Full wwPDB EM Validation Report (i)

Mar 7, 2026 – 04:08 AM UTC

PDB ID	:	6SD1 / pdb_00006sd1
EMDB ID	:	EMD-10145
Title	:	Structure of the RBM3/collar region of the Salmonella flagella MS-ring protein FliF with 33-fold symmetry applied
Authors	:	Johnson, S.; Fong, Y.H.; Deme, J.C.; Furlong, E.J.; Kuhlen, L.; Lea, S.M.
Deposited on	:	2019-07-26
Resolution	:	2.60 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

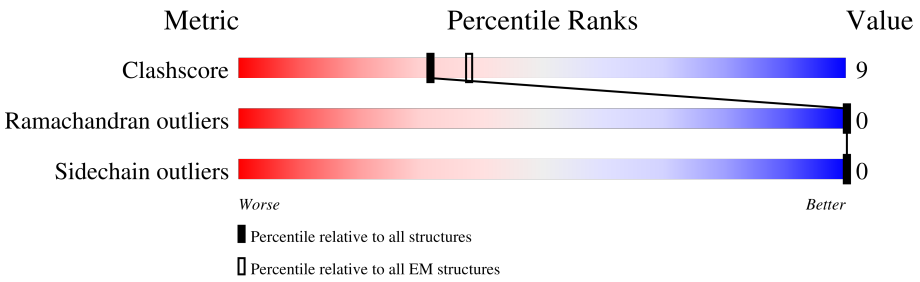
EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh &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

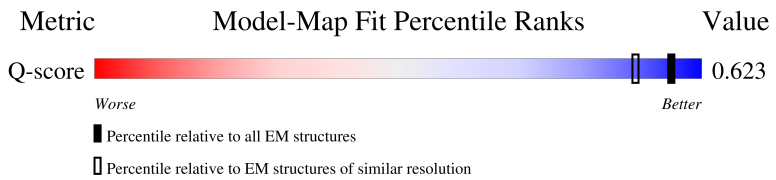
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 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	8728 (2.10 - 3.10)

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 <=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	A	560	21% 6% 73%
1	B	560	20% 7% 73%
1	C	560	22% 5% 73%
1	D	560	21% 6% 73%

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Mol	Chain	Length	Quality of chain
1	E	560	22% 5% 73%
1	F	560	21% 6% 73%
1	G	560	21% 6% 73%
1	H	560	20% 7% 73%
1	I	560	21% 6% 73%
1	J	560	21% 6% 73%
1	K	560	22% 5% 73%
1	L	560	20% 7% 73%
1	M	560	20% 7% 73%
1	N	560	21% 6% 73%
1	O	560	20% 7% 73%
1	P	560	20% 7% 73%
1	Q	560	20% 7% 73%
1	R	560	21% 6% 73%
1	S	560	21% 6% 73%
1	T	560	21% 6% 73%
1	U	560	21% 6% 73%
1	V	560	21% 6% 73%
1	W	560	21% 6% 73%
1	X	560	20% 7% 73%
1	Y	560	20% 7% 73%
1	Z	560	21% 6% 73%
1	a	560	21% 6% 73%
1	b	560	20% 7% 73%
1	c	560	21% 6% 73%

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Mol	Chain	Length	Quality of chain
1	d	560	21% 6% 73%
1	e	560	21% 6% 73%
1	f	560	21% 6% 73%
1	g	560	21% 6% 73%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 39369 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 M-ring protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	151	1193	726	223	241	3	0	0
1	B	151	1193	726	223	241	3	0	0
1	C	151	1193	726	223	241	3	0	0
1	D	151	1193	726	223	241	3	0	0
1	E	151	1193	726	223	241	3	0	0
1	F	151	1193	726	223	241	3	0	0
1	G	151	1193	726	223	241	3	0	0
1	H	151	1193	726	223	241	3	0	0
1	I	151	1193	726	223	241	3	0	0
1	J	151	1193	726	223	241	3	0	0
1	K	151	1193	726	223	241	3	0	0
1	L	151	1193	726	223	241	3	0	0
1	M	151	1193	726	223	241	3	0	0
1	N	151	1193	726	223	241	3	0	0
1	O	151	1193	726	223	241	3	0	0
1	P	151	1193	726	223	241	3	0	0
1	Q	151	1193	726	223	241	3	0	0

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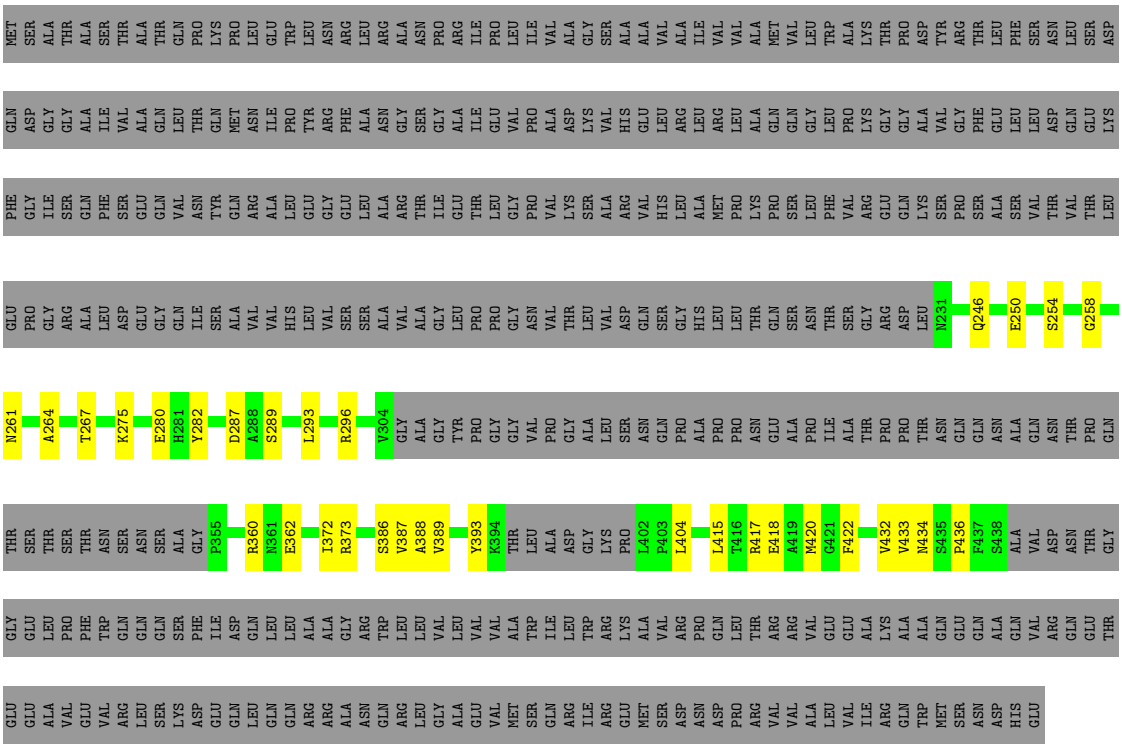
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	R	151	1193	726	223	241	3	0	0
1	S	151	1193	726	223	241	3	0	0
1	T	151	1193	726	223	241	3	0	0
1	U	151	1193	726	223	241	3	0	0
1	V	151	1193	726	223	241	3	0	0
1	W	151	1193	726	223	241	3	0	0
1	X	151	1193	726	223	241	3	0	0
1	Y	151	1193	726	223	241	3	0	0
1	Z	151	1193	726	223	241	3	0	0
1	a	151	1193	726	223	241	3	0	0
1	b	151	1193	726	223	241	3	0	0
1	c	151	1193	726	223	241	3	0	0
1	d	151	1193	726	223	241	3	0	0
1	e	151	1193	726	223	241	3	0	0
1	f	151	1193	726	223	241	3	0	0
1	g	151	1193	726	223	241	3	0	0

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.

