



Full wwPDB EM Validation Report ⓘ

Oct 14, 2025 – 04:51 PM JST

PDB ID : 8Z5W / pdb_00008z5w
EMDB ID : EMD-39786
Title : Cryo-EM structure of the LRR protein within the polar flagellar motor
Authors : Zhang, L.; Tan, J.X.; Zhou, Y.; Zhu, Y.Q.
Deposited on : 2024-04-18
Resolution : 3.46 Å (reported)
Based on initial model : .

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

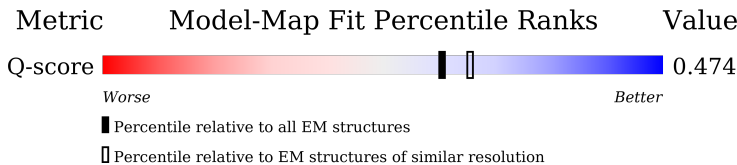
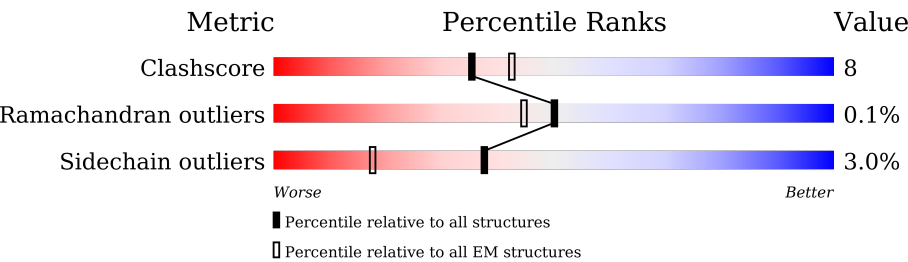
EMDB validation analysis : 0.0.1.dev129
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.46 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	13788 (2.96 - 3.96)

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

Mol	Chain	Length	Quality of chain
1	0	199	<div><div>47%</div><div><div></div><div>66%</div><div>23%</div><div>10%</div></div><div></div></div>
1	9	199	<div><div>23%</div><div><div></div><div>73%</div><div>17%</div><div>10%</div></div><div></div></div>
2	A	262	<div><div>32%</div><div><div></div><div>81%</div><div>18%</div><div></div></div><div></div></div>
2	AP	262	<div><div>18%</div><div><div></div><div>82%</div><div>17%</div><div></div></div><div></div></div>






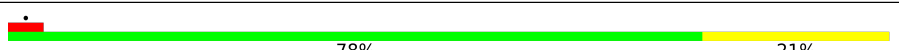
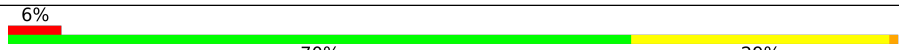
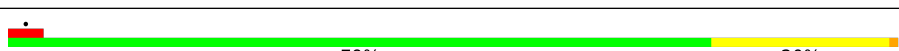
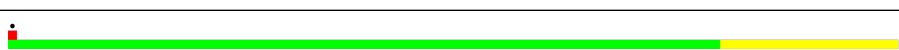

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Mol	Chain	Length	Quality of chain
2	AQ	262	
2	AR	262	
2	B	262	
2	C	262	
3	AA	580	
3	AB	580	
3	AC	580	
3	AD	580	
3	AE	580	
3	AF	580	
3	AG	580	
3	AH	580	
3	AI	580	
3	AJ	580	
3	AK	580	
3	AL	580	
3	AM	580	
3	AN	580	
3	AO	580	
4	b	131	
4	c	131	
4	d	131	
4	e	131	
4	f	131	
5	g	137	

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Mol	Chain	Length	Quality of chain
5	h	137	
5	i	137	
5	j	137	
5	k	137	
5	l	137	
6	m	249	
6	n	249	
6	o	249	
6	p	249	
6	q	249	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 36128 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 Leucine-rich repeat protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	180	Total	C	N	O	S	0	0
			1361	876	231	253	1		
1	9	180	Total	C	N	O	S	0	0
			1361	876	231	253	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	262	Total	C	N	O	S	0	0
			1956	1208	334	405	9		
2	B	262	Total	C	N	O	S	0	0
			1956	1208	334	405	9		
2	C	262	Total	C	N	O	S	0	0
			1956	1208	334	405	9		
2	AP	262	Total	C	N	O	S	0	0
			1956	1208	334	405	9		
2	AQ	262	Total	C	N	O	S	0	0
			1956	1208	334	405	9		
2	AR	248	Total	C	N	O	S	0	0
			1858	1151	317	382	8		

- Molecule 3 is a protein called Flagellar M-ring protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AA	19	Total	C	N	O	S	0	0
			135	82	23	29	1		
3	AB	19	Total	C	N	O	S	0	0
			135	82	23	29	1		
3	AC	20	Total	C	N	O	S	0	0
			139	84	24	30	1		
3	AD	19	Total	C	N	O	S	0	0
			135	82	23	29	1		
3	AE	19	Total	C	N	O	S	0	0
			135	82	23	29	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	AF	23	Total	C	N	O	S	0	0
			158	97	27	33	1		
3	AG	11	Total	C	N	O		0	0
			73	46	13	14			
3	AH	11	Total	C	N	O		0	0
			73	46	13	14			
3	AI	11	Total	C	N	O		0	0
			73	46	13	14			
3	AJ	24	Total	C	N	O	S	0	0
			163	100	28	34	1		
3	AK	25	Total	C	N	O	S	0	0
			169	104	29	35	1		
3	AL	32	Total	C	N	O	S	0	0
			220	134	38	46	2		
3	AM	33	Total	C	N	O	S	0	0
			224	136	39	47	2		
3	AN	33	Total	C	N	O	S	0	0
			224	136	39	47	2		
3	AO	32	Total	C	N	O	S	0	0
			220	134	38	46	2		

- Molecule 4 is a protein called Flagellar basal body rod protein FlgB.

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

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

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

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

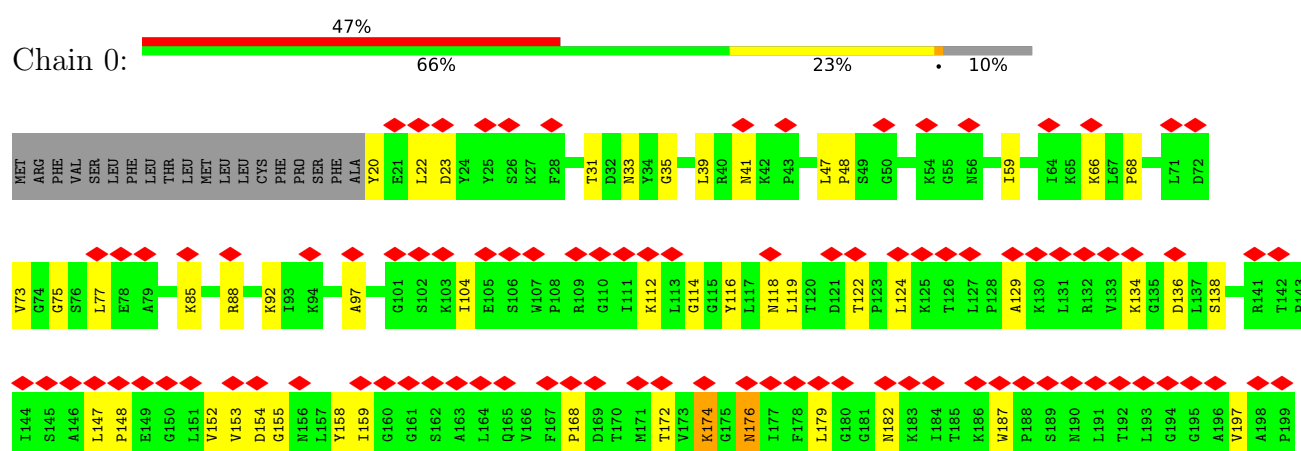
- Molecule 6 is a protein called Flagellar basal-body rod protein FlgF.

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

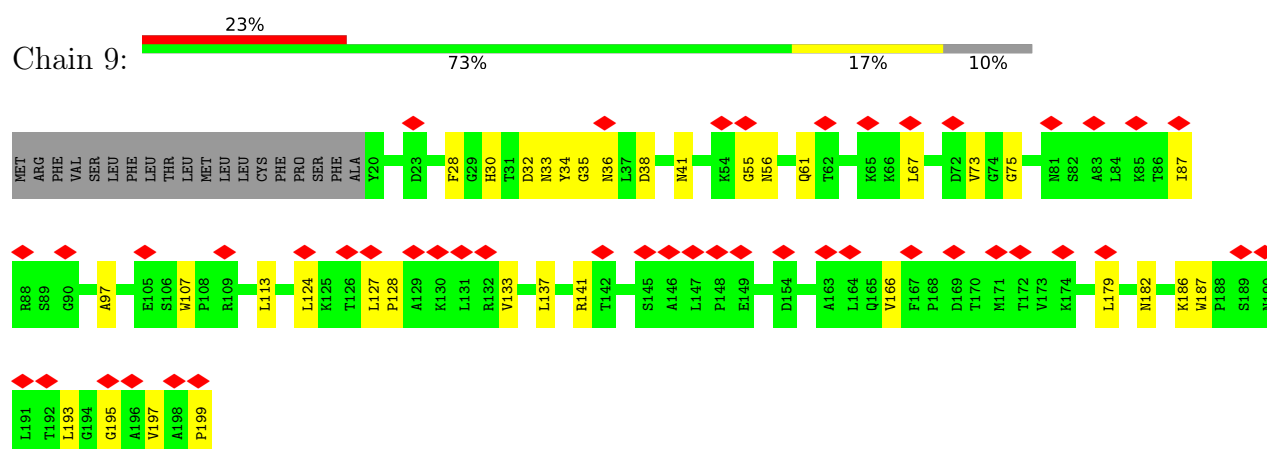
3 Residue-property plots

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

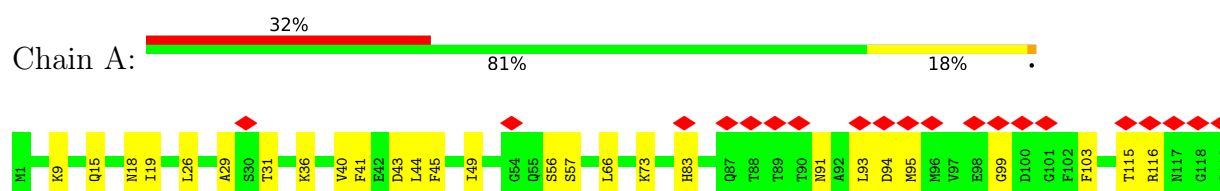
• Molecule 1: Leucine-rich repeat protein

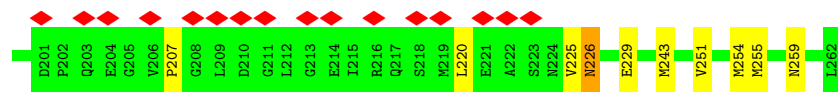


• Molecule 1: Leucine-rich repeat protein

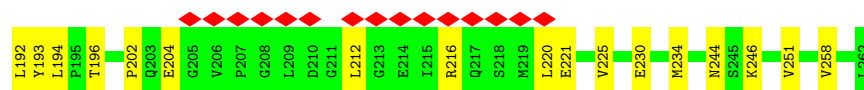
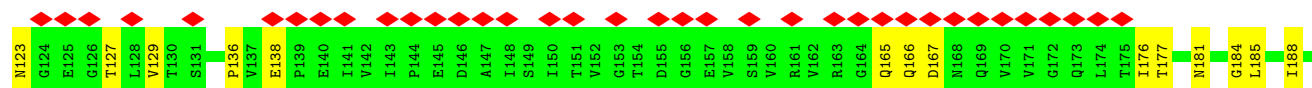
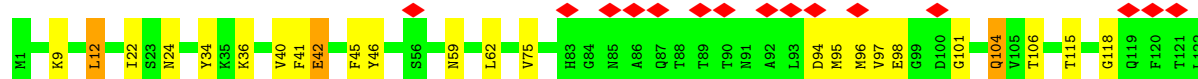
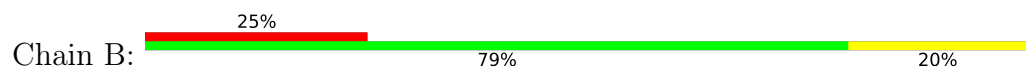


• Molecule 2: Flagellar basal-body rod protein FlgG

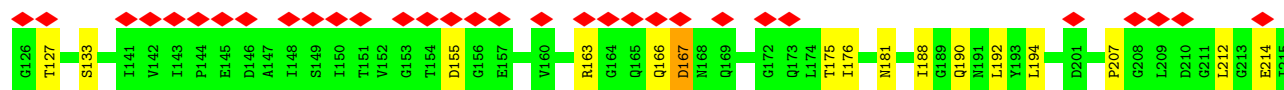
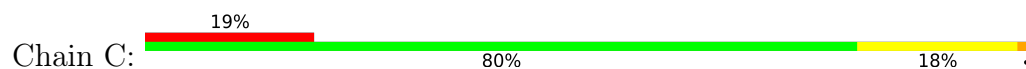




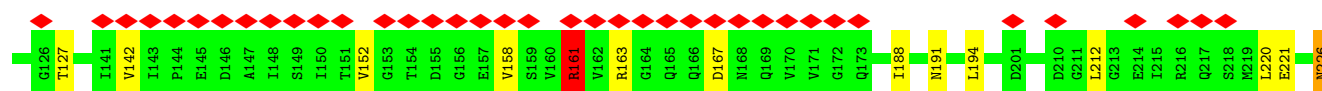
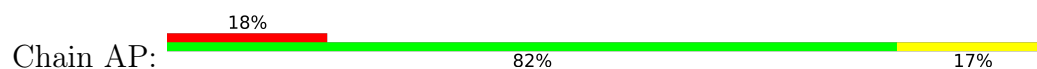
• Molecule 2: Flagellar basal-body rod protein FlgG



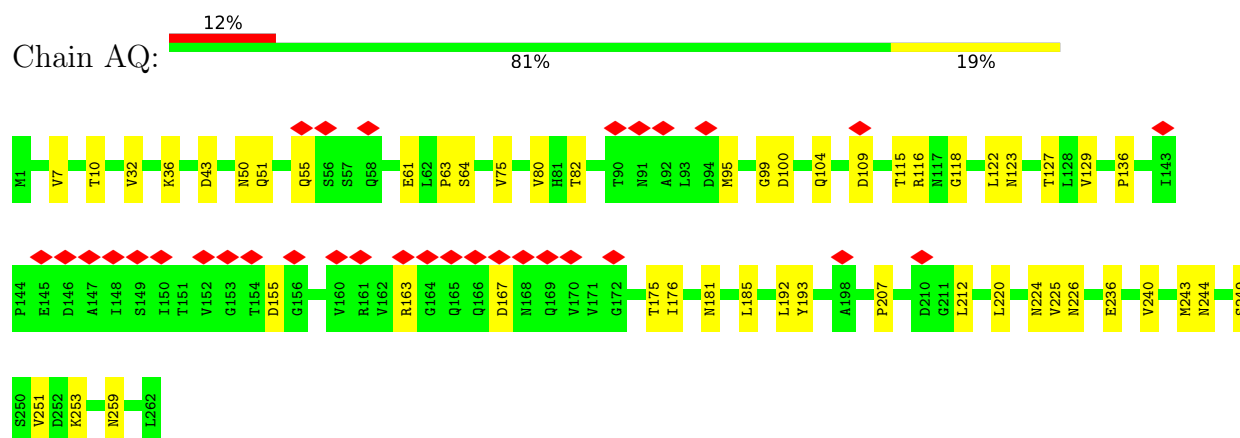
• Molecule 2: Flagellar basal-body rod protein FlgG



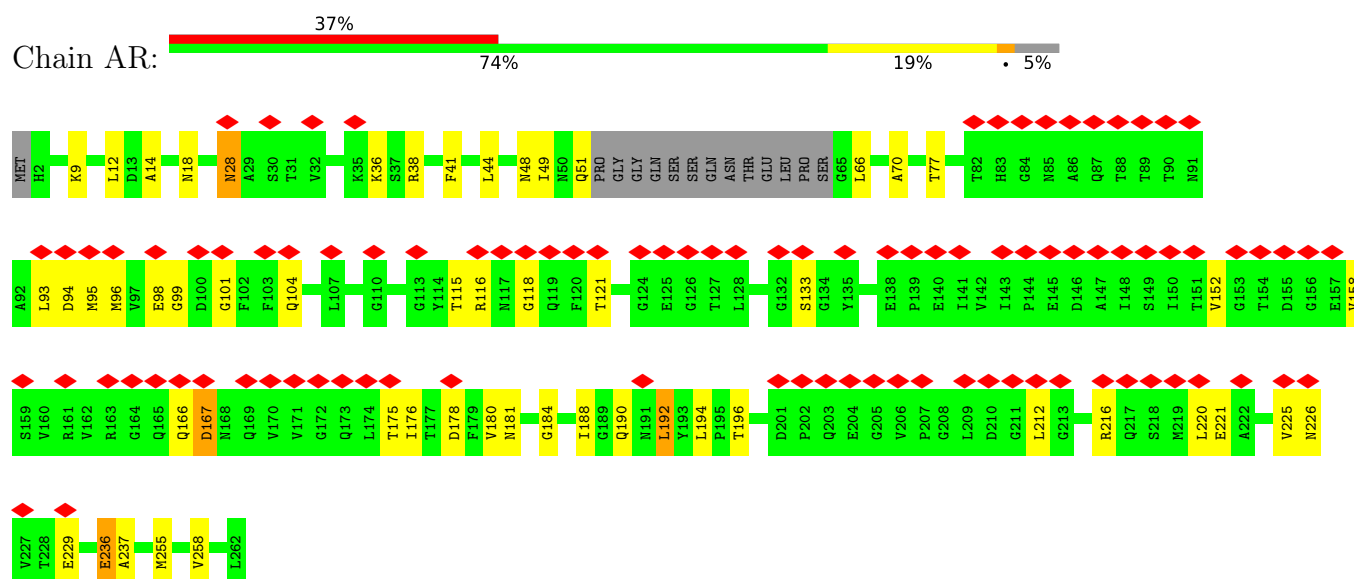
• Molecule 2: Flagellar basal-body rod protein FlgG



