.68
3:8:92:MET:HE2	3:8:248:GLY:HA3	1.77	0.67
7:q:86:GLY:O	7:q:101:ARG:NH1	2.28	0.67
6:i:36:SER:HB2	7:n:43:SER:HB2	1.77	0.67
2:5:54:ARG:NH1	2:7:48:THR:OG1	2.28	0.67
7:n:24:ASN:O	7:n:28:ASN:ND2	2.24	0.66
1:2:244:VAL:HG11	1:2:262:SER:HB2	1.78	0.66
4:AA:355:GLN:O	4:AA:356:MET:HB3	1.94	0.66
7:o:65:ASN:O	7:o:208:ASN:ND2	2.29	0.66
1:2:141:LEU:HG	1:z:198:MET:HE1	1.78	0.66
6:i:53:LEU:O	6:i:54:SER:C	2.38	0.65
6:j:75:LYS:O	6:j:98:ASN:ND2	2.29	0.65
1:y:103:VAL:O	1:y:107:THR:OG1	2.15	0.65
6:h:22:ASN:HD22	7:o:54:ARG:HE	1.45	0.65
7:o:135:LEU:HD13	7:o:138:ILE:HD11	1.78	0.64
1:1:239:ILE:HG23	2:6:17:VAL:HG12	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:6:9:LEU:HD21	2:6:80:LEU:HD21	1.80	0.64
1:3:198:MET:HE2	1:y:144:PHE:HB2	1.80	0.64
1:z:244:VAL:HG11	1:z:262:SER:HB3	1.79	0.64
7:n:83:GLU:OE2	7:n:142:ARG:NH1	2.30	0.64
3:8:186:SER:HA	3:8:189:LEU:HD23	1.80	0.63
1:2:184:LEU:HG	1:2:214:LEU:HD11	1.81	0.63
2:7:50:SER:O	2:7:54:ARG:NH1	2.31	0.63
4:AI:335:ILE:HG13	4:AI:338:ALA:HB2	1.78	0.63
5:c:85:GLN:OE1	7:n:54:ARG:NH2	2.31	0.63
1:1:85:VAL:HA	1:1:88:GLN:HE21	1.63	0.63
1:1:183:MET:HE1	1:1:215:ILE:HG12	1.80	0.63
6:i:108:MET:HE2	7:n:231:MET:HE2	1.79	0.63
6:i:43:LYS:HG2	6:i:77:LEU:HD21	1.80	0.63
7:m:91:LEU:HD23	7:m:122:LEU:HD21	1.80	0.62
7:p:137:LYS:NZ	7:p:139:GLU:OE2	2.33	0.62
5:f:30:ILE:HG23	5:f:96:LEU:HD11	1.80	0.62
1:2:103:VAL:O	1:2:107:THR:OG1	2.18	0.62
4:AI:334:GLY:O	4:AI:335:ILE:C	2.40	0.62
6:i:61:ASP:OD1	6:i:61:ASP:N	2.33	0.62
7:m:11:GLY:O	7:m:15:ASN:ND2	2.31	0.62
1:z:103:VAL:O	1:z:107:THR:OG1	2.17	0.61
5:d:35:THR:O	5:d:92:ASN:ND2	2.33	0.61
8:w:71:MET:O	8:w:75:ASN:ND2	2.30	0.61
4:AH:335:ILE:HB	4:AH:338:ALA:HB2	1.82	0.61
1:1:104:ILE:O	1:1:110:THR:OG1	2.19	0.61
1:1:141:LEU:HD11	1:1:280:LEU:HD22	1.82	0.61
2:4:59:LEU:HD13	9:x:90:LEU:HD22	1.82	0.61
6:k:108:MET:HE2	7:p:231:MET:HE2	1.83	0.61
1:1:244:VAL:HG11	1:1:262:SER:HB3	1.81	0.61
2:4:1:MET:SD	2:4:1:MET:N	2.73	0.61
6:h:17:GLU:OE1	6:h:20:ARG:NH2	2.32	0.61
2:7:31:ILE:HG13	2:7:57:VAL:HG11	1.81	0.60
7:p:11:GLY:O	7:p:15:ASN:ND2	2.30	0.60
7:n:76:ARG:NH1	7:n:79:ASP:OD1	2.34	0.60
1:y:88:GLN:OE1	1:y:161:TYR:OH	2.14	0.60
4:AI:335:ILE:HD12	6:h:71:VAL:HG23	1.82	0.60
6:l:35:SER:OG	7:q:40:GLN:NE2	2.35	0.60
6:i:22:ASN:HD22	7:n:54:ARG:HE	1.49	0.60
5:e:15:THR:HG23	5:e:45:PHE:HZ	1.67	0.60
6:k:22:ASN:HD22	7:p:54:ARG:HE	1.48	0.60
6:l:37:SER:HB3	7:q:44:MET:HA	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:h:135:MET:HE2	8:t:75:ASN:HD22	1.66	0.60
6:i:100:ASN:HD22	6:i:103:GLU:H	1.49	0.60
6:k:75:LYS:O	6:k:98:ASN:ND2	2.34	0.60
1:y:112:ILE:HG23	1:y:283:LEU:HD23	1.84	0.60
7:q:65:ASN:O	7:q:208:ASN:ND2	2.34	0.59
6:j:133:LEU:HD23	8:u:71:MET:HE3	1.83	0.59
7:m:86:GLY:O	7:m:101:ARG:NH1	2.35	0.59
5:f:86:PRO:O	7:p:54:ARG:NH1	2.36	0.59
6:l:113:ARG:NH2	6:l:116:GLN:OE1	2.36	0.59
4:AF:350:PRO:HA	4:AF:353:VAL:HG22	1.83	0.59
7:q:102:ASN:HD21	7:q:116:ALA:HB3	1.66	0.59
6:j:22:ASN:HD22	7:m:54:ARG:HE	1.51	0.59
7:o:91:LEU:HD23	7:o:122:LEU:HD21	1.85	0.59
5:d:108:ILE:HD11	6:h:126:LYS:HG3	1.85	0.58
2:4:31:ILE:HG13	2:4:57:VAL:HG21	1.85	0.58
4:AH:341:ASN:ND2	7:m:50:GLY:O	2.36	0.58
5:f:35:THR:O	5:f:92:ASN:ND2	2.37	0.58
6:j:61:ASP:N	6:j:61:ASP:OD1	2.35	0.58
8:s:90:LYS:HE3	8:w:74:ARG:HH21	1.68	0.58
7:o:22:ARG:HE	7:o:39:ALA:HB3	1.69	0.58
1:z:183:MET:HE1	1:z:215:ILE:HG12	1.86	0.58
5:f:41:ARG:HG2	5:f:78:LYS:HE2	1.85	0.58
3:8:70:ARG:HA	3:8:73:MET:HE2	1.85	0.57
2:4:54:ARG:NH1	2:5:46:GLU:OE2	2.38	0.57
4:AG:335:ILE:HB	4:AG:338:ALA:HB2	1.86	0.57
5:e:86:PRO:O	7:m:54:ARG:NH1	2.35	0.57
1:y:248:LEU:HD11	1:y:261:VAL:HG11	1.86	0.57
4:AO:335:ILE:O	4:AO:340:SER:OG	2.14	0.57
7:q:22:ARG:HE	7:q:39:ALA:HB3	1.68	0.57
7:n:104:ASN:HB3	7:n:116:ALA:HB2	1.87	0.57
4:AJ:341:ASN:ND2	7:n:48:GLY:O	2.38	0.57
5:b:86:PRO:O	7:q:54:ARG:NH1	2.38	0.57
5:d:20:GLU:OE2	8:u:68:SER:OG	2.20	0.57
7:o:86:GLY:O	7:o:101:ARG:NH1	2.37	0.57
8:v:66:SER:OG	8:v:69:ASP:OD1	2.23	0.57
3:8:187:MET:HE2	3:8:240:HIS:HB3	1.86	0.57
6:h:35:SER:OG	7:o:40:GLN:NE2	2.38	0.57
7:o:40:GLN:NE2	7:o:60:GLU:OE2	2.35	0.57
6:k:61:ASP:OD1	6:k:61:ASP:N	2.38	0.57
1:3:239:ILE:HG23	9:x:89:LEU:HD22	1.87	0.57
4:AK:331:MET:HE3	6:g:52:GLU:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AN:352:ASP:OD1	4:AN:352:ASP:N	2.38	0.57
6:g:75:LYS:O	6:g:98:ASN:ND2	2.33	0.57
6:l:34:VAL:HG12	6:l:96:LYS:HG2	1.87	0.57
6:h:61:ASP:OD1	6:h:61:ASP:N	2.36	0.56
1:l:228:GLN:HA	3:8:136:MET:HE1	1.85	0.56
1:3:136:GLY:HA3	3:8:87:MET:HE2	1.87	0.56
2:5:31:ILE:HG13	2:5:57:VAL:HG21	1.88	0.56
4:AI:335:ILE:HD11	6:h:69:GLY:HA3	1.86	0.56
6:j:108:MET:HE2	7:m:231:MET:HE2	1.87	0.56
7:m:83:GLU:OE2	7:m:142:ARG:NH2	2.39	0.56
7:p:82:ILE:HD11	7:p:88:ILE:HG13	1.88	0.56
6:i:17:GLU:OE1	6:i:20:ARG:NH2	2.34	0.56
6:h:108:MET:HE2	7:o:231:MET:HE2	1.87	0.56
6:l:22:ASN:HD22	7:q:54:ARG:HE	1.53	0.56
1:2:144:PHE:HB2	1:z:198:MET:HE2	1.86	0.56
7:n:126:ASP:OD1	7:n:165:LYS:NZ	2.31	0.56
7:p:86:GLY:O	7:p:101:ARG:NH1	2.39	0.56
1:y:220:THR:HG23	1:z:276:TRP:HB3	1.88	0.55
5:c:20:GLU:OE2	8:t:68:SER:OG	2.24	0.55
4:AF:350:PRO:O	4:AF:351:GLN:C	2.50	0.55
4:AH:335:ILE:HD12	4:AN:356:MET:HE1	1.88	0.55
6:g:20:ARG:HH21	6:g:111:ALA:HA	1.71	0.55
7:p:76:ARG:NH1	7:p:79:ASP:OD1	2.39	0.55
1:l:103:VAL:O	1:l:107:THR:HG22	2.06	0.55
1:2:115:VAL:HG11	1:2:283:LEU:HD11	1.87	0.55
2:6:40:ALA:HA	3:8:211:GLN:HG3	1.87	0.55
6:k:135:MET:HE1	8:r:72:ILE:HG12	1.89	0.55
2:5:13:ALA:HB1	1:z:239:ILE:HD11	1.89	0.55
6:g:129:LEU:HD22	8:w:67:LEU:HD12	1.88	0.55
7:p:244:SER:HA	7:p:247:ARG:HG3	1.89	0.55
1:l:268:MET:HE1	2:7:1:MET:HG3	1.88	0.55
2:6:84:LEU:N	2:6:85:PRO:HD2	2.21	0.55
6:k:3:LEU:HD21	6:k:128:MET:HE3	1.89	0.55
7:p:91:LEU:HD23	7:p:122:LEU:HD21	1.89	0.55
1:z:104:ILE:O	1:z:110:THR:OG1	2.24	0.55
1:3:103:VAL:O	1:3:107:THR:OG1	2.23	0.54
1:3:112:ILE:HD13	1:3:141:LEU:HB3	1.89	0.54
4:AD:348:SER:HB2	4:AD:356:MET:HE3	1.89	0.54
8:u:66:SER:OG	8:u:69:ASP:OD1	2.25	0.54
4:AF:352:ASP:O	4:AF:353:VAL:C	2.51	0.54
6:g:108:MET:HE2	6:i:121:VAL:HG22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:k:3:LEU:HB3	6:k:129:LEU:HD21	1.89	0.54
7:m:154:PRO:HG2	7:m:157:GLU:HG3	1.89	0.54
6:k:43:LYS:HG2	6:k:77:LEU:HD21	1.90	0.54
2:4:6:PHE:HB2	1:z:268:MET:HE2	1.89	0.54
1:3:198:MET:HE1	1:y:141:LEU:HD22	1.90	0.54
5:c:30:ILE:HG23	5:c:96:LEU:HD11	1.89	0.54
7:p:18:ALA:HB2	7:p:59:THR:HG21	1.90	0.54
1:3:239:ILE:HD12	9:x:89:LEU:HD22	1.90	0.54
6:g:84:ASP:OD1	6:i:73:SER:OG	2.23	0.54
6:g:9:VAL:HG21	6:g:62:THR:HB	1.90	0.53
6:l:126:LYS:HD3	7:q:248:MET:HG2	1.91	0.53
6:l:108:MET:HE2	7:q:231:MET:HE2	1.89	0.53
8:t:66:SER:OG	8:t:69:ASP:OD1	2.26	0.53
3:8:54:MET:HE2	8:s:26:GLY:HA3	1.90	0.53
7:m:65:ASN:O	7:m:208:ASN:ND2	2.36	0.53
8:r:94:ALA:HA	1:z:100:PRO:HG3	1.90	0.53
4:AI:339:LEU:HD11	6:h:72:GLU:HG3	1.91	0.53
6:h:133:LEU:HA	8:t:71:MET:HE3	1.89	0.53
7:o:76:ARG:NH1	7:o:79:ASP:OD1	2.39	0.53
4:AJ:335:ILE:HG22	6:g:87:LEU:HD11	1.89	0.53
5:d:31:ALA:HA	6:j:118:ASN:HD21	1.73	0.53
5:c:85:GLN:HE21	6:i:19:VAL:HG22	1.73	0.53
5:e:36:PRO:HB3	5:e:90:ASP:HB2	1.91	0.53
3:8:64:ILE:HG22	3:8:70:ARG:HG2	1.91	0.53
5:f:37:GLY:N	5:f:90:ASP:O	2.42	0.53
6:l:133:LEU:HD23	8:v:71:MET:HE3	1.91	0.53
1:3:85:VAL:HG13	5:b:3:ILE:HA	1.90	0.52
2:5:81:ILE:HG13	1:z:278:LEU:HD21	1.91	0.52
1:3:125:LEU:HB3	1:3:128:THR:HB	1.91	0.52
3:8:97:VAL:HG22	3:8:131:MET:HB2	1.90	0.52
5:b:128:ILE:HG13	5:b:129:LYS:HG3	1.91	0.52
7:m:18:ALA:HB2	7:m:59:THR:HG21	1.90	0.52
7:n:82:ILE:HD11	7:n:88:ILE:HG13	1.92	0.52
4:AM:340:SER:HA	4:AM:349:ILE:HD11	1.90	0.52
7:q:77:ASP:OD1	7:q:77:ASP:N	2.43	0.52
5:e:41:ARG:NH2	5:e:80:TYR:OH	2.38	0.52
1:y:208:ASP:OD1	1:y:208:ASP:N	2.42	0.52
2:5:81:ILE:HG21	1:z:278:LEU:HD11	1.91	0.52
3:8:150:LEU:HD13	3:8:252:ILE:HG21	1.92	0.52
4:AE:351:GLN:O	7:n:42:ARG:NH1	2.38	0.52
1:2:248:LEU:HD11	1:2:261:VAL:HG11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:8:28:VAL:HB	3:8:86:GLY:HA3	1.91	0.51
7:o:18:ALA:HB2	7:o:59:THR:HG21	1.91	0.51
1:2:112:ILE:HD13	1:2:141:LEU:HB3	1.92	0.51
7:n:86:GLY:O	7:n:101:ARG:NH1	2.44	0.51
6:l:9:VAL:HG21	6:l:62:THR:HB	1.92	0.51
7:n:70:SER:O	7:n:206:GLY:N	2.30	0.51
7:o:82:ILE:HD11	7:o:88:ILE:HG13	1.92	0.51
1:1:198:MET:HE2	3:8:53:VAL:HG11	1.92	0.51
1:3:139:LEU:HD21	8:w:98:LEU:HD13	1.93	0.51
4:AF:347:ALA:O	4:AF:353:VAL:HG13	2.10	0.51
7:q:84:GLY:O	7:q:101:ARG:NH2	2.42	0.51
1:3:255:MET:HB2	3:8:214:ILE:HG12	1.93	0.51
5:c:119:SER:OG	8:s:74:ARG:NH2	2.44	0.51
7:o:84:GLY:O	7:o:101:ARG:NH2	2.43	0.51
4:AI:339:LEU:HD11	6:h:72:GLU:CG	2.41	0.51
1:1:282:THR:HG21	2:6:81:ILE:HG23	1.93	0.51
1:2:112:ILE:HG22	1:2:116:MET:HE2	1.93	0.51
7:q:14:GLN:HG3	7:q:58:MET:HA	1.92	0.51
7:o:1:MET:HG3	7:o:239:ASP:HB2	1.93	0.50
2:6:52:LEU:HB2	2:7:25:ILE:HG21	1.94	0.50
4:AH:342:GLN:HG3	4:AH:343:PRO:HD2	1.92	0.50
5:b:35:THR:O	5:b:92:ASN:ND2	2.44	0.50
5:e:88:THR:HG22	7:m:56:PHE:HZ	1.74	0.50
3:8:81:ILE:HG22	3:8:85:MET:HE1	1.94	0.50
4:AG:336:PRO:HG2	4:AO:352:ASP:HB3	1.92	0.50
3:8:204:VAL:HG23	9:x:39:LEU:HD22	1.93	0.50
6:l:70:ILE:HD13	7:q:51:HIS:HB3	1.93	0.50
4:AK:330:ASN:N	4:AK:330:ASN:HD22	2.10	0.50
5:c:104:MET:SD	6:i:126:LYS:NZ	2.80	0.50
4:AF:347:ALA:HA	4:AF:353:VAL:CG1	2.42	0.50
7:n:21:LEU:HD23	7:n:39:ALA:HB2	1.94	0.50
1:2:276:TRP:HB3	1:z:220:THR:HG23	1.93	0.50
4:AK:353:VAL:HG21	6:g:71:VAL:HG11	1.94	0.50
1:3:183:MET:HE1	1:3:211:MET:HG3	1.92	0.50
6:i:37:SER:O	6:i:38:ALA:HB3	2.11	0.50
1:1:104:ILE:HD12	3:8:44:TYR:HE2	1.77	0.50