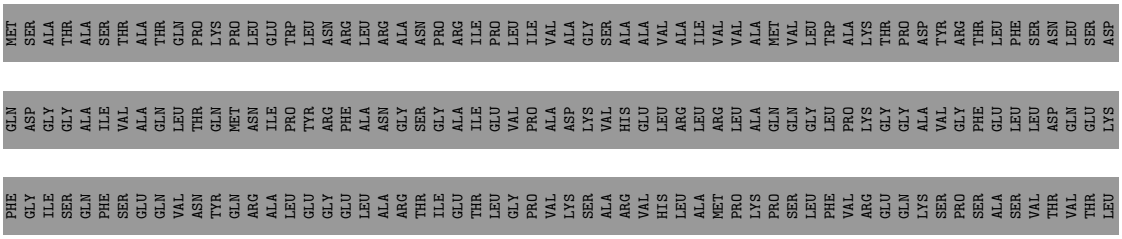
- Molecule 1: Flagellar M-ring protein

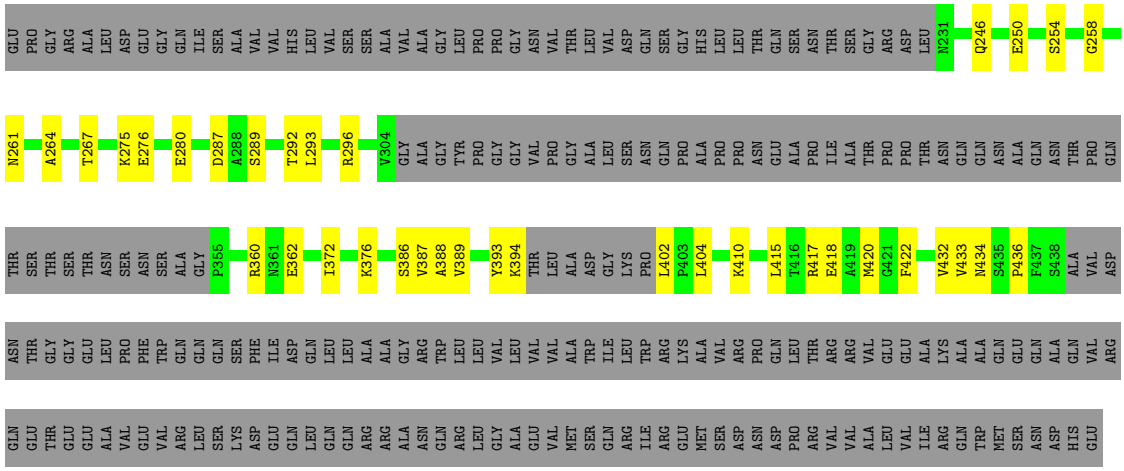
Chain A: 21% 6% 73%



- Molecule 1: Flagellar M-ring protein

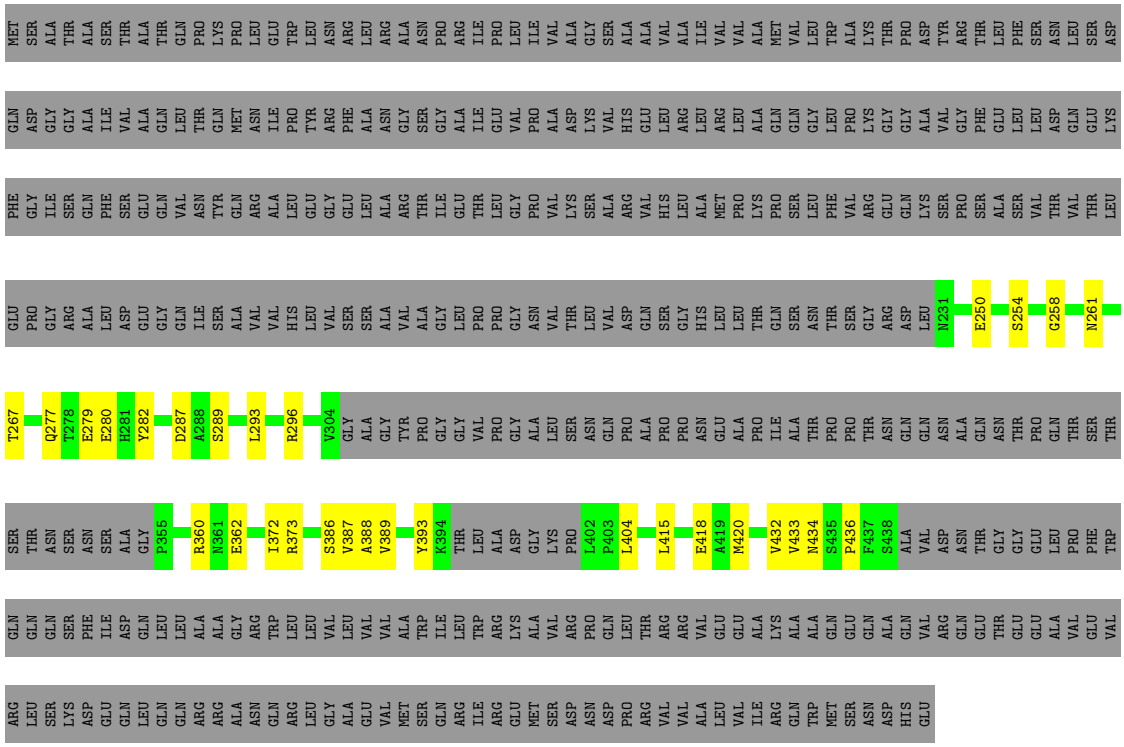
Chain B: 20% 7% 73%





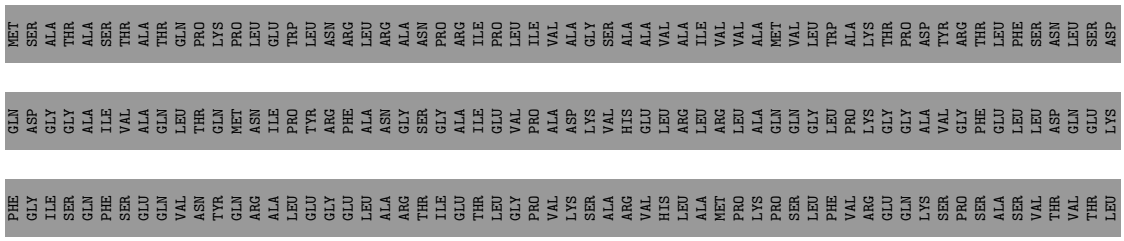
• Molecule 1: Flagellar M-ring protein

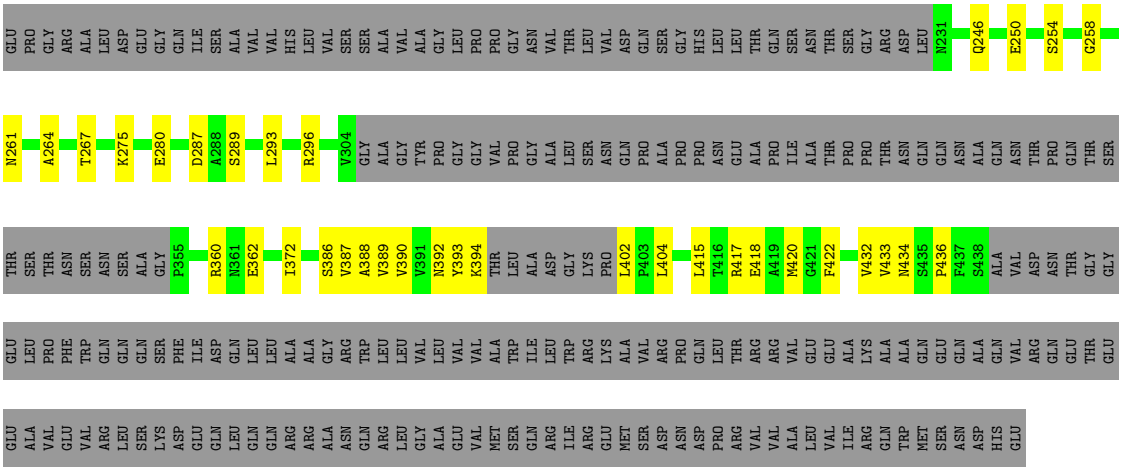
Chain C: 22% 5% 73%



• Molecule 1: Flagellar M-ring protein

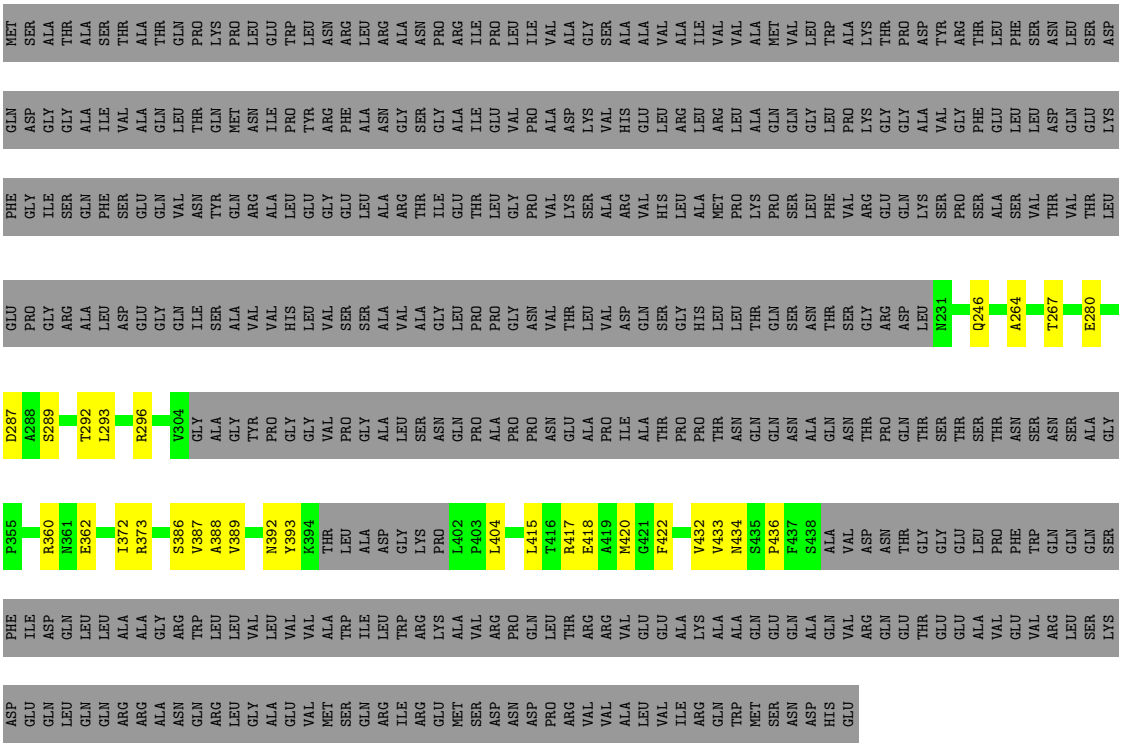
Chain D: 21% 6% 73%





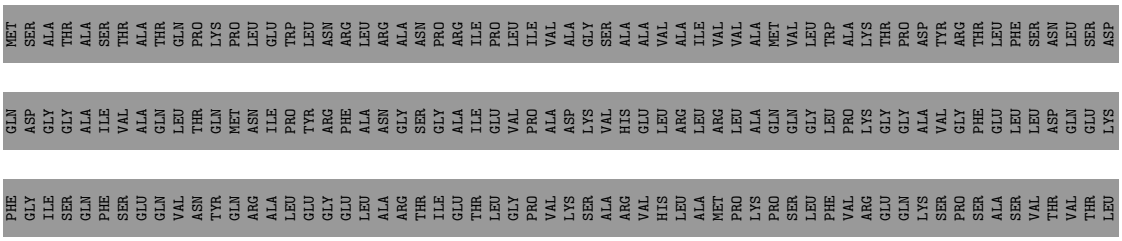
• Molecule 1: Flagellar M-ring protein

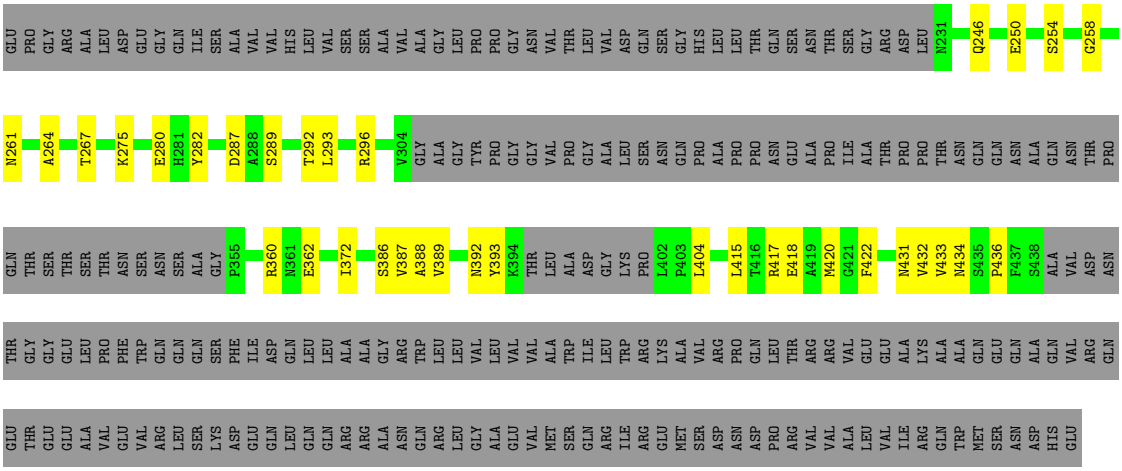
Chain E: 22% 5% 73%



• Molecule 1: Flagellar M-ring protein

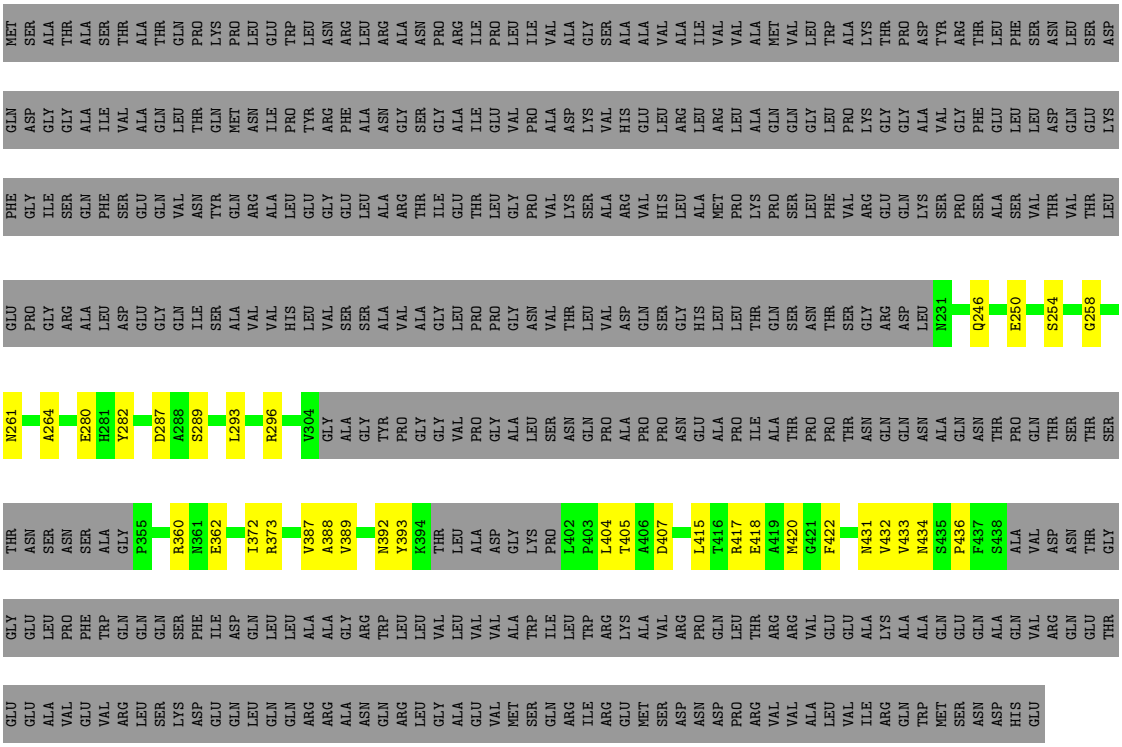
Chain F: 21% 6% 73%





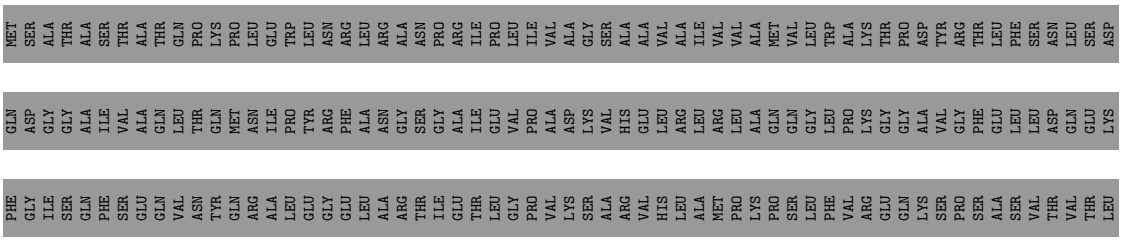
• Molecule 1: Flagellar M-ring protein

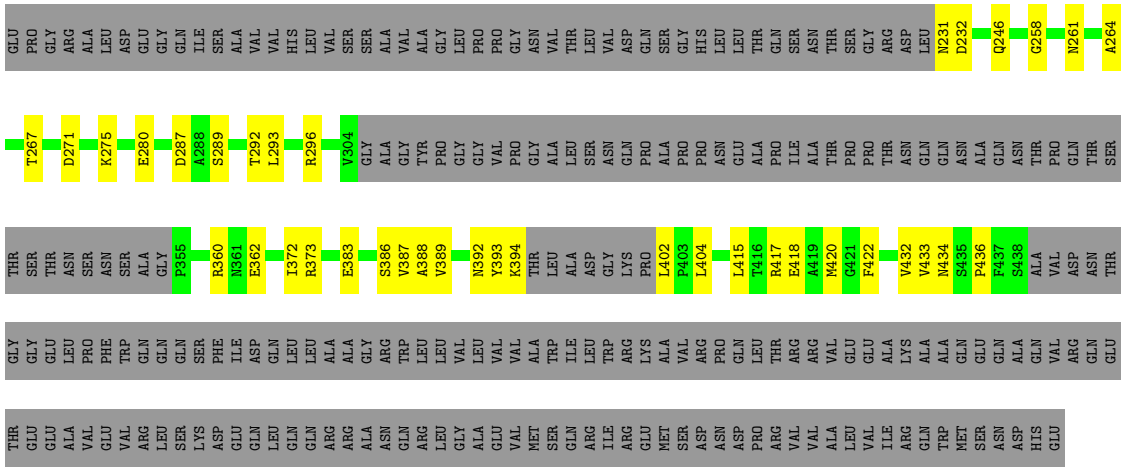
Chain G: 21% 6% 73%



• Molecule 1: Flagellar M-ring protein

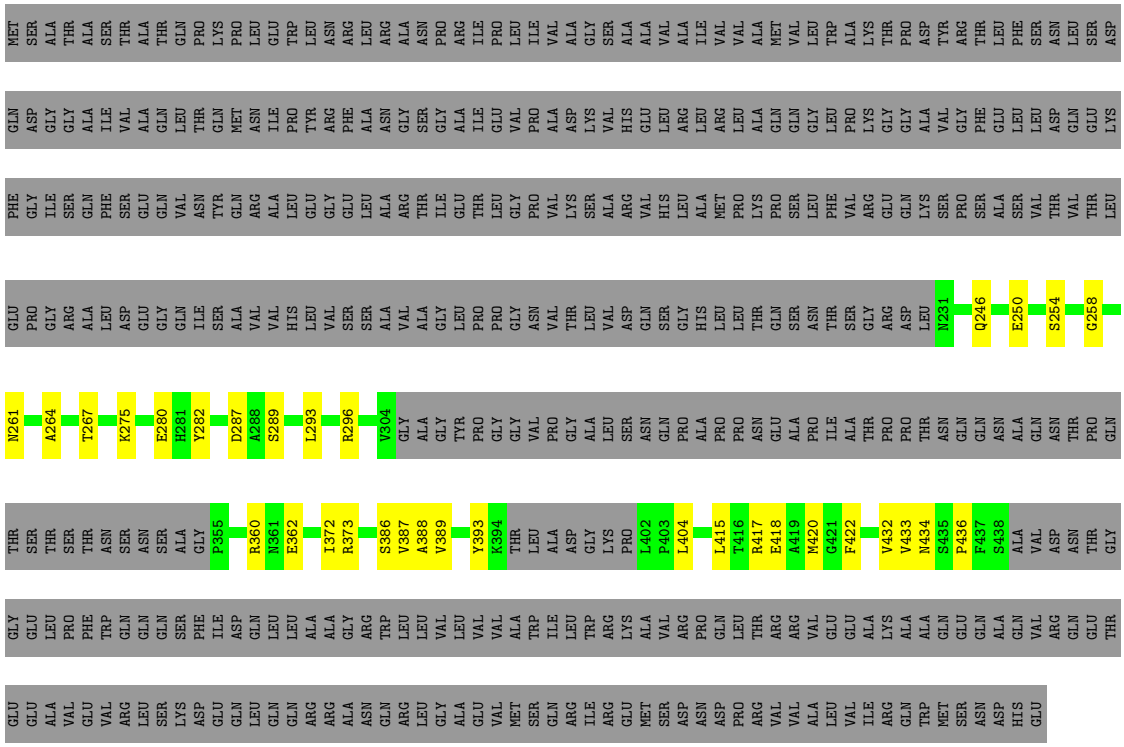
Chain H: 20% 7% 73%





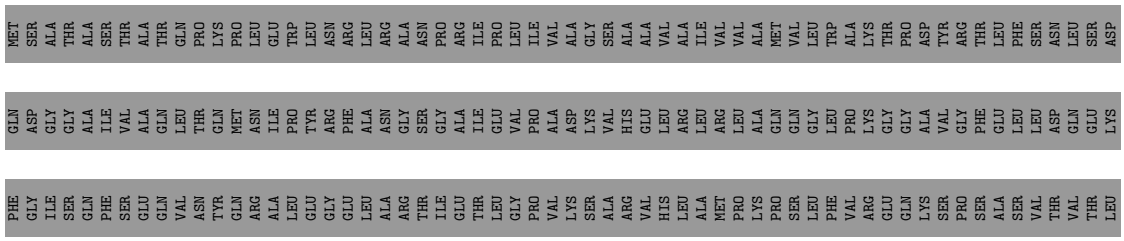
- Molecule 1: Flagellar M-ring protein

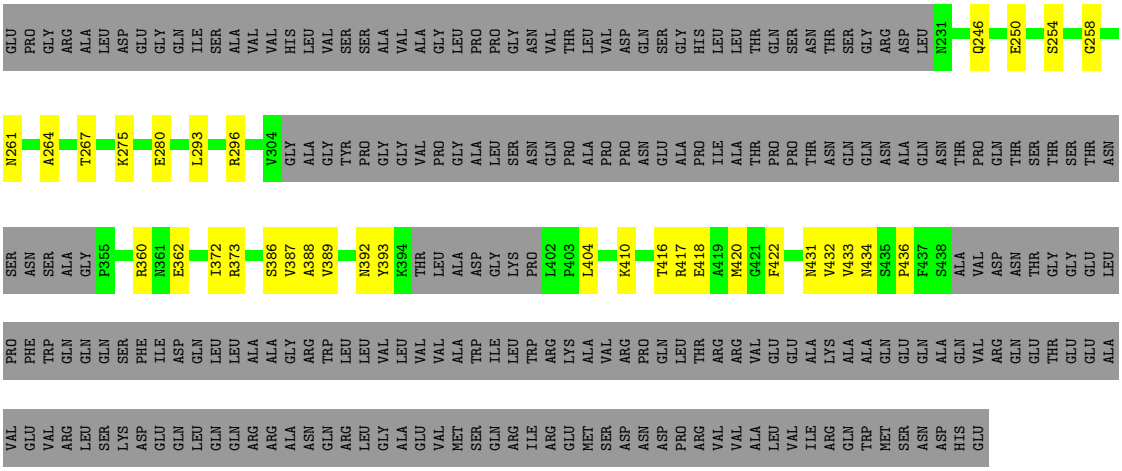
Chain I: 21% 6% 73%



- Molecule 1: Flagellar M-ring protein

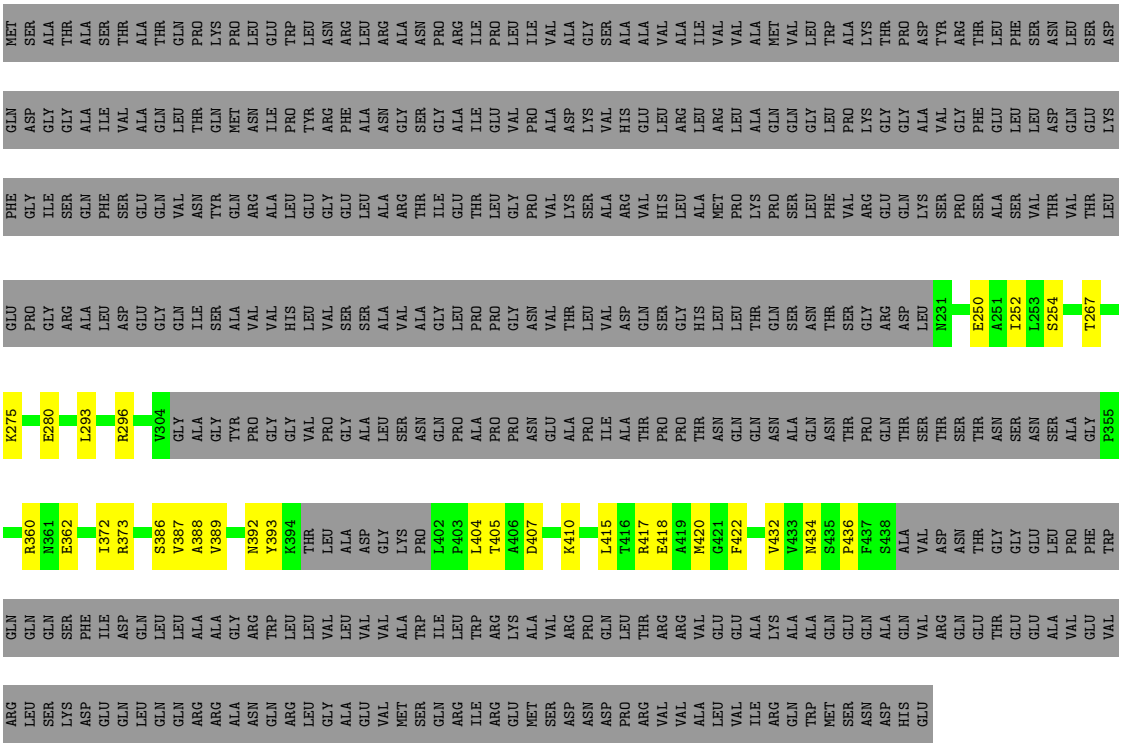
Chain J: 21% 6% 73%





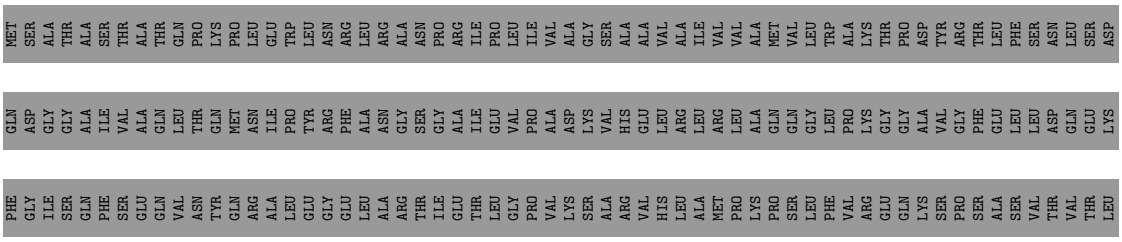
- Molecule 1: Flagellar M-ring protein

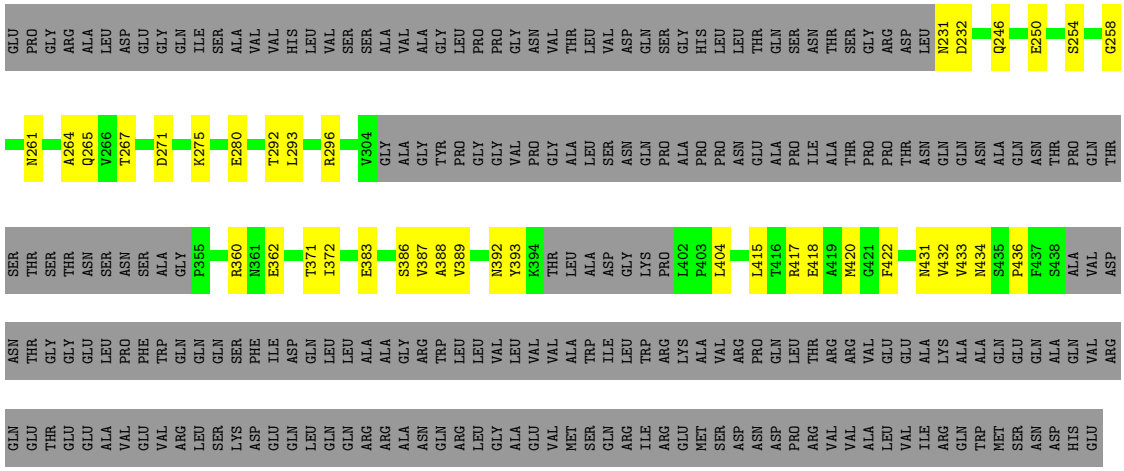
Chain K:



- Molecule 1: Flagellar M-ring protein

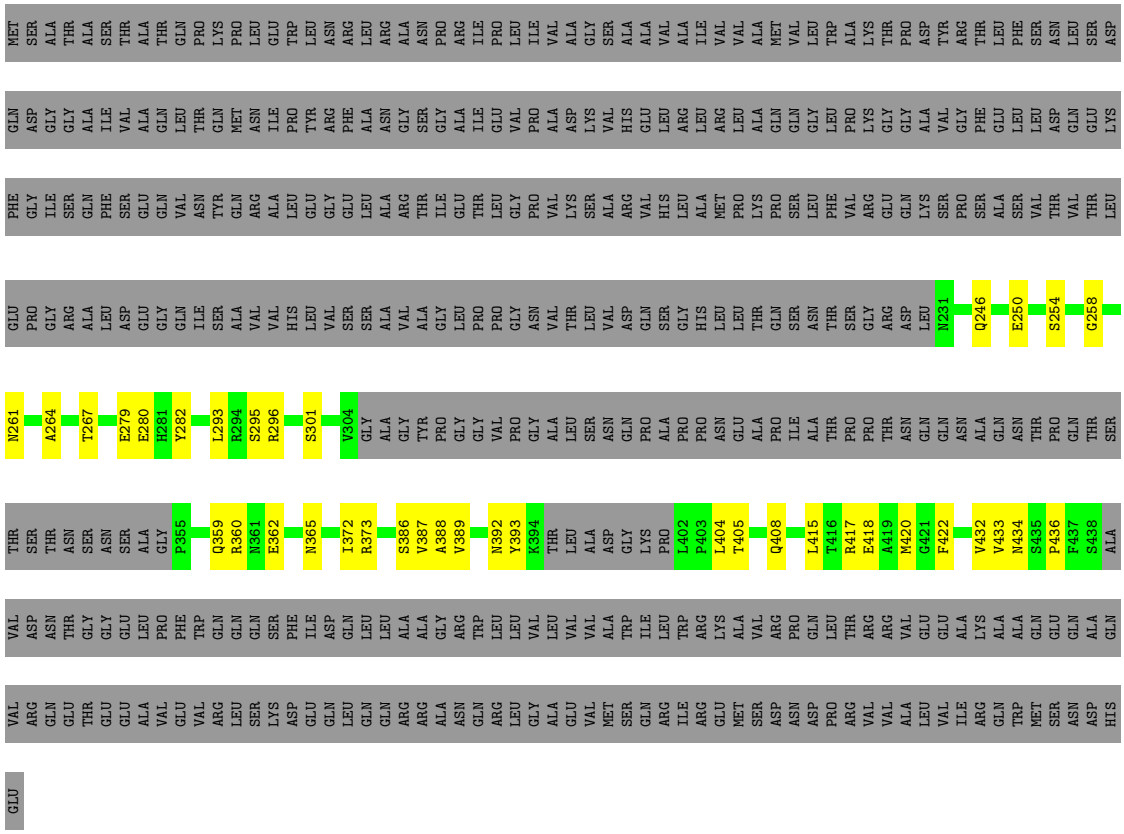
Chain L:





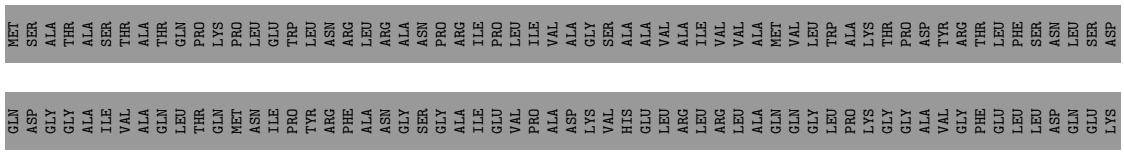
• Molecule 1: Flagellar M-ring protein

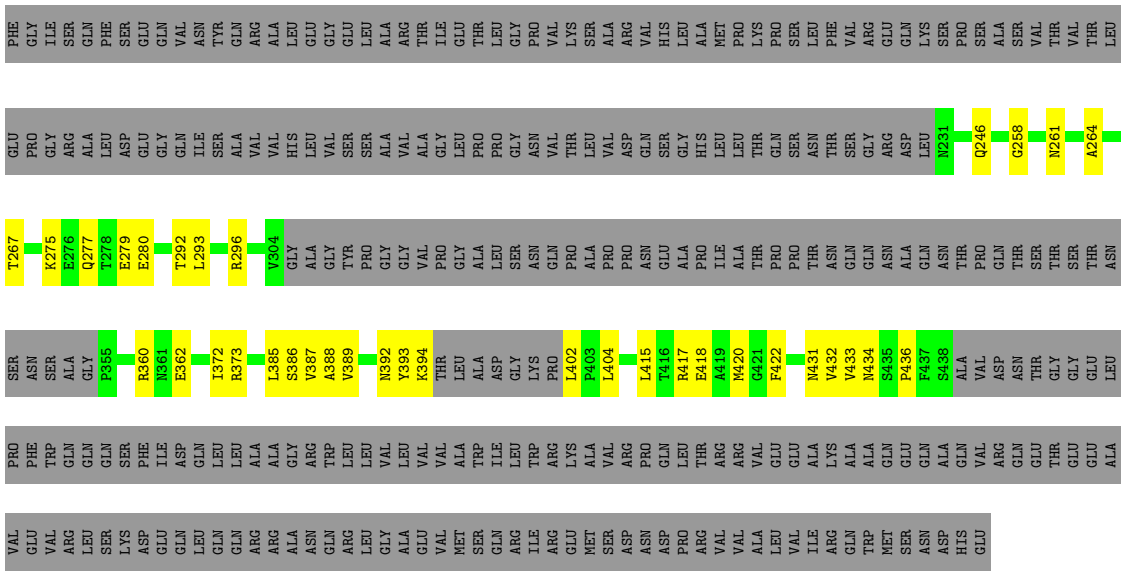
Chain M: 20% 7% 73%



• Molecule 1: Flagellar M-ring protein

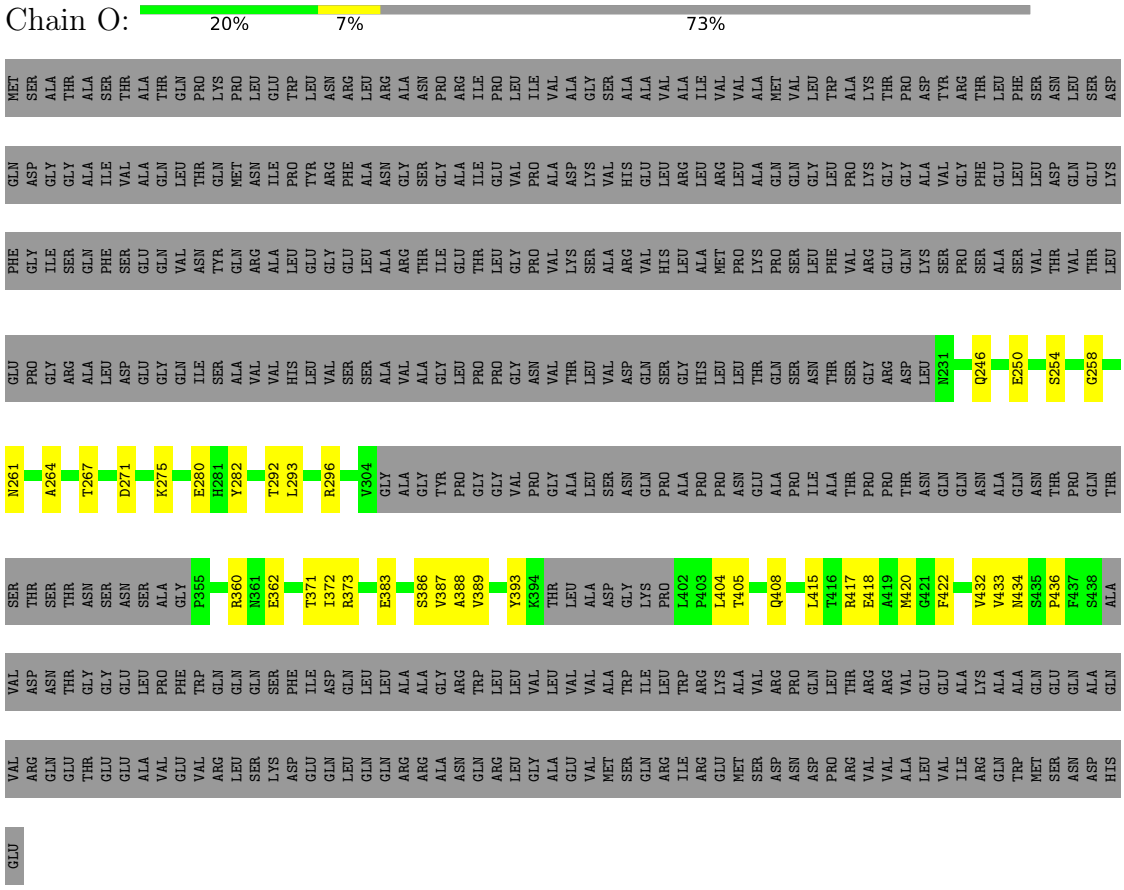
Chain N: 21% 6% 73%





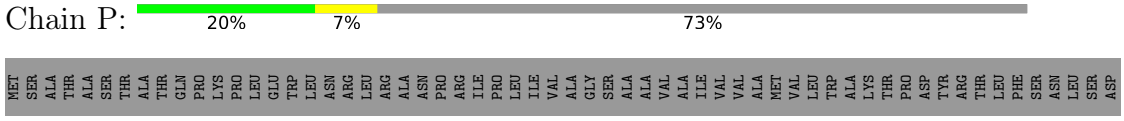
- Molecule 1: Flagellar M-ring protein

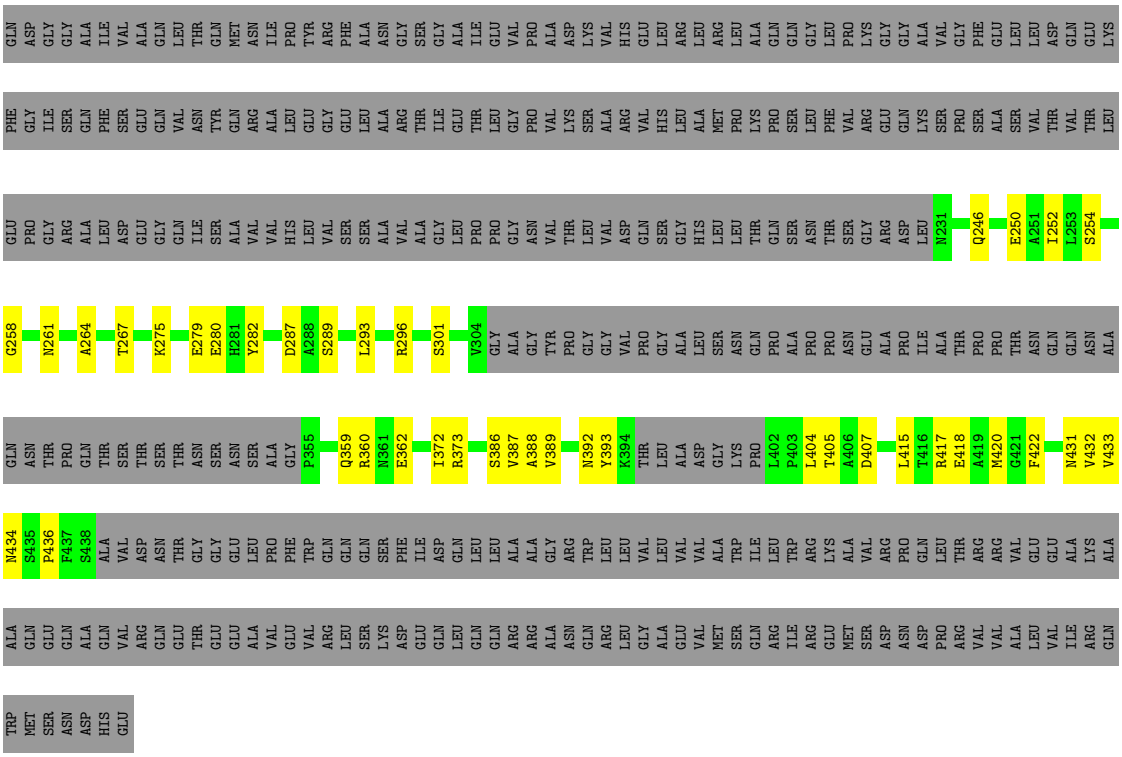
Chain O:



- Molecule 1: Flagellar M-ring protein

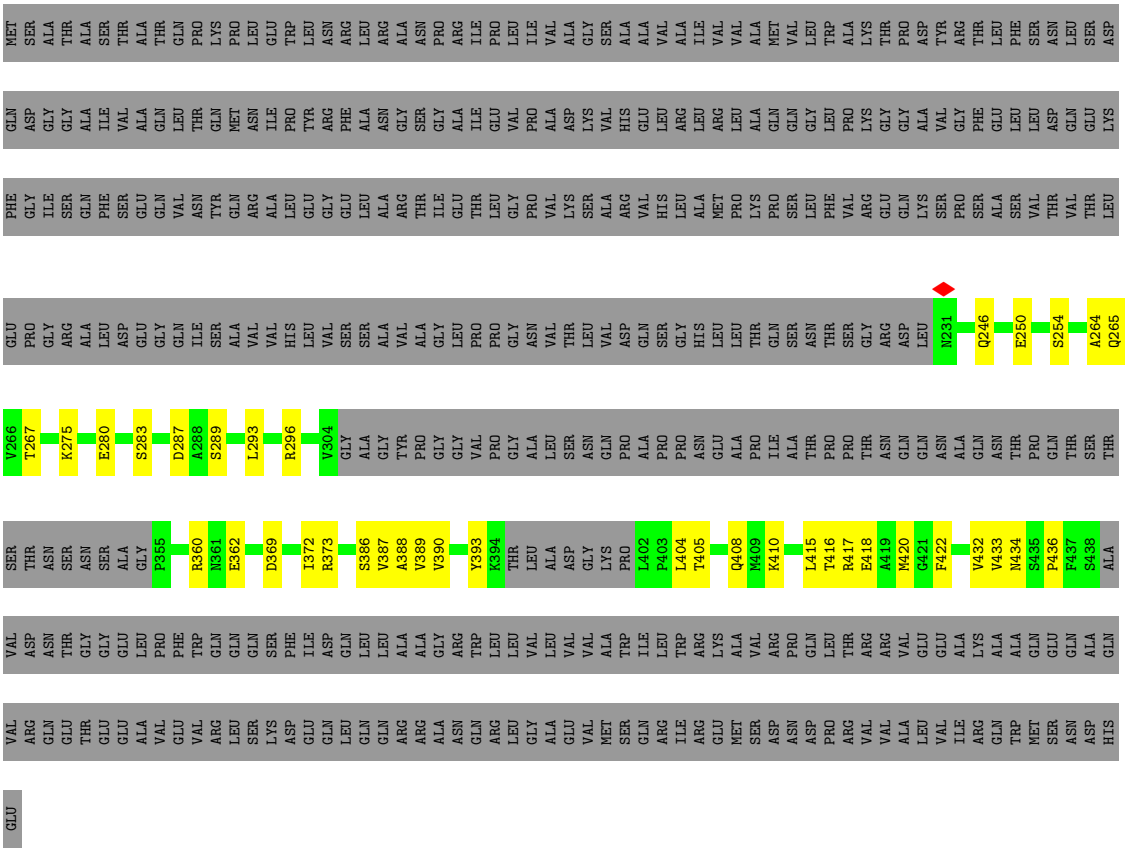
Chain P:





- Molecule 1: Flagellar M-ring protein

Chain Q: 20% 7% 73%



• Molecule 1: Flagellar M-ring protein

Chain R: 21% 6% 73%

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

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

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

GLU PRO GLY ARG ALA LEU ASP GLU GLY GLN ILE SER ALA VAL VAL HIS LEU VAL SER SER ALA VAL ALA GLY LEU PRO PRO GLY ASN VAL THR LEU VAL ASP GLN SER GLY HIS LEU LEU THR GLN SER ASN THR SER GLY ARG ASP LEU N231 Q246 E250 A261 I252 L253 S254

G258 N261 A264 T267 K275 E280 T292 L293 R296 V304 GLY ALA GLY TYR PRO GLY GLY VAL PRO GLY ALA LEU SER ASN GLN PRO ALA PRO PRO GLU ALA PRO ILE ALA THR PRO PRO THR ASN GLN GLN ASN ALA GLN ASN THR PRO GLN THR SER THR

SER THR ASN SER ASN SER ALA GLY P355 R360 N361 E362 I372 R373 S386 V387 A388 V389 N392 Y393 K394 THR LEU ALA ASP GLY LYS PRO L402 P403 L404 L415 T416 R417 E418 A419 M420 G421 F422 N431 V432 V433 N434 S435 P436 F437 S438 ALA VAL ASP ASN THR GLY GLY

GLU LEU PRO PHE TRP GLN GLN GLN SER PHE ILE ASP GLN LEU LEU ALA ALA GLY ARG TRP LEU LEU LEU VAL LEU VAL VAL ALA ALA TRP ILE LEU TRP ARG LYS ALA VAL ARG PRO GLN LEU THR ARG ARG VAL GLU GLU ALA LYS ALA ALA GLN GLN GLU GLN ALA GLN VAL ARG GLN GLU THR GLU

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

• Molecule 1: Flagellar M-ring protein

Chain S: 21% 6% 73%

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

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

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

GLU PRO GLY ARG ALA LEU ASP GLU GLY GLN ILE SER ALA VAL VAL HIS LEU VAL SER SER ALA VAL ALA GLY LEU PRO PRO GLY ASN VAL THR LEU VAL ASP GLN SER GLY HIS LEU LEU THR GLN SER ASN THR SER GLY ARG ASP LEU N231 Q246 E250 S254 G258

N261 A264 Q265 V266 T267 K275 Y282 D287 A288 S289 L293 R296 V304 GLY ALA GLY TYR PRO GLY GLY VAL PRO GLY ALA LEU SER ASN GLN PRO ALA PRO PRO GLU ALA PRO ILE ALA THR PRO PRO THR ASN GLN GLN ASN ALA GLN ASN THR PRO GLN THR

SER THR SER THR ASN SER ASN SER ALA GLY P355 R360 N361 E362 R373 S386 V387 A388 V389 N392 Y393 K394 THR LEU ALA ASP GLY LYS PRO L402 P403 L404 L415 T416 R417 E418 A419 M420 G421 F422 N431 V432 V433 N434 S435 P436 F437 S438 ALA VAL ASP ASN THR GLY

GLY GLU LEU PRO PHE TRP GLN GLN GLN SER PHE ILE ASP GLN LEU LEU ALA ALA GLY ARG TRP LEU LEU LEU VAL LEU VAL VAL ALA ALA TRP ILE LEU TRP ARG LYS ALA VAL ARG PRO GLN LEU THR ARG ARG VAL GLU GLU ALA LYS ALA ALA GLN GLN GLU GLN ALA GLN VAL ARG GLN GLU THR

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

• Molecule 1: Flagellar M-ring protein

Chain T: 21% 6% 73%

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

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

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

GLU PRO GLY ARG ALA LEU ASP GLU GLY GLN ILE SER ALA VAL VAL HIS LEU VAL SER SER ALA VAL ALA GLY LEU PRO PRO GLY ASN VAL THR LEU VAL ASP GLN SER GLY HIS LEU LEU THR GLN SER ASN THR SER GLY ARG ASP LEU N231 Q246 E250 S254 G258

N261 A264 T267 K275 E280 D287 A288 S289 L293 R296 V304 GLY ALA GLY TYR PRO GLY GLY VAL PRO GLY ALA LEU SER ASN GLN PRO ALA PRO ASN GLU ALA PRO ILE ALA THR PRO PRO THR ASN GLN GLN ASN ALA GLN ASN THR PRO GLN THR SER

THR SER THR ASN SER ASN SER ALA GLY P355 E362 I372 S386 V387 A388 V389 V390 V391 N392 Y393 K394 THR LEU ALA ASP GLY LYS PRO L402 P403 L404 L415 T416 R417 E418 A419 M420 G421 F422 V432 V433 N434 S435 P436 F437 S438 ALA VAL ASP ASN THR GLY GLY GLU LEU

PRO PHE TRP GLN GLN GLN SER PHE ILE ASP GLN LEU LEU ALA ALA GLY ARG TRP LEU LEU VAL LEU VAL VAL ALA TRP ILE LEU TRP ARG LYS ALA VAL ARG PRO GLN LEU THR ARG ARG VAL GLU GLU ALA LYS ALA ALA GLN GLN GLN ALA GLN VAL ARG GLN GLU THR GLU GLU ALA

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

• Molecule 1: Flagellar M-ring protein

Chain U: 21% 6% 73%

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

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

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

GLU PRO GLY ARG ALA LEU ASP GLU GLY GLN ILE SER ALA VAL VAL HIS LEU VAL SER SER ALA VAL ALA GLY LEU PRO PRO GLY ASN VAL THR LEU VAL ASP GLN SER GLY HIS LEU LEU THR GLN SER ASN THR SER GLY ARG ASP LEU N231 Q246 E250 A251 I252 L253 S254

G258 N261 A264 T267 E280 D287 A288 S289 T292 L293 R296 V304 GLY ALA GLY TYR PRO GLY GLY GLY VAL PRO GLY ALA LEU SER ASN GLN PRO ALA PRO PRO ASN GLU ALA PRO ILE ALA THR PRO PRO THR ASN GLN GLN ASN ALA GLN ASN THR PRO GLN THR

SER THR SER THR ASN SER ASN SER ALA GLY P355 R360 N361 E362 I372 S386 V387 A388 V389 N392 Y393 K394 THR LEU ALA ASP GLY LYS PRO L402 P403 L404 T405 Q408 E413 D414 L415 T416 R417 E418 A419 M420 G421 F422 V432 V433 N434 S435 P436 F437 S438 ALA VAL

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

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

• Molecule 1: Flagellar M-ring protein

Chain V: 21% 6% 73%

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

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

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

GLU PRO GLY ARG ALA LEU ASP GLU GLY GLN ILE SER ALA VAL VAL HIS LEU VAL SER SER ALA VAL ALA GLY LEU PRO PRO GLY ASN VAL THR LEU VAL ASP GLN SER GLY HIS LEU LEU THR GLN SER ASN THR SER GLY ARG ASP LEU N231 Q246 E250 S254 G258

N261 A264 Q265 V266 T267 Y282 D287 A288 S289 L293 R296 V304 GLY ALA GLY TYR PRO GLY GLY VAL PRO GLY ALA LEU SER ASN GLN PRO GLN GLU GLN ASN ALA GLN ASN THR PRO GLN THR SER THR

SER THR ASN SER ASN SER ALA GLY P355 R360 N361 E362 R373 S386 V387 A388 V389 N392 Y393 K394 THR LEU ALA ASP GLY LYS PRO L402 P403 L404 K410 L415 T416 R417 E418 A419 M420 G421 F422 V432 V433 N434 S435 P436 F437 S438 ALA VAL ASP ASN THR GLY GLY

GLU LEU PRO PHE TRP GLN GLN GLN SER PHE ILE ASP GLN LEU LEU ALA ALA GLY ARG TRP LEU LEU LEU VAL VAL LEU ALA ALA TRP ILE LEU TRP ARG LYS ALA VAL ARG PRO GLN LEU THR ARG ARG VAL GLU GLU ALA LYS ALA ALA GLN GLN GLU GLN ALA GLN VAL ARG GLN GLU THR GLU

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

• Molecule 1: Flagellar M-ring protein

Chain W: 21% 6% 73%

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

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

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

GLU PRO GLY ARG ALA LEU ASP GLU GLY GLN ILE SER ALA VAL VAL HIS LEU VAL SER SER ALA VAL ALA GLY LEU PRO PRO GLY ASN VAL THR LEU VAL ASP GLN SER GLY HIS LEU LEU THR GLN SER ASN THR SER GLY ARG ASP LEU N231 Q246 E250 S254 G258

N261 A264 T267 K275 D287 A288 S289 L293 R296 V304 GLY ALA GLY TYR PRO GLY GLY VAL PRO GLY ALA LEU SER ASN GLN PRO GLN GLU GLN ASN ALA GLN ASN THR PRO GLN THR SER THR

THR ASN SER ASN SER ALA GLY P355 R360 N361 E362 R373 S386 V387 A388 V389 N392 Y393 K394 THR LEU ALA ASP GLY LYS PRO L402 P403 L404 T405 Q408 M409 K410 L415 E418 A419 M420 V432 V433 N434 S435 P436 F437 S438 ALA VAL ASP ASN THR GLY GLY GLU

LEU PRO PHE TRP GLN GLN GLN SER PHE ILE ASP GLN LEU LEU ALA ALA GLY ARG TRP LEU LEU LEU VAL VAL LEU VAL VAL ALA TRP ILE LEU TRP ARG LYS ALA VAL ARG ARG PRO GLN LEU THR ARG ARG VAL GLU GLU ALA LYS ALA ALA GLN GLU GLN ALA GLN VAL ARG GLN GLU THR GLU GLU

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

• Molecule 1: Flagellar M-ring protein

Chain X: 20% 7% 73%

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

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

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

GLU PRO GLY ARG ALA LEU ASP GLU GLY GLN ILE SER ALA VAL VAL HIS LEU VAL SER SER ALA VAL ALA GLY LEU PRO PRO GLY ASN VAL THR LEU VAL ASP GLN SER GLY HIS LEU LEU THR GLN SER ASN THR SER GLY ARG ASP LEU N231 Q246 E250 A251 I252 L253 S254

G258 N261 A264 K275 E276 Q277 T278 E279 E280 D287 A288 S289 L293 R296 S301 V304 GLY ALA GLY TYR PRO GLY GLY VAL PRO GLY ALA LEU SER ASN GLN PRO L402 P403 L404 T405 Q408 L415 E418 A419 M420 V432 V433 N434 S435 P436 F437 S438 ALA

THR PRO GLN THR SER THR SER THR ASN SER ASN SER ALA GLY P355 Q359 R360 N361 E362 T371 I372 R373 V387 A388 V389 N392 Y393 K394 THR LEU ALA ASP GLY LYS PRO L402 P403 L404 T405 Q408 L415 E418 A419 M420 V432 V433 N434 S435 P436 F437 S438 ALA

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

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

GLU

• Molecule 1: Flagellar M-ring protein

Chain Y: 20% 7% 73%

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

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

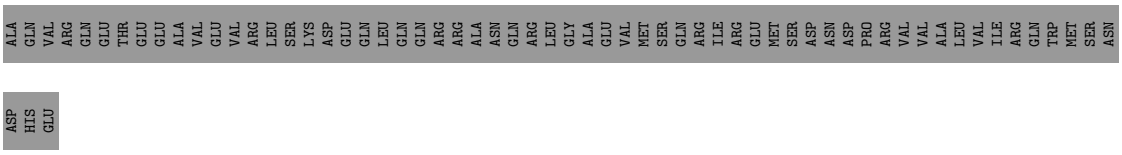
PHE GLY ILE SER GLN PHE SER GLU GLN VAL ASN TYR GLN ARG ALA LEU GLU GLY GLU LEU ALA ARG THR ILE GLU THR LEU GLY PRO VAL LYS SER ALA ARG VAL HIS LEU ALA MET PRO LYS PRO SER LEU PHE VAL ARG GLU GLN LYS SER PRO SER ALA SER VAL THR VAL THR LEU

GLU PRO GLY ARG ALA LEU ASP GLU GLY GLN ILE SER ALA VAL VAL HIS LEU VAL SER SER ALA VAL ALA GLY LEU PRO PRO GLY ASN VAL THR LEU VAL ASP GLN SER GLY HIS LEU LEU THR GLN SER ASN THR SER GLY ARG ASP LEU N231 Q246 E250 S254 G258

N261 A264 Q265 V266 T267 K275 E279 E280 S283 D287 A288 S289 T292 L293 R296 V304 GLY ALA GLY TYR PRO GLY GLY VAL PRO GLY ALA LEU SER ASN GLN PRO ALA PRO PRO ASN GLU ALA PRO ILE ALA THR PRO PRO THR ASN GLN GLN ASN ASN GLN ASN

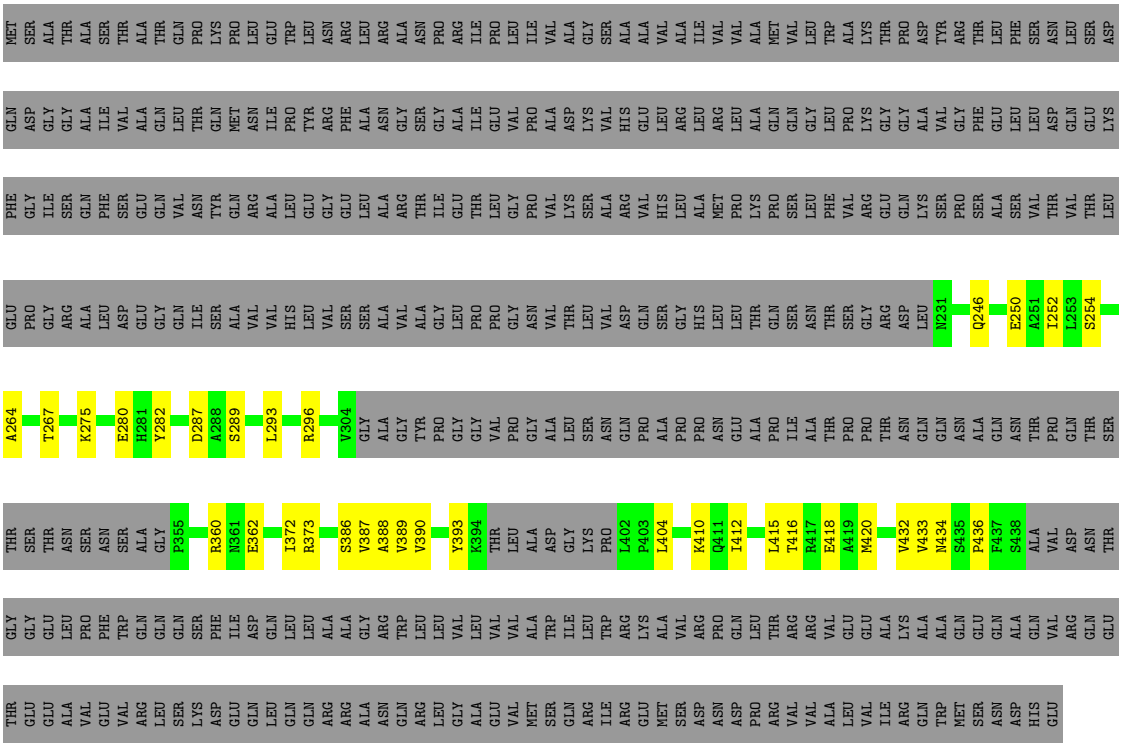
THR PRO GLN THR SER THR SER THR ASN SER ASN SER ALA GLY P355 R360 N361 E362 D369 I372 R373 S386 V387 A388 V389 N392 Y393 K394 THR LEU ALA ASP GLY LYS PRO L402 P403 L404 K410 R417 E418 A419 M420 G421 F422 N431 V432 V433 N434 S435 P436 F437

S438 ALA VAL ASP ASN THR GLY GLY GLU LEU PRO PHE TRP GLN GLN GLN SER PHE ILE ASP GLN LEU LEU ALA ALA GLY ARG TRP LEU LEU VAL LEU VAL VAL ALA TRP ILE LEU TRP ARG LYS ALA VAL ARG PRO GLN LEU THR ARG ARG VAL GLU GLU ALA LYS ALA ALA GLN GLU GLN



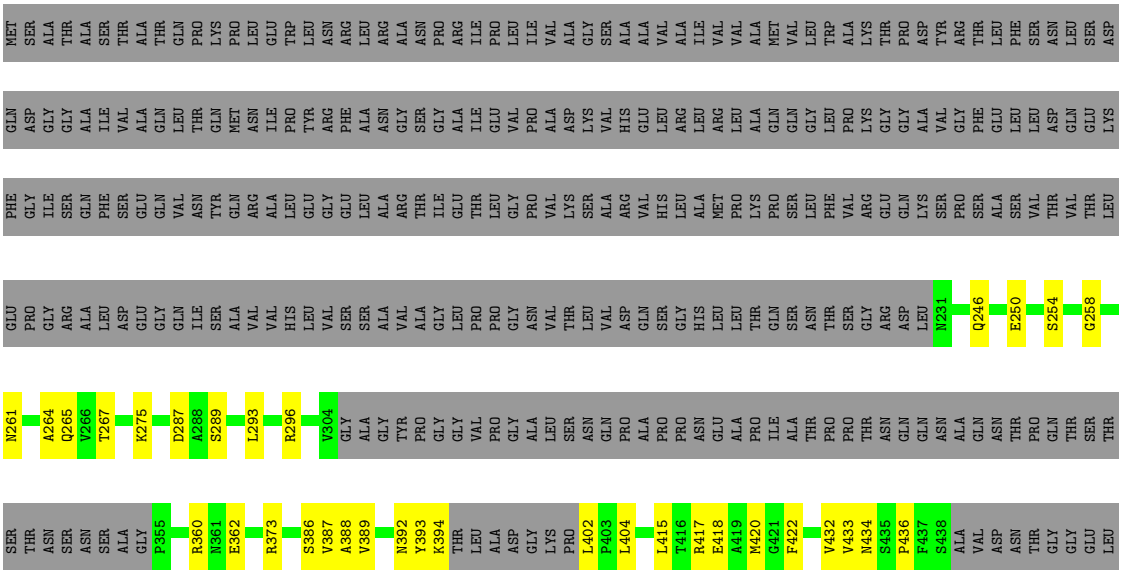
• Molecule 1: Flagellar M-ring protein

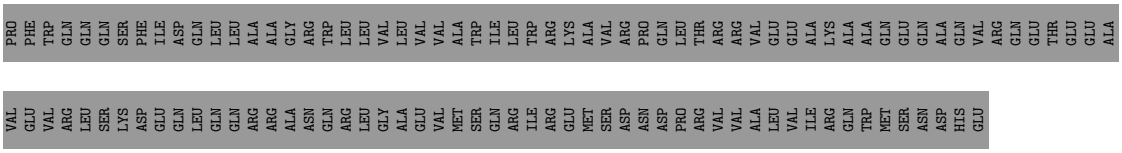
Chain Z:



