



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 07:07 PM UTC

PDB ID : 8WK3 / pdb_00008wk3
EMDB ID : EMD-37594
Title : Cryo-EM structure of the proximal rod-export apparatus and FlgF within the motor-hook complex in the CW state
Authors : Tan, J.X.; Zhang, L.; Zhou, Y.; Zhu, Y.Q.
Deposited on : 2023-09-26
Resolution : 3.30 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.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

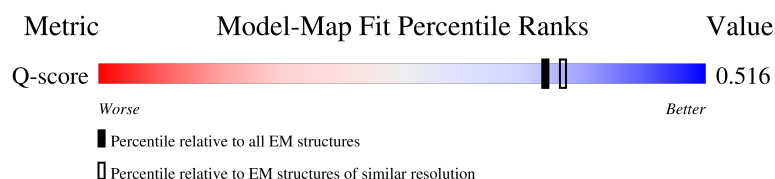
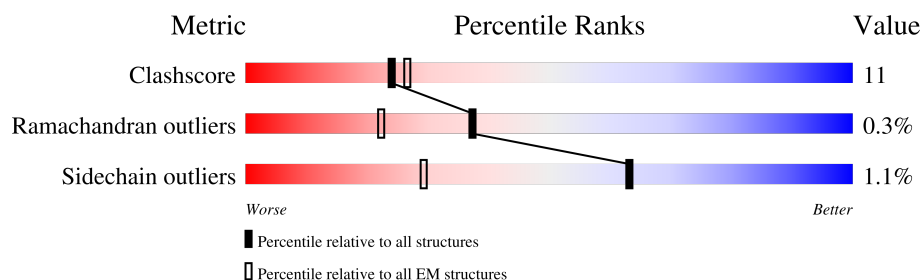
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

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



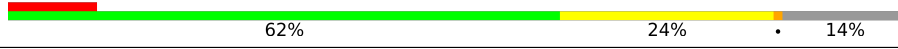
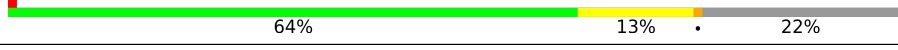
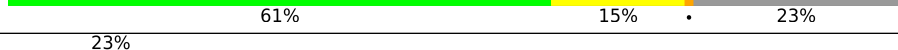
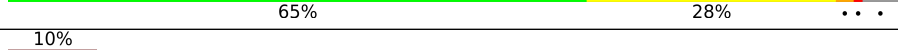
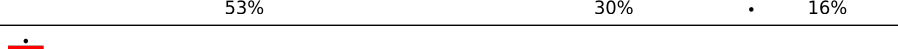
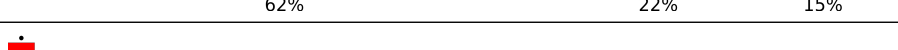
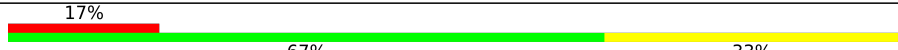
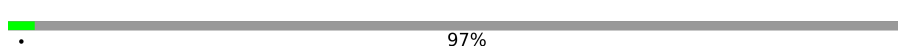
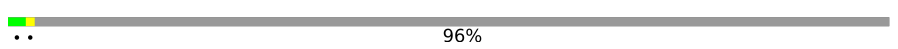
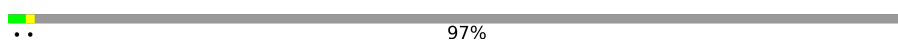
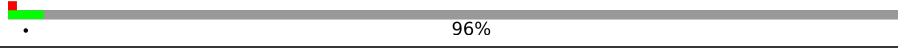
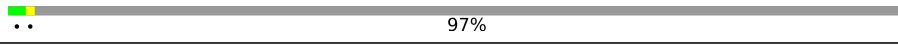
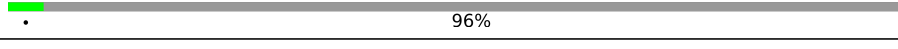
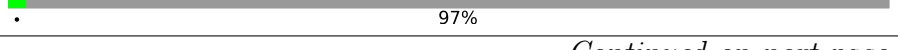
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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

Mol	Chain	Length	Quality of chain
1	K	104	
1	L	104	
1	M	104	
1	N	104	

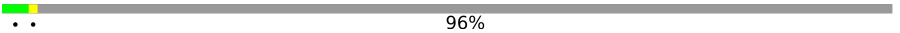
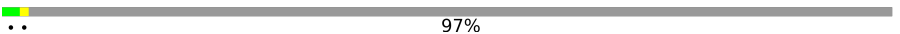
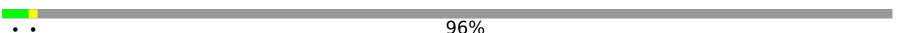
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Mol	Chain	Length	Quality of chain
1	O	104	
1	P	104	
2	Q	138	
2	R	138	
2	S	138	
2	T	138	
2	U	138	
3	E	264	
4	F	245	
4	G	245	
4	H	245	
4	I	245	
4	J	245	
5	A	89	
5	B	89	
5	C	89	
5	D	89	
6	b	560	
6	c	560	
6	d	560	
6	e	560	
6	f	560	
6	g	560	
6	h	560	
6	i	560	

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Mol	Chain	Length	Quality of chain
6	j	560	 96%
6	k	560	 97%
6	l	560	 96%
7	V	134	 81% 13% 18%
7	W	134	 74% 25%
7	X	134	 78% 21%
7	Y	134	 77% 22%
7	Z	134	 71% 28%
7	a	134	 78% 21%
8	m	251	 76% 21%
8	n	251	 75% 24%
8	o	251	 79% 20%
8	p	251	 77% 23%
8	q	251	 77% 22%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 36243 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 hook-basal body complex protein FliE.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	K	40	Total	C	N	O	S	0	0
			300	185	52	57	6		
1	L	72	Total	C	N	O	S	0	0
			543	335	99	103	6		
1	M	74	Total	C	N	O	S	0	0
			557	344	101	106	6		
1	N	74	Total	C	N	O	S	0	0
			557	344	101	106	6		
1	O	74	Total	C	N	O	S	0	0
			557	344	101	106	6		
1	P	73	Total	C	N	O	S	0	0
			550	340	100	104	6		

- Molecule 2 is a protein called Flagellar basal body rod protein FlgB.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Q	119	Total	C	N	O	S	0	0
			922	565	169	183	5		
2	R	108	Total	C	N	O	S	0	0
			848	523	155	165	5		
2	S	108	Total	C	N	O	S	0	0
			848	523	155	165	5		
2	T	110	Total	C	N	O	S	0	0
			863	531	160	167	5		
2	U	106	Total	C	N	O	S	0	0
			832	514	150	163	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	253	Total	C	N	O	S	0	0
			1945	1305	307	318	15		

- Molecule 4 is a protein called Flagellar biosynthetic protein FliP.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	208	Total	C	N	O	S	0	0
			1614	1077	251	274	12		
4	H	208	Total	C	N	O	S	0	0
			1614	1077	251	274	12		
4	G	209	Total	C	N	O	S	0	0
			1626	1086	252	276	12		
4	F	207	Total	C	N	O	S	0	0
			1605	1072	249	272	12		
4	J	209	Total	C	N	O	S	0	0
			1623	1084	251	276	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	89	Total	C	N	O	S	0	0
			670	449	100	114	7		
5	A	89	Total	C	N	O	S	0	0
			670	449	100	114	7		
5	B	89	Total	C	N	O	S	0	0
			670	449	100	114	7		
5	D	89	Total	C	N	O	S	0	0
			670	449	100	114	7		

- Molecule 6 is a protein called Flagellar M-ring protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	c	16	Total	C	N	O	0	0
			103	64	19	20		
6	e	16	Total	C	N	O	0	0
			103	64	19	20		
6	g	16	Total	C	N	O	0	0
			103	64	19	20		
6	i	16	Total	C	N	O	0	0
			103	64	19	20		
6	k	16	Total	C	N	O	0	0
			103	64	19	20		
6	b	13	Total	C	N	O	0	0
			81	50	15	16		
6	h	21	Total	C	N	O	0	0
			140	88	24	28		
6	d	20	Total	C	N	O	0	0
			133	83	23	27		
6	f	21	Total	C	N	O	0	0
			140	88	24	28		

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Mol	Chain	Residues	Atoms				AltConf	Trace
6	j	20	Total	C	N	O	0	0
			133	83	23	27		
6	l	21	Total	C	N	O	0	0
			140	88	24	28		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	a	133	Total	C	N	O	S	0	0
			969	604	167	193	5		
7	Y	133	Total	C	N	O	S	0	0
			969	604	167	193	5		
7	Z	133	Total	C	N	O	S	0	0
			969	604	167	193	5		
7	V	133	Total	C	N	O	S	0	0
			969	604	167	193	5		
7	X	133	Total	C	N	O	S	0	0
			969	604	167	193	5		
7	W	132	Total	C	N	O	S	0	0
			964	601	166	192	5		

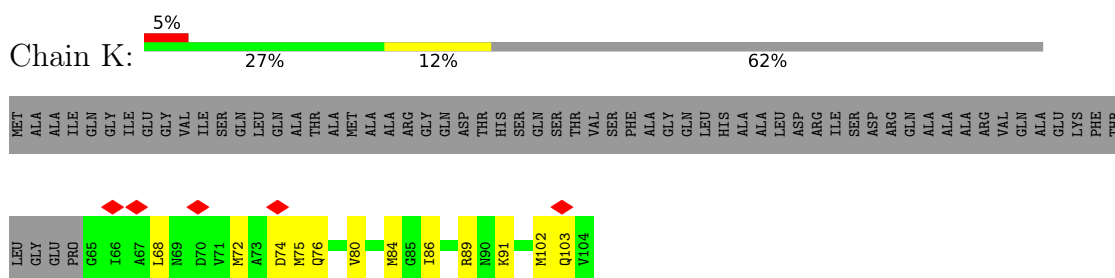
- Molecule 8 is a protein called Flagellar basal-body rod protein FlgF.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	m	248	Total	C	N	O	S	0	0
			1804	1106	324	367	7		
8	n	249	Total	C	N	O	S	0	0
			1812	1111	325	368	8		
8	o	250	Total	C	N	O	S	0	0
			1820	1116	326	369	9		
8	p	250	Total	C	N	O	S	0	0
			1820	1116	326	369	9		
8	q	249	Total	C	N	O	S	0	0
			1812	1111	325	368	8		

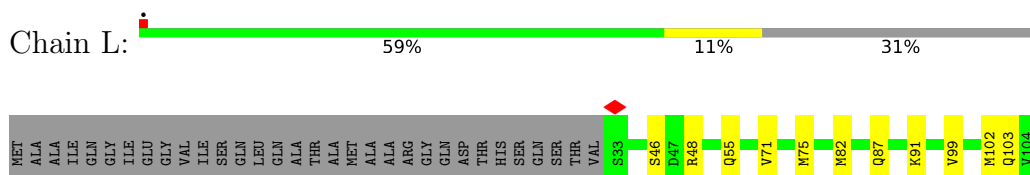
3 Residue-property plots [i](#)

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

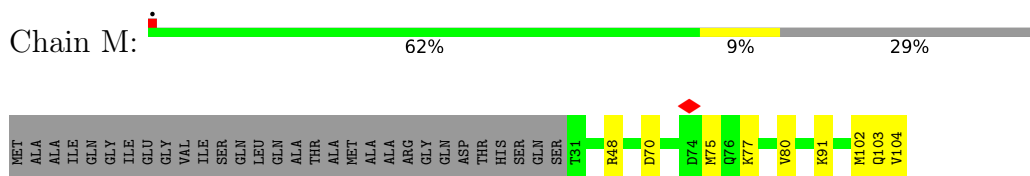
- Molecule 1: Flagellar hook-basal body complex protein FliE



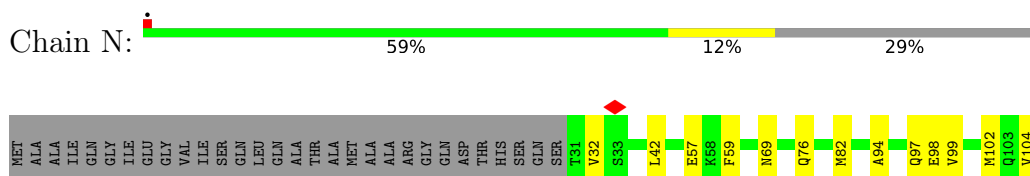
- Molecule 1: Flagellar hook-basal body complex protein FliE



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- Molecule 1: Flagellar hook-basal body complex protein FliE

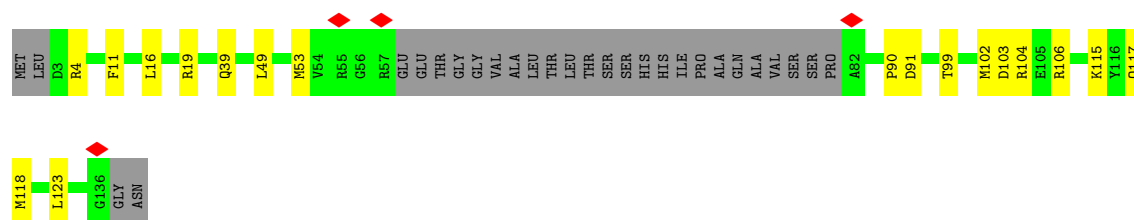


- Molecule 1: Flagellar hook-basal body complex protein FliE



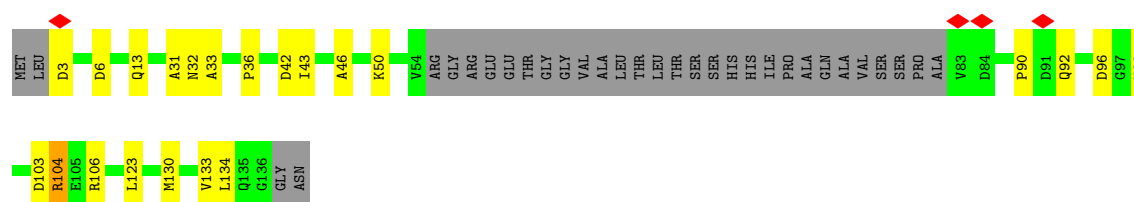
- Molecule 2: Flagellar basal body rod protein FlgB

Chain T: 



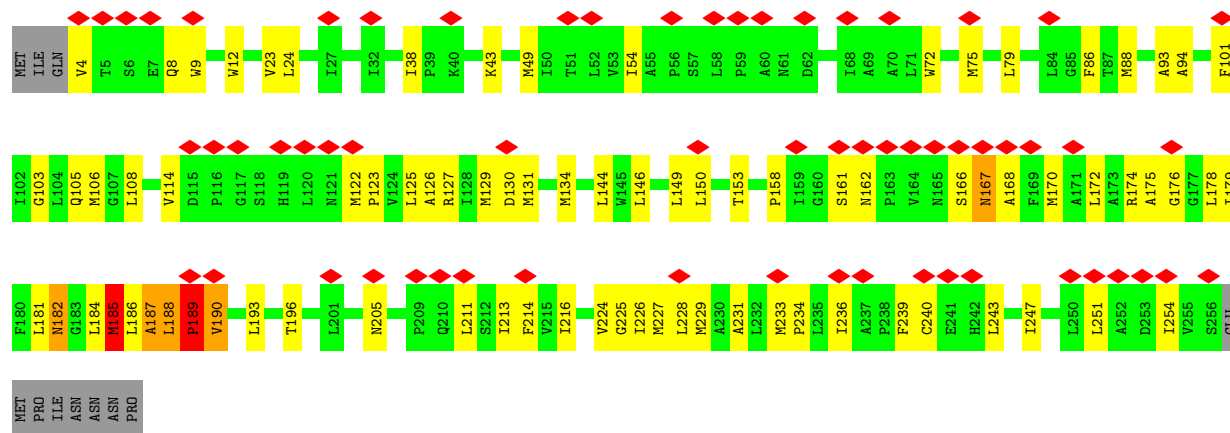
- Molecule 2: Flagellar basal body rod protein FlgB

Chain U: 



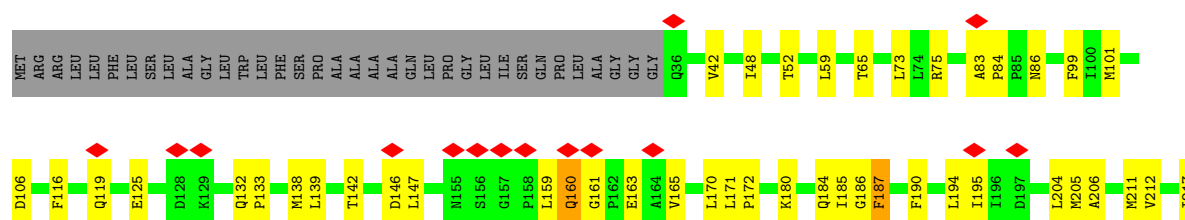
- Molecule 3: Flagellar biosynthetic protein FliR

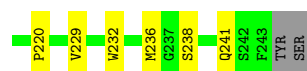
Chain E: 



- Molecule 4: Flagellar biosynthetic protein FliP

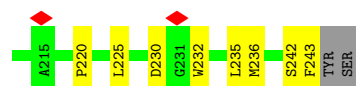
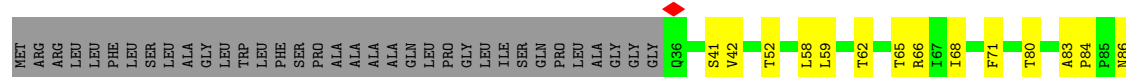
Chain I: 





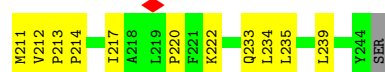
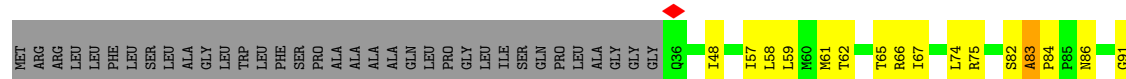
• Molecule 4: Flagellar biosynthetic protein FlpP

Chain H: 64% 20% 15%



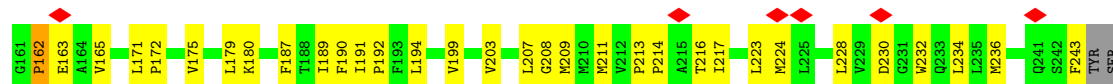
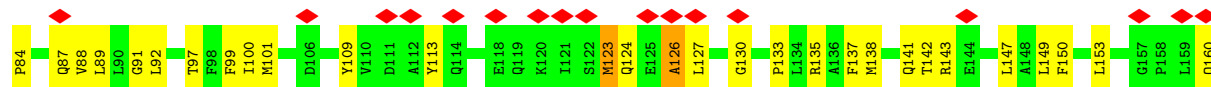
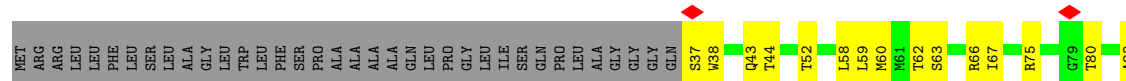
• Molecule 4: Flagellar biosynthetic protein FlpP

Chain G: 62% 22% 15%

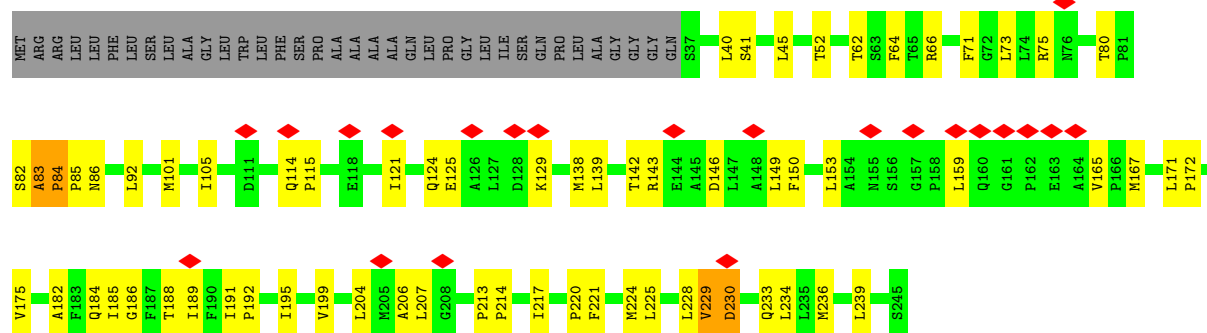


• Molecule 4: Flagellar biosynthetic protein FlpP

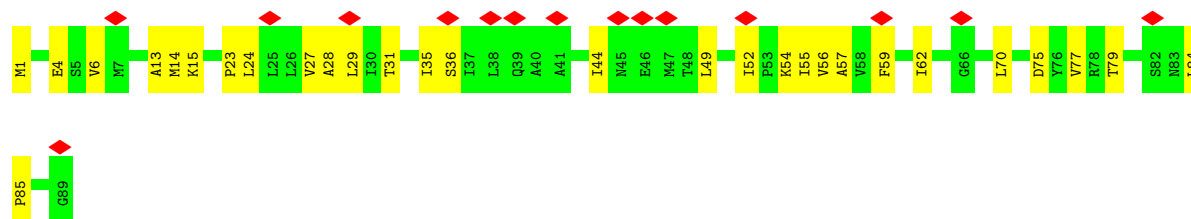
Chain F: 10% 53% 30% 16%



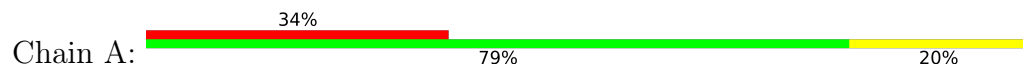
• Molecule 4: Flagellar biosynthetic protein FlpP



