



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 02:56 PM UTC

PDB ID : 8ZDS / pdb_00008zds
EMDB ID : EMD-60007
Title : Structure of the Salmonella flagellar MS-ring with C11 symmetry applied
Authors : Kinoshita, M.; Makino, F.; Miyata, T.; Imada, K.; Minamino, T.; Namba, K.
Deposited on : 2024-05-03
Resolution : 3.10 Å(reported)
Based on initial models : 7D84, ., 7CIK

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

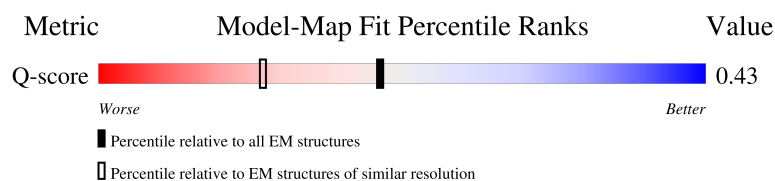
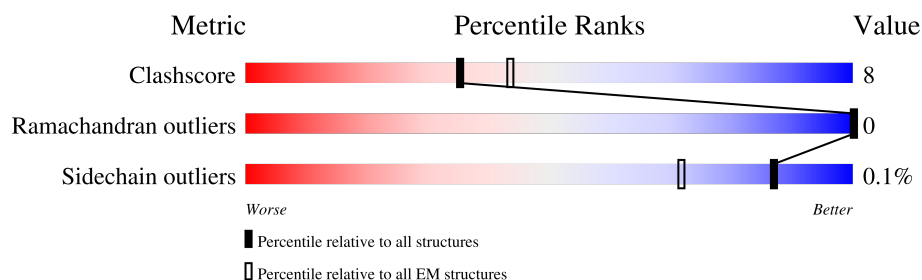
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.10 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	14724 (2.60 - 3.60)

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	A	560	38% 38% 8% 54%
1	B	560	47% 44% 11% 45%
1	C	560	38% 37% 9% 54%
1	D	560	38% 38% 8% 54%

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Mol	Chain	Length	Quality of chain
1	E	560	47% 46%10%45%
1	F	560	37% 36%9%54%
1	G	560	38% 38%8%54%
1	H	560	47% 44%11%45%
1	I	560	37% 37%9%54%
1	J	560	37% 39%7%54%
1	K	560	47% 45%10%45%
1	L	560	38% 37%9%54%
1	M	560	38% 39%7%54%
1	N	560	47% 44%11%45%
1	O	560	38% 38%8%54%
1	P	560	37% 39%7%54%
1	Q	560	47% 44%12%45%
1	R	560	38% 38%8%54%
1	S	560	38% 38%8%54%
1	T	560	47% 44%11%45%
1	U	560	38% 36%10%54%
1	V	560	38% 38%8%54%
1	W	560	47% 45%10%45%
1	X	560	38% 37%9%54%
1	Y	560	38% 37%9%54%
1	Z	560	47% 45%10%45%
1	a	560	37% 36%10%54%
1	b	560	38% 38%8%54%
1	c	560	47% 46%9%45%

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Mol	Chain	Length	Quality of chain
1	d	560	38% 8% 54%
1	e	560	38% 7% 54%
1	f	560	47% 12% 45%
1	g	560	38% 10% 54%

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 69498 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
1	A	257	Total	C	N	O	S	1	0
			1977	1212	365	396	4		
1	B	309	Total	C	N	O	S	1	0
			2363	1454	437	467	5		
1	C	257	Total	C	N	O	S	1	0
			1978	1213	365	396	4		
1	D	257	Total	C	N	O	S	1	0
			1977	1212	365	396	4		
1	E	309	Total	C	N	O	S	1	0
			2363	1454	437	467	5		
1	F	257	Total	C	N	O	S	1	0
			1978	1213	365	396	4		
1	G	257	Total	C	N	O	S	1	0
			1977	1212	365	396	4		
1	H	309	Total	C	N	O	S	1	0
			2363	1454	437	467	5		
1	I	257	Total	C	N	O	S	1	0
			1978	1213	365	396	4		
1	J	257	Total	C	N	O	S	1	0
			1977	1212	365	396	4		
1	K	309	Total	C	N	O	S	1	0
			2363	1454	437	467	5		
1	L	257	Total	C	N	O	S	1	0
			1978	1213	365	396	4		
1	M	257	Total	C	N	O	S	1	0
			1977	1212	365	396	4		
1	N	309	Total	C	N	O	S	1	0
			2363	1454	437	467	5		
1	O	257	Total	C	N	O	S	1	0
			1978	1213	365	396	4		
1	P	257	Total	C	N	O	S	1	0
			1977	1212	365	396	4		
1	Q	309	Total	C	N	O	S	1	0
			2363	1454	437	467	5		