• Molecule 1: Flagellar M-ring protein

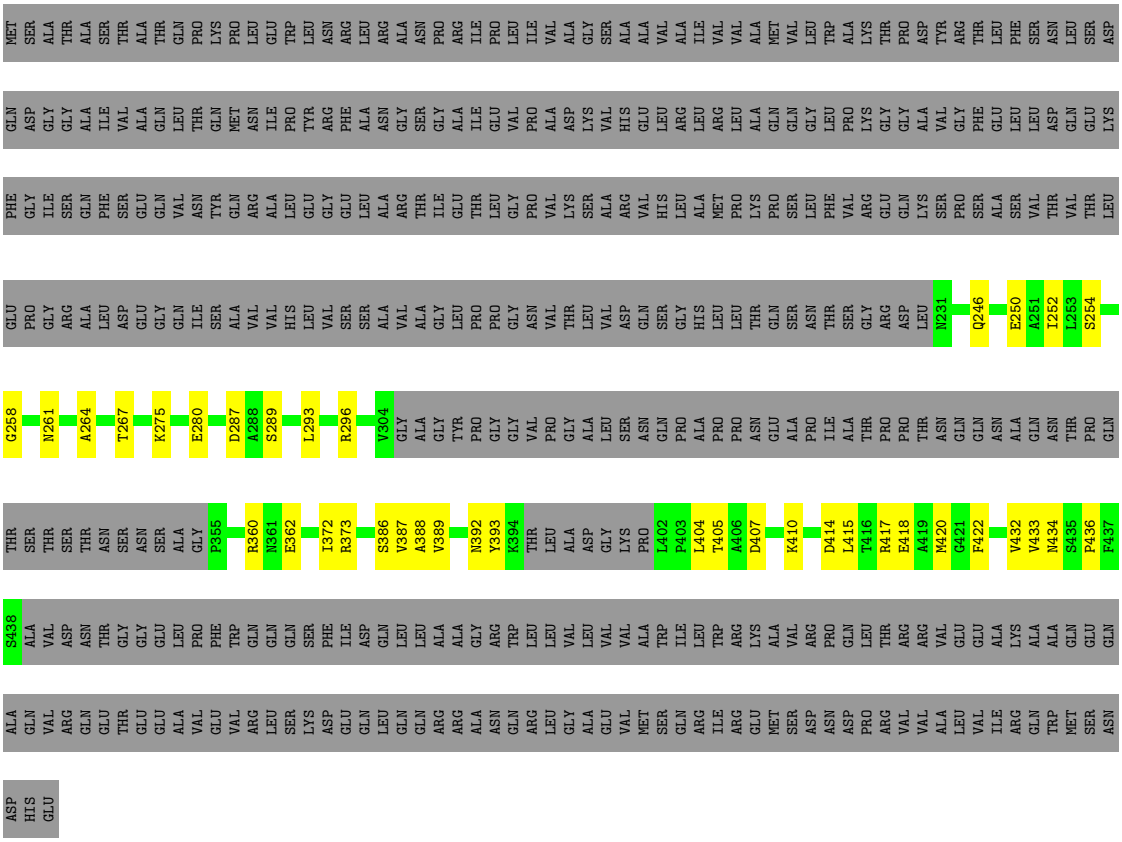
Chain a:





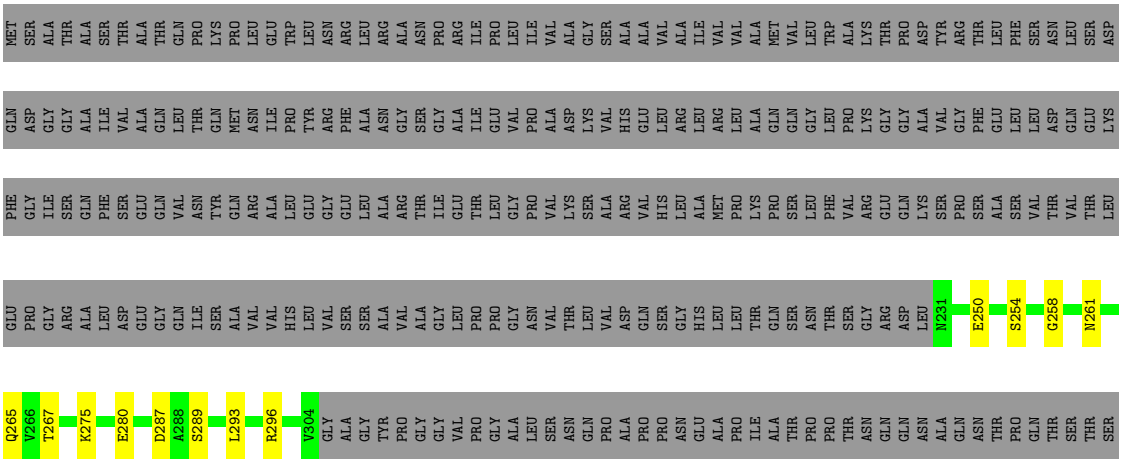
• Molecule 1: Flagellar M-ring protein

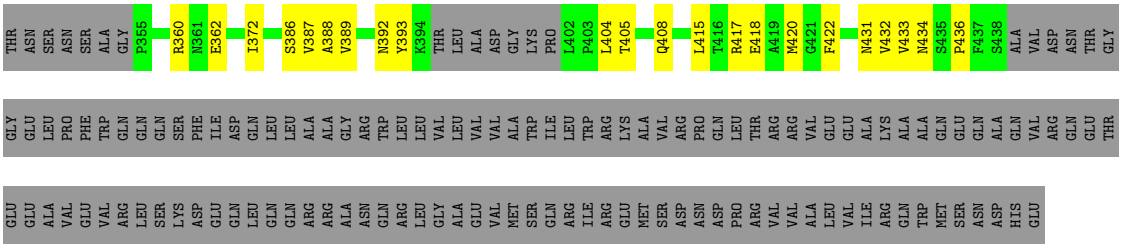
Chain b: 20% 7% 73%



• Molecule 1: Flagellar M-ring protein

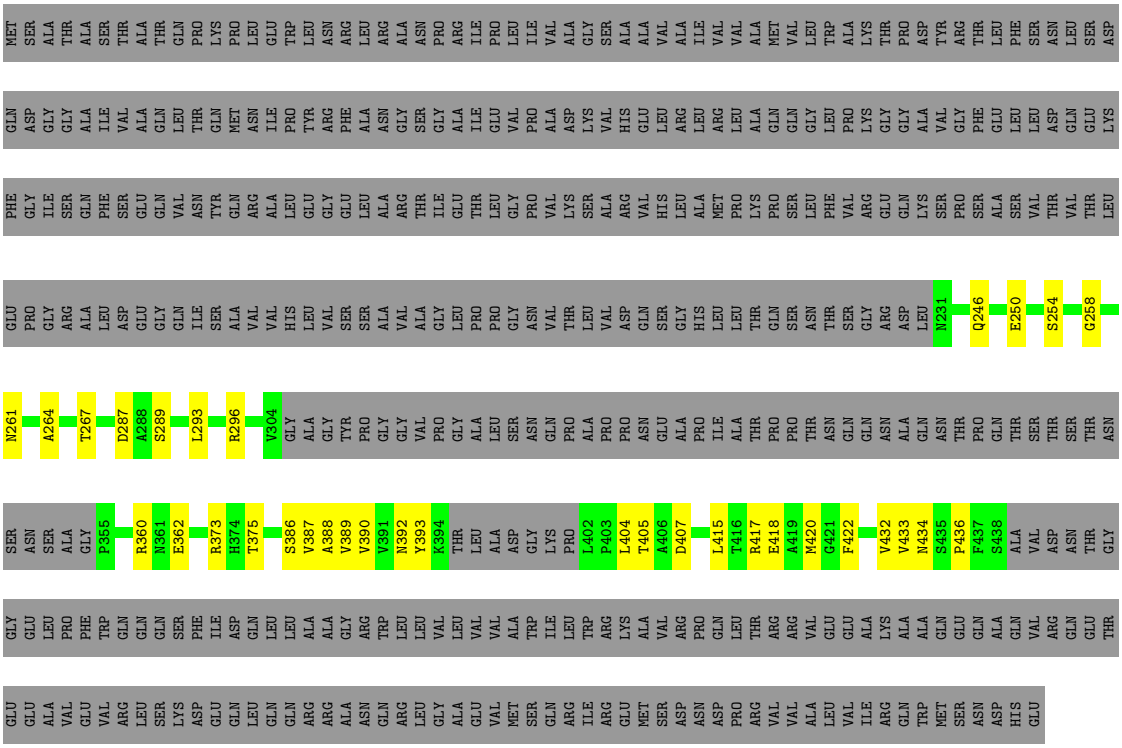
Chain c: 21% 6% 73%





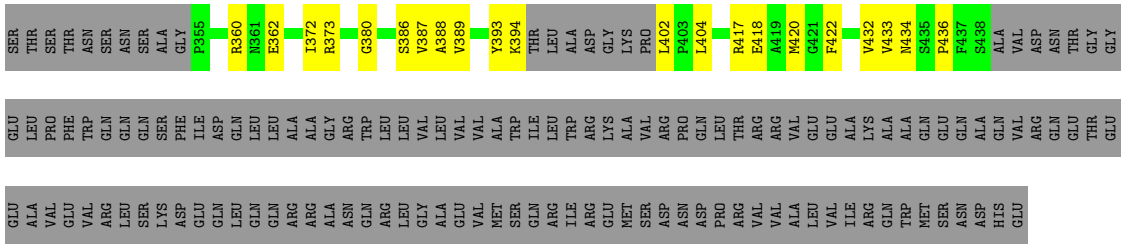
• Molecule 1: Flagellar M-ring protein

Chain d:



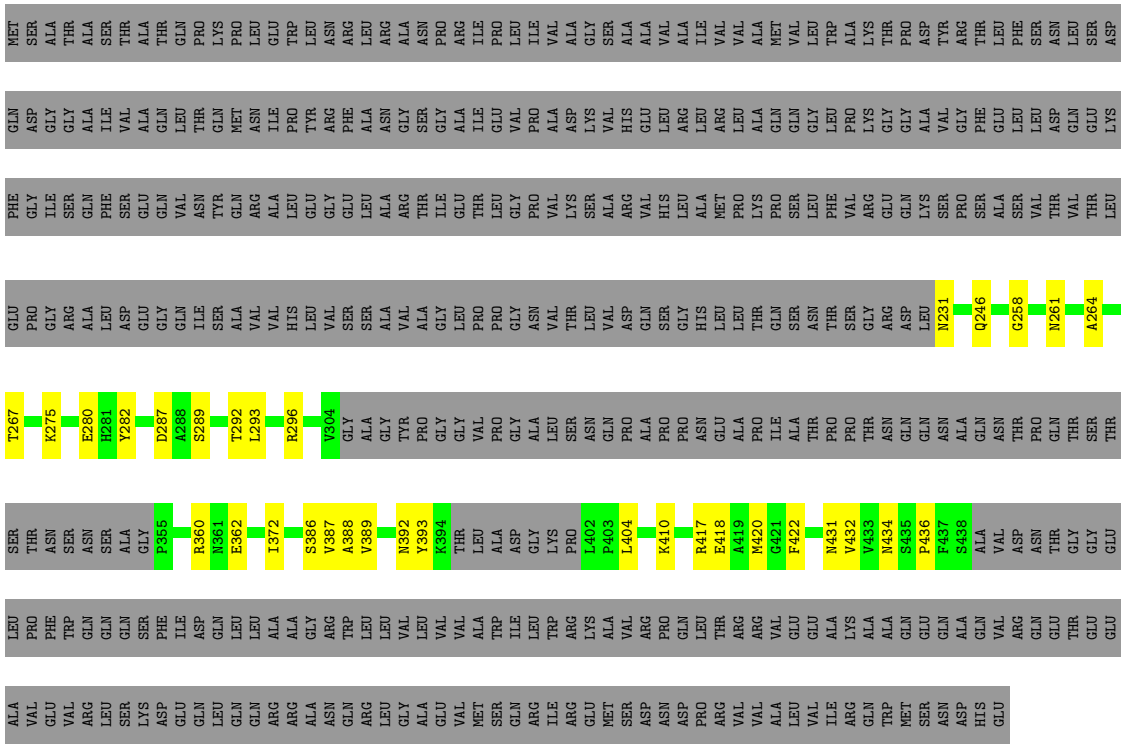
• Molecule 1: Flagellar M-ring protein

Chain e:



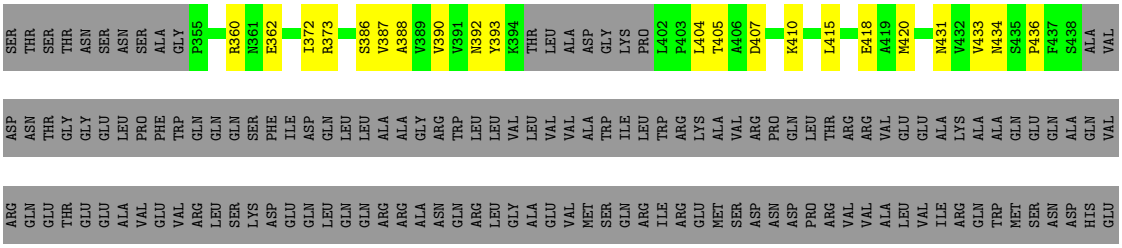
• Molecule 1: Flagellar M-ring protein

Chain f: 21% 6% 73%



• Molecule 1: Flagellar M-ring protein

Chain g: 21% 6% 73%


SER THR SER THR ASN SER ASN SER ALA GLY P355 R360 N361 E362 I372 R373 S386 V387 A388 V389 V390 V391 N392 Y393 K394 THR LEU ALA ASP GLY LYS PRO L402 P403 L404 T405 A406 D407 K410 L415 E418 A419 M420 N431 V432 V433 N434 S435 P436 F437 S438 ALA VAL
ASP ASN THR GLY GLY GLU LEU PRO PHE TRP GLN GLN GLN SER PHE ILE ASP GLN LEU LEU ALA ALA GLY ARG TRP LEU LEU VAL LEU VAL VAL ALA ASP TRP ILE LEU TRP ARG LYS ALA VAL ARG PRO GLN LEU THR ARG ARG VAL GLU GLU ALA LYS ALA ALA GLN GLU GLN ALA GLN VAL
ARG GLN GLU THR GLU GLU ALA VAL GLU VAL ARG LEU SER LYS ASP GLU GLN LEU GLN GLN ARG ARG ALA ASN GLN ARG LEU GLY ALA GLU VAL MET SER GLN ARG ILE ARG GLU MET SER ASP ASN ASP PRO ARG VAL VAL ALA LEU VAL ILE ARG GLN TRP MET SER ASN ASP HIS GLU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C33	Depositor
Number of particles used	77849	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 ($e^-/Å^2$)	48	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.100	Depositor
Minimum map value	-0.057	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	355.104, 355.104, 355.104	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.822, 0.822, 0.822	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	A	0.16	0/1205	0.34	0/1624
1	B	0.16	0/1205	0.33	0/1624
1	C	0.16	0/1205	0.34	0/1624
1	D	0.16	0/1205	0.33	0/1624
1	E	0.16	0/1205	0.34	0/1624
1	F	0.17	0/1205	0.33	0/1624
1	G	0.16	0/1205	0.34	0/1624
1	H	0.17	0/1205	0.33	0/1624
1	I	0.16	0/1205	0.33	0/1624
1	J	0.16	0/1205	0.33	0/1624
1	K	0.16	0/1205	0.33	0/1624
1	L	0.16	0/1205	0.33	0/1624
1	M	0.16	0/1205	0.32	0/1624
1	N	0.16	0/1205	0.33	0/1624
1	O	0.16	0/1205	0.33	0/1624
1	P	0.16	0/1205	0.32	0/1624
1	Q	0.16	0/1205	0.34	0/1624
1	R	0.17	0/1205	0.33	0/1624
1	S	0.16	0/1205	0.33	0/1624
1	T	0.17	0/1205	0.33	0/1624
1	U	0.16	0/1205	0.32	0/1624
1	V	0.16	0/1205	0.33	0/1624
1	W	0.16	0/1205	0.33	0/1624
1	X	0.16	0/1205	0.33	0/1624
1	Y	0.17	0/1205	0.33	0/1624
1	Z	0.16	0/1205	0.34	0/1624
1	a	0.16	0/1205	0.32	0/1624
1	b	0.16	0/1205	0.33	0/1624
1	c	0.16	0/1205	0.34	0/1624
1	d	0.16	0/1205	0.33	0/1624
1	e	0.17	0/1205	0.33	0/1624
1	f	0.17	0/1205	0.33	0/1624
1	g	0.16	0/1205	0.33	0/1624
All	All	0.16	0/39765	0.33	0/53592

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1193	0	1173	22	0
1	B	1193	0	1173	24	0
1	C	1193	0	1173	19	0
1	D	1193	0	1173	23	0
1	E	1193	0	1173	21	0
1	F	1193	0	1173	25	0
1	G	1193	0	1173	23	0
1	H	1193	0	1173	26	0
1	I	1193	0	1173	23	0
1	J	1193	0	1173	24	0
1	K	1193	0	1173	22	0
1	L	1193	0	1173	26	0
1	M	1193	0	1173	26	0
1	N	1193	0	1173	25	0
1	O	1193	0	1173	26	0
1	P	1193	0	1173	28	0
1	Q	1193	0	1173	27	0
1	R	1193	0	1173	25	0
1	S	1193	0	1173	26	0
1	T	1193	0	1173	22	0
1	U	1193	0	1173	24	0
1	V	1193	0	1173	23	0
1	W	1193	0	1173	24	0
1	X	1193	0	1173	27	0
1	Y	1193	0	1173	27	0
1	Z	1193	0	1173	23	0
1	a	1193	0	1173	24	0
1	b	1193	0	1173	26	0
1	c	1193	0	1173	23	0
1	d	1193	0	1173	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	e	1193	0	1173	24	0
1	f	1193	0	1173	23	0
1	g	1193	0	1173	26	0
All	All	39369	0	38709	676	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 9.

