



wwPDB EM Validation Summary Report ⓘ

May 7, 2026 – 02:44 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 wwPDB EM Validation Summary 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
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

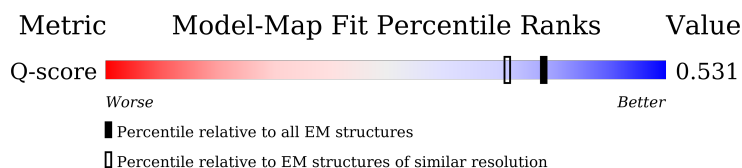
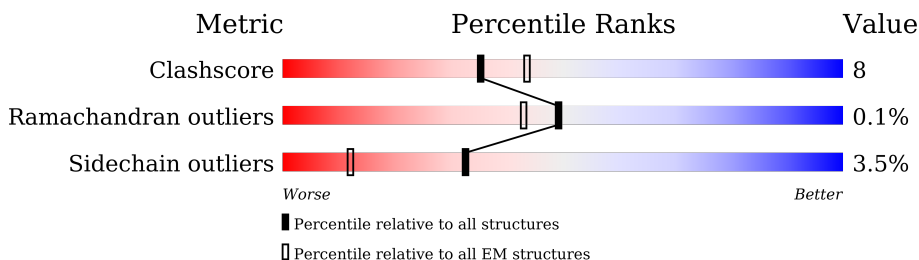
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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.



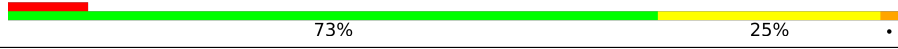
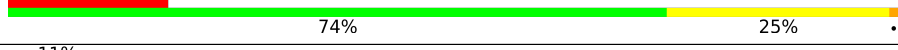
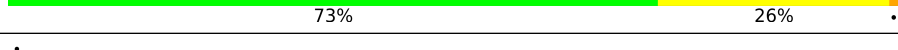
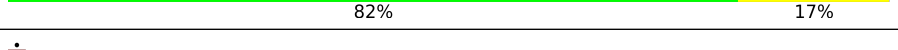
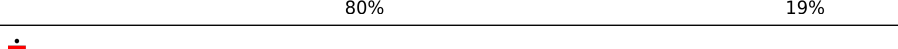
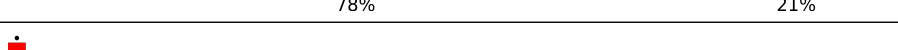
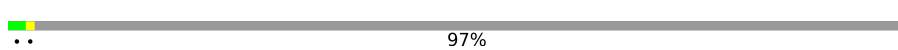
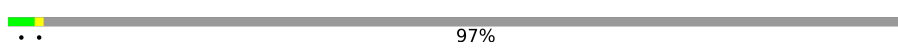
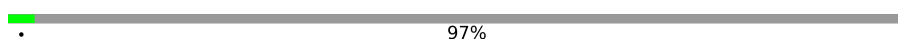
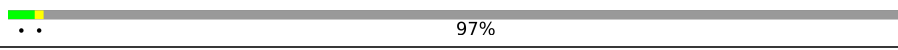
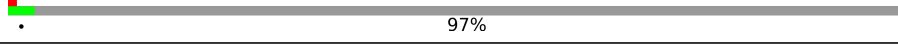
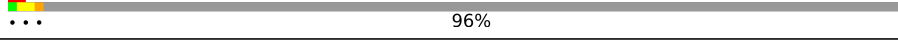
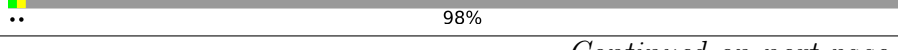
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13929 (2.53 - 3.53)

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	

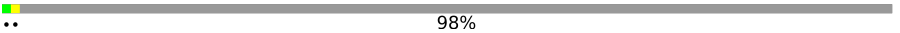
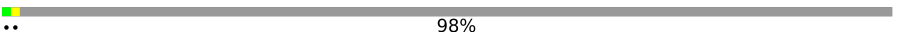
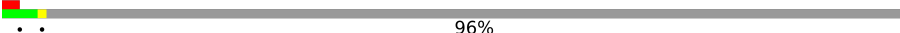
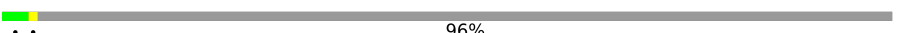
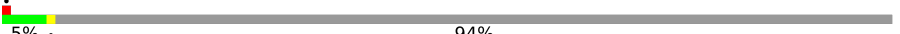
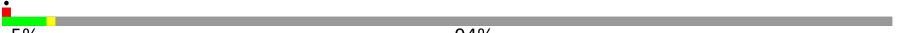
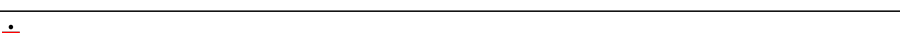
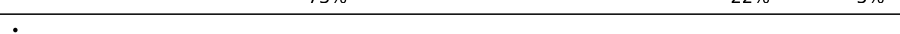
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Mol	Chain	Length	Quality of chain
1	z	289	
2	4	89	
2	5	89	
2	6	89	
2	7	89	
3	m	249	
3	n	249	
3	o	249	
3	p	249	
3	q	249	
4	r	103	
4	s	103	
4	t	103	
4	u	103	
4	v	103	
4	w	103	
5	x	376	
6	8	260	
7	AA	580	
7	AB	580	
7	AC	580	
7	AD	580	
7	AE	580	
7	AF	580	
7	AG	580	

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Mol	Chain	Length	Quality of chain
7	AH	580	 98%
7	AI	580	 98%
7	AJ	580	 96%
7	AK	580	 96%
7	AL	580	 5% 94%
7	AM	580	 5% 94%
7	AN	580	 5% 94%
7	AO	580	 94%
8	b	131	 69% 14% 17%
8	c	131	 8% 66% 16% 18%
8	d	131	 69% 14% 17%
8	e	131	 66% 16% 18%
8	f	131	 68% 15% 18%
9	g	137	 79% 16% 5%
9	h	137	 73% 22% 5%
9	i	137	 67% 24% 5%
9	j	137	 81% 13% 5%
9	k	137	 75% 20% 5%
9	l	137	 75% 18% 5%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 38700 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		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	26	SER	THR	conflict	UNP A0A1W6TTE6
1	204	ASP	GLU	conflict	UNP A0A1W6TTE6
2	26	SER	THR	conflict	UNP A0A1W6TTE6
2	204	ASP	GLU	conflict	UNP A0A1W6TTE6
3	26	SER	THR	conflict	UNP A0A1W6TTE6
3	204	ASP	GLU	conflict	UNP A0A1W6TTE6
y	26	SER	THR	conflict	UNP A0A1W6TTE6
y	204	ASP	GLU	conflict	UNP A0A1W6TTE6
z	26	SER	THR	conflict	UNP A0A1W6TTE6
z	204	ASP	GLU	conflict	UNP A0A1W6TTE6

- 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		

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

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	34	ILE	VAL	conflict	UNP A0A0H0YAF4
5	34	ILE	VAL	conflict	UNP A0A0H0YAF4
6	34	ILE	VAL	conflict	UNP A0A0H0YAF4
7	34	ILE	VAL	conflict	UNP A0A0H0YAF4

- Molecule 3 is a protein called Flagellar basal-body rod protein FlgF.

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

- Molecule 4 is a protein called Flagellar hook-basal body complex protein FliE.

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

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
r	3	VAL	ILE	conflict	UNP A0A0H0Y9C1
s	3	VAL	ILE	conflict	UNP A0A0H0Y9C1
t	3	VAL	ILE	conflict	UNP A0A0H0Y9C1
u	3	VAL	ILE	conflict	UNP A0A0H0Y9C1
v	3	VAL	ILE	conflict	UNP A0A0H0Y9C1
w	3	VAL	ILE	conflict	UNP A0A0H0Y9C1

- Molecule 5 is a protein called Flagellar biosynthetic protein FlhB.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
x	87	THR	SER	conflict	UNP A0A0H0YB55

- Molecule 6 is a protein called Flagellar biosynthetic protein FliR.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	8	242	Total	C	N	O	S	0	0
			1896	1265	295	315	21		

- Molecule 7 is a protein called Flagellar M-ring protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AA	19	Total	C	N	O	S	0	0
			135	82	23	29	1		
7	AB	19	Total	C	N	O	S	0	0
			135	82	23	29	1		
7	AC	20	Total	C	N	O	S	0	0
			139	84	24	30	1		
7	AD	19	Total	C	N	O	S	0	0
			135	82	23	29	1		
7	AE	19	Total	C	N	O	S	0	0
			135	82	23	29	1		
7	AF	23	Total	C	N	O	S	0	0
			158	97	27	33	1		
7	AG	11	Total	C	N	O		0	0
			73	46	13	14			
7	AH	11	Total	C	N	O		0	0
			73	46	13	14			

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	AI	11	Total	C	N	O		0	0
			73	46	13	14			
7	AJ	24	Total	C	N	O	S	0	0
			163	100	28	34	1		
7	AK	25	Total	C	N	O	S	0	0
			169	104	29	35	1		
7	AL	32	Total	C	N	O	S	0	0
			220	134	38	46	2		
7	AM	33	Total	C	N	O	S	0	0
			224	136	39	47	2		
7	AN	33	Total	C	N	O	S	0	0
			224	136	39	47	2		
7	AO	32	Total	C	N	O	S	0	0
			220	134	38	46	2		

- Molecule 8 is a protein called Flagellar basal body rod protein FlgB.

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

- Molecule 9 is a protein called Flagellar basal-body rod protein FlgC.

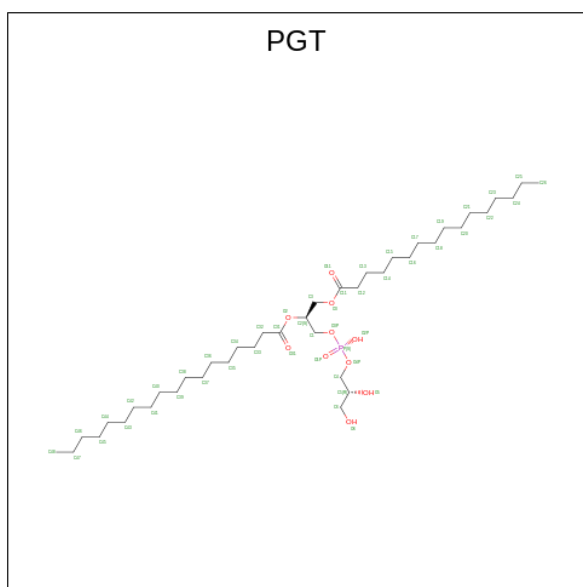
Mol	Chain	Residues	Atoms					AltConf	Trace
9	g	130	Total	C	N	O	S	0	0
			983	605	168	203	7		
9	h	130	Total	C	N	O	S	0	0
			983	605	168	203	7		
9	i	130	Total	C	N	O	S	0	0
			983	605	168	203	7		
9	j	130	Total	C	N	O	S	0	0
			983	605	168	203	7		
9	k	130	Total	C	N	O	S	0	0
			983	605	168	203	7		

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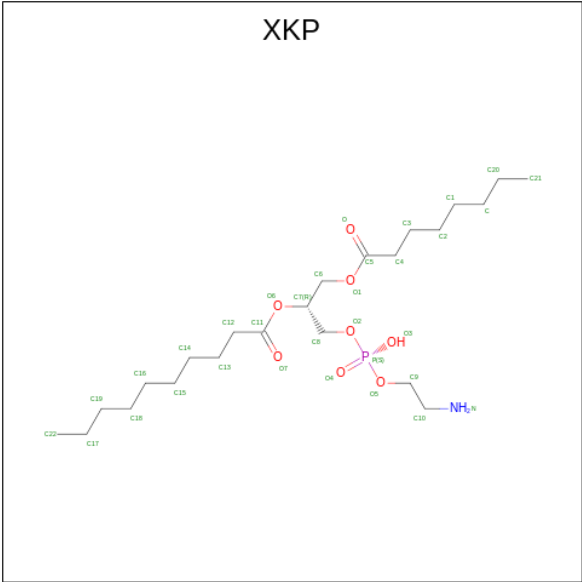
Mol	Chain	Residues	Atoms					AltConf	Trace
9	1	130	Total	C	N	O	S	0	0
			983	605	168	203	7		

- Molecule 10 is (1S)-2-{{[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (CCD ID: PGT) (formula: C₄₀H₇₉O₁₀P) (labeled as "Ligand of Interest" by depositor).

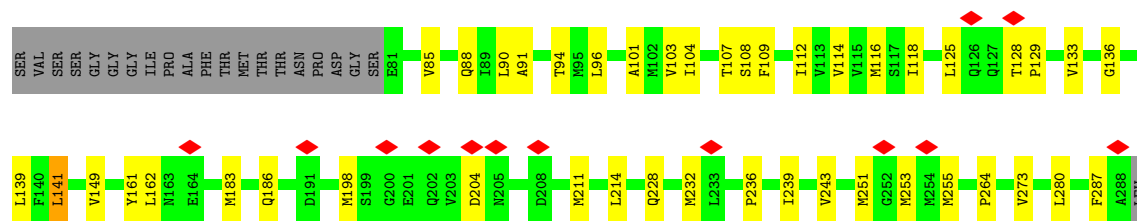


Mol	Chain	Residues	Atoms				AltConf
10	2	1	Total	C	O	P	0
			51	40	10	1	
10	t	1	Total	C	O	P	0
			51	40	10	1	
10	v	1	Total	C	O	P	0
			51	40	10	1	
10	e	1	Total	C	O	P	0
			51	40	10	1	

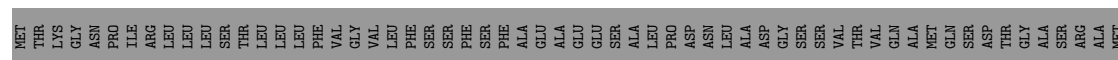
- Molecule 11 is (11R,14S)-17-amino-14-hydroxy-8,14-dioxo-9,13,15-trioxa-14lambda 5 -phosphahaheptadecan-11-yl decanoate (CCD ID: XKP) (formula: C₂₃H₄₆NO₈P) (labeled as "Ligand of Interest" by depositor).