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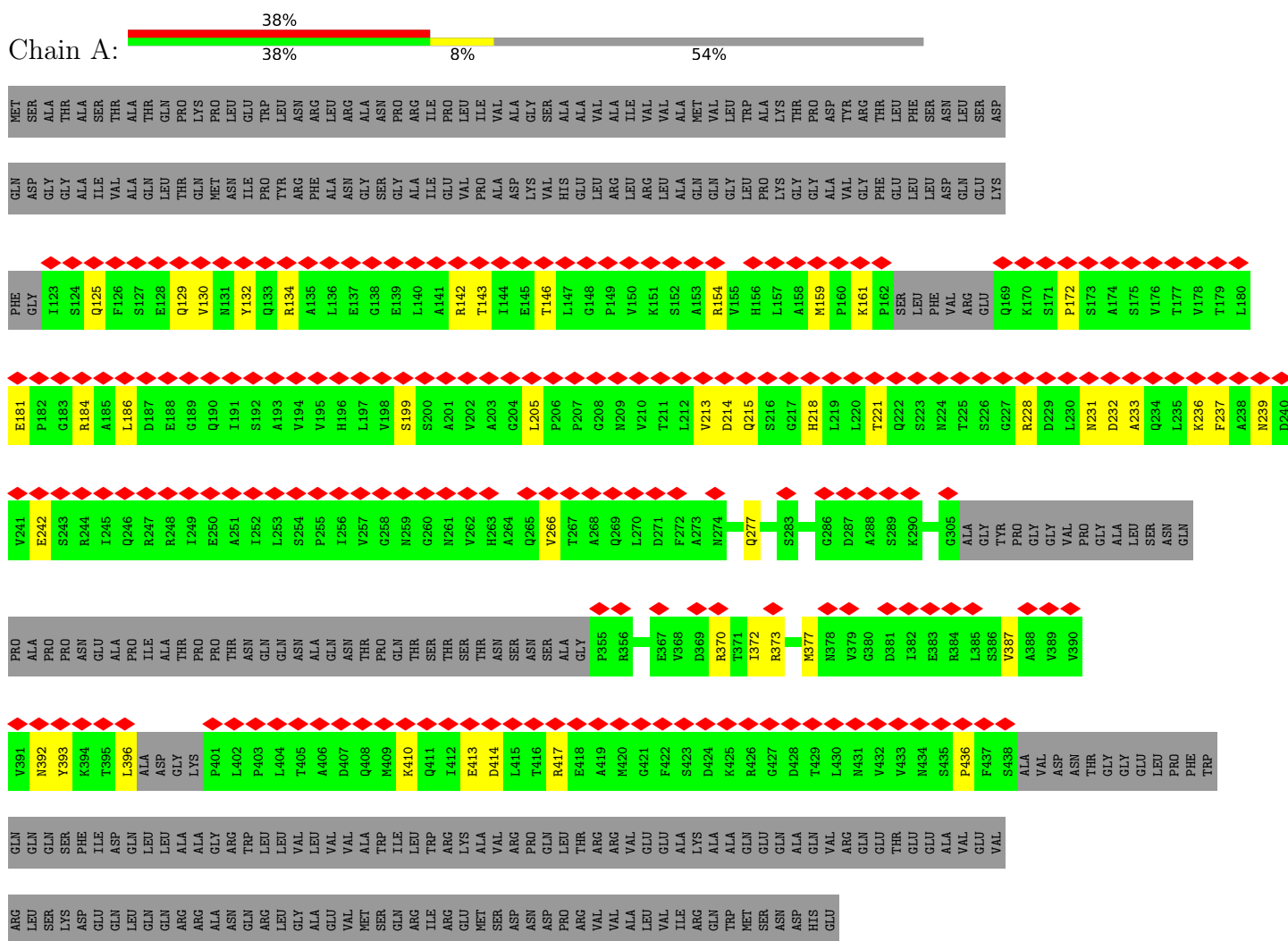
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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	257	Total	C	N	O	S	1	0
			1978	1213	365	396	4		
1	S	257	Total	C	N	O	S	1	0
			1977	1212	365	396	4		
1	T	309	Total	C	N	O	S	1	0
			2363	1454	437	467	5		
1	U	257	Total	C	N	O	S	1	0
			1978	1213	365	396	4		
1	V	257	Total	C	N	O	S	1	0
			1977	1212	365	396	4		
1	W	309	Total	C	N	O	S	1	0
			2363	1454	437	467	5		
1	X	257	Total	C	N	O	S	1	0
			1978	1213	365	396	4		
1	Y	257	Total	C	N	O	S	1	0
			1977	1212	365	396	4		
1	Z	309	Total	C	N	O	S	1	0
			2363	1454	437	467	5		
1	a	257	Total	C	N	O	S	1	0
			1978	1213	365	396	4		
1	b	257	Total	C	N	O	S	1	0
			1977	1212	365	396	4		
1	c	309	Total	C	N	O	S	1	0
			2363	1454	437	467	5		
1	d	257	Total	C	N	O	S	1	0
			1978	1213	365	396	4		
1	e	257	Total	C	N	O	S	1	0
			1977	1212	365	396	4		
1	f	309	Total	C	N	O	S	1	0
			2363	1454	437	467	5		
1	g	257	Total	C	N	O	S	1	0
			1978	1213	365	396	4		