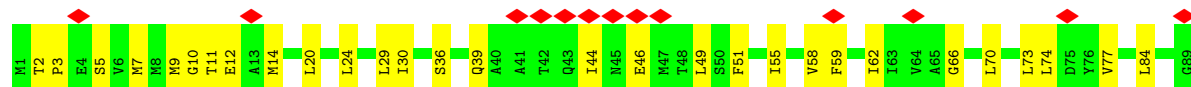
• Molecule 5: Flagellar biosynthetic protein FliQ



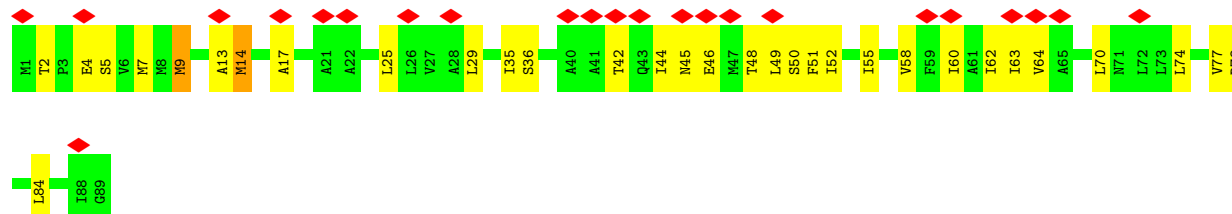
• Molecule 5: Flagellar biosynthetic protein FliQ



• Molecule 5: Flagellar biosynthetic protein FliQ



• Molecule 5: Flagellar biosynthetic protein FliQ



[illegible]

- Molecule 6: Flagellar M-ring protein

Chain d: 96%

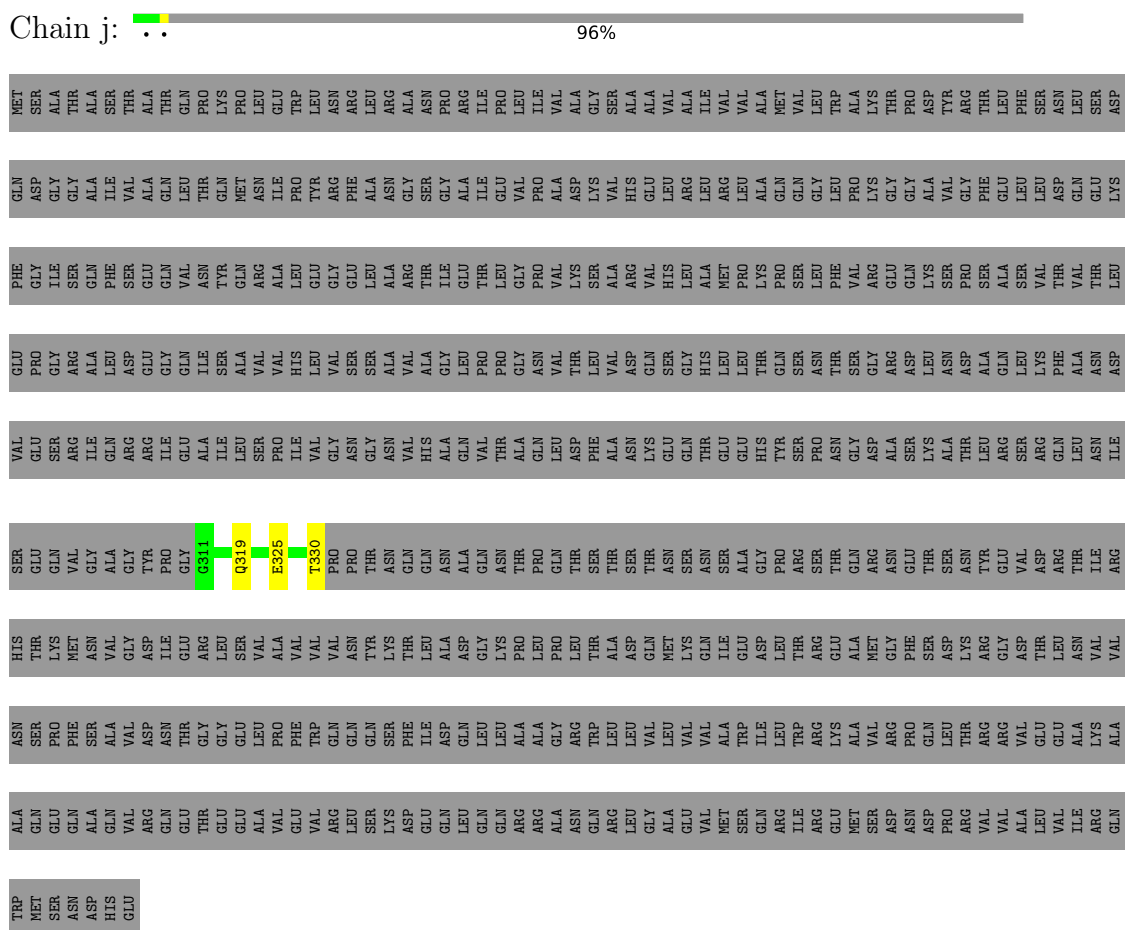
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ILE	VAL	GLU	ASN	THR	THR	ARG	THR	ARG	GLN	VAL	ARG	ARG	SER	ILE	ILE	ILE	ILE	ALA
ARG	GLN	LYS	VAL	VAL	VAL	VAL	VAL	ARG	ALA	GLY	GLN	GLN	PHE	ILE	VAL	VAL	SER	SER
ALA	ALA	VAL	ASN	ASN	HIS	GLY	HIS	ARG	GLY	ARG	ARG	ASP	SER	VAL	VAL	VAL	THR	THR
TRP	ALA	ALA	SER	THR	THR	GLN	THR	THR	TYR	ARG	ARG	GLU	GLN	ALA	ALA	ALA	ALA	THR
MET	GLU	GLU	PRO	LYS	PRO	LYS	PRO	ILE	GLY	ILE	ILE	GLY	GLN	VAL	VAL	GLN	GLN	THR
ASN	ASN	GLN	SER	ASN	ASN	ASN	ASN	ASN	G311	G311	ALA	ILE	ILE	ASN	ASN	THR	PRO	PRO
HIS	HIS	GLN	VAL	VAL	GLY	GLY	VAL	GLY	L316	L316	LEU	ILE	ILE	SER	TYR	GLN	MET	PRO
GLU	GLU	VAL	VAL	ASP	GLY	ASP	VAL	GLY	G317	G317	VAL	VAL	ARG	ASN	GLN	MET	GLU	LEU
	ARG	GLN	ASN	ASN	ILE	ASN	ILE	ILE	N318	N318	PRO	PRO	ALA	ILE	ALA	ILE	GLU	PRO
	GLU	GLU	THR	THR	GLU	THR	GLU	GLU	O319	O319	ILE	HIS	LEU	LEU	LEU	PRO	TYR	ASN
	THR	THR	GLY	GLY	ARG	GLY	LEU	VAL	P320	P320	VAL	VAL	GLY	VAL	GLY	ARG	ASN	ASN
	GLU	GLU	GLY	GLY	SER	GLY	SER	ASN	ASN	ASN	SER	SER	GLY	SER	GLU	PHE	ARG	ARG
	GLU	ALA	LEU	VAL	VAL	VAL	VAL	VAL	N324	N324	GLY	GLY	LEU	SER	LEU	ALA	LEU	ARG
	VAL	GLU	PHE	PHE	VAL	VAL	VAL	VAL	E325	E325	ASN	ALA	ASN	ALA	ALA	ASN	LEU	ARG
	VAL	GLU	GLY	GLY	VAL	VAL	VAL	VAL	A326	A326	VAL	VAL	VAL	VAL	VAL	VAL	GLY	GLY
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	LEU	LEU	GLN	ASN	ASN	ASN	ASN	ASN	PRO	PRO	GLN	LEU	GLY	ASN	ASN	PRO	PRO	VAL
	SER	SER	GLN	TYR	TYR	TYR	TYR	VAL	THR	THR	VAL	PRO	THR	ILE	THR	GLU	GLU	ILE
	LYS	LYS	LYS	LYS	THR	LYS	THR	THR	ASN	ASN	ALA	ALA	GLY	GLY	GLY	GLY	GLY	GLY
	ASP	ASP	PHE	PHE	THR	THR	THR	THR	GLN	GLN	ALA	GLY	GLY	GLY	GLY	GLY	GLY	GLY
	GLU	GLU	ILE	ILE	ILE	ILE	ILE	LEU	GLN	GLN	GLN	SER	HIS	GLY	GLY	GLY	GLY	GLY
	GLN	GLN	ASP	ASP	GLY	GLY	ASP	ALA	ASN	ASN	LEU	THR	VAL	LEU	VAL	VAL	VAL	VAL
	GLN	GLN	GLN	GLN	ARG	GLY	GLY	ASP	GLN	GLN	GLN	GLN	GLY	GLY	GLY	GLY	GLY	GLY
	ARG	ARG	ALA	ALA	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
	ALA	ALA	PRO	PRO	ASP	ASP	ASP	GLN	SER	SER	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN
	ASN	ASN	GLY	GLY	VAL	VAL	VAL	MET	ASN	ASN	THR	THR	THR	THR	THR	THR	THR	THR
	VAL	VAL	VAL	VAL	VAL	VAL	VAL	LYS	SER	SER	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN
	MET	MET	ALA	ALA	ILE	ILE	ILE	ILE	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN
	SER	SER	TRP	TRP	ILE	ILE	ILE	ASP	ALA	ALA	ASP	GLY	ARG	GLY	GLY	GLY	GLY	GLY
	GLN	GLN	GLN	GLN	LEU	LEU	LEU	LEU	PRO	PRO	ALA	ASP	ARG	ARG	GLU	GLY	GLY	GLY
	ARG	ARG	ILE	THR	THR	THR	THR	THR	ASN	ASN	LYS	ALA	ALA	ALA	ALA	ALA	ALA	ALA
	ILE																	

- Molecule 6: Flagellar M-ring protein

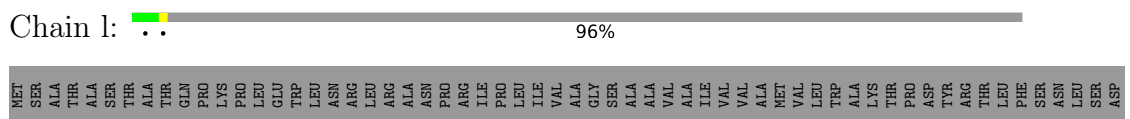
Chain f: . 96%

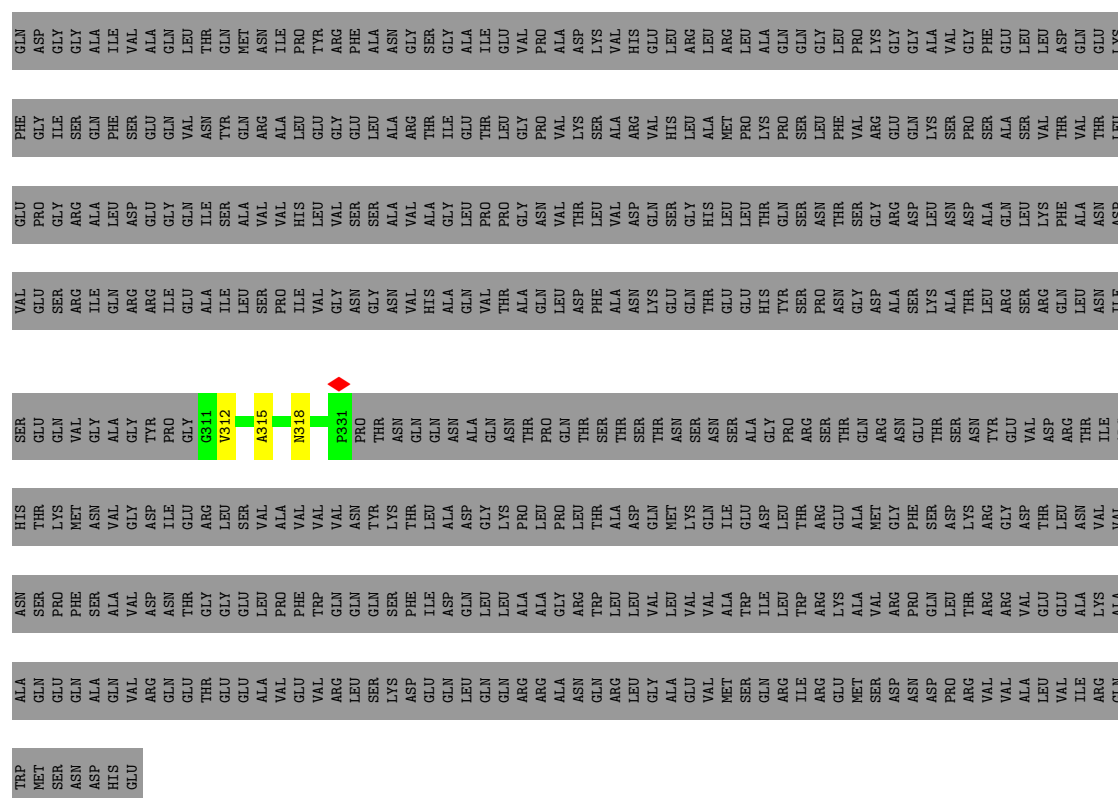
[illegible]

- Molecule 6: Flagellar M-ring protein

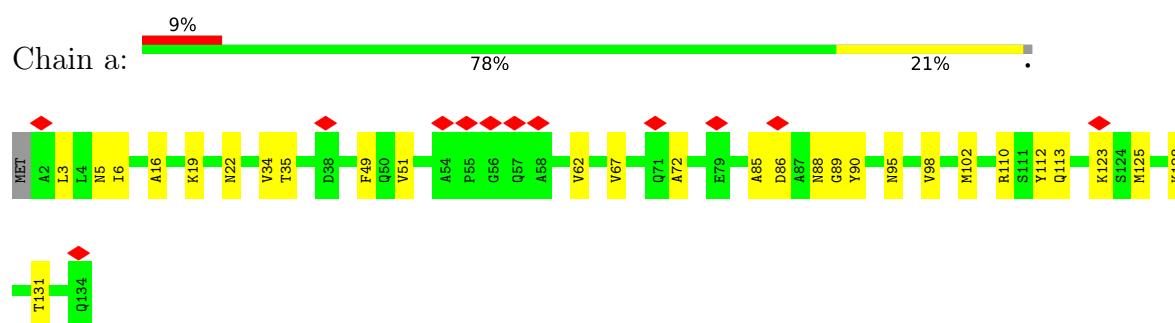


- Molecule 6: Flagellar M-ring protein

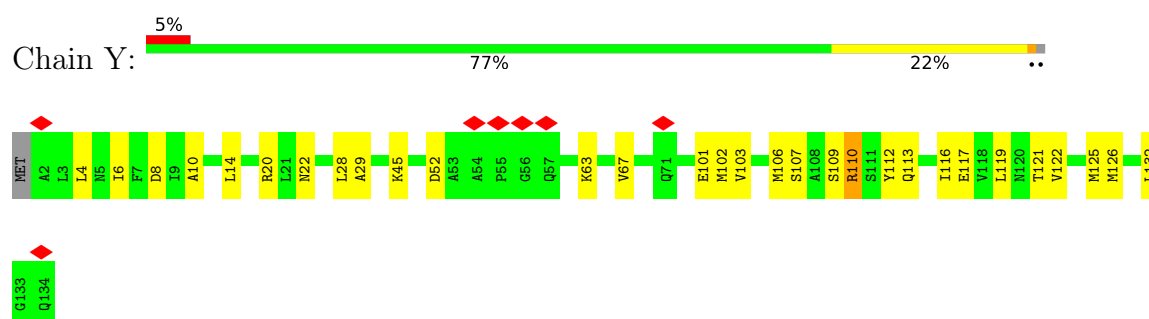




- Molecule 7: Flagellar basal-body rod protein FlgC

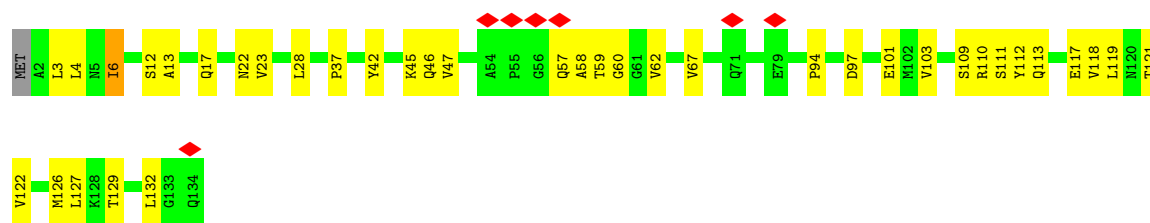


- Molecule 7: Flagellar basal-body rod protein FlgC

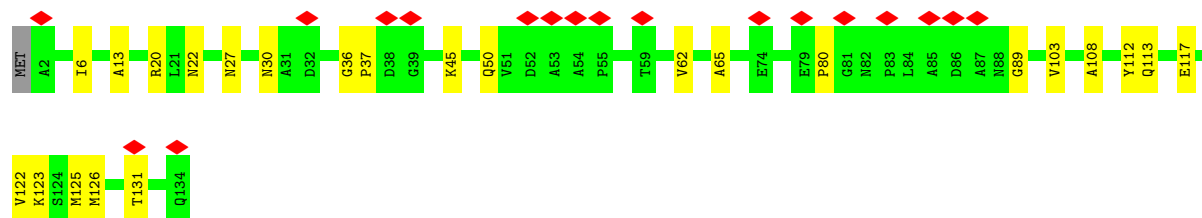
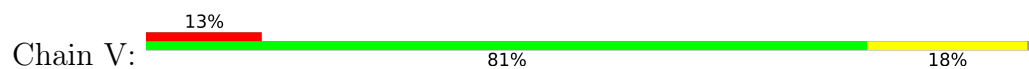


- Molecule 7: Flagellar basal-body rod protein FlgC

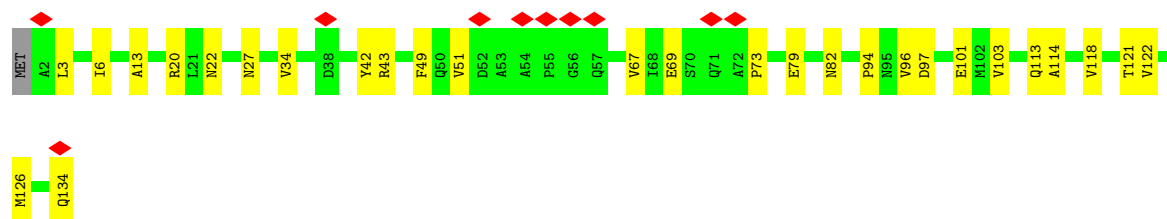
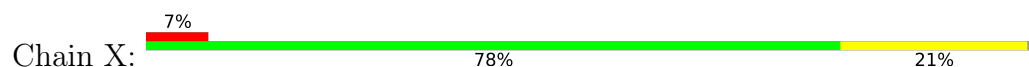




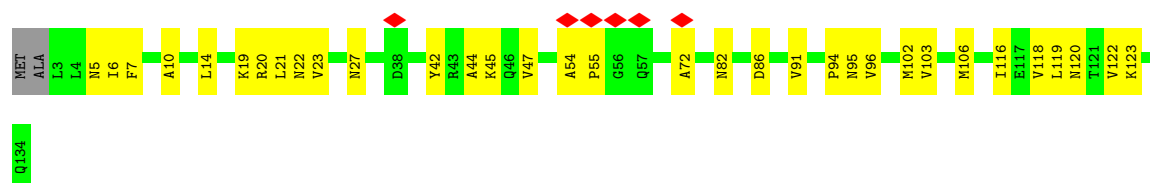
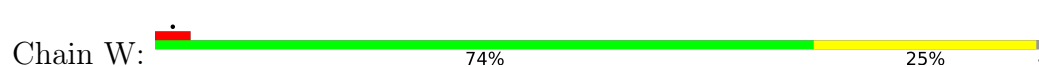
- Molecule 7: Flagellar basal-body rod protein FlgC



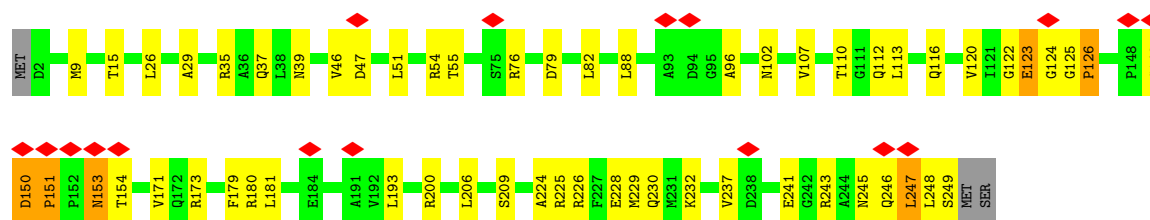
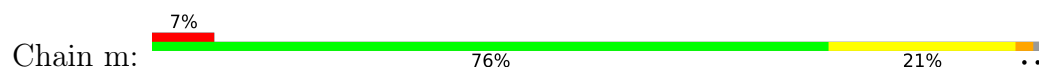
- Molecule 7: Flagellar basal-body rod protein FlgC