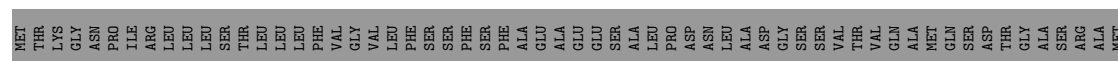
Mol	Chain	Residues	Atoms					AltConf
11	s	1	Total	C	N	O	P	0
			32	22	1	8	1	
11	t	1	Total	C	N	O	P	0
			32	22	1	8	1	
11	u	1	Total	C	N	O	P	0
			32	22	1	8	1	
11	v	1	Total	C	N	O	P	0
			32	22	1	8	1	
11	e	1	Total	C	N	O	P	0
			32	22	1	8	1	



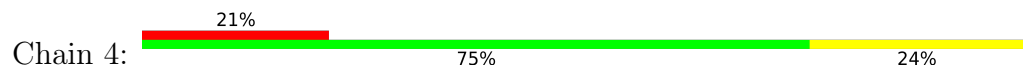
• Molecule 1: Flagellar biosynthetic protein FliP



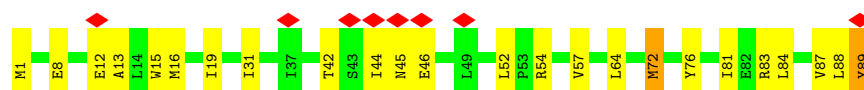
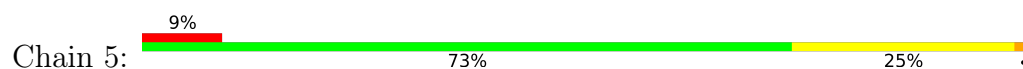
• Molecule 1: Flagellar biosynthetic protein FliP



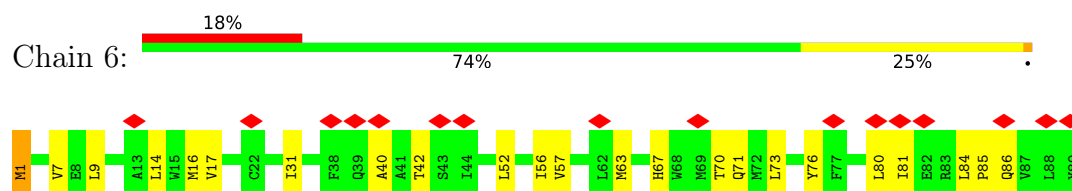
• Molecule 2: Flagellar biosynthetic protein FliQ



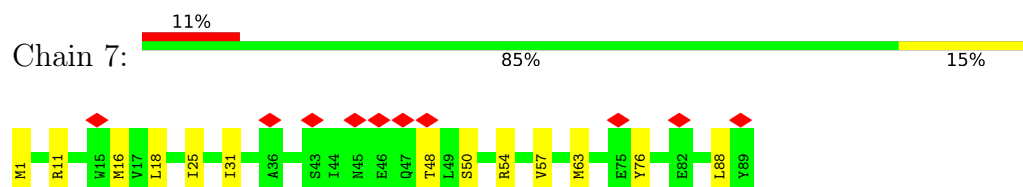
• Molecule 2: Flagellar biosynthetic protein FliQ



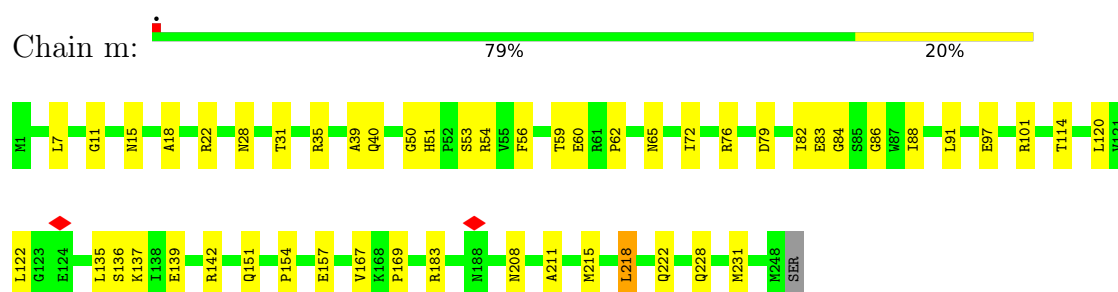
- Molecule 2: Flagellar biosynthetic protein FliQ



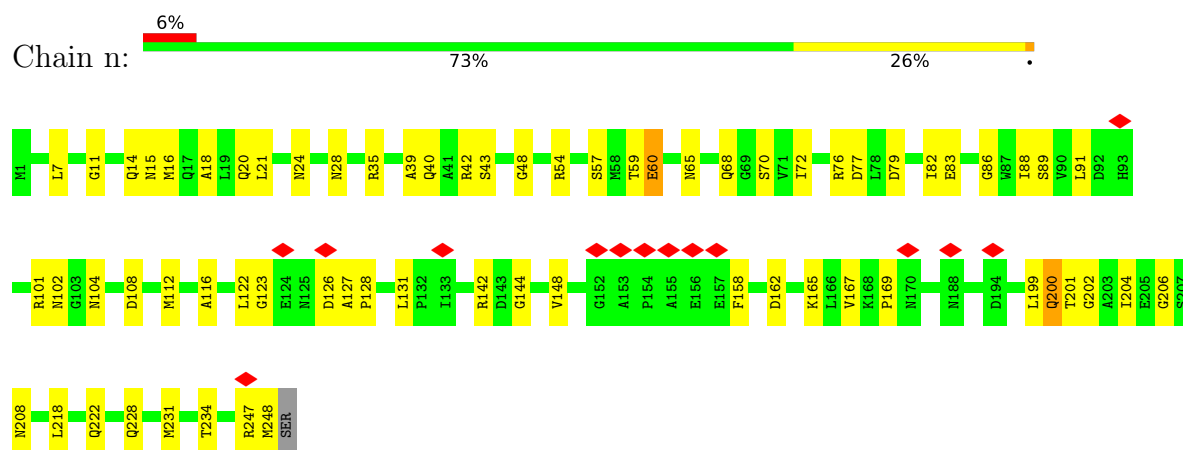
- Molecule 2: Flagellar biosynthetic protein FliQ



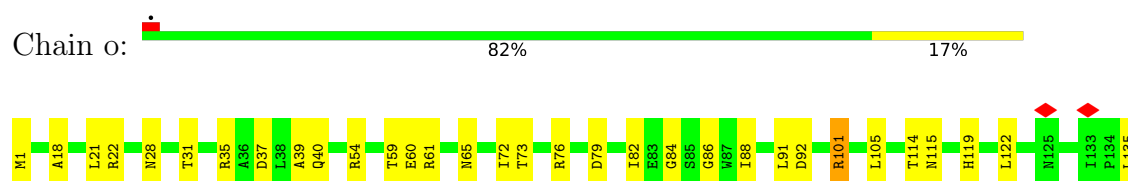
- Molecule 3: Flagellar basal-body rod protein FlgF



- Molecule 3: Flagellar basal-body rod protein FlgF

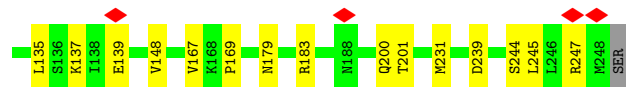
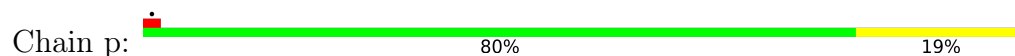


- Molecule 3: Flagellar basal-body rod protein FlgF

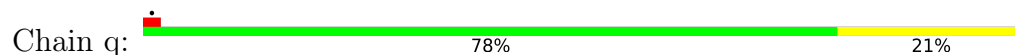




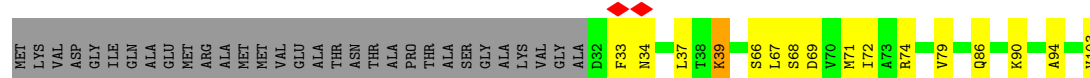
- Molecule 3: Flagellar basal-body rod protein FlgF



- Molecule 3: Flagellar basal-body rod protein FlgF



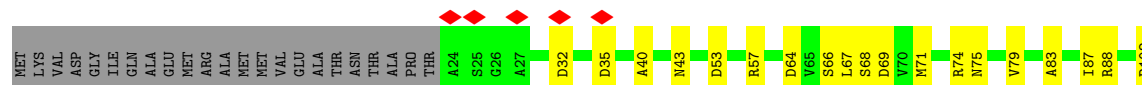
- Molecule 4: Flagellar hook-basal body complex protein FliE



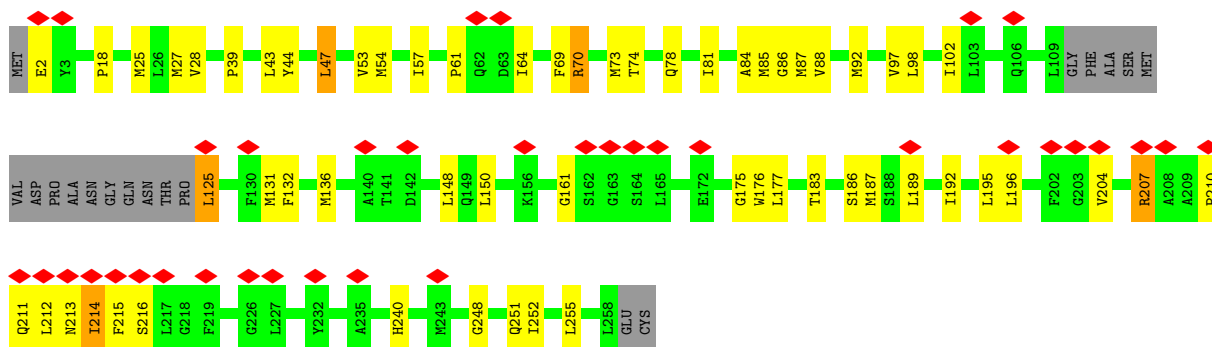
- Molecule 4: Flagellar hook-basal body complex protein FliE



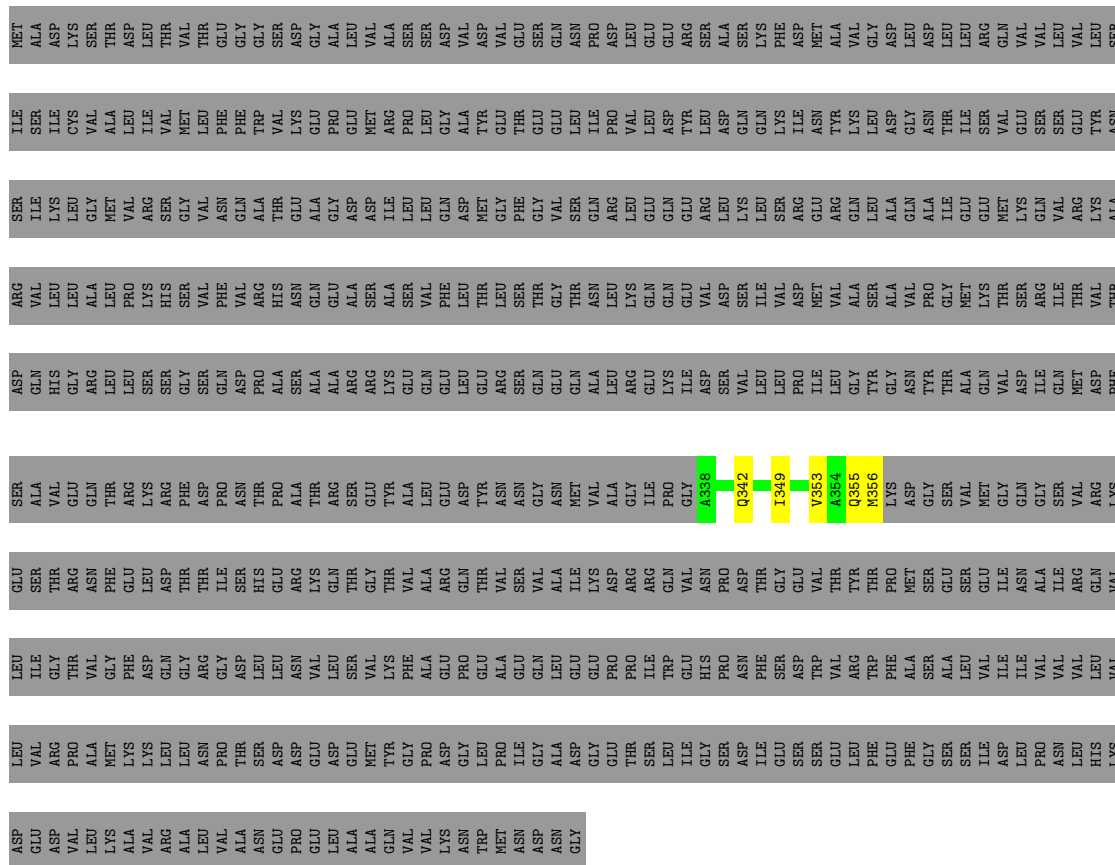
- Molecule 4: Flagellar hook-basal body complex protein FliE



- Molecule 6: Flagellar biosynthetic protein FliR



- Molecule 7: Flagellar M-ring protein



- Molecule 7: Flagellar M-ring protein

97%

[illegible]

97%

[illegible]

[illegible]

- Molecule 7: Flagellar M-ring protein

Chain AD: 97%

[illegible]

- Molecule 7: Flagellar M-ring protein

Chain AE: 97%

[illegible]

[illegible]

- Molecule 7: Flagellar M-ring protein

Chain AI: 98%

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

ARG	VAL	LEU	LEU	ALA	LEU	PRO	LYS	HIS	SER	HIS	PHE	VAL	VAL	ARG	ASN	GLN	GLU	ALA	SER	ALA	ALA	SER	SER	PHE	LEU	THR	LEU	LEU	THR	THR	GLY	THR	ASN	ASN	LYS	LYS	GLN	GLN	GLU	GLN	VAL	ASP	SER	ILE	VAL	ASP	MET	VAL	VAL	ALA	SER	VAL	ALA	PRO	GLY	GLY	MET	LYS	THR	SER	ARG	ILE	THR	VAL
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ASP	GLN	HIS	GLY	ARG	LEU	LEU	SER	SER	SER	SER	GLN	ASP	PRD	ALA	ALA	ALA	ALA	ARG	ARG	LYS	GLU	GLN	GLU	LEU	GLU	ARG	ARG	SER	SER	GLN	GLU	GLN	GLA	ALA	LEU	ARG	GLY	LYS	GLY	LEU	LEU	PRO	ILE	ILE	ASP	ASP	ILE	THR	THR	ALA	ALA	GLN	VAL	VAL	ASP	MET	ASP
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SER	ALA	VAL	GLU	GLN	THR	ARG	LYS	ARG	PHE	ASP	PRO	ASN	THR	PRO	ALA	THR	ARG	SER	GLU	TYR	ALA	LEU	GLU	ASP	TYR	ASN	ASN	GLY	ASN	MET	VAL	ALA	G334	1335	P336	G337	A338	L339	G342	P343	P344	ALA	ASP	ALA	SER	ILE	PRO	GLN	ASP	VAL	ALA	GLN	MET	LYS	ASP	GLY	SER
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MET	GLY	GLN	GLY	SER	VAL	ARG	LYS	GLU	SER	THR	ARG	ASN	PHE	GLU	LEU	ASP	THR	THR	ILE	SER	HIS	GLU	ARG	LYS	GLN	THR	THR	GLY	VAL	ALA	ARG	GLN	THR	THR	VAL	SER	VAL	ALA	ILE	LYS	ASP	ARG	ARG	GLN	ASN	VAL	PRO	ASP	THR	THR	TYR	THR	PRO	MET	SER	GLU
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ASP
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TRP
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ALA