3 Residue-property plots

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

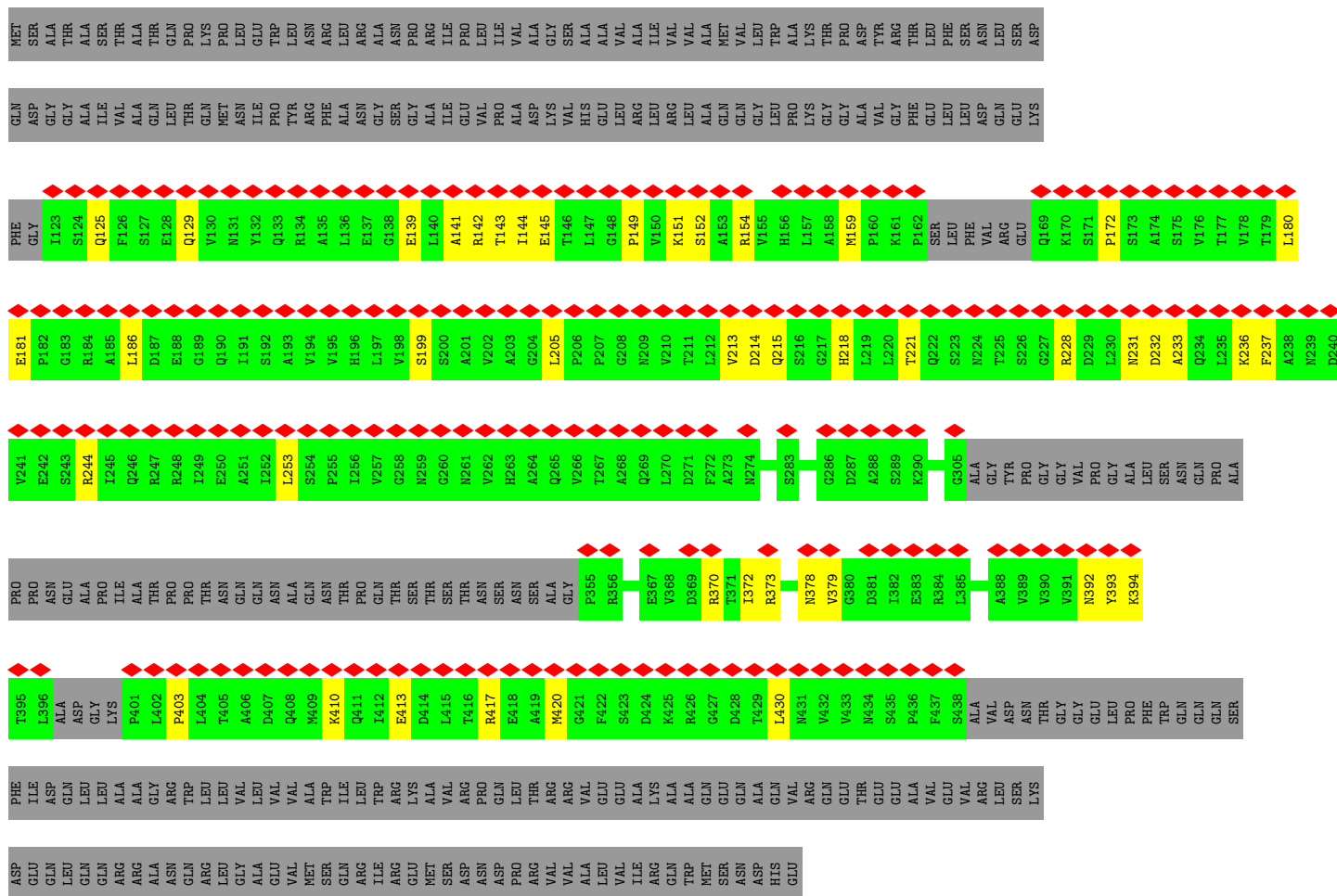
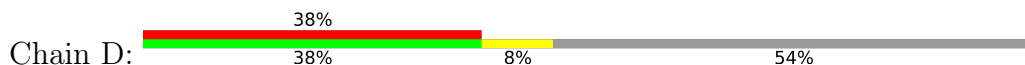
• Molecule 1: Flagellar M-ring protein