All (676) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:280:GLU:HG3	1:Q:372:ILE:HG12	1.80	0.64
1:B:250:GLU:O	1:B:254:SER:OG	2.15	0.63
1:H:360:ARG:NH1	1:H:362:GLU:OE1	2.31	0.63
1:P:405:THR:HG22	1:P:407:ASP:H	1.64	0.62
1:G:405:THR:HG22	1:G:407:ASP:H	1.64	0.61
1:Y:387:VAL:HG21	1:Y:420:MET:HG2	1.82	0.61
1:d:405:THR:HG22	1:d:407:ASP:H	1.65	0.61
1:U:404:LEU:H	1:U:434:ASN:HD21	1.47	0.61
1:P:360:ARG:NH1	1:P:362:GLU:OE1	2.34	0.61
1:b:405:THR:HG22	1:b:407:ASP:H	1.65	0.61
1:K:405:THR:HG22	1:K:407:ASP:H	1.66	0.61
1:N:277:GLN:NE2	1:N:279:GLU:OE2	2.33	0.61
1:P:404:LEU:H	1:P:434:ASN:HD21	1.49	0.60
1:L:387:VAL:HG21	1:L:420:MET:HG2	1.84	0.60
1:f:387:VAL:HG21	1:f:420:MET:HG2	1.82	0.60
1:g:405:THR:HG22	1:g:407:ASP:H	1.66	0.60
1:M:405:THR:HG23	1:M:408:GLN:H	1.67	0.60
1:d:404:LEU:H	1:d:434:ASN:HD21	1.49	0.60
1:F:387:VAL:HG21	1:F:420:MET:HG2	1.84	0.60
1:M:404:LEU:H	1:M:434:ASN:HD21	1.47	0.60
1:J:404:LEU:H	1:J:434:ASN:HD21	1.47	0.60
1:S:258:GLY:HA3	1:S:261:ASN:HD22	1.67	0.60
1:R:258:GLY:HA3	1:R:261:ASN:HD22	1.66	0.60
1:W:404:LEU:H	1:W:434:ASN:HD21	1.50	0.60
1:a:404:LEU:H	1:a:434:ASN:HD21	1.49	0.60
1:X:404:LEU:H	1:X:434:ASN:HD21	1.50	0.59
1:g:387:VAL:HG21	1:g:420:MET:HG2	1.84	0.59
1:A:404:LEU:H	1:A:434:ASN:HD21	1.50	0.59
1:O:293:LEU:HD11	1:O:296:ARG:HH11	1.67	0.59
1:X:293:LEU:HD11	1:X:296:ARG:HH11	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:387:VAL:HG21	1:b:420:MET:HG2	1.83	0.59
1:U:293:LEU:HD11	1:U:296:ARG:HH11	1.67	0.59
1:c:387:VAL:HG21	1:c:420:MET:HG2	1.83	0.59
1:e:404:LEU:H	1:e:434:ASN:HD21	1.49	0.59
1:D:404:LEU:H	1:D:434:ASN:HD21	1.49	0.59
1:d:293:LEU:HD11	1:d:296:ARG:HH11	1.68	0.59
1:W:405:THR:HG23	1:W:408:GLN:H	1.67	0.59
1:H:258:GLY:HA3	1:H:261:ASN:HD22	1.66	0.59
1:S:404:LEU:H	1:S:434:ASN:HD21	1.50	0.59
1:I:293:LEU:HD11	1:I:296:ARG:HH11	1.67	0.59
1:O:387:VAL:HG21	1:O:420:MET:HG2	1.84	0.59
1:O:404:LEU:H	1:O:434:ASN:HD21	1.51	0.59
1:N:404:LEU:H	1:N:434:ASN:HD21	1.51	0.58
1:P:387:VAL:HG21	1:P:420:MET:HG2	1.86	0.58
1:G:404:LEU:H	1:G:434:ASN:ND2	2.00	0.58
1:J:258:GLY:HA3	1:J:261:ASN:HD22	1.69	0.58
1:T:250:GLU:O	1:T:254:SER:OG	2.16	0.58
1:F:404:LEU:H	1:F:434:ASN:HD21	1.52	0.58
1:L:258:GLY:HA3	1:L:261:ASN:HD22	1.68	0.58
1:c:404:LEU:H	1:c:434:ASN:HD21	1.49	0.58
1:P:293:LEU:HD11	1:P:296:ARG:HH11	1.68	0.58
1:V:404:LEU:H	1:V:434:ASN:HD21	1.50	0.58
1:W:250:GLU:O	1:W:254:SER:OG	2.20	0.58
1:c:293:LEU:HD11	1:c:296:ARG:HH11	1.69	0.58
1:c:405:THR:HG23	1:c:408:GLN:H	1.68	0.58
1:F:415:LEU:HD11	1:G:433:VAL:HG21	1.86	0.58
1:J:293:LEU:HD11	1:J:296:ARG:HH11	1.69	0.58
1:D:258:GLY:HA3	1:D:261:ASN:HD22	1.68	0.57
1:I:258:GLY:HA3	1:I:261:ASN:HD22	1.70	0.57
1:Q:405:THR:HG23	1:Q:408:GLN:H	1.68	0.57
1:W:293:LEU:HD11	1:W:296:ARG:HH11	1.69	0.57
1:C:250:GLU:O	1:C:254:SER:OG	2.18	0.57
1:I:404:LEU:H	1:I:434:ASN:HD21	1.52	0.57
1:N:258:GLY:HA3	1:N:261:ASN:HD22	1.69	0.57
1:X:387:VAL:HG21	1:X:420:MET:HG2	1.86	0.57
1:H:404:LEU:H	1:H:434:ASN:HD21	1.52	0.57
1:J:404:LEU:H	1:J:434:ASN:ND2	2.02	0.57
1:H:293:LEU:HD11	1:H:296:ARG:HH11	1.68	0.57
1:L:404:LEU:H	1:L:434:ASN:HD21	1.51	0.57
1:d:387:VAL:HG21	1:d:420:MET:HG2	1.86	0.57
1:E:404:LEU:H	1:E:434:ASN:HD21	1.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:387:VAL:HG21	1:Q:420:MET:HG2	1.87	0.57
1:V:387:VAL:HG21	1:V:420:MET:HG2	1.86	0.57
1:X:258:GLY:HA3	1:X:261:ASN:HD22	1.69	0.57
1:E:293:LEU:HD11	1:E:296:ARG:HH11	1.70	0.57
1:P:404:LEU:H	1:P:434:ASN:ND2	2.01	0.57
1:W:258:GLY:HA3	1:W:261:ASN:HD22	1.69	0.57
1:G:387:VAL:HG21	1:G:420:MET:HG2	1.85	0.56
1:M:293:LEU:HD11	1:M:296:ARG:HH11	1.69	0.56
1:V:293:LEU:HD11	1:V:296:ARG:HH11	1.69	0.56
1:K:293:LEU:HD11	1:K:296:ARG:HH11	1.71	0.56
1:D:293:LEU:HD11	1:D:296:ARG:HH11	1.70	0.56
1:F:293:LEU:HD11	1:F:296:ARG:HH11	1.71	0.56
1:K:250:GLU:O	1:K:254:SER:OG	2.21	0.56
1:T:293:LEU:HD11	1:T:296:ARG:HH11	1.68	0.56
1:X:405:THR:HG23	1:X:408:GLN:H	1.70	0.56
1:e:287:ASP:OD2	1:e:289:SER:OG	2.23	0.56
1:B:293:LEU:HD11	1:B:296:ARG:HH11	1.70	0.56
1:C:387:VAL:HG21	1:C:420:MET:HG2	1.87	0.56
1:I:387:VAL:HG21	1:I:420:MET:HG2	1.87	0.56
1:T:404:LEU:H	1:T:434:ASN:HD21	1.51	0.56
1:O:405:THR:HG23	1:O:408:GLN:H	1.69	0.56
1:U:405:THR:HG23	1:U:408:GLN:H	1.70	0.56
1:Y:293:LEU:HD11	1:Y:296:ARG:HH11	1.70	0.56
1:Z:293:LEU:HD11	1:Z:296:ARG:HH11	1.69	0.56
1:N:387:VAL:HG21	1:N:420:MET:HG2	1.87	0.56
1:Q:404:LEU:H	1:Q:434:ASN:HD21	1.52	0.56
1:R:404:LEU:H	1:R:434:ASN:HD21	1.52	0.56
1:a:258:GLY:HA3	1:a:261:ASN:HD22	1.70	0.56
1:b:404:LEU:H	1:b:434:ASN:HD21	1.53	0.56
1:A:293:LEU:HD11	1:A:296:ARG:HH11	1.71	0.56
1:B:404:LEU:H	1:B:434:ASN:HD21	1.52	0.56
1:K:387:VAL:HG21	1:K:420:MET:HG2	1.88	0.56
1:V:404:LEU:H	1:V:434:ASN:ND2	2.03	0.56
1:d:404:LEU:H	1:d:434:ASN:ND2	2.03	0.56
1:f:404:LEU:H	1:f:434:ASN:HD21	1.51	0.56
1:D:250:GLU:O	1:D:254:SER:OG	2.20	0.56
1:H:387:VAL:HG21	1:H:420:MET:HG2	1.86	0.56
1:T:387:VAL:HG21	1:T:420:MET:HG2	1.85	0.56
1:R:387:VAL:HG21	1:R:420:MET:HG2	1.88	0.56
1:S:387:VAL:HG21	1:S:420:MET:HG2	1.87	0.56
1:B:387:VAL:HG21	1:B:420:MET:HG2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:404:LEU:H	1:K:434:ASN:ND2	2.04	0.56
1:Y:258:GLY:HA3	1:Y:261:ASN:HD22	1.70	0.56
1:M:250:GLU:O	1:M:254:SER:OG	2.20	0.55
1:N:293:LEU:HD11	1:N:296:ARG:HH11	1.69	0.55
1:b:404:LEU:H	1:b:434:ASN:ND2	2.03	0.55
1:g:250:GLU:O	1:g:254:SER:OG	2.21	0.55
1:C:293:LEU:HD11	1:C:296:ARG:HH11	1.71	0.55
1:K:404:LEU:H	1:K:434:ASN:HD21	1.54	0.55
1:g:404:LEU:H	1:g:434:ASN:HD21	1.54	0.55
1:A:404:LEU:H	1:A:434:ASN:ND2	2.04	0.55
1:B:404:LEU:H	1:B:434:ASN:ND2	2.05	0.55
1:O:258:GLY:HA3	1:O:261:ASN:HD22	1.71	0.55
1:b:250:GLU:O	1:b:254:SER:OG	2.19	0.55
1:J:280:GLU:HG3	1:J:372:ILE:HG12	1.88	0.55
1:L:250:GLU:O	1:L:254:SER:OG	2.18	0.55
1:P:258:GLY:HA3	1:P:261:ASN:HD22	1.72	0.55
1:F:287:ASP:OD2	1:F:289:SER:OG	2.24	0.55
1:e:250:GLU:O	1:e:254:SER:OG	2.20	0.55
1:E:387:VAL:HG21	1:E:420:MET:HG2	1.88	0.55
1:X:277:GLN:NE2	1:X:279:GLU:OE2	2.40	0.55
1:b:258:GLY:HA3	1:b:261:ASN:HD22	1.70	0.55
1:e:258:GLY:HA3	1:e:261:ASN:HD22	1.71	0.55
1:V:287:ASP:OD2	1:V:289:SER:OG	2.24	0.55
1:c:250:GLU:O	1:c:254:SER:OG	2.20	0.55
1:Z:387:VAL:HG21	1:Z:420:MET:HG2	1.87	0.55
1:V:250:GLU:O	1:V:254:SER:OG	2.19	0.55
1:a:387:VAL:HG21	1:a:420:MET:HG2	1.87	0.55
1:e:387:VAL:HG21	1:e:420:MET:HG2	1.89	0.55
1:H:404:LEU:H	1:H:434:ASN:ND2	2.05	0.55
1:a:293:LEU:HD11	1:a:296:ARG:HH11	1.71	0.55
1:N:404:LEU:H	1:N:434:ASN:ND2	2.05	0.54
1:U:250:GLU:O	1:U:254:SER:OG	2.18	0.54
1:U:417:ARG:HG3	1:U:422:PHE:HB3	1.89	0.54
1:Z:250:GLU:O	1:Z:254:SER:OG	2.19	0.54
1:e:293:LEU:HD11	1:e:296:ARG:HH11	1.72	0.54
1:f:258:GLY:HA3	1:f:261:ASN:HD22	1.71	0.54
1:C:258:GLY:HA3	1:C:261:ASN:HD22	1.71	0.54
1:E:404:LEU:H	1:E:434:ASN:ND2	2.06	0.54
1:W:387:VAL:HG21	1:W:420:MET:HG2	1.88	0.54
1:Z:404:LEU:H	1:Z:434:ASN:HD21	1.53	0.54
1:g:287:ASP:OD2	1:g:289:SER:OG	2.26	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:g:293:LEU:HD11	1:g:296:ARG:HH11	1.72	0.54
1:X:287:ASP:OD2	1:X:289:SER:OG	2.24	0.54
1:Y:360:ARG:NH1	1:Y:362:GLU:OE1	2.39	0.54
1:B:287:ASP:OD2	1:B:289:SER:OG	2.26	0.54
1:P:280:GLU:HG3	1:P:372:ILE:HG12	1.90	0.54
1:X:404:LEU:H	1:X:434:ASN:ND2	2.05	0.54
1:b:293:LEU:HD11	1:b:296:ARG:HH11	1.72	0.54
1:b:360:ARG:NH1	1:b:362:GLU:OE1	2.36	0.54
1:d:287:ASP:OD2	1:d:289:SER:OG	2.26	0.54
1:C:287:ASP:OD2	1:C:289:SER:OG	2.26	0.54
1:S:293:LEU:HD11	1:S:296:ARG:HH11	1.72	0.54
1:W:404:LEU:H	1:W:434:ASN:ND2	2.04	0.54
1:C:404:LEU:H	1:C:434:ASN:HD21	1.54	0.54
1:f:287:ASP:OD2	1:f:289:SER:OG	2.26	0.54
1:C:280:GLU:HG3	1:C:372:ILE:HG12	1.90	0.54
1:D:287:ASP:OD2	1:D:289:SER:OG	2.23	0.54
1:D:387:VAL:HG21	1:D:420:MET:HG2	1.90	0.54
1:G:287:ASP:OD2	1:G:289:SER:OG	2.26	0.54
1:W:287:ASP:OD2	1:W:289:SER:OG	2.24	0.54
1:Y:404:LEU:H	1:Y:434:ASN:HD21	1.55	0.54
1:H:417:ARG:HG3	1:H:422:PHE:HB3	1.90	0.53
1:Z:280:GLU:HG3	1:Z:372:ILE:HG12	1.90	0.53
1:A:287:ASP:OD2	1:A:289:SER:OG	2.27	0.53
1:G:250:GLU:O	1:G:254:SER:OG	2.21	0.53
1:J:389:VAL:HB	1:J:432:VAL:HG22	1.90	0.53
1:Q:250:GLU:O	1:Q:254:SER:OG	2.20	0.53
1:R:293:LEU:HD11	1:R:296:ARG:HH11	1.73	0.53
1:O:404:LEU:H	1:O:434:ASN:ND2	2.05	0.53
1:F:246:GLN:NE2	1:F:264:ALA:O	2.42	0.53
1:M:404:LEU:H	1:M:434:ASN:ND2	2.07	0.53
1:P:287:ASP:OD2	1:P:289:SER:OG	2.25	0.53
1:Q:293:LEU:HD11	1:Q:296:ARG:HH11	1.73	0.53
1:D:404:LEU:H	1:D:434:ASN:ND2	2.07	0.53
1:L:360:ARG:NH1	1:L:362:GLU:OE1	2.36	0.53
1:Y:418:GLU:HB2	1:Z:388:ALA:HB2	1.91	0.53
1:a:360:ARG:NH1	1:a:362:GLU:OE1	2.37	0.53
1:G:404:LEU:H	1:G:434:ASN:HD21	1.57	0.53
1:e:404:LEU:H	1:e:434:ASN:ND2	2.07	0.53
1:g:404:LEU:H	1:g:434:ASN:ND2	2.07	0.53
1:J:387:VAL:HG21	1:J:420:MET:HG2	1.90	0.53
1:O:360:ARG:NH1	1:O:362:GLU:OE1	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:287:ASP:OD2	1:Q:289:SER:OG	2.26	0.53
1:Q:360:ARG:NH1	1:Q:362:GLU:OE1	2.41	0.53
1:U:258:GLY:HA3	1:U:261:ASN:HD22	1.74	0.53
1:X:360:ARG:NH1	1:X:362:GLU:OE1	2.40	0.52
1:Y:287:ASP:OD2	1:Y:289:SER:OG	2.27	0.52
1:N:417:ARG:HG3	1:N:422:PHE:HB3	1.91	0.52
1:E:287:ASP:OD2	1:E:289:SER:OG	2.28	0.52
1:A:280:GLU:HG3	1:A:372:ILE:HG12	1.91	0.52
1:G:258:GLY:HA3	1:G:261:ASN:HD22	1.75	0.52
1:L:389:VAL:HB	1:L:432:VAL:HG22	1.91	0.52
1:R:360:ARG:NH1	1:R:362:GLU:OE1	2.39	0.52
1:N:280:GLU:HG3	1:N:372:ILE:HG12	1.91	0.52
1:c:404:LEU:H	1:c:434:ASN:ND2	2.08	0.52
1:f:293:LEU:HD11	1:f:296:ARG:HH11	1.73	0.52
1:Z:360:ARG:NH1	1:Z:362:GLU:OE1	2.42	0.52
1:D:417:ARG:HG3	1:D:422:PHE:HB3	1.92	0.52
1:O:417:ARG:HG3	1:O:422:PHE:HB3	1.91	0.52
1:Q:267:THR:HB	1:Q:386:SER:HB2	1.92	0.52
1:Y:280:GLU:HG3	1:Y:372:ILE:HG12	1.92	0.52
1:C:404:LEU:H	1:C:434:ASN:ND2	2.08	0.52
1:F:258:GLY:HA3	1:F:261:ASN:HD22	1.75	0.52
1:I:250:GLU:O	1:I:254:SER:OG	2.18	0.52
1:L:293:LEU:HD11	1:L:296:ARG:HH11	1.75	0.52
1:c:280:GLU:HG3	1:c:372:ILE:HG12	1.92	0.52
1:G:389:VAL:HB	1:G:432:VAL:HG22	1.92	0.51
1:c:258:GLY:HA3	1:c:261:ASN:HD22	1.75	0.51
1:e:380:GLY:HA3	1:f:231:ASN:HD21	1.76	0.51
1:f:404:LEU:H	1:f:434:ASN:ND2	2.08	0.51
1:A:246:GLN:NE2	1:A:264:ALA:O	2.44	0.51
1:a:287:ASP:OD2	1:a:289:SER:OG	2.29	0.51
1:f:360:ARG:NH1	1:f:362:GLU:OE1	2.40	0.51
1:S:287:ASP:OD2	1:S:289:SER:OG	2.28	0.51
1:U:404:LEU:H	1:U:434:ASN:ND2	2.09	0.51
1:Q:417:ARG:HG3	1:Q:422:PHE:HB3	1.92	0.51
1:O:250:GLU:O	1:O:254:SER:OG	2.21	0.51
1:N:360:ARG:NH1	1:N:362:GLU:OE1	2.42	0.51
1:Z:267:THR:HB	1:Z:386:SER:HB2	1.93	0.51
1:C:373:ARG:NH2	1:D:275:LYS:HD3	2.26	0.51
1:T:258:GLY:HA3	1:T:261:ASN:HD22	1.75	0.51
1:Y:417:ARG:HG3	1:Y:422:PHE:HB3	1.93	0.51
1:b:393:TYR:CE2	1:b:436:PRO:HD3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:GLY:HA3	1:B:261:ASN:HD22	1.73	0.51
1:S:373:ARG:NH2	1:T:275:LYS:HD3	2.26	0.51
1:a:373:ARG:NH2	1:b:275:LYS:HD3	2.26	0.51
1:A:360:ARG:NH1	1:A:362:GLU:OE1	2.38	0.50
1:R:250:GLU:O	1:R:254:SER:OG	2.21	0.50
1:f:418:GLU:HB2	1:g:388:ALA:HB2	1.93	0.50
1:R:389:VAL:HB	1:R:432:VAL:HG22	1.93	0.50
1:a:250:GLU:O	1:a:254:SER:OG	2.25	0.50
1:Q:373:ARG:NH2	1:R:275:LYS:HD3	2.25	0.50
1:a:404:LEU:H	1:a:434:ASN:ND2	2.08	0.50
1:d:258:GLY:HA3	1:d:261:ASN:HD22	1.77	0.50
1:A:417:ARG:HG3	1:A:422:PHE:HB3	1.93	0.50
1:B:280:GLU:HG3	1:B:372:ILE:HG12	1.93	0.50
1:I:287:ASP:OD2	1:I:289:SER:OG	2.29	0.50
1:b:287:ASP:OD2	1:b:289:SER:OG	2.27	0.50
1:D:360:ARG:NH1	1:D:362:GLU:OE1	2.43	0.50
1:L:404:LEU:H	1:L:434:ASN:ND2	2.10	0.50
1:A:275:LYS:HD3	1:g:373:ARG:NH2	2.27	0.50
1:D:393:TYR:CE2	1:D:436:PRO:HD3	2.47	0.50
1:M:417:ARG:HG3	1:M:422:PHE:HB3	1.94	0.50
1:U:246:GLN:NE2	1:U:264:ALA:O	2.44	0.50
1:G:293:LEU:HD11	1:G:296:ARG:HH11	1.76	0.50
1:E:393:TYR:CE2	1:E:436:PRO:HD3	2.47	0.50
1:J:373:ARG:NH2	1:K:275:LYS:HD3	2.27	0.50
1:M:258:GLY:HA3	1:M:261:ASN:HD22	1.76	0.49
1:R:373:ARG:NH2	1:S:275:LYS:HD3	2.27	0.49
1:U:287:ASP:OD2	1:U:289:SER:OG	2.27	0.49
1:A:373:ARG:NH2	1:B:275:LYS:HD3	2.27	0.49
1:G:417:ARG:HG3	1:G:422:PHE:HB3	1.94	0.49
1:F:360:ARG:NH1	1:F:362:GLU:OE1	2.43	0.49
1:M:267:THR:HB	1:M:386:SER:HB2	1.94	0.49
1:M:373:ARG:NH2	1:N:275:LYS:HD3	2.27	0.49
1:M:387:VAL:HG21	1:M:420:MET:HG2	1.93	0.49
1:P:246:GLN:NE2	1:P:264:ALA:O	2.45	0.49
1:R:417:ARG:HG3	1:R:422:PHE:HB3	1.93	0.49
1:S:404:LEU:H	1:S:434:ASN:ND2	2.08	0.49
1:T:267:THR:HB	1:T:386:SER:HB2	1.94	0.49
1:U:387:VAL:HG21	1:U:420:MET:HG2	1.93	0.49
1:Z:418:GLU:HB2	1:a:388:ALA:HB2	1.95	0.49
1:c:360:ARG:NH1	1:c:362:GLU:OE1	2.41	0.49
1:c:393:TYR:CE2	1:c:436:PRO:HD3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:417:ARG:HG3	1:E:422:PHE:HB3	1.95	0.49
1:H:373:ARG:NH2	1:I:275:LYS:HD3	2.27	0.49
1:Q:283:SER:HB2	1:Q:369:ASP:HB2	1.95	0.49
1:V:373:ARG:NH2	1:W:275:LYS:HD3	2.27	0.49
1:f:417:ARG:HG3	1:f:422:PHE:HB3	1.95	0.49
1:B:360:ARG:NH1	1:B:362:GLU:OE1	2.41	0.49
1:C:360:ARG:NH1	1:C:362:GLU:OE1	2.42	0.49
1:I:373:ARG:NH2	1:J:275:LYS:HD3	2.28	0.49
1:P:373:ARG:NH2	1:Q:275:LYS:HD3	2.27	0.49
1:d:393:TYR:CE2	1:d:436:PRO:HD3	2.48	0.49
1:e:417:ARG:HG3	1:e:422:PHE:HB3	1.94	0.49
1:g:393:TYR:CE2	1:g:436:PRO:HD3	2.48	0.49
1:I:360:ARG:NH1	1:I:362:GLU:OE1	2.44	0.49
1:K:373:ARG:NH2	1:L:275:LYS:HD3	2.27	0.49
1:I:267:THR:HB	1:I:386:SER:HB2	1.94	0.49
1:U:360:ARG:NH1	1:U:362:GLU:OE1	2.39	0.49
1:W:418:GLU:HB2	1:X:388:ALA:HB2	1.94	0.49
1:d:267:THR:HB	1:d:386:SER:HB2	1.94	0.49
1:g:360:ARG:NH1	1:g:362:GLU:OE1	2.41	0.49
1:D:415:LEU:HD11	1:E:433:VAL:HG21	1.95	0.49
1:G:373:ARG:NH2	1:H:275:LYS:HD3	2.28	0.49
1:W:373:ARG:NH2	1:X:275:LYS:HD3	2.27	0.49
1:I:393:TYR:CE2	1:I:436:PRO:HD3	2.48	0.48
1:S:267:THR:HB	1:S:386:SER:HB2	1.95	0.48
1:S:393:TYR:CE2	1:S:436:PRO:HD3	2.48	0.48
1:V:393:TYR:CE2	1:V:436:PRO:HD3	2.48	0.48
1:X:415:LEU:HD11	1:Y:433:VAL:HG21	1.94	0.48
1:U:393:TYR:CE2	1:U:436:PRO:HD3	2.48	0.48
1:X:280:GLU:HG3	1:X:372:ILE:HG12	1.94	0.48
1:A:258:GLY:HA3	1:A:261:ASN:HD22	1.78	0.48
1:G:393:TYR:CE2	1:G:436:PRO:HD3	2.47	0.48
1:T:404:LEU:H	1:T:434:ASN:ND2	2.11	0.48
1:Y:410:LYS:HE2	1:Y:410:LYS:HB3	1.67	0.48
1:Z:373:ARG:NH2	1:a:275:LYS:HD3	2.28	0.48
1:b:389:VAL:HB	1:b:432:VAL:HG22	1.95	0.48
1:f:246:GLN:NE2	1:f:264:ALA:O	2.47	0.48
1:g:267:THR:HB	1:g:386:SER:HB2	1.95	0.48
1:A:393:TYR:CE2	1:A:436:PRO:HD3	2.48	0.48
1:H:287:ASP:OD2	1:H:289:SER:OG	2.31	0.48
1:X:418:GLU:HB2	1:Y:388:ALA:HB2	1.96	0.48
1:c:287:ASP:OD2	1:c:289:SER:OG	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:393:TYR:CE2	1:O:436:PRO:HD3	2.49	0.48
1:H:267:THR:HB	1:H:386:SER:HB2	1.95	0.48
1:K:280:GLU:HG3	1:K:372:ILE:HG12	1.95	0.48
1:Q:393:TYR:CE2	1:Q:436:PRO:HD3	2.49	0.48
1:B:389:VAL:HB	1:B:432:VAL:HG22	1.95	0.48
1:H:393:TYR:CE2	1:H:436:PRO:HD3	2.49	0.48
1:M:393:TYR:CE2	1:M:436:PRO:HD3	2.48	0.48
1:O:418:GLU:HB2	1:P:388:ALA:HB2	1.96	0.48
1:Q:404:LEU:H	1:Q:434:ASN:ND2	2.12	0.48
1:T:393:TYR:CE2	1:T:436:PRO:HD3	2.48	0.48
1:V:258:GLY:HA3	1:V:261:ASN:HD22	1.77	0.48
1:Y:404:LEU:H	1:Y:434:ASN:ND2	2.11	0.48
1:F:404:LEU:H	1:F:434:ASN:ND2	2.11	0.48
1:I:246:GLN:NE2	1:I:264:ALA:O	2.46	0.48
1:I:280:GLU:HG3	1:I:372:ILE:HG12	1.96	0.48
1:N:415:LEU:HD11	1:O:433:VAL:HG21	1.95	0.48
1:T:287:ASP:OD2	1:T:289:SER:OG	2.29	0.48
1:b:417:ARG:HG3	1:b:422:PHE:HB3	1.95	0.48
1:e:393:TYR:CE2	1:e:436:PRO:HD3	2.49	0.48
1:A:250:GLU:O	1:A:254:SER:OG	2.22	0.48
1:P:250:GLU:O	1:P:254:SER:OG	2.27	0.48
1:X:373:ARG:NH2	1:Y:275:LYS:HD3	2.28	0.48
1:Z:246:GLN:NE2	1:Z:264:ALA:O	2.46	0.48
1:d:418:GLU:HB2	1:e:388:ALA:HB2	1.96	0.48
1:f:393:TYR:CE2	1:f:436:PRO:HD3	2.49	0.48
1:A:387:VAL:HG21	1:A:420:MET:HG2	1.95	0.48
1:E:418:GLU:HB2	1:F:388:ALA:HB2	1.96	0.48
1:J:250:GLU:O	1:J:254:SER:OG	2.20	0.48
1:L:393:TYR:CE2	1:L:436:PRO:HD3	2.49	0.48
1:a:418:GLU:HB2	1:b:388:ALA:HB2	1.96	0.48
1:C:267:THR:HB	1:C:386:SER:HB2	1.95	0.47
1:C:393:TYR:CE2	1:C:436:PRO:HD3	2.49	0.47
1:V:267:THR:HB	1:V:386:SER:HB2	1.95	0.47
1:B:417:ARG:HG3	1:B:422:PHE:HB3	1.96	0.47
1:D:280:GLU:HG3	1:D:372:ILE:HG12	1.96	0.47
1:H:389:VAL:HB	1:H:432:VAL:HG22	1.96	0.47
1:J:393:TYR:CE2	1:J:436:PRO:HD3	2.50	0.47
1:P:418:GLU:HB2	1:Q:388:ALA:HB2	1.96	0.47
1:a:267:THR:HB	1:a:386:SER:HB2	1.96	0.47
1:I:404:LEU:H	1:I:434:ASN:ND2	2.12	0.47
1:W:360:ARG:NH1	1:W:362:GLU:OE1	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:246:GLN:NE2	1:X:264:ALA:O	2.47	0.47
1:X:250:GLU:O	1:X:254:SER:OG	2.21	0.47
1:Y:393:TYR:CE2	1:Y:436:PRO:HD3	2.49	0.47
1:F:418:GLU:HB2	1:G:388:ALA:HB2	1.97	0.47
1:J:267:THR:HB	1:J:386:SER:HB2	1.96	0.47
1:E:392:ASN:OD1	1:E:393:TYR:N	2.48	0.47
1:G:415:LEU:HD11	1:H:433:VAL:HG21	1.97	0.47
1:H:231:ASN:CG	1:H:232:ASP:H	2.22	0.47
1:O:292:THR:HG21	1:P:282:TYR:HB3	1.97	0.47
1:g:246:GLN:NE2	1:g:264:ALA:O	2.47	0.47
1:I:389:VAL:HB	1:I:432:VAL:HG22	1.96	0.47
1:K:418:GLU:HB2	1:L:388:ALA:HB2	1.97	0.47
1:S:418:GLU:HB2	1:T:388:ALA:HB2	1.96	0.47
1:V:246:GLN:NE2	1:V:264:ALA:O	2.47	0.47
1:Z:404:LEU:H	1:Z:434:ASN:ND2	2.13	0.47
1:f:389:VAL:HB	1:f:432:VAL:HG22	1.97	0.47
1:N:267:THR:HB	1:N:386:SER:HB2	1.95	0.47
1:P:389:VAL:HB	1:P:432:VAL:HG22	1.96	0.47