5:d:128:ILE:HD13	8:u:83:ALA:HB2	1.94	0.50
3:8:43:LEU:HD21	8:s:99:MET:HA	1.95	0.49
8:u:60:ARG:NH1	8:u:62:ASP:OD1	2.45	0.49
1:z:142:THR:HA	1:z:145:VAL:HG22	1.93	0.49
6:l:120:GLN:HE22	7:p:247:ARG:HG2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:5:MET:SD	2:4:83:ARG:NH2	2.85	0.49
5:e:85:GLN:NE2	7:m:53:SER:OG	2.34	0.49
7:q:35:ARG:NH1	7:q:101:ARG:HD3	2.27	0.49
1:2:112:ILE:HG23	1:2:283:LEU:HD23	1.94	0.49
1:1:195:PHE:HB3	1:1:213:VAL:HG22	1.95	0.49
1:y:144:PHE:O	1:y:147:SER:OG	2.27	0.49
1:2:116:MET:HE3	1:2:134:ILE:HG23	1.94	0.49
7:p:84:GLY:O	7:p:101:ARG:NH2	2.32	0.49
6:h:75:LYS:O	6:h:98:ASN:ND2	2.43	0.49
6:k:133:LEU:HD23	8:r:71:MET:HE3	1.95	0.49
5:f:33:ALA:O	5:f:92:ASN:ND2	2.45	0.49
1:2:253:MET:HA	1:z:249:MET:HE3	1.95	0.49
2:6:1:MET:SD	2:6:1:MET:N	2.70	0.48
7:p:200:GLN:NE2	7:p:201:THR:O	2.45	0.48
1:1:184:LEU:HD11	1:1:207:GLU:HA	1.95	0.48
4:AL:353:VAL:HG21	6:h:71:VAL:HG11	1.94	0.48
5:c:97:ASP:OD1	6:i:115:TYR:OH	2.32	0.48
7:q:40:GLN:NE2	7:q:60:GLU:OE2	2.40	0.48
9:x:49:PHE:HB3	9:x:96:VAL:HG22	1.95	0.48
7:m:35:ARG:NH1	7:m:101:ARG:HD3	2.29	0.48
7:n:89:SER:HB3	7:n:122:LEU:HD12	1.95	0.48
7:p:22:ARG:HE	7:p:39:ALA:HB3	1.78	0.48
1:3:236:PRO:HB2	9:x:61:MET:HG2	1.95	0.48
3:8:183:THR:HG22	3:8:187:MET:HE3	1.95	0.48
6:g:61:ASP:N	6:g:61:ASP:OD1	2.45	0.48
1:y:82:ASP:OD1	1:y:82:ASP:N	2.45	0.48
1:y:183:MET:HE1	1:y:215:ILE:HG12	1.95	0.48
5:d:39:LYS:NZ	5:d:91:GLY:O	2.40	0.48
1:z:111:ARG:NE	1:z:222:GLU:OE1	2.44	0.48
1:1:119:LEU:HD21	1:1:270:PHE:CE1	2.49	0.47
2:5:8:GLU:HG2	2:5:83:ARG:NH2	2.29	0.47
7:n:40:GLN:NE2	7:n:60:GLU:OE2	2.39	0.47
6:h:13:ALA:O	6:h:17:GLU:HG2	2.14	0.47
7:m:76:ARG:NH1	7:m:79:ASP:OD1	2.44	0.47
1:y:149:VAL:HG23	1:y:178:PRO:HB2	1.96	0.47
7:n:14:GLN:HB3	7:n:59:THR:HG23	1.95	0.47
2:5:42:THR:HG23	2:5:44:ILE:HG12	1.96	0.47
5:f:85:GLN:OE1	6:k:22:ASN:ND2	2.47	0.47
3:8:27:MET:HE1	8:w:92:VAL:HG13	1.96	0.47
5:d:30:ILE:HG23	5:d:96:LEU:HD11	1.97	0.47
8:s:71:MET:SD	8:s:74:ARG:NH1	2.85	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:154:ASN:HA	1:2:158:VAL:HB	1.95	0.47
5:b:9:LEU:HD12	5:b:120:LYS:HB3	1.97	0.47
5:c:24:GLU:OE2	6:h:2:SER:N	2.47	0.47
6:i:126:LYS:HD3	7:n:248:MET:HA	1.96	0.47
8:u:71:MET:O	8:u:75:ASN:ND2	2.28	0.47
8:w:88:ARG:HH11	8:w:92:VAL:HG21	1.80	0.47
1:2:264:PRO:HG3	1:z:234:PHE:CG	2.50	0.47
5:b:30:ILE:HG23	5:b:96:LEU:HD11	1.96	0.47
7:m:114:THR:HG22	7:m:120:LEU:HD13	1.96	0.47
7:o:35:ARG:NH1	7:o:101:ARG:HD3	2.30	0.47
1:1:105:LEU:HD23	3:8:44:TYR:HB3	1.97	0.47
5:f:21:ARG:NH1	5:f:48:GLU:OE1	2.48	0.47
1:2:258:PRO:HA	1:2:261:VAL:HG12	1.98	0.46
2:5:87:VAL:C	2:5:89:TYR:H	2.23	0.46
4:AF:349:ILE:O	4:AF:350:PRO:C	2.58	0.46
4:AM:341:ASN:ND2	5:f:88:THR:OG1	2.48	0.46
5:e:43:LEU:HG	5:e:48:GLU:HG3	1.96	0.46
6:i:84:ASP:OD1	6:i:84:ASP:N	2.32	0.46
7:o:21:LEU:HD23	7:o:39:ALA:HB2	1.97	0.46
4:AK:340:SER:HA	4:AK:349:ILE:HD11	1.97	0.46
5:c:35:THR:O	5:c:92:ASN:ND2	2.48	0.46
6:j:20:ARG:HH21	6:j:111:ALA:HA	1.79	0.46
8:s:90:LYS:HG3	8:w:74:ARG:HE	1.80	0.46
1:z:81:GLU:O	1:z:169:ARG:NH2	2.49	0.46
1:3:264:PRO:HG2	3:8:196:LEU:HD11	1.98	0.46
3:8:43:LEU:HB2	8:s:103:VAL:HG11	1.98	0.46
6:h:66:LYS:HE3	6:h:68:MET:SD	2.56	0.46
6:j:100:ASN:O	6:j:104:GLU:HG2	2.16	0.46
6:k:70:ILE:HD13	7:p:51:HIS:HB3	1.97	0.46
1:1:208:ASP:OD1	1:1:208:ASP:N	2.49	0.46
3:8:85:MET:HG3	3:8:252:ILE:HG23	1.98	0.46
5:d:15:THR:HG23	5:d:45:PHE:HZ	1.81	0.46
6:j:100:ASN:HB3	6:j:103:GLU:HG2	1.98	0.46
7:o:28:ASN:O	7:o:31:THR:OG1	2.34	0.46
1:y:141:LEU:HD11	1:y:280:LEU:HD22	1.98	0.46
7:p:28:ASN:O	7:p:31:THR:OG1	2.32	0.46
1:2:186:GLN:NE2	1:2:287:PHE:O	2.49	0.46
4:AI:342:GLN:O	4:AI:343:PRO:C	2.59	0.46
7:n:91:LEU:HD21	7:n:128:PRO:HG3	1.96	0.46
7:p:9:MET:HE3	7:p:9:MET:HB3	1.82	0.46
2:6:16:MET:HE1	2:6:76:TYR:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:p:131:LEU:HD23	7:p:148:VAL:HG11	1.97	0.46
1:3:128:THR:HG22	3:8:98:LEU:HG	1.98	0.45
3:8:25:MET:HE1	3:8:148:LEU:HD23	1.98	0.45
4:AF:344:PRO:O	4:AF:345:ALA:C	2.57	0.45
7:n:91:LEU:HD23	7:n:122:LEU:HD21	1.98	0.45
1:2:263:LEU:HD23	1:z:234:PHE:HE2	1.80	0.45
5:e:30:ILE:HG23	5:e:96:LEU:HD11	1.98	0.45
8:t:53:ASP:OD2	8:t:57:ARG:NH1	2.50	0.45
2:5:19:ILE:HG21	2:5:72:MET:HE1	1.98	0.45
3:8:74:THR:O	3:8:78:GLN:HG2	2.17	0.45
5:b:39:LYS:NZ	5:b:91:GLY:O	2.42	0.45
5:b:126:LYS:HE2	8:v:82:ASP:OD1	2.16	0.45
1:y:183:MET:HE2	1:y:214:LEU:HG	1.98	0.45
6:i:39:LYS:HA	6:i:39:LYS:HD3	1.74	0.45
4:AF:336:PRO:HG2	4:AM:352:ASP:HB3	1.98	0.45
6:i:30:ASN:OD1	7:n:57:SER:HB3	2.17	0.45
6:i:52:GLU:O	6:i:53:LEU:C	2.59	0.45
7:q:18:ALA:HB2	7:q:59:THR:HG21	1.99	0.45
1:3:90:LEU:O	1:3:94:THR:OG1	2.34	0.45
1:3:116:MET:HE3	3:8:177:LEU:HD22	1.98	0.45
1:2:204:ASP:OD1	1:2:204:ASP:N	2.49	0.45
6:h:27:ASN:OD1	6:h:42:TYR:OH	2.27	0.45
1:1:144:PHE:HD2	1:2:198:MET:HE3	1.82	0.45
2:6:31:ILE:HG13	2:6:57:VAL:HG11	1.99	0.45
5:e:20:GLU:OE2	8:r:68:SER:OG	2.34	0.45
7:p:114:THR:HG22	7:p:120:LEU:HD13	1.99	0.45
7:q:244:SER:HA	7:q:247:ARG:HB2	1.98	0.45
8:r:86:GLN:O	8:r:90:LYS:HG2	2.17	0.45
1:z:116:MET:SD	1:z:134:ILE:HG23	2.57	0.45
1:3:108:SER:HB2	1:3:287:PHE:CZ	2.51	0.44
2:5:1:MET:HE2	2:5:87:VAL:HG11	1.98	0.44
4:AJ:341:ASN:HD21	5:c:86:PRO:HG3	1.82	0.44
4:AM:331:MET:HE2	4:AM:331:MET:HB3	1.87	0.44
5:c:26:ILE:HG21	5:c:103:PHE:HB2	1.99	0.44
7:n:18:ALA:HB2	7:n:59:THR:HG21	1.98	0.44
7:p:21:LEU:HD23	7:p:39:ALA:HB2	1.98	0.44
1:3:251:MET:HE2	9:x:39:LEU:HD23	1.99	0.44
2:5:87:VAL:C	2:5:89:TYR:N	2.74	0.44
4:AF:339:LEU:HD11	6:l:72:GLU:HG3	1.99	0.44
7:m:137:LYS:NZ	7:m:139:GLU:OE2	2.48	0.44
7:n:167:VAL:HG12	7:n:169:PRO:HD3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:z:125:LEU:HD22	1:z:263:LEU:HD11	1.98	0.44
3:8:18:PRO:HB3	3:8:57:ILE:HD13	2.00	0.44
3:8:215:PHE:HD2	3:8:216:SER:H	1.66	0.44
6:i:22:ASN:ND2	7:n:54:ARG:HE	2.15	0.44
7:n:131:LEU:HD23	7:n:148:VAL:HG11	1.99	0.44
5:b:85:GLN:OE1	6:l:22:ASN:ND2	2.51	0.44
6:l:129:LEU:HD22	8:v:67:LEU:HD12	1.99	0.44
7:q:82:ILE:HD11	7:q:88:ILE:HG13	2.00	0.44
8:s:48:GLN:HE21	8:s:81:PHE:HB2	1.81	0.44
2:6:63:MET:HG2	2:7:11:ARG:HA	1.98	0.44
4:AA:349:ILE:HG12	7:q:46:ALA:HA	1.99	0.44
7:o:105:LEU:HA	7:o:115:ASN:HA	2.00	0.44
8:w:96:LYS:O	8:w:100:ASN:ND2	2.45	0.44
9:x:71:GLU:HA	9:x:77:LYS:HD2	1.99	0.44
4:AF:348:SER:O	4:AF:349:ILE:HB	2.17	0.44
6:i:66:LYS:HE3	6:i:68:MET:HG2	1.99	0.44
7:p:40:GLN:HG2	7:p:62:PRO:HD3	1.99	0.44
4:AA:353:VAL:O	4:AA:356:MET:HG2	2.18	0.44
7:m:211:ALA:O	7:m:215:MET:HG2	2.18	0.44
7:q:21:LEU:HD23	7:q:39:ALA:HB2	2.00	0.44
7:q:37:ASP:OD1	7:q:176:LYS:NZ	2.42	0.44
2:4:20:MET:HE1	2:4:69:MET:HB3	2.00	0.43
5:b:21:ARG:NH1	5:b:48:GLU:OE1	2.51	0.43
7:q:91:LEU:HD21	7:q:128:PRO:HG3	1.98	0.43
8:v:64:ASP:OD1	8:v:64:ASP:N	2.48	0.43
2:5:8:GLU:HG2	2:5:83:ARG:HH22	1.82	0.43
2:6:67:HIS:HD2	2:7:11:ARG:HH22	1.65	0.43
6:k:39:LYS:HD2	6:k:39:LYS:HA	1.85	0.43
1:y:238:LEU:HD11	1:z:261:VAL:HG13	2.00	0.43
2:5:12:GLU:OE1	2:5:83:ARG:NH1	2.50	0.43
6:j:70:ILE:HD13	7:m:51:HIS:HB3	1.99	0.43
1:y:204:ASP:OD1	1:y:204:ASP:N	2.46	0.43
6:g:100:ASN:O	6:g:104:GLU:HG2	2.18	0.43
6:j:22:ASN:ND2	7:m:54:ARG:HE	2.14	0.43
7:n:15:ASN:ND2	7:n:228:GLN:HE22	2.16	0.43
1:y:108:SER:HB2	1:y:287:PHE:CZ	2.53	0.43
5:e:35:THR:O	5:e:92:ASN:ND2	2.52	0.43
7:o:92:ASP:OD1	7:o:92:ASP:N	2.46	0.43
7:o:154:PRO:HG2	7:o:157:GLU:HG3	1.99	0.43
8:v:55:GLN:NE2	8:v:74:ARG:HE	2.16	0.43
5:e:41:ARG:HD3	5:e:78:LYS:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:m:97:GLU:O	7:m:183:ARG:NH1	2.52	0.43
5:b:33:ALA:O	5:b:92:ASN:ND2	2.51	0.43
6:k:100:ASN:HB3	6:k:103:GLU:HG2	1.99	0.43
7:q:91:LEU:HD23	7:q:122:LEU:HD21	2.01	0.43
3:8:132:PHE:O	3:8:136:MET:HG2	2.19	0.43
5:b:36:PRO:HB3	5:b:90:ASP:HB2	2.01	0.43
5:f:15:THR:HG23	5:f:45:PHE:HZ	1.84	0.43
6:l:115:TYR:CG	7:q:238:MET:HE3	2.53	0.43
7:m:218:LEU:O	7:m:222:GLN:HG3	2.18	0.43
1:1:255:MET:HG2	1:2:257:SER:HA	2.01	0.43
1:3:114:VAL:O	1:3:118:ILE:HG12	2.17	0.43
2:4:81:ILE:HG13	1:y:278:LEU:HD21	2.01	0.43
4:AE:343:PRO:HG3	5:c:80:TYR:CZ	2.54	0.43
5:d:36:PRO:HB3	5:d:90:ASP:HB2	2.01	0.43
6:i:75:LYS:HB2	6:i:98:ASN:HD22	1.84	0.43
6:l:37:SER:N	7:q:43:SER:O	2.52	0.43
7:m:136:SER:HB2	7:m:151:GLN:HA	2.00	0.43
7:n:77:ASP:OD1	7:n:77:ASP:N	2.51	0.43
1:z:203:VAL:HG11	1:z:209:VAL:HG12	1.99	0.43
1:1:275:GLY:O	1:1:279:ILE:HG12	2.19	0.43
2:5:84:LEU:HD11	1:z:229:ILE:HG12	2.01	0.43
8:t:64:ASP:OD1	8:t:64:ASP:N	2.46	0.43
1:y:195:PHE:HB3	1:y:213:VAL:HG13	2.01	0.43
2:7:16:MET:HE1	2:7:76:TYR:HB2	2.01	0.42
3:8:207:ARG:HH12	3:8:210:PRO:HA	1.84	0.42
6:l:13:ALA:O	6:l:17:GLU:HG2	2.19	0.42
1:3:204:ASP:OD1	1:3:204:ASP:N	2.52	0.42
1:3:228:GLN:O	1:3:232:MET:HG2	2.18	0.42
6:i:100:ASN:O	6:i:104:GLU:HG2	2.19	0.42
1:3:243:VAL:HG21	9:x:89:LEU:HD11	2.01	0.42
3:8:176:TRP:HE1	3:8:251:GLN:HG2	1.83	0.42
6:h:115:TYR:CG	7:o:238:MET:HE3	2.54	0.42
6:l:22:ASN:ND2	7:q:54:ARG:HE	2.17	0.42
2:4:49:LEU:HD23	2:4:49:LEU:H	1.84	0.42
4:AL:338:ALA:HB1	6:h:103:GLU:HB2	2.01	0.42
6:i:44:ALA:O	6:i:73:SER:N	2.46	0.42
6:k:119:VAL:HG13	7:p:245:LEU:HG	2.00	0.42
1:3:101:ALA:HB2	8:v:95:TYR:OH	2.19	0.42
6:k:126:LYS:HE2	6:k:126:LYS:HB3	1.86	0.42
7:n:200:GLN:NE2	7:n:201:THR:O	2.53	0.42
2:5:15:TRP:HE3	2:7:63:MET:HE1	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:6:70:THR:O	2:6:71:GLN:C	2.63	0.42
3:8:84:ALA:HB1	3:8:255:LEU:HD13	2.01	0.42
6:g:127:GLN:O	6:g:131:ARG:HG2	2.20	0.42
6:i:41:THR:O	6:i:42:TYR:C	2.62	0.42
6:k:133:LEU:HA	8:r:71:MET:HE3	2.01	0.42
1:z:110:THR:HG21	1:z:219:ILE:HD11	2.01	0.42