• Molecule 1: Flagellar M-ring protein

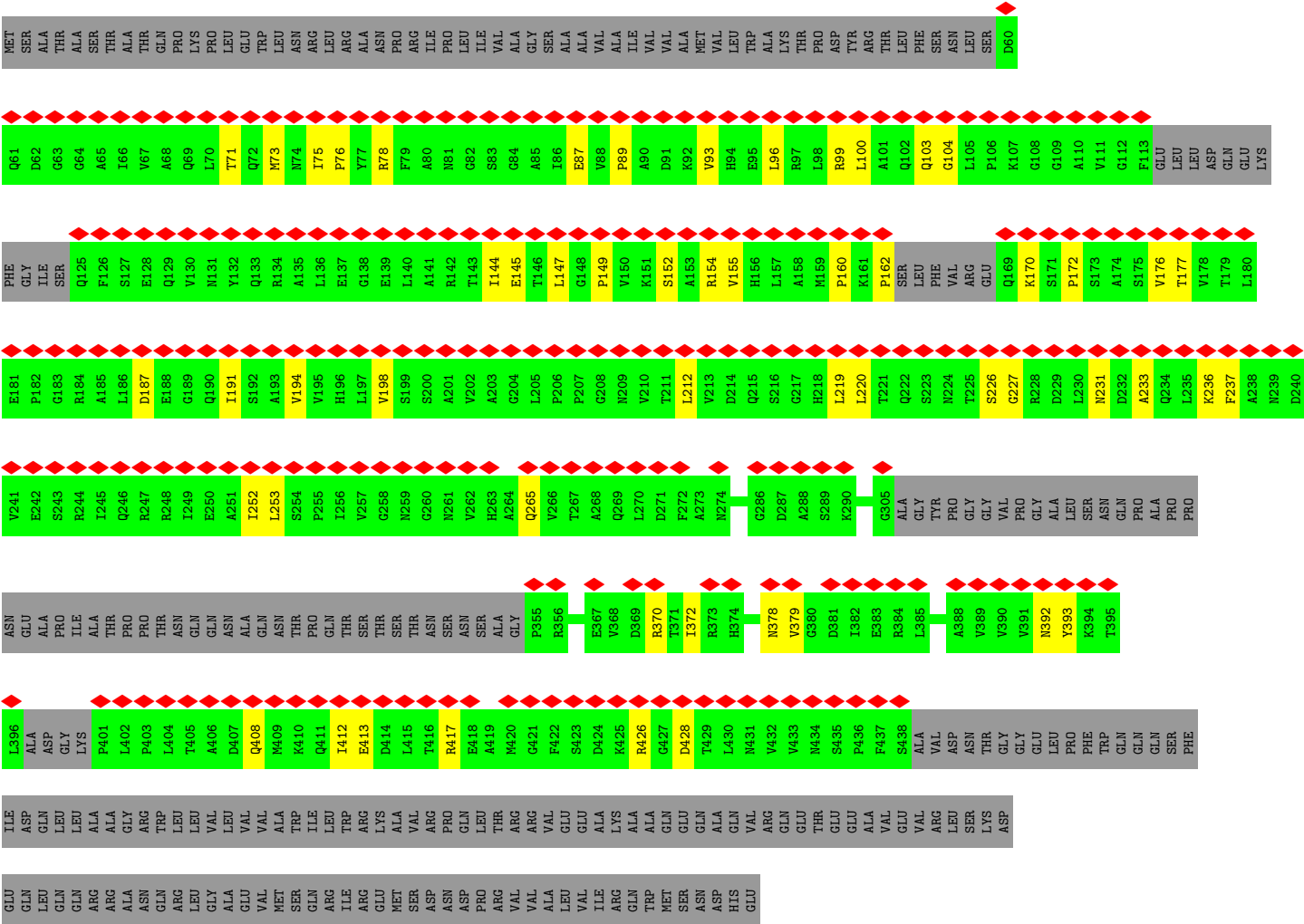


- Molecule 1: Flagellar