VAL	ILE	ILE	VAL	VAL	VAL	VAL	LEU	VAL	VAL	VAL	ARG	PRO	ALA	MET	LYS	LYS	LEU	LEU	ASN	PRO	THR	SER	SER	ASP	ASP	GLU	GLU	GLY	PRO	ASP	ASP	GLY	GLY	ILE	GLY	ALA	ASP	GLY	GLY	THR	SER	LEU	ILE	GLY	SER	ASP	ILE	GLU	PHE	GLY	PHE	GLY	SER
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ILE	ASP	LEU	PRO	ASN	LEU	HIS	LYS	ASP	GLU	ASP	VAL	LEU	LYS	ALA	VAL	ARG	ALA	LEU	VAL	ALA	ASN	GLU	PRO	GLU	LEU	ALA	ALA	GLN	VAL	VAL	VAL	LYS	ASN	TRP	MET	ASN	ASP	ASN	GLY
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- Molecule 7: Flagellar M-ring protein

Chain AJ: 96%

MET ASP ASP LYS SER THR ASP LEU THR VAL THR GLU GLY GLY SER ASP GLY ALA LEU VAL VAL ALA SER ASP ASP ASP GLU GLU GLN ASN PRO ASP ASP LEU LEU GLU GLU ARG SER SER LYS PHE ASP MET VAL VAL VAL GLY ASP LEU ASP ASP LEU LEU ARG GLN VAL VAL VAL VAL LEU LEU

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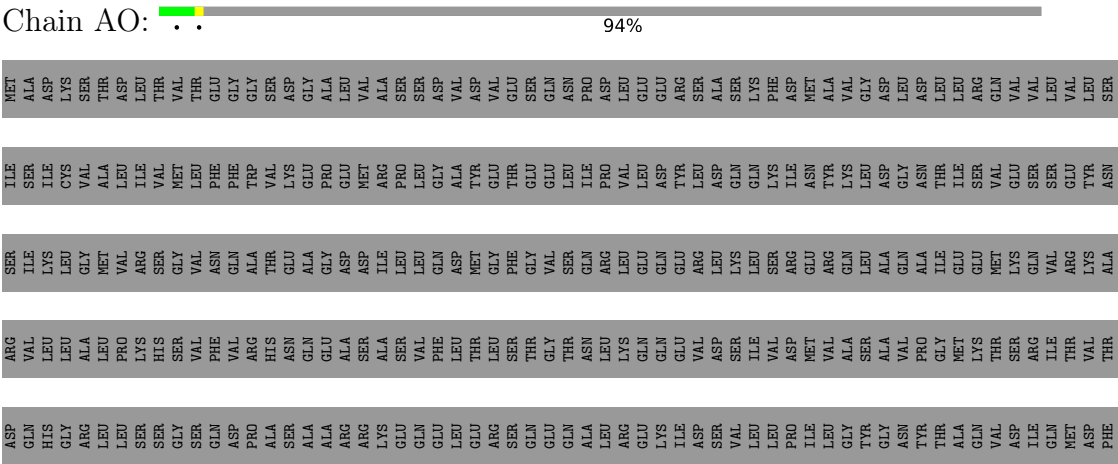


ALA
LEU
VAL
ALA
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GLU
PRO
GLU
LEU
ALA
ALA
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VAL
LYS
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MET
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GLY

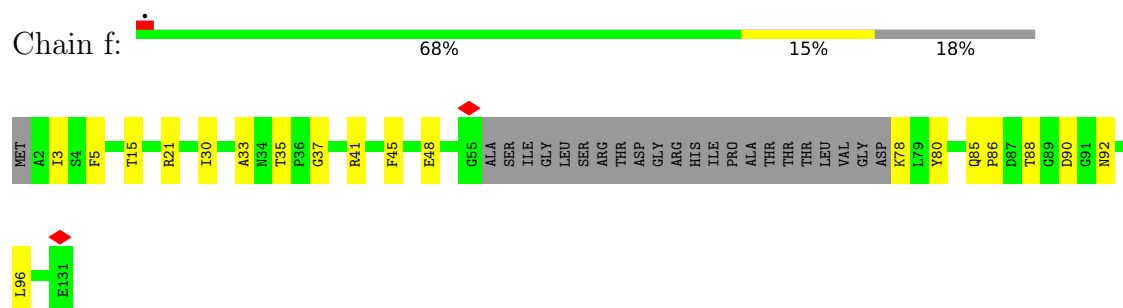
● Molecule 7: Flagellar M-ring protein



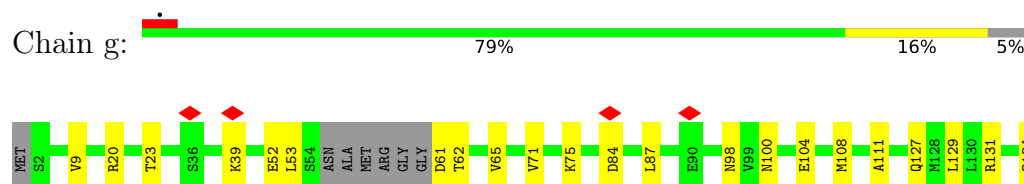
● Molecule 7: Flagellar M-ring protein



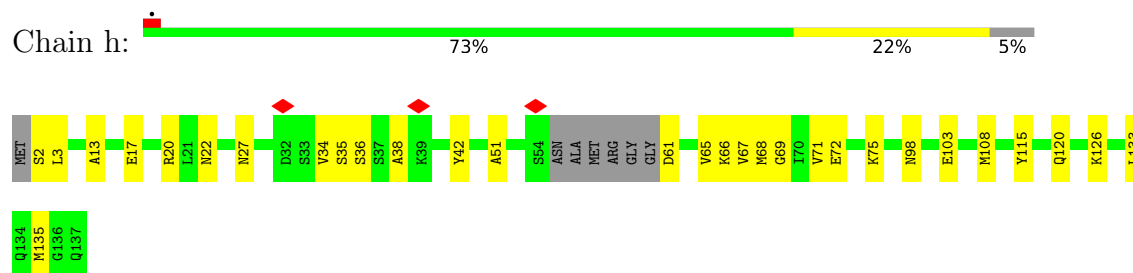
- Molecule 8: Flagellar basal body rod protein FlgB



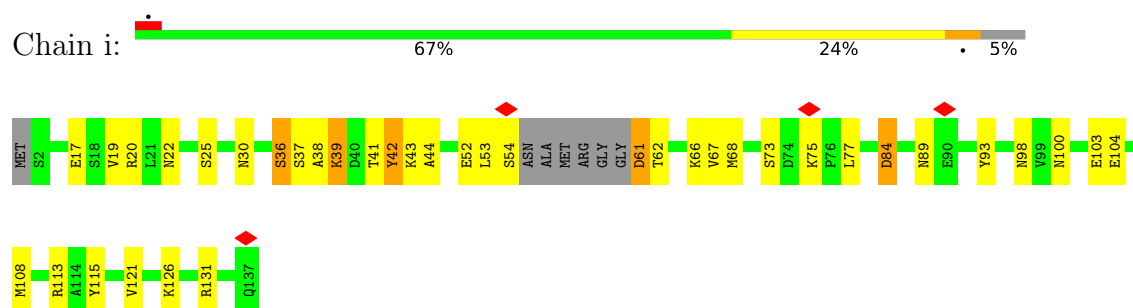
- Molecule 9: Flagellar basal-body rod protein FlgC



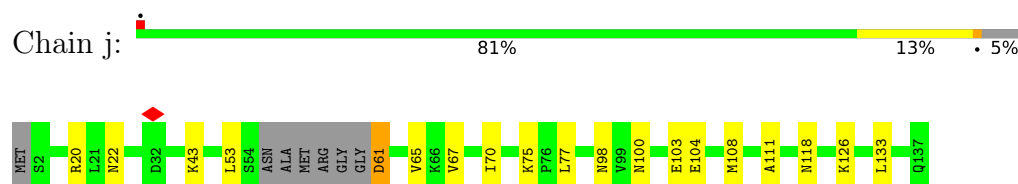
- Molecule 9: Flagellar basal-body rod protein FlgC



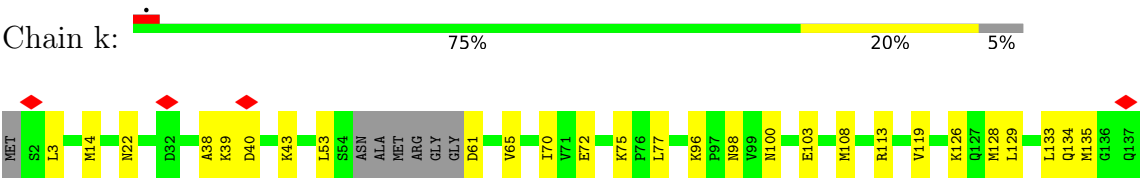
- Molecule 9: Flagellar basal-body rod protein FlgC



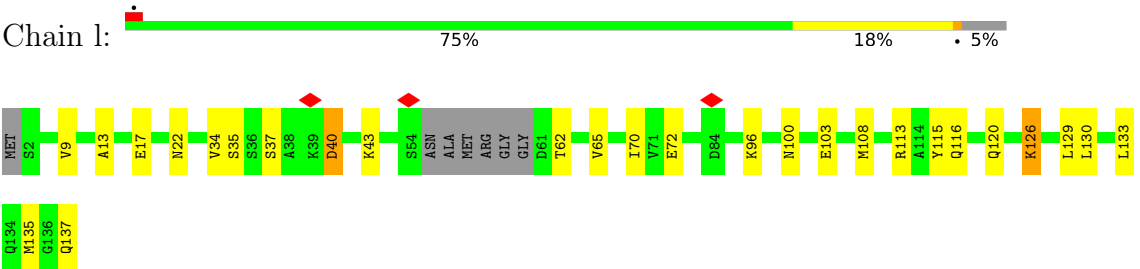
- Molecule 9: Flagellar basal-body rod protein FlgC



- Molecule 9: Flagellar basal-body rod protein FlgC



• Molecule 9: Flagellar basal-body rod protein FlgC



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	TFS 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

5.1 Standard geometry

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

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	m	0.11	0/1905	0.26	0/2572
3	n	0.13	0/1905	0.26	0/2572
3	o	0.10	0/1905	0.26	0/2572
3	p	0.11	0/1905	0.26	0/2572
3	q	0.10	0/1905	0.25	0/2572
4	r	0.32	0/564	0.43	0/759
4	s	0.08	0/609	0.20	0/819
4	t	0.07	0/609	0.17	0/819
4	u	0.07	0/564	0.16	0/759
4	v	0.07	0/564	0.18	0/759
4	w	0.09	0/313	0.19	0/420
5	x	0.08	0/562	0.19	0/760
6	8	0.09	0/1941	0.25	0/2631
7	AA	0.35	0/137	0.45	0/188
7	AB	0.29	0/137	0.43	0/188
7	AC	0.14	0/141	0.31	0/193
7	AD	0.30	0/137	0.46	0/188
7	AE	0.12	0/137	0.28	0/188
7	AF	0.92	0/161	1.23	0/221
7	AG	0.16	0/75	0.32	0/103
7	AH	0.20	0/75	0.42	0/103
7	AI	0.94	0/75	1.34	0/103
7	AJ	0.37	0/166	0.57	0/228

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
7	AK	0.31	0/172	0.70	0/237
7	AL	0.39	0/223	0.62	0/304
7	AM	0.20	0/227	0.44	0/309
7	AN	0.23	0/227	0.49	0/309
7	AO	0.16	0/223	0.40	0/304
8	b	0.22	0/856	0.36	0/1151
8	c	0.22	0/846	0.30	0/1138
8	d	0.23	0/856	0.31	0/1151
8	e	0.19	0/848	0.31	0/1140
8	f	0.22	0/848	0.35	0/1140
9	g	0.11	0/996	0.26	0/1348
9	h	0.10	0/996	0.26	0/1348
9	i	0.30	0/996	0.46	0/1348
9	j	0.10	0/996	0.24	0/1348
9	k	0.11	0/996	0.28	0/1348
9	l	0.13	0/996	0.30	0/1348
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	27	0
1	2	1608	0	1691	32	0
1	3	1608	0	1691	34	0
1	y	1608	0	1691	26	0
1	z	1608	0	1691	36	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	m	1879	0	1864	31	0
3	n	1879	0	1864	46	0
3	o	1879	0	1864	24	0
3	p	1879	0	1864	30	0
3	q	1879	0	1864	37	0
4	r	560	0	561	12	0
4	s	605	0	609	11	0
4	t	605	0	609	19	0
4	u	560	0	561	10	0
4	v	560	0	561	21	0
4	w	311	0	320	8	0
5	x	552	0	577	13	0
6	8	1896	0	1968	44	0
7	AA	135	0	128	3	0
7	AB	135	0	128	2	0
7	AC	139	0	131	0	0
7	AD	135	0	128	2	0
7	AE	135	0	128	2	0
7	AF	158	0	152	13	0
7	AG	73	0	72	4	0
7	AH	73	0	72	4	0
7	AI	73	0	72	8	0
7	AJ	163	0	157	4	0
7	AK	169	0	164	5	0
7	AL	220	0	215	3	0
7	AM	224	0	218	4	0
7	AN	224	0	218	2	0
7	AO	220	0	215	3	0
8	b	845	0	833	12	0
8	c	835	0	825	19	0
8	d	845	0	833	11	0
8	e	837	0	829	15	0
8	f	837	0	829	14	0
9	g	983	0	958	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	h	983	0	958	23	0
9	i	983	0	958	30	0
9	j	983	0	958	12	0
9	k	983	0	958	20	0
9	l	983	0	958	23	0
10	2	51	0	78	10	0
10	e	51	0	78	4	0
10	t	51	0	78	15	0
10	v	51	0	78	12	0
11	e	32	0	0	1	0
11	s	32	0	0	1	0
11	t	32	0	0	2	0
11	u	32	0	0	3	0
11	v	32	0	0	6	0
All	All	38700	0	39014	610	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 8.