1:R:404:LEU:H	1:R:434:ASN:ND2	2.12	0.47
1:c:389:VAL:HB	1:c:432:VAL:HG22	1.97	0.47
1:d:417:ARG:HG3	1:d:422:PHE:HB3	1.95	0.47
1:F:417:ARG:HG3	1:F:422:PHE:HB3	1.97	0.47
1:M:246:GLN:NE2	1:M:264:ALA:O	2.47	0.47
1:N:389:VAL:HB	1:N:432:VAL:HG22	1.96	0.47
1:Z:287:ASP:OD2	1:Z:289:SER:OG	2.29	0.47
1:g:258:GLY:HA3	1:g:261:ASN:HD22	1.80	0.47
1:E:389:VAL:HB	1:E:432:VAL:HG22	1.97	0.47
1:F:392:ASN:OD1	1:F:393:TYR:N	2.48	0.47
1:J:410:LYS:HB3	1:J:410:LYS:HE2	1.68	0.47
1:K:360:ARG:NH1	1:K:362:GLU:OE1	2.47	0.47
1:b:414:ASP:HB3	1:c:431:ASN:ND2	2.29	0.47
1:N:373:ARG:NH2	1:O:275:LYS:HD3	2.29	0.47
1:Y:373:ARG:NH2	1:Z:275:LYS:HD3	2.30	0.47
1:H:246:GLN:NE2	1:H:264:ALA:O	2.48	0.46
1:H:418:GLU:HB2	1:I:388:ALA:HB2	1.98	0.46
1:T:280:GLU:HG3	1:T:372:ILE:HG12	1.97	0.46
1:T:417:ARG:HG3	1:T:422:PHE:HB3	1.96	0.46
1:d:373:ARG:NH2	1:e:275:LYS:HD3	2.30	0.46
1:e:267:THR:HB	1:e:386:SER:HB2	1.97	0.46
1:C:389:VAL:HB	1:C:432:VAL:HG22	1.97	0.46
1:D:389:VAL:HB	1:D:432:VAL:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:417:ARG:HG3	1:J:422:PHE:HB3	1.97	0.46
1:c:418:GLU:HB2	1:d:388:ALA:HB2	1.97	0.46
1:Q:389:VAL:HB	1:Q:432:VAL:HG22	1.96	0.46
1:V:360:ARG:NH1	1:V:362:GLU:OE1	2.44	0.46
1:a:246:GLN:NE2	1:a:264:ALA:O	2.48	0.46
1:A:267:THR:HB	1:A:386:SER:HB2	1.97	0.46
1:G:360:ARG:NH1	1:G:362:GLU:OE1	2.43	0.46
1:P:415:LEU:HD11	1:Q:433:VAL:HG21	1.97	0.46
1:Z:393:TYR:CE2	1:Z:436:PRO:HD3	2.50	0.46
1:N:418:GLU:HB2	1:O:388:ALA:HB2	1.98	0.46
1:O:280:GLU:HG3	1:O:372:ILE:HG12	1.98	0.46
1:O:373:ARG:NH2	1:P:275:LYS:HD3	2.30	0.46
1:R:393:TYR:CE2	1:R:436:PRO:HD3	2.50	0.46
1:U:389:VAL:HB	1:U:432:VAL:HG22	1.97	0.46
1:V:410:LYS:HE2	1:V:410:LYS:HB3	1.68	0.46
1:W:389:VAL:HB	1:W:432:VAL:HG22	1.98	0.46
1:G:246:GLN:NE2	1:G:264:ALA:O	2.48	0.46
1:L:246:GLN:NE2	1:L:264:ALA:O	2.49	0.46
1:A:418:GLU:HB2	1:B:388:ALA:HB2	1.97	0.46
1:B:410:LYS:HE2	1:B:410:LYS:HB3	1.70	0.46
1:B:418:GLU:HB2	1:C:388:ALA:HB2	1.98	0.46
1:U:280:GLU:HG3	1:U:372:ILE:HG12	1.97	0.46
1:W:267:THR:HB	1:W:386:SER:HB2	1.98	0.46
1:X:394:LYS:O	1:X:402:LEU:N	2.48	0.46
1:E:415:LEU:HD11	1:F:433:VAL:HG21	1.97	0.46
1:I:418:GLU:HB2	1:J:388:ALA:HB2	1.98	0.46
1:K:417:ARG:HG3	1:K:422:PHE:HB3	1.98	0.46
1:b:373:ARG:NH2	1:c:275:LYS:HD3	2.30	0.46
1:b:415:LEU:HD11	1:c:433:VAL:HG21	1.97	0.46
1:C:418:GLU:HB2	1:D:388:ALA:HB2	1.98	0.46
1:R:280:GLU:HG3	1:R:372:ILE:HG12	1.98	0.46
1:S:360:ARG:NH1	1:S:362:GLU:OE1	2.43	0.46
1:a:417:ARG:HG3	1:a:422:PHE:HB3	1.98	0.46
1:P:301:SER:HB3	1:P:359:GLN:HB3	1.97	0.46
1:Q:418:GLU:HB2	1:R:388:ALA:HB2	1.98	0.46
1:V:418:GLU:HB2	1:W:388:ALA:HB2	1.98	0.46
1:A:388:ALA:HB2	1:g:418:GLU:HB2	1.98	0.45
1:L:267:THR:HB	1:L:386:SER:HB2	1.98	0.45
1:N:393:TYR:CE2	1:N:436:PRO:HD3	2.52	0.45
1:Q:415:LEU:HD11	1:R:433:VAL:HG21	1.97	0.45
1:V:389:VAL:HB	1:V:432:VAL:HG22	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:252:ILE:HD13	1:Y:265:GLN:HG2	1.98	0.45
1:Y:250:GLU:O	1:Y:254:SER:OG	2.23	0.45
1:C:415:LEU:HD11	1:D:433:VAL:HG21	1.98	0.45
1:M:389:VAL:HB	1:M:432:VAL:HG22	1.98	0.45
1:P:417:ARG:HG3	1:P:422:PHE:HB3	1.98	0.45
1:X:389:VAL:HB	1:X:432:VAL:HG22	1.97	0.45
1:Z:410:LYS:HB3	1:Z:410:LYS:HE2	1.68	0.45
1:a:392:ASN:OD1	1:a:393:TYR:N	2.48	0.45
1:b:418:GLU:HB2	1:c:388:ALA:HB2	1.99	0.45
1:J:360:ARG:NH1	1:J:362:GLU:OE1	2.48	0.45
1:T:389:VAL:HB	1:T:432:VAL:HG22	1.97	0.45
1:T:415:LEU:HD11	1:U:433:VAL:HG21	1.98	0.45
1:B:292:THR:HG21	1:C:282:TYR:HB3	1.99	0.45
1:P:267:THR:HB	1:P:386:SER:HB2	1.98	0.45
1:Y:246:GLN:NE2	1:Y:264:ALA:O	2.50	0.45
1:D:246:GLN:NE2	1:D:264:ALA:O	2.50	0.45
1:M:418:GLU:HG3	1:N:431:ASN:HB2	1.97	0.45
1:U:292:THR:HG21	1:V:282:TYR:HB3	1.99	0.45
1:B:394:LYS:O	1:B:402:LEU:N	2.50	0.45
1:I:417:ARG:HG3	1:I:422:PHE:HB3	1.99	0.45
1:L:415:LEU:HD11	1:M:433:VAL:HG21	1.97	0.45
1:X:371:THR:HG23	1:Y:279:GLU:HG3	1.99	0.45
1:Y:267:THR:HB	1:Y:386:SER:HB2	1.98	0.45
1:A:389:VAL:HB	1:A:432:VAL:HG22	1.99	0.45
1:B:267:THR:HB	1:B:386:SER:HB2	1.98	0.45
1:K:392:ASN:OD1	1:K:393:TYR:N	2.50	0.45
1:R:415:LEU:HD11	1:S:433:VAL:HG21	1.98	0.45
1:W:246:GLN:NE2	1:W:264:ALA:O	2.50	0.45
1:U:392:ASN:OD1	1:U:393:TYR:N	2.50	0.45
1:a:394:LYS:O	1:a:402:LEU:N	2.50	0.45
1:f:267:THR:HB	1:f:386:SER:HB2	1.98	0.45
1:D:296:ARG:NH2	1:D:362:GLU:OE2	2.50	0.45
1:I:415:LEU:HD11	1:J:433:VAL:HG21	1.98	0.45
1:L:418:GLU:HB2	1:M:388:ALA:HB2	1.99	0.45
1:P:393:TYR:CE2	1:P:436:PRO:HD3	2.52	0.45
1:e:292:THR:HG21	1:f:282:TYR:HB3	1.99	0.45
1:e:418:GLU:HB2	1:f:388:ALA:HB2	1.99	0.45
1:f:392:ASN:OD1	1:f:393:TYR:N	2.50	0.45
1:P:392:ASN:OD1	1:P:393:TYR:N	2.50	0.45
1:Z:389:VAL:HB	1:Z:432:VAL:HG22	1.99	0.45
1:D:394:LYS:O	1:D:402:LEU:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:392:ASN:OD1	1:X:393:TYR:N	2.50	0.44
1:L:231:ASN:CG	1:L:232:ASP:H	2.25	0.44
1:U:252:ILE:HD13	1:V:265:GLN:HG2	2.00	0.44
1:e:373:ARG:NH2	1:f:275:LYS:HD3	2.31	0.44
1:F:267:THR:HB	1:F:386:SER:HB2	2.00	0.44
1:J:418:GLU:HB2	1:K:388:ALA:HB2	2.00	0.44
1:L:392:ASN:OD1	1:L:393:TYR:N	2.51	0.44
1:Q:389:VAL:HG21	1:Q:416:THR:HG21	1.98	0.44
1:R:292:THR:HG21	1:S:282:TYR:HB3	2.00	0.44
1:T:246:GLN:NE2	1:T:264:ALA:O	2.51	0.44
1:V:417:ARG:HG3	1:V:422:PHE:HB3	1.98	0.44
1:a:389:VAL:HB	1:a:432:VAL:HG22	1.99	0.44
1:g:296:ARG:NH2	1:g:362:GLU:OE2	2.50	0.44
1:R:246:GLN:NE2	1:R:264:ALA:O	2.51	0.44
1:W:415:LEU:HD11	1:X:433:VAL:HG21	1.99	0.44
1:O:267:THR:HB	1:O:386:SER:HB2	2.00	0.44
1:c:417:ARG:HG3	1:c:422:PHE:HB3	1.98	0.44
1:d:246:GLN:NE2	1:d:264:ALA:O	2.51	0.44
1:d:360:ARG:NH1	1:d:362:GLU:OE1	2.43	0.44
1:B:415:LEU:HD11	1:C:433:VAL:HG21	1.98	0.44
1:E:267:THR:HB	1:E:386:SER:HB2	2.00	0.44
1:O:389:VAL:HB	1:O:432:VAL:HG22	1.98	0.44
1:S:415:LEU:HD11	1:T:433:VAL:HG21	2.00	0.44
1:X:393:TYR:CE2	1:X:436:PRO:HD3	2.52	0.44
1:f:410:LYS:HB3	1:f:410:LYS:HE2	1.67	0.44
1:B:276:GLU:HG2	1:B:376:LYS:HG3	1.99	0.44
1:D:418:GLU:HB2	1:E:388:ALA:HB2	2.00	0.44
1:E:292:THR:HG21	1:F:282:TYR:HB3	2.00	0.44
1:Q:390:VAL:HG12	1:Q:433:VAL:HG22	1.99	0.44
1:c:415:LEU:HD11	1:d:433:VAL:HG21	2.00	0.44
1:E:246:GLN:NE2	1:E:264:ALA:O	2.50	0.44
1:F:389:VAL:HB	1:F:432:VAL:HG22	1.99	0.44
1:L:417:ARG:HG3	1:L:422:PHE:HB3	1.99	0.44
1:U:418:GLU:HB2	1:V:388:ALA:HB2	1.99	0.44
1:d:389:VAL:HB	1:d:432:VAL:HG22	1.99	0.44
1:D:390:VAL:HG12	1:D:433:VAL:HG22	2.00	0.44
1:f:280:GLU:HG3	1:f:372:ILE:HG12	2.00	0.44
1:A:296:ARG:NH2	1:A:362:GLU:OE2	2.51	0.43
1:W:394:LYS:O	1:W:402:LEU:N	2.51	0.43
1:A:433:VAL:HG21	1:g:415:LEU:HD11	1.99	0.43
1:K:393:TYR:CE2	1:K:436:PRO:HD3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:275:LYS:HB2	1:R:275:LYS:HE3	1.71	0.43
1:R:418:GLU:HB2	1:S:388:ALA:HB2	2.00	0.43
1:V:296:ARG:NH2	1:V:362:GLU:OE2	2.50	0.43
1:Y:389:VAL:HB	1:Y:432:VAL:HG22	1.99	0.43
1:b:392:ASN:OD1	1:b:393:TYR:N	2.51	0.43
1:K:296:ARG:NH2	1:K:362:GLU:OE2	2.51	0.43
1:M:392:ASN:OD1	1:M:393:TYR:N	2.51	0.43
1:O:271:ASP:HB2	1:O:383:GLU:HG3	2.00	0.43
1:e:246:GLN:NE2	1:e:264:ALA:O	2.50	0.43
1:B:296:ARG:NH2	1:B:362:GLU:OE2	2.52	0.43
1:B:393:TYR:CE2	1:B:436:PRO:HD3	2.53	0.43
1:G:418:GLU:HB2	1:H:388:ALA:HB2	2.01	0.43
1:S:394:LYS:O	1:S:402:LEU:N	2.52	0.43
1:W:393:TYR:CE2	1:W:436:PRO:HD3	2.53	0.43
1:b:296:ARG:NH2	1:b:362:GLU:OE2	2.51	0.43
1:G:280:GLU:HG3	1:G:372:ILE:HG12	2.00	0.43
1:K:415:LEU:HD11	1:L:433:VAL:HG21	1.99	0.43
1:K:418:GLU:HG3	1:L:431:ASN:HB2	2.00	0.43
1:N:392:ASN:OD1	1:N:393:TYR:N	2.52	0.43
1:V:415:LEU:HD11	1:W:433:VAL:HG21	2.00	0.43
1:b:410:LYS:HB3	1:b:410:LYS:HE2	1.70	0.43
1:A:415:LEU:HD11	1:B:433:VAL:HG21	2.01	0.43
1:X:301:SER:HB2	1:X:359:GLN:HB3	2.00	0.43
1:H:271:ASP:HB2	1:H:383:GLU:HG2	2.01	0.43
1:a:415:LEU:HD11	1:b:433:VAL:HG21	2.00	0.43
1:e:360:ARG:NH1	1:e:362:GLU:OE1	2.44	0.43
1:e:418:GLU:HG3	1:f:431:ASN:HB2	2.00	0.43
1:F:418:GLU:HG3	1:G:431:ASN:HB2	2.00	0.43
1:H:275:LYS:HE3	1:H:275:LYS:HB2	1.74	0.43
1:H:292:THR:HG21	1:I:282:TYR:HB3	2.01	0.43
1:M:418:GLU:HB2	1:N:388:ALA:HB2	2.01	0.43
1:N:394:LYS:O	1:N:402:LEU:N	2.52	0.43
1:R:418:GLU:HG3	1:S:431:ASN:HB2	2.01	0.43
1:T:390:VAL:HG12	1:T:433:VAL:HG22	2.01	0.43
1:T:418:GLU:HB2	1:U:388:ALA:HB2	2.01	0.43
1:Y:296:ARG:NH2	1:Y:362:GLU:OE2	2.52	0.43
1:F:296:ARG:NH2	1:F:362:GLU:OE2	2.52	0.43
1:Q:410:LYS:HB3	1:Q:410:LYS:HE2	1.70	0.43
1:W:410:LYS:HE2	1:W:410:LYS:HB3	1.67	0.43
1:E:360:ARG:NH1	1:E:362:GLU:OE1	2.44	0.43
1:S:275:LYS:HB2	1:S:275:LYS:HE3	1.73	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:275:LYS:HE3	1:T:275:LYS:HB2	1.74	0.43
1:T:296:ARG:NH2	1:T:362:GLU:OE2	2.52	0.43
1:b:246:GLN:NE2	1:b:264:ALA:O	2.52	0.43
1:e:280:GLU:HG3	1:e:372:ILE:HG12	2.00	0.43
1:O:371:THR:HG23	1:P:279:GLU:HG3	2.01	0.42
1:S:389:VAL:HB	1:S:432:VAL:HG22	1.99	0.42
1:a:296:ARG:NH2	1:a:362:GLU:OE2	2.52	0.42
1:d:250:GLU:O	1:d:254:SER:OG	2.33	0.42
1:d:392:ASN:OD1	1:d:393:TYR:N	2.52	0.42
1:e:394:LYS:O	1:e:402:LEU:N	2.52	0.42
1:g:280:GLU:HG3	1:g:372:ILE:HG12	2.01	0.42
1:K:267:THR:HB	1:K:386:SER:HB2	2.01	0.42
1:M:280:GLU:HG3	1:M:372:ILE:HG12	2.02	0.42
1:M:296:ARG:NH2	1:M:362:GLU:OE2	2.52	0.42
1:D:267:THR:HB	1:D:386:SER:HB2	2.02	0.42
1:K:389:VAL:HB	1:K:432:VAL:HG22	2.01	0.42
1:L:371:THR:HG23	1:M:279:GLU:HG3	2.02	0.42
1:M:415:LEU:HD11	1:N:433:VAL:HG21	2.01	0.42
1:N:246:GLN:NE2	1:N:264:ALA:O	2.52	0.42
1:R:267:THR:HB	1:R:386:SER:HB2	2.00	0.42
1:E:296:ARG:NH2	1:E:362:GLU:OE2	2.52	0.42
1:S:250:GLU:O	1:S:254:SER:OG	2.32	0.42
1:V:392:ASN:OD1	1:V:393:TYR:N	2.52	0.42
1:g:410:LYS:HE2	1:g:410:LYS:HB3	1.65	0.42
1:H:392:ASN:OD1	1:H:393:TYR:N	2.52	0.42
1:H:394:LYS:O	1:H:402:LEU:N	2.52	0.42
1:I:296:ARG:NH2	1:I:362:GLU:OE2	2.52	0.42
1:L:280:GLU:HG3	1:L:372:ILE:HG12	2.02	0.42
1:S:246:GLN:NE2	1:S:264:ALA:O	2.52	0.42
1:S:392:ASN:OD1	1:S:393:TYR:N	2.53	0.42
1:b:280:GLU:HG3	1:b:372:ILE:HG12	2.01	0.42
1:c:296:ARG:NH2	1:c:362:GLU:OE2	2.53	0.42
1:c:392:ASN:OD1	1:c:393:TYR:N	2.52	0.42
1:d:296:ARG:NH2	1:d:362:GLU:OE2	2.52	0.42
1:D:392:ASN:OD1	1:D:393:TYR:N	2.52	0.42
1:J:296:ARG:NH2	1:J:362:GLU:OE2	2.53	0.42
1:P:275:LYS:HE3	1:P:275:LYS:HB2	1.75	0.42
1:Q:418:GLU:HG3	1:R:431:ASN:HB2	2.02	0.42
1:e:389:VAL:HB	1:e:432:VAL:HG22	2.02	0.42
1:E:373:ARG:NH2	1:F:275:LYS:HD3	2.35	0.42
1:L:271:ASP:HB2	1:L:383:GLU:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:417:ARG:HG3	1:S:422:PHE:HB3	2.00	0.42
1:T:392:ASN:OD1	1:T:393:TYR:N	2.52	0.42
1:Z:296:ARG:NH2	1:Z:362:GLU:OE2	2.53	0.42
1:K:410:LYS:HB3	1:K:410:LYS:HE2	1.66	0.42
1:M:360:ARG:NH1	1:M:362:GLU:OE1	2.48	0.42
1:X:418:GLU:HG3	1:Y:431:ASN:HB2	2.02	0.42
1:c:267:THR:HB	1:c:386:SER:HB2	2.02	0.42
1:F:280:GLU:HG3	1:F:372:ILE:HG12	2.01	0.42
1:S:296:ARG:NH2	1:S:362:GLU:OE2	2.52	0.42
1:Y:283:SER:HB2	1:Y:369:ASP:HB2	2.01	0.42
1:a:393:TYR:CE2	1:a:436:PRO:HD3	2.55	0.42
1:g:392:ASN:OD1	1:g:393:TYR:N	2.52	0.42
1:H:280:GLU:HG3	1:H:372:ILE:HG12	2.02	0.41
1:W:392:ASN:OD1	1:W:393:TYR:N	2.53	0.41
1:F:393:TYR:CE2	1:F:436:PRO:HD3	2.54	0.41
1:K:252:ILE:HD13	1:L:265:GLN:HG2	2.02	0.41
1:U:415:LEU:HD11	1:V:433:VAL:HG21	2.02	0.41
1:Z:390:VAL:HG12	1:Z:433:VAL:HG22	2.02	0.41
1:d:415:LEU:HD11	1:e:433:VAL:HG21	2.01	0.41
1:f:418:GLU:HG3	1:g:431:ASN:HB2	2.00	0.41
1:E:418:GLU:HG3	1:F:431:ASN:HB2	2.01	0.41
1:H:415:LEU:HD11	1:I:433:VAL:HG21	2.02	0.41
1:J:246:GLN:NE2	1:J:264:ALA:O	2.53	0.41
1:Q:296:ARG:NH2	1:Q:362:GLU:OE2	2.53	0.41
1:U:267:THR:HB	1:U:386:SER:HB2	2.03	0.41
1:J:389:VAL:HG21	1:J:416:THR:HG21	2.03	0.41
1:O:418:GLU:HG3	1:P:431:ASN:HB2	2.02	0.41
1:P:252:ILE:HD13	1:Q:265:GLN:HG2	2.03	0.41
1:J:392:ASN:OD1	1:J:393:TYR:N	2.53	0.41
1:N:292:THR:HG21	1:O:282:TYR:HB3	2.03	0.41
1:g:390:VAL:HG12	1:g:433:VAL:HG22	2.02	0.41
1:G:392:ASN:OD1	1:G:393:TYR:N	2.54	0.41
1:W:296:ARG:NH2	1:W:362:GLU:OE2	2.53	0.41
1:a:275:LYS:HB2	1:a:275:LYS:HE3	1.70	0.41
1:d:375:THR:HG23	1:e:275:LYS:HE2	2.02	0.41
1:g:231:ASN:N	1:g:231:ASN:OD1	2.52	0.41
1:C:277:GLN:NE2	1:C:279:GLU:OE2	2.54	0.41
1:E:280:GLU:HG3	1:E:372:ILE:HG12	2.03	0.41
1:G:293:LEU:HD13	1:G:296:ARG:HD2	2.03	0.41
1:M:295:SER:HB2	1:M:365:ASN:HD22	1.86	0.41
1:R:252:ILE:HD13	1:S:265:GLN:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:252:ILE:HD13	1:c:265:GLN:HG2	2.03	0.41
1:I:418:GLU:HG3	1:J:431:ASN:HB2	2.02	0.41
1:U:413:GLU:HG2	1:U:417:ARG:HH12	1.86	0.41
1:b:267:THR:HB	1:b:386:SER:HB2	2.01	0.41
1:H:296:ARG:NH2	1:H:362:GLU:OE2	2.54	0.41
1:M:301:SER:HB3	1:M:359:GLN:HB3	2.03	0.41
1:Y:292:THR:HG21	1:Z:282:TYR:HB3	2.03	0.41
1:d:390:VAL:HG12	1:d:433:VAL:HG22	2.02	0.41
1:A:282:TYR:HB3	1:g:292:THR:HG21	2.03	0.41
1:O:415:LEU:HD11	1:P:433:VAL:HG21	2.03	0.41
1:f:292:THR:HG21	1:g:282:TYR:HB3	2.03	0.41
1:O:296:ARG:NH2	1:O:362:GLU:OE2	2.53	0.40
1:Q:246:GLN:NE2	1:Q:264:ALA:O	2.54	0.40
1:W:275:LYS:HE3	1:W:275:LYS:HB2	1.89	0.40
1:Y:392:ASN:OD1	1:Y:393:TYR:N	2.54	0.40
1:J:275:LYS:HE3	1:J:275:LYS:HB2	1.70	0.40
1:O:246:GLN:NE2	1:O:264:ALA:O	2.54	0.40
1:U:296:ARG:NH2	1:U:362:GLU:OE2	2.54	0.40
1:X:275:LYS:HB2	1:X:275:LYS:HE3	1.72	0.40
1:Z:412:ILE:O	1:Z:416:THR:HG22	2.21	0.40
1:Z:415:LEU:HD11	1:a:433:VAL:HG21	2.03	0.40
1:L:292:THR:HG21	1:M:282:TYR:HB3	2.04	0.40
1:N:296:ARG:NH2	1:N:362:GLU:OE2	2.54	0.40
1:R:392:ASN:OD1	1:R:393:TYR:N	2.54	0.40
1:Z:252:ILE:HD13	1:a:265:GLN:HG2	2.04	0.40
1:g:293:LEU:HD13	1:g:296:ARG:HD2	2.03	0.40
1:B:246:GLN:NE2	1:B:264:ALA:O	2.55	0.40
1:F:250:GLU:O	1:F:254:SER:OG	2.21	0.40
1:F:292:THR:HG21	1:G:282:TYR:HB3	2.04	0.40
1:L:296:ARG:NH2	1:L:362:GLU:OE2	2.54	0.40
1:N:385:LEU:HD23	1:N:385:LEU:HA	1.96	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	A	145/560 (26%)	138 (95%)	7 (5%)	0	100	100
1	B	145/560 (26%)	139 (96%)	6 (4%)	0	100	100
1	C	145/560 (26%)	139 (96%)	6 (4%)	0	100	100
1	D	145/560 (26%)	138 (95%)	7 (5%)	0	100	100
1	E	145/560 (26%)	139 (96%)	6 (4%)	0	100	100
1	F	145/560 (26%)	138 (95%)	7 (5%)	0	100	100
1	G	145/560 (26%)	139 (96%)	6 (4%)	0	100	100
1	H	145/560 (26%)	138 (95%)	7 (5%)	0	100	100
1	I	145/560 (26%)	139 (96%)	6 (4%)	0	100	100
1	J	145/560 (26%)	139 (96%)	6 (4%)	0	100	100
1	K	145/560 (26%)	136 (94%)	9 (6%)	0	100	100
1	L	145/560 (26%)	139 (96%)	6 (4%)	0	100	100
1	M	145/560 (26%)	140 (97%)	5 (3%)	0	100	100
1	N	145/560 (26%)	139 (96%)	6 (4%)	0	100	100
1	O	145/560 (26%)	140 (97%)	5 (3%)	0	100	100
1	P	145/560 (26%)	139 (96%)	6 (4%)	0	100	100
1	Q	145/560 (26%)	139 (96%)	6 (4%)	0	100	100
1	R	145/560 (26%)	138 (95%)	7 (5%)	0	100	100
1	S	145/560 (26%)	139 (96%)	6 (4%)	0	100	100
1	T	145/560 (26%)	138 (95%)	7 (5%)	0	100	100
1	U	145/560 (26%)	140 (97%)	5 (3%)	0	100	100
1	V	145/560 (26%)	138 (95%)	7 (5%)	0	100	100
1	W	145/560 (26%)	140 (97%)	5 (3%)	0	100	100
1	X	145/560 (26%)	137 (94%)	8 (6%)	0	100	100
1	Y	145/560 (26%)	140 (97%)	5 (3%)	0	100	100
1	Z	145/560 (26%)	140 (97%)	5 (3%)	0	100	100
1	a	145/560 (26%)	138 (95%)	7 (5%)	0	100	100
1	b	145/560 (26%)	139 (96%)	6 (4%)	0	100	100
1	c	145/560 (26%)	139 (96%)	6 (4%)	0	100	100
1	d	145/560 (26%)	139 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	e	145/560 (26%)	138 (95%)	7 (5%)	0	100	100
1	f	145/560 (26%)	139 (96%)	6 (4%)	0	100	100
1	g	145/560 (26%)	139 (96%)	6 (4%)	0	100	100
All	All	4785/18480 (26%)	4579 (96%)	206 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	A	134/467 (29%)	134 (100%)	0	100	100
1	B	134/467 (29%)	134 (100%)	0	100	100
1	C	134/467 (29%)	134 (100%)	0	100	100
1	D	134/467 (29%)	134 (100%)	0	100	100
1	E	134/467 (29%)	134 (100%)	0	100	100
1	F	134/467 (29%)	134 (100%)	0	100	100
1	G	134/467 (29%)	134 (100%)	0	100	100
1	H	134/467 (29%)	134 (100%)	0	100	100
1	I	134/467 (29%)	134 (100%)	0	100	100
1	J	134/467 (29%)	134 (100%)	0	100	100
1	K	134/467 (29%)	134 (100%)	0	100	100
1	L	134/467 (29%)	134 (100%)	0	100	100
1	M	134/467 (29%)	134 (100%)	0	100	100
1	N	134/467 (29%)	134 (100%)	0	100	100
1	O	134/467 (29%)	134 (100%)	0	100	100
1	P	134/467 (29%)	134 (100%)	0	100	100
1	Q	134/467 (29%)	134 (100%)	0	100	100
1	R	134/467 (29%)	134 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	S	134/467 (29%)	134 (100%)	0	100	100
1	T	134/467 (29%)	134 (100%)	0	100	100
1	U	134/467 (29%)	134 (100%)	0	100	100
1	V	134/467 (29%)	134 (100%)	0	100	100
1	W	134/467 (29%)	134 (100%)	0	100	100
1	X	134/467 (29%)	134 (100%)	0	100	100
1	Y	134/467 (29%)	134 (100%)	0	100	100
1	Z	134/467 (29%)	134 (100%)	0	100	100
1	a	134/467 (29%)	134 (100%)	0	100	100
1	b	134/467 (29%)	134 (100%)	0	100	100
1	c	134/467 (29%)	134 (100%)	0	100	100
1	d	134/467 (29%)	134 (100%)	0	100	100
1	e	134/467 (29%)	134 (100%)	0	100	100
1	f	134/467 (29%)	134 (100%)	0	100	100
1	g	134/467 (29%)	134 (100%)	0	100	100
All	All	4422/15411 (29%)	4422 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (114) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	261	ASN
1	A	434	ASN
1	B	261	ASN
1	B	434	ASN
1	C	261	ASN
1	C	277	GLN
1	C	434	ASN
1	D	261	ASN
1	D	361	ASN
1	D	365	ASN
1	D	434	ASN
1	E	259	ASN
1	E	261	ASN
1	E	434	ASN