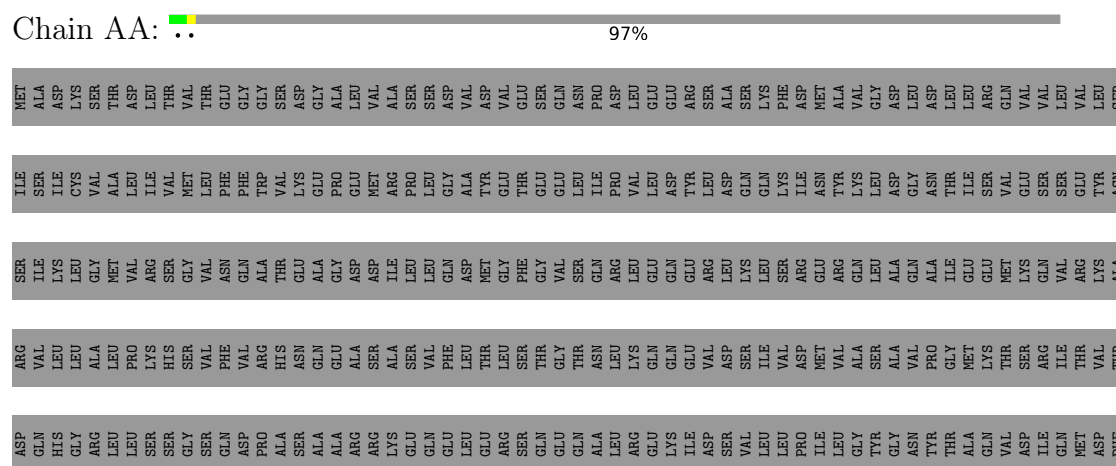
- Molecule 2: Flagellar basal-body rod protein FlgG

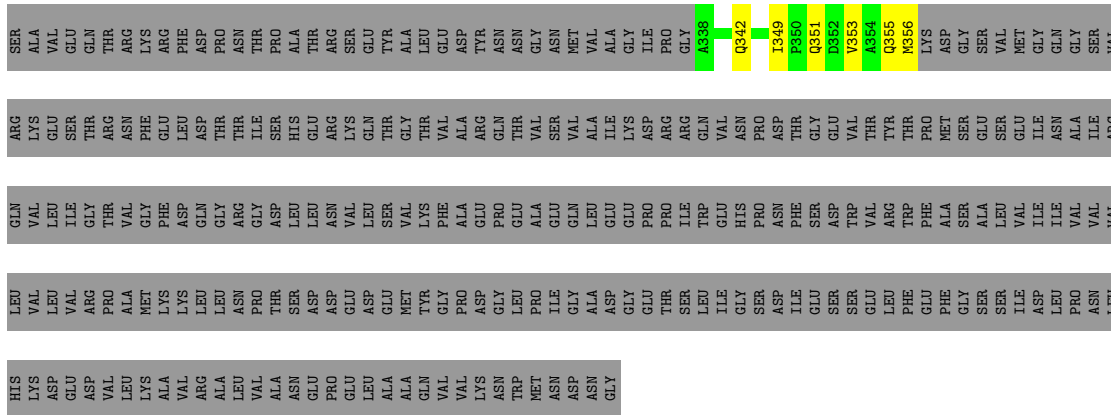


- Molecule 2: Flagellar basal-body rod protein FlgG



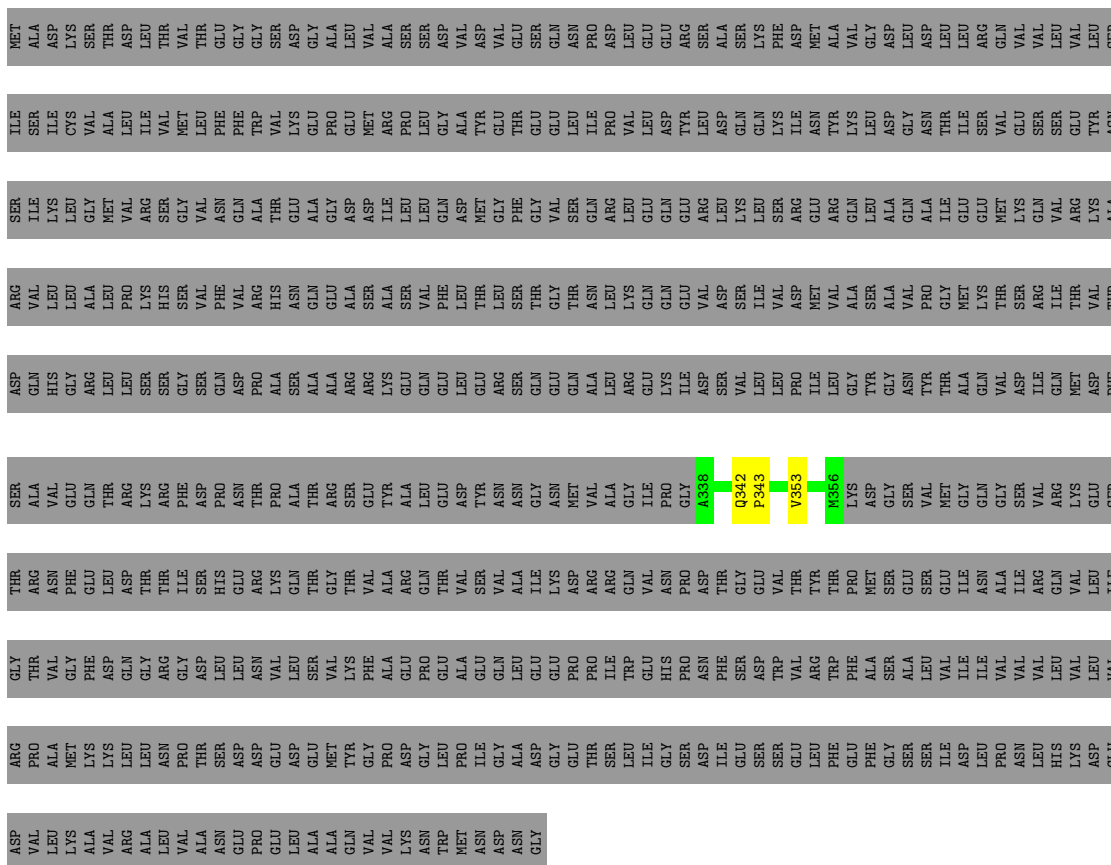
- Molecule 3: Flagellar M-ring protein





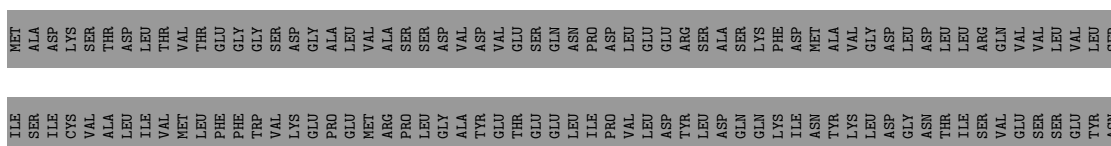
- Molecule 3: Flagellar M-ring protein

Chain AB:  97%

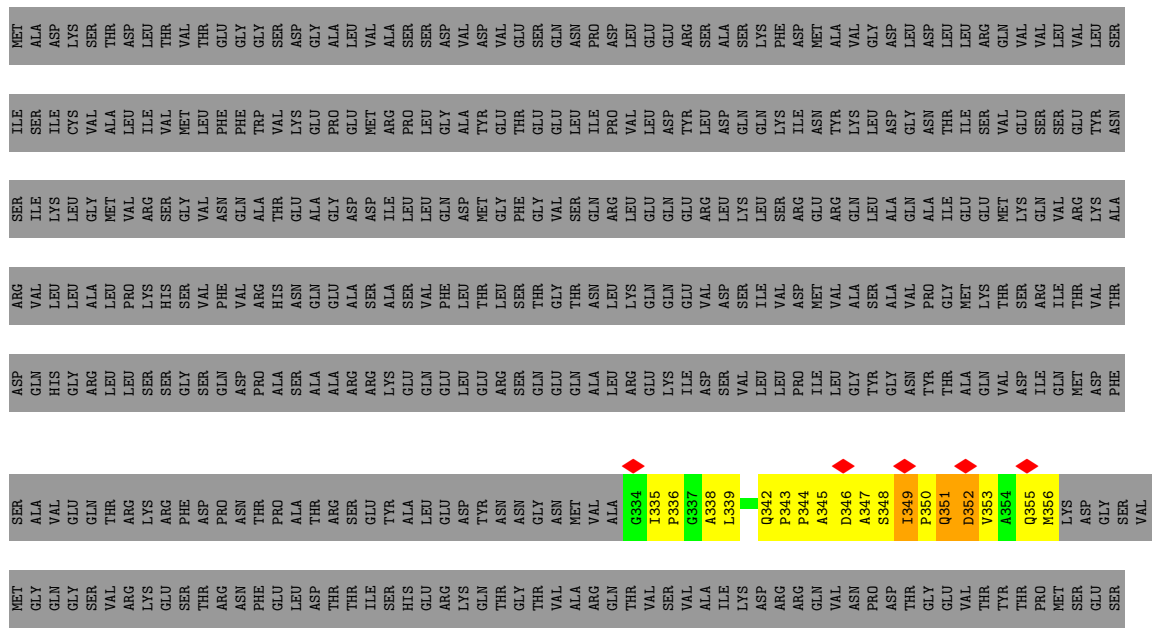


- Molecule 3: Flagellar M-ring protein

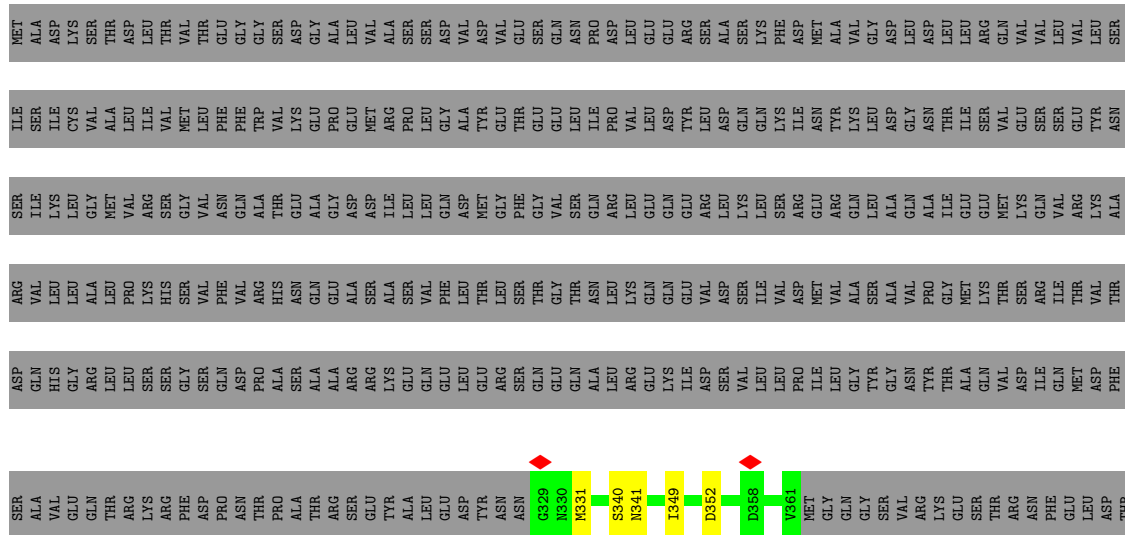
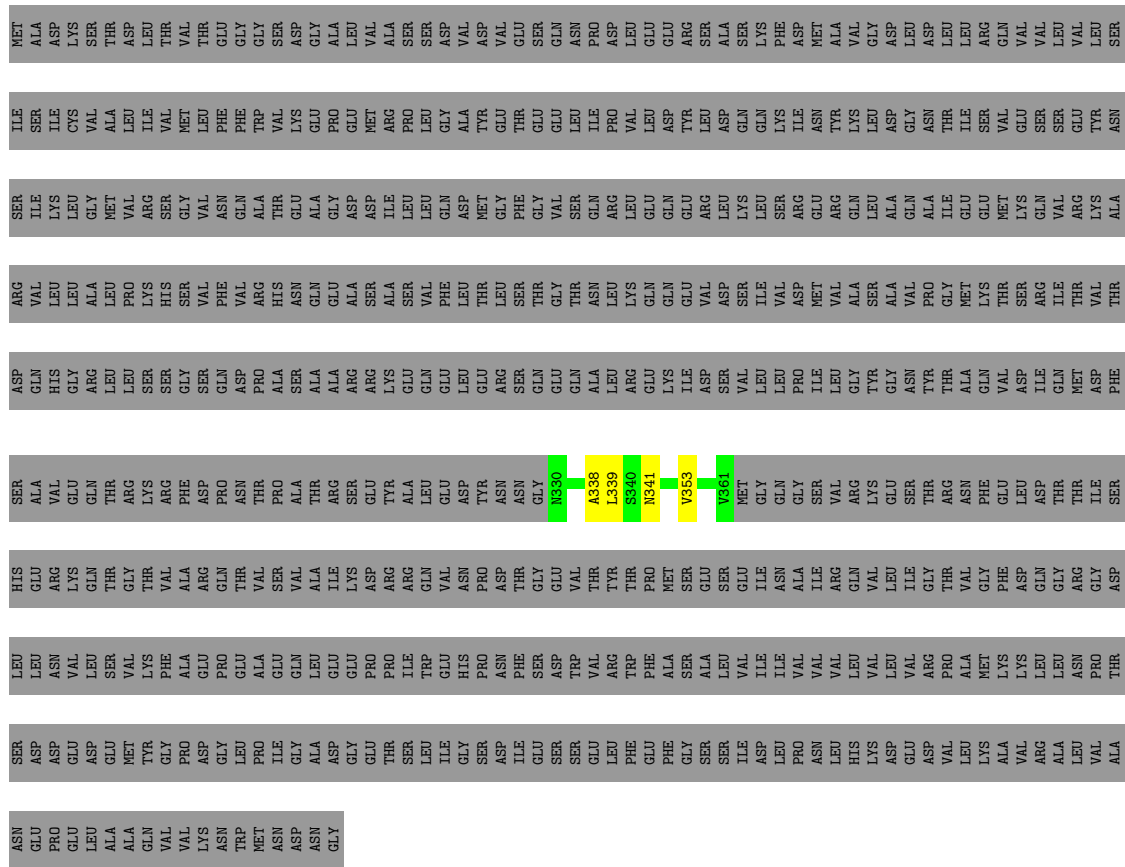
Chain AC:  97%



Chain AE: 97%







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

- Molecule 3: Flagellar M-ring protein

Chain AN:  5% 94%

[illegible]

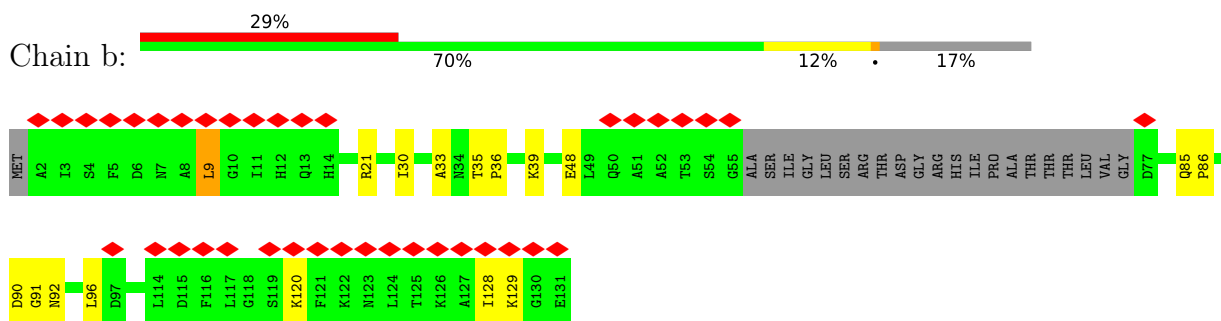
- Molecule 3: Flagellar M-ring protein

Chain AO: 94%

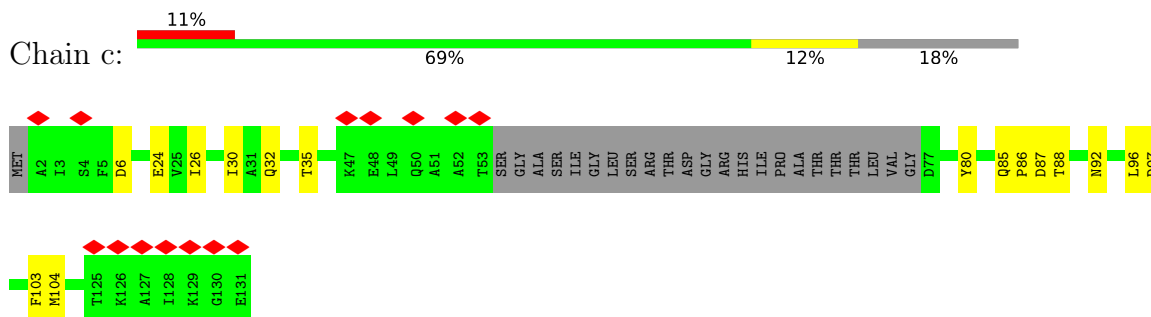
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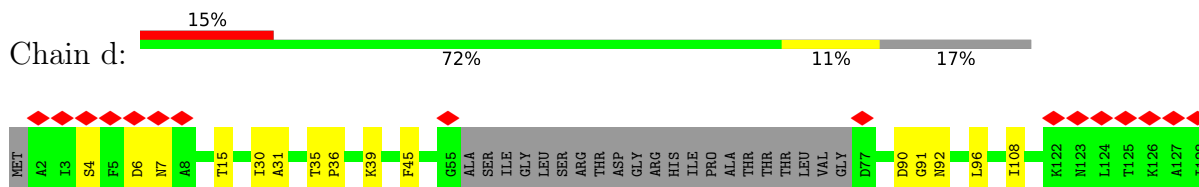
- Molecule 4: Flagellar basal body rod protein FlgB



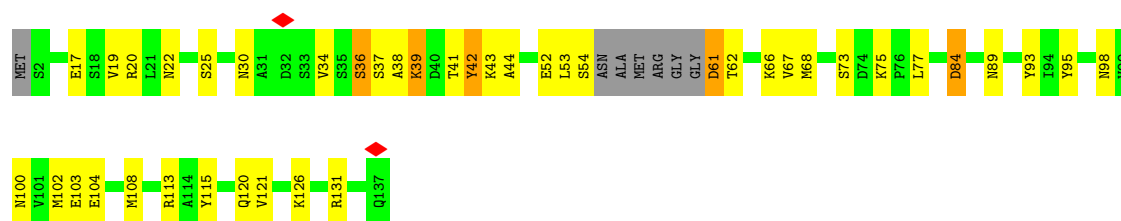
- Molecule 4: Flagellar basal body rod protein FlgB



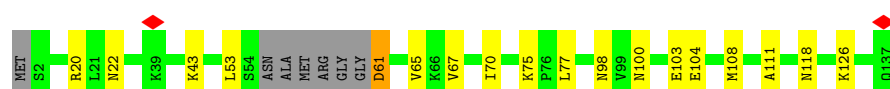
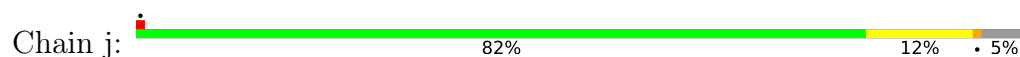
- Molecule 4: Flagellar basal body rod protein FlgB