The worst 5 of 610 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)
4:v:40:ALA:HB2	11:v:201:XKP:O	1.46	1.15
9:i:52:GLU:HG3	9:i:52:GLU:O	1.47	1.06
9:i:52:GLU:O	9:i:52:GLU:CG	2.15	0.94
1:z:96:LEU:HD21	10:e:202:PGT:H222	1.52	0.90
4:t:87:ILE:HD11	10:t:202:PGT:H182	1.55	0.86

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	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%)	11	39
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	m	246/249 (99%)	242 (98%)	4 (2%)	0	100	100
3	n	246/249 (99%)	242 (98%)	4 (2%)	0	100	100
3	o	246/249 (99%)	241 (98%)	5 (2%)	0	100	100
3	p	246/249 (99%)	242 (98%)	4 (2%)	0	100	100
3	q	246/249 (99%)	240 (98%)	6 (2%)	0	100	100
4	r	70/103 (68%)	70 (100%)	0	0	100	100
4	s	78/103 (76%)	78 (100%)	0	0	100	100
4	t	78/103 (76%)	77 (99%)	1 (1%)	0	100	100
4	u	70/103 (68%)	69 (99%)	1 (1%)	0	100	100
4	v	70/103 (68%)	69 (99%)	1 (1%)	0	100	100
4	w	38/103 (37%)	38 (100%)	0	0	100	100
5	x	69/376 (18%)	69 (100%)	0	0	100	100
6	8	238/260 (92%)	232 (98%)	6 (2%)	0	100	100
7	AA	17/580 (3%)	17 (100%)	0	0	100	100
7	AB	17/580 (3%)	15 (88%)	2 (12%)	0	100	100
7	AC	18/580 (3%)	18 (100%)	0	0	100	100
7	AD	17/580 (3%)	17 (100%)	0	0	100	100
7	AE	17/580 (3%)	17 (100%)	0	0	100	100
7	AF	21/580 (4%)	14 (67%)	6 (29%)	1 (5%)	2	9
7	AG	9/580 (2%)	7 (78%)	2 (22%)	0	100	100
7	AH	9/580 (2%)	9 (100%)	0	0	100	100
7	AI	9/580 (2%)	8 (89%)	1 (11%)	0	100	100
7	AJ	22/580 (4%)	18 (82%)	4 (18%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	AK	23/580 (4%)	23 (100%)	0	0	100	100
7	AL	30/580 (5%)	26 (87%)	4 (13%)	0	100	100
7	AM	31/580 (5%)	31 (100%)	0	0	100	100
7	AN	31/580 (5%)	31 (100%)	0	0	100	100
7	AO	30/580 (5%)	30 (100%)	0	0	100	100
8	b	105/131 (80%)	104 (99%)	1 (1%)	0	100	100
8	c	103/131 (79%)	102 (99%)	1 (1%)	0	100	100
8	d	105/131 (80%)	103 (98%)	2 (2%)	0	100	100
8	e	104/131 (79%)	104 (100%)	0	0	100	100
8	f	104/131 (79%)	103 (99%)	1 (1%)	0	100	100
9	g	126/137 (92%)	122 (97%)	4 (3%)	0	100	100
9	h	126/137 (92%)	123 (98%)	3 (2%)	0	100	100
9	i	126/137 (92%)	122 (97%)	3 (2%)	1 (1%)	16	46
9	j	126/137 (92%)	125 (99%)	1 (1%)	0	100	100
9	k	126/137 (92%)	120 (95%)	6 (5%)	0	100	100
9	l	126/137 (92%)	121 (96%)	5 (4%)	0	100	100
All	All	4896/14477 (34%)	4795 (98%)	98 (2%)	3 (0%)	49	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	5	88	LEU
9	i	42	TYR
7	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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2	182/247 (74%)	176 (97%)	6 (3%)	33	64
1	3	182/247 (74%)	177 (97%)	5 (3%)	39	68
1	y	182/247 (74%)	175 (96%)	7 (4%)	29	60
1	z	182/247 (74%)	175 (96%)	7 (4%)	29	60
2	4	80/80 (100%)	77 (96%)	3 (4%)	29	60
2	5	80/80 (100%)	76 (95%)	4 (5%)	22	53
2	6	80/80 (100%)	75 (94%)	5 (6%)	16	45
2	7	80/80 (100%)	79 (99%)	1 (1%)	61	79
3	m	204/205 (100%)	199 (98%)	5 (2%)	42	69
3	n	204/205 (100%)	198 (97%)	6 (3%)	37	67
3	o	204/205 (100%)	198 (97%)	6 (3%)	37	67
3	p	204/205 (100%)	202 (99%)	2 (1%)	68	81
3	q	204/205 (100%)	200 (98%)	4 (2%)	48	73
4	r	63/84 (75%)	59 (94%)	4 (6%)	16	45
4	s	66/84 (79%)	64 (97%)	2 (3%)	36	66
4	t	66/84 (79%)	63 (96%)	3 (4%)	24	56
4	u	63/84 (75%)	62 (98%)	1 (2%)	55	76
4	v	63/84 (75%)	63 (100%)	0	100	100
4	w	36/84 (43%)	35 (97%)	1 (3%)	38	67
5	x	58/317 (18%)	55 (95%)	3 (5%)	21	51
6	8	204/218 (94%)	194 (95%)	10 (5%)	22	53
7	AA	15/500 (3%)	14 (93%)	1 (7%)	15	43
7	AB	15/500 (3%)	14 (93%)	1 (7%)	15	43
7	AC	15/500 (3%)	15 (100%)	0	100	100
7	AD	15/500 (3%)	14 (93%)	1 (7%)	15	43
7	AE	15/500 (3%)	15 (100%)	0	100	100
7	AF	17/500 (3%)	13 (76%)	4 (24%)	1	4
7	AG	8/500 (2%)	8 (100%)	0	100	100
7	AH	8/500 (2%)	7 (88%)	1 (12%)	4	18
7	AI	8/500 (2%)	8 (100%)	0	100	100
7	AJ	17/500 (3%)	16 (94%)	1 (6%)	18	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	AK	18/500 (4%)	15 (83%)	3 (17%)	2	10
7	AL	24/500 (5%)	23 (96%)	1 (4%)	26	58
7	AM	24/500 (5%)	24 (100%)	0	100	100
7	AN	24/500 (5%)	22 (92%)	2 (8%)	10	34
7	AO	24/500 (5%)	23 (96%)	1 (4%)	26	58
8	b	89/106 (84%)	88 (99%)	1 (1%)	65	80
8	c	88/106 (83%)	86 (98%)	2 (2%)	44	70
8	d	89/106 (84%)	86 (97%)	3 (3%)	32	63
8	e	88/106 (83%)	85 (97%)	3 (3%)	32	63
8	f	88/106 (83%)	88 (100%)	0	100	100
9	g	111/115 (96%)	106 (96%)	5 (4%)	24	56
9	h	111/115 (96%)	107 (96%)	4 (4%)	31	62
9	i	111/115 (96%)	103 (93%)	8 (7%)	13	40
9	j	111/115 (96%)	106 (96%)	5 (4%)	24	56
9	k	111/115 (96%)	105 (95%)	6 (5%)	20	50
9	l	111/115 (96%)	106 (96%)	5 (4%)	24	56
All	All	4223/12339 (34%)	4074 (96%)	149 (4%)	32	62

5 of 149 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	e	88	THR
9	k	134	GLN
9	g	65	VAL
9	i	84	ASP
3	p	135	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 96 such sidechains are listed below:

Mol	Chain	Res	Type
7	AL	351	GLN
8	e	85	GLN
7	AN	342	GLN
8	c	110	HIS
8	f	14	HIS

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 ⓘ

9 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
11	XKP	t	201	-	31,31,32	0.36	0	34,36,37	0.38	0
11	XKP	s	201	-	31,31,32	0.37	0	34,36,37	0.35	0
11	XKP	e	201	-	31,31,32	0.36	0	34,36,37	0.43	0
10	PGT	v	202	-	50,50,50	0.30	0	53,56,56	0.38	0
11	XKP	u	201	-	31,31,32	0.38	0	34,36,37	0.43	0
10	PGT	2	301	-	50,50,50	0.31	0	53,56,56	0.47	0
11	XKP	v	201	-	31,31,32	0.37	0	34,36,37	0.49	0
10	PGT	t	202	-	50,50,50	0.30	0	53,56,56	0.37	0
10	PGT	e	202	-	50,50,50	0.33	0	53,56,56	0.45	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	XKP	t	201	-	-	25/35/35/36	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	XKP	s	201	-	-	20/35/35/36	-
11	XKP	e	201	-	-	17/35/35/36	-
10	PGT	v	202	-	-	39/55/55/55	-
11	XKP	u	201	-	-	18/35/35/36	-
10	PGT	2	301	-	-	34/55/55/55	-
11	XKP	v	201	-	-	20/35/35/36	-
10	PGT	t	202	-	-	37/55/55/55	-
10	PGT	e	202	-	-	32/55/55/55	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 242 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	2	301	PGT	C32-C31-O2-C2
10	2	301	PGT	C1-O3P-P-O1P
10	2	301	PGT	C4-O4P-P-O3P
10	2	301	PGT	C4-O4P-P-O1P
10	2	301	PGT	C5-C4-O4P-P

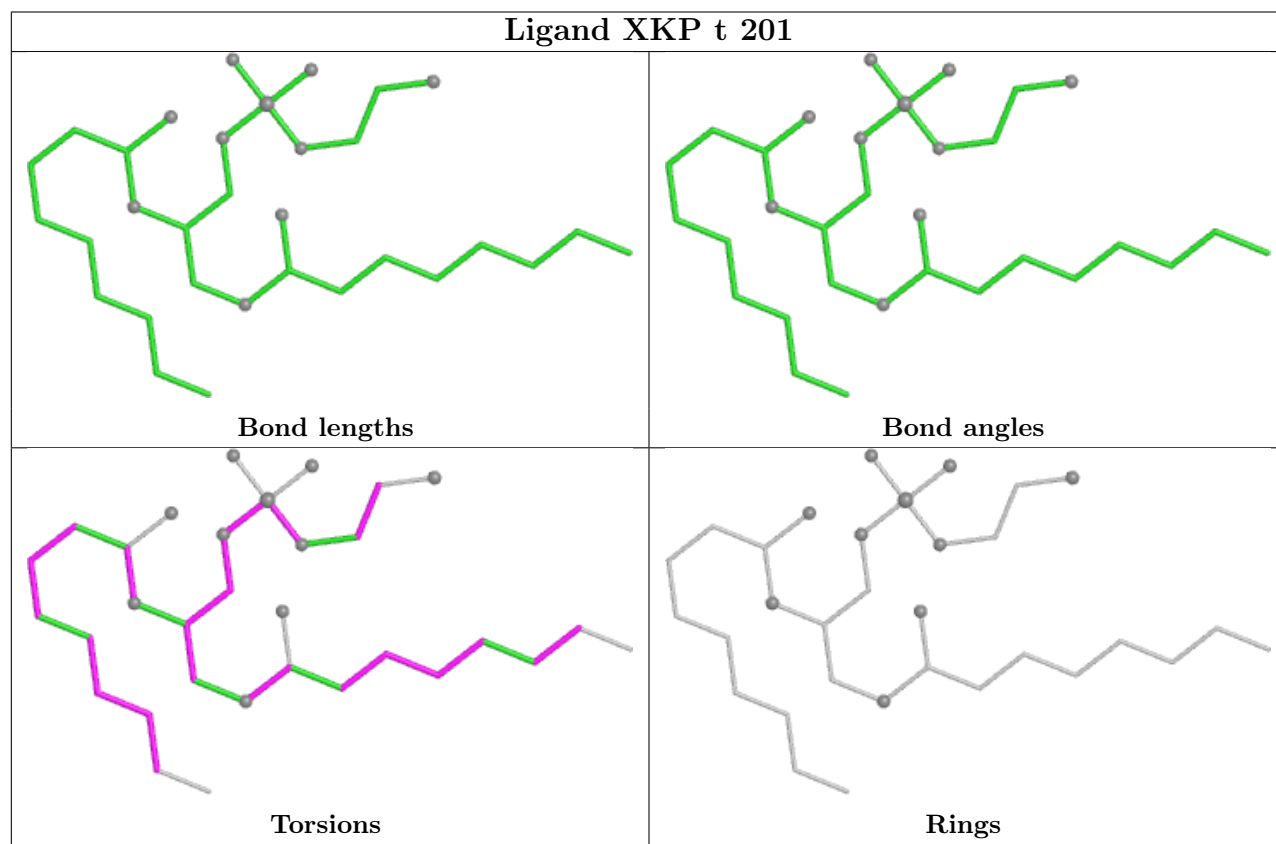
There are no ring outliers.

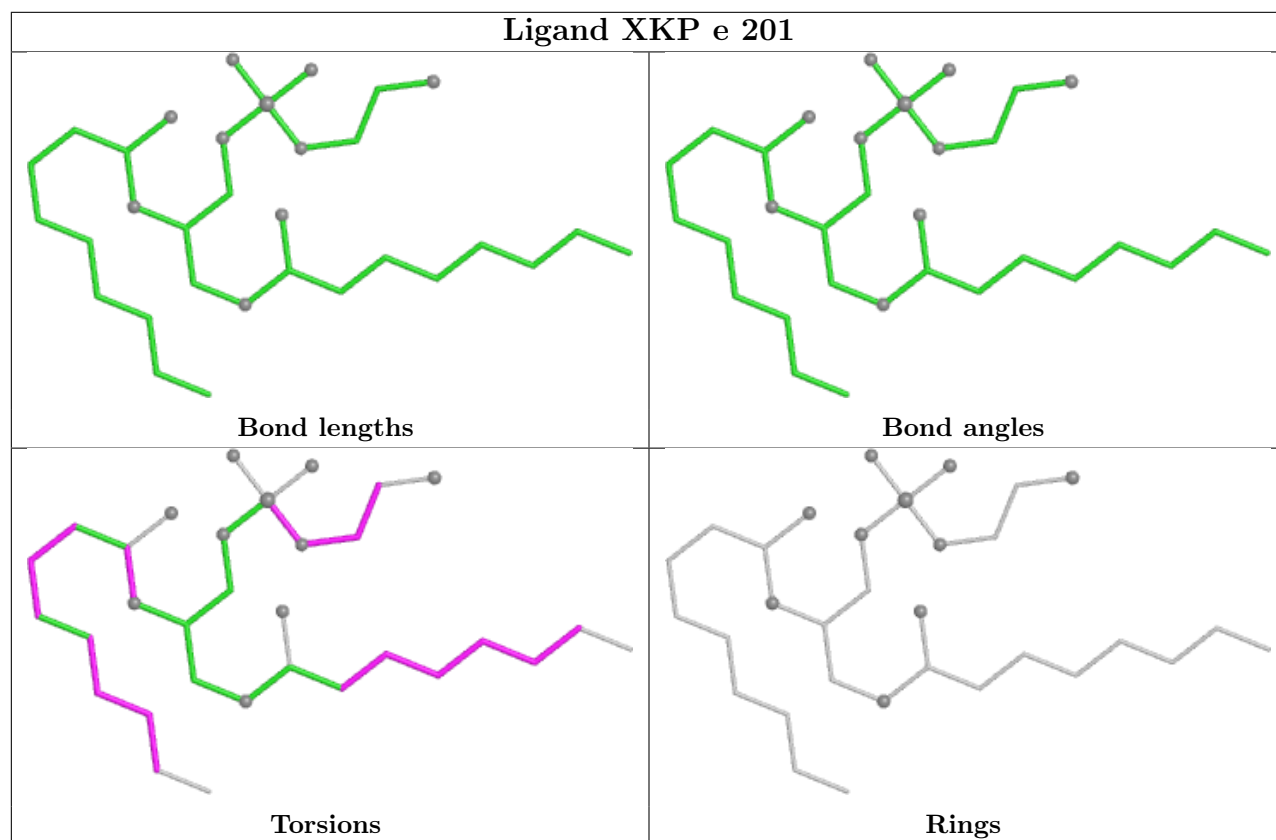
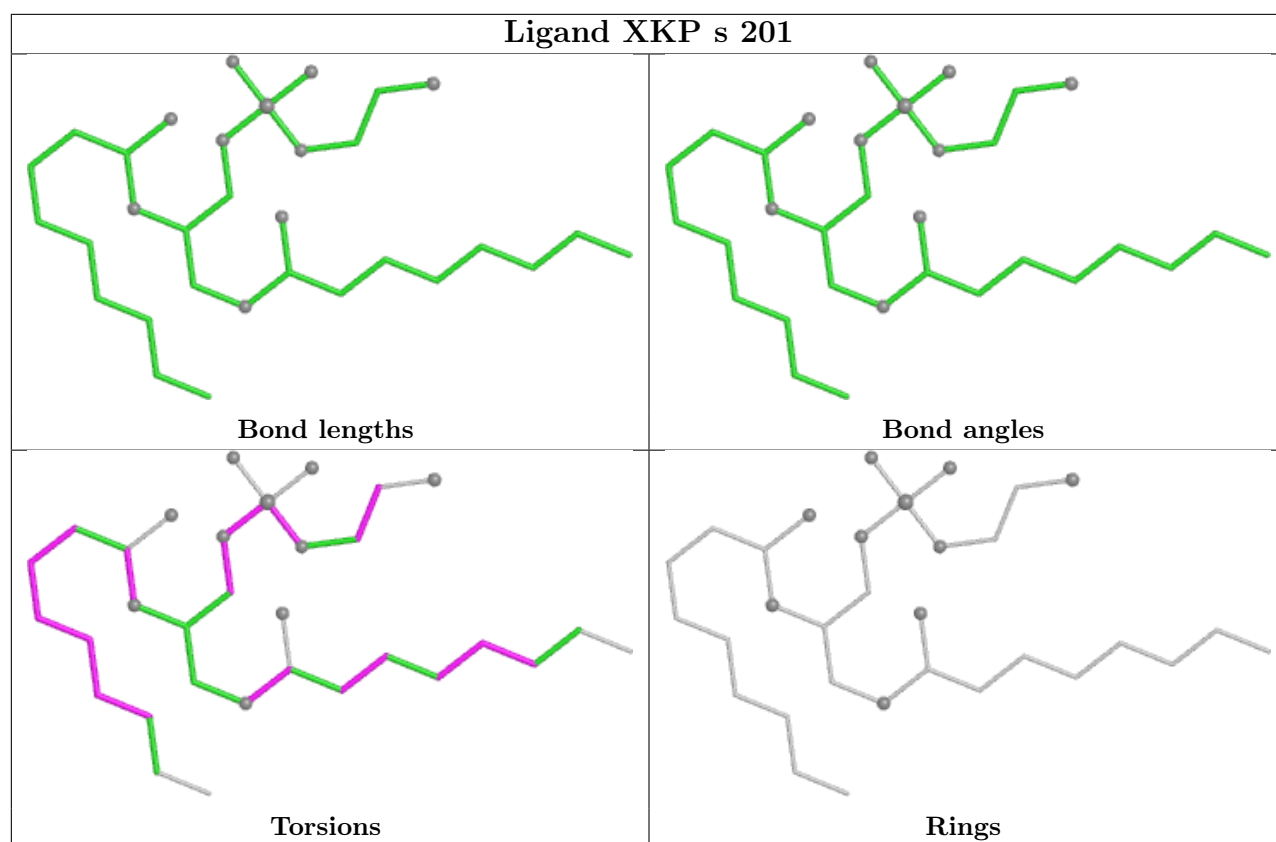
9 monomers are involved in 52 short contacts:

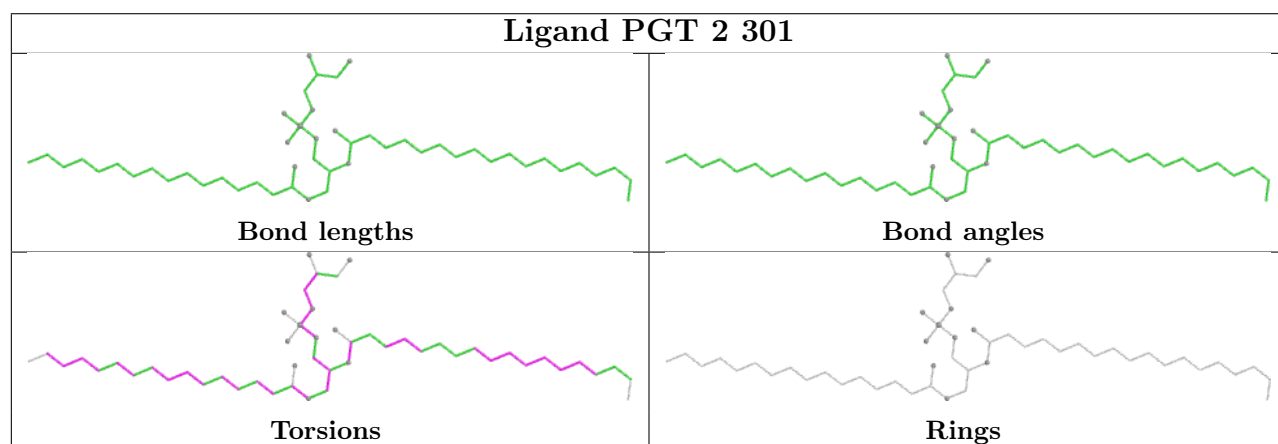
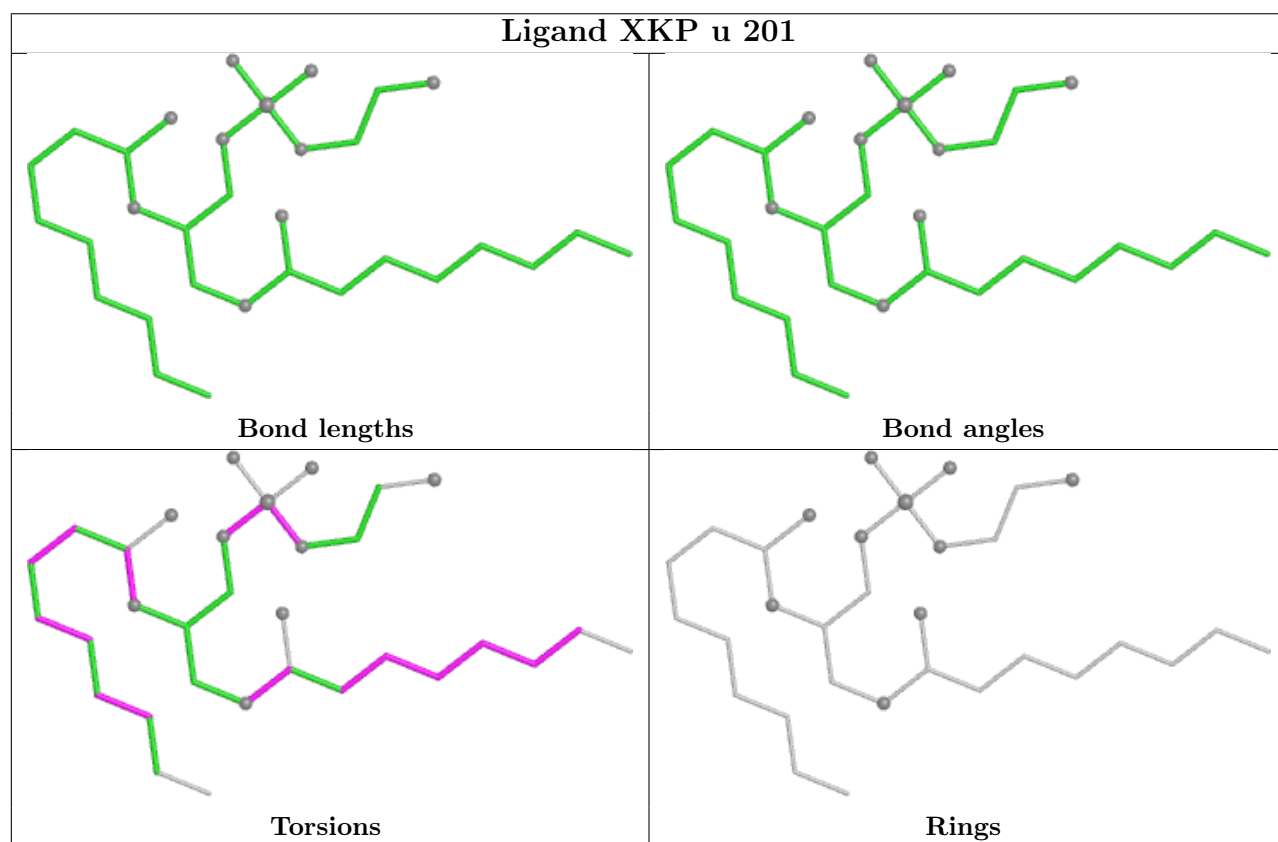
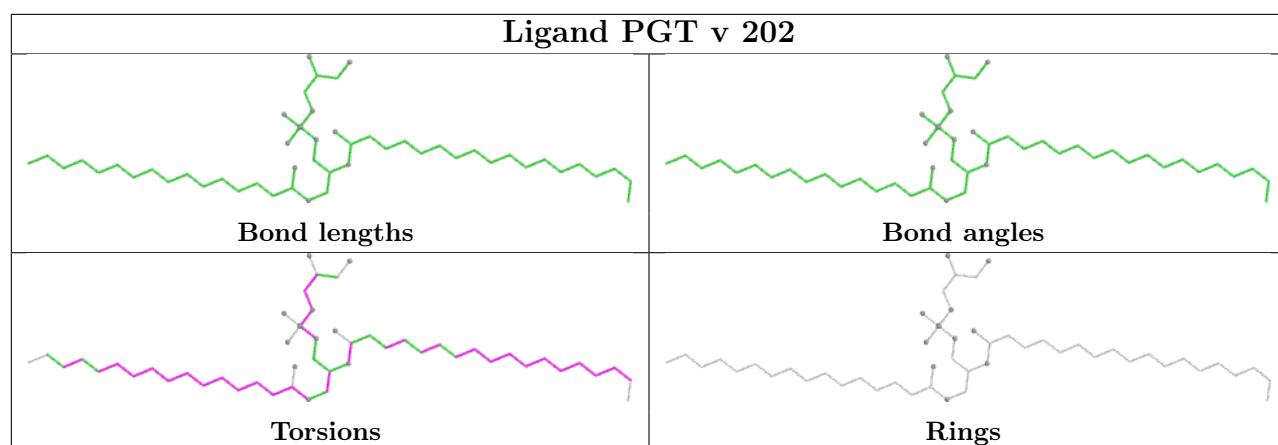
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	t	201	XKP	2	0
11	s	201	XKP	1	0
11	e	201	XKP	1	0
10	v	202	PGT	12	0
11	u	201	XKP	3	0
10	2	301	PGT	10	0
11	v	201	XKP	6	0
10	t	202	PGT	15	0
10	e	202	PGT	4	0

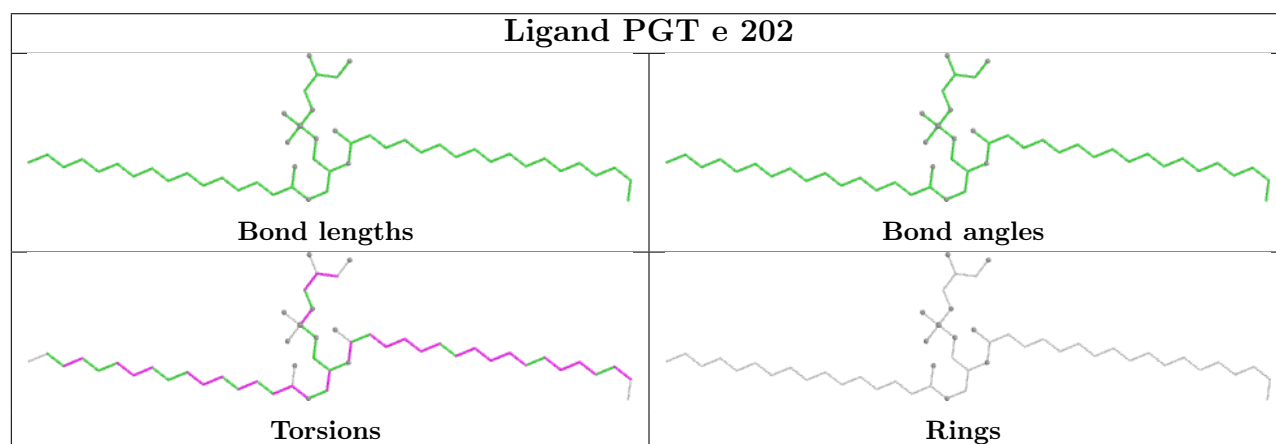
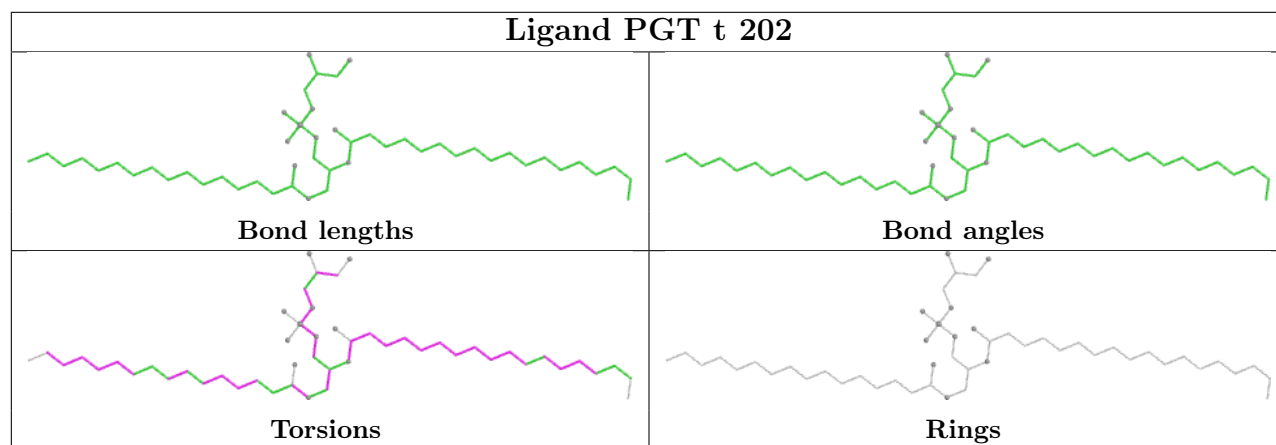
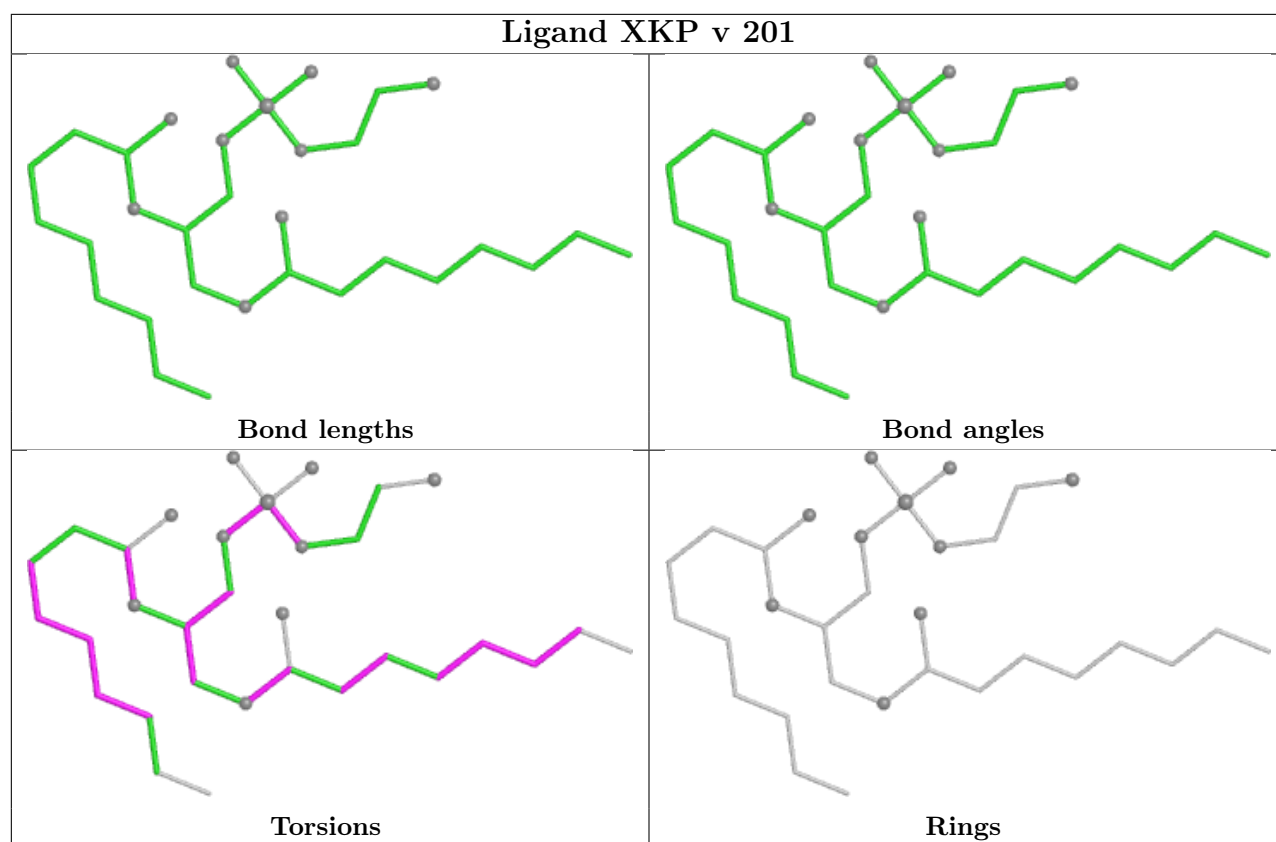
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