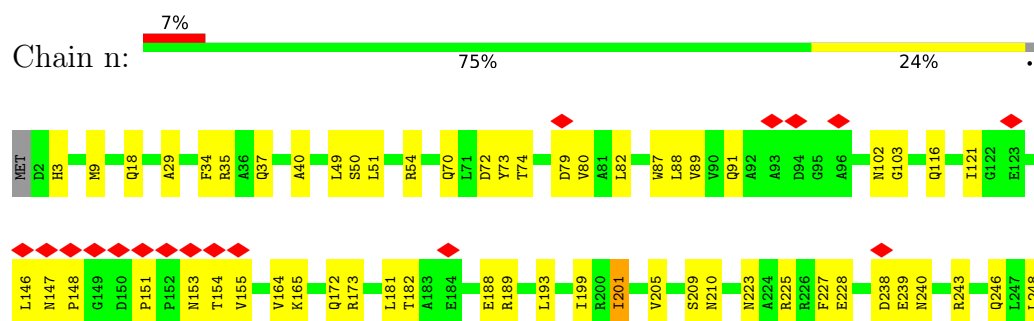
- Molecule 7: Flagellar basal-body rod protein FlgC



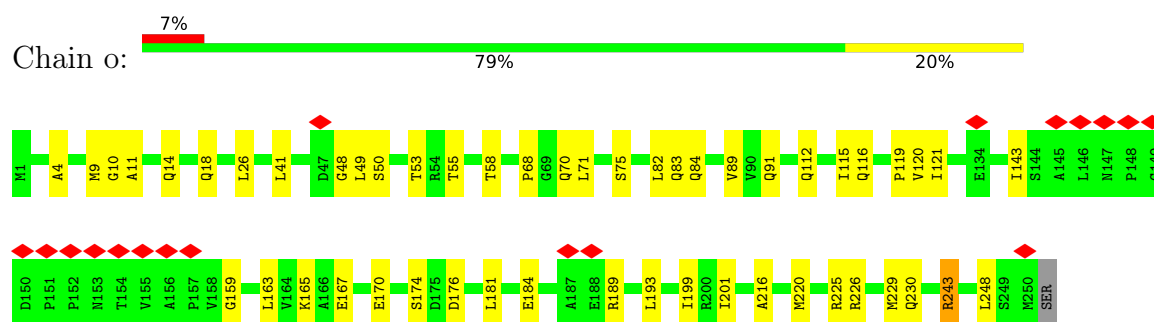
- Molecule 8: Flagellar basal-body rod protein FlgF



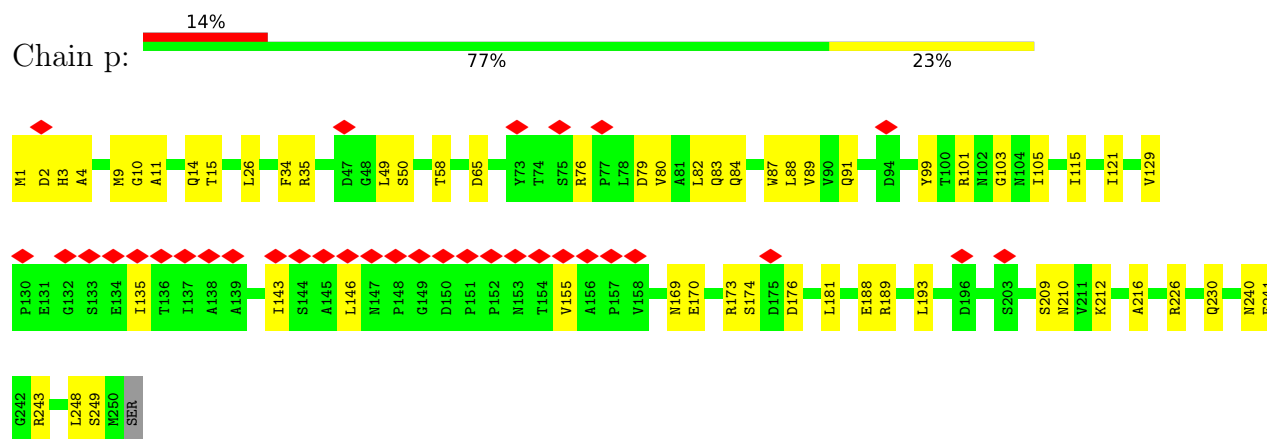
- Molecule 8: Flagellar basal-body rod protein FlgF



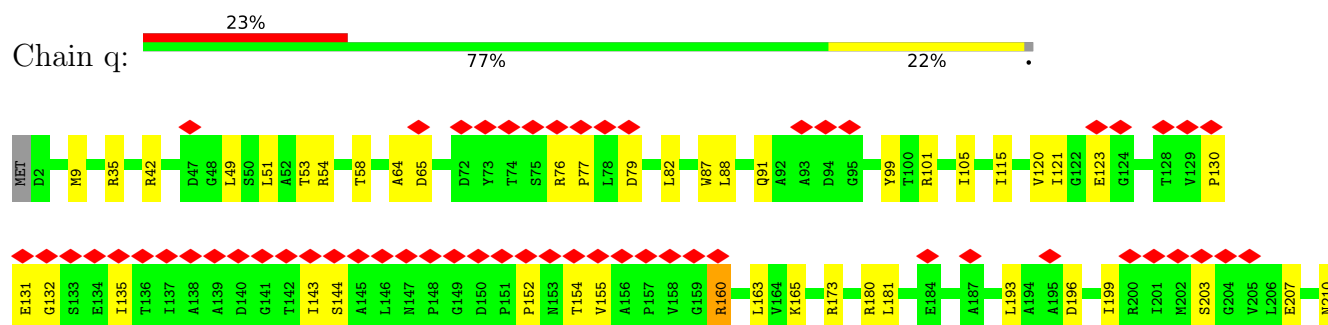
- Molecule 8: Flagellar basal-body rod protein FlgF



- Molecule 8: Flagellar basal-body rod protein FlgF



- Molecule 8: Flagellar basal-body rod protein FlgF





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	24190	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	1.839	Depositor
Minimum map value	-1.172	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	0.082	Depositor
Recommended contour level	0.35	Depositor
Map size ($\text{\AA}$)	614.4, 614.4, 614.4	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.2, 1.2, 1.2	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	K	0.17	0/300	0.43	0/400
1	L	0.11	0/547	0.24	0/733
1	M	0.17	0/561	0.29	0/753
1	N	0.13	0/561	0.27	0/753
1	O	0.13	0/561	0.31	0/753
1	P	0.16	0/554	0.32	0/743
2	Q	0.21	0/930	0.46	0/1251
2	R	0.16	0/855	0.34	0/1150
2	S	0.18	0/855	0.39	0/1150
2	T	0.16	0/870	0.33	0/1169
2	U	0.18	0/839	0.35	0/1129
3	E	0.45	3/1994 (0.2%)	0.61	3/2724 (0.1%)
4	F	0.33	0/1643	0.61	4/2237 (0.2%)
4	G	0.26	0/1665	0.46	2/2267 (0.1%)
4	H	0.22	0/1652	0.42	0/2249
4	I	0.22	0/1652	0.40	0/2249
4	J	0.30	0/1662	0.53	1/2263 (0.0%)
5	A	0.26	0/681	0.49	0/930
5	B	0.16	0/681	0.42	0/930
5	C	0.23	0/681	0.44	0/930
5	D	0.26	0/681	0.55	0/930
6	b	0.70	0/83	0.97	0/114
6	c	0.16	0/107	0.37	0/148
6	d	0.27	0/137	0.52	0/191
6	e	0.20	0/107	0.44	0/148
6	f	1.32	1/145 (0.7%)	1.50	3/203 (1.5%)
6	g	0.22	0/107	0.57	0/148
6	h	0.13	0/145	0.29	0/203
6	i	0.14	0/107	0.41	0/148
6	j	0.25	0/137	0.66	0/191
6	k	0.16	0/107	0.30	0/148
6	l	0.26	0/145	0.44	0/203
7	V	0.15	0/981	0.31	0/1334
7	W	0.13	0/976	0.32	0/1327

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
7	X	0.52	2/981 (0.2%)	0.98	3/1334 (0.2%)
7	Y	0.16	0/981	0.36	0/1334
7	Z	0.15	0/981	0.35	0/1334
7	a	0.19	0/981	0.36	0/1334
8	m	0.36	0/1828	0.56	1/2492 (0.0%)
8	n	0.26	0/1836	0.47	0/2502
8	o	0.22	0/1844	0.44	0/2512
8	p	0.17	0/1844	0.37	0/2512
8	q	0.29	0/1836	0.49	1/2502 (0.0%)
All	All	0.27	6/36821 (0.0%)	0.48	18/50055 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	Q	0	1
2	U	0	1
4	H	0	1
7	Y	0	1
7	a	0	1
8	m	0	2
8	n	0	1
8	o	0	1
8	q	0	1
All	All	0	10

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	f	331	PRO	CG-CD	-13.86	1.03	1.50
7	X	73	PRO	CG-CD	-12.38	1.08	1.50
3	E	185	MET	C-O	9.78	1.35	1.24
7	X	73	PRO	CB-CG	-7.58	1.11	1.49
3	E	182	ASN	C-O	6.64	1.32	1.24
3	E	184	LEU	C-O	-5.47	1.17	1.24

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	X	73	PRO	CB-CG-CD	23.05	179.87	106.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	X	73	PRO	N-CD-CG	-18.79	75.01	103.20
6	f	331	PRO	N-CD-CG	-16.10	79.05	103.20
7	X	73	PRO	CA-CB-CG	-14.25	77.42	104.50
4	F	162	PRO	CA-N-CD	-12.38	94.66	112.00
6	f	331	PRO	CA-CB-CG	-9.27	86.89	104.50
4	J	84	PRO	N-CA-C	-7.75	101.25	110.70
6	f	331	PRO	N-CA-CB	-7.42	94.84	103.00
4	F	162	PRO	N-CD-CG	-6.55	93.37	103.20
4	G	162	PRO	N-CA-CB	-6.19	96.75	103.25
3	E	185	MET	CA-C-N	-6.16	112.23	120.54
3	E	185	MET	C-N-CA	-6.16	112.23	120.54
3	E	189	PRO	CA-N-CD	-5.85	103.81	112.00
4	G	120	LYS	N-CA-C	-5.59	104.28	113.50
4	F	126	ALA	CA-C-N	-5.37	113.03	120.38
4	F	126	ALA	C-N-CA	-5.37	113.03	120.38
8	m	153	ASN	N-CA-C	-5.21	106.70	113.16
8	q	246	GLN	N-CA-C	-5.13	107.69	114.31

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	H	143	ARG	Sidechain
2	Q	106	ARG	Sidechain
2	U	104	ARG	Sidechain
7	Y	110	ARG	Sidechain
7	a	110	ARG	Sidechain
8	m	200	ARG	Sidechain
8	m	243	ARG	Sidechain
8	n	225	ARG	Sidechain
8	o	243	ARG	Sidechain
8	q	160	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	300	0	311	15	0
1	L	543	0	550	10	0
1	M	557	0	566	10	0
1	N	557	0	566	13	0
1	O	557	0	566	18	0
1	P	550	0	559	18	0
2	Q	922	0	914	26	0
2	R	848	0	847	16	0
2	S	848	0	847	25	0
2	T	863	0	863	17	0
2	U	832	0	829	24	0
3	E	1945	0	2063	81	0
4	F	1605	0	1701	63	0
4	G	1626	0	1718	48	0
4	H	1614	0	1709	40	0
4	I	1614	0	1709	43	0
4	J	1623	0	1715	65	0
5	A	670	0	739	15	0
5	B	670	0	739	28	0
5	C	670	0	739	28	0
5	D	670	0	739	40	0
6	b	81	0	78	6	0
6	c	103	0	99	1	0
6	d	133	0	129	5	0
6	e	103	0	99	5	0
6	f	140	0	136	0	0
6	g	103	0	99	4	0
6	h	140	0	136	2	0
6	i	103	0	99	2	0
6	j	133	0	129	2	0
6	k	103	0	99	3	0
6	l	140	0	136	1	0
7	V	969	0	981	22	0
7	W	964	0	976	27	0
7	X	969	0	981	24	0
7	Y	969	0	981	30	0
7	Z	969	0	981	33	0
7	a	969	0	981	26	0
8	m	1804	0	1791	42	0
8	n	1812	0	1800	46	0
8	o	1820	0	1812	40	0
8	p	1820	0	1812	45	0
8	q	1812	0	1800	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	36243	0	37124	792	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 11.