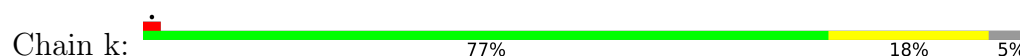




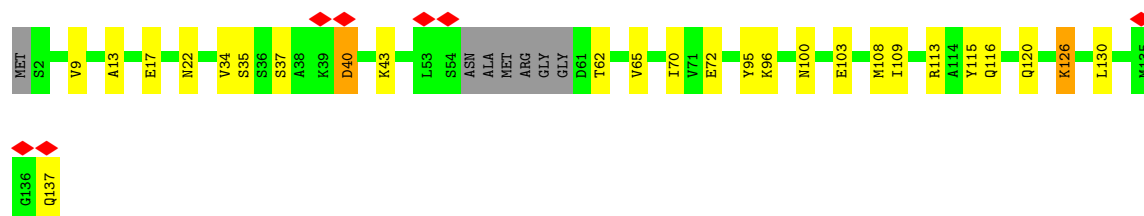
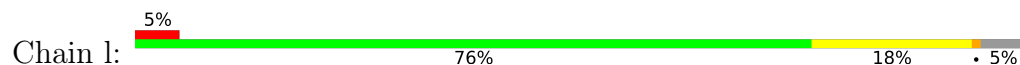
- Molecule 5: Flagellar basal-body rod protein FlgC



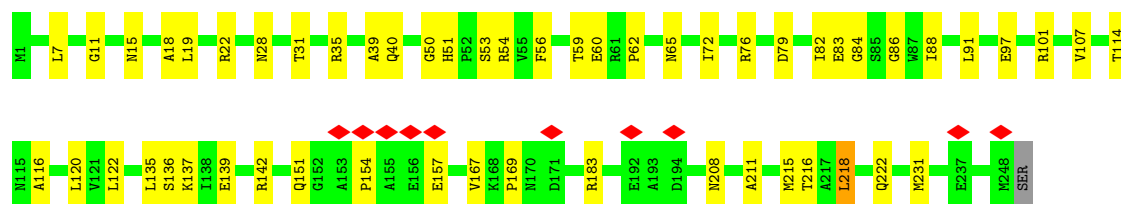
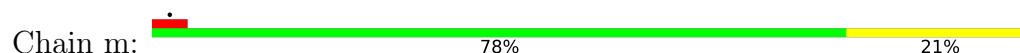
- Molecule 5: Flagellar basal-body rod protein FlgC



- Molecule 5: Flagellar basal-body rod protein FlgC

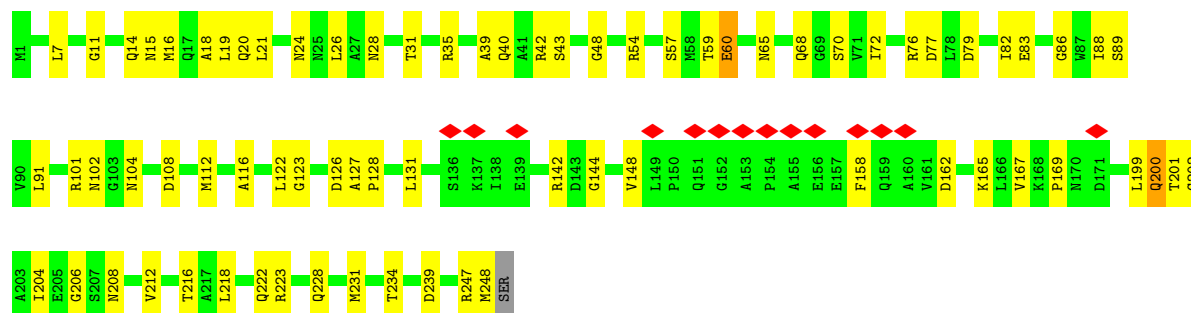


- Molecule 6: Flagellar basal-body rod protein FlgF

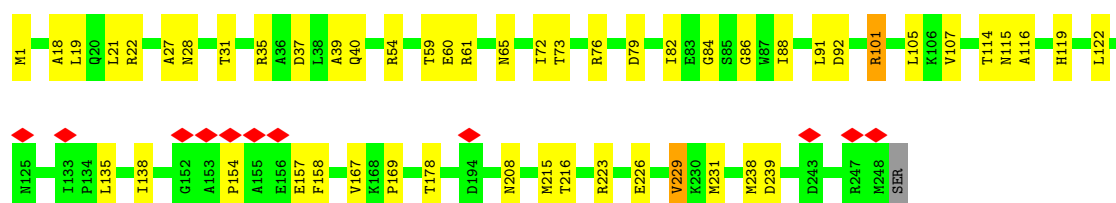
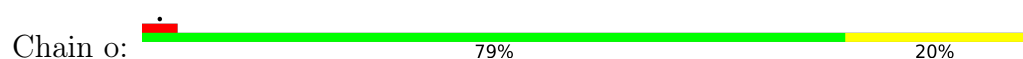


- Molecule 6: Flagellar basal-body rod protein FlgF

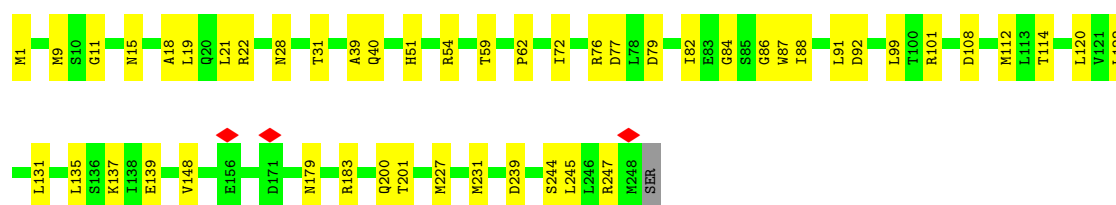
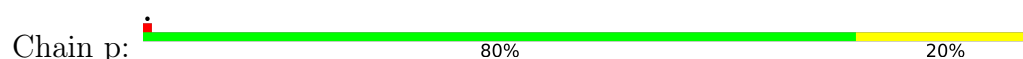




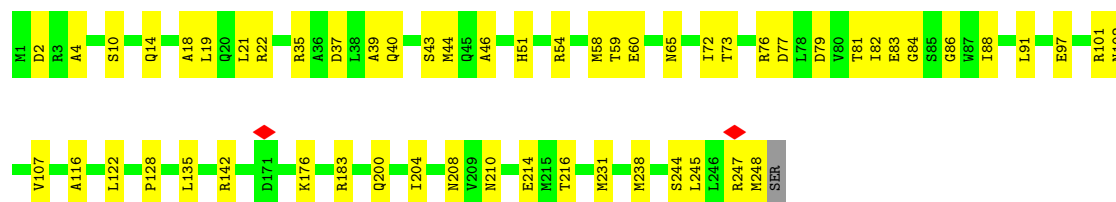
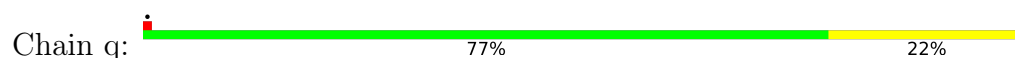
- Molecule 6: Flagellar basal-body rod protein FlgF



- Molecule 6: Flagellar basal-body rod protein FlgF



- Molecule 6: 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	19450	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	105000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.014	Depositor
Minimum map value	-1.257	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.073	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	744.0, 744.0, 744.0	wwPDB
Map dimensions	620, 620, 620	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2, 1.2, 1.2	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	0	0.10	0/1389	0.27	0/1884
1	9	0.10	0/1389	0.28	0/1884
2	A	0.17	0/1985	0.33	0/2697
2	AP	0.15	0/1985	0.34	1/2697 (0.0%)
2	AQ	0.10	0/1985	0.24	0/2697
2	AR	0.14	0/1884	0.28	0/2558
2	B	0.14	0/1985	0.32	0/2697
2	C	0.10	0/1985	0.24	0/2697
3	AA	0.35	0/137	0.45	0/188
3	AB	0.29	0/137	0.43	0/188
3	AC	0.15	0/141	0.31	0/193
3	AD	0.31	0/137	0.46	0/188
3	AE	0.12	0/137	0.28	0/188
3	AF	0.92	0/161	1.23	0/221
3	AG	0.21	0/75	0.37	0/103
3	AH	0.21	0/75	0.42	0/103
3	AI	0.94	0/75	1.33	0/103
3	AJ	0.37	0/166	0.58	0/228
3	AK	0.31	0/172	0.70	0/237
3	AL	0.40	0/223	0.61	0/304
3	AM	0.20	0/227	0.44	0/309
3	AN	0.24	0/227	0.49	0/309
3	AO	0.17	0/223	0.40	0/304
4	b	0.22	0/856	0.36	0/1151
4	c	0.22	0/846	0.31	0/1138
4	d	0.24	0/856	0.31	0/1151
4	e	0.19	0/848	0.31	0/1140
4	f	0.22	0/848	0.35	0/1140
5	g	0.11	0/996	0.26	0/1348
5	h	0.11	0/996	0.26	0/1348
5	i	0.30	0/996	0.46	0/1348
5	j	0.10	0/996	0.24	0/1348
5	k	0.11	0/996	0.28	0/1348
5	l	0.13	0/996	0.30	0/1348

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	m	0.11	0/1905	0.26	0/2572
6	n	0.13	0/1905	0.26	0/2572
6	o	0.11	0/1905	0.26	0/2572
6	p	0.17	0/1905	0.36	1/2572 (0.0%)
6	q	0.10	0/1905	0.25	0/2572
All	All	0.17	0/36655	0.33	2/49645 (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	AP	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	p	227	MET	N-CA-C	-8.13	103.49	113.41
2	AP	161	ARG	CB-CA-C	-7.48	97.41	109.75

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AP	161	ARG	Sidechain
2	AP	163	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	0	1361	0	1418	29	0
1	9	1361	0	1418	23	0
2	A	1956	0	1907	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	AP	1956	0	1907	28	0
2	AQ	1956	0	1907	28	0
2	AR	1858	0	1813	35	0
2	B	1956	0	1907	34	0
2	C	1956	0	1907	30	0
3	AA	135	0	128	4	0
3	AB	135	0	128	2	0
3	AC	139	0	131	0	0
3	AD	135	0	128	2	0
3	AE	135	0	128	2	0
3	AF	158	0	152	16	0
3	AG	73	0	72	4	0
3	AH	73	0	72	4	0
3	AI	73	0	72	8	0
3	AJ	163	0	157	5	0
3	AK	169	0	164	5	0
3	AL	220	0	215	3	0
3	AM	224	0	218	5	0
3	AN	224	0	218	2	0
3	AO	220	0	215	3	0
4	b	845	0	833	10	0
4	c	835	0	825	14	0
4	d	845	0	833	8	0
4	e	837	0	829	11	0
4	f	837	0	829	11	0
5	g	983	0	958	11	0
5	h	983	0	958	23	0
5	i	983	0	958	37	0
5	j	983	0	958	11	0
5	k	983	0	958	17	0
5	l	983	0	958	22	0
6	m	1879	0	1864	35	0
6	n	1879	0	1864	55	0
6	o	1879	0	1864	35	0
6	p	1879	0	1864	32	0
6	q	1879	0	1864	40	0
All	All	36128	0	35599	552	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.