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Mol	Chain	Res	Type
1	F	261	ASN
1	F	365	ASN
1	F	434	ASN
1	G	261	ASN
1	G	365	ASN
1	G	434	ASN
1	H	261	ASN
1	H	434	ASN
1	I	231	ASN
1	I	261	ASN
1	I	434	ASN
1	J	261	ASN
1	J	361	ASN
1	J	434	ASN
1	K	263	HIS
1	K	277	GLN
1	K	434	ASN
1	L	259	ASN
1	L	261	ASN
1	L	365	ASN
1	L	434	ASN
1	M	261	ASN
1	M	365	ASN
1	M	434	ASN
1	N	261	ASN
1	N	361	ASN
1	N	365	ASN
1	N	434	ASN
1	O	261	ASN
1	O	269	GLN
1	O	365	ASN
1	P	261	ASN
1	P	263	HIS
1	P	365	ASN
1	P	434	ASN
1	Q	261	ASN
1	Q	274	ASN
1	Q	277	GLN
1	Q	365	ASN
1	Q	434	ASN
1	R	261	ASN
1	R	263	HIS

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Mol	Chain	Res	Type
1	R	365	ASN
1	R	434	ASN
1	S	261	ASN
1	S	263	HIS
1	S	274	ASN
1	S	365	ASN
1	S	434	ASN
1	T	259	ASN
1	T	261	ASN
1	T	277	GLN
1	U	261	ASN
1	U	277	GLN
1	U	431	ASN
1	U	434	ASN
1	V	259	ASN
1	V	261	ASN
1	V	365	ASN
1	V	434	ASN
1	W	261	ASN
1	W	277	GLN
1	W	434	ASN
1	X	261	ASN
1	X	263	HIS
1	X	277	GLN
1	X	365	ASN
1	X	434	ASN
1	Y	261	ASN
1	Y	277	GLN
1	Y	434	ASN
1	Z	261	ASN
1	Z	365	ASN
1	Z	434	ASN
1	a	261	ASN
1	a	263	HIS
1	a	434	ASN
1	b	261	ASN
1	b	277	GLN
1	b	365	ASN
1	c	259	ASN
1	c	261	ASN
1	c	365	ASN
1	c	434	ASN

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Mol	Chain	Res	Type
1	d	259	ASN
1	d	261	ASN
1	d	434	ASN
1	e	259	ASN
1	e	261	ASN
1	e	434	ASN
1	f	231	ASN
1	f	261	ASN
1	f	277	GLN
1	f	434	ASN
1	g	231	ASN
1	g	259	ASN
1	g	261	ASN
1	g	263	HIS
1	g	365	ASN
1	g	434	ASN

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.

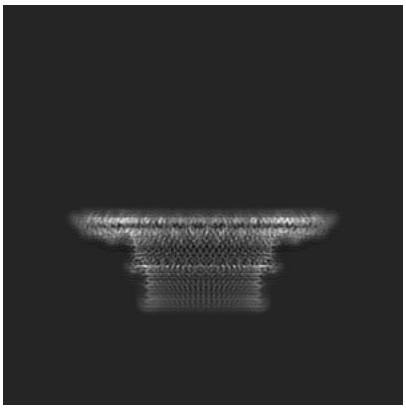
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-10145. These allow visual inspection of the internal detail of the map and identification of artifacts.

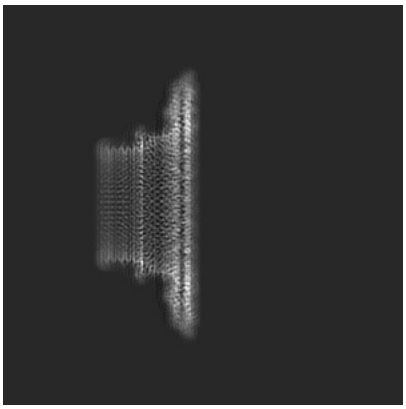
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

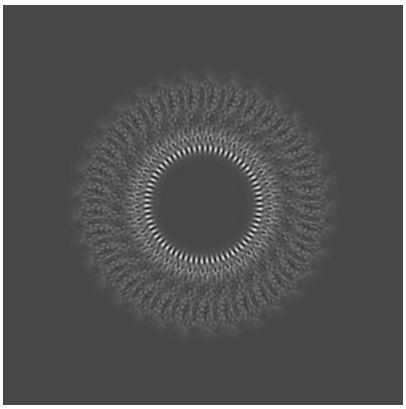
6.1.1 Primary map



X

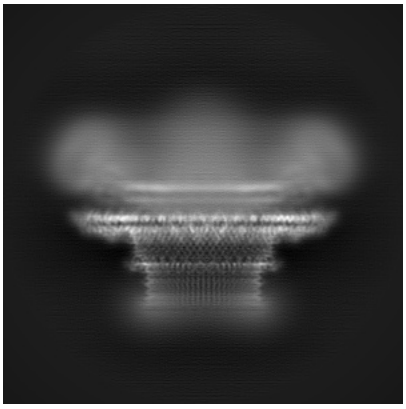


Y

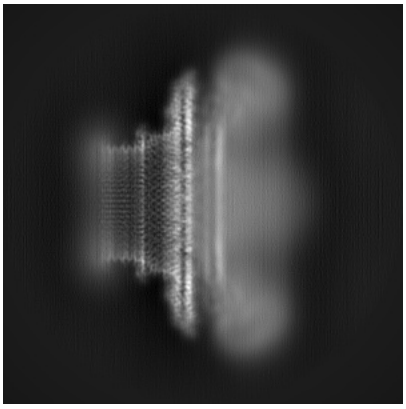


Z

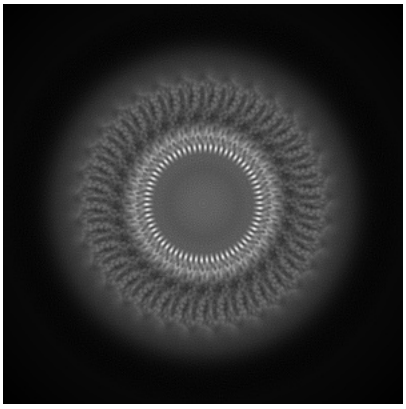
6.1.2 Raw map



X



Y



Z

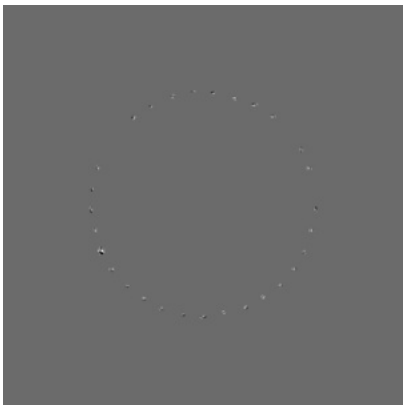
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map

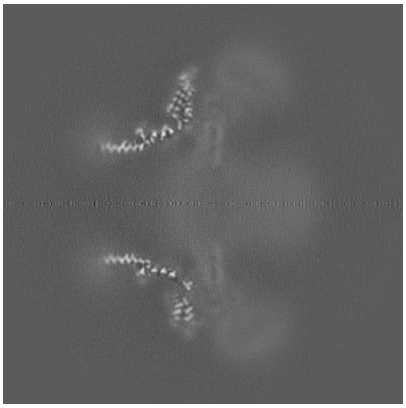
X Index: 216

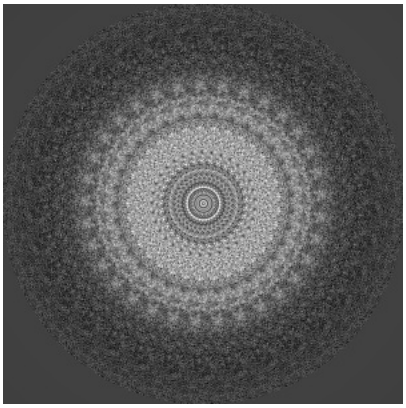
Y Index: 216


Z Index: 216

6.2.2 Raw map

X Index: 216


Y Index: 216


Z Index: 216

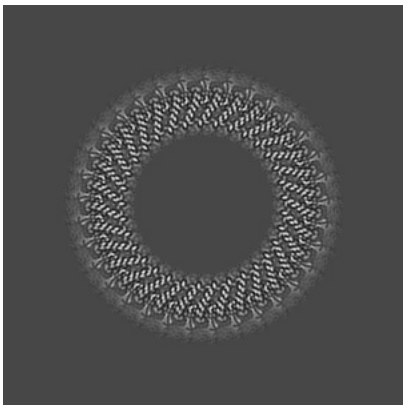
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

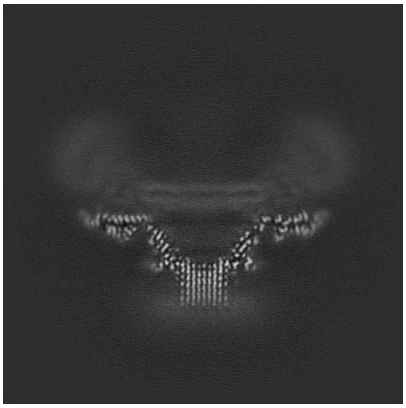
X Index: 274

Y Index: 156

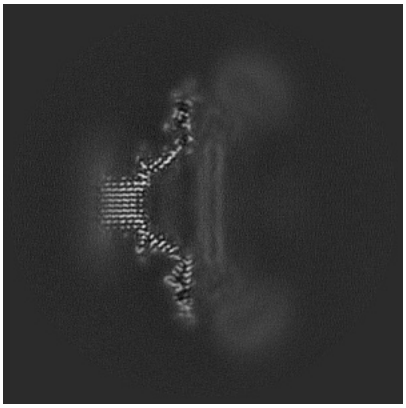


Z Index: 197

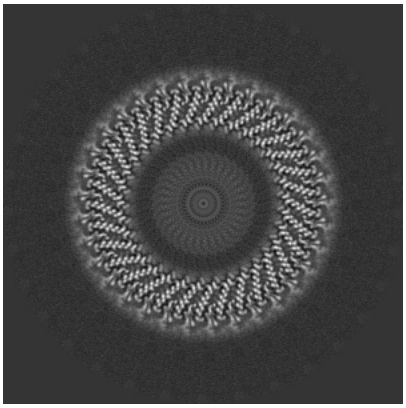
6.3.2 Raw map



X Index: 275



Y Index: 157

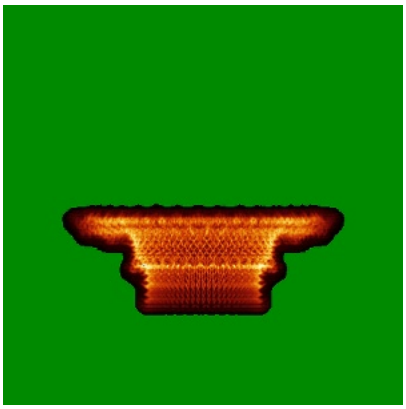


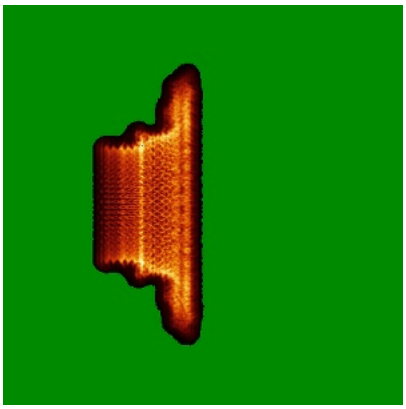
Z Index: 199

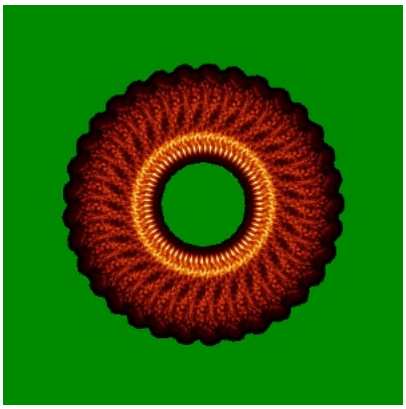
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

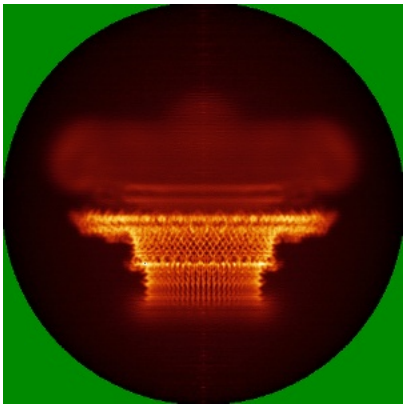
6.4.1 Primary map

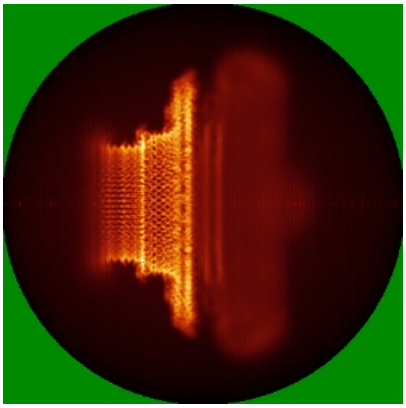

X

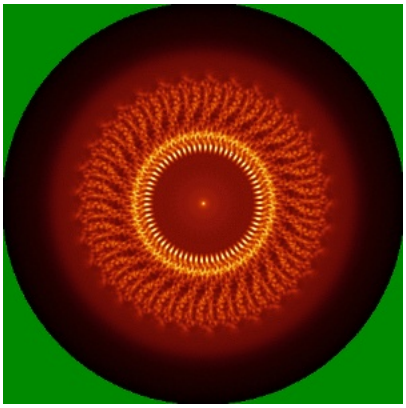

Y


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)

This section was not generated.