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









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.

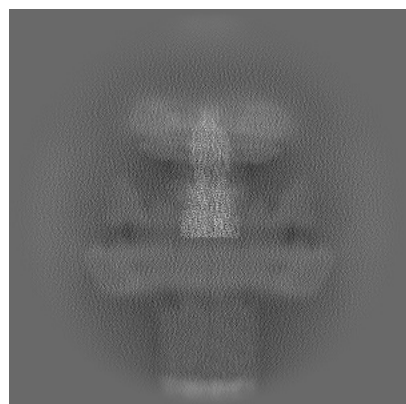
6 Map visualisation [i](#)

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.

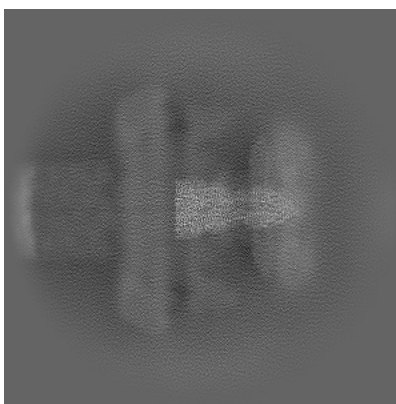
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

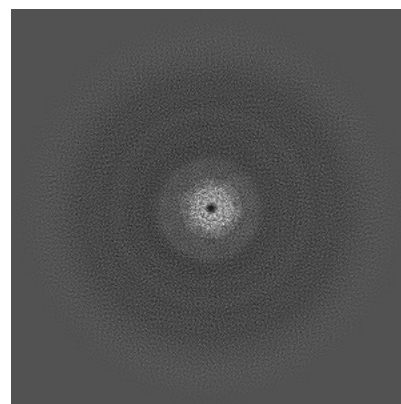
6.1.1 Primary map



X

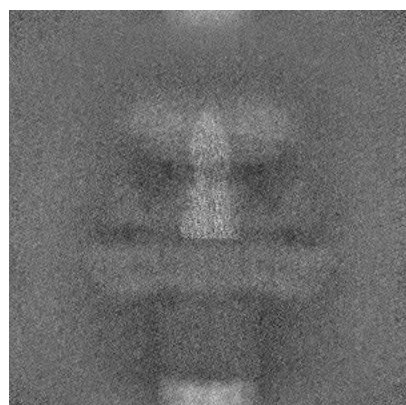


Y

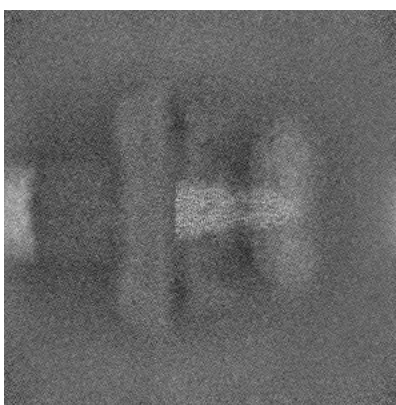


Z

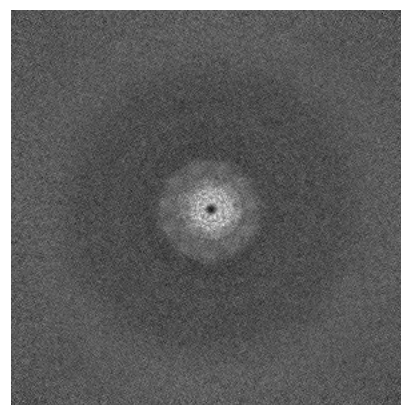
6.1.2 Raw map



X



Y

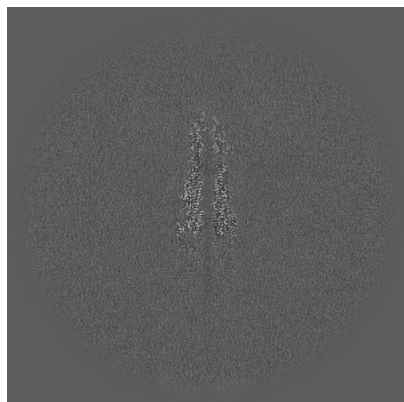


Z

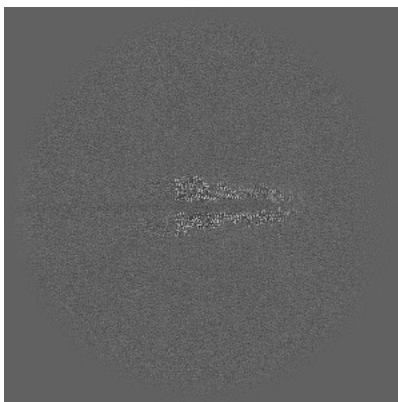
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

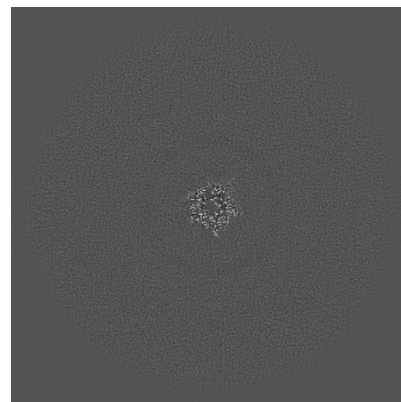
6.2.1 Primary map



X Index: 310

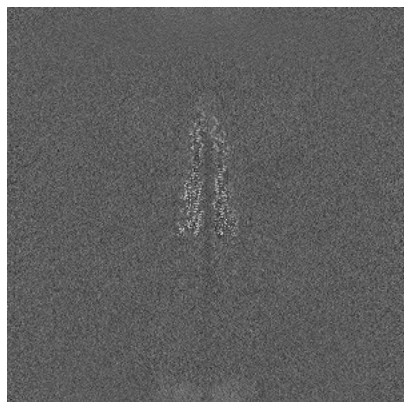


Y Index: 310

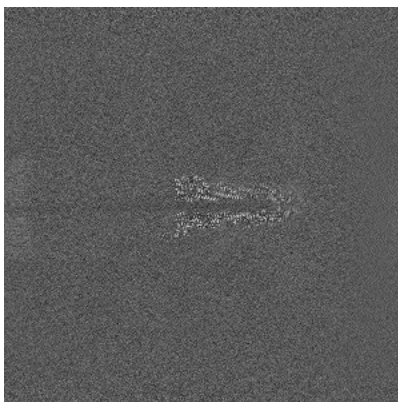


Z Index: 310

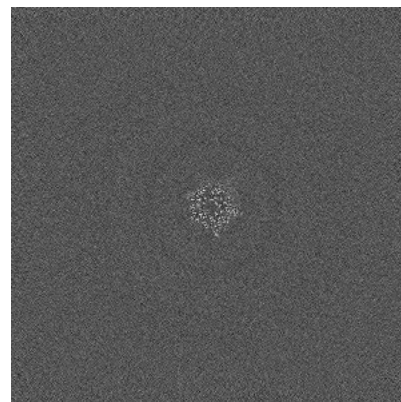
6.2.2 Raw map



X Index: 310



Y Index: 310

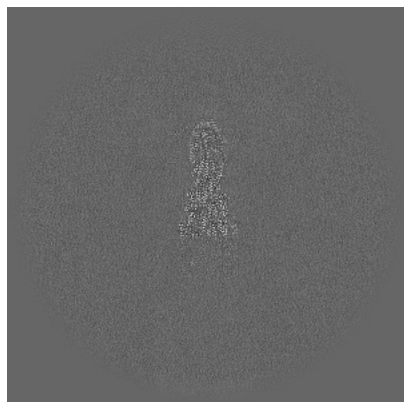


Z Index: 310

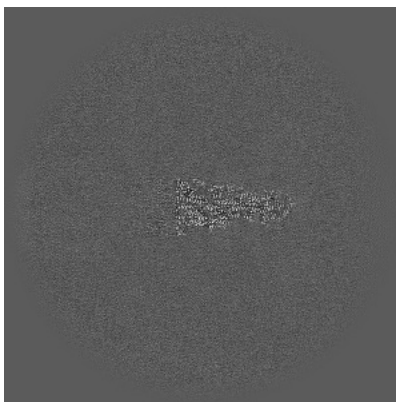
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

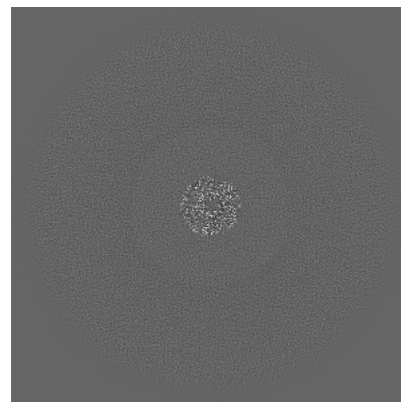
6.3.1 Primary map



X Index: 297

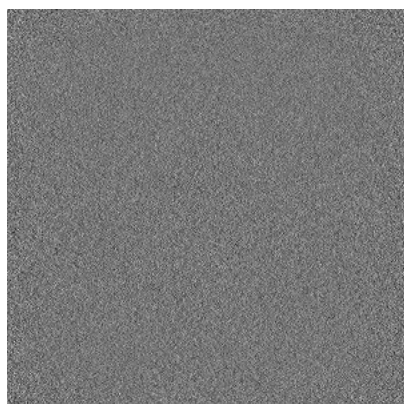


Y Index: 296

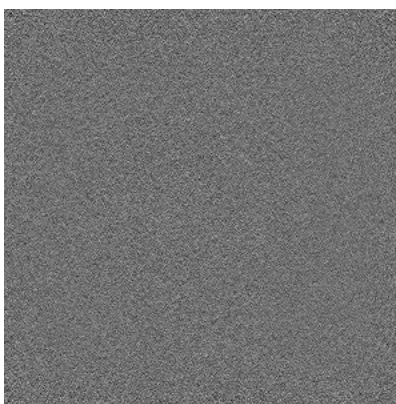


Z Index: 276

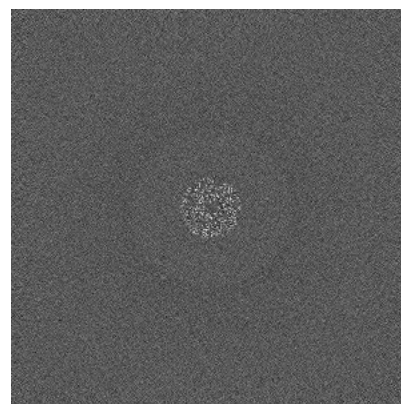
6.3.2 Raw map



X Index: 0



Y Index: 0

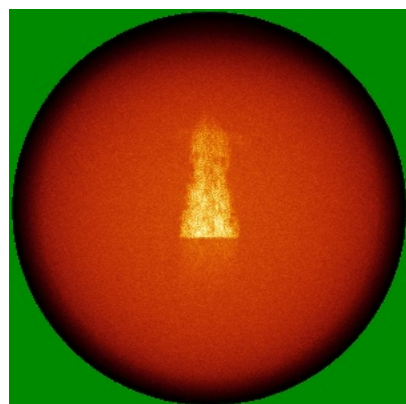


Z Index: 276

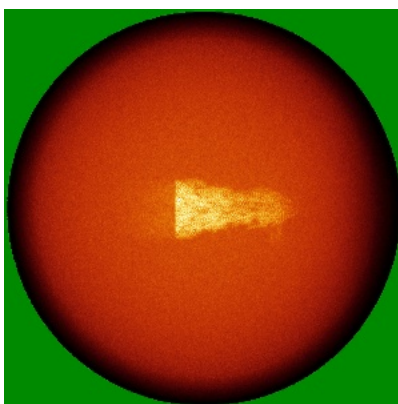
The images above show the largest variance slices of the map in three orthogonal directions.