All (552) 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)
5:i:52:GLU:HG3	5:i:52:GLU:O	1.47	1.06
5:i:52:GLU:O	5:i:52:GLU:CG	2.15	0.94
1:9:34:TYR:HD2	5:i:39:LYS:HA	1.51	0.73
1:0:138:SER:OG	3:AF:356:MET:HE1	1.88	0.73
6:n:102:ASN:HD21	6:n:116:ALA:HB3	1.55	0.72
1:9:179:LEU:O	1:9:182:ASN:ND2	2.22	0.71
1:0:119:LEU:HD13	1:0:124:LEU:HD22	1.71	0.71
1:9:34:TYR:CD2	5:i:39:LYS:HA	2.24	0.71
4:c:86:PRO:O	6:n:54:ARG:NH1	2.24	0.71
2:AR:98:GLU:HG3	2:AR:216:ARG:HG3	1.74	0.69
6:m:22:ARG:HE	6:m:39:ALA:HB3	1.58	0.69
2:AR:133:SER:OG	2:AR:190:GLN:NE2	2.25	0.68
3:AL:341:ASN:ND2	4:c:88:THR:OG1	2.27	0.68
5:l:40:ASP:N	5:l:40:ASP:OD1	2.27	0.68
3:AF:335:ILE:HG13	3:AF:338:ALA:HB2	1.74	0.68
2:AP:117:ASN:HD21	2:AP:119:GLN:HE21	1.42	0.67
2:AQ:99:GLY:O	2:AQ:116:ARG:NH2	2.28	0.67
2:A:99:GLY:O	2:A:116:ARG:NH2	2.27	0.67
5:i:36:SER:HB2	6:n:43:SER:HB2	1.77	0.67
6:q:86:GLY:O	6:q:101:ARG:NH1	2.28	0.67
6:n:24:ASN:O	6:n:28:ASN:ND2	2.24	0.66
6:o:65:ASN:O	6:o:208:ASN:ND2	2.29	0.66
3:AA:355:GLN:O	3:AA:356:MET:HB3	1.94	0.66
5:i:53:LEU:O	5:i:54:SER:C	2.38	0.65
5:j:75:LYS:O	5:j:98:ASN:ND2	2.29	0.65
5:h:22:ASN:HD22	6:o:54:ARG:HE	1.45	0.65
6:o:135:LEU:HD13	6:o:138:ILE:HD11	1.78	0.64
2:B:42:GLU:HG2	2:B:75:VAL:HB	1.78	0.64
6:n:83:GLU:OE2	6:n:142:ARG:NH1	2.30	0.64
3:AI:335:ILE:HG13	3:AI:338:ALA:HB2	1.78	0.63
2:AQ:176:ILE:HD11	2:AQ:212:LEU:HB3	1.79	0.63
4:c:85:GLN:OE1	6:n:54:ARG:NH2	2.31	0.63
5:i:108:MET:HE2	6:n:231:MET:HE2	1.80	0.63
5:i:43:LYS:HG2	5:i:77:LEU:HD21	1.80	0.62
6:m:91:LEU:HD23	6:m:122:LEU:HD21	1.80	0.62
6:p:137:LYS:NZ	6:p:139:GLU:OE2	2.32	0.62
4:f:30:ILE:HG23	4:f:96:LEU:HD11	1.80	0.62
3:AI:334:GLY:O	3:AI:335:ILE:C	2.40	0.62
5:i:61:ASP:OD1	5:i:61:ASP:N	2.33	0.62
6:m:11:GLY:O	6:m:15:ASN:ND2	2.31	0.62
2:A:133:SER:OG	2:A:190:GLN:NE2	2.33	0.61
4:d:35:THR:O	4:d:92:ASN:ND2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:136:ASP:HB2	3:AF:356:MET:HE3	1.82	0.61
3:AH:335:ILE:HB	3:AH:338:ALA:HB2	1.82	0.61
5:k:108:MET:HE2	6:p:231:MET:HE2	1.83	0.61
2:B:246:LYS:HE3	6:o:215:MET:HE2	1.81	0.61
5:h:17:GLU:OE1	5:h:20:ARG:NH2	2.32	0.61
2:C:249:SER:OG	2:C:253:LYS:NZ	2.33	0.60
6:p:84:GLY:O	6:p:101:ARG:NH2	2.32	0.60
2:B:123:ASN:HD21	2:B:127:THR:HB	1.66	0.60
6:n:76:ARG:NH1	6:n:79:ASP:OD1	2.34	0.60
6:p:11:GLY:O	6:p:15:ASN:ND2	2.30	0.60
5:l:35:SER:OG	6:q:40:GLN:NE2	2.35	0.60
3:AI:335:ILE:HD12	5:h:71:VAL:HG23	1.82	0.60
5:k:75:LYS:O	5:k:98:ASN:ND2	2.34	0.60
4:e:15:THR:HG23	4:e:45:PHE:HZ	1.67	0.60
5:k:22:ASN:HD22	6:p:54:ARG:HE	1.48	0.60
5:i:22:ASN:HD22	6:n:54:ARG:HE	1.49	0.60
1:O:22:LEU:HB3	1:O:48:PRO:HD3	1.84	0.60
2:AR:36:LYS:HB3	2:AR:225:VAL:HG12	1.84	0.60
5:i:100:ASN:HD22	5:i:103:GLU:H	1.49	0.60
5:l:37:SER:HB3	6:q:44:MET:HA	1.84	0.59
6:q:65:ASN:O	6:q:208:ASN:ND2	2.34	0.59
6:m:86:GLY:O	6:m:101:ARG:NH1	2.35	0.59
4:f:86:PRO:O	6:p:54:ARG:NH1	2.36	0.59
5:l:113:ARG:NH2	5:l:116:GLN:OE1	2.36	0.59
3:AF:350:PRO:HA	3:AF:353:VAL:HG22	1.83	0.59
6:q:102:ASN:HD21	6:q:116:ALA:HB3	1.66	0.59
2:AP:127:THR:HG22	2:AP:142:VAL:HG22	1.84	0.59
4:d:108:ILE:HD11	5:h:126:LYS:HG3	1.85	0.59
6:o:91:LEU:HD23	6:o:122:LEU:HD21	1.85	0.58
5:j:22:ASN:HD22	6:m:54:ARG:HE	1.52	0.58
2:C:28:ASN:HD22	2:C:31:THR:HG21	1.68	0.58
2:AR:176:ILE:HG13	2:AR:212:LEU:HD22	1.83	0.58
4:f:35:THR:O	4:f:92:ASN:ND2	2.37	0.58
3:AH:341:ASN:ND2	6:m:50:GLY:O	2.36	0.58
5:j:61:ASP:N	5:j:61:ASP:OD1	2.35	0.58
2:C:109:ASP:N	2:C:109:ASP:OD1	2.36	0.58
2:A:94:ASP:HB2	2:A:220:LEU:HD21	1.84	0.58
4:f:41:ARG:HG2	4:f:78:LYS:HE2	1.85	0.58
6:o:22:ARG:HE	6:o:39:ALA:HB3	1.69	0.58
2:AR:101:GLY:O	2:AR:116:ARG:NH1	2.37	0.57
4:e:86:PRO:O	6:m:54:ARG:NH1	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AO:335:ILE:O	3:AO:340:SER:OG	2.14	0.57
3:AG:335:ILE:HB	3:AG:338:ALA:HB2	1.86	0.57
6:q:22:ARG:HE	6:q:39:ALA:HB3	1.68	0.57
3:AJ:341:ASN:ND2	6:n:48:GLY:O	2.38	0.57
2:C:99:GLY:O	2:C:116:ARG:NH2	2.37	0.57
4:b:86:PRO:O	6:q:54:ARG:NH1	2.38	0.57
6:n:104:ASN:HB3	6:n:116:ALA:HB2	1.87	0.57
6:o:86:GLY:O	6:o:101:ARG:NH1	2.37	0.57
5:g:75:LYS:O	5:g:98:ASN:ND2	2.33	0.57
5:h:35:SER:OG	6:o:40:GLN:NE2	2.38	0.57
5:k:61:ASP:OD1	5:k:61:ASP:N	2.38	0.57
6:o:40:GLN:NE2	6:o:60:GLU:OE2	2.35	0.57
2:C:251:VAL:HG22	6:m:19:LEU:HD21	1.87	0.57
1:9:166:VAL:HG13	1:9:186:LYS:HB3	1.86	0.57
2:A:152:VAL:HG22	2:A:158:VAL:HG22	1.87	0.57
3:AK:331:MET:HE3	5:g:52:GLU:HB2	1.87	0.57
3:AN:352:ASP:OD1	3:AN:352:ASP:N	2.38	0.57
5:h:61:ASP:OD1	5:h:61:ASP:N	2.36	0.56
5:l:34:VAL:HG12	5:l:96:LYS:HG2	1.87	0.56
2:AP:188:ILE:HD13	2:AP:194:LEU:HG	1.88	0.56
3:AI:335:ILE:HD11	5:h:69:GLY:HA3	1.86	0.56
5:i:17:GLU:OE1	5:i:20:ARG:NH2	2.34	0.56
6:m:83:GLU:OE2	6:m:142:ARG:NH2	2.39	0.56
6:p:82:ILE:HD11	6:p:88:ILE:HG13	1.88	0.56
5:j:108:MET:HE2	6:m:231:MET:HE2	1.87	0.56
2:AP:94:ASP:HB2	2:AP:220:LEU:HD21	1.88	0.56
5:h:108:MET:HE2	6:o:231:MET:HE2	1.87	0.56
2:B:166:GLN:HG2	2:B:167:ASP:OD1	2.06	0.56
2:AP:251:VAL:HG22	6:p:19:LEU:HD21	1.88	0.56
5:l:22:ASN:HD22	6:q:54:ARG:HE	1.53	0.56
6:p:86:GLY:O	6:p:101:ARG:NH1	2.39	0.56
6:n:126:ASP:OD1	6:n:165:LYS:NZ	2.31	0.56
3:AH:335:ILE:HD12	3:AN:356:MET:HE1	1.88	0.55
3:AF:350:PRO:O	3:AF:351:GLN:C	2.50	0.55
5:g:20:ARG:HH21	5:g:111:ALA:HA	1.71	0.55
6:p:76:ARG:NH1	6:p:79:ASP:OD1	2.39	0.55
2:AP:101:GLY:O	2:AP:116:ARG:NH1	2.35	0.55
2:AQ:259:ASN:O	5:i:120:GLN:NE2	2.39	0.55
2:A:36:LYS:HB3	2:A:225:VAL:HG12	1.89	0.55
5:k:3:LEU:HD21	5:k:128:MET:HE3	1.89	0.55
2:A:162:VAL:HG23	2:A:165:GLN:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:p:91:LEU:HD23	6:p:122:LEU:HD21	1.89	0.55
6:p:244:SER:HA	6:p:247:ARG:HG3	1.89	0.55
3:AD:348:SER:HB2	3:AD:356:MET:HE3	1.89	0.54
5:g:108:MET:HE2	5:i:121:VAL:HG22	1.89	0.54
6:m:154:PRO:HG2	6:m:157:GLU:HG3	1.89	0.54
2:B:36:LYS:HB3	2:B:225:VAL:HG12	1.89	0.54
3:AF:352:ASP:O	3:AF:353:VAL:C	2.51	0.54
2:AQ:249:SER:OG	2:AQ:253:LYS:NZ	2.40	0.54
5:k:3:LEU:HB3	5:k:129:LEU:HD21	1.89	0.54
2:AQ:123:ASN:HD21	2:AQ:127:THR:HB	1.71	0.54
5:k:43:LYS:HG2	5:k:77:LEU:HD21	1.90	0.54
2:A:43:ASP:OD1	2:A:43:ASP:N	2.41	0.54
2:AQ:115:THR:HB	2:AQ:192:LEU:HD12	1.90	0.54
4:c:30:ILE:HG23	4:c:96:LEU:HD11	1.89	0.54
6:p:18:ALA:HB2	6:p:59:THR:HG21	1.90	0.54
5:g:9:VAL:HG21	5:g:62:THR:HB	1.90	0.54
2:AR:99:GLY:O	2:AR:116:ARG:NH2	2.38	0.53
2:AR:184:GLY:O	2:AR:196:THR:OG1	2.24	0.53
5:l:108:MET:HE2	6:q:231:MET:HE2	1.89	0.53
5:l:126:LYS:HD3	6:q:248:MET:HG2	1.91	0.53
2:C:214:GLU:OE1	2:C:216:ARG:NH1	2.32	0.53
1:9:97:ALA:HB2	1:9:113:LEU:HD11	1.90	0.53
3:AJ:335:ILE:HG22	5:g:87:LEU:HD11	1.89	0.53
2:AQ:36:LYS:HB3	2:AQ:225:VAL:HG12	1.89	0.53
6:m:65:ASN:O	6:m:208:ASN:ND2	2.36	0.53
6:o:76:ARG:NH1	6:o:79:ASP:OD1	2.39	0.53
2:A:41:PHE:HB2	6:n:31:THR:HA	1.89	0.53
2:B:24:ASN:ND2	2:B:34:TYR:OH	2.41	0.53
2:AP:9:LYS:HD2	6:q:216:THR:HG21	1.90	0.53
3:AI:339:LEU:HD11	5:h:72:GLU:HG3	1.91	0.53
4:d:31:ALA:HA	5:j:118:ASN:HD21	1.73	0.53
1:9:179:LEU:HB2	1:9:199:PRO:HA	1.91	0.53
4:e:36:PRO:HB3	4:e:90:ASP:HB2	1.91	0.53
2:AP:83:HIS:HE1	2:AP:96:MET:HE2	1.74	0.52
4:c:85:GLN:HE21	5:i:19:VAL:HG22	1.74	0.52
4:f:37:GLY:N	4:f:90:ASP:O	2.42	0.52
2:AQ:185:LEU:HB3	2:AQ:193:TYR:HB3	1.92	0.52
4:b:128:ILE:HG13	4:b:129:LYS:HG3	1.91	0.52
4:e:41:ARG:NH2	4:e:80:TYR:OH	2.38	0.52
1:0:152:VAL:HG13	1:0:172:THR:HB	1.90	0.52
1:9:67:LEU:HD12	1:9:87:ILE:HG12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AM:340:SER:HA	3:AM:349:ILE:HD11	1.90	0.52
6:m:18:ALA:HB2	6:m:59:THR:HG21	1.90	0.52
6:n:82:ILE:HD11	6:n:88:ILE:HG13	1.92	0.52
6:q:77:ASP:OD1	6:q:77:ASP:N	2.43	0.52
3:AE:351:GLN:O	6:n:42:ARG:NH1	2.38	0.52
2:AQ:240:VAL:HA	2:AQ:243:MET:HE2	1.92	0.52
1:0:73:VAL:HG12	1:0:75:GLY:H	1.74	0.52
2:C:41:PHE:HB2	6:m:31:THR:HA	1.92	0.52
2:C:123:ASN:HD21	2:C:127:THR:HB	1.75	0.52
2:C:181:ASN:ND2	6:m:107:VAL:O	2.42	0.52
6:o:18:ALA:HB2	6:o:59:THR:HG21	1.91	0.52
2:A:93:LEU:HD13	2:A:121:THR:HA	1.92	0.51
2:C:94:ASP:HB2	2:C:220:LEU:HD21	1.90	0.51
2:A:95:MET:HE2	2:A:152:VAL:HG21	1.92	0.51
2:AP:152:VAL:HG22	2:AP:158:VAL:HG22	1.91	0.51
5:g:84:ASP:OD1	5:i:73:SER:OG	2.23	0.51
2:AQ:181:ASN:ND2	6:q:107:VAL:O	2.44	0.51
2:AR:115:THR:HB	2:AR:192:LEU:HD12	1.92	0.51
5:l:9:VAL:HG21	5:l:62:THR:HB	1.92	0.51
6:n:86:GLY:O	6:n:101:ARG:NH1	2.44	0.51
6:o:82:ILE:HD11	6:o:88:ILE:HG13	1.92	0.51
6:n:70:SER:O	6:n:206:GLY:N	2.30	0.51
2:B:98:GLU:OE1	2:B:216:ARG:NH1	2.40	0.51
3:AF:347:ALA:O	3:AF:353:VAL:HG13	2.10	0.51
1:9:141:ARG:HH22	3:AJ:356:MET:HB3	1.75	0.51
2:AP:41:PHE:HB2	6:p:31:THR:HA	1.91	0.51
6:o:84:GLY:O	6:o:101:ARG:NH2	2.43	0.51
6:q:84:GLY:O	6:q:101:ARG:NH2	2.43	0.51
2:A:44:LEU:HD21	2:A:73:LYS:HD3	1.92	0.51
3:AI:339:LEU:HD11	5:h:72:GLU:CG	2.41	0.51
2:AP:226:ASN:HB3	2:AP:229:GLU:HB2	1.93	0.51
6:q:14:GLN:HG3	6:q:58:MET:HA	1.92	0.51
2:AR:49:ILE:HD11	2:AR:66:LEU:HD13	1.93	0.51
2:C:59:ASN:HB3	2:C:62:LEU:HB2	1.93	0.50
4:b:35:THR:O	4:b:92:ASN:ND2	2.44	0.50
2:AQ:122:LEU:O	2:AR:181:ASN:ND2	2.44	0.50
6:o:1:MET:HG3	6:o:239:ASP:HB2	1.93	0.50
3:AH:342:GLN:HG3	3:AH:343:PRO:HD2	1.92	0.50
2:B:184:GLY:O	2:B:196:THR:OG1	2.30	0.50
4:e:88:THR:HG22	6:m:56:PHE:HZ	1.75	0.50
1:9:32:ASP:OD1	1:9:36:ASN:N	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AG:336:PRO:HG2	3:AO:352:ASP:HB3	1.92	0.50
5:l:70:ILE:HD13	6:q:51:HIS:HB3	1.93	0.50
1:9:193:LEU:HG	1:9:195:GLY:H	1.76	0.50
3:AK:330:ASN:N	3:AK:330:ASN:HD22	2.10	0.50
2:B:94:ASP:HB2	2:B:220:LEU:HD21	1.94	0.50
2:C:133:SER:OG	2:C:190:GLN:NE2	2.45	0.50
4:c:104:MET:SD	5:i:126:LYS:NZ	2.80	0.50
1:9:33:ASN:ND2	5:i:95:TYR:O	2.40	0.50
2:A:56:SER:OG	2:A:57:SER:N	2.42	0.50
2:AR:258:VAL:HG11	5:i:102:MET:HE1	1.93	0.50
6:n:21:LEU:HD23	6:n:39:ALA:HB2	1.94	0.50
3:AK:353:VAL:HG21	5:g:71:VAL:HG11	1.94	0.50
2:B:104:GLN:HE22	2:B:204:GLU:HG3	1.77	0.50
2:AR:94:ASP:HB2	2:AR:220:LEU:HD21	1.92	0.50
2:AR:255:MET:HE3	6:n:223:ARG:HG3	1.93	0.50
3:AF:347:ALA:HA	3:AF:353:VAL:CG1	2.42	0.50
2:C:188:ILE:HD13	2:C:194:LEU:HG	1.94	0.50
2:AQ:43:ASP:OD1	2:AQ:43:ASP:N	2.45	0.50
5:i:37:SER:O	5:i:38:ALA:HB3	2.11	0.50
1:0:153:VAL:HG12	1:0:155:GLY:H	1.77	0.49
1:9:33:ASN:ND2	5:i:34:VAL:O	2.45	0.49
2:AQ:82:THR:OG1	2:AQ:224:ASN:ND2	2.37	0.49
5:l:120:GLN:HE22	6:p:247:ARG:HG2	1.77	0.49
2:AQ:129:VAL:HG12	2:AQ:136:PRO:HA	1.94	0.49
2:AR:166:GLN:O	2:AR:167:ASP:HB2	2.12	0.49
4:e:85:GLN:NE2	6:m:53:SER:OG	2.34	0.49
1:9:32:ASP:HB2	5:i:41:THR:HB	1.94	0.49
1:9:41:ASN:ND2	1:9:61:GLN:OE1	2.45	0.49
6:q:35:ARG:NH1	6:q:101:ARG:HD3	2.28	0.49
2:B:46:TYR:HB2	6:o:178:THR:HA	1.94	0.49
2:A:226:ASN:HB3	2:A:229:GLU:HB3	1.95	0.49
2:C:31:THR:OG1	2:C:34:TYR:HB2	2.12	0.49
4:f:33:ALA:O	4:f:92:ASN:ND2	2.45	0.49
5:h:75:LYS:O	5:h:98:ASN:ND2	2.43	0.49
2:B:96:MET:HG3	2:B:221:GLU:HB2	1.95	0.49
1:0:66:LYS:HD3	1:0:88:ARG:HE	1.78	0.48
2:A:251:VAL:HG22	6:n:19:LEU:HD21	1.96	0.48
2:AP:123:ASN:ND2	2:AP:127:THR:OG1	2.46	0.48
6:p:200:GLN:NE2	6:p:201:THR:O	2.45	0.48
6:q:40:GLN:NE2	6:q:60:GLU:OE2	2.40	0.48
2:AQ:240:VAL:O	2:AQ:244:ASN:ND2	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:255:MET:HE3	6:o:223:ARG:HG3	1.94	0.48
3:AL:353:VAL:HG21	5:h:71:VAL:HG11	1.94	0.48
1:0:41:ASN:ND2	3:AM:352:ASP:OD1	2.47	0.48
1:9:187:TRP:HH2	1:9:197:VAL:HG11	1.78	0.48
2:A:18:ASN:HB2	2:A:41:PHE:HZ	1.78	0.48
2:AQ:104:GLN:NE2	2:AQ:175:THR:OG1	2.47	0.48
2:AR:12:LEU:HD13	6:n:212:VAL:HG11	1.96	0.48
4:c:97:ASP:OD1	5:i:115:TYR:OH	2.32	0.48
6:m:35:ARG:NH1	6:m:101:ARG:HD3	2.29	0.48
6:p:22:ARG:HE	6:p:39:ALA:HB3	1.78	0.48
1:0:114:GLY:HA2	1:0:134:LYS:HD2	1.95	0.48
2:B:176:ILE:HD11	2:B:212:LEU:HB3	1.96	0.48
5:g:61:ASP:N	5:g:61:ASP:OD1	2.45	0.48
6:n:89:SER:HB3	6:n:122:LEU:HD12	1.95	0.48
2:B:9:LYS:HG3	6:m:216:THR:HG21	1.94	0.48
2:B:101:GLY:HA3	2:B:176:ILE:HD12	1.95	0.48
2:AP:24:ASN:ND2	2:AP:34:TYR:OH	2.47	0.48
2:AR:176:ILE:HD11	2:AR:212:LEU:HB3	1.95	0.48
4:d:39:LYS:NZ	4:d:91:GLY:O	2.40	0.48
2:A:243:MET:HE3	6:n:26:LEU:HD22	1.96	0.48
1:0:187:TRP:HH2	1:0:197:VAL:HG11	1.79	0.47
2:A:259:ASN:ND2	6:o:226:GLU:OE1	2.47	0.47
6:n:40:GLN:NE2	6:n:60:GLU:OE2	2.39	0.47
1:0:31:THR:HG23	1:0:35:GLY:HA2	1.96	0.47
5:h:13:ALA:O	5:h:17:GLU:HG2	2.14	0.47
6:m:76:ARG:NH1	6:m:79:ASP:OD1	2.44	0.47
2:A:40:VAL:HG11	6:n:116:ALA:HB1	1.95	0.47
4:b:9:LEU:HD12	4:b:120:LYS:HB3	1.96	0.47
6:n:14:GLN:HB3	6:n:59:THR:HG23	1.95	0.47
2:B:177:THR:HG21	2:B:202:PRO:HB3	1.96	0.47
4:d:30:ILE:HG23	4:d:96:LEU:HD11	1.97	0.47
4:f:85:GLN:OE1	5:k:22:ASN:ND2	2.47	0.47
1:0:119:LEU:O	1:0:122:THR:OG1	2.28	0.47
4:c:24:GLU:OE2	5:h:2:SER:N	2.47	0.47
1:0:39:LEU:HD12	1:0:59:ILE:HG22	1.97	0.47
2:A:49:ILE:HD11	2:A:66:LEU:HD23	1.96	0.47
4:b:30:ILE:HG23	4:b:96:LEU:HD11	1.96	0.47
5:i:126:LYS:HD3	6:n:248:MET:HA	1.96	0.47
6:m:114:THR:HG22	6:m:120:LEU:HD13	1.96	0.47
6:o:35:ARG:NH1	6:o:101:ARG:HD3	2.30	0.47
2:AQ:251:VAL:HG22	6:q:19:LEU:HD21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AR:18:ASN:HB2	2:AR:41:PHE:HZ	1.80	0.47
5:i:84:ASP:OD1	5:i:84:ASP:N	2.32	0.47
1:9:107:TRP:HD1	1:9:128:PRO:HG3	1.79	0.47
2:A:83:HIS:CD2	2:A:99:GLY:H	2.33	0.47
4:f:21:ARG:NH1	4:f:48:GLU:OE1	2.48	0.47
3:AF:349:ILE:O	3:AF:350:PRO:C	2.58	0.46
5:j:20:ARG:HH21	5:j:111:ALA:HA	1.79	0.46
6:o:21:LEU:HD23	6:o:39:ALA:HB2	1.97	0.46
3:AM:341:ASN:ND2	4:f:88:THR:OG1	2.48	0.46
4:e:43:LEU:HG	4:e:48:GLU:HG3	1.96	0.46
3:AK:340:SER:HA	3:AK:349:ILE:HD11	1.97	0.46
2:AR:44:LEU:HB2	2:AR:70:ALA:HB3	1.98	0.46
4:c:35:THR:O	4:c:92:ASN:ND2	2.48	0.46
5:h:66:LYS:HE3	5:h:68:MET:SD	2.56	0.46
5:j:100:ASN:O	5:j:104:GLU:HG2	2.16	0.46
5:j:100:ASN:HB3	5:j:103:GLU:HG2	1.97	0.46
2:B:185:LEU:HB3	2:B:193:TYR:HB3	1.97	0.46
4:d:15:THR:HG23	4:d:45:PHE:HZ	1.81	0.46
5:k:70:ILE:HD13	6:p:51:HIS:HB3	1.97	0.46
1:0:179:LEU:O	1:0:182:ASN:ND2	2.48	0.46
2:B:40:VAL:HG11	6:o:116:ALA:HB1	1.98	0.46
5:h:36:SER:OG	5:h:38:ALA:O	2.27	0.46
6:o:28:ASN:O	6:o:31:THR:OG1	2.34	0.46
2:A:44:LEU:HD13	5:h:81:TYR:HB2	1.98	0.46
3:AI:342:GLN:O	3:AI:343:PRO:C	2.59	0.46
6:p:9:MET:HE3	6:p:9:MET:HB3	1.81	0.46
6:p:28:ASN:O	6:p:31:THR:OG1	2.32	0.46
6:p:131:LEU:HD23	6:p:148:VAL:HG11	1.97	0.46
1:0:129:ALA:HA	1:0:148:PRO:HB2	1.97	0.45
2:B:123:ASN:ND2	2:B:127:THR:HB	2.31	0.45
2:AR:36:LYS:HD3	2:AR:225:VAL:HA	1.98	0.45
2:AR:188:ILE:HD13	2:AR:194:LEU:HG	1.97	0.45
6:n:91:LEU:HD21	6:n:128:PRO:HG3	1.97	0.45
2:B:181:ASN:ND2	6:o:107:VAL:O	2.49	0.45
1:0:92:LYS:HG2	1:0:112:LYS:HD2	1.97	0.45
3:AF:344:PRO:O	3:AF:345:ALA:C	2.57	0.45
4:e:30:ILE:HG23	4:e:96:LEU:HD11	1.98	0.45
6:n:91:LEU:HD23	6:n:122:LEU:HD21	1.98	0.45
2:B:251:VAL:HG22	6:o:19:LEU:HD21	1.97	0.45
4:b:39:LYS:NZ	4:b:91:GLY:O	2.42	0.45
5:i:39:LYS:HA	5:i:39:LYS:HD3	1.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AF:336:PRO:HG2	3:AM:352:ASP:HB3	1.98	0.45
2:C:115:THR:HB	2:C:192:LEU:HD12	1.98	0.45
2:AP:83:HIS:CD2	2:AP:99:GLY:H	2.35	0.45
2:AR:48:ASN:HB3	2:AR:51:GLN:HG3	1.98	0.45
5:i:30:ASN:OD1	6:n:57:SER:HB3	2.17	0.45
6:q:18:ALA:HB2	6:q:59:THR:HG21	1.99	0.45
2:C:49:ILE:HD11	2:C:66:LEU:HD23	1.99	0.45
5:i:52:GLU:O	5:i:53:LEU:C	2.59	0.45
5:h:27:ASN:OD1	5:h:42:TYR:OH	2.27	0.45
6:p:114:THR:HG22	6:p:120:LEU:HD13	1.99	0.45
6:q:244:SER:HA	6:q:247:ARG:HB2	1.98	0.45
3:AM:331:MET:HE2	3:AM:331:MET:HB3	1.87	0.45
2:AP:18:ASN:HB2	2:AP:41:PHE:HZ	1.81	0.45
2:AQ:7:VAL:O	2:AQ:10:THR:OG1	2.34	0.45
4:c:26:ILE:HG21	4:c:103:PHE:HB2	1.99	0.45
6:n:167:VAL:HG12	6:n:169:PRO:HD3	1.98	0.45
3:AJ:341:ASN:HD21	4:c:86:PRO:HG3	1.82	0.44
6:p:21:LEU:HD23	6:p:39:ALA:HB2	1.98	0.44
6:n:18:ALA:HB2	6:n:59:THR:HG21	1.98	0.44
3:AF:339:LEU:HD11	5:l:72:GLU:HG3	1.99	0.44
2:AR:104:GLN:NE2	2:AR:175:THR:OG1	2.49	0.44
2:AR:152:VAL:HG22	2:AR:158:VAL:HG22	1.99	0.44
6:m:137:LYS:NZ	6:m:139:GLU:OE2	2.48	0.44
1:0:154:ASP:HA	1:0:174:LYS:HB2	1.99	0.44
1:0:176:ASN:N	1:0:176:ASN:OD1	2.49	0.44
2:AP:80:VAL:HG12	2:AP:82:THR:HG23	2.00	0.44
5:h:113:ARG:NH1	6:n:239:ASP:OD2	2.46	0.44
5:i:22:ASN:ND2	6:n:54:ARG:HE	2.16	0.44
6:n:131:LEU:HD23	6:n:148:VAL:HG11	1.99	0.44
2:AR:178:ASP:HB2	2:AR:212:LEU:HD23	1.99	0.44
4:b:85:GLN:OE1	5:l:22:ASN:ND2	2.51	0.44
2:A:29:ALA:HA	2:A:225:VAL:HG21	1.99	0.44
2:B:115:THR:HB	2:B:192:LEU:HD12	1.99	0.44
6:q:82:ILE:HD11	6:q:88:ILE:HG13	2.00	0.44
2:AR:226:ASN:HB3	2:AR:229:GLU:HB2	2.00	0.44
1:0:47:LEU:HB2	1:0:68:PRO:HG3	1.99	0.44
3:AA:349:ILE:HG12	6:q:46:ALA:HA	1.99	0.44
3:AA:353:VAL:O	3:AA:356:MET:HG2	2.17	0.44
3:AF:348:SER:O	3:AF:349:ILE:HB	2.17	0.44
2:C:93:LEU:HD23	2:C:121:THR:HA	1.99	0.44
2:AR:93:LEU:HD13	2:AR:121:THR:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:i:66:LYS:HE3	5:i:68:MET:HG2	1.99	0.44
6:o:105:LEU:HA	6:o:115:ASN:HA	2.00	0.44
6:p:40:GLN:HG2	6:p:62:PRO:HD3	1.99	0.44
1:0:92:LYS:HA	1:0:112:LYS:HB2	1.99	0.44
1:0:136:ASP:CB	3:AF:356:MET:HE3	2.47	0.44
2:B:12:LEU:HD13	2:B:244:ASN:HB2	2.00	0.44
2:B:129:VAL:HG12	2:B:136:PRO:HA	2.00	0.44
2:AR:9:LYS:HG3	6:n:216:THR:HG21	1.99	0.44
6:q:37:ASP:OD1	6:q:176:LYS:NZ	2.42	0.44
6:q:91:LEU:HD21	6:q:128:PRO:HG3	1.98	0.44
2:A:115:THR:HB	2:A:192:LEU:HD12	2.00	0.43
2:AP:262:LEU:HG	5:l:109:ILE:HD11	1.99	0.43
4:b:21:ARG:NH1	4:b:48:GLU:OE1	2.51	0.43
5:j:70:ILE:HD13	6:m:51:HIS:HB3	1.99	0.43
6:m:211:ALA:O	6:m:215:MET:HG2	2.18	0.43
6:q:21:LEU:HD23	6:q:39:ALA:HB2	2.00	0.43
2:B:96:MET:HG2	2:B:97:VAL:N	2.33	0.43
2:C:166:GLN:O	2:C:167:ASP:HB2	2.18	0.43
5:g:100:ASN:O	5:g:104:GLU:HG2	2.18	0.43
5:k:39:LYS:HD2	5:k:39:LYS:HA	1.85	0.43
2:B:106:THR:OG1	2:B:138:GLU:OE2	2.36	0.43
6:n:15:ASN:ND2	6:n:228:GLN:HE22	2.16	0.43
6:o:92:ASP:OD1	6:o:92:ASP:N	2.46	0.43
6:q:91:LEU:HD23	6:q:122:LEU:HD21	2.01	0.43
1:0:33:ASN:ND2	5:l:95:TYR:O	2.34	0.43
2:A:103:PHE:HB2	2:A:115:THR:HG23	2.00	0.43
4:b:33:ALA:O	4:b:92:ASN:ND2	2.51	0.43
4:e:35:THR:O	4:e:92:ASN:ND2	2.52	0.43
4:e:41:ARG:HD3	4:e:78:LYS:HD2	2.00	0.43
5:j:22:ASN:ND2	6:m:54:ARG:HE	2.14	0.43
6:o:154:PRO:HG2	6:o:157:GLU:HG3	1.99	0.43
1:9:133:VAL:HG21	1:9:137:LEU:HD13	2.01	0.43
2:B:95:MET:O	2:B:118:GLY:HA3	2.18	0.43
2:AP:116:ARG:NH2	2:AP:221:GLU:OE2	2.41	0.43
2:AR:28:ASN:OD1	2:AR:28:ASN:N	2.51	0.43
5:k:100:ASN:HB3	5:k:103:GLU:HG2	1.99	0.43
6:m:97:GLU:O	6:m:183:ARG:NH1	2.52	0.43
6:m:218:LEU:O	6:m:222:GLN:HG3	2.18	0.43
3:AE:343:PRO:HG3	4:c:80:TYR:CZ	2.54	0.43
2:AQ:50:ASN:ND2	2:AQ:63:PRO:O	2.36	0.43
4:b:36:PRO:HB3	4:b:90:ASP:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:f:15:THR:HG23	4:f:45:PHE:HZ	1.84	0.43
5:l:115:TYR:CG	6:q:238:MET:HE3	2.53	0.43
5:i:75:LYS:HB2	5:i:98:ASN:HD22	1.84	0.43
1:9:30:HIS:HB3	1:9:38:ASP:O	2.19	0.43
1:9:32:ASP:CG	1:9:36:ASN:HD22	2.26	0.43
2:C:247:VAL:O	2:C:251:VAL:HG23	2.19	0.43
5:l:13:ALA:O	5:l:17:GLU:HG2	2.19	0.43
5:l:37:SER:N	6:q:43:SER:O	2.52	0.43
6:m:136:SER:HB2	6:m:151:GLN:HA	2.00	0.43
6:n:77:ASP:OD1	6:n:77:ASP:N	2.51	0.43
2:AQ:80:VAL:HG12	2:AQ:82:THR:HG23	2.01	0.42
2:AQ:95:MET:O	2:AQ:118:GLY:HA3	2.19	0.42
4:d:36:PRO:HB3	4:d:90:ASP:HB2	2.01	0.42
5:h:115:TYR:CG	6:o:238:MET:HE3	2.54	0.42
5:i:44:ALA:O	5:i:73:SER:N	2.46	0.42
5:i:100:ASN:O	5:i:104:GLU:HG2	2.19	0.42
1:9:73:VAL:HG12	1:9:75:GLY:H	1.84	0.42
2:A:254:MET:SD	6:n:222:GLN:HG2	2.59	0.42
3:AL:338:ALA:HB1	5:h:103:GLU:HB2	2.01	0.42
2:C:50:ASN:ND2	2:C:63:PRO:O	2.40	0.42
2:C:176:ILE:HD11	2:C:212:LEU:HB3	2.01	0.42
2:AQ:109:ASP:OD1	2:AQ:109:ASP:N	2.49	0.42
5:k:126:LYS:HE2	5:k:126:LYS:HB3	1.86	0.42
5:l:22:ASN:ND2	6:q:54:ARG:HE	2.17	0.42
2:A:31:THR:HG21	2:A:191:ASN:HD21	1.85	0.42
2:B:22:ILE:HG21	2:B:234:MET:HG2	2.01	0.42
2:AQ:32:VAL:HG11	2:AQ:220:LEU:HD22	2.00	0.42
1:0:138:SER:HA	1:0:158:TYR:HB2	2.02	0.42
2:AP:21:THR:HG21	2:AP:39:ALA:HB2	2.01	0.42
5:k:119:VAL:HG13	6:p:245:LEU:HG	2.01	0.42
6:n:200:GLN:NE2	6:n:201:THR:O	2.53	0.42
3:AO:333:ALA:HB3	3:AO:356:MET:HB3	2.02	0.42
2:AQ:123:ASN:ND2	2:AQ:127:THR:HB	2.34	0.42
1:0:85:LYS:HA	1:0:104:ILE:HA	2.00	0.42
3:AF:342:GLN:O	3:AF:343:PRO:C	2.61	0.42
2:C:155:ASP:C	2:C:207:PRO:HG2	2.44	0.42
2:AQ:51:GLN:NE2	2:AQ:64:SER:OG	2.52	0.42
2:AR:14:ALA:HB1	2:AR:41:PHE:HE1	1.84	0.42
5:i:41:THR:O	5:i:42:TYR:C	2.62	0.42
6:q:210:ASN:O	6:q:214:GLU:HG2	2.20	0.42
3:AK:337:GLY:O	3:AK:341:ASN:ND2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:g:127:GLN:O	5:g:131:ARG:HG2	2.20	0.42
5:k:22:ASN:ND2	6:p:54:ARG:HE	2.14	0.42
6:n:40:GLN:HE21	6:n:60:GLU:CD	2.27	0.42
2:B:41:PHE:HB2	6:o:31:THR:HA	2.02	0.42
4:e:85:GLN:HE21	6:m:53:SER:HG	1.61	0.42
6:n:35:ARG:NH1	6:n:101:ARG:HD3	2.34	0.42
6:o:37:ASP:HB3	6:o:61:ARG:HD2	2.02	0.42
6:q:76:ARG:NH1	6:q:79:ASP:OD1	2.47	0.42
5:l:100:ASN:HB3	5:l:103:GLU:HG2	2.01	0.42
6:n:218:LEU:O	6:n:222:GLN:HG3	2.20	0.42
1:9:36:ASN:OD1	1:9:56:ASN:N	2.41	0.41
3:AB:353:VAL:HG21	5:k:38:ALA:HB2	2.01	0.41
3:AD:346:ASP:OD1	4:d:39:LYS:NZ	2.44	0.41
2:B:258:VAL:HG22	6:o:229:VAL:HG21	2.00	0.41
2:C:18:ASN:HB2	2:C:41:PHE:HZ	1.84	0.41
2:AP:31:THR:HG21	2:AP:191:ASN:HD21	1.85	0.41
2:AQ:155:ASP:C	2:AQ:207:PRO:HG2	2.45	0.41
2:AR:94:ASP:OD1	2:AR:94:ASP:N	2.53	0.41
6:n:65:ASN:O	6:n:208:ASN:ND2	2.51	0.41
6:n:123:GLY:N	6:n:127:ALA:O	2.53	0.41
6:p:87:TRP:HB3	6:p:99:LEU:HB3	2.01	0.41
6:q:97:GLU:O	6:q:183:ARG:NH1	2.53	0.41
2:A:15:GLN:O	2:A:19:ILE:HG12	2.19	0.41
2:A:123:ASN:OD1	2:A:127:THR:N	2.53	0.41
2:A:155:ASP:C	2:A:207:PRO:HG2	2.46	0.41
6:m:82:ILE:HD11	6:m:88:ILE:HG13	2.02	0.41
6:q:81:THR:HG23	6:q:200:GLN:HB3	2.02	0.41
2:AR:181:ASN:OD1	2:AR:184:GLY:N	2.53	0.41
6:m:28:ASN:O	6:m:31:THR:OG1	2.37	0.41
6:m:84:GLY:O	6:m:101:ARG:NH2	2.31	0.41
6:m:167:VAL:HG12	6:m:169:PRO:HD3	2.03	0.41
6:n:11:GLY:O	6:n:15:ASN:ND2	2.45	0.41
6:n:142:ARG:HH12	6:n:200:GLN:HG2	1.86	0.41
1:9:124:LEU:HD21	1:9:127:LEU:HD21	2.02	0.41
3:AB:343:PRO:HG3	4:f:80:TYR:CZ	2.55	0.41
2:C:104:GLN:NE2	2:C:175:THR:OG1	2.54	0.41
6:n:68:GLN:OE1	6:n:101:ARG:NH2	2.53	0.41
1:9:35:GLY:O	1:9:55:GLY:N	2.53	0.41
3:AF:346:ASP:HB3	3:AF:347:ALA:H	1.61	0.41
2:AP:22:ILE:HD11	2:AP:233:ASN:HB2	2.03	0.41
4:c:32:GLN:NE2	5:h:51:ALA:HB2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:k:96:LYS:HE3	5:k:96:LYS:HB3	1.90	0.41
1:0:147:LEU:HB2	1:0:168:PRO:HD3	2.03	0.41
3:AA:351:GLN:OE1	2:AQ:64:SER:N	2.49	0.41
2:AP:246:LYS:HE2	2:AP:246:LYS:HB3	1.93	0.41
6:n:16:MET:O	6:n:20:GLN:HG3	2.20	0.41
6:q:14:GLN:HB3	6:q:59:THR:HG23	2.02	0.41
2:C:36:LYS:HB3	2:C:225:VAL:HG12	2.03	0.41
2:AP:96:MET:HE3	2:AP:221:GLU:HA	2.02	0.41
2:AR:95:MET:O	2:AR:118:GLY:HA3	2.20	0.41
5:j:43:LYS:HG2	5:j:77:LEU:HD21	2.03	0.41
6:p:1:MET:HG3	6:p:239:ASP:HB2	2.03	0.41
2:A:9:LYS:HG3	6:o:216:THR:HG21	2.01	0.41
2:AR:95:MET:HE2	2:AR:95:MET:HB3	2.00	0.41
5:l:130:LEU:HD11	6:q:248:MET:HE3	2.03	0.41
1:0:159:ILE:HG13	1:0:182:ASN:HD21	1.86	0.41
3:AG:339:LEU:HD11	5:k:72:GLU:HG3	2.03	0.41
3:AG:343:PRO:HA	3:AG:344:PRO:HD3	1.92	0.41
3:AI:335:ILE:O	3:AI:336:PRO:C	2.61	0.41
3:AJ:341:ASN:ND2	4:c:86:PRO:HG3	2.36	0.41
2:B:188:ILE:HD13	2:B:194:LEU:HG	2.02	0.41
2:C:40:VAL:HG11	6:m:116:ALA:HB1	2.02	0.41
2:AP:59:ASN:HB3	2:AP:62:LEU:HB2	2.02	0.41
2:AP:212:LEU:HD23	2:AP:212:LEU:HA	1.93	0.41
5:i:89:ASN:OD1	5:i:93:TYR:N	2.51	0.41
6:p:77:ASP:OD1	6:p:77:ASP:N	2.53	0.41
6:p:92:ASP:OD1	6:p:92:ASP:N	2.54	0.41
6:p:108:ASP:OD1	6:p:112:MET:N	2.54	0.41
6:q:83:GLU:OE1	6:q:142:ARG:NH2	2.54	0.41
2:B:22:ILE:HG23	2:B:230:GLU:HB3	2.01	0.41
2:B:244:ASN:HD21	6:o:27:ALA:HA	1.84	0.41
2:C:163:ARG:HD2	2:C:163:ARG:HA	1.98	0.41
6:n:108:ASP:OD1	6:n:112:MET:N	2.54	0.41
6:n:231:MET:HA	6:n:234:THR:HG22	2.03	0.41
6:p:179:ASN:HD21	6:p:183:ARG:HH21	1.69	0.41
2:B:59:ASN:HB3	2:B:62:LEU:HB2	2.03	0.40
2:C:123:ASN:ND2	2:C:127:THR:HB	2.34	0.40
2:AR:236:GLU:HG3	2:AR:237:ALA:N	2.36	0.40
5:i:53:LEU:N	5:i:53:LEU:HD23	2.36	0.40
6:m:40:GLN:HG2	6:m:62:PRO:HD3	2.01	0.40
6:o:115:ASN:OD1	6:o:119:HIS:N	2.54	0.40
6:o:167:VAL:HG12	6:o:169:PRO:HD3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:26:LEU:HD23	2:A:26:LEU:HA	1.93	0.40
2:AQ:155:ASP:HA	2:AQ:207:PRO:O	2.21	0.40
2:AR:96:MET:HG3	2:AR:221:GLU:HB2	2.03	0.40
5:l:126:LYS:NZ	6:q:245:LEU:O	2.54	0.40
6:n:144:GLY:HA2	6:n:199:LEU:HD12	2.03	0.40
6:q:2:ASP:C	6:q:4:ALA:H	2.29	0.40
2:C:32:VAL:HG21	2:C:220:LEU:HD13	2.03	0.40
2:C:258:VAL:O	2:C:262:LEU:HB2	2.21	0.40
2:AP:102:PHE:HB3	2:AP:114:TYR:HB3	2.03	0.40
6:q:10:SER:O	6:q:14:GLN:HG2	2.22	0.40
1:0:77:LEU:HB3	1:0:97:ALA:HA	2.04	0.40
2:A:91:ASN:HB3	2:A:94:ASP:OD2	2.21	0.40
2:AP:161:ARG:HA	2:AP:161:ARG:HD2	1.96	0.40
2:AP:226:ASN:O	2:AP:230:GLU:HG2	2.21	0.40
5:h:120:GLN:HE22	6:n:247:ARG:NE	2.18	0.40
5:i:25:SER:HB2	6:n:7:LEU:HD23	2.04	0.40
6:n:76:ARG:O	6:n:202:GLY:HA2	2.20	0.40
1:0:116:TYR:HE2	1:0:118:ASN:HB2	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	178/199 (89%)	173 (97%)	5 (3%)	0	100	100
1	9	178/199 (89%)	174 (98%)	4 (2%)	0	100	100
2	A	260/262 (99%)	251 (96%)	9 (4%)	0	100	100
2	AP	260/262 (99%)	253 (97%)	6 (2%)	1 (0%)	30	64
2	AQ	260/262 (99%)	248 (95%)	11 (4%)	1 (0%)	30	64
2	AR	244/262 (93%)	240 (98%)	3 (1%)	1 (0%)	30	64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	260/262 (99%)	250 (96%)	10 (4%)	0	100	100
2	C	260/262 (99%)	252 (97%)	7 (3%)	1 (0%)	30	64
3	AA	17/580 (3%)	17 (100%)	0	0	100	100
3	AB	17/580 (3%)	15 (88%)	2 (12%)	0	100	100
3	AC	18/580 (3%)	18 (100%)	0	0	100	100
3	AD	17/580 (3%)	17 (100%)	0	0	100	100
3	AE	17/580 (3%)	17 (100%)	0	0	100	100
3	AF	21/580 (4%)	14 (67%)	6 (29%)	1 (5%)	2	17
3	AG	9/580 (2%)	7 (78%)	2 (22%)	0	100	100
3	AH	9/580 (2%)	9 (100%)	0	0	100	100
3	AI	9/580 (2%)	8 (89%)	1 (11%)	0	100	100
3	AJ	22/580 (4%)	18 (82%)	4 (18%)	0	100	100
3	AK	23/580 (4%)	23 (100%)	0	0	100	100
3	AL	30/580 (5%)	26 (87%)	4 (13%)	0	100	100
3	AM	31/580 (5%)	31 (100%)	0	0	100	100
3	AN	31/580 (5%)	31 (100%)	0	0	100	100
3	AO	30/580 (5%)	30 (100%)	0	0	100	100
4	b	105/131 (80%)	104 (99%)	1 (1%)	0	100	100
4	c	103/131 (79%)	102 (99%)	1 (1%)	0	100	100
4	d	105/131 (80%)	103 (98%)	2 (2%)	0	100	100
4	e	104/131 (79%)	104 (100%)	0	0	100	100
4	f	104/131 (79%)	103 (99%)	1 (1%)	0	100	100
5	g	126/137 (92%)	122 (97%)	4 (3%)	0	100	100
5	h	126/137 (92%)	123 (98%)	3 (2%)	0	100	100
5	i	126/137 (92%)	122 (97%)	3 (2%)	1 (1%)	16	50
5	j	126/137 (92%)	125 (99%)	1 (1%)	0	100	100
5	k	126/137 (92%)	120 (95%)	6 (5%)	0	100	100
5	l	126/137 (92%)	121 (96%)	5 (4%)	0	100	100
6	m	246/249 (99%)	242 (98%)	4 (2%)	0	100	100
6	n	246/249 (99%)	242 (98%)	4 (2%)	0	100	100
6	o	246/249 (99%)	241 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	p	246/249 (99%)	242 (98%)	4 (2%)	0	100	100
6	q	246/249 (99%)	240 (98%)	6 (2%)	0	100	100
All	All	4708/13392 (35%)	4578 (97%)	124 (3%)	6 (0%)	50	79