4:AO:333:ALA:HB3	4:AO:356:MET:HB3	2.02	0.42
6:h:36:SER:OG	6:h:38:ALA:O	2.27	0.42
7:q:210:ASN:O	7:q:214:GLU:HG2	2.20	0.42
1:y:167:THR:HG22	1:y:169:ARG:H	1.84	0.42
1:z:166:VAL:HB	1:z:170:GLU:HB2	2.00	0.42
1:2:272:LEU:HD12	1:2:273:VAL:HG23	2.02	0.42
2:4:17:VAL:HG23	1:y:243:VAL:HG23	2.01	0.42
2:4:21:VAL:O	2:4:25:ILE:HG12	2.20	0.42
4:AK:337:GLY:O	4:AK:341:ASN:ND2	2.53	0.42
7:n:40:GLN:HE21	7:n:60:GLU:CD	2.27	0.42
8:r:33:PHE:HE1	1:z:154:ASN:HB2	1.84	0.42
8:r:66:SER:OG	8:r:69:ASP:OD1	2.38	0.42
1:3:280:LEU:HD11	3:8:175:GLY:HA2	2.02	0.42
4:AD:346:ASP:OD1	5:d:39:LYS:NZ	2.44	0.42
4:AF:342:GLN:O	4:AF:343:PRO:C	2.61	0.42
5:e:85:GLN:HE21	7:m:53:SER:HG	1.61	0.42
6:k:22:ASN:ND2	7:p:54:ARG:HE	2.14	0.42
7:n:35:ARG:NH1	7:n:101:ARG:HD3	2.34	0.42
7:o:37:ASP:HB3	7:o:61:ARG:HD2	2.02	0.42
8:r:71:MET:HA	8:r:74:ARG:HG2	2.02	0.42
1:3:162:LEU:HD21	3:8:69:PHE:HB3	2.02	0.42
2:4:80:LEU:HA	2:4:83:ARG:HG2	2.01	0.42
2:5:16:MET:HE2	2:5:76:TYR:HB2	2.02	0.42
5:c:128:ILE:HD13	8:t:83:ALA:HB2	2.02	0.42
7:p:87:TRP:HB3	7:p:99:LEU:HB3	2.01	0.42
7:q:76:ARG:NH1	7:q:79:ASP:OD1	2.47	0.42
7:q:97:GLU:O	7:q:183:ARG:NH1	2.53	0.42
9:x:105:MET:HE2	9:x:105:MET:HB3	1.98	0.42
1:3:255:MET:HE3	3:8:214:ILE:HG12	2.01	0.41
4:AB:343:PRO:HG3	5:f:80:TYR:CZ	2.55	0.41
6:l:100:ASN:HB3	6:l:103:GLU:HG2	2.01	0.41
7:m:84:GLY:O	7:m:101:ARG:NH2	2.31	0.41
7:n:123:GLY:N	7:n:127:ALA:O	2.53	0.41
7:n:218:LEU:O	7:n:222:GLN:HG3	2.20	0.41
2:4:8:GLU:OE1	2:4:83:ARG:NH2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:m:82:ILE:HD11	7:m:88:ILE:HG13	2.02	0.41
7:n:65:ASN:O	7:n:208:ASN:ND2	2.51	0.41
9:x:77:LYS:HE3	9:x:77:LYS:HB2	1.89	0.41
1:z:183:MET:HB2	1:z:214:LEU:HD21	2.02	0.41
1:2:274:ASP:OD2	1:2:277:ASN:ND2	2.52	0.41
3:8:88:VAL:HG12	3:8:92:MET:HE3	2.02	0.41
3:8:207:ARG:HD3	3:8:207:ARG:O	2.20	0.41
7:m:28:ASN:O	7:m:31:THR:OG1	2.37	0.41
7:m:167:VAL:HG12	7:m:169:PRO:HD3	2.03	0.41
7:n:142:ARG:HH12	7:n:200:GLN:HG2	1.86	0.41
7:q:81:THR:HG23	7:q:200:GLN:HB3	2.03	0.41
1:3:88:GLN:OE1	1:3:161:TYR:OH	2.29	0.41
4:AB:353:VAL:HG21	6:k:38:ALA:HB2	2.01	0.41
6:k:96:LYS:HE3	6:k:96:LYS:HB3	1.89	0.41
7:n:11:GLY:O	7:n:15:ASN:ND2	2.45	0.41
1:1:188:ARG:NH1	1:1:225:THR:OG1	2.46	0.41
1:3:104:ILE:HG22	1:3:109:PHE:CD2	2.56	0.41
1:3:253:MET:H	1:3:253:MET:HG2	1.69	0.41
4:AF:346:ASP:HB3	4:AF:347:ALA:H	1.61	0.41
5:c:32:GLN:NE2	6:h:51:ALA:HB2	2.35	0.41
7:n:16:MET:O	7:n:20:GLN:HG3	2.20	0.41
7:q:14:GLN:HB3	7:q:59:THR:HG23	2.01	0.41
1:3:273:VAL:HG22	9:x:58:PHE:CE2	2.56	0.41
3:8:61:PRO:HG3	3:8:161:GLY:HA3	2.03	0.41
6:j:43:LYS:HG2	6:j:77:LEU:HD21	2.02	0.41
7:n:68:GLN:OE1	7:n:101:ARG:NH2	2.53	0.41
2:4:44:ILE:HG22	2:4:46:GLU:H	1.86	0.41
3:8:39:PRO:HD2	8:t:102:PRO:HG2	2.01	0.41
6:l:130:LEU:HD11	7:q:248:MET:HE3	2.03	0.41
7:p:1:MET:HG3	7:p:239:ASP:HB2	2.03	0.41
3:8:213:ASN:HB2	3:8:215:PHE:CE1	2.55	0.41
1:z:184:LEU:O	1:z:187:THR:HG22	2.21	0.41
1:1:189:ILE:HD12	1:1:189:ILE:H	1.85	0.41
2:6:73:LEU:HD13	2:6:73:LEU:HA	1.97	0.41
4:AG:343:PRO:HA	4:AG:344:PRO:HD3	1.92	0.41
4:AI:335:ILE:O	4:AI:336:PRO:C	2.61	0.41
4:AJ:341:ASN:ND2	5:c:86:PRO:HG3	2.36	0.41
5:c:124:LEU:HD23	8:t:79:VAL:HG11	2.03	0.41
6:i:89:ASN:OD1	6:i:93:TYR:N	2.51	0.41
6:l:135:MET:HE2	8:v:75:ASN:HD22	1.85	0.41
7:p:77:ASP:OD1	7:p:77:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:p:108:ASP:OD1	7:p:112:MET:N	2.54	0.41
7:p:179:ASN:HD21	7:p:183:ARG:HH21	1.69	0.41
1:2:104:ILE:O	1:2:110:THR:OG1	2.38	0.41
1:3:128:THR:HB	1:3:129:PRO:HD3	2.03	0.41
2:6:81:ILE:HA	2:6:84:LEU:HD13	2.02	0.41
4:AG:339:LEU:HD11	6:k:72:GLU:HG3	2.03	0.41
5:e:124:LEU:HD23	8:r:79:VAL:HG11	2.03	0.41
6:i:53:LEU:N	6:i:53:LEU:HD23	2.36	0.41
7:n:231:MET:HA	7:n:234:THR:HG22	2.03	0.41
7:q:83:GLU:OE1	7:q:142:ARG:NH2	2.54	0.41
8:v:71:MET:SD	8:v:74:ARG:HD3	2.61	0.41
1:2:270:PHE:HE2	1:2:276:TRP:CD1	2.38	0.40
6:l:126:LYS:NZ	7:q:245:LEU:O	2.53	0.40
7:n:108:ASP:OD1	7:n:112:MET:N	2.54	0.40
7:o:167:VAL:HG12	7:o:169:PRO:HD3	2.04	0.40
9:x:69:ARG:CZ	9:x:69:ARG:H	2.34	0.40
1:2:96:LEU:HB3	8:u:90:LYS:HB3	2.03	0.40
1:3:186:GLN:HE22	1:3:287:PHE:HA	1.85	0.40
6:h:120:GLN:HE22	7:n:247:ARG:NE	2.18	0.40
7:m:40:GLN:HG2	7:m:62:PRO:HD3	2.01	0.40
7:o:115:ASN:OD1	7:o:119:HIS:N	2.54	0.40
7:q:10:SER:O	7:q:14:GLN:HG2	2.22	0.40
1:y:254:MET:HB2	1:z:254:MET:SD	2.61	0.40
1:1:242:LEU:HD13	3:8:125:LEU:HD12	2.01	0.40
1:2:111:ARG:NE	1:2:222:GLU:OE1	2.50	0.40
2:5:84:LEU:HD13	1:z:232:MET:HG3	2.04	0.40
2:6:56:ILE:HG12	2:7:18:LEU:HD11	2.04	0.40
6:i:25:SER:HB2	7:n:7:LEU:HD23	2.04	0.40
7:m:15:ASN:ND2	7:m:228:GLN:HE22	2.18	0.40
7:n:76:ARG:O	7:n:202:GLY:HA2	2.20	0.40
7:n:144:GLY:HA2	7:n:199:LEU:HD12	2.03	0.40
7:q:2:ASP:C	7:q:4:ALA:H	2.29	0.40
8:t:71:MET:SD	8:t:74:ARG:HD3	2.61	0.40
1:z:152:GLU:CD	1:z:178:PRO:HB3	2.46	0.40
7:p:167:VAL:HG12	7:p:169:PRO:HD3	2.04	0.40
2:4:14:LEU:HA	2:4:17:VAL:HG12	2.03	0.40
5:e:127:ALA:HB2	1:z:86:THR:HG22	2.02	0.40
8:s:57:ARG:HB3	8:s:65:VAL:HG21	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	205/289 (71%)	202 (98%)	3 (2%)	0	100	100
1	2	206/289 (71%)	203 (98%)	3 (2%)	0	100	100
1	3	206/289 (71%)	204 (99%)	2 (1%)	0	100	100
1	y	206/289 (71%)	202 (98%)	4 (2%)	0	100	100
1	z	206/289 (71%)	202 (98%)	4 (2%)	0	100	100
2	4	87/89 (98%)	87 (100%)	0	0	100	100
2	5	87/89 (98%)	86 (99%)	0	1 (1%)	12	40
2	6	87/89 (98%)	84 (97%)	3 (3%)	0	100	100
2	7	87/89 (98%)	86 (99%)	1 (1%)	0	100	100
3	8	238/260 (92%)	232 (98%)	6 (2%)	0	100	100
4	AA	17/580 (3%)	17 (100%)	0	0	100	100
4	AB	17/580 (3%)	15 (88%)	2 (12%)	0	100	100
4	AC	18/580 (3%)	18 (100%)	0	0	100	100
4	AD	17/580 (3%)	17 (100%)	0	0	100	100
4	AE	17/580 (3%)	17 (100%)	0	0	100	100
4	AF	21/580 (4%)	14 (67%)	6 (29%)	1 (5%)	2	9
4	AG	9/580 (2%)	7 (78%)	2 (22%)	0	100	100
4	AH	9/580 (2%)	9 (100%)	0	0	100	100
4	AI	9/580 (2%)	8 (89%)	1 (11%)	0	100	100
4	AJ	22/580 (4%)	18 (82%)	4 (18%)	0	100	100
4	AK	23/580 (4%)	23 (100%)	0	0	100	100
4	AL	30/580 (5%)	26 (87%)	4 (13%)	0	100	100
4	AM	31/580 (5%)	31 (100%)	0	0	100	100
4	AN	31/580 (5%)	31 (100%)	0	0	100	100
4	AO	30/580 (5%)	30 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	b	105/131 (80%)	104 (99%)	1 (1%)	0	100	100
5	c	103/131 (79%)	102 (99%)	1 (1%)	0	100	100
5	d	105/131 (80%)	103 (98%)	2 (2%)	0	100	100
5	e	104/131 (79%)	104 (100%)	0	0	100	100
5	f	104/131 (79%)	103 (99%)	1 (1%)	0	100	100
6	g	126/137 (92%)	122 (97%)	4 (3%)	0	100	100
6	h	126/137 (92%)	123 (98%)	3 (2%)	0	100	100
6	i	126/137 (92%)	122 (97%)	3 (2%)	1 (1%)	16	47
6	j	126/137 (92%)	125 (99%)	1 (1%)	0	100	100
6	k	126/137 (92%)	120 (95%)	6 (5%)	0	100	100
6	l	126/137 (92%)	121 (96%)	5 (4%)	0	100	100
7	m	246/249 (99%)	242 (98%)	4 (2%)	0	100	100
7	n	246/249 (99%)	242 (98%)	4 (2%)	0	100	100
7	o	246/249 (99%)	241 (98%)	5 (2%)	0	100	100
7	p	246/249 (99%)	242 (98%)	4 (2%)	0	100	100
7	q	246/249 (99%)	240 (98%)	6 (2%)	0	100	100
8	r	70/103 (68%)	70 (100%)	0	0	100	100
8	s	78/103 (76%)	78 (100%)	0	0	100	100
8	t	78/103 (76%)	77 (99%)	1 (1%)	0	100	100
8	u	70/103 (68%)	69 (99%)	1 (1%)	0	100	100
8	v	70/103 (68%)	69 (99%)	1 (1%)	0	100	100
8	w	38/103 (37%)	38 (100%)	0	0	100	100
9	x	69/376 (18%)	69 (100%)	0	0	100	100
All	All	4896/14477 (34%)	4795 (98%)	98 (2%)	3 (0%)	50	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	5	88	LEU
6	i	42	TYR
4	AF	349	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	181/247 (73%)	175 (97%)	6 (3%)	33	64
1	2	182/247 (74%)	176 (97%)	6 (3%)	33	64
1	3	182/247 (74%)	177 (97%)	5 (3%)	40	68
1	y	182/247 (74%)	175 (96%)	7 (4%)	28	59
1	z	182/247 (74%)	175 (96%)	7 (4%)	28	59
2	4	80/80 (100%)	77 (96%)	3 (4%)	28	59
2	5	80/80 (100%)	76 (95%)	4 (5%)	20	50
2	6	80/80 (100%)	75 (94%)	5 (6%)	15	42
2	7	80/80 (100%)	79 (99%)	1 (1%)	65	83
3	8	204/218 (94%)	194 (95%)	10 (5%)	21	51
4	AA	15/500 (3%)	14 (93%)	1 (7%)	13	40
4	AB	15/500 (3%)	14 (93%)	1 (7%)	13	40
4	AC	15/500 (3%)	15 (100%)	0	100	100
4	AD	15/500 (3%)	14 (93%)	1 (7%)	13	40
4	AE	15/500 (3%)	15 (100%)	0	100	100
4	AF	17/500 (3%)	13 (76%)	4 (24%)	0	2
4	AG	8/500 (2%)	8 (100%)	0	100	100
4	AH	8/500 (2%)	7 (88%)	1 (12%)	3	15
4	AI	8/500 (2%)	8 (100%)	0	100	100
4	AJ	17/500 (3%)	16 (94%)	1 (6%)	16	44
4	AK	18/500 (4%)	15 (83%)	3 (17%)	2	8
4	AL	24/500 (5%)	23 (96%)	1 (4%)	25	56
4	AM	24/500 (5%)	24 (100%)	0	100	100
4	AN	24/500 (5%)	22 (92%)	2 (8%)	9	31
4	AO	24/500 (5%)	23 (96%)	1 (4%)	25	56
5	b	89/106 (84%)	88 (99%)	1 (1%)	70	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	c	88/106 (83%)	86 (98%)	2 (2%)	45	72
5	d	89/106 (84%)	86 (97%)	3 (3%)	32	63
5	e	88/106 (83%)	85 (97%)	3 (3%)	32	63
5	f	88/106 (83%)	88 (100%)	0	100	100
6	g	111/115 (96%)	106 (96%)	5 (4%)	23	54
6	h	111/115 (96%)	107 (96%)	4 (4%)	30	61
6	i	111/115 (96%)	103 (93%)	8 (7%)	12	37
6	j	111/115 (96%)	106 (96%)	5 (4%)	23	54
6	k	111/115 (96%)	105 (95%)	6 (5%)	18	47
6	l	111/115 (96%)	106 (96%)	5 (4%)	23	54
7	m	204/205 (100%)	199 (98%)	5 (2%)	42	70
7	n	204/205 (100%)	198 (97%)	6 (3%)	37	67
7	o	204/205 (100%)	198 (97%)	6 (3%)	37	67
7	p	204/205 (100%)	202 (99%)	2 (1%)	73	87
7	q	204/205 (100%)	200 (98%)	4 (2%)	50	75
8	r	63/84 (75%)	59 (94%)	4 (6%)	15	42
8	s	66/84 (79%)	64 (97%)	2 (3%)	36	66
8	t	66/84 (79%)	63 (96%)	3 (4%)	23	54
8	u	63/84 (75%)	62 (98%)	1 (2%)	58	79
8	v	63/84 (75%)	63 (100%)	0	100	100
8	w	36/84 (43%)	35 (97%)	1 (3%)	38	67
9	x	58/317 (18%)	55 (95%)	3 (5%)	19	49
All	All	4223/12339 (34%)	4074 (96%)	149 (4%)	33	62