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

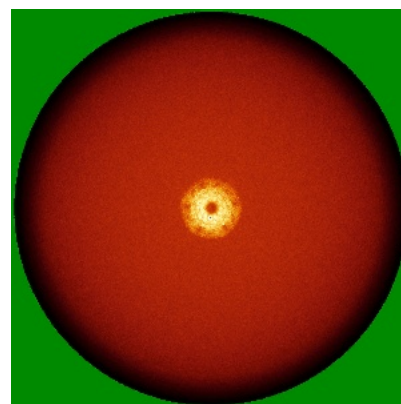
6.4.1 Primary map



X

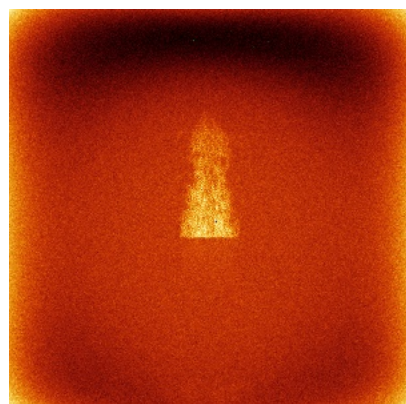


Y

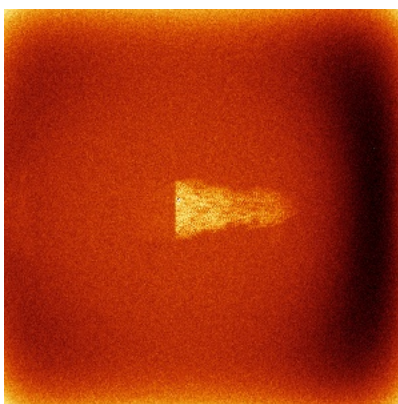


Z

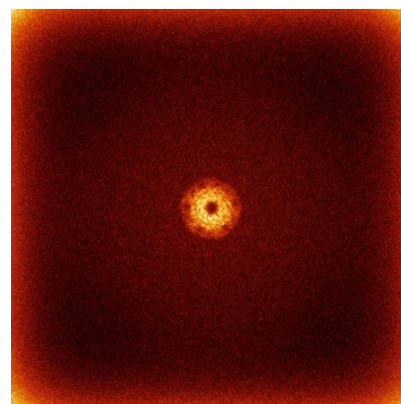
6.4.2 Raw map



X



Y

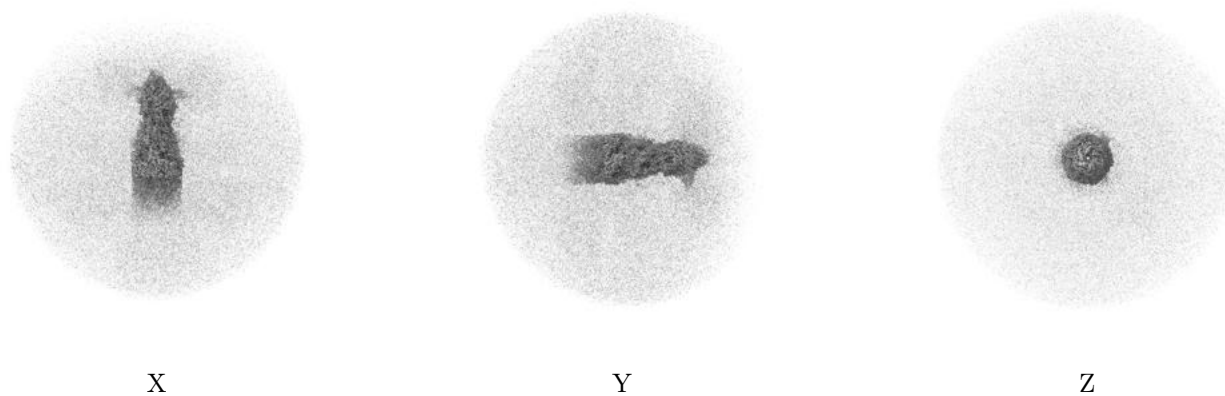


Z

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.

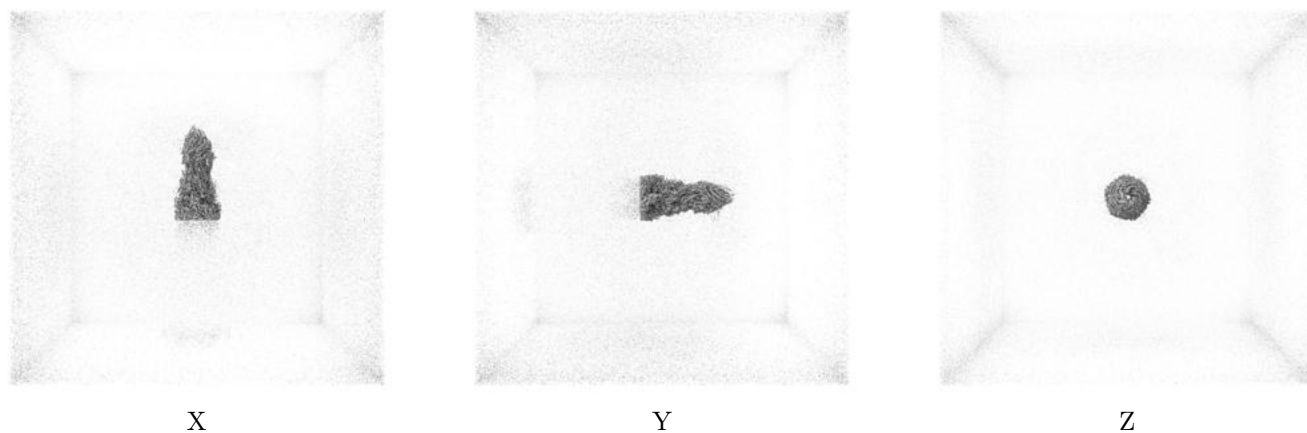
6.5 Orthogonal surface views [i](#)

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.

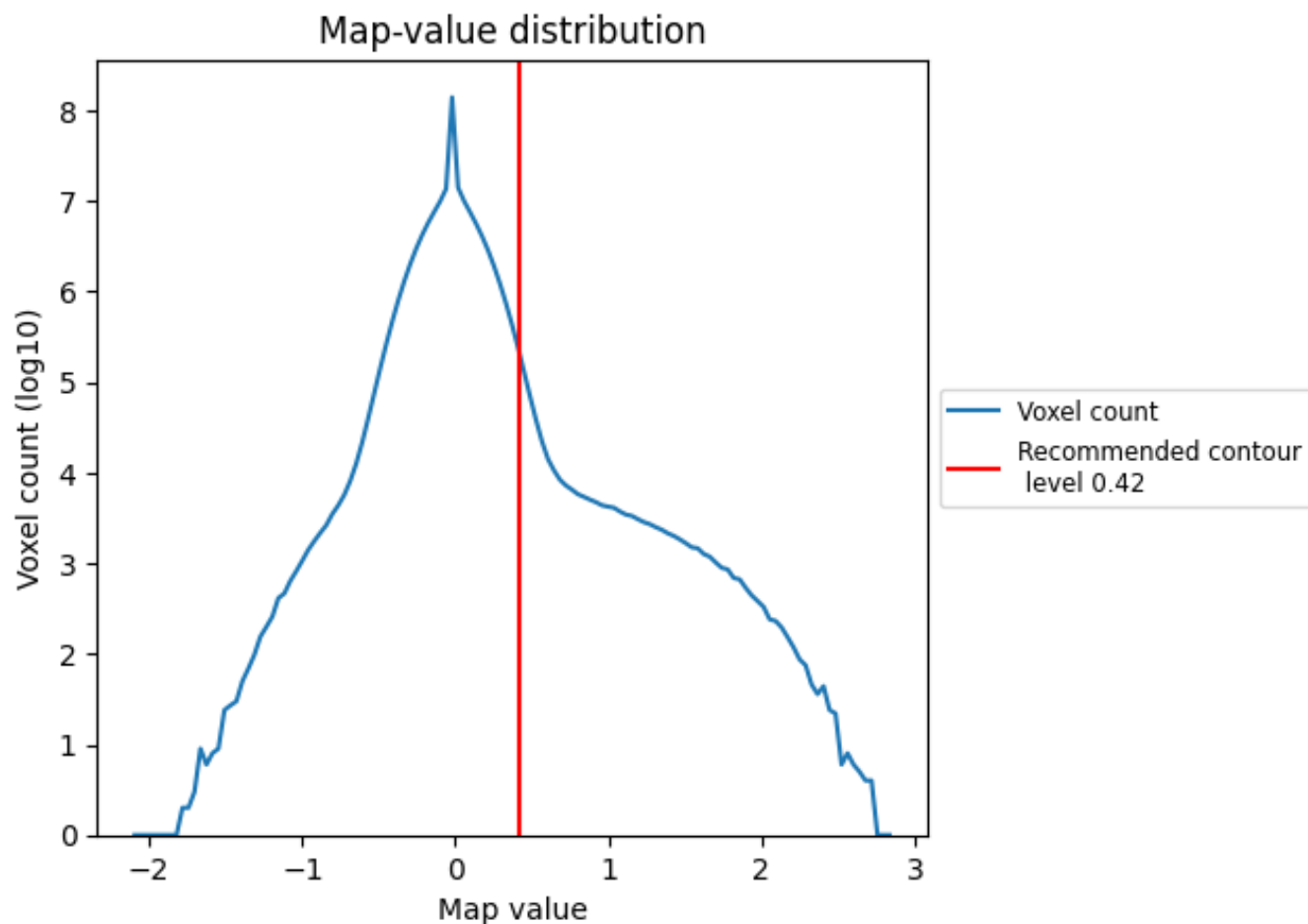
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

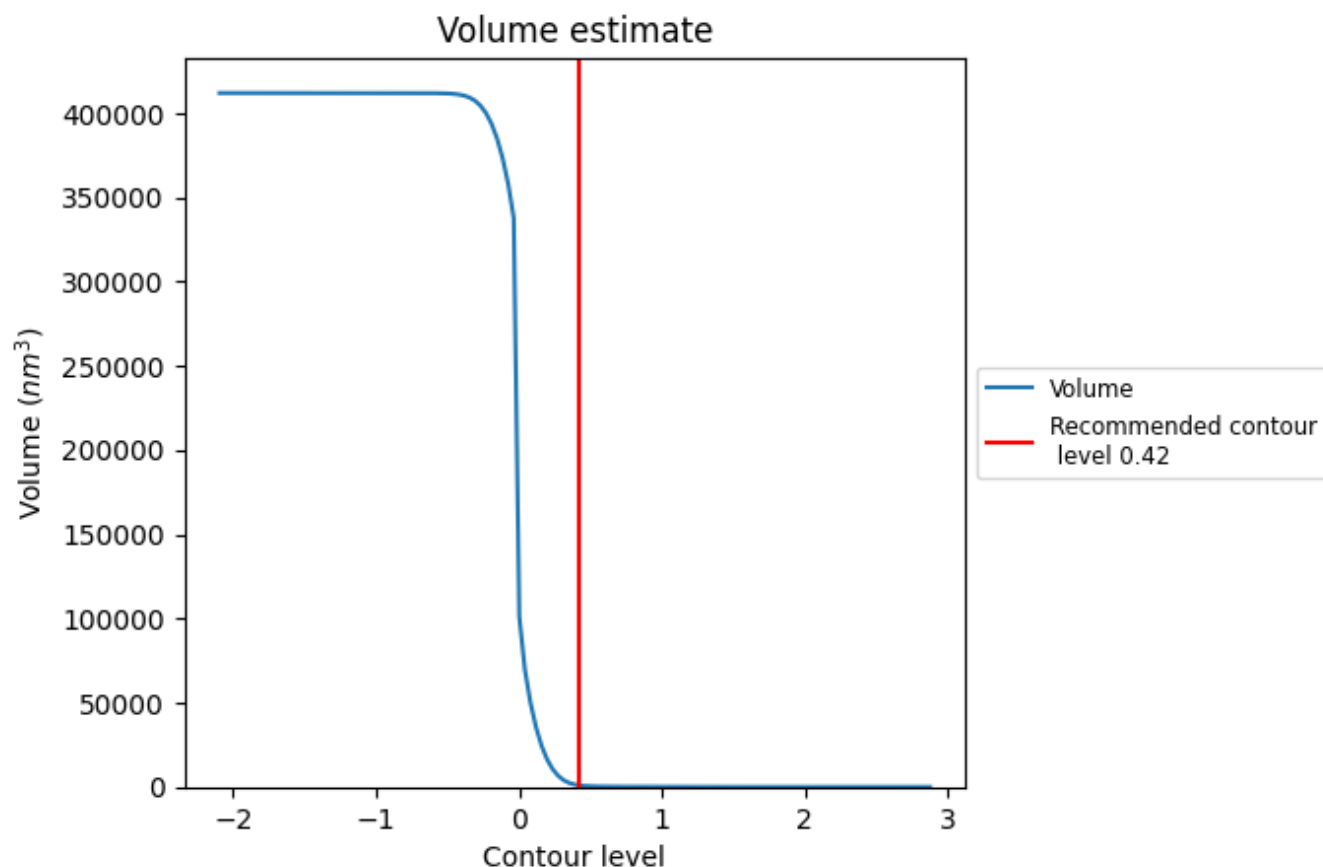
This section contains the results of statistical analysis of the map.

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.

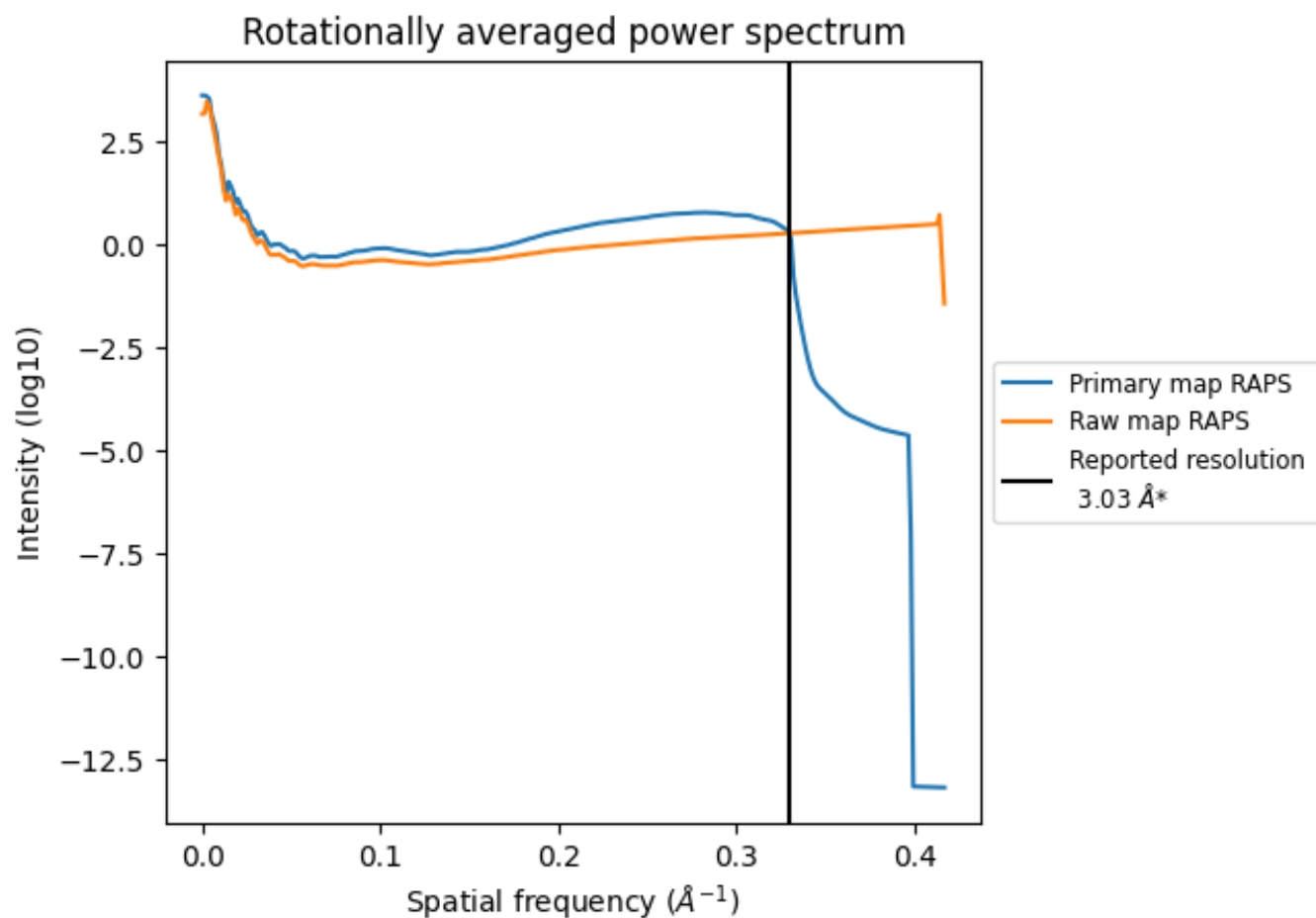
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 972 nm³; 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 ⓘ