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	i	42	TYR
2	C	167	ASP
2	AR	167	ASP
2	AP	167	ASP
2	AQ	167	ASP
3	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	0	149/167 (89%)	145 (97%)	4 (3%)	40	67
1	9	149/167 (89%)	148 (99%)	1 (1%)	81	89
2	A	218/218 (100%)	214 (98%)	4 (2%)	54	75
2	AP	218/218 (100%)	214 (98%)	4 (2%)	54	75
2	AQ	218/218 (100%)	211 (97%)	7 (3%)	34	63
2	AR	206/218 (94%)	200 (97%)	6 (3%)	37	65
2	B	218/218 (100%)	213 (98%)	5 (2%)	45	71
2	C	218/218 (100%)	211 (97%)	7 (3%)	34	63
3	AA	15/500 (3%)	14 (93%)	1 (7%)	13	42
3	AB	15/500 (3%)	14 (93%)	1 (7%)	13	42
3	AC	15/500 (3%)	15 (100%)	0	100	100
3	AD	15/500 (3%)	14 (93%)	1 (7%)	13	42
3	AE	15/500 (3%)	15 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	AF	17/500 (3%)	14 (82%)	3 (18%)	1	8
3	AG	8/500 (2%)	8 (100%)	0	100	100
3	AH	8/500 (2%)	7 (88%)	1 (12%)	3	20
3	AI	8/500 (2%)	8 (100%)	0	100	100
3	AJ	17/500 (3%)	16 (94%)	1 (6%)	16	45
3	AK	18/500 (4%)	15 (83%)	3 (17%)	2	10
3	AL	24/500 (5%)	23 (96%)	1 (4%)	25	55
3	AM	24/500 (5%)	24 (100%)	0	100	100
3	AN	24/500 (5%)	22 (92%)	2 (8%)	9	33
3	AO	24/500 (5%)	23 (96%)	1 (4%)	25	55
4	b	89/106 (84%)	88 (99%)	1 (1%)	70	83
4	c	88/106 (83%)	86 (98%)	2 (2%)	45	71
4	d	89/106 (84%)	86 (97%)	3 (3%)	32	61
4	e	88/106 (83%)	85 (97%)	3 (3%)	32	61
4	f	88/106 (83%)	88 (100%)	0	100	100
5	g	111/115 (96%)	106 (96%)	5 (4%)	23	54
5	h	111/115 (96%)	107 (96%)	4 (4%)	30	60
5	i	111/115 (96%)	103 (93%)	8 (7%)	12	39
5	j	111/115 (96%)	106 (96%)	5 (4%)	23	54
5	k	111/115 (96%)	105 (95%)	6 (5%)	18	47
5	l	111/115 (96%)	106 (96%)	5 (4%)	23	54
6	m	204/205 (100%)	199 (98%)	5 (2%)	42	69
6	n	204/205 (100%)	198 (97%)	6 (3%)	37	65
6	o	204/205 (100%)	198 (97%)	6 (3%)	37	65
6	p	204/205 (100%)	202 (99%)	2 (1%)	73	84
6	q	204/205 (100%)	200 (98%)	4 (2%)	50	73
All	All	3969/11387 (35%)	3851 (97%)	118 (3%)	37	65