All (149) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	127	GLN
1	1	146	MET
1	1	166	VAL
1	1	202	GLN
1	1	208	ASP
1	1	259	MET
1	2	86	THR

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Mol	Chain	Res	Type
1	2	95	MET
1	2	149	VAL
1	2	214	LEU
1	2	220	THR
1	2	272	LEU
1	3	96	LEU
1	3	133	VAL
1	3	141	LEU
1	3	149	VAL
1	3	214	LEU
2	4	1	MET
2	4	16	MET
2	4	55	LEU
2	5	45	ASN
2	5	64	LEU
2	5	72	MET
2	5	89	TYR
2	6	1	MET
2	6	7	VAL
2	6	14	LEU
2	6	42	THR
2	6	86	GLN
2	7	88	LEU
3	8	2	GLU
3	8	47	LEU
3	8	70	ARG
3	8	102	ILE
3	8	125	LEU
3	8	192	ILE
3	8	195	LEU
3	8	207	ARG
3	8	212	LEU
3	8	214	ILE
4	AA	342	GLN
4	AB	342	GLN
4	AD	349	ILE
4	AF	346	ASP
4	AF	351	GLN
4	AF	352	ASP
4	AF	355	GLN
4	AH	342	GLN
4	AJ	349	ILE

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Mol	Chain	Res	Type
4	AK	330	ASN
4	AK	331	MET
4	AK	332	VAL
4	AL	339	LEU
4	AN	339	LEU
4	AN	352	ASP
4	AO	330	ASN
5	b	9	LEU
5	c	6	ASP
5	c	87	ASP
5	d	4	SER
5	d	6	ASP
5	d	7	ASN
5	e	6	ASP
5	e	7	ASN
5	e	88	THR
6	g	23	THR
6	g	39	LYS
6	g	53	LEU
6	g	65	VAL
6	g	134	GLN
6	h	3	LEU
6	h	34	VAL
6	h	65	VAL
6	h	67	VAL
6	i	36	SER
6	i	39	LYS
6	i	61	ASP
6	i	62	THR
6	i	67	VAL
6	i	84	ASP
6	i	113	ARG
6	i	131	ARG
6	j	53	LEU
6	j	61	ASP
6	j	65	VAL
6	j	67	VAL
6	j	126	LYS
6	k	14	MET
6	k	40	ASP
6	k	53	LEU
6	k	65	VAL