All (792) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:185:MET:O	3:E:189:PRO:HD2	1.64	0.98
3:E:158:PRO:HG2	3:E:162:ASN:HD21	1.35	0.89
8:m:247:LEU:HB3	7:W:120:ASN:HD21	1.37	0.88
2:Q:88:ARG:NH1	2:Q:105:GLU:OE1	2.10	0.84
3:E:182:ASN:HB3	3:E:239:PHE:HZ	1.43	0.83
7:Z:6:ILE:HG21	7:Z:122:VAL:HG11	1.59	0.82
5:C:28:ALA:HB1	5:C:54:LYS:HE3	1.60	0.81
8:m:247:LEU:HB3	7:W:120:ASN:ND2	1.94	0.81
2:U:33:ALA:O	2:U:98:ASN:ND2	2.13	0.81
7:Y:6:ILE:HG21	7:Y:122:VAL:HG21	1.63	0.79
4:J:83:ALA:HB3	4:J:84:PRO:HD3	1.62	0.79
5:B:39:GLN:NE2	5:B:46:GLU:O	2.13	0.79
2:S:35:THR:HG22	7:X:49:PHE:HB3	1.65	0.78
4:F:141:GLN:HE22	4:F:243:PHE:HB3	1.47	0.78
4:J:62:THR:HG23	4:J:101:MET:HE2	1.66	0.77
4:I:205:MET:HE1	5:D:55:ILE:HD11	1.67	0.75
6:e:312:VAL:O	6:e:317:SER:OG	2.05	0.74
4:G:135:ARG:NH2	4:G:165:VAL:O	2.21	0.74
7:X:6:ILE:HG21	7:X:122:VAL:HG21	1.69	0.74
3:E:23:VAL:HA	3:E:150:LEU:HD21	1.69	0.74
8:m:248:LEU:O	8:m:249:SER:C	2.28	0.74
1:K:75:MET:HE1	1:P:88:VAL:HG22	1.69	0.74
2:Q:93:PRO:O	8:m:54:ARG:NH1	2.21	0.74
1:N:94:ALA:O	1:N:98:GLU:HG3	1.89	0.73
7:Z:6:ILE:HD13	7:Z:122:VAL:HG21	1.70	0.73
1:K:89:ARG:NH1	1:P:102:MET:SD	2.62	0.73
5:C:29:LEU:HB2	5:D:52:ILE:HG13	1.71	0.73
7:X:79:GLU:HG2	7:X:82:ASN:HB2	1.69	0.73
2:S:42:ASP:OD2	2:S:43:ILE:N	2.22	0.73
7:X:3:LEU:HB2	7:X:126:MET:HE3	1.70	0.73
7:W:6:ILE:HG21	7:W:122:VAL:HG21	1.72	0.72
2:R:46:ALA:O	2:R:50:LYS:HG3	1.90	0.72
1:P:76:GLN:HE21	7:V:123:LYS:HB2	1.54	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:139:LEU:O	4:J:142:THR:HG22	1.89	0.71
4:I:206:ALA:O	5:D:48:THR:OG1	2.08	0.71
3:E:187:ALA:O	3:E:188:LEU:C	2.34	0.71
5:B:39:GLN:HE21	5:B:49:LEU:HD12	1.56	0.71
4:J:185:ILE:HG23	5:D:84:LEU:HD21	1.72	0.70
4:J:195:ILE:HD11	5:D:13:ALA:HB1	1.73	0.70
3:E:182:ASN:HB3	3:E:239:PHE:CZ	2.26	0.70
8:q:180:ARG:HG3	8:q:180:ARG:HH11	1.56	0.69
2:T:91:ASP:OD2	2:T:104:ARG:NH1	2.25	0.69
1:M:77:LYS:NZ	2:S:13:GLN:OE1	2.26	0.69
3:E:188:LEU:HB3	3:E:189:PRO:CD	2.23	0.69
4:J:143:ARG:HB3	4:J:146:ASP:OD2	1.92	0.69
2:R:36:PRO:HG2	6:e:311:GLY:H	1.56	0.69
4:I:99:PHE:HB3	4:H:153:LEU:HD22	1.74	0.69
4:I:195:ILE:HD11	5:C:13:ALA:HB1	1.75	0.69
8:p:170:GLU:OE2	8:p:189:ARG:NH1	2.25	0.69
8:p:249:SER:OG	7:Y:117:GLU:OE1	2.11	0.69
8:p:1:MET:HG2	8:p:241:GLU:CD	2.18	0.68
8:m:51:LEU:HD12	7:W:19:LYS:HE2	1.75	0.68
4:F:109:TYR:HA	4:F:113:TYR:HB2	1.74	0.68
7:a:123:LYS:HD2	8:q:250:MET:O	1.93	0.68
8:n:102:ASN:ND2	8:n:116:GLN:OE1	2.26	0.68
4:H:207:LEU:HD11	5:B:58:VAL:HG21	1.75	0.67
1:K:102:MET:HE1	4:F:59:LEU:HD21	1.75	0.67
5:C:59:PHE:HE1	5:B:14:MET:HG3	1.58	0.67
8:m:35:ARG:O	8:m:173:ARG:NH2	2.28	0.67
3:E:166:SER:O	3:E:168:ALA:N	2.26	0.67
8:n:35:ARG:HA	8:n:210:ASN:HD21	1.60	0.67
2:U:36:PRO:HB3	2:U:96:ASP:HB2	1.77	0.67
1:M:104:VAL:HG22	4:H:68:ILE:HD11	1.76	0.66
2:Q:4:ARG:NH1	4:F:43:GLN:OE1	2.28	0.66
8:q:238:ASP:OD1	7:Z:110:ARG:NH1	2.28	0.66
3:E:193:LEU:HD22	3:E:228:LEU:HD11	1.77	0.66
4:I:194:LEU:HD11	4:J:220:PRO:HG2	1.77	0.66
6:k:312:VAL:O	6:k:317:SER:OG	2.11	0.66
7:V:6:ILE:HG21	7:V:122:VAL:HG21	1.76	0.66
8:n:151:PRO:HB2	8:n:154:THR:HG23	1.77	0.66
7:Z:37:PRO:HB2	6:j:330:THR:HG23	1.78	0.66
2:U:123:LEU:HD23	7:Z:132:LEU:HD11	1.77	0.66
4:H:66:ARG:NH2	4:H:242:SER:OG	2.30	0.65
8:o:165:LYS:HG3	8:o:199:ILE:HD11	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:135:ARG:NH1	4:H:165:VAL:O	2.30	0.65
4:J:138:MET:HE1	4:J:171:LEU:HD23	1.78	0.65
4:F:58:LEU:O	4:F:62:THR:OG1	2.14	0.64
2:R:36:PRO:HB3	2:R:96:ASP:HB2	1.79	0.64
1:P:55:GLN:NE2	1:P:74:ASP:OD2	2.31	0.64
4:I:204:LEU:HD22	4:I:212:VAL:HG11	1.78	0.64
8:p:76:ARG:NH2	8:p:79:ASP:OD1	2.31	0.64
1:K:89:ARG:NH2	3:E:24:LEU:HB3	2.12	0.64
3:E:158:PRO:CG	3:E:162:ASN:HD21	2.09	0.63
5:C:75:ASP:O	5:C:79:THR:HG23	1.98	0.63
8:p:243:ARG:NH2	7:Z:109:SER:O	2.31	0.63
2:S:22:ARG:NH2	2:S:108:GLN:OE1	2.31	0.63
4:J:207:LEU:HD11	5:D:58:VAL:HG11	1.79	0.63
8:q:165:LYS:HB2	8:q:199:ILE:HD11	1.81	0.63
2:S:4:ARG:NH2	4:H:116:PHE:O	2.30	0.63
6:g:313:PRO:O	7:X:20:ARG:NH1	2.32	0.63
8:q:91:GLN:HB2	8:q:121:ILE:HD11	1.80	0.63
5:C:23:PRO:O	5:C:27:VAL:HG12	1.99	0.62
8:n:37:GLN:OE1	8:n:173:ARG:NH1	2.30	0.62
4:J:229:VAL:O	4:J:230:ASP:C	2.41	0.62
4:G:91:GLY:HA3	4:F:60:MET:HE1	1.81	0.62
8:n:239:GLU:OE1	7:X:113:GLN:NE2	2.31	0.62
5:B:24:LEU:HD22	5:B:58:VAL:HG13	1.81	0.62
4:F:162:PRO:HD2	4:F:163:GLU:N	2.14	0.62
4:G:67:ILE:HD12	4:G:239:LEU:HD13	1.81	0.62
3:E:105:GLN:NE2	4:F:216:THR:O	2.33	0.62
8:o:165:LYS:O	8:o:189:ARG:NH2	2.33	0.62
1:P:89:ARG:HD3	4:J:45:LEU:HG	1.81	0.62
1:M:91:LYS:NZ	4:H:52:THR:OG1	2.28	0.62
1:M:75:MET:HE1	2:R:122:VAL:HG13	1.82	0.61
3:E:185:MET:O	3:E:186:LEU:C	2.42	0.61
5:D:70:LEU:O	5:D:74:LEU:HG	2.00	0.61
3:E:114:VAL:HG12	4:G:213:PRO:HB3	1.81	0.61
5:D:46:GLU:HB2	5:D:49:LEU:HD23	1.82	0.61
4:J:83:ALA:O	4:J:84:PRO:C	2.39	0.61
4:J:191:ILE:HG13	5:D:9:MET:HE2	1.81	0.61
8:n:133:SER:HA	8:n:148:PRO:HD3	1.82	0.61
2:Q:23:GLN:NE2	7:V:125:MET:HE1	2.15	0.61
8:p:146:LEU:HD13	8:p:155:VAL:HG22	1.83	0.61
1:K:103:GLN:NE2	4:G:82:SER:HA	2.15	0.61
5:A:66:GLY:HA2	5:A:69:MET:HE2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:91:LYS:NZ	4:F:52:THR:OG1	2.34	0.61
2:R:51:LYS:NZ	2:R:84:ASP:OD1	2.34	0.61
7:W:27:ASN:OD1	7:W:42:TYR:OH	2.19	0.61
5:A:56:VAL:O	5:A:60:ILE:HG12	2.01	0.61
4:G:66:ARG:NE	4:G:178:GLU:OE1	2.33	0.61
2:R:94:SER:OG	8:n:3:HIS:ND1	2.33	0.60
3:E:106:MET:SD	3:E:225:GLY:HA3	2.40	0.60
8:m:181:LEU:HD21	8:m:193:LEU:HD11	1.81	0.60
4:F:123:MET:HE3	4:F:124:GLN:HG2	1.81	0.60
7:Z:12:SER:OG	7:Z:62:VAL:O	2.20	0.60
4:I:83:ALA:HB3	4:I:84:PRO:HD3	1.84	0.60
4:J:228:LEU:HD13	5:D:74:LEU:HD11	1.83	0.60
5:C:59:PHE:CE1	5:B:14:MET:HG3	2.37	0.60
7:Y:109:SER:O	7:Y:113:GLN:HG3	2.02	0.60
4:J:83:ALA:CB	4:J:84:PRO:HD3	2.30	0.60
4:I:232:TRP:O	4:I:236:MET:HG2	2.02	0.59
5:C:52:ILE:O	5:C:56:VAL:HG22	2.02	0.59
4:J:184:GLN:O	4:J:188:THR:HG23	2.02	0.59
2:Q:94:SER:O	6:d:324:ASN:ND2	2.35	0.59
2:U:32:ASN:ND2	7:Z:60:GLY:O	2.35	0.59
8:n:51:LEU:HD22	7:X:67:VAL:HG23	1.83	0.59
7:V:20:ARG:HD3	7:V:108:ALA:HB2	1.84	0.59
2:S:115:LYS:HE3	7:Y:4:LEU:HD11	1.84	0.59
8:n:91:GLN:HB2	8:n:121:ILE:HD11	1.83	0.59
2:Q:46:ALA:O	2:Q:50:LYS:HG3	2.02	0.59
5:A:84:LEU:HD13	4:G:188:THR:HG21	1.84	0.59
5:B:51:PHE:CZ	5:B:55:ILE:HD11	2.38	0.59
4:F:66:ARG:NH2	4:F:243:PHE:O	2.36	0.59
8:o:170:GLU:OE1	8:o:189:ARG:NH1	2.36	0.59
8:m:122:GLY:O	8:m:124:GLY:N	2.35	0.59
8:p:174:SER:OG	8:p:176:ASP:OD2	2.16	0.59
8:m:96:ALA:HB3	8:m:180:ARG:HH21	1.68	0.58
8:m:122:GLY:O	8:m:123:GLU:C	2.47	0.58
6:i:313:PRO:HG2	7:Y:20:ARG:HD2	1.85	0.58
8:q:226:ARG:O	8:q:230:GLN:HG2	2.03	0.58
2:Q:127:LEU:O	2:Q:131:MET:HG2	2.03	0.58
1:N:104:VAL:O	4:J:82:SER:OG	2.20	0.58
2:S:42:ASP:OD1	2:S:88:ARG:NH2	2.36	0.58
7:a:51:VAL:HG12	7:V:36:GLY:HA2	1.85	0.58
8:m:150:ASP:O	8:m:151:PRO:C	2.47	0.58
4:I:146:ASP:OD1	4:J:233:GLN:NE2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:29:LEU:HD22	5:D:52:ILE:HG21	1.84	0.58
8:o:91:GLN:HB3	8:o:119:PRO:HG2	1.86	0.58
5:A:35:ILE:HD11	5:A:53:PRO:HB2	1.85	0.58
4:H:83:ALA:HB3	4:H:84:PRO:HD3	1.85	0.58
3:E:187:ALA:O	3:E:190:VAL:HG12	2.04	0.58
7:V:50:GLN:HG3	7:V:65:ALA:HB2	1.85	0.58
3:E:167:ASN:HD21	3:E:174:ARG:HH12	1.52	0.57
8:p:26:LEU:HD21	8:p:216:ALA:HB1	1.86	0.57
3:E:176:GLY:HA2	3:E:179:ILE:HD12	1.86	0.57
8:n:165:LYS:HG3	8:n:199:ILE:HD11	1.85	0.57
8:o:226:ARG:O	8:o:230:GLN:HG2	2.04	0.57
4:G:58:LEU:O	4:G:62:THR:OG1	2.22	0.57
2:T:103:ASP:OD1	7:Z:112:TYR:OH	2.14	0.57
8:o:55:THR:OG1	7:Y:45:LYS:NZ	2.36	0.57
1:M:102:MET:HE1	4:H:59:LEU:HD11	1.87	0.57
1:P:76:GLN:HG3	7:V:123:LYS:HD2	1.87	0.57
2:U:42:ASP:OD1	2:U:43:ILE:N	2.38	0.57
3:E:170:MET:O	3:E:174:ARG:N	2.26	0.57
8:n:243:ARG:HD2	7:X:113:GLN:HG2	1.86	0.57
7:W:94:PRO:HB2	7:W:96:VAL:HG23	1.86	0.57
3:E:149:LEU:O	3:E:153:THR:HG23	2.05	0.56
8:p:9:MET:HB2	7:Y:103:VAL:HG21	1.85	0.56
8:o:181:LEU:HD11	8:o:193:LEU:HG	1.86	0.56
2:R:114:LEU:HD21	7:X:126:MET:SD	2.45	0.56
5:C:4:GLU:C	5:C:6:VAL:H	2.13	0.56
8:m:226:ARG:O	8:m:230:GLN:HG2	2.05	0.56
5:B:9:MET:HA	5:B:12:GLU:OE1	2.05	0.56
8:q:248:LEU:HD13	7:Z:118:VAL:HG23	1.88	0.56
2:Q:23:GLN:HE22	7:V:125:MET:HE1	1.69	0.56
8:o:9:MET:HB2	7:X:103:VAL:HG21	1.86	0.56
3:E:93:ALA:HB2	4:F:88:VAL:HG21	1.87	0.56
4:J:206:ALA:HB2	5:D:25:LEU:HD23	1.86	0.56
3:E:205:ASN:HD21	4:F:211:MET:HB2	1.71	0.56
4:H:66:ARG:HG3	4:H:182:ALA:HB2	1.87	0.56
8:p:2:ASP:OD2	8:p:4:ALA:N	2.31	0.56
7:W:72:ALA:O	7:W:95:ASN:ND2	2.38	0.56
1:L:87:GLN:O	1:L:91:LYS:HG2	2.06	0.55
2:Q:42:ASP:HB3	6:d:316:LEU:HD21	1.88	0.55
3:E:166:SER:C	3:E:168:ALA:N	2.64	0.55
4:H:58:LEU:O	4:H:62:THR:OG1	2.23	0.55
1:P:89:ARG:NH2	1:P:90:ASN:OD1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:q:196:ASP:HB3	8:q:199:ILE:HD12	1.88	0.55
4:J:75:ARG:NH1	4:J:86:ASN:OD1	2.36	0.55
1:L:46:SER:OG	4:F:38:TRP:HB2	2.06	0.55
8:o:75:SER:O	8:o:75:SER:OG	2.23	0.55
3:E:233:MET:O	3:E:236:ILE:HG12	2.06	0.55
4:J:230:ASP:OD2	4:J:230:ASP:N	2.40	0.55
7:Z:17:GLN:NE2	7:Z:111:SER:OG	2.39	0.55
4:J:80:THR:HB	4:J:83:ALA:HB2	1.88	0.55
1:O:59:PHE:CD2	2:T:118:MET:HE2	2.42	0.55
8:n:54:ARG:HH21	7:X:22:ASN:HD21	1.55	0.55
7:Z:3:LEU:HB3	7:Z:126:MET:HE3	1.88	0.55
8:o:14:GLN:HG3	8:o:58:THR:HA	1.89	0.55
8:p:243:ARG:NE	7:Z:113:GLN:HB2	2.21	0.55
8:q:248:LEU:HB2	7:Z:117:GLU:HB3	1.89	0.55
1:K:72:MET:O	1:K:76:GLN:HG2	2.06	0.54
8:q:76:ARG:NH2	8:q:105:ILE:O	2.35	0.54
3:E:166:SER:O	3:E:167:ASN:C	2.49	0.54
4:F:83:ALA:HB3	4:F:84:PRO:HD3	1.89	0.54
7:V:113:GLN:O	7:V:117:GLU:HG2	2.07	0.54
2:R:90:PRO:HB3	2:R:99:THR:HB	1.88	0.54
1:O:77:LYS:HE3	2:U:13:GLN:HE22	1.73	0.54
2:S:36:PRO:HB3	2:S:96:ASP:HB2	1.89	0.54
8:o:248:LEU:O	7:X:121:THR:OG1	2.19	0.54
4:F:37:SER:HA	4:F:123:MET:HE2	1.90	0.54
3:E:38:ILE:HB	3:E:43:LYS:HE2	1.90	0.54
5:C:54:LYS:HZ3	5:D:48:THR:HG21	1.72	0.54
1:O:77:LYS:HE3	2:U:13:GLN:NE2	2.23	0.54
3:E:236:ILE:O	3:E:240:CYS:N	2.36	0.54
5:C:44:ILE:HG23	5:B:36:SER:HB3	1.89	0.54
4:I:205:MET:HE3	5:D:51:PHE:HB3	1.90	0.54
7:a:85:ALA:HB1	7:a:89:GLY:HA2	1.89	0.54
8:m:151:PRO:HB2	8:m:154:THR:HG23	1.90	0.54
8:n:243:ARG:O	8:n:246:GLN:HG2	2.08	0.54
8:o:216:ALA:O	8:o:220:MET:HG3	2.08	0.54
8:p:243:ARG:HE	7:Z:113:GLN:HB2	1.72	0.54
8:o:115:ILE:HG22	8:o:116:GLN:HG3	1.90	0.54
8:p:87:TRP:HB3	8:p:99:TYR:HB3	1.90	0.54
4:F:126:ALA:O	4:F:127:LEU:C	2.48	0.54
1:N:76:GLN:NE2	7:Y:132:LEU:O	2.41	0.53
8:q:87:TRP:HB3	8:q:99:TYR:HB3	1.90	0.53
2:U:103:ASP:OD1	7:a:112:TYR:OH	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:188:LEU:O	3:E:190:VAL:N	2.39	0.53
1:N:102:MET:HE1	4:I:59:LEU:HD11	1.90	0.53
3:E:186:LEU:HD21	3:E:236:ILE:HG22	1.90	0.53
4:I:139:LEU:HG	4:I:170:LEU:HD21	1.90	0.53
4:I:163:GLU:OE2	4:I:163:GLU:N	2.39	0.53
8:o:18:GLN:NE2	8:o:41:LEU:HG	2.22	0.53
4:G:211:MET:HE3	4:F:211:MET:SD	2.49	0.53
5:D:42:THR:HG22	5:D:44:ILE:HG12	1.91	0.53
8:p:76:ARG:HB3	8:p:79:ASP:OD2	2.09	0.53
2:U:106:ARG:HG2	8:q:248:LEU:HD21	1.91	0.53
8:o:89:VAL:HG12	8:o:121:ILE:HB	1.91	0.53
8:q:250:MET:HE2	7:Z:121:THR:HA	1.90	0.53
4:F:75:ARG:HD2	4:F:84:PRO:HD2	1.89	0.53
4:F:207:LEU:HD23	4:F:209:MET:HE1	1.91	0.53
4:J:188:THR:HA	5:D:9:MET:HE1	1.90	0.53
3:E:54:ILE:HD11	4:J:153:LEU:HB3	1.91	0.53
4:H:225:LEU:HD11	5:B:77:VAL:HG21	1.91	0.53
2:Q:50:LYS:O	2:Q:54:VAL:HG22	2.09	0.53
3:E:101:PHE:CE2	4:F:223:LEU:HD11	2.43	0.53
8:m:76:ARG:HB3	8:m:79:ASP:OD1	2.09	0.53
8:m:107:VAL:HG12	8:m:113:LEU:HD23	1.91	0.53
8:m:151:PRO:C	8:m:153:ASN:H	2.17	0.53
8:q:180:ARG:HG3	8:q:180:ARG:NH1	2.21	0.53
7:W:23:VAL:HG21	7:W:47:VAL:HG13	1.91	0.53
2:T:90:PRO:HG2	8:p:49:LEU:HB2	1.91	0.53
5:B:62:ILE:O	5:B:66:GLY:N	2.39	0.53
7:Z:57:GLN:O	7:Z:59:THR:N	2.40	0.53
3:E:127:ARG:O	3:E:131:MET:HE3	2.08	0.53
8:n:137:ILE:HG12	8:n:143:ILE:HG12	1.91	0.53
8:q:76:ARG:NH1	8:q:79:ASP:OD1	2.40	0.53
4:I:180:LYS:O	4:I:184:GLN:HG3	2.09	0.52
4:I:217:ILE:HA	4:H:194:LEU:HD11	1.91	0.52
1:P:76:GLN:NE2	7:V:123:LYS:HB2	2.24	0.52
2:T:4:ARG:NH2	4:I:116:PHE:O	2.42	0.52
3:E:188:LEU:HB3	3:E:189:PRO:HD2	1.91	0.52
7:a:113:GLN:NE2	8:q:239:GLU:OE2	2.39	0.52
7:Y:10:ALA:HB3	7:Y:119:LEU:HD13	1.89	0.52
4:H:232:TRP:O	4:H:236:MET:HG3	2.10	0.52
7:V:80:PRO:HB3	7:V:89:GLY:HA3	1.90	0.52
1:O:91:LYS:NZ	4:J:52:THR:OG1	2.32	0.52
2:U:133:VAL:HG21	4:J:41:SER:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:p:35:ARG:HH11	8:p:101:ARG:HG3	1.74	0.52
1:O:73:ALA:HB1	2:U:13:GLN:HE21	1.74	0.52
8:n:40:ALA:HB1	7:X:34:VAL:HG21	1.92	0.52
8:o:48:GLY:HA3	6:h:324:ASN:HD21	1.75	0.52
4:H:209:MET:HA	4:G:205:MET:HE3	1.91	0.52
7:V:131:THR:HG22	7:V:131:THR:O	2.09	0.52
8:m:79:ASP:HB3	8:m:206:LEU:HD13	1.92	0.52
4:G:233:GLN:HG3	4:F:149:LEU:HD22	1.92	0.52
1:O:48:ARG:NH1	2:U:3:ASP:OD2	2.43	0.52
8:n:89:VAL:HG12	8:n:121:ILE:HB	1.91	0.52
8:q:115:ILE:HD12	8:q:120:VAL:HG22	1.91	0.52
4:F:199:VAL:O	4:F:203:VAL:HG23	2.10	0.52
5:D:35:ILE:HG21	5:D:50:SER:HA	1.92	0.52
2:S:46:ALA:O	2:S:50:LYS:HG3	2.09	0.52
8:m:102:ASN:HD22	8:m:116:GLN:HE21	1.57	0.52
7:Y:20:ARG:NH2	7:Y:107:SER:HB2	2.24	0.52
5:B:3:PRO:O	5:B:7:MET:HG2	2.09	0.52
4:J:229:VAL:HG21	5:D:77:VAL:HG11	1.90	0.52
4:H:80:THR:O	4:H:80:THR:OG1	2.26	0.52
7:a:67:VAL:HG11	8:q:53:THR:HG22	1.91	0.52
8:q:42:ARG:HG3	8:q:58:THR:HG23	1.91	0.52
6:j:325:GLU:N	6:j:325:GLU:OE1	2.43	0.52
4:I:73:LEU:HD13	4:I:186:GLY:HA3	1.92	0.51
8:p:135:ILE:HG23	8:p:143:ILE:HG23	1.92	0.51
5:A:65:ALA:O	5:A:69:MET:HG3	2.09	0.51
4:G:83:ALA:HB1	4:G:84:PRO:HD2	1.92	0.51
3:E:227:MET:SD	3:E:228:LEU:N	2.83	0.51
7:Z:23:VAL:HG21	7:Z:47:VAL:HG13	1.91	0.51
4:G:74:LEU:HD22	4:G:235:LEU:HD22	1.91	0.51
5:C:4:GLU:C	5:C:6:VAL:N	2.67	0.51
4:F:67:ILE:HD12	4:F:67:ILE:H	1.75	0.51
1:N:42:LEU:HD22	4:H:42:VAL:HG13	1.93	0.51
7:a:72:ALA:HB3	7:a:95:ASN:HD22	1.74	0.51
8:q:248:LEU:O	7:Z:121:THR:OG1	2.19	0.51
7:Z:28:LEU:HD21	7:Z:101:GLU:HB2	1.91	0.51
4:J:234:LEU:HD11	5:D:78:ARG:HG3	1.91	0.51
4:I:75:ARG:NH1	4:I:86:ASN:OD1	2.36	0.51
7:W:7:PHE:HZ	7:W:123:LYS:HB2	1.76	0.51
1:O:53:ARG:O	1:O:57:GLU:HG2	2.11	0.51
2:Q:29:ASN:ND2	2:Q:41:ARG:O	2.36	0.51
3:E:130:ASP:O	3:E:134:MET:HG2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:p:240:ASN:ND2	7:Z:109:SER:OG	2.42	0.51
5:B:59:PHE:HZ	4:G:198:LEU:HD21	1.75	0.51
4:J:195:ILE:HG23	5:D:17:ALA:HB2	1.92	0.51
3:E:88:MET:HG2	3:E:146:LEU:HD11	1.93	0.51
3:E:86:PHE:CZ	4:F:91:GLY:HA3	2.45	0.51
4:G:193:PHE:HB3	4:G:222:LYS:HD3	1.92	0.51
5:D:2:THR:HG23	5:D:5:SER:H	1.76	0.51
2:U:92:GLN:HE21	7:a:19:LYS:HG2	1.76	0.51
8:m:55:THR:OG1	7:W:45:LYS:NZ	2.44	0.51
5:B:10:GLY:O	5:B:14:MET:HE2	2.11	0.51
4:F:135:ARG:NH2	4:F:165:VAL:O	2.44	0.51
1:O:84:MET:O	1:O:88:VAL:HG23	2.11	0.50
3:E:205:ASN:ND2	4:F:211:MET:HB2	2.25	0.50
5:D:58:VAL:O	5:D:62:ILE:HD12	2.11	0.50
2:T:4:ARG:HE	4:I:119:GLN:HG3	1.75	0.50
4:I:161:GLY:C	4:I:163:GLU:N	2.69	0.50
7:a:19:LYS:HD3	8:q:51:LEU:HD12	1.93	0.50
4:H:65:THR:O	4:H:68:ILE:HG22	2.12	0.50
8:n:248:LEU:HD13	7:W:118:VAL:HG23	1.93	0.50
8:p:129:VAL:HG11	8:p:135:ILE:HD11	1.92	0.50
5:D:2:THR:O	5:D:5:SER:OG	2.24	0.50
4:I:204:LEU:HD11	4:I:217:ILE:HD12	1.93	0.50
8:p:1:MET:HE2	7:Y:107:SER:HA	1.94	0.50
7:W:54:ALA:HB3	7:W:55:PRO:HD3	1.93	0.50
3:E:106:MET:HE1	3:E:226:ILE:HG13	1.93	0.50
8:q:35:ARG:O	8:q:173:ARG:NH2	2.44	0.50
2:T:123:LEU:HD23	7:Y:132:LEU:HD11	1.92	0.50
8:n:172:GLN:HB2	8:n:182:THR:HG22	1.93	0.50
4:F:143:ARG:HH21	4:F:180:LYS:HB3	1.77	0.50
1:K:86:ILE:HG12	1:P:102:MET:HE2	1.93	0.50
1:L:103:GLN:HA	4:G:86:ASN:HD21	1.77	0.50
3:E:229:MET:O	3:E:233:MET:HG2	2.12	0.50
7:Y:10:ALA:O	7:Y:14:LEU:HG	2.12	0.50
4:H:230:ASP:OD1	4:G:180:LYS:NZ	2.27	0.50
4:G:75:ARG:NH2	4:G:84:PRO:O	2.44	0.50
1:N:57:GLU:HG2	2:S:11:PHE:CE2	2.47	0.50
8:n:147:ASN:O	8:n:148:PRO:C	2.54	0.50
4:F:224:MET:O	4:F:228:LEU:HB2	2.11	0.50
4:J:167:MET:HG3	4:J:171:LEU:HG	1.93	0.50
3:E:185:MET:HE3	3:E:188:LEU:HD22	1.94	0.50
8:o:174:SER:OG	8:o:176:ASP:OD1	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:q:101:ARG:NH1	8:q:207:GLU:OE1	2.45	0.50
7:Y:106:MET:O	7:Y:110:ARG:HG2	2.12	0.49
1:P:55:GLN:HG2	1:P:71:VAL:HG22	1.94	0.49
2:U:46:ALA:O	2:U:50:LYS:HG2	2.11	0.49
4:I:161:GLY:C	4:I:163:GLU:H	2.20	0.49
8:q:154:THR:O	8:q:155:VAL:C	2.55	0.49
8:o:229:MET:HG2	7:Y:102:MET:HE3	1.94	0.49
8:o:243:ARG:HD2	7:Y:113:GLN:CD	2.38	0.49
2:U:130:MET:HE1	4:J:40:LEU:HD23	1.94	0.49
4:I:59:LEU:O	4:I:65:THR:OG1	2.28	0.49
8:n:188:GLU:HG3	8:n:189:ARG:HG2	1.94	0.49
4:F:232:TRP:NE1	4:F:236:MET:HE3	2.27	0.49
2:Q:106:ARG:NH1	8:m:241:GLU:OE2	2.45	0.49
8:m:54:ARG:HE	7:W:22:ASN:ND2	2.10	0.49
8:o:48:GLY:HA3	6:h:324:ASN:ND2	2.28	0.49
8:p:91:GLN:HB2	8:p:121:ILE:HD11	1.94	0.49
4:G:66:ARG:NH2	4:G:178:GLU:OE1	2.45	0.49
4:F:101:MET:HE1	4:F:137:PHE:CZ	2.47	0.49
1:P:34:PHE:HB2	3:E:12:TRP:CZ3	2.48	0.49
4:J:229:VAL:HG21	5:D:77:VAL:CG1	2.42	0.49
1:L:82:MET:HE3	2:Q:133:VAL:CG2	2.43	0.49
2:Q:17:ASN:HD22	2:Q:57:ARG:NH1	2.10	0.49
2:T:102:MET:HB3	2:T:106:ARG:HH21	1.77	0.49
8:p:188:GLU:HG3	8:p:189:ARG:HG2	1.95	0.49
5:C:36:SER:OG	5:D:44:ILE:HG23	2.12	0.49
4:G:84:PRO:HG3	4:F:179:LEU:HD22	1.95	0.49
2:T:49:LEU:O	2:T:53:MET:HG2	2.13	0.48
4:F:92:LEU:HD13	4:F:232:TRP:HZ2	1.77	0.48
7:a:51:VAL:HG13	7:V:37:PRO:HD3	1.95	0.48
4:F:130:GLY:O	4:F:133:PRO:HD2	2.13	0.48
7:X:97:ASP:O	7:X:101:GLU:HG2	2.13	0.48
1:O:42:LEU:HD22	4:I:42:VAL:HG13	1.95	0.48
2:S:32:ASN:ND2	7:X:51:VAL:HG12	2.28	0.48
5:A:48:THR:HG21	4:F:208:GLY:HA2	1.95	0.48
4:J:73:LEU:HD13	4:J:186:GLY:HA3	1.94	0.48
7:X:94:PRO:HB2	7:X:96:VAL:HG23	1.94	0.48
1:N:99:VAL:O	1:N:102:MET:HG2	2.13	0.48
3:E:211:LEU:O	5:D:36:SER:OG	2.24	0.48
8:m:232:LYS:HG2	7:W:102:MET:CE	2.43	0.48
8:m:237:VAL:HG22	7:W:21:LEU:HD21	1.94	0.48
8:p:11:ALA:HB3	8:p:230:GLN:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:114:VAL:HG21	4:I:211:MET:HE1	1.96	0.48
3:E:178:LEU:HD13	3:E:181:LEU:HD23	1.95	0.48
8:n:34:PHE:HB3	8:n:209:SER:HB3	1.96	0.48
8:q:181:LEU:HD21	8:q:193:LEU:HD11	1.96	0.48
1:L:55:GLN:HG2	1:L:71:VAL:HG22	1.95	0.48
2:T:11:PHE:CD1	2:T:53:MET:HE2	2.48	0.48
3:E:101:PHE:CE2	4:F:80:THR:HG21	2.48	0.48
4:I:159:LEU:O	4:I:160:GLN:HB2	2.14	0.48
8:q:123:GLU:OE2	8:q:160:ARG:HD3	2.14	0.48
4:J:71:PHE:CZ	4:J:236:MET:HE1	2.49	0.48
4:J:150:PHE:CE1	4:J:172:PRO:HB2	2.48	0.48
7:X:27:ASN:OD1	7:X:42:TYR:OH	2.27	0.48
3:E:158:PRO:HG2	3:E:162:ASN:ND2	2.16	0.48
5:C:14:MET:HE3	5:D:63:ILE:HD11	1.96	0.48
7:V:27:ASN:ND2	7:V:45:LYS:O	2.33	0.48
3:E:86:PHE:CZ	4:F:88:VAL:HA	2.48	0.48
4:F:99:PHE:C	4:F:99:PHE:CD2	2.91	0.48