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	20	TYR
1	0	23	ASP

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Mol	Chain	Res	Type
1	0	174	LYS
1	0	176	ASN
1	9	28	PHE
2	A	45	PHE
2	A	167	ASP
2	A	192	LEU
2	A	226	ASN
3	AA	342	GLN
3	AB	342	GLN
3	AD	349	ILE
3	AF	351	GLN
3	AF	352	ASP
3	AF	355	GLN
3	AH	342	GLN
3	AJ	349	ILE
3	AK	330	ASN
3	AK	331	MET
3	AK	332	VAL
3	AL	339	LEU
3	AN	339	LEU
3	AN	352	ASP
3	AO	330	ASN
2	B	12	LEU
2	B	42	GLU
2	B	45	PHE
2	B	104	GLN
2	B	165	GLN
2	C	31	THR
2	C	55	GLN
2	C	60	THR
2	C	109	ASP
2	C	112	ILE
2	C	259	ASN
2	C	262	LEU
2	AP	55	GLN
2	AP	106	THR
2	AP	109	ASP
2	AP	226	ASN
2	AQ	55	GLN
2	AQ	61	GLU
2	AQ	75	VAL
2	AQ	100	ASP

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Mol	Chain	Res	Type
2	AQ	163	ARG
2	AQ	226	ASN
2	AQ	236	GLU
2	AR	28	ASN
2	AR	38	ARG
2	AR	77	THR
2	AR	180	VAL
2	AR	192	LEU
2	AR	236	GLU
4	b	9	LEU
4	c	6	ASP
4	c	87	ASP
4	d	4	SER
4	d	6	ASP
4	d	7	ASN
4	e	6	ASP
4	e	7	ASN
4	e	88	THR
5	g	23	THR
5	g	39	LYS
5	g	53	LEU
5	g	65	VAL
5	g	134	GLN
5	h	3	LEU
5	h	34	VAL
5	h	65	VAL
5	h	67	VAL
5	i	36	SER
5	i	39	LYS
5	i	61	ASP
5	i	62	THR
5	i	67	VAL
5	i	84	ASP
5	i	113	ARG
5	i	131	ARG
5	j	53	LEU
5	j	61	ASP
5	j	65	VAL
5	j	67	VAL
5	j	126	LYS
5	k	14	MET
5	k	40	ASP

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Mol	Chain	Res	Type
5	k	53	LEU
5	k	65	VAL
5	k	113	ARG
5	k	134	GLN
5	l	40	ASP
5	l	43	LYS
5	l	65	VAL
5	l	126	LYS
5	l	137	GLN
6	m	7	LEU
6	m	60	GLU
6	m	72	ILE
6	m	135	LEU
6	m	218	LEU
6	n	60	GLU
6	n	72	ILE
6	n	158	PHE
6	n	162	ASP
6	n	200	GLN
6	n	204	ILE
6	o	72	ILE
6	o	73	THR
6	o	101	ARG
6	o	114	THR
6	o	158	PHE
6	o	229	VAL
6	p	72	ILE
6	p	135	LEU
6	q	72	ILE
6	q	73	THR
6	q	135	LEU
6	q	204	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (135) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	41	ASN
1	0	118	ASN
1	0	182	ASN
1	9	41	ASN
1	9	182	ASN
2	A	15	GLN

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Mol	Chain	Res	Type
2	A	16	GLN
2	A	28	ASN
2	A	58	GLN
2	A	104	GLN
2	A	168	ASN
2	A	190	GLN
2	A	191	ASN
2	A	217	GLN
2	A	226	ASN
3	AH	342	GLN
3	AK	330	ASN
3	AL	341	ASN
3	AL	351	GLN
3	AM	341	ASN
3	AN	342	GLN
3	AO	330	ASN
3	AO	355	GLN
2	B	24	ASN
2	B	48	ASN
2	B	55	GLN
2	B	104	GLN
2	B	181	ASN
2	B	191	ASN
2	B	203	GLN
2	B	217	GLN
2	B	226	ASN
2	B	244	ASN
2	C	28	ASN
2	C	51	GLN
2	C	104	GLN
2	C	119	GLN
2	C	166	GLN
2	C	168	ASN
2	C	169	GLN
2	C	190	GLN
2	C	217	GLN
2	C	226	ASN
2	AP	15	GLN
2	AP	24	ASN
2	AP	47	GLN
2	AP	51	GLN
2	AP	87	GLN

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Mol	Chain	Res	Type
2	AP	119	GLN
2	AP	191	ASN
2	AP	217	GLN
2	AP	259	ASN
2	AQ	16	GLN
2	AQ	24	ASN
2	AQ	51	GLN
2	AQ	58	GLN
2	AQ	81	HIS
2	AQ	104	GLN
2	AQ	165	GLN
2	AQ	168	ASN
2	AQ	190	GLN
2	AQ	191	ASN
2	AQ	203	GLN
2	AQ	217	GLN
2	AQ	226	ASN
2	AR	2	HIS
2	AR	16	GLN
2	AR	24	ASN
2	AR	104	GLN
2	AR	165	GLN
2	AR	168	ASN
2	AR	190	GLN
2	AR	203	GLN
2	AR	217	GLN
2	AR	226	ASN
2	AR	260	GLN
4	b	50	GLN
4	c	32	GLN
4	c	106	ASN
4	c	110	HIS
4	d	14	HIS
4	d	105	GLN
4	d	106	ASN
4	d	107	GLN
4	d	110	HIS
4	e	85	GLN
4	e	101	ASN
4	e	107	GLN
4	e	110	HIS
4	f	12	HIS

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Mol	Chain	Res	Type
4	f	14	HIS
4	f	34	ASN
4	f	50	GLN
4	f	107	GLN
4	f	110	HIS
5	g	100	ASN
5	g	118	ASN
5	g	134	GLN
5	h	127	GLN
5	i	22	ASN
5	i	46	HIS
5	i	100	ASN
5	i	118	ASN
5	j	22	ASN
5	j	118	ASN
5	k	22	ASN
5	k	100	ASN
5	k	120	GLN
5	l	22	ASN
5	l	100	ASN
5	l	120	GLN
6	m	24	ASN
6	m	125	ASN
6	m	179	ASN
6	m	200	GLN
6	m	228	GLN
6	n	15	ASN
6	n	24	ASN
6	n	102	ASN
6	n	188	ASN
6	n	200	GLN
6	o	14	GLN
6	o	40	GLN
6	o	102	ASN
6	o	200	GLN
6	o	222	GLN
6	p	17	GLN
6	p	119	HIS
6	p	200	GLN
6	p	228	GLN
6	q	15	ASN
6	q	20	GLN

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Mol	Chain	Res	Type
6	q	40	GLN
6	q	102	ASN
6	q	200	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

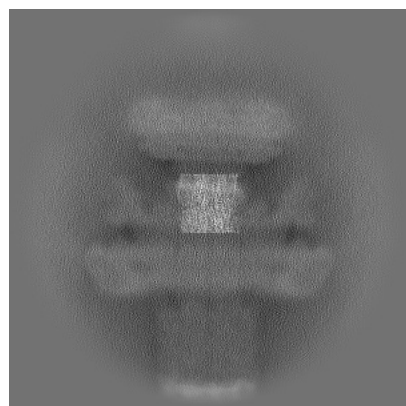
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39786. These allow visual inspection of the internal detail of the map and identification of artifacts.

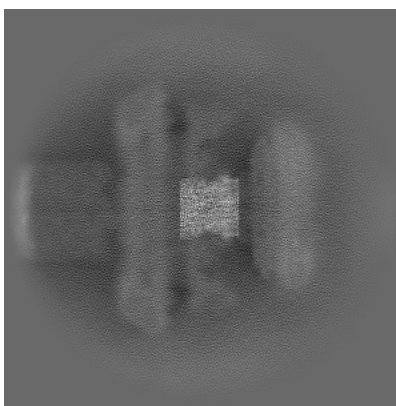
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

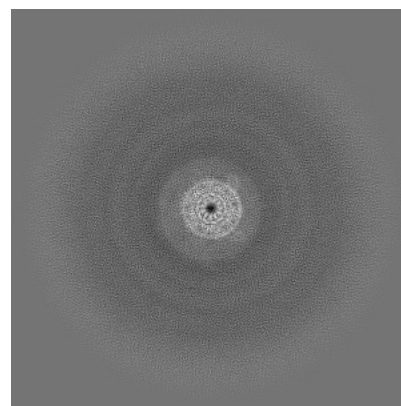
6.1.1 Primary map



X

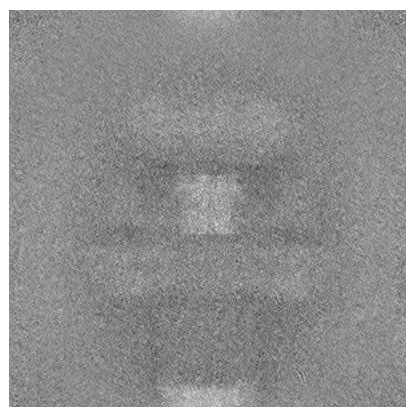


Y

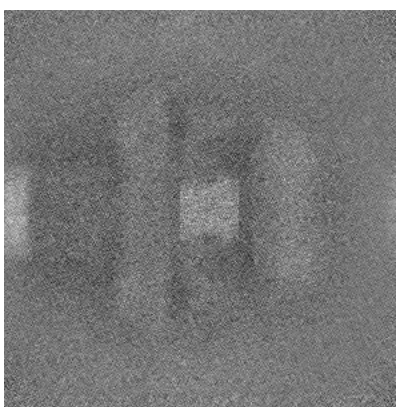


Z

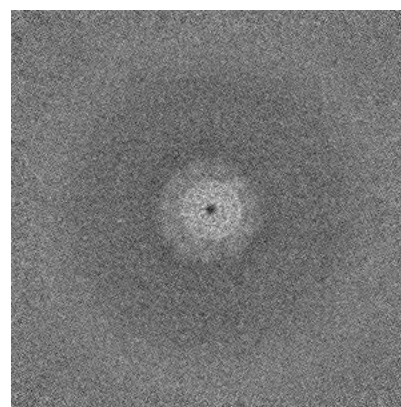
6.1.2 Raw map



X



Y

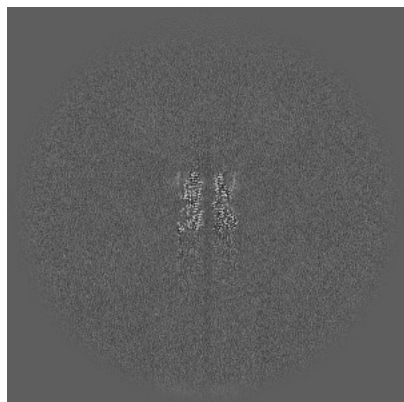


Z

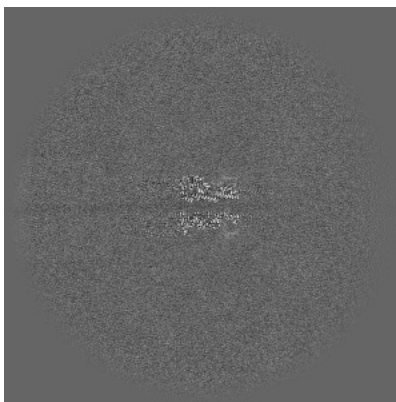
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