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Mol	Chain	Res	Type
6	k	113	ARG
6	k	134	GLN
6	l	40	ASP
6	l	43	LYS
6	l	65	VAL
6	l	126	LYS
6	l	137	GLN
7	m	7	LEU
7	m	60	GLU
7	m	72	ILE
7	m	135	LEU
7	m	218	LEU
7	n	60	GLU
7	n	72	ILE
7	n	158	PHE
7	n	162	ASP
7	n	200	GLN
7	n	204	ILE
7	o	72	ILE
7	o	73	THR
7	o	101	ARG
7	o	114	THR
7	o	158	PHE
7	o	229	VAL
7	p	72	ILE
7	p	135	LEU
7	q	72	ILE
7	q	73	THR
7	q	135	LEU
7	q	204	ILE
8	r	34	ASN
8	r	37	LEU
8	r	39	LYS
8	r	67	LEU
8	s	67	LEU
8	s	98	LEU
8	t	32	ASP
8	t	35	ASP
8	t	67	LEU
8	u	67	LEU
8	w	91	LEU
9	x	48	TRP

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Mol	Chain	Res	Type
9	x	69	ARG
9	x	86	MET
1	y	86	THR
1	y	99	LEU
1	y	113	VAL
1	y	141	LEU
1	y	254	MET
1	y	261	VAL
1	y	283	LEU
1	z	86	THR
1	z	87	LEU
1	z	113	VAL
1	z	128	THR
1	z	184	LEU
1	z	192	LEU
1	z	272	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (95) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	88	GLN
1	1	127	GLN
1	1	228	GLN
1	2	127	GLN
1	3	186	GLN
1	3	205	ASN
2	4	47	GLN
2	4	71	GLN
2	6	47	GLN
2	6	67	HIS
2	7	39	GLN
2	7	67	HIS
3	8	90	GLN
3	8	106	GLN
3	8	182	GLN
3	8	199	ASN
3	8	211	GLN
4	AH	342	GLN
4	AK	330	ASN
4	AL	341	ASN
4	AL	351	GLN
4	AM	341	ASN

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Mol	Chain	Res	Type
4	AN	342	GLN
4	AO	330	ASN
4	AO	355	GLN
5	b	50	GLN
5	c	32	GLN
5	c	106	ASN
5	c	110	HIS
5	d	14	HIS
5	d	105	GLN
5	d	106	ASN
5	d	107	GLN
5	d	110	HIS
5	e	85	GLN
5	e	101	ASN
5	e	107	GLN
5	e	110	HIS
5	f	14	HIS
5	f	34	ASN
5	f	50	GLN
5	f	107	GLN
5	f	110	HIS
6	g	100	ASN
6	g	118	ASN
6	g	134	GLN
6	h	127	GLN
6	i	22	ASN
6	i	46	HIS
6	i	100	ASN
6	i	118	ASN
6	j	22	ASN
6	j	118	ASN
6	k	22	ASN
6	k	100	ASN
6	k	120	GLN
6	l	22	ASN
6	l	100	ASN
6	l	120	GLN
7	m	179	ASN
7	m	200	GLN
7	m	228	GLN
7	n	15	ASN
7	n	24	ASN

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Mol	Chain	Res	Type
7	n	102	ASN
7	n	188	ASN
7	n	200	GLN
7	o	40	GLN
7	o	102	ASN
7	o	200	GLN
7	p	14	GLN
7	p	119	HIS
7	p	179	ASN
7	p	200	GLN
7	p	228	GLN
7	q	15	ASN
7	q	20	GLN
7	q	40	GLN
7	q	102	ASN
7	q	200	GLN
8	r	42	ASN
8	r	86	GLN
8	s	45	ASN
8	s	86	GLN
8	s	89	ASN
8	t	45	ASN
8	t	75	ASN
8	t	86	GLN
8	u	86	GLN
8	v	55	GLN
8	v	75	ASN
1	y	186	GLN
1	z	126	GLN
1	z	127	GLN
1	z	165	GLN

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 [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.

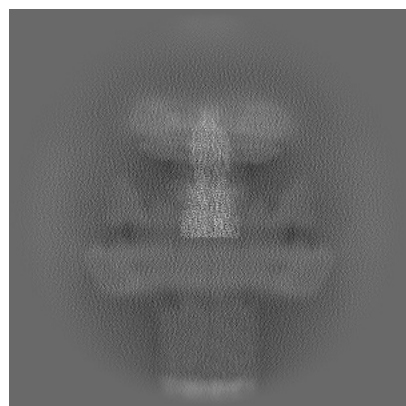
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39780. These allow visual inspection of the internal detail of the map and identification of artifacts.

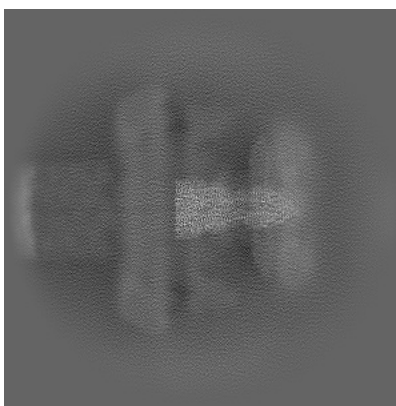
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

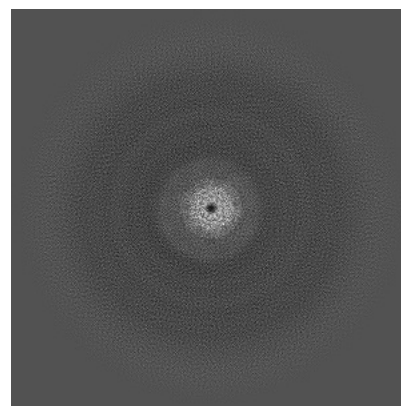
6.1.1 Primary map



X

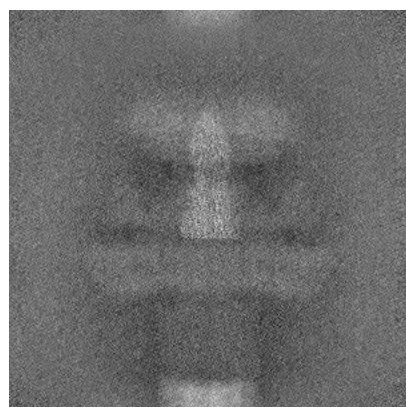


Y

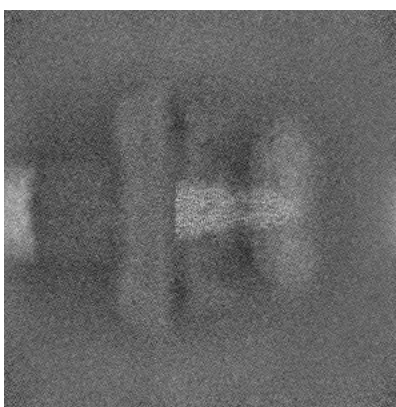


Z

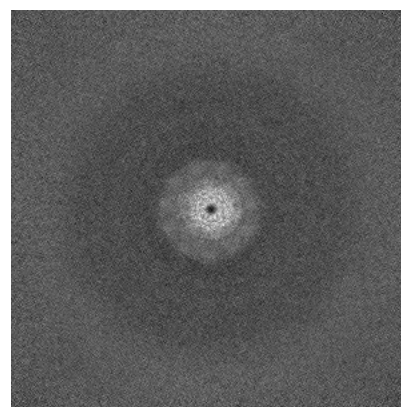
6.1.2 Raw map



X



Y

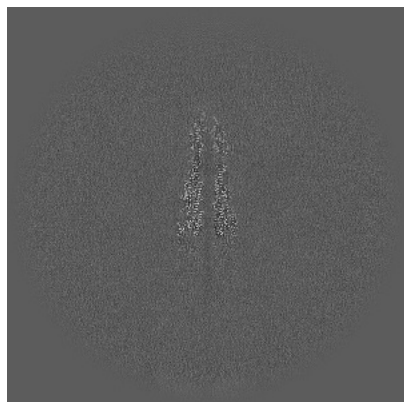


Z

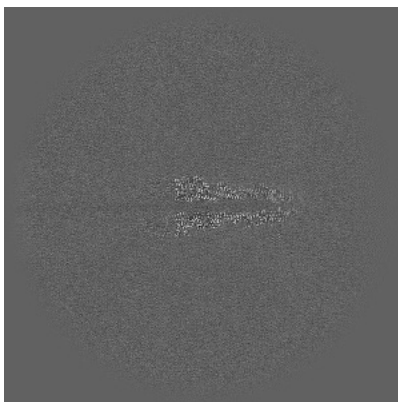
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