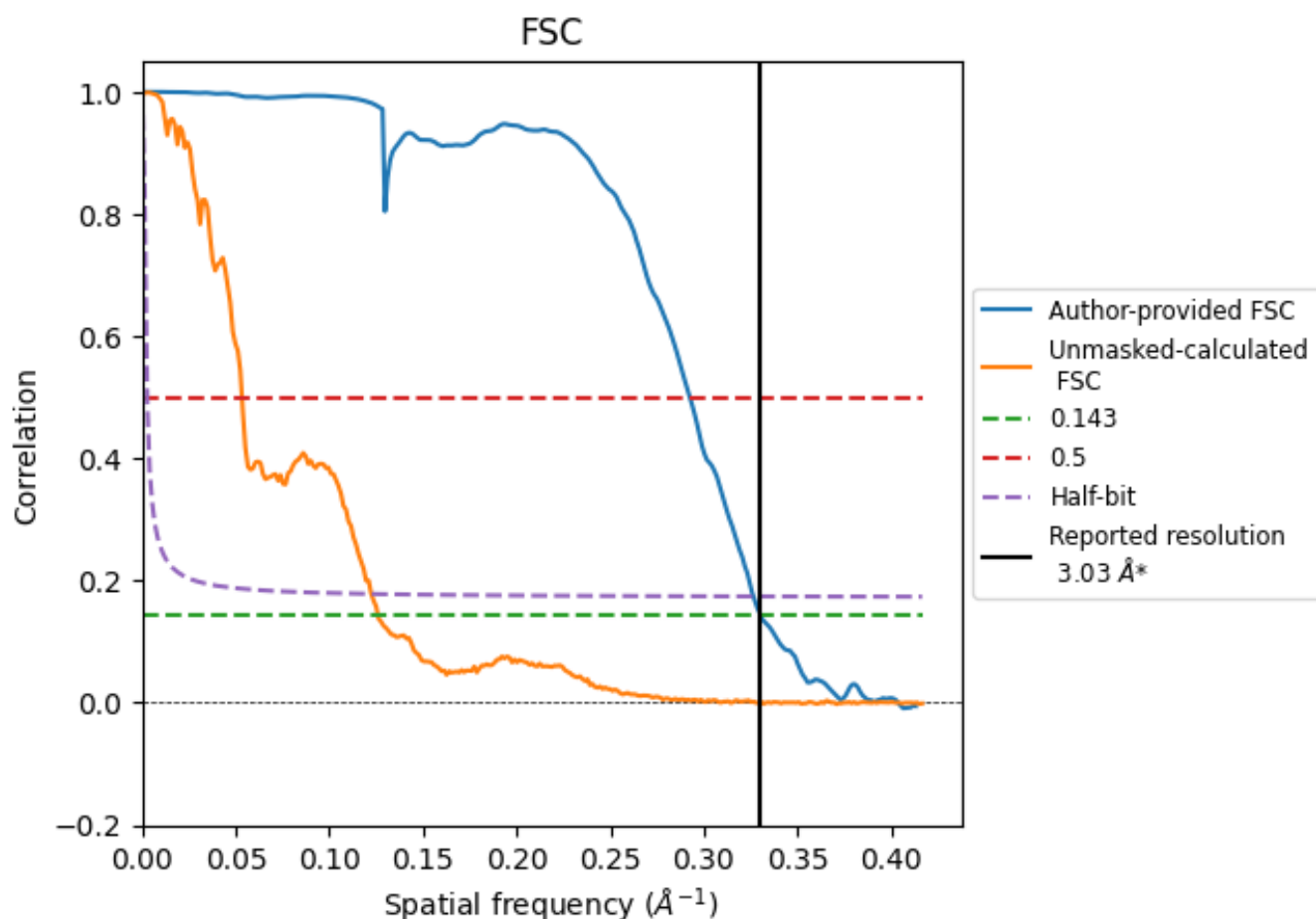


*Reported resolution corresponds to spatial frequency of 0.330 $\text{\AA}^{-1}$

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

8.2 Resolution estimates [i](#)

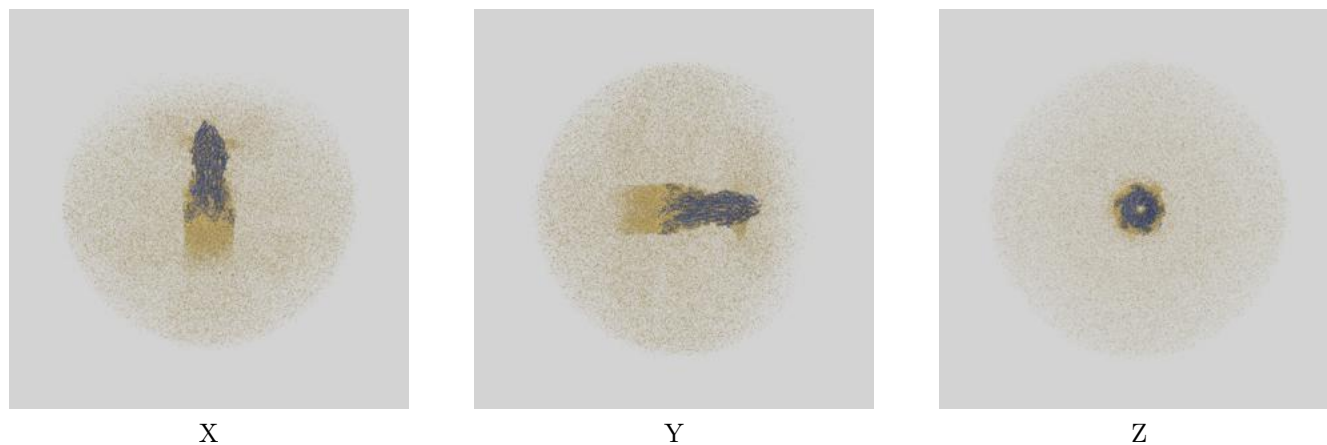
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.03	-	-
Author-provided FSC curve	3.03	3.42	3.06
Unmasked-calculated*	7.94	18.76	8.17

*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](#)

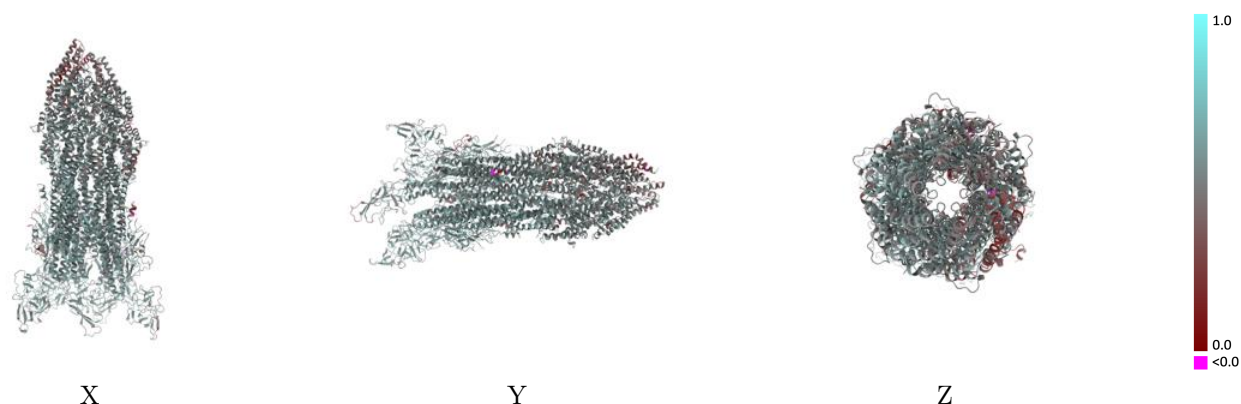
This section contains information regarding the fit between EMDB map EMD-39780 and PDB model 8Z5S. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



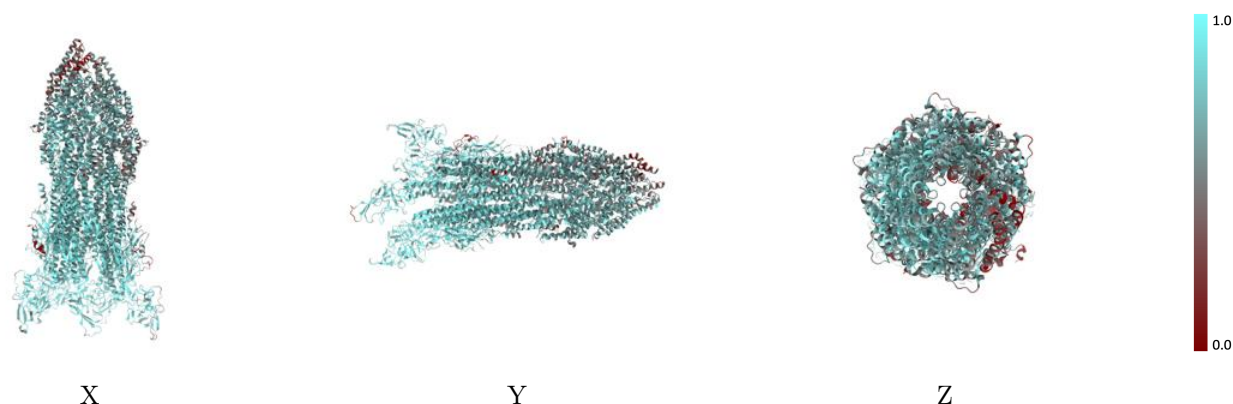
The images above show the 3D surface view of the map at the recommended contour level 0.42 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



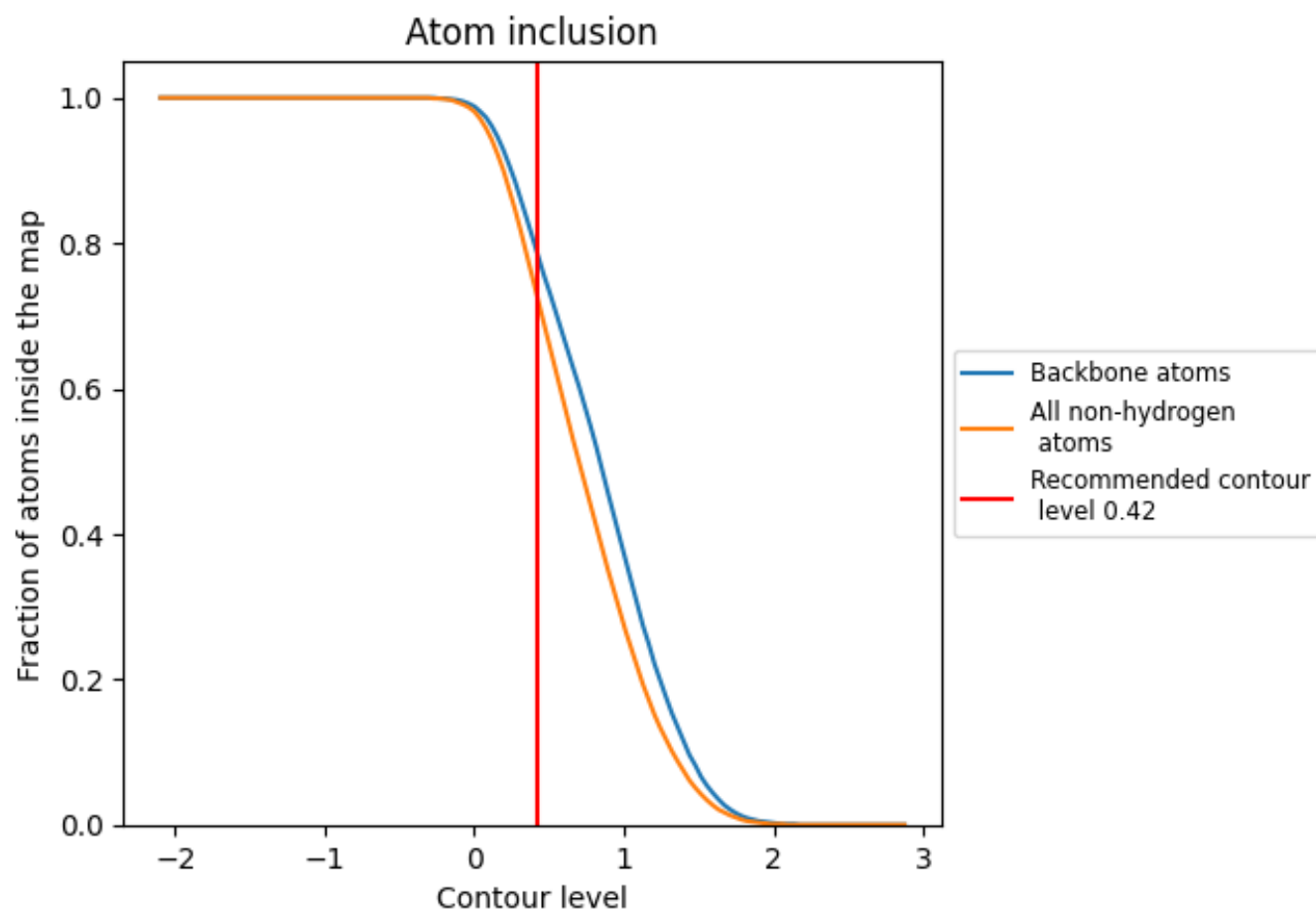
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.42).

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	 0.5310
1	 0.6080	 0.4950
2	 0.6940	 0.5170
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	 0.8110	 0.5720
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	 0.6670	 0.5070
t	 0.6880	 0.5290
u	 0.7480	 0.5500
v	 0.7400	 0.5560
w	 0.7480	 0.5480
x	 0.2790	 0.3340
y	 0.7330	 0.5340
z	 0.7410	 0.5360