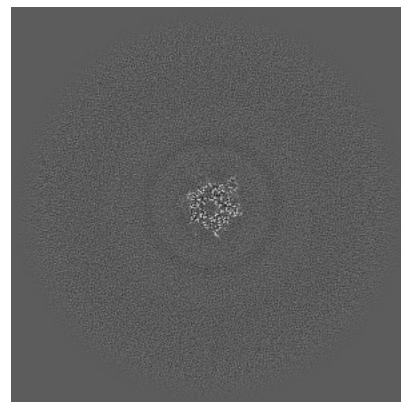
6.2.1 Primary map



X Index: 310

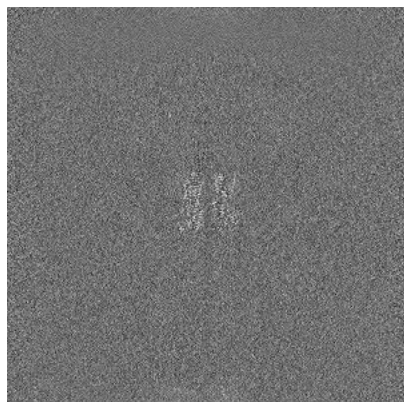


Y Index: 310



Z Index: 310

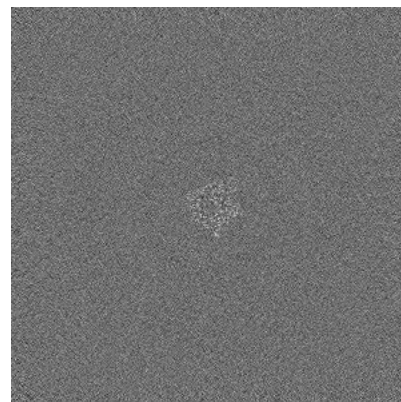
6.2.2 Raw map



X Index: 310



Y Index: 310

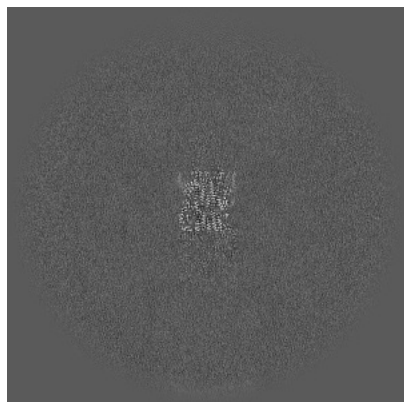


Z Index: 310

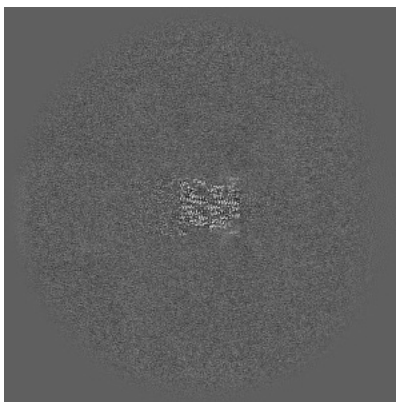
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

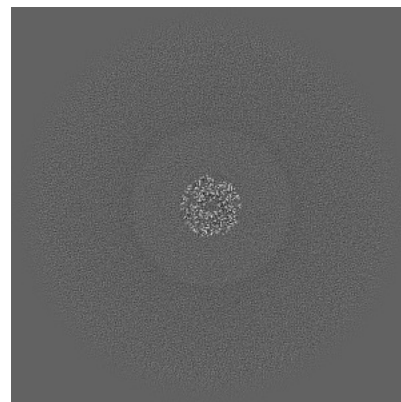
6.3.1 Primary map



X Index: 322

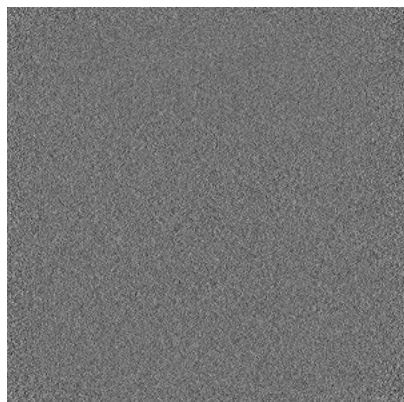


Y Index: 296

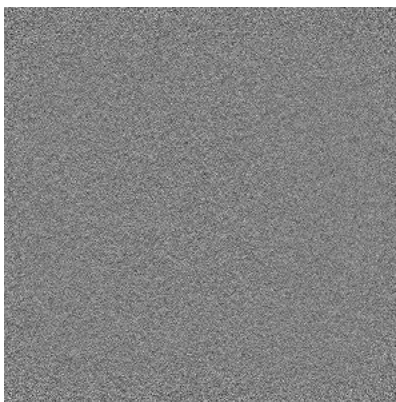


Z Index: 276

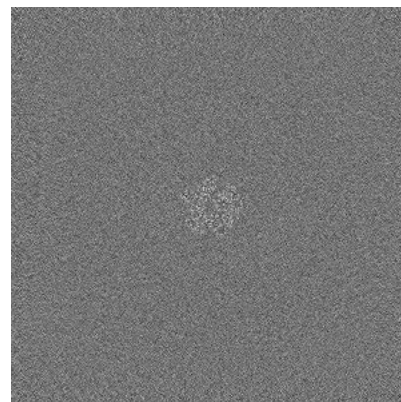
6.3.2 Raw map



X Index: 0



Y Index: 0

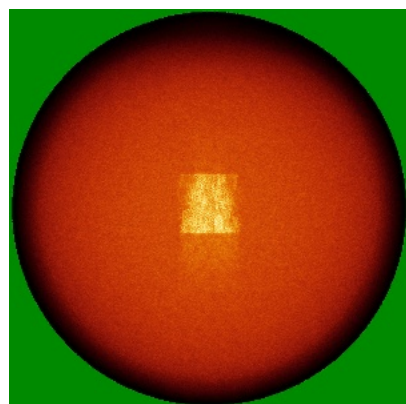


Z Index: 289

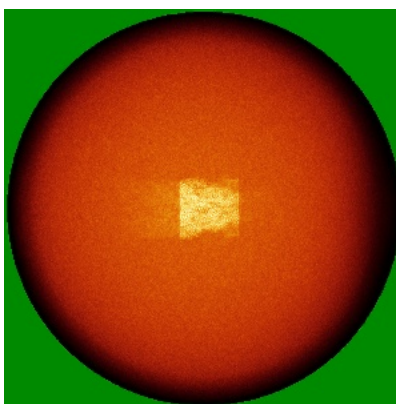
The images above show the largest variance slices of the map in three orthogonal directions.

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

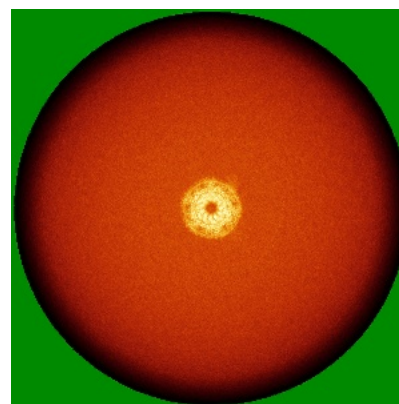
6.4.1 Primary map



X

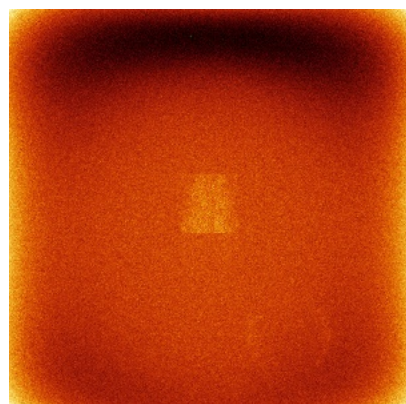


Y

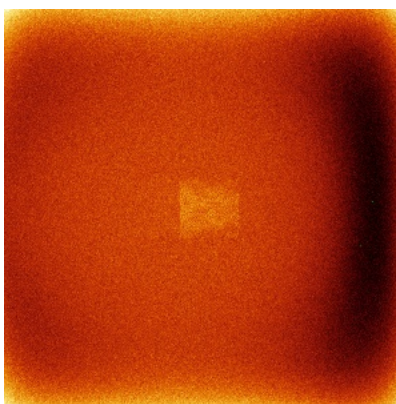


Z

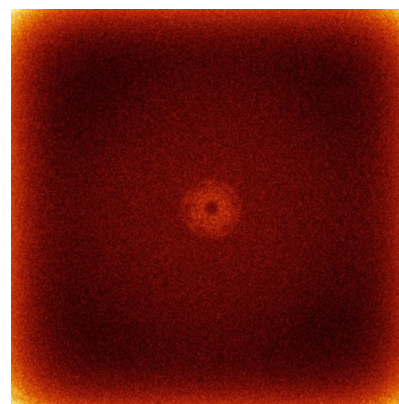
6.4.2 Raw map



X



Y

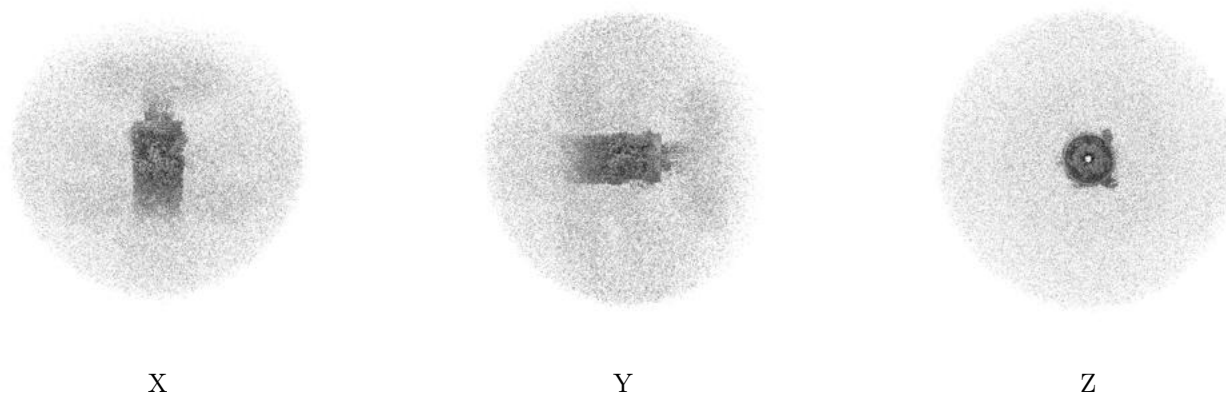


Z

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.

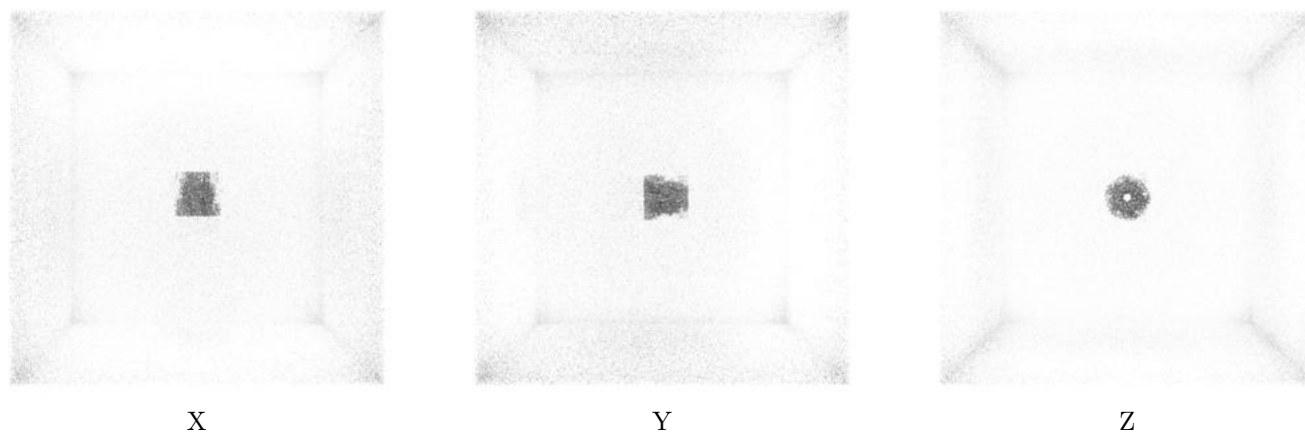
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. 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.

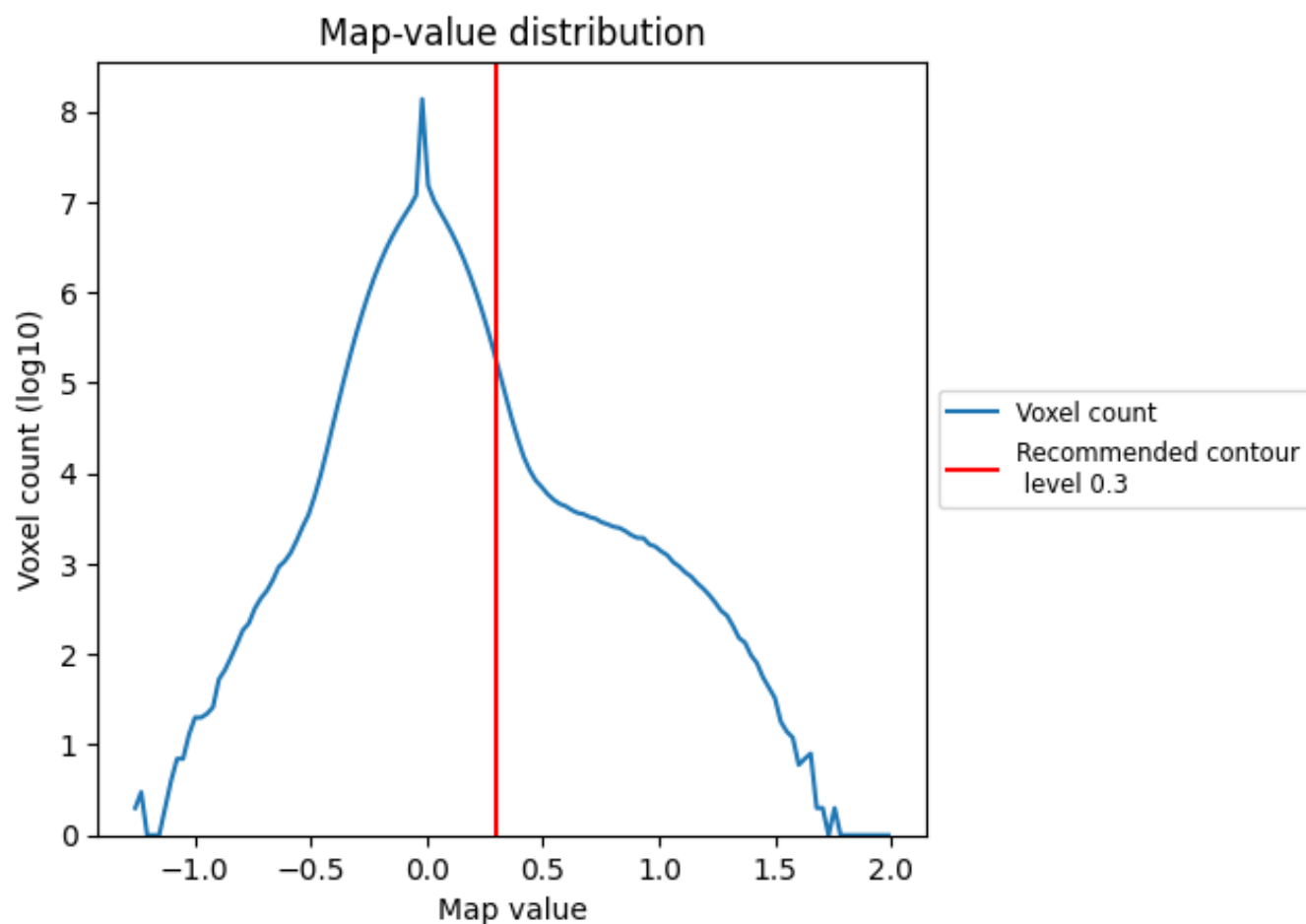
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

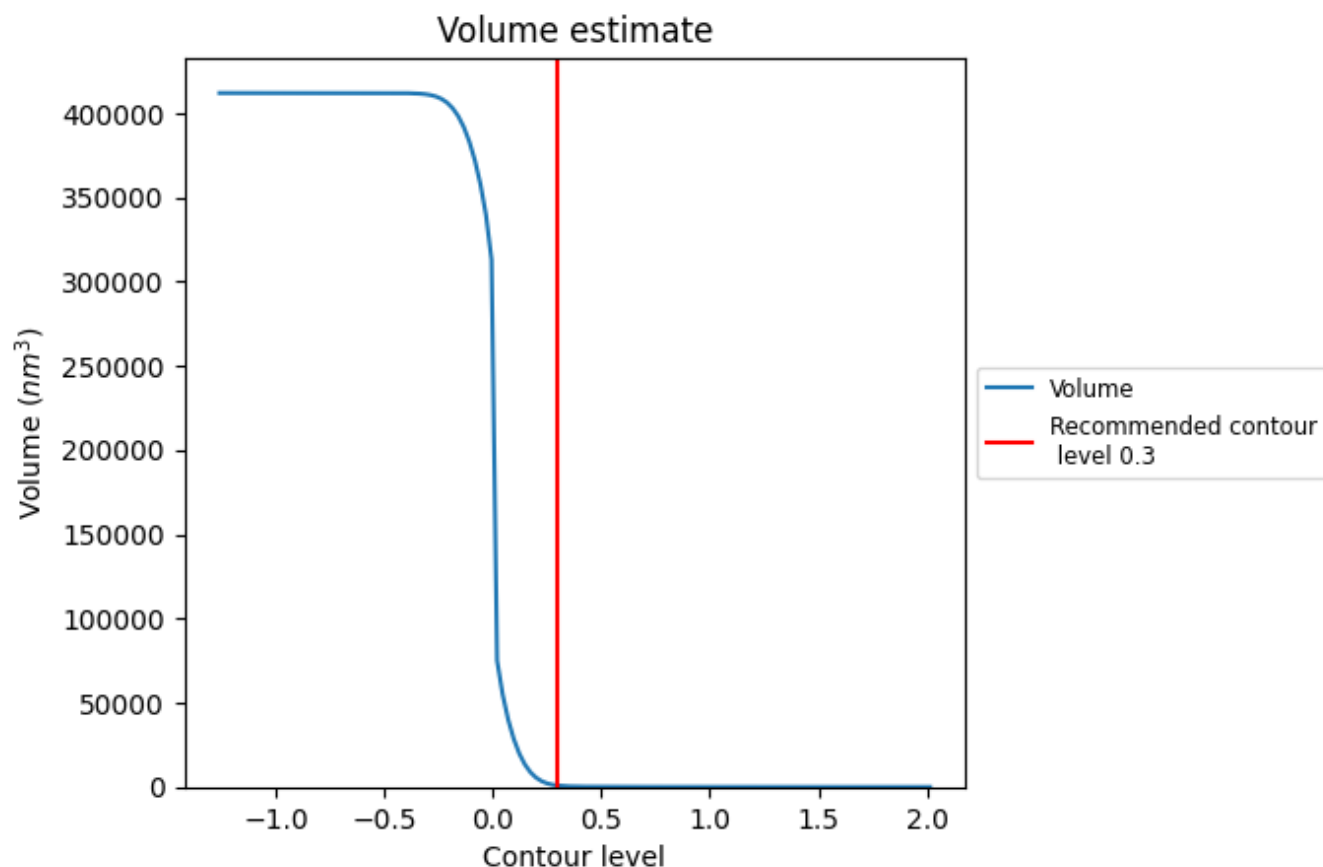
This section contains the results of statistical analysis of the map.