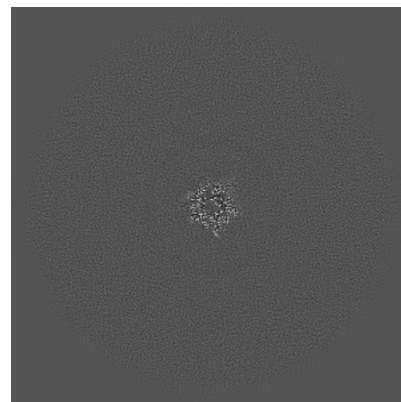
6.2.1 Primary map



X Index: 310

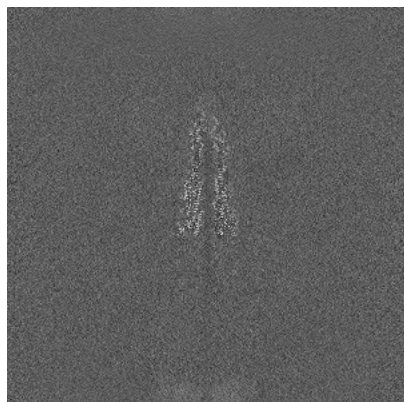


Y Index: 310

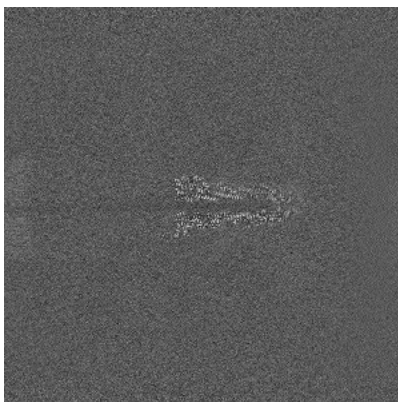


Z Index: 310

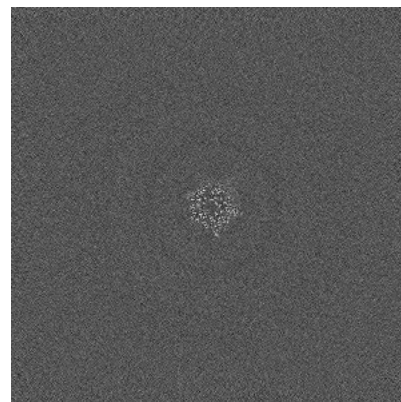
6.2.2 Raw map



X Index: 310



Y Index: 310

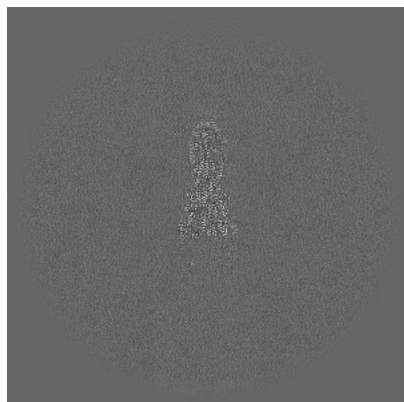


Z Index: 310

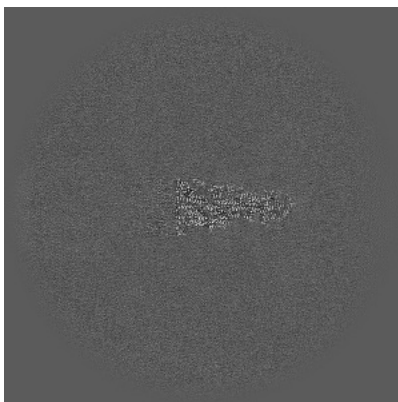
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

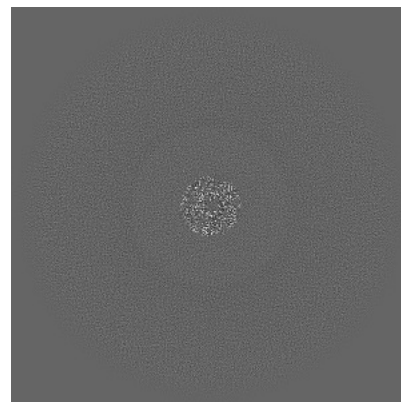
6.3.1 Primary map



X Index: 297

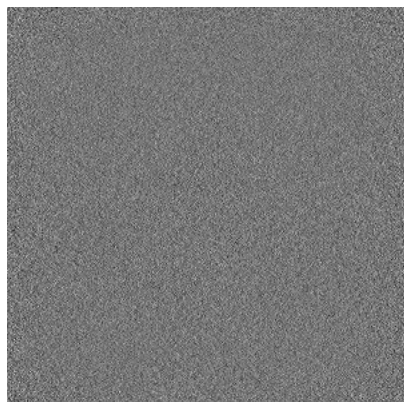


Y Index: 296

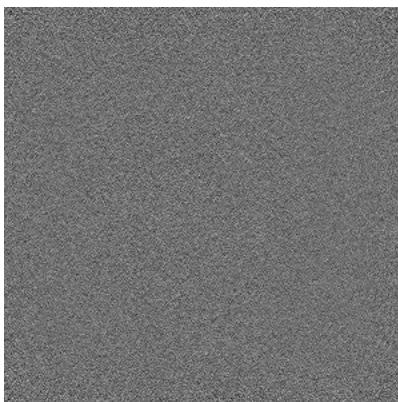


Z Index: 276

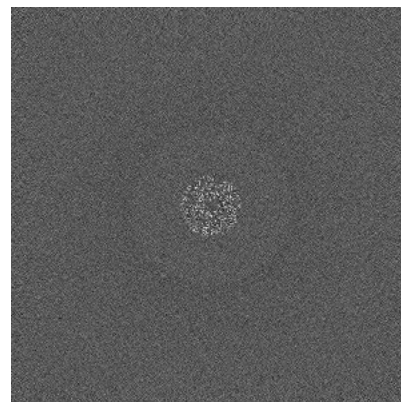
6.3.2 Raw map



X Index: 0



Y Index: 0

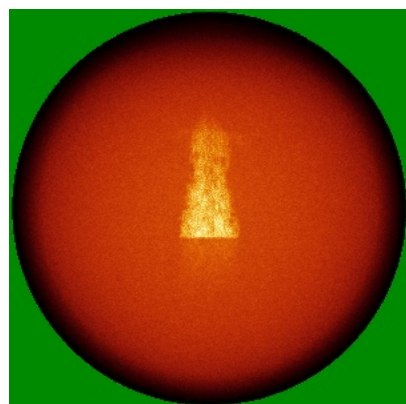


Z Index: 276

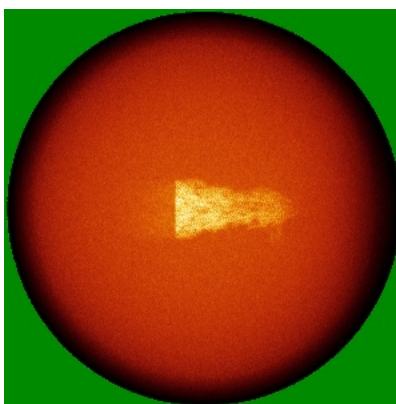
The images above show the largest variance slices of the map in three orthogonal directions.

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

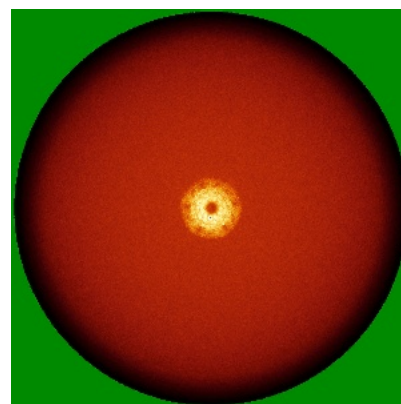
6.4.1 Primary map



X

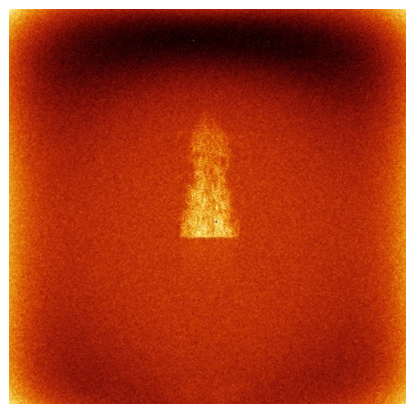


Y

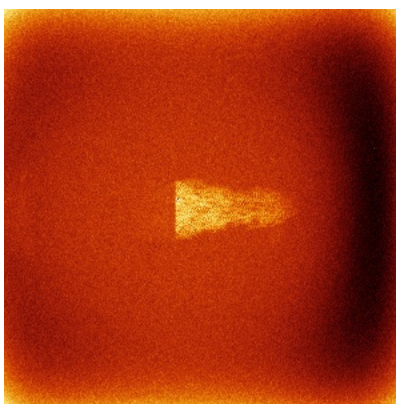


Z

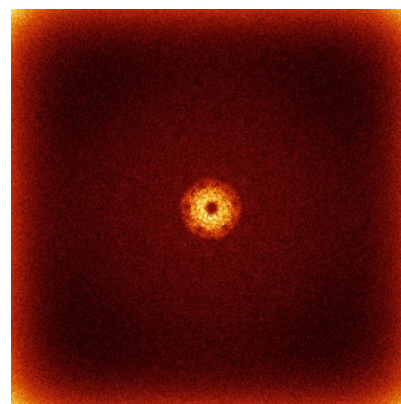
6.4.2 Raw map



X



Y

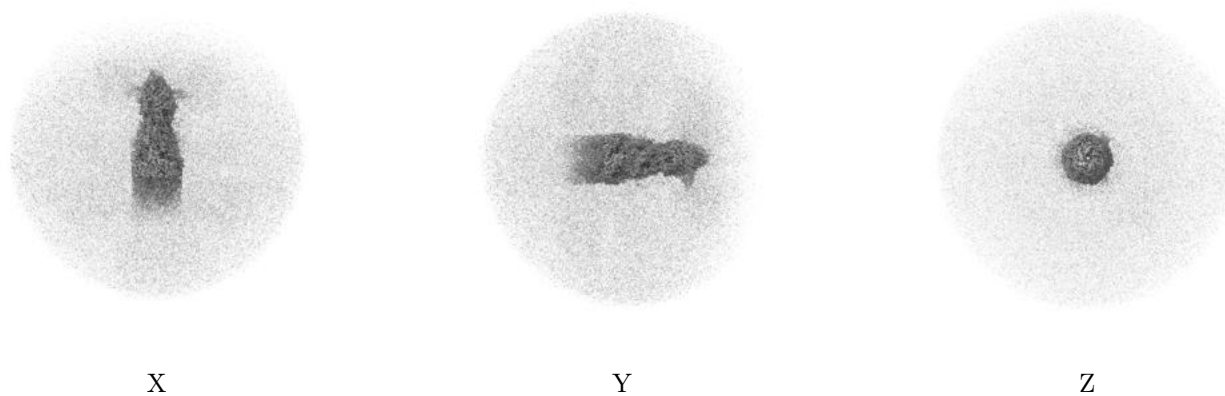


Z

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.

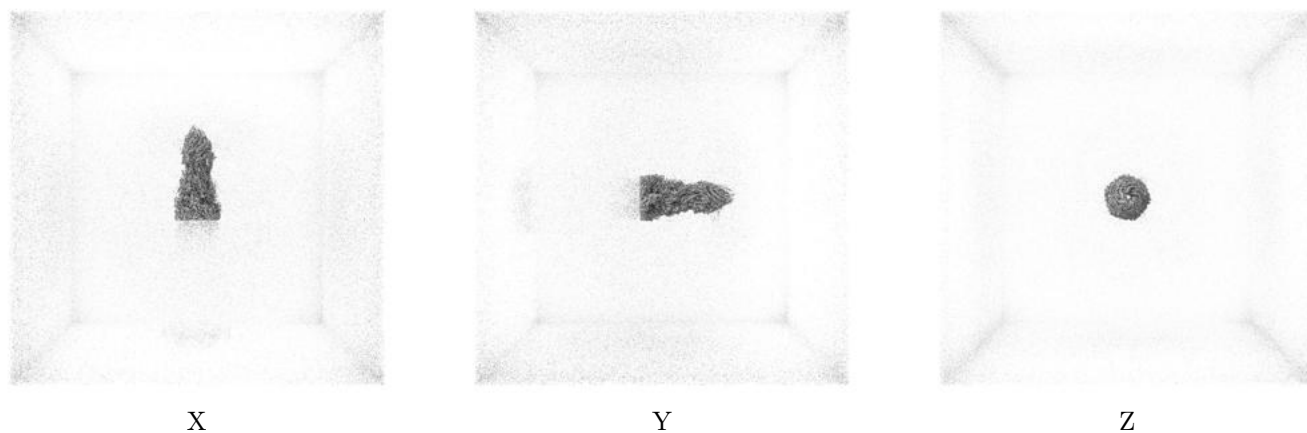
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.42. 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.