M-ring protein

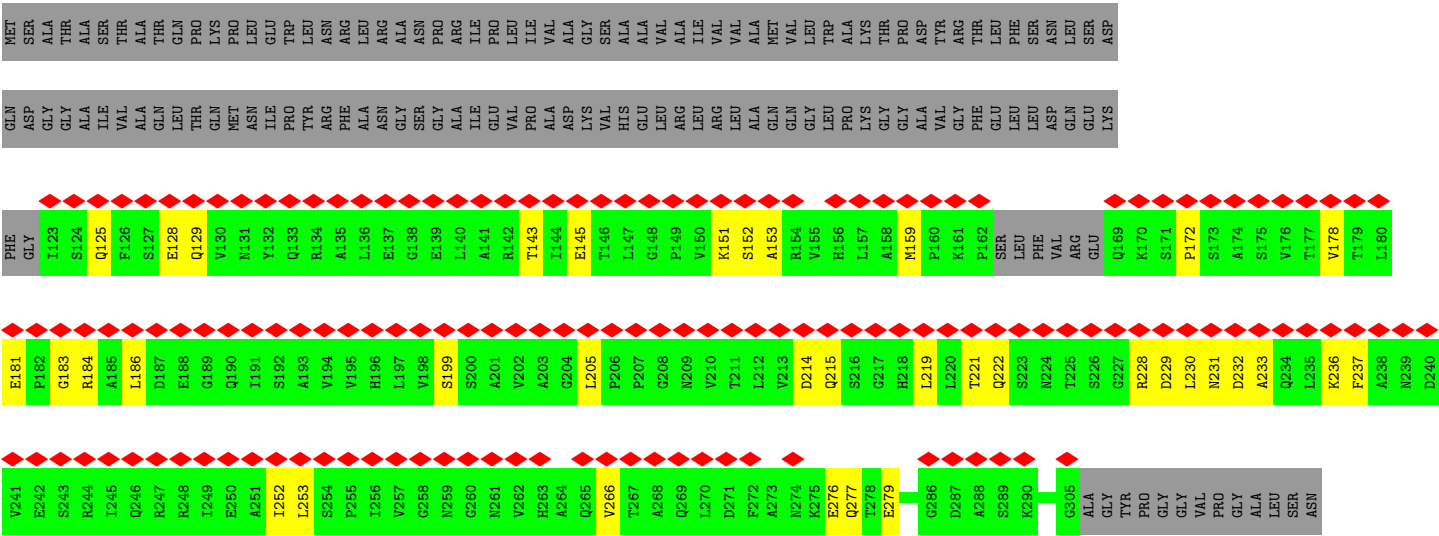
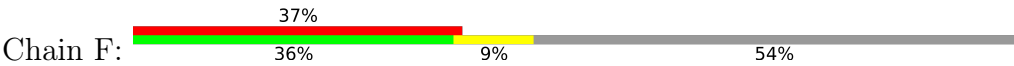