5:D:60:ILE:HA	5:D:63:ILE:HG12	1.96	0.48
3:E:94:ALA:HB2	3:E:179:ILE:HA	1.96	0.47
5:C:54:LYS:NZ	5:D:48:THR:HG21	2.29	0.47
8:n:18:GLN:NE2	8:n:223:ASN:OD1	2.46	0.47
8:p:35:ARG:HA	8:p:210:ASN:HD21	1.78	0.47
5:B:11:THR:HA	5:B:14:MET:HE3	1.96	0.47
7:Z:42:TYR:O	7:Z:94:PRO:HB3	2.14	0.47
7:W:44:ALA:HB2	7:W:96:VAL:HG22	1.96	0.47
2:R:29:ASN:HD21	2:R:41:ARG:H	1.61	0.47
4:I:220:PRO:HG3	4:H:190:PHE:CD1	2.49	0.47
8:q:65:ASP:O	8:q:210:ASN:ND2	2.45	0.47
7:Y:28:LEU:HD21	7:Y:102:MET:HE2	1.96	0.47
2:R:24:GLU:OE1	7:W:5:ASN:HB2	2.14	0.47
8:m:225:ARG:O	8:m:229:MET:HG3	2.14	0.47
8:n:238:ASP:HB2	7:W:106:MET:HE3	1.95	0.47
5:B:44:ILE:HD13	5:B:44:ILE:HA	1.74	0.47
2:S:10:ARG:HE	2:S:53:MET:HE1	1.79	0.47
7:Y:52:ASP:OD1	7:Y:63:LYS:HD3	2.13	0.47
5:B:70:LEU:O	5:B:74:LEU:HG	2.14	0.47
5:D:2:THR:OG1	5:D:4:GLU:OE1	2.29	0.47
1:K:103:GLN:HE21	4:G:82:SER:HA	1.79	0.47
1:L:99:VAL:HA	1:L:102:MET:HE3	1.96	0.47
2:R:96:ASP:OD1	2:R:96:ASP:N	2.39	0.47
2:T:11:PHE:HD1	2:T:53:MET:HE2	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:106:ARG:NH1	8:q:245:ASN:OD1	2.47	0.47
5:C:70:LEU:HD22	5:B:7:MET:SD	2.54	0.47
8:m:224:ALA:O	8:m:228:GLU:HG2	2.14	0.47
8:o:243:ARG:HD2	7:Y:113:GLN:HG2	1.96	0.47
8:p:35:ARG:O	8:p:173:ARG:NH2	2.37	0.47
1:K:80:VAL:HG22	2:Q:131:MET:SD	2.54	0.47
2:T:102:MET:HE3	2:T:106:ARG:HE	1.78	0.47
3:E:9:TRP:H	3:E:9:TRP:CD1	2.31	0.47
8:p:248:LEU:O	7:Y:121:THR:OG1	2.19	0.47
8:q:152:PRO:C	8:q:154:THR:H	2.22	0.47
4:F:189:ILE:O	4:F:192:PRO:HD2	2.15	0.47
7:a:86:ASP:OD1	7:a:86:ASP:N	2.38	0.47
8:m:151:PRO:C	8:m:153:ASN:N	2.73	0.47
8:n:82:LEU:HD11	8:n:88:LEU:HG	1.97	0.47
8:o:18:GLN:HE21	8:o:41:LEU:HG	1.79	0.47
6:b:318:ASN:O	6:b:319:GLN:C	2.58	0.47
1:L:48:ARG:HH22	2:R:6:ASP:CG	2.22	0.47
3:E:72:TRP:HE1	3:E:161:SER:HB2	1.80	0.47
1:M:48:ARG:NH2	2:S:6:ASP:OD2	2.48	0.47
1:N:59:PHE:CD2	2:S:118:MET:HE1	2.50	0.47
5:C:31:THR:O	5:C:35:ILE:HG12	2.14	0.47
2:Q:22:ARG:NH2	2:Q:108:GLN:OE1	2.47	0.46
7:a:88:ASN:HB2	7:a:90:TYR:CD2	2.50	0.46
4:H:138:MET:HE2	4:H:170:LEU:HG	1.98	0.46
5:A:17:ALA:HB2	4:G:195:ILE:HD12	1.96	0.46
4:F:230:ASP:O	4:F:234:LEU:HG	2.15	0.46
7:W:14:LEU:HD21	7:W:116:ILE:HG13	1.97	0.46
1:O:34:PHE:HZ	4:J:105:ILE:HD13	1.80	0.46
2:S:114:LEU:HD21	7:Y:126:MET:CE	2.45	0.46
3:E:103:GLY:O	3:E:106:MET:HB2	2.16	0.46
7:a:5:ASN:ND2	7:V:22:ASN:HD21	2.12	0.46
5:B:29:LEU:HD23	5:B:30:ILE:HD13	1.96	0.46
6:d:319:GLN:HG2	6:d:320:PRO:HD2	1.95	0.46
4:J:83:ALA:HB3	4:J:84:PRO:CD	2.38	0.46
4:G:59:LEU:O	4:G:65:THR:OG1	2.21	0.46
1:O:48:ARG:NH2	2:U:6:ASP:OD1	2.49	0.46
7:Z:47:VAL:HG12	7:Z:67:VAL:HG22	1.96	0.46
4:F:75:ARG:HD3	4:F:89:LEU:HD11	1.97	0.46
4:J:159:LEU:HD13	4:J:165:VAL:HG22	1.98	0.46
7:X:114:ALA:O	7:X:118:VAL:HG23	2.16	0.46
6:c:315:ALA:HA	8:m:9:MET:HE1	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:100:ILE:HG23	4:F:101:MET:HE2	1.98	0.46
5:C:15:LYS:HB2	5:C:15:LYS:HE2	1.70	0.46
4:F:150:PHE:CZ	4:F:172:PRO:HB2	2.51	0.46
7:X:43:ARG:HD2	7:X:69:GLU:OE2	2.14	0.46
2:Q:113:SER:O	2:Q:117:GLN:HG3	2.15	0.46
2:R:51:LYS:O	2:R:55:ARG:HG2	2.16	0.46
3:E:86:PHE:HZ	4:F:87:GLN:O	1.97	0.46
4:I:138:MET:O	4:I:142:THR:OG1	2.28	0.46
6:i:315:ALA:HA	8:p:9:MET:HE1	1.97	0.46
5:C:24:LEU:HD11	5:C:62:ILE:HD11	1.96	0.46
7:a:123:LYS:HD2	8:q:250:MET:C	2.40	0.46
3:E:108:LEU:HD23	3:E:108:LEU:HA	1.76	0.46
4:G:97:THR:O	4:G:101:MET:HG2	2.16	0.46
4:G:171:LEU:HB3	4:G:172:PRO:HD3	1.97	0.46
1:O:89:ARG:HH12	4:I:48:ILE:HD11	1.81	0.45
4:I:238:SER:HA	5:C:85:PRO:HG3	1.98	0.45
7:a:3:LEU:HB2	6:b:319:GLN:HE21	1.80	0.45
8:n:151:PRO:HB2	8:n:154:THR:CG2	2.44	0.45
8:o:225:ARG:HA	8:o:225:ARG:HD3	1.66	0.45
4:H:109:TYR:HA	4:H:113:TYR:HB3	1.98	0.45
5:A:84:LEU:HD21	4:G:185:ILE:HG23	1.97	0.45
5:D:7:MET:HA	5:D:7:MET:HE3	1.97	0.45
1:K:86:ILE:HG12	1:P:102:MET:CE	2.46	0.45
2:U:130:MET:HE2	2:U:130:MET:HB2	1.87	0.45
3:E:229:MET:SD	5:D:14:MET:HE2	2.56	0.45
4:I:190:PHE:CD1	4:J:220:PRO:HG3	2.52	0.45
8:q:9:MET:HB2	7:Z:103:VAL:HG21	1.97	0.45
4:H:209:MET:HA	4:G:205:MET:CE	2.45	0.45
1:N:69:ASN:HB2	2:T:16:LEU:HD23	1.99	0.45
2:S:33:ALA:O	2:S:98:ASN:ND2	2.50	0.45
2:T:115:LYS:HE2	7:Z:4:LEU:HD21	1.97	0.45
3:E:158:PRO:HD2	3:E:162:ASN:ND2	2.32	0.45
8:o:53:THR:HG22	7:Y:67:VAL:HG21	1.98	0.45
4:H:66:ARG:HB2	4:H:178:GLU:OE1	2.17	0.45
2:Q:104:ARG:O	2:Q:108:GLN:HG2	2.17	0.45
5:A:58:VAL:HG21	4:G:207:LEU:HD21	1.97	0.45
4:J:188:THR:HB	5:D:9:MET:HE1	1.99	0.45
1:L:102:MET:HE1	4:G:59:LEU:HD11	1.99	0.45
1:P:61:LEU:HD21	2:U:50:LYS:NZ	2.31	0.45
2:Q:11:PHE:HD1	2:Q:53:MET:HE2	1.82	0.45
2:S:128:LYS:HE2	7:X:134:GLN:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:m:110:THR:HG23	8:m:112:GLN:HG2	1.97	0.45
8:n:240:ASN:ND2	7:X:113:GLN:HE21	2.14	0.45
8:o:82:LEU:HD13	8:o:201:ILE:HG22	1.97	0.45
3:E:254:ILE:HD13	3:E:254:ILE:HA	1.86	0.45
4:G:204:LEU:HD12	4:G:214:PRO:HB3	1.99	0.45
1:P:64:PRO:CG	6:b:322:PRO:HB3	2.47	0.45
8:q:64:ALA:HB2	8:q:173:ARG:HH21	1.80	0.45
5:A:10:GLY:O	5:A:14:MET:HG2	2.16	0.45
5:D:60:ILE:O	5:D:64:VAL:HG22	2.17	0.45
7:W:86:ASP:OD1	7:W:86:ASP:N	2.41	0.45
1:M:104:VAL:CG2	4:H:90:LEU:HG	2.47	0.45
7:a:125:MET:HG3	7:V:112:TYR:CD1	2.51	0.45
7:a:128:LYS:O	7:a:131:THR:HG22	2.17	0.45
8:n:80:VAL:O	8:n:103:GLY:HA3	2.17	0.45
4:J:239:LEU:HD12	4:J:239:LEU:HA	1.84	0.45
3:E:144:LEU:HB3	4:J:149:LEU:HD22	1.98	0.45
6:e:313:PRO:HG2	7:W:20:ARG:HD3	1.99	0.45
6:g:313:PRO:HG3	7:X:49:PHE:CG	2.52	0.45
8:q:144:SER:HB3	8:q:155:VAL:HG22	1.99	0.45
4:J:221:PHE:O	4:J:224:MET:HE2	2.17	0.45
2:S:31:ALA:HB1	7:X:13:ALA:HB2	1.98	0.44
2:S:109:PHE:CZ	7:X:118:VAL:HG13	2.53	0.44
3:E:8:GLN:O	3:E:12:TRP:HD1	2.01	0.44
5:C:27:VAL:HG22	5:C:57:ALA:HB1	1.98	0.44
8:m:171:VAL:HG13	8:m:179:PHE:HB3	1.98	0.44
8:p:10:GLY:O	8:p:14:GLN:HG2	2.16	0.44
4:G:57:ILE:O	4:G:61:MET:HB2	2.17	0.44
4:J:114:GLN:HB3	4:J:115:PRO:HD3	2.00	0.44
1:L:75:MET:HE3	1:L:75:MET:HB3	1.83	0.44
1:M:70:ASP:OD1	2:S:13:GLN:NE2	2.49	0.44
8:o:4:ALA:HB2	7:Y:22:ASN:OD1	2.18	0.44
8:o:10:GLY:O	8:o:14:GLN:HG2	2.17	0.44
8:p:14:GLN:HG3	8:p:58:THR:HA	1.98	0.44
8:p:26:LEU:HD21	8:p:216:ALA:CB	2.48	0.44
5:B:2:THR:HG23	5:B:5:SER:H	1.82	0.44
5:B:20:LEU:HD11	5:B:73:LEU:HD13	2.00	0.44
4:H:101:MET:HE3	4:H:101:MET:HB3	1.77	0.44
4:H:127:LEU:HD23	4:H:127:LEU:HA	1.88	0.44
2:Q:49:LEU:O	2:Q:53:MET:HG2	2.17	0.44
3:E:75:MET:O	3:E:79:LEU:HG	2.17	0.44
3:E:123:PRO:HB2	3:E:126:ALA:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:233:MET:O	5:D:7:MET:HE2	2.17	0.44
8:q:130:PRO:O	8:q:131:GLU:C	2.60	0.44
8:q:227:PHE:O	8:q:231:MET:HG2	2.17	0.44
4:J:204:LEU:HD11	4:J:217:ILE:HD12	1.99	0.44
4:I:147:LEU:HD21	4:I:165:VAL:HG11	2.00	0.44
8:m:9:MET:HB2	7:V:103:VAL:HG21	1.98	0.44
8:m:120:VAL:O	8:m:126:PRO:HA	2.16	0.44
4:F:100:ILE:HG23	4:F:101:MET:CE	2.47	0.44
4:F:213:PRO:HA	4:F:214:PRO:HD3	1.91	0.44
8:n:34:PHE:O	8:n:210:ASN:ND2	2.51	0.44
8:n:87:TRP:HB2	8:n:164:VAL:HG23	1.99	0.44
8:p:49:LEU:HA	8:p:50:SER:HA	1.72	0.44
8:p:105:ILE:HG12	8:p:115:ILE:HD11	2.00	0.44
4:I:212:VAL:HG21	4:I:217:ILE:HD11	2.00	0.44
7:a:3:LEU:H	6:b:319:GLN:HE21	1.66	0.44
8:n:29:ALA:O	8:n:209:SER:OG	2.36	0.44
8:o:167:GLU:OE1	8:o:167:GLU:N	2.50	0.44
8:q:77:PRO:O	8:q:203:SER:OG	2.34	0.44
3:E:193:LEU:O	3:E:196:THR:OG1	2.25	0.44
5:D:52:ILE:HD13	5:D:52:ILE:HA	1.83	0.44
2:S:88:ARG:HH12	2:S:108:GLN:HG3	1.83	0.43
7:a:3:LEU:O	6:b:319:GLN:HG3	2.18	0.43
8:n:18:GLN:HG2	8:n:223:ASN:HD21	1.82	0.43
4:H:210:MET:CE	4:G:211:MET:HE1	2.48	0.43
7:Z:97:ASP:O	7:Z:101:GLU:HG2	2.18	0.43
4:J:80:THR:CB	4:J:83:ALA:HB2	2.48	0.43
7:a:6:ILE:HG22	6:b:315:ALA:O	2.18	0.43
8:o:143:ILE:HB	8:o:159:GLY:O	2.18	0.43
4:J:124:GLN:H	4:J:124:GLN:HG2	1.67	0.43
4:J:195:ILE:O	4:J:199:VAL:HG13	2.18	0.43
3:E:251:LEU:HD23	3:E:251:LEU:HA	1.84	0.43
8:m:125:GLY:O	8:m:126:PRO:C	2.60	0.43
8:p:243:ARG:CZ	7:Z:113:GLN:HB2	2.48	0.43
4:F:123:MET:HE3	4:F:123:MET:HB3	1.84	0.43
3:E:205:ASN:HB3	4:F:209:MET:HG3	2.00	0.43
6:e:315:ALA:HA	8:n:9:MET:HE1	2.00	0.43
8:n:72:ASP:OD1	8:n:72:ASP:C	2.61	0.43
8:p:34:PHE:HB3	8:p:209:SER:HB2	2.00	0.43
5:A:37:ILE:HD13	5:B:44:ILE:HD11	2.00	0.43
1:K:84:MET:HE2	2:Q:134:LEU:HD21	2.00	0.43
2:T:19:ARG:NH2	2:T:115:LYS:HD3	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:117:GLN:HE22	7:Y:125:MET:CG	2.32	0.43
3:E:179:ILE:H	3:E:179:ILE:HG13	1.69	0.43
4:I:229:VAL:HG11	5:C:77:VAL:HG12	2.00	0.43
7:a:22:ASN:OD1	8:q:54:ARG:NH1	2.51	0.43
8:p:4:ALA:HB2	7:Z:22:ASN:OD1	2.19	0.43
4:H:143:ARG:HH22	4:H:177:SER:HA	1.83	0.43
1:N:59:PHE:CD2	1:N:59:PHE:C	2.97	0.43
1:N:102:MET:HE1	4:I:59:LEU:HD21	2.01	0.43
8:m:245:ASN:OD1	8:m:246:GLN:N	2.51	0.43
8:n:9:MET:HB2	7:W:103:VAL:HG21	1.99	0.43
8:n:73:TYR:HD1	8:n:205:VAL:HG12	1.83	0.43
8:n:193:LEU:HD23	8:n:193:LEU:HA	1.87	0.43
8:p:65:ASP:OD2	8:p:212:LYS:NZ	2.52	0.43
4:F:63:SER:HB2	4:F:66:ARG:HH21	1.84	0.43
3:E:216:ILE:HG13	5:D:29:LEU:HD12	2.01	0.43
3:E:224:VAL:O	3:E:228:LEU:HB2	2.18	0.43
4:H:114:GLN:O	4:H:118:GLU:HG2	2.19	0.43
4:H:121:ILE:HD12	4:H:121:ILE:HA	1.90	0.43
4:G:217:ILE:O	4:G:220:PRO:HD2	2.18	0.43
7:W:82:ASN:HD22	7:W:91:VAL:HG21	1.83	0.43
1:N:32:VAL:HG23	4:I:106:ASP:OD2	2.19	0.43
2:R:4:ARG:HG2	4:G:119:GLN:HE22	1.84	0.43
3:E:166:SER:C	3:E:168:ALA:H	2.27	0.43
8:n:74:THR:OG1	8:n:79:ASP:OD2	2.34	0.43
4:H:141:GLN:NE2	4:H:243:PHE:HA	2.33	0.43
4:F:97:THR:HA	4:F:100:ILE:HG22	2.00	0.43
7:W:7:PHE:CD2	7:W:119:LEU:HD11	2.54	0.43
8:o:11:ALA:HB2	7:Y:29:ALA:HB1	2.01	0.43
8:p:82:LEU:HD11	8:p:88:LEU:HG	2.01	0.43
4:H:220:PRO:HG3	4:G:190:PHE:CD1	2.54	0.43
5:B:2:THR:O	5:B:5:SER:OG	2.35	0.43
4:F:147:LEU:HD23	4:F:147:LEU:HA	1.87	0.43
7:V:122:VAL:O	7:V:126:MET:HG2	2.18	0.43
3:E:49:MET:HE1	4:J:175:VAL:HG21	2.01	0.43
1:K:74:ASP:OD2	1:K:74:ASP:N	2.52	0.42
3:E:88:MET:HA	3:E:247:ILE:HG21	1.99	0.42
6:e:322:PRO:HA	6:e:323:PRO:HD3	1.94	0.42
8:n:72:ASP:OD1	8:n:74:THR:HG23	2.18	0.42
8:n:80:VAL:HB	8:n:201:ILE:HD11	2.01	0.42
8:n:181:LEU:HD23	8:n:181:LEU:HA	1.90	0.42
8:p:169:ASN:OD1	8:p:169:ASN:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:p:181:LEU:HD11	8:p:193:LEU:HG	2.00	0.42
4:F:63:SER:O	4:F:67:ILE:HD12	2.19	0.42
2:Q:114:LEU:HD21	7:W:123:LYS:HG3	2.00	0.42
2:U:31:ALA:HB1	7:Z:13:ALA:HB2	2.00	0.42
6:g:315:ALA:HA	8:o:9:MET:HE1	1.99	0.42
8:n:240:ASN:HD22	8:n:240:ASN:HA	1.61	0.42
7:Z:3:LEU:HD12	7:Z:3:LEU:HA	1.92	0.42
4:G:161:GLY:O	4:G:162:PRO:C	2.61	0.42
5:D:45:ASN:OD1	5:D:45:ASN:N	2.50	0.42
3:E:243:LEU:HD23	3:E:243:LEU:HA	1.81	0.42
4:G:114:GLN:HB3	4:G:115:PRO:HD3	2.01	0.42
4:J:82:SER:OG	4:J:82:SER:O	2.37	0.42
7:V:13:ALA:HA	7:V:62:VAL:HG12	2.02	0.42
1:O:73:ALA:HB1	2:U:13:GLN:NE2	2.33	0.42
2:Q:62:GLY:HA2	2:Q:79:SER:HB3	2.02	0.42
2:S:103:ASP:OD1	7:Y:112:TYR:OH	2.36	0.42
3:E:125:LEU:O	3:E:129:MET:HG3	2.20	0.42
4:I:171:LEU:HB3	4:I:172:PRO:HD3	2.01	0.42
4:I:185:ILE:HG23	5:C:84:LEU:HD21	2.01	0.42
4:G:212:VAL:HG22	4:F:214:PRO:HG2	2.01	0.42
1:M:103:GLN:HA	4:H:86:ASN:HD22	1.83	0.42
1:N:82:MET:HE3	4:H:41:SER:HB2	2.00	0.42
2:Q:85:LEU:HD23	2:Q:85:LEU:HA	1.81	0.42
2:U:36:PRO:HG2	6:k:311:GLY:H	1.84	0.42
3:E:167:ASN:ND2	3:E:174:ARG:HH12	2.18	0.42
5:C:52:ILE:O	5:C:55:ILE:HG22	2.18	0.42
5:C:54:LYS:HB3	5:C:54:LYS:HE2	1.83	0.42
8:n:181:LEU:HD11	8:n:193:LEU:HD21	2.01	0.42
8:o:83:GLN:HG2	8:o:84:GLN:N	2.34	0.42
8:o:115:ILE:HG13	8:o:120:VAL:HG22	2.01	0.42
7:Y:112:TYR:CE2	7:Y:116:ILE:HD11	2.55	0.42
7:a:16:ALA:HB1	7:a:49:PHE:CE1	2.55	0.42
8:m:15:THR:OG1	8:m:226:ARG:NH1	2.52	0.42
8:p:15:THR:OG1	8:p:226:ARG:NH1	2.53	0.42
4:G:121:ILE:HG12	4:G:125:GLU:HB3	2.02	0.42
4:F:171:LEU:HB3	4:F:172:PRO:HD3	2.01	0.42
4:J:121:ILE:HG23	4:J:125:GLU:HB3	2.02	0.42
4:F:162:PRO:CD	4:F:163:GLU:N	2.82	0.42
3:E:122:MET:HG3	4:J:214:PRO:HG2	2.01	0.42
5:C:1:MET:HE2	5:C:1:MET:HB3	1.90	0.42
6:g:316:LEU:HD12	6:g:316:LEU:HA	1.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:a:123:LYS:HE2	7:a:123:LYS:HA	2.02	0.42
8:m:29:ALA:O	8:m:209:SER:OG	2.37	0.42
8:m:249:SER:CB	7:V:117:GLU:HB3	2.50	0.42
8:n:146:LEU:HB2	8:n:155:VAL:HG22	2.01	0.42
8:p:1:MET:HG2	8:p:241:GLU:CG	2.49	0.42
8:p:80:VAL:O	8:p:103:GLY:HA3	2.19	0.42
4:J:92:LEU:HD12	4:J:92:LEU:HA	1.78	0.42
1:O:69:ASN:OD1	1:O:69:ASN:N	2.52	0.42
3:E:175:ALA:HA	3:E:178:LEU:HD23	2.02	0.42
7:a:34:VAL:HG13	7:a:35:THR:HG22	2.02	0.42
8:m:47:ASP:O	6:d:324:ASN:HB2	2.19	0.42
8:n:49:LEU:HA	8:n:50:SER:HA	1.64	0.42
8:o:82:LEU:HD11	8:o:163:LEU:HD22	2.02	0.42
4:J:66:ARG:HA	4:J:182:ALA:HB2	2.02	0.42
4:J:189:ILE:O	4:J:192:PRO:HD2	2.19	0.42
7:W:10:ALA:HB3	7:W:119:LEU:HD13	2.02	0.42
1:O:84:MET:SD	2:U:134:LEU:HD21	2.59	0.42
1:P:75:MET:HE2	1:P:75:MET:HB2	1.81	0.42
2:R:29:ASN:ND2	2:R:40:ALA:HA	2.34	0.42
8:q:135:ILE:HG23	8:q:143:ILE:HG23	2.01	0.42
4:G:91:GLY:HA3	4:F:60:MET:CE	2.47	0.42
1:L:82:MET:HE3	2:Q:133:VAL:HG22	2.02	0.41
2:T:39:GLN:HA	2:T:99:THR:HB	2.01	0.41
8:o:68:PRO:CD	8:o:84:GLN:HE21	2.32	0.41
6:l:312:VAL:HG12	6:l:315:ALA:HB2	2.01	0.41
1:M:80:VAL:HG22	2:S:131:MET:HG2	2.01	0.41
1:P:82:MET:HE2	1:P:82:MET:HA	2.02	0.41
3:E:176:GLY:HA2	3:E:179:ILE:CD1	2.49	0.41
4:I:190:PHE:CG	4:J:220:PRO:HG3	2.55	0.41
8:p:2:ASP:OD2	8:p:3:HIS:N	2.54	0.41
4:J:85:PRO:O	4:J:86:ASN:C	2.62	0.41
4:J:129:LYS:HB3	4:J:129:LYS:HE3	1.87	0.41
4:I:101:MET:HE3	4:I:101:MET:HB3	1.76	0.41
8:n:227:PHE:O	8:n:228:GLU:C	2.62	0.41
4:J:217:ILE:O	4:J:220:PRO:HD2	2.20	0.41
4:J:225:LEU:HD12	4:J:229:VAL:HG22	2.01	0.41
1:K:84:MET:HE1	4:F:44:THR:HG23	2.01	0.41
8:q:35:ARG:NH1	8:q:101:ARG:HG3	2.35	0.41
4:H:95:PHE:CZ	4:G:171:LEU:HD23	2.55	0.41
7:Z:119:LEU:HD23	7:Z:119:LEU:HA	1.67	0.41
4:J:83:ALA:O	4:J:85:PRO:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:97:GLN:HE21	4:I:52:THR:HG23	1.85	0.41
2:S:16:LEU:HD11	2:S:120:LEU:HG	2.02	0.41
2:U:90:PRO:HG2	8:q:49:LEU:HB2	2.02	0.41
7:a:62:VAL:HB	7:V:30:ASN:ND2	2.36	0.41
4:G:194:LEU:HD23	4:G:194:LEU:HA	1.83	0.41
4:G:220:PRO:HG2	4:F:194:LEU:HD12	2.03	0.41
2:S:106:ARG:HG2	8:o:248:LEU:HD21	2.02	0.41
6:k:322:PRO:HA	6:k:323:PRO:HD3	1.98	0.41
7:a:98:VAL:O	7:a:102:MET:HG2	2.21	0.41
8:m:26:LEU:HD23	8:m:26:LEU:HA	1.87	0.41
8:m:46:VAL:HA	6:d:326:ALA:HB2	2.03	0.41
8:n:153:ASN:OD1	8:n:153:ASN:N	2.52	0.41
8:p:89:VAL:HG22	8:p:99:TYR:CD1	2.56	0.41
8:q:82:LEU:HD11	8:q:88:LEU:HD12	2.03	0.41
5:A:18:LEU:HD12	5:A:18:LEU:HA	1.91	0.41
5:A:52:ILE:HD12	5:A:52:ILE:N	2.35	0.41
5:B:51:PHE:CE2	5:B:55:ILE:HD11	2.56	0.41
4:G:234:LEU:HD12	4:G:234:LEU:HA	1.92	0.41
4:I:187:PHE:CD2	4:J:224:MET:HB2	2.56	0.41
8:o:49:LEU:HA	8:o:50:SER:HA	1.69	0.41
7:Y:8:ASP:OD2	7:Y:8:ASP:C	2.64	0.41
5:B:39:GLN:NE2	5:B:49:LEU:HD12	2.31	0.41
7:Z:126:MET:O	7:Z:129:THR:HG22	2.21	0.41
4:F:175:VAL:O	4:F:179:LEU:HG	2.20	0.41
4:F:217:ILE:HD13	4:F:217:ILE:HA	1.89	0.41
1:P:69:ASN:OD1	7:V:112:TYR:OH	2.11	0.41
2:R:29:ASN:HD22	2:R:38:TYR:HE2	1.68	0.41
3:E:231:ALA:O	3:E:234:PRO:HD2	2.21	0.41
5:A:15:LYS:HE2	5:A:15:LYS:HB3	1.88	0.41
4:G:171:LEU:O	4:G:175:VAL:HG23	2.21	0.41
4:J:213:PRO:HA	4:J:214:PRO:HD3	1.91	0.41
4:H:189:ILE:HD13	4:H:235:LEU:HD11	2.03	0.41
5:B:59:PHE:CZ	4:G:198:LEU:HD21	2.55	0.41
7:Z:45:LYS:C	7:Z:46:GLN:HG2	2.46	0.41
4:G:204:LEU:HD11	4:G:217:ILE:HD12	2.01	0.41
1:P:44:ARG:HH12	3:E:4:VAL:HB	1.86	0.40
8:m:247:LEU:CB	7:W:120:ASN:HD21	2.21	0.40
8:o:243:ARG:HD2	7:Y:113:GLN:CG	2.51	0.40
4:H:189:ILE:O	4:H:192:PRO:HD2	2.21	0.40
4:F:138:MET:O	4:F:142:THR:OG1	2.16	0.40
4:F:153:LEU:HD23	4:F:153:LEU:HA	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:187:PHE:CZ	4:F:191:ILE:HD11	2.56	0.40
4:J:225:LEU:HD11	5:D:77:VAL:HG11	2.03	0.40
5:D:35:ILE:HD13	5:D:35:ILE:HA	1.98	0.40
1:O:102:MET:HE1	4:J:64:PHE:HE2	1.85	0.40
1:O:103:GLN:CD	1:O:103:GLN:H	2.30	0.40
5:C:49:LEU:HD23	5:C:49:LEU:HA	1.94	0.40
8:o:26:LEU:HD23	8:o:26:LEU:HA	1.91	0.40
8:p:83:GLN:HG2	8:p:84:GLN:N	2.36	0.40
4:H:185:ILE:HG23	5:B:84:LEU:HD22	2.03	0.40
4:G:75:ARG:HB2	4:G:83:ALA:CB	2.52	0.40
2:Q:128:LYS:HD2	2:Q:128:LYS:HA	1.62	0.40
4:H:71:PHE:HD1	4:H:71:PHE:HA	1.80	0.40
5:A:50:SER:OG	5:B:46:GLU:OE2	2.25	0.40
3:E:146:LEU:HA	3:E:146:LEU:HD23	1.80	0.40
4:I:132:GLN:HB2	4:I:133:PRO:HD3	2.04	0.40
8:m:82:LEU:HD21	8:m:88:LEU:HD12	2.03	0.40
1:K:68:LEU:H	1:K:68:LEU:HD12	1.85	0.40
3:E:172:LEU:O	3:E:175:ALA:HB3	2.21	0.40
8:m:79:ASP:HB3	8:m:206:LEU:CD1	2.51	0.40
8:o:112:GLN:H	8:o:112:GLN:HG2	1.58	0.40
7:Y:119:LEU:HD12	7:Y:119:LEU:HA	1.84	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	K	38/104 (36%)	36 (95%)	2 (5%)	0	100	100
1	L	70/104 (67%)	70 (100%)	0	0	100	100
1	M	72/104 (69%)	70 (97%)	2 (3%)	0	100	100
1	N	72/104 (69%)	72 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	72/104 (69%)	72 (100%)	0	0	100	100
1	P	71/104 (68%)	71 (100%)	0	0	100	100
2	Q	115/138 (83%)	115 (100%)	0	0	100	100
2	R	104/138 (75%)	103 (99%)	1 (1%)	0	100	100
2	S	104/138 (75%)	103 (99%)	1 (1%)	0	100	100
2	T	106/138 (77%)	104 (98%)	2 (2%)	0	100	100
2	U	102/138 (74%)	101 (99%)	1 (1%)	0	100	100
3	E	251/264 (95%)	231 (92%)	14 (6%)	6 (2%)	4	24
4	F	205/245 (84%)	195 (95%)	10 (5%)	0	100	100
4	G	207/245 (84%)	199 (96%)	6 (3%)	2 (1%)	12	40
4	H	206/245 (84%)	201 (98%)	5 (2%)	0	100	100
4	I	206/245 (84%)	199 (97%)	6 (3%)	1 (0%)	24	55
4	J	207/245 (84%)	200 (97%)	5 (2%)	2 (1%)	12	40
5	A	87/89 (98%)	85 (98%)	2 (2%)	0	100	100
5	B	87/89 (98%)	86 (99%)	1 (1%)	0	100	100
5	C	87/89 (98%)	86 (99%)	1 (1%)	0	100	100
5	D	87/89 (98%)	85 (98%)	2 (2%)	0	100	100
6	b	11/560 (2%)	10 (91%)	1 (9%)	0	100	100
6	c	14/560 (2%)	12 (86%)	2 (14%)	0	100	100
6	d	18/560 (3%)	18 (100%)	0	0	100	100
6	e	14/560 (2%)	14 (100%)	0	0	100	100
6	f	19/560 (3%)	19 (100%)	0	0	100	100
6	g	14/560 (2%)	13 (93%)	1 (7%)	0	100	100
6	h	19/560 (3%)	19 (100%)	0	0	100	100
6	i	14/560 (2%)	14 (100%)	0	0	100	100
6	j	18/560 (3%)	17 (94%)	1 (6%)	0	100	100
6	k	14/560 (2%)	14 (100%)	0	0	100	100
6	l	19/560 (3%)	19 (100%)	0	0	100	100
7	V	131/134 (98%)	123 (94%)	8 (6%)	0	100	100
7	W	130/134 (97%)	124 (95%)	6 (5%)	0	100	100
7	X	131/134 (98%)	126 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	Y	131/134 (98%)	127 (97%)	4 (3%)	0	100	100
7	Z	131/134 (98%)	125 (95%)	5 (4%)	1 (1%)	16	45
7	a	131/134 (98%)	125 (95%)	6 (5%)	0	100	100
8	m	246/251 (98%)	232 (94%)	11 (4%)	3 (1%)	10	37
8	n	247/251 (98%)	241 (98%)	6 (2%)	0	100	100
8	o	248/251 (99%)	239 (96%)	9 (4%)	0	100	100
8	p	248/251 (99%)	240 (97%)	8 (3%)	0	100	100
8	q	247/251 (98%)	233 (94%)	13 (5%)	1 (0%)	30	60
All	All	4751/11378 (42%)	4588 (97%)	147 (3%)	16 (0%)	37	65