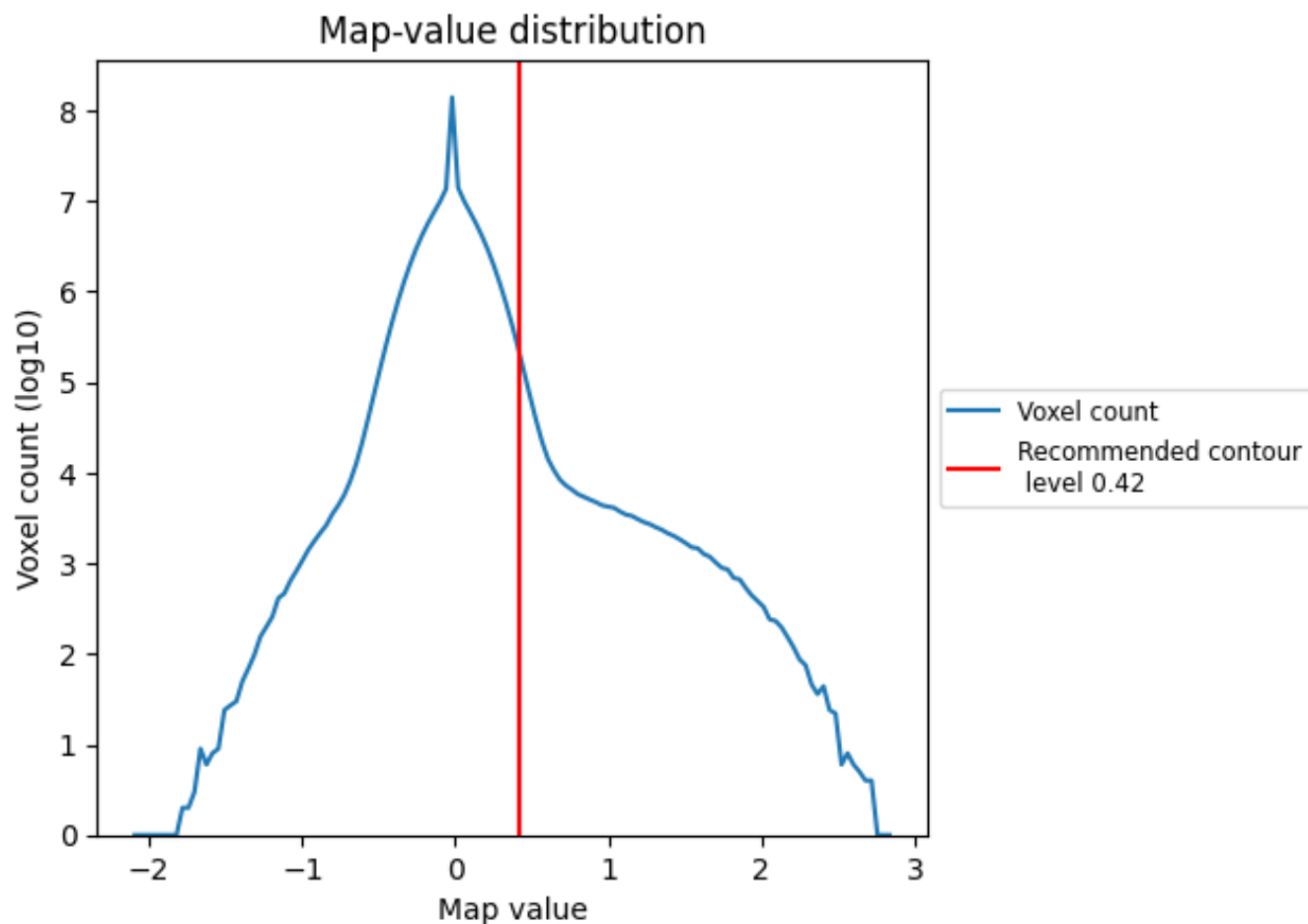
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

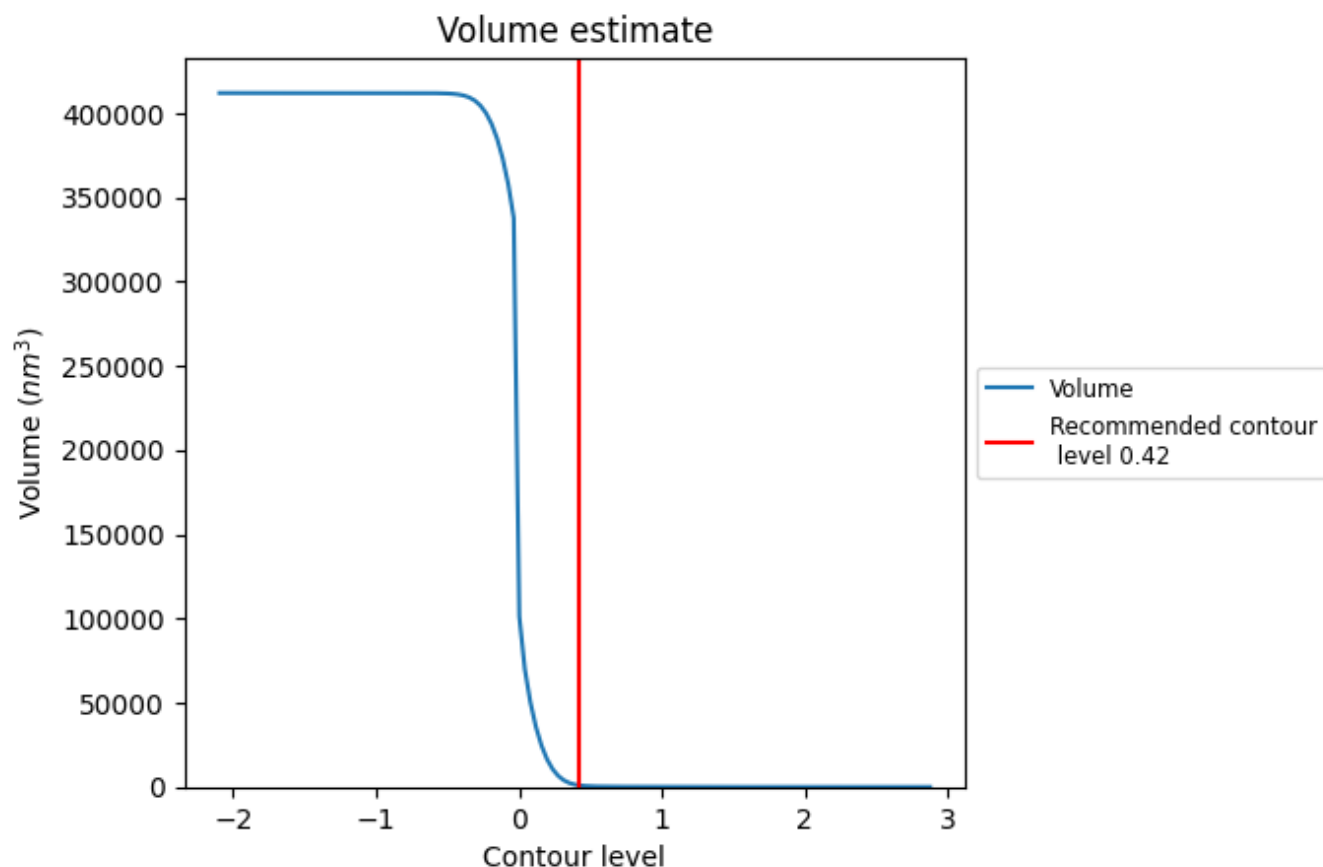
This section contains the results of statistical analysis of the map.

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.

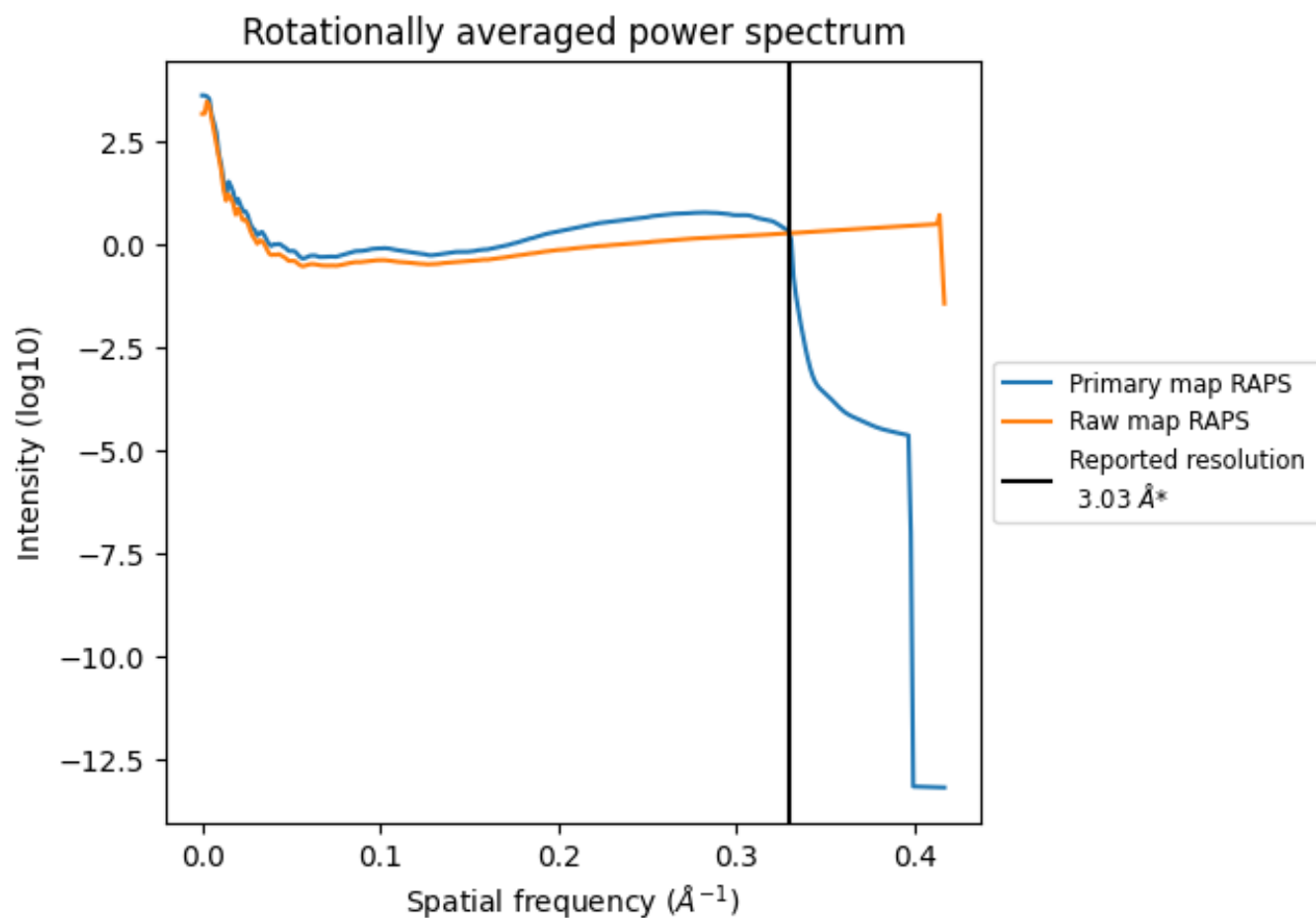
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 972 nm^3 ; this corresponds to an approximate mass of 878 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 ⓘ