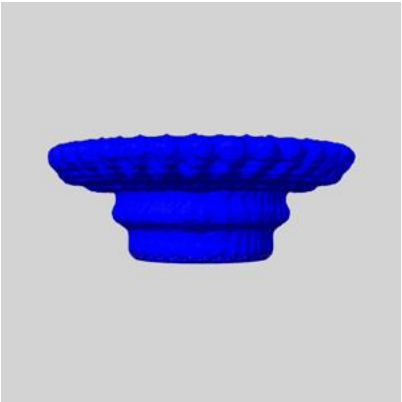
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

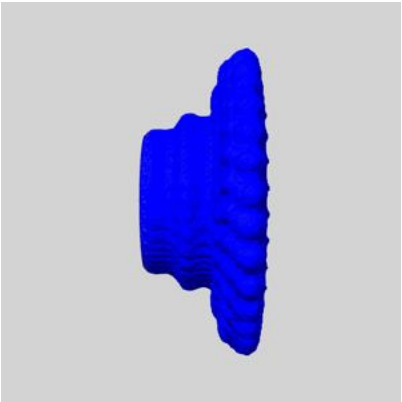
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

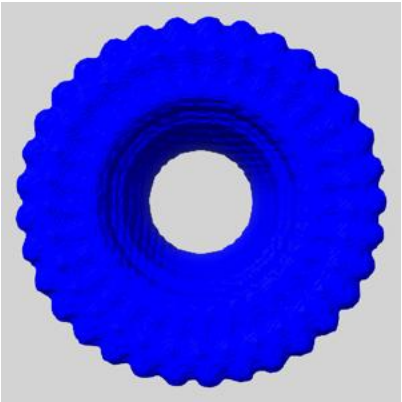
6.6.1 emd_10145_msk_1.map (i)



X



Y

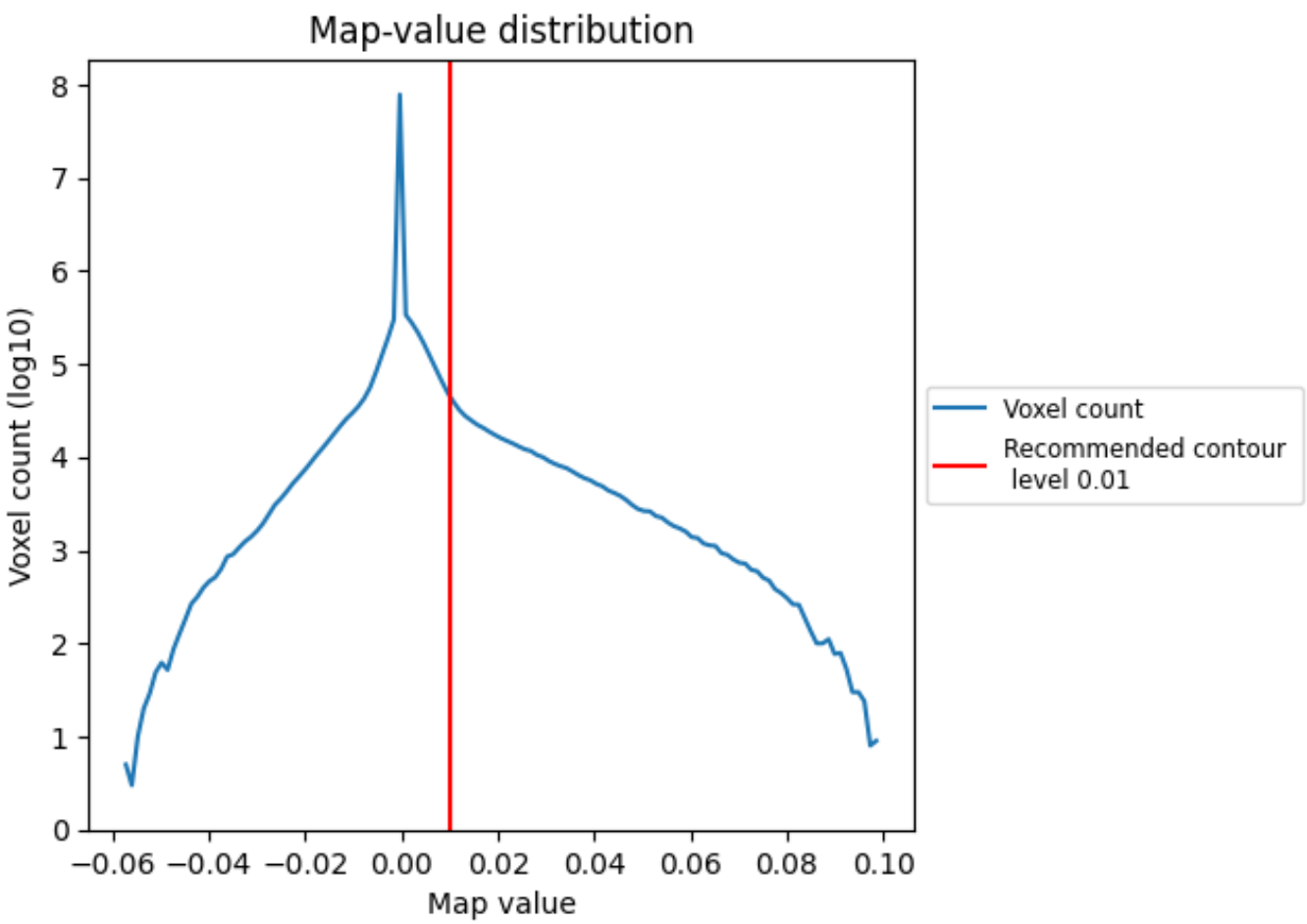


Z

7 Map analysis (i)

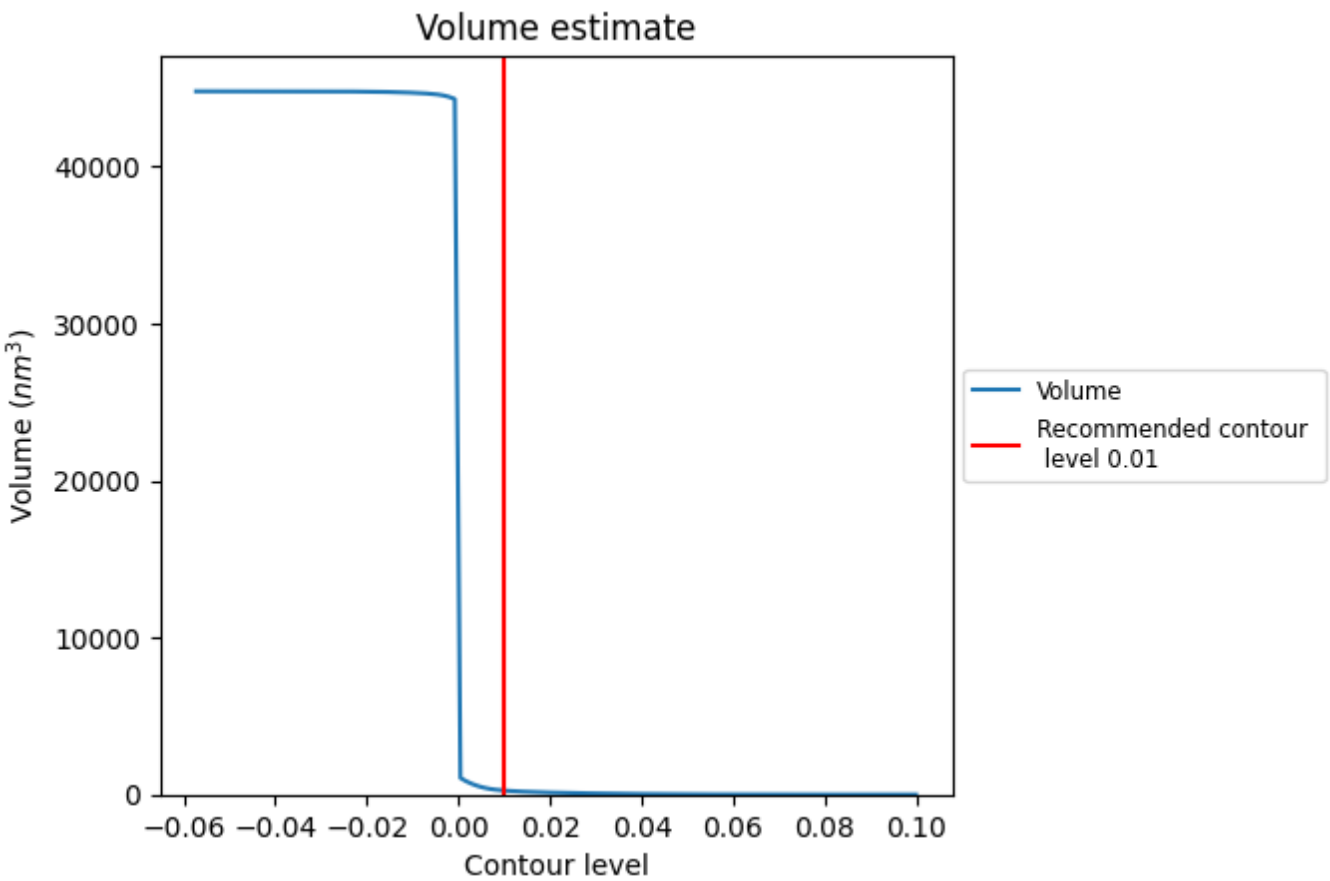
This section contains the results of statistical analysis of the map.

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.

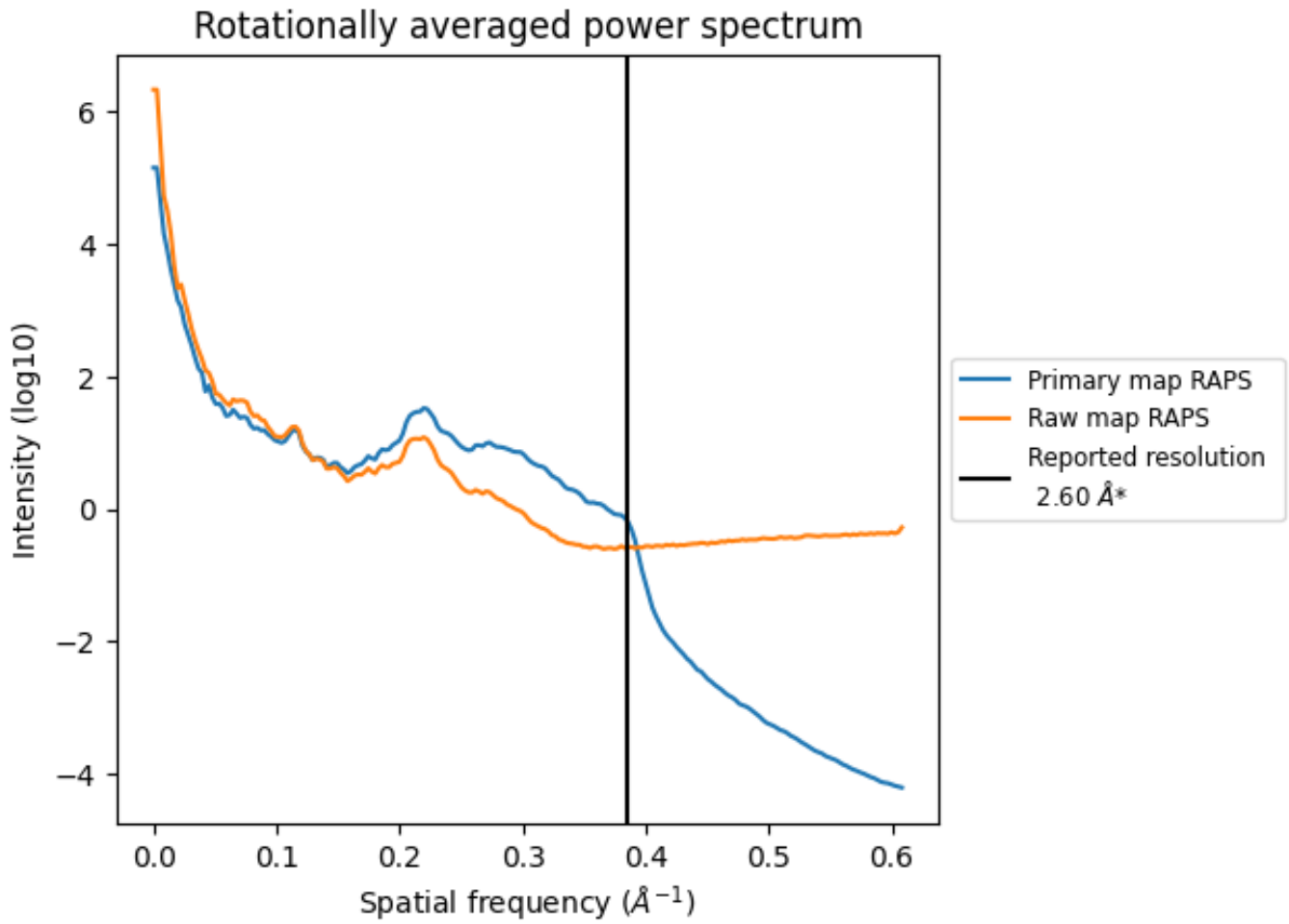
7.2 Volume estimate (i)



The volume at the recommended contour level is 254 nm^3; this corresponds to an approximate mass of 229 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 (i)

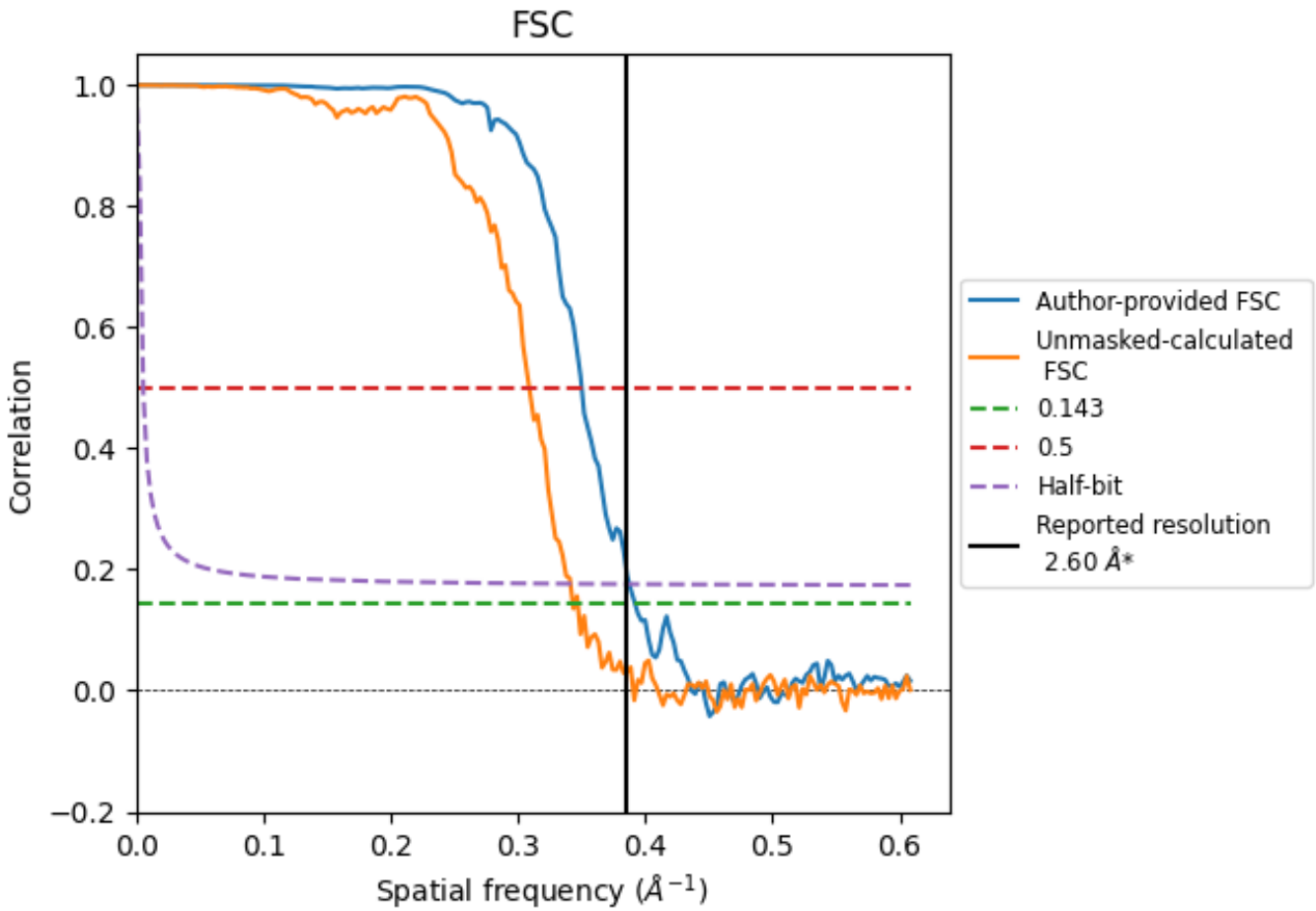


*Reported resolution corresponds to spatial frequency of 0.385 Å^{-1}

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 0.385 Å^{-1}

8.2 Resolution estimates (i)

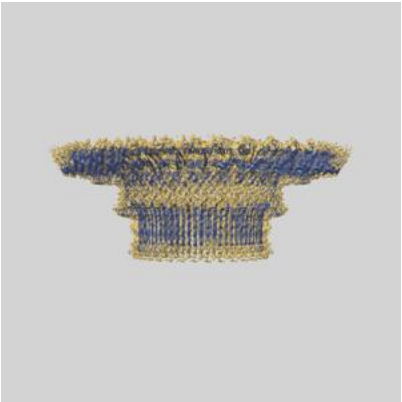
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.55	2.86	2.58
Unmasked-calculated*	2.91	3.24	2.93

*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 2.91 differs from the reported value 2.6 by more than 10 %

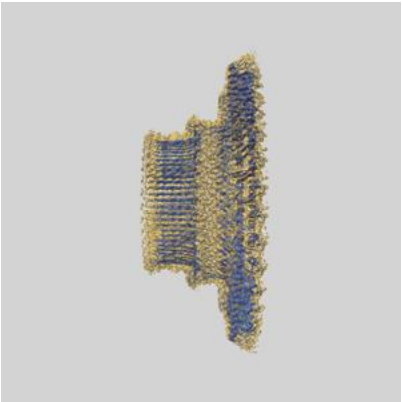
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-10145 and PDB model 6SD1. Per-residue inclusion information can be found in section 3 on page 7.

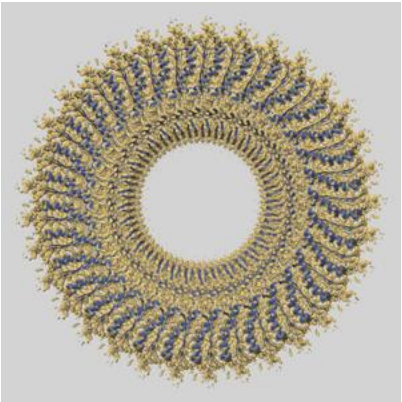
9.1 Map-model overlay (i)



X



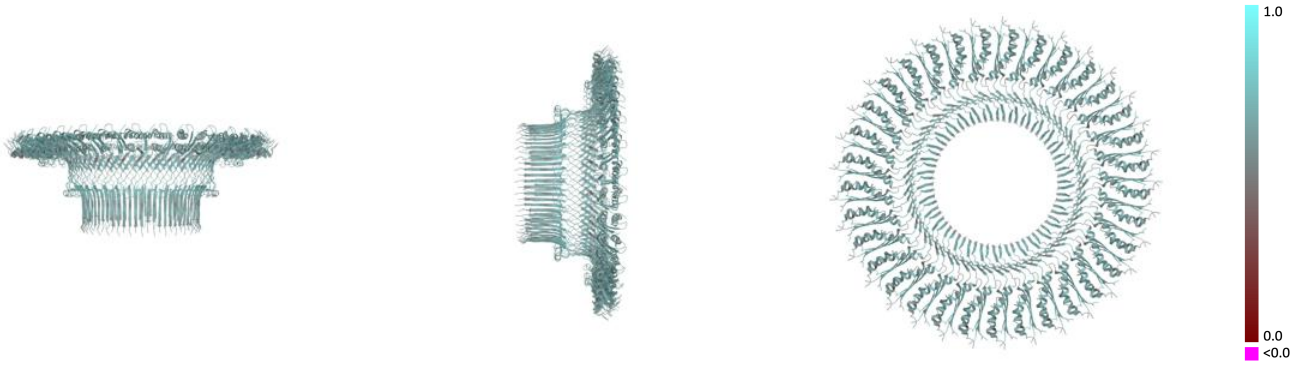
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01 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.

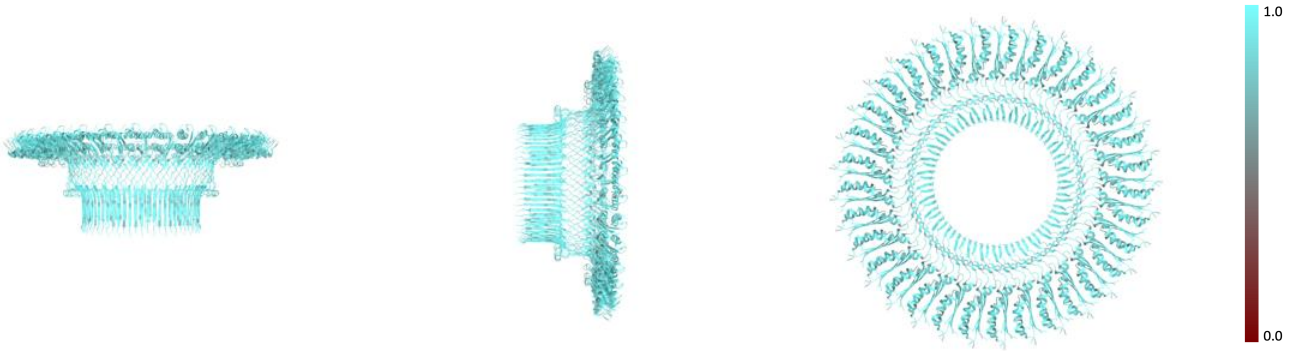
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

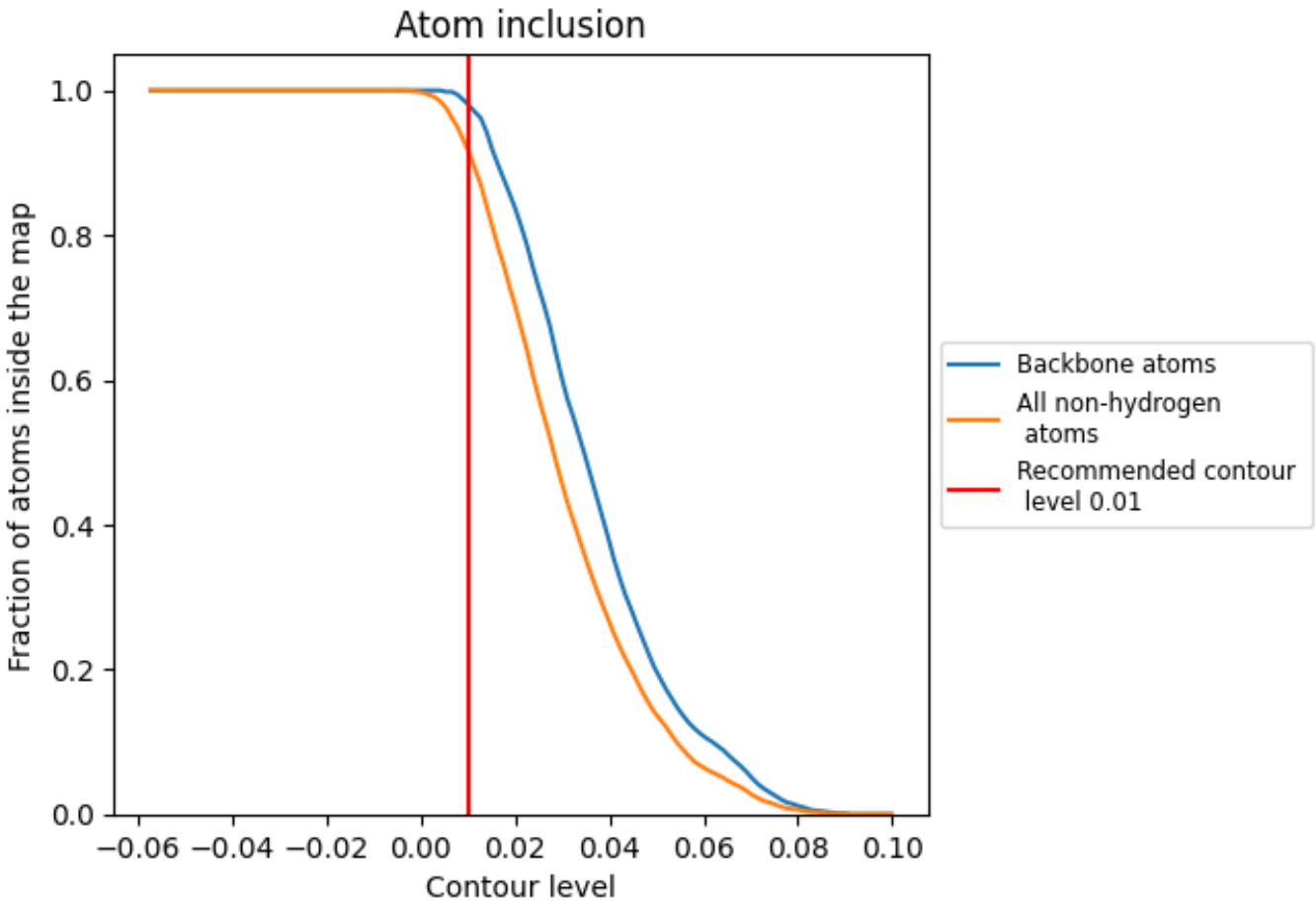
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.01).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9180	0.6230
A	0.9170	0.6230
B	0.9200	0.6220
C	0.9150	0.6210
D	0.9190	0.6220
E	0.9170	0.6210
F	0.9190	0.6230
G	0.9190	0.6260
H	0.9190	0.6240
I	0.9180	0.6220
J	0.9180	0.6240
K	0.9140	0.6230
L	0.9230	0.6230
M	0.9190	0.6210
N	0.9180	0.6230
O	0.9150	0.6230
P	0.9180	0.6240
Q	0.9150	0.6240
R	0.9160	0.6240
S	0.9150	0.6230
T	0.9190	0.6220
U	0.9180	0.6220
V	0.9130	0.6230
W	0.9180	0.6240
X	0.9180	0.6220
Y	0.9200	0.6260
Z	0.9170	0.6250
a	0.9170	0.6220
b	0.9220	0.6250
c	0.9150	0.6220
d	0.9190	0.6180
e	0.9170	0.6250
f	0.9160	0.6250
g	0.9160	0.6240