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.

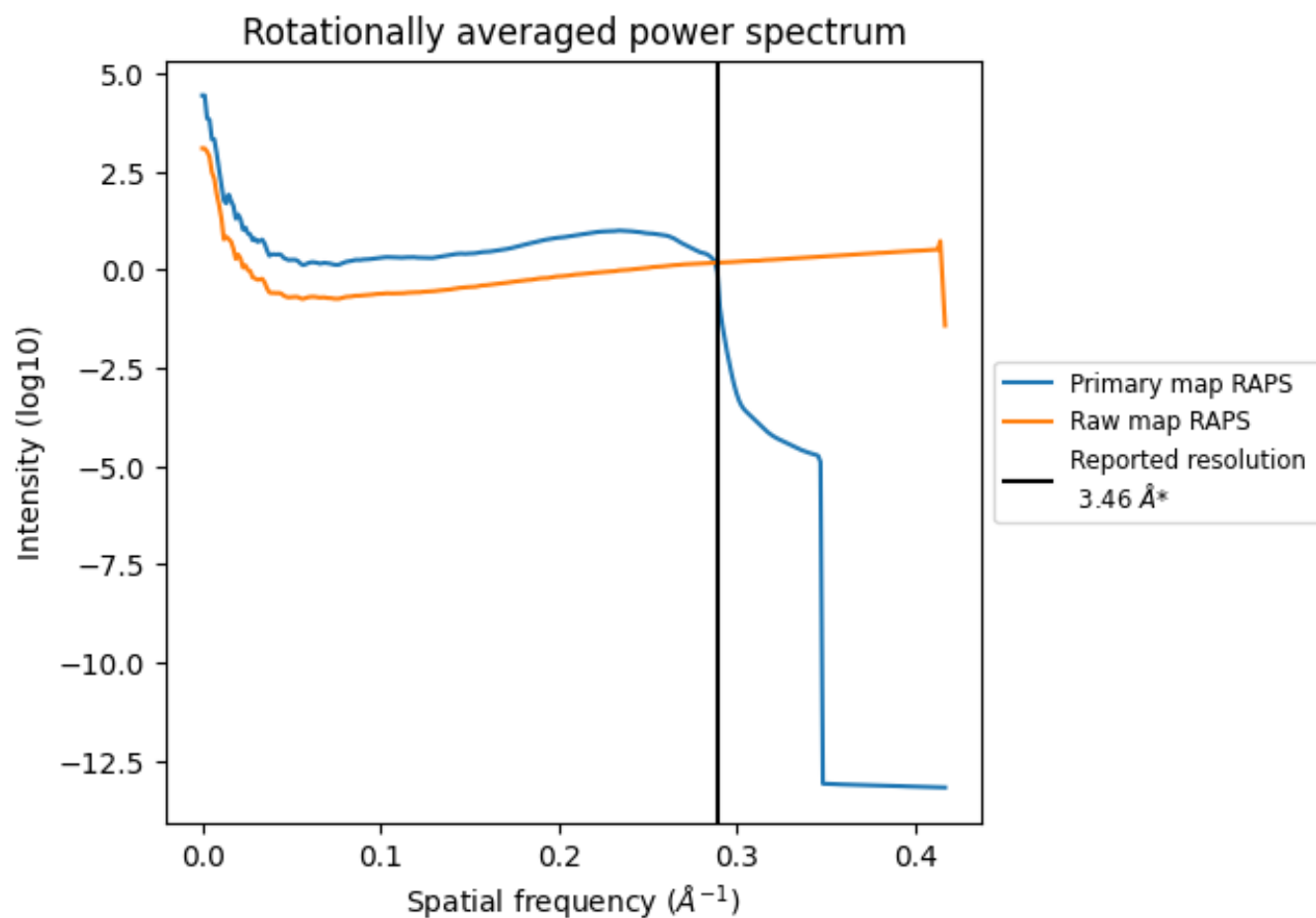
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 837 nm^3 ; this corresponds to an approximate mass of 756 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 ⓘ

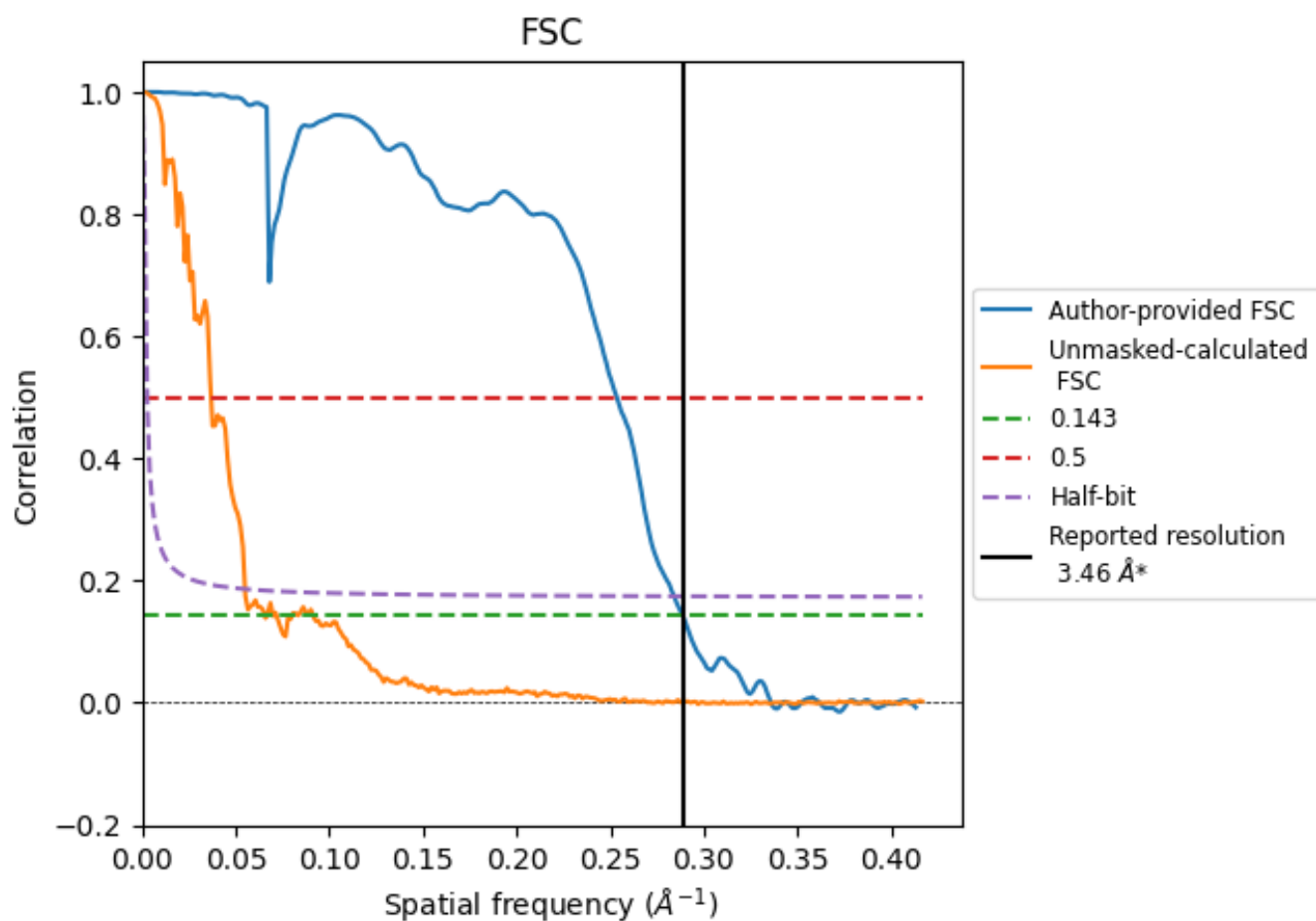


*Reported resolution corresponds to spatial frequency of 0.289 \AA^{-1}

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 0.289 \AA^{-1}

8.2 Resolution estimates [i](#)

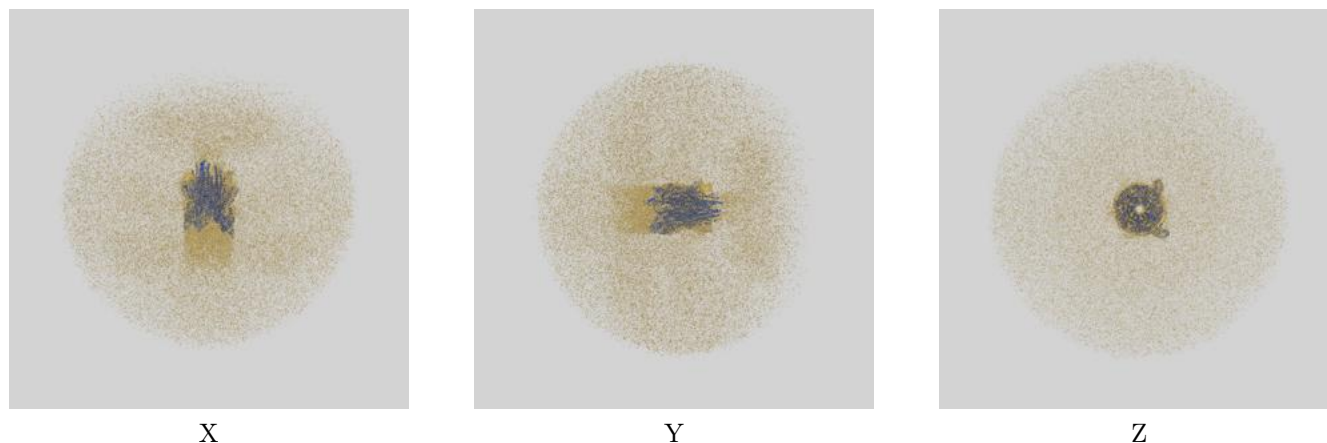
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.46	-	-
Author-provided FSC curve	3.46	3.94	3.52
Unmasked-calculated*	15.29	27.17	18.21

*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 15.29 differs from the reported value 3.46 by more than 10 %

9 Map-model fit [i](#)

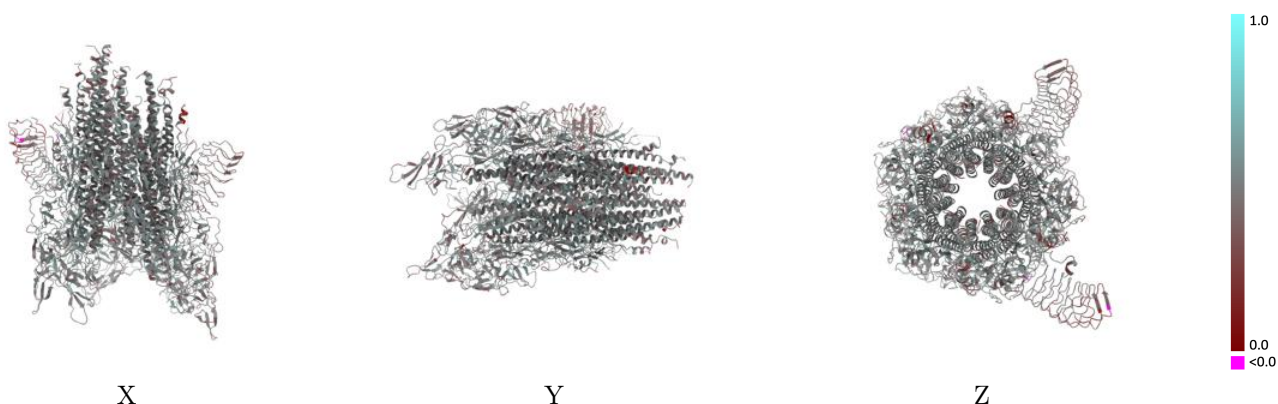
This section contains information regarding the fit between EMDB map EMD-39786 and PDB model 8Z5W. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



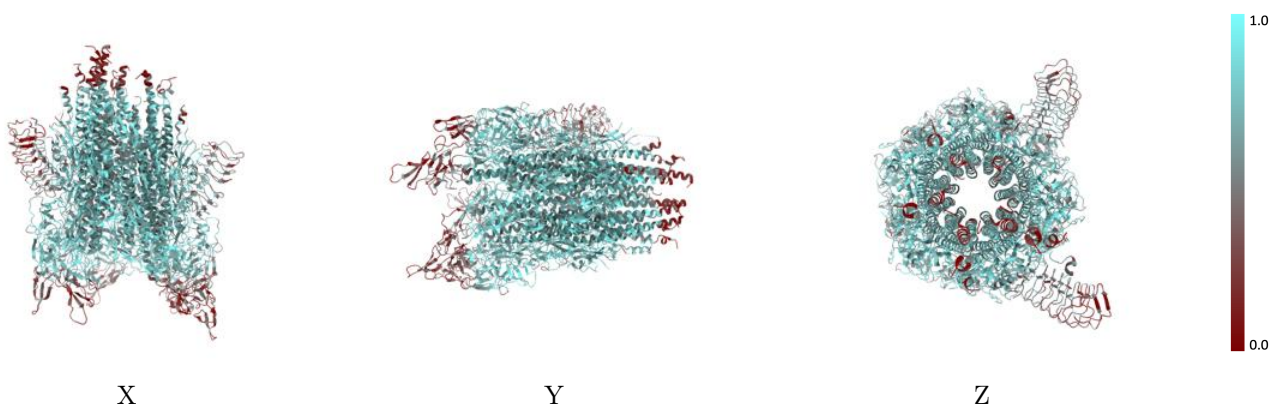
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



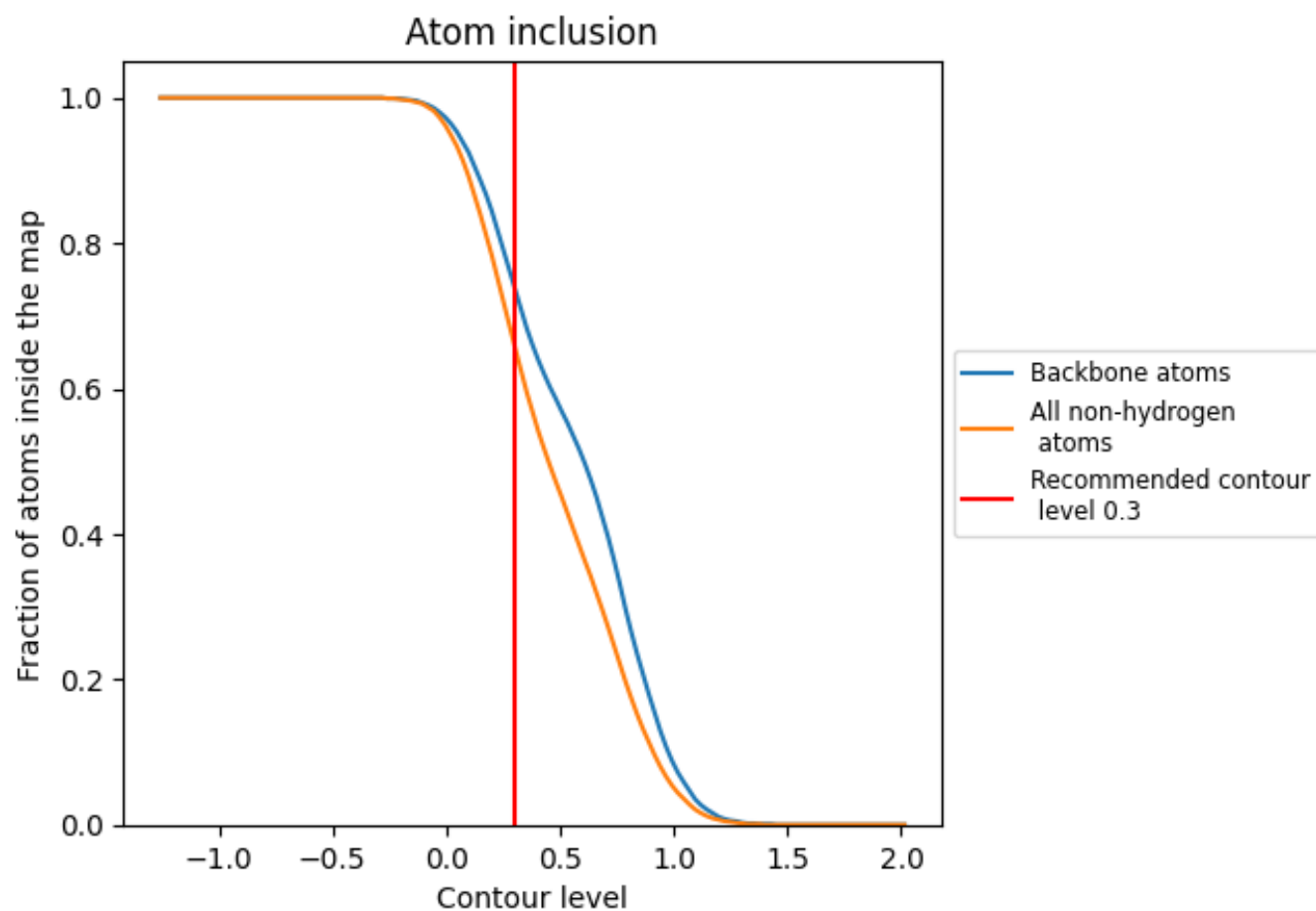
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 66% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6580	 0.4740
0	 0.3860	 0.4000
9	 0.5090	 0.4220
A	 0.5540	 0.4730
AA	 0.7110	 0.4600
AB	 0.7410	 0.4830
AC	 0.6690	 0.4800
AD	 0.7190	 0.4880
AE	 0.7110	 0.4760
AF	 0.5820	 0.4390
AG	 0.8360	 0.5070
AH	 0.7670	 0.4810
AI	 0.8080	 0.5300
AJ	 0.6070	 0.4550
AK	 0.6690	 0.4660
AL	 0.7640	 0.4770
AM	 0.7230	 0.4890
AN	 0.7410	 0.4830
AO	 0.7730	 0.5050
AP	 0.6510	 0.4830
AQ	 0.6730	 0.4780
AR	 0.4890	 0.4680
B	 0.6010	 0.4770
C	 0.6350	 0.4880
b	 0.5380	 0.4660
c	 0.6610	 0.4540
d	 0.6680	 0.4680
e	 0.6350	 0.4890
f	 0.5930	 0.4680
g	 0.7070	 0.4680
h	 0.7700	 0.4840
i	 0.7490	 0.4800
j	 0.7640	 0.4920
k	 0.7460	 0.4870
l	 0.7340	 0.4760



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Chain	Atom inclusion	Q-score
m	 0.7320	 0.4830
n	 0.7100	 0.4780
o	 0.7450	 0.4850
p	 0.7570	 0.4910
q	 0.7510	 0.4730