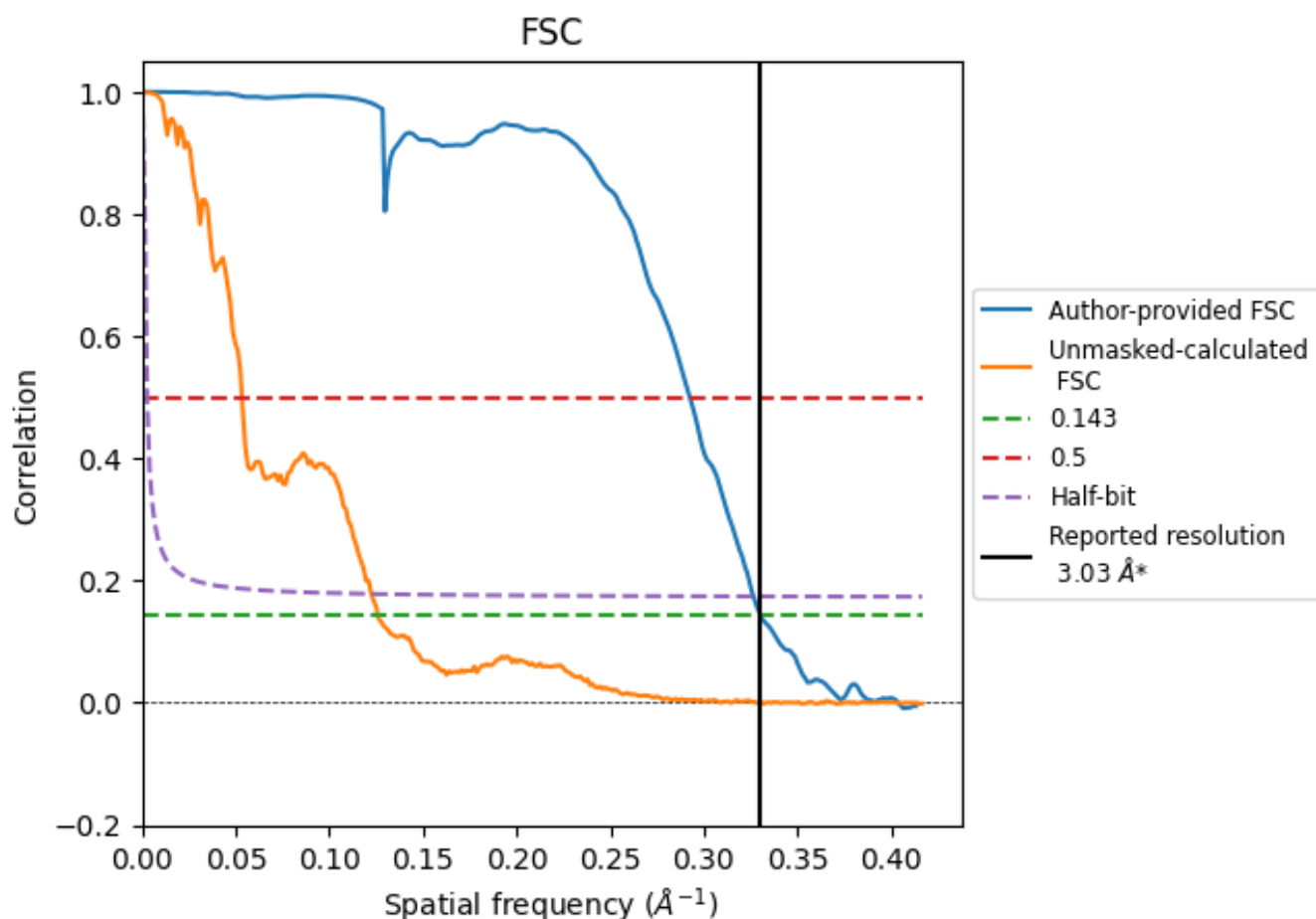


*Reported resolution corresponds to spatial frequency of 0.330 \AA^{-1}

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 0.330 \AA^{-1}

8.2 Resolution estimates [i](#)

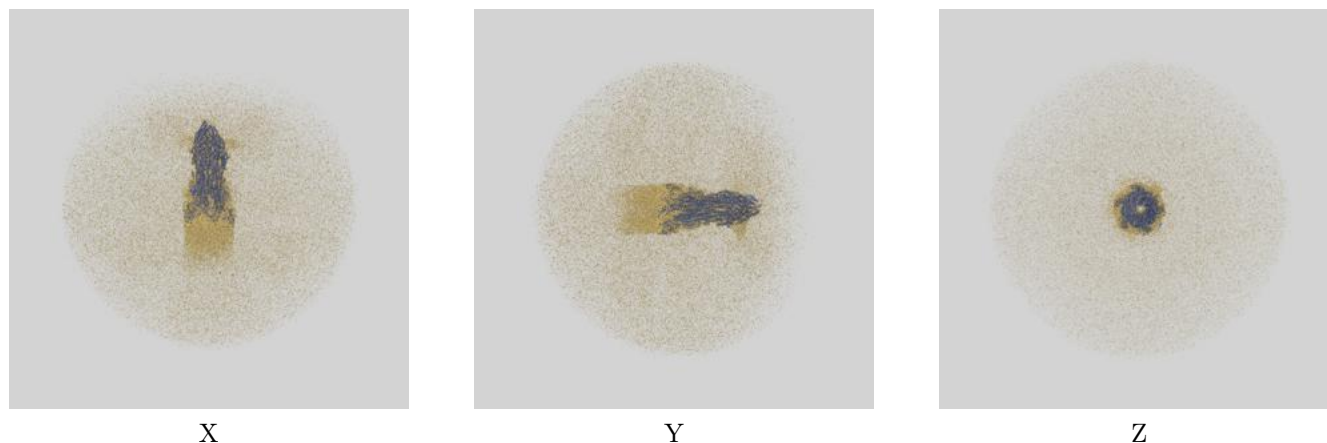
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.03	-	-
Author-provided FSC curve	3.03	3.42	3.06
Unmasked-calculated*	7.94	18.76	8.17

*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 7.94 differs from the reported value 3.03 by more than 10 %

9 Map-model fit [i](#)

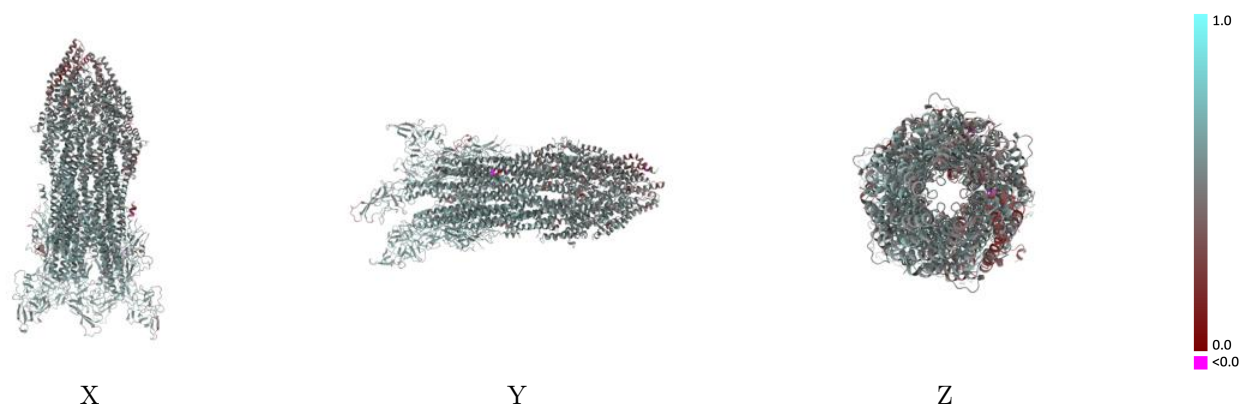
This section contains information regarding the fit between EMDB map EMD-39780 and PDB model 8Z5S. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



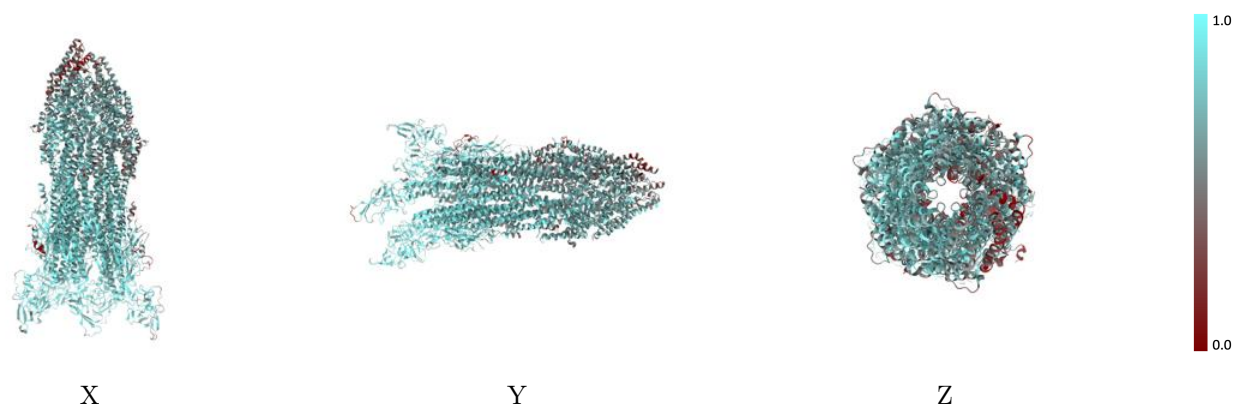
The images above show the 3D surface view of the map at the recommended contour level 0.42 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



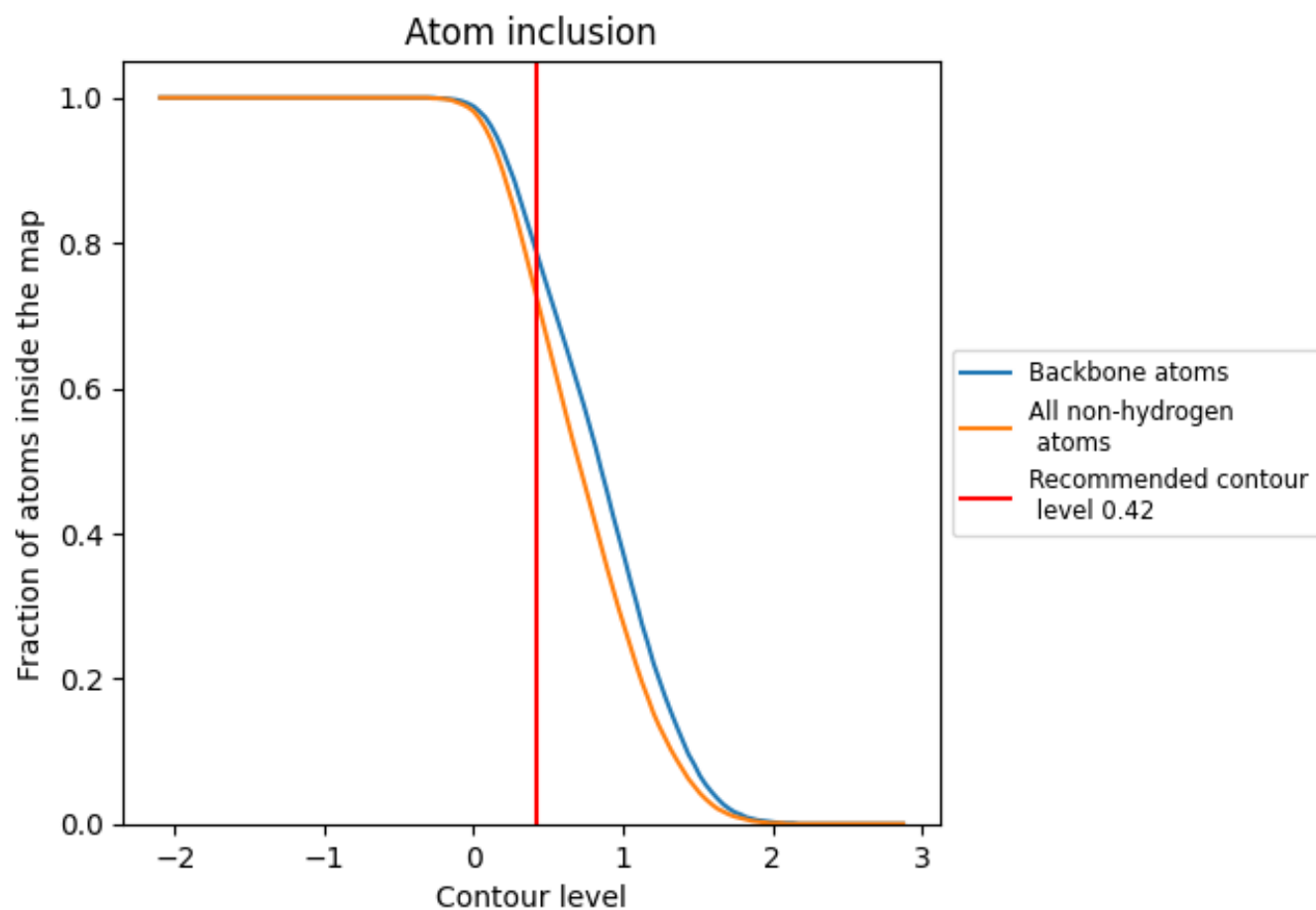
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.42).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 73% 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 (0.42) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7270	 0.5300
1	 0.6080	 0.4950
2	 0.6920	 0.5140
3	 0.6770	 0.5050
4	 0.5410	 0.4620
5	 0.6410	 0.4880
6	 0.5880	 0.4760
7	 0.6130	 0.4910
8	 0.6090	 0.4830
AA	 0.7330	 0.5090
AB	 0.7780	 0.5510
AC	 0.7700	 0.5490
AD	 0.7560	 0.5690
AE	 0.6220	 0.5130
AF	 0.3990	 0.4030
AG	 0.7940	 0.5320
AH	 0.7940	 0.5470
AI	 0.6850	 0.4850
AJ	 0.3370	 0.4000
AK	 0.7340	 0.5370
AL	 0.6640	 0.4930
AM	 0.6920	 0.5050
AN	 0.7720	 0.5490
AO	 0.7730	 0.5520
b	 0.7970	 0.5610
c	 0.7330	 0.5200
d	 0.7890	 0.5640
e	 0.8100	 0.5660
f	 0.8190	 0.5720
g	 0.7630	 0.5440
h	 0.8030	 0.5560
i	 0.7700	 0.5380
j	 0.8250	 0.5670
k	 0.8220	 0.5600
l	 0.8060	 0.5550



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Chain	Atom inclusion	Q-score
m	 0.8210	 0.5650
n	 0.7430	 0.5330
o	 0.8120	 0.5620
p	 0.8090	 0.5610
q	 0.7740	 0.5480
r	 0.7330	 0.5470
s	 0.6640	 0.5060
t	 0.7080	 0.5180
u	 0.7440	 0.5450
v	 0.7300	 0.5440
w	 0.7480	 0.5480
x	 0.2790	 0.3340
y	 0.7330	 0.5340
z	 0.7410	 0.5360