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	188	LEU
3	E	190	VAL
8	m	123	GLU
4	J	83	ALA
3	E	167	ASN
3	E	213	ILE
4	I	160	GLN
4	G	83	ALA
3	E	189	PRO
8	m	151	PRO
4	G	162	PRO
3	E	187	ALA
7	Z	58	ALA
8	m	149	GLY
8	q	132	GLY
4	J	229	VAL

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	K	33/79 (42%)	33 (100%)	0	100	100
1	L	56/79 (71%)	56 (100%)	0	100	100
1	M	58/79 (73%)	58 (100%)	0	100	100
1	N	58/79 (73%)	57 (98%)	1 (2%)	53	71
1	O	58/79 (73%)	58 (100%)	0	100	100
1	P	57/79 (72%)	56 (98%)	1 (2%)	51	70
2	Q	98/113 (87%)	96 (98%)	2 (2%)	48	68
2	R	90/113 (80%)	89 (99%)	1 (1%)	65	76
2	S	90/113 (80%)	90 (100%)	0	100	100
2	T	91/113 (80%)	91 (100%)	0	100	100
2	U	89/113 (79%)	88 (99%)	1 (1%)	65	76
3	E	210/221 (95%)	208 (99%)	2 (1%)	68	76
4	F	177/204 (87%)	174 (98%)	3 (2%)	53	71
4	G	179/204 (88%)	174 (97%)	5 (3%)	38	62
4	H	178/204 (87%)	176 (99%)	2 (1%)	65	76
4	I	178/204 (87%)	175 (98%)	3 (2%)	53	71
4	J	179/204 (88%)	178 (99%)	1 (1%)	78	81
5	A	74/74 (100%)	72 (97%)	2 (3%)	39	63
5	B	74/74 (100%)	74 (100%)	0	100	100
5	C	74/74 (100%)	74 (100%)	0	100	100
5	D	74/74 (100%)	72 (97%)	2 (3%)	39	63
6	b	8/467 (2%)	8 (100%)	0	100	100
6	c	11/467 (2%)	11 (100%)	0	100	100
6	d	14/467 (3%)	12 (86%)	2 (14%)	3	14
6	e	11/467 (2%)	11 (100%)	0	100	100
6	f	15/467 (3%)	15 (100%)	0	100	100
6	g	11/467 (2%)	11 (100%)	0	100	100
6	h	15/467 (3%)	15 (100%)	0	100	100
6	i	11/467 (2%)	11 (100%)	0	100	100
6	j	14/467 (3%)	13 (93%)	1 (7%)	13	40
6	k	11/467 (2%)	11 (100%)	0	100	100
6	l	15/467 (3%)	14 (93%)	1 (7%)	15	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	V	104/105 (99%)	104 (100%)	0	100	100
7	W	104/105 (99%)	104 (100%)	0	100	100
7	X	104/105 (99%)	104 (100%)	0	100	100
7	Y	104/105 (99%)	103 (99%)	1 (1%)	68	76
7	Z	104/105 (99%)	102 (98%)	2 (2%)	50	68
7	a	104/105 (99%)	104 (100%)	0	100	100
8	m	190/193 (98%)	185 (97%)	5 (3%)	40	64
8	n	191/193 (99%)	189 (99%)	2 (1%)	68	76
8	o	192/193 (100%)	189 (98%)	3 (2%)	55	72
8	p	192/193 (100%)	192 (100%)	0	100	100
8	q	191/193 (99%)	190 (100%)	1 (0%)	81	83
All	All	3891/9308 (42%)	3847 (99%)	44 (1%)	63	76

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	97	GLN
1	P	91	LYS
2	Q	101	ASP
2	Q	125	SER
2	R	55	ARG
2	U	104	ARG
3	E	185	MET
3	E	214	PHE
4	I	125	GLU
4	I	187	PHE
4	I	241	GLN
8	m	37	GLN
8	m	39	ASN
8	m	126	PRO
8	m	150	ASP
8	m	247	LEU
8	n	70	GLN
8	n	201	ILE
8	o	70	GLN
8	o	71	LEU
8	o	184	GLU
8	q	163	LEU

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Mol	Chain	Res	Type
7	Y	101	GLU
4	H	143	ARG
4	H	152	ARG
5	A	7	MET
5	A	15	LYS
7	Z	6	ILE
7	Z	127	LEU
4	G	48	ILE
4	G	140	ARG
4	G	160	GLN
4	G	162	PRO
4	G	209	MET
4	F	123	MET
4	F	160	GLN
4	F	190	PHE
6	d	318	ASN
6	d	319	GLN
6	j	319	GLN
6	l	318	ASN
4	J	230	ASP
5	D	9	MET
5	D	14	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

Mol	Chain	Res	Type
1	K	103	GLN
1	M	83	GLN
1	M	103	GLN
1	O	39	HIS
1	O	55	GLN
1	O	83	GLN
1	O	87	GLN
1	O	97	GLN
1	P	55	GLN
1	P	76	GLN
1	P	87	GLN
2	Q	17	ASN
2	R	21	GLN
2	R	29	ASN
2	R	92	GLN
2	R	98	ASN

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Mol	Chain	Res	Type
2	R	117	GLN
2	S	32	ASN
2	S	92	GLN
2	S	135	GLN
2	T	21	GLN
2	T	32	ASN
2	T	98	ASN
2	T	117	GLN
2	U	13	GLN
2	U	112	ASN
3	E	162	ASN
3	E	182	ASN
3	E	205	ASN
4	I	160	GLN
4	I	184	GLN
4	I	241	GLN
6	e	324	ASN
6	i	318	ASN
7	a	5	ASN
7	a	57	GLN
7	a	115	ASN
8	m	18	GLN
8	m	37	GLN
8	m	91	GLN
8	m	102	ASN
8	m	112	GLN
8	n	18	GLN
8	n	210	ASN
8	n	223	ASN
8	n	230	GLN
8	n	240	ASN
8	o	18	GLN
8	o	83	GLN
8	o	84	GLN
8	o	186	GLN
8	p	14	GLN
8	p	210	ASN
8	p	240	ASN
8	q	18	GLN
8	q	112	GLN
8	q	116	GLN
7	Y	82	ASN

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Mol	Chain	Res	Type
4	H	184	GLN
7	Z	17	GLN
7	Z	115	ASN
4	G	86	ASN
4	G	241	GLN
6	b	319	GLN
4	F	119	GLN
4	F	141	GLN
4	F	160	GLN
6	h	324	ASN
6	f	324	ASN
6	l	318	ASN
4	J	87	GLN
4	J	114	GLN
4	J	155	ASN
7	V	30	ASN
7	V	115	ASN
5	D	39	GLN
7	X	40	GLN
7	X	50	GLN
7	X	57	GLN
7	X	134	GLN
7	W	22	ASN
7	W	30	ASN
7	W	120	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

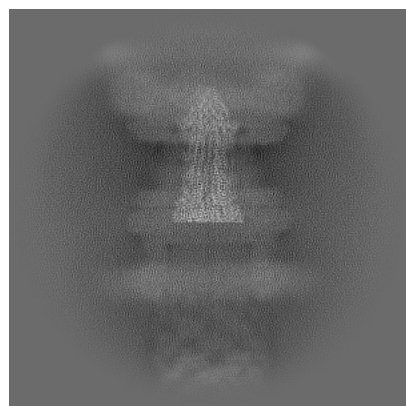
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37594. These allow visual inspection of the internal detail of the map and identification of artifacts.

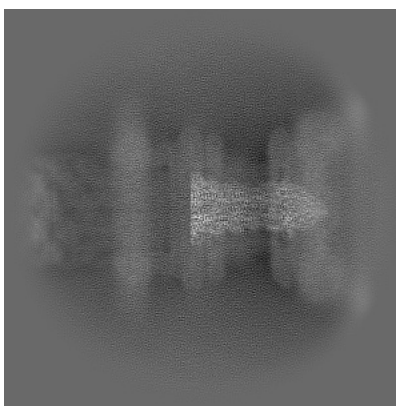
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

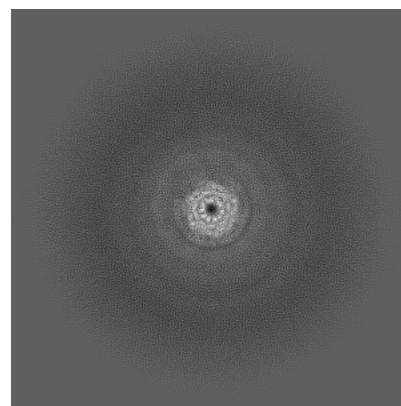
6.1.1 Primary map



X

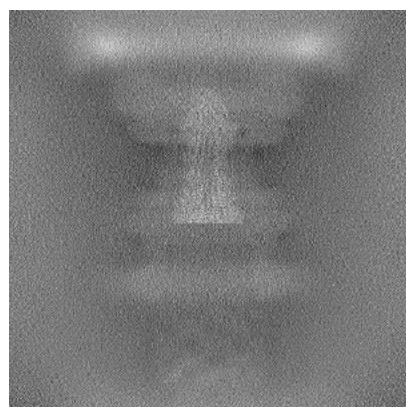


Y

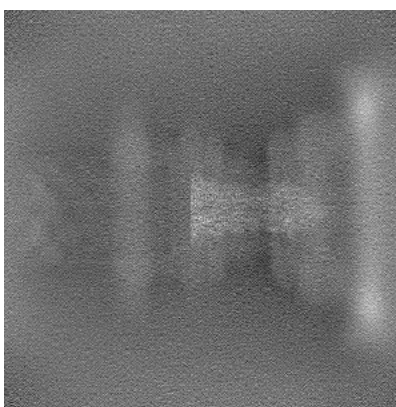


Z

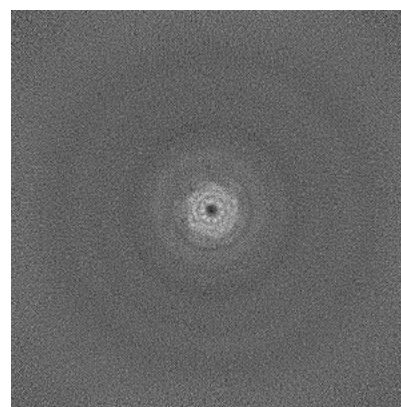
6.1.2 Raw map



X



Y

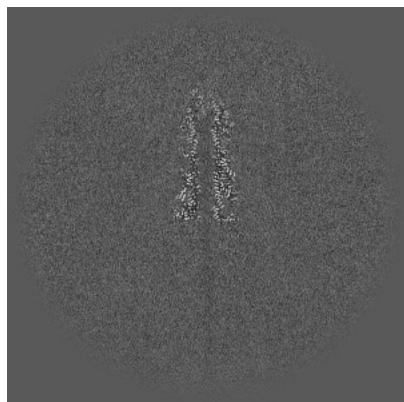


Z

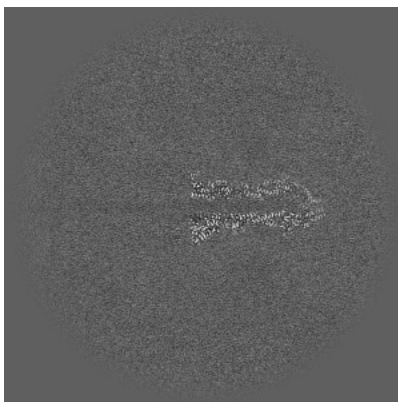
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

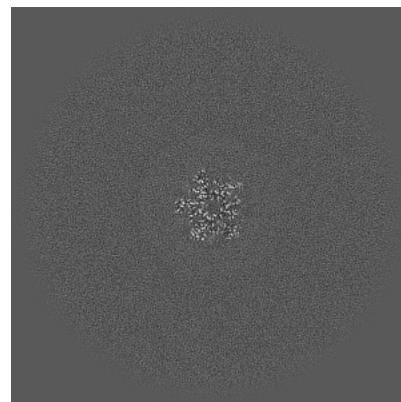
6.2.1 Primary map



X Index: 256

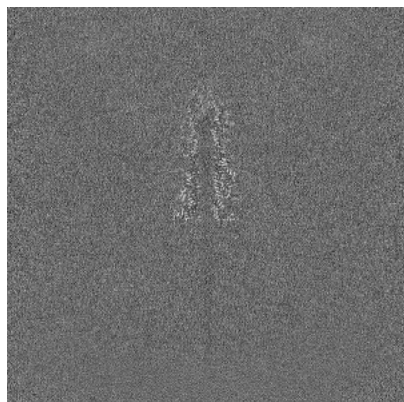


Y Index: 256

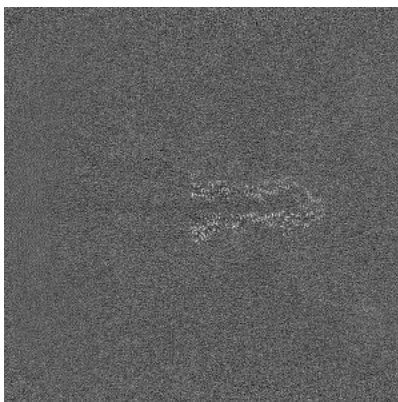


Z Index: 256

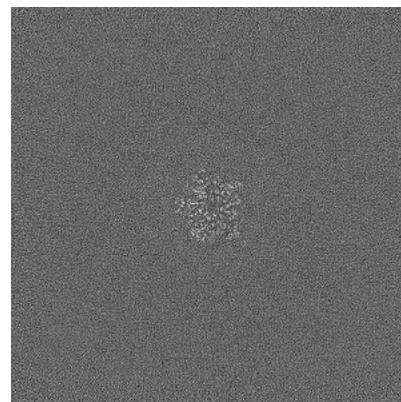
6.2.2 Raw map



X Index: 256



Y Index: 256

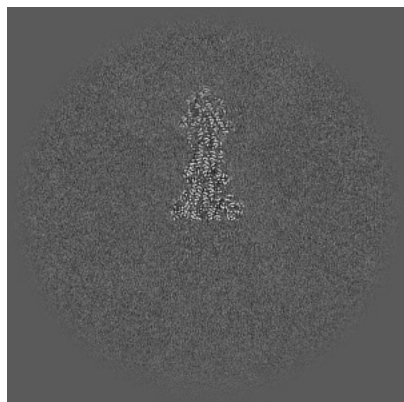


Z Index: 256

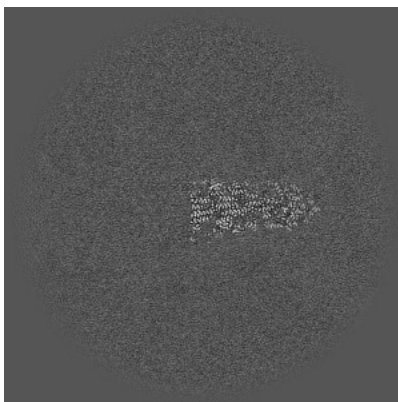
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

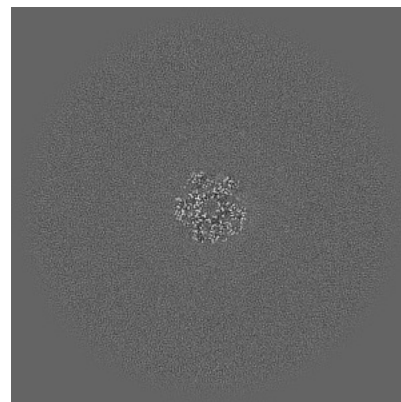
6.3.1 Primary map



X Index: 244

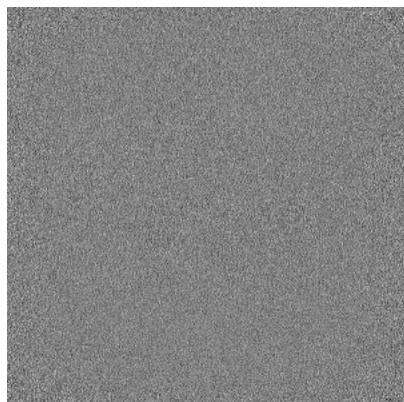


Y Index: 268

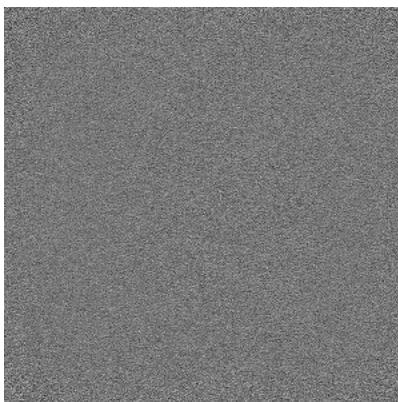


Z Index: 247

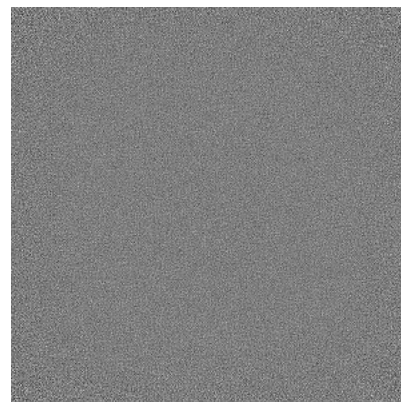
6.3.2 Raw map



X Index: 0



Y Index: 0

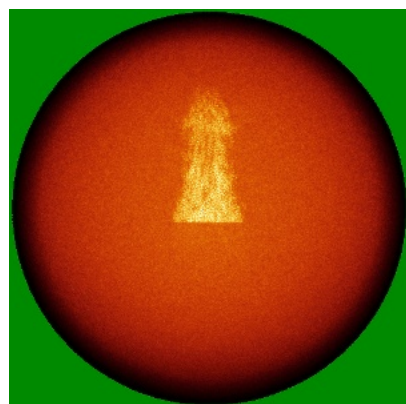


Z Index: 0

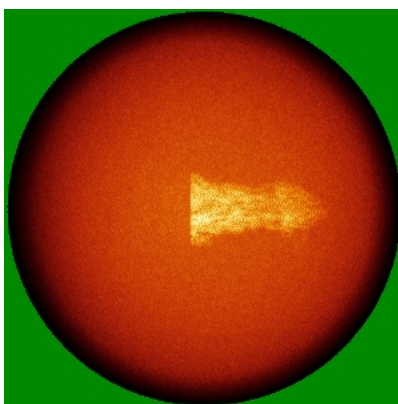
The images above show the largest variance slices of the map in three orthogonal directions.

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

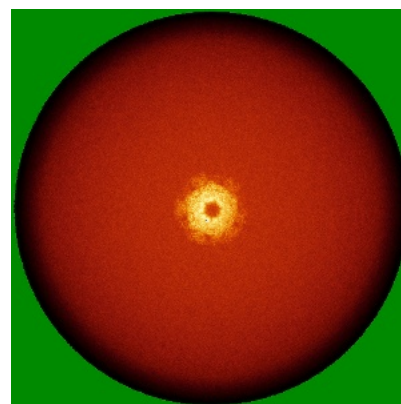
6.4.1 Primary map



X

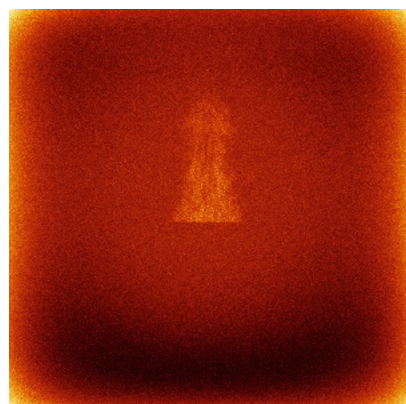


Y

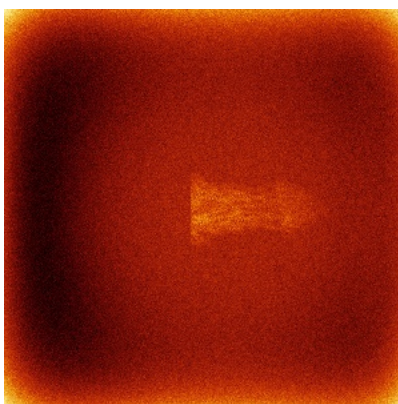


Z

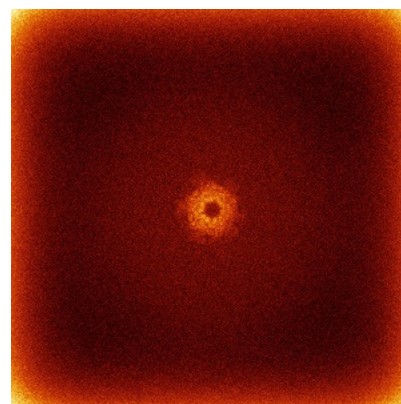
6.4.2 Raw map



X



Y

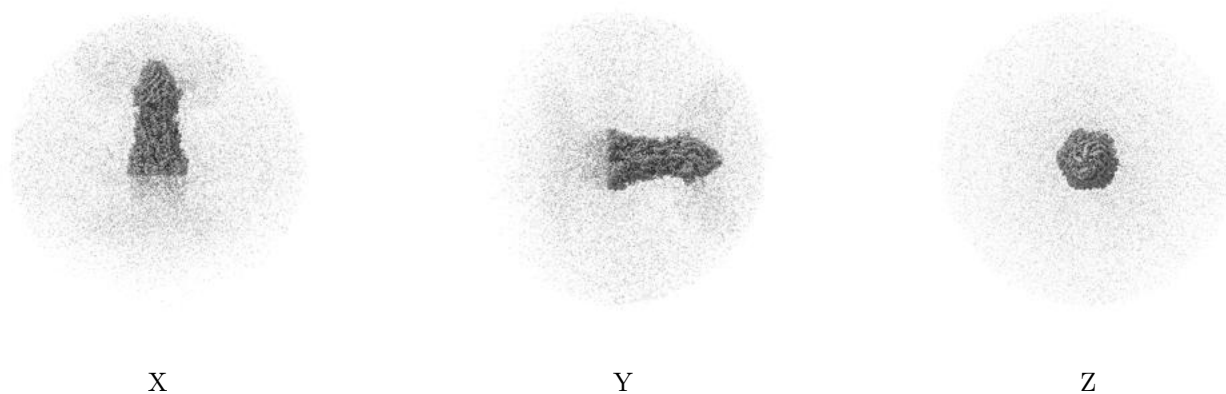


Z

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

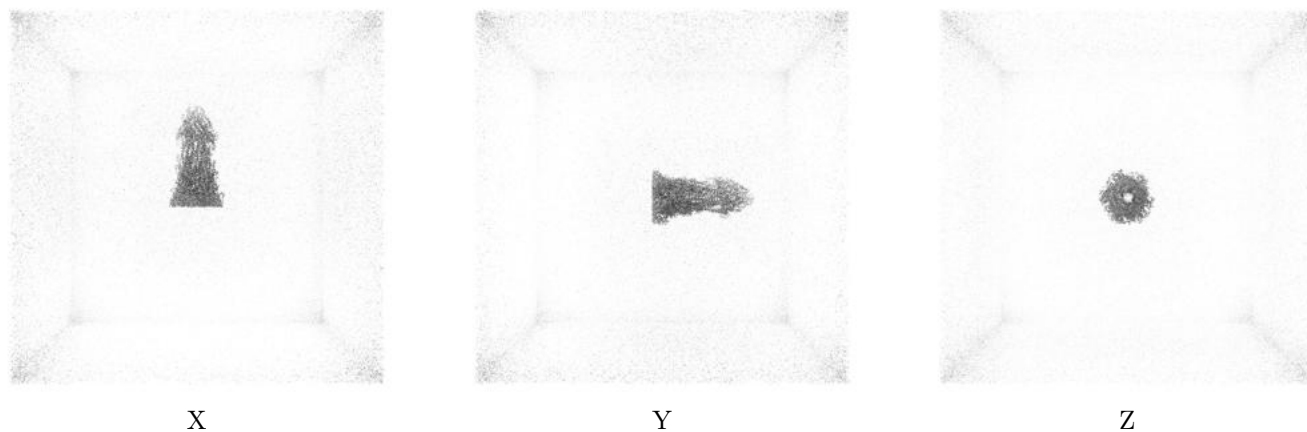
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

6.5.2 Raw map



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

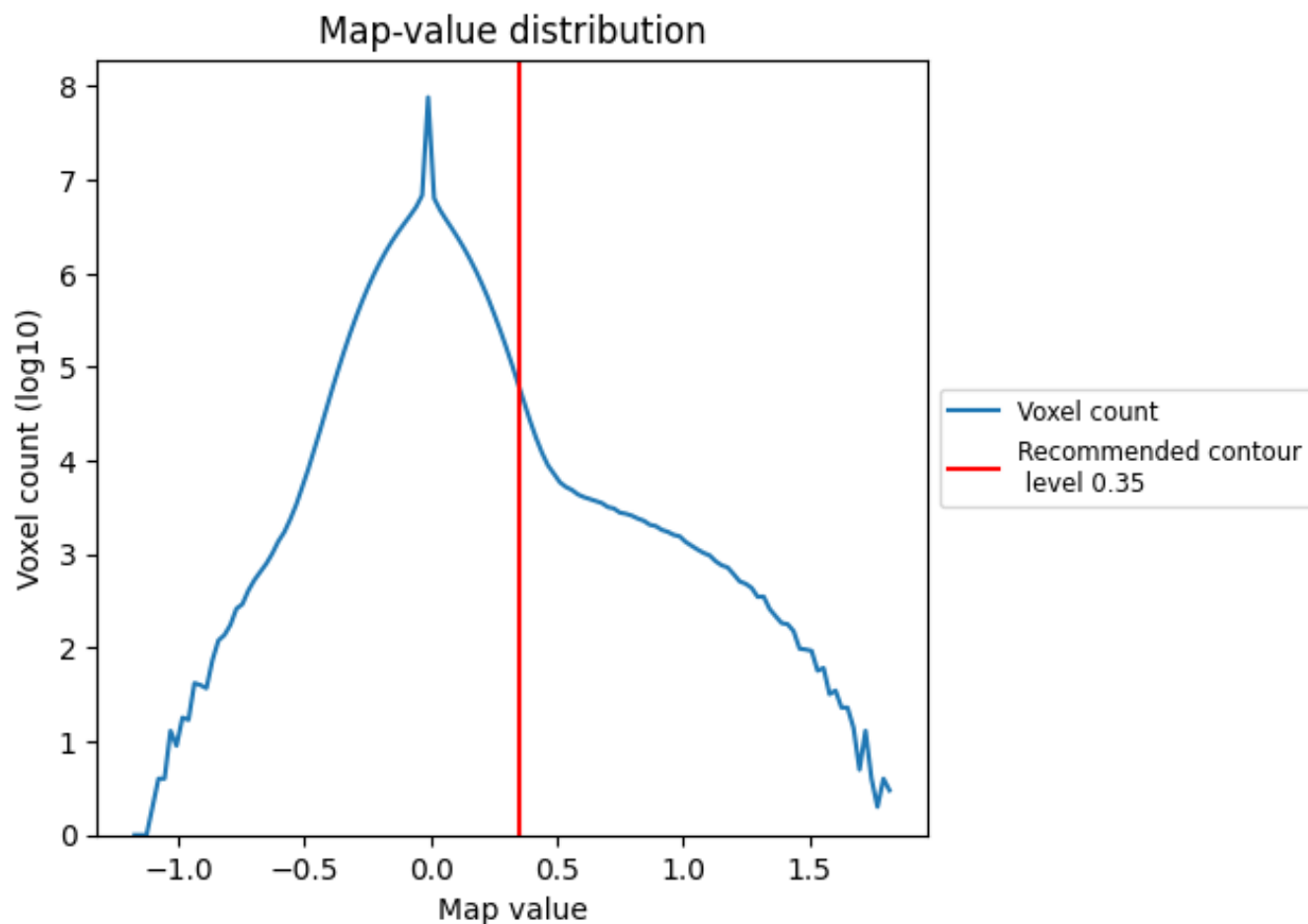
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

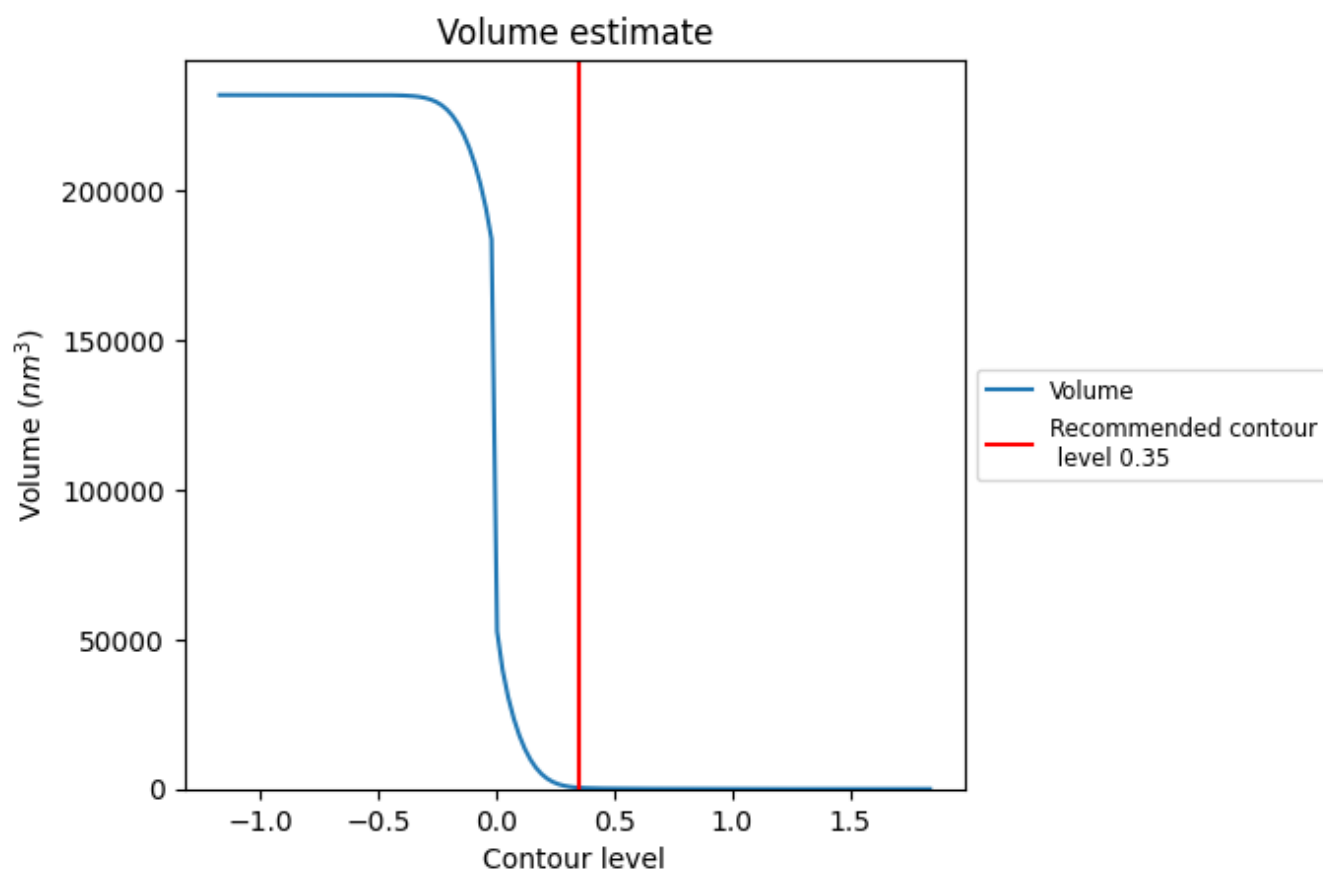
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

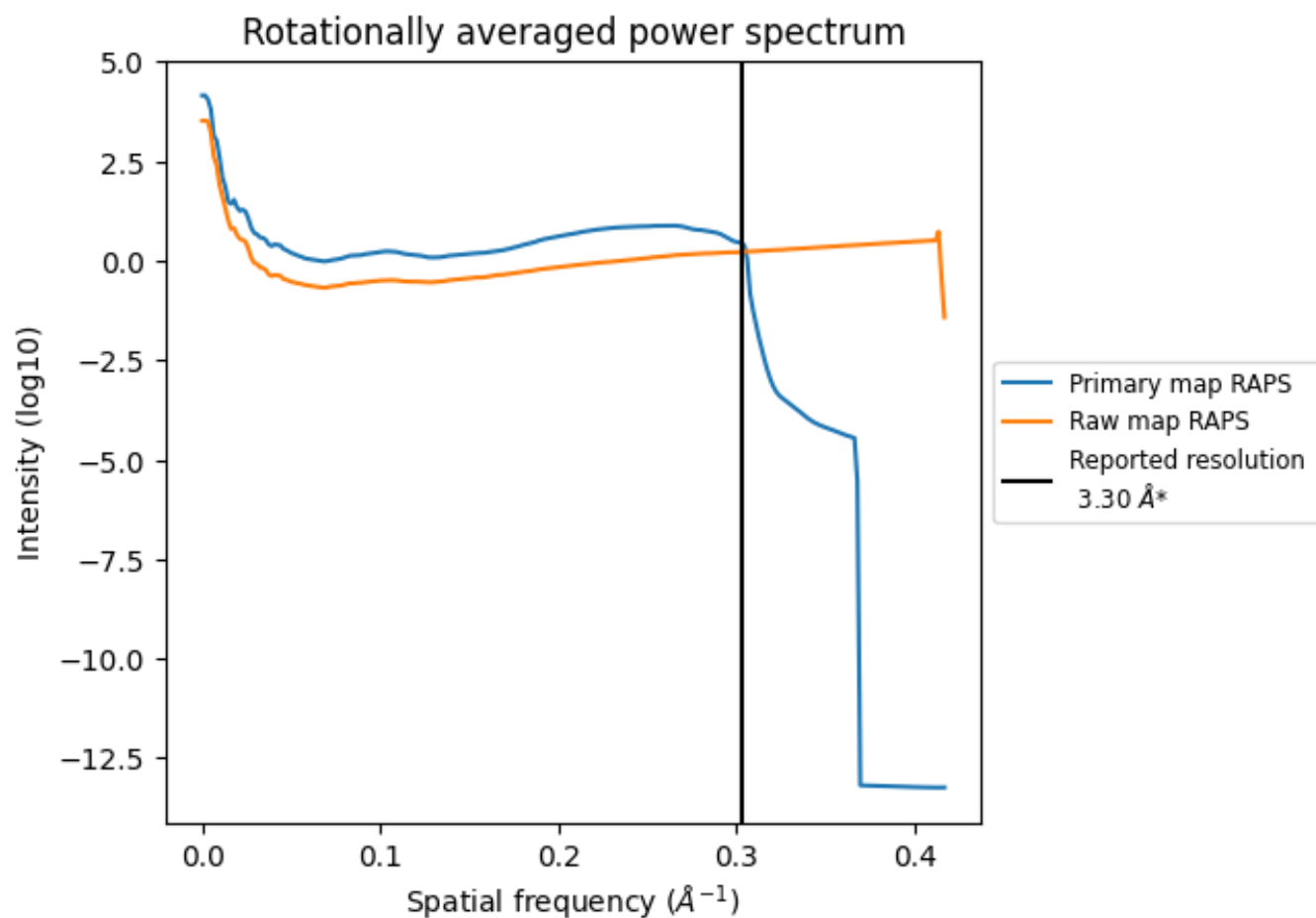
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 429 nm^3 ; this corresponds to an approximate mass of 387 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

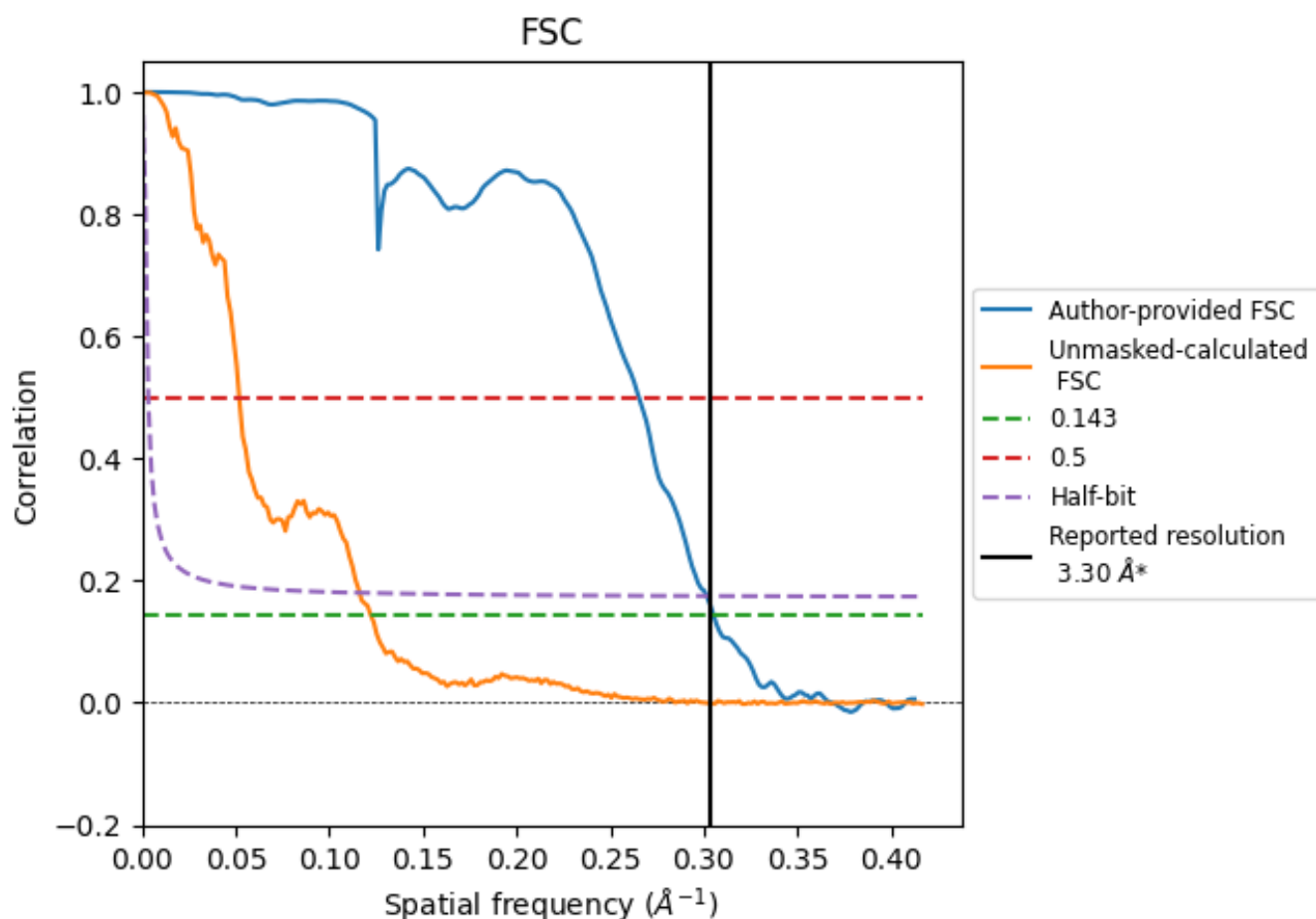


*Reported resolution corresponds to spatial frequency of 0.303 $\text{\AA}^{-1}$

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 0.303 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.28	3.77	3.32
Unmasked-calculated*	8.19	19.31	8.61

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

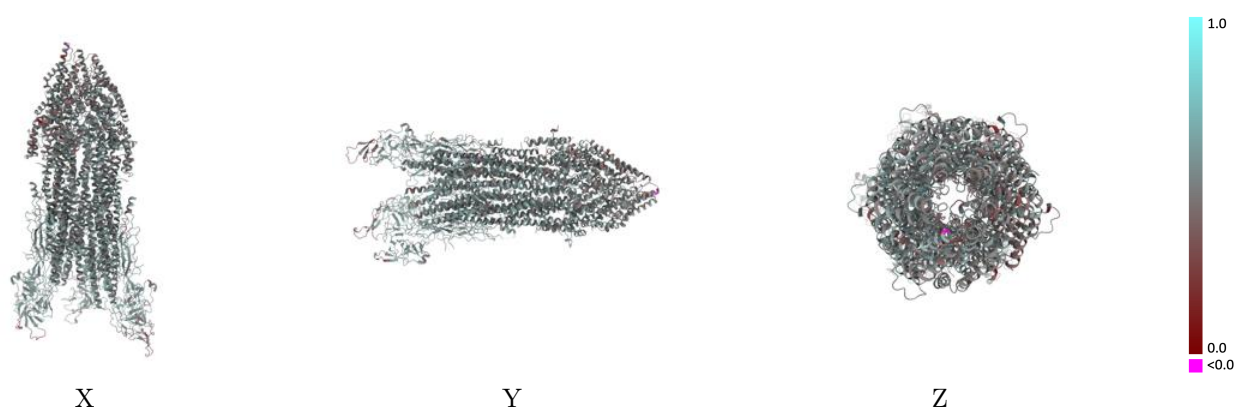
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-37594 and PDB model 8WK3. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)

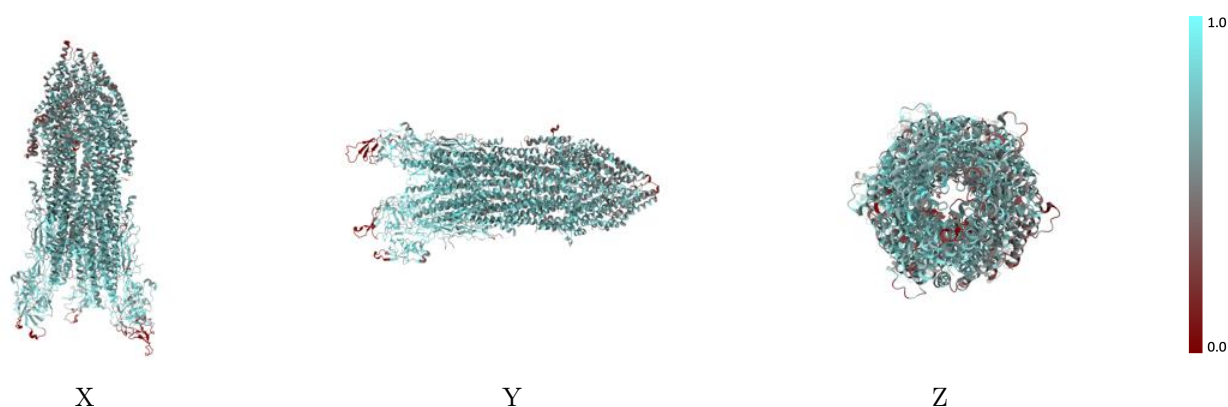
This section was not generated.

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



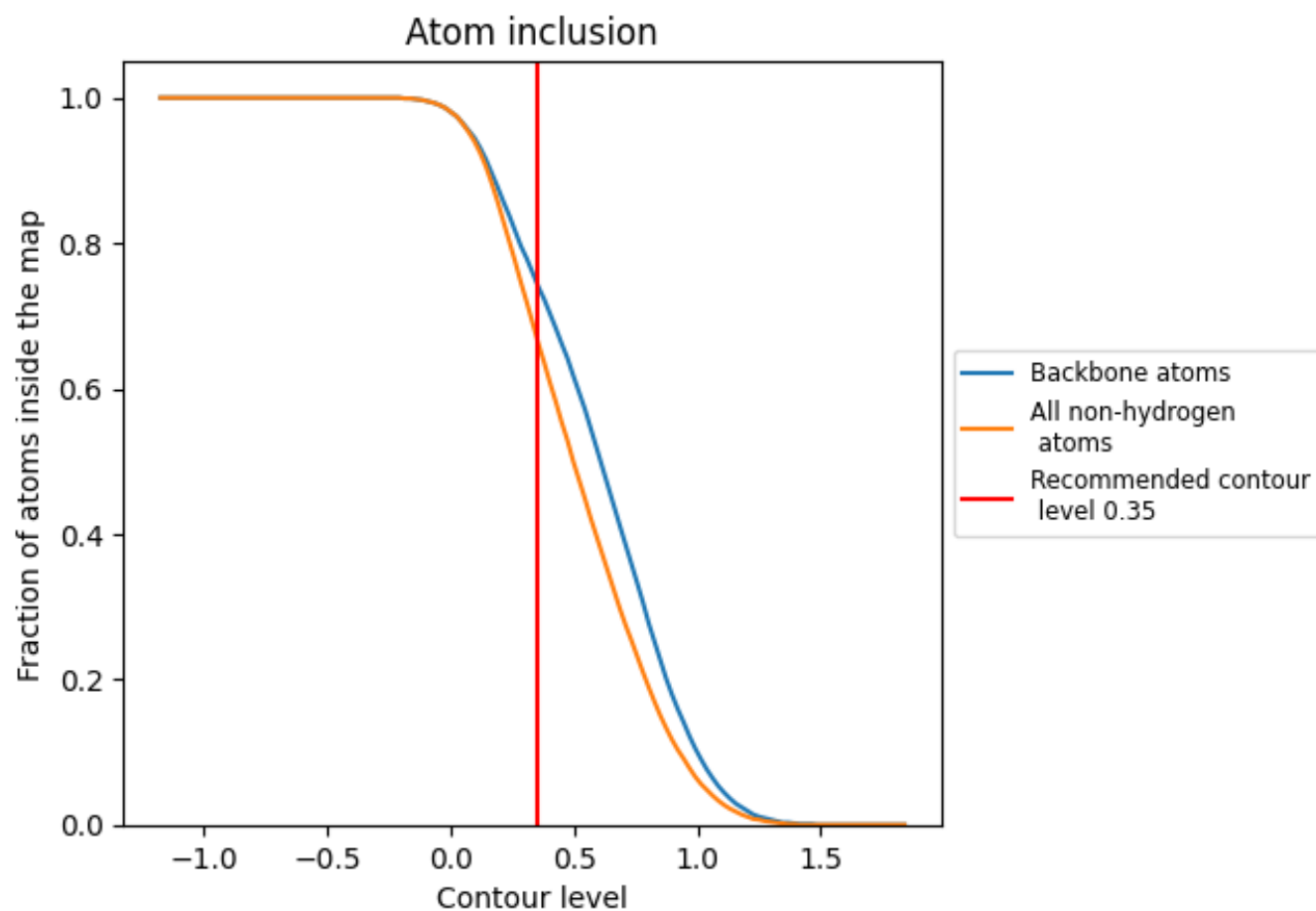
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 67% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6700	 0.5160
A	 0.5010	 0.4560
B	 0.5990	 0.4880
C	 0.5990	 0.4730
D	 0.5430	 0.4670
E	 0.5210	 0.4510
F	 0.6250	 0.4920
G	 0.7090	 0.5160
H	 0.7270	 0.5200
I	 0.6900	 0.5170
J	 0.6310	 0.5020
K	 0.6330	 0.5210
L	 0.7060	 0.5220
M	 0.7280	 0.5360
N	 0.7250	 0.5390
O	 0.6840	 0.5160
P	 0.6750	 0.5030
Q	 0.6710	 0.5230
R	 0.7420	 0.5320
S	 0.7510	 0.5420
T	 0.7290	 0.5330
U	 0.7120	 0.5230
V	 0.6750	 0.5200
W	 0.7320	 0.5390
X	 0.7400	 0.5430
Y	 0.7260	 0.5310
Z	 0.7160	 0.5310
a	 0.6750	 0.5220
b	 0.4940	 0.4790
c	 0.6210	 0.5170
d	 0.6320	 0.5250
e	 0.6990	 0.5460
f	 0.6710	 0.5110
g	 0.6990	 0.5260
h	 0.6790	 0.5470



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Chain	Atom inclusion	Q-score
i	 0.6210	 0.5070
j	 0.6920	 0.5080
k	 0.6210	 0.5170
l	 0.6290	 0.5150
m	 0.6720	 0.5270
n	 0.7170	 0.5390
o	 0.7250	 0.5380
p	 0.6710	 0.5280
q	 0.5840	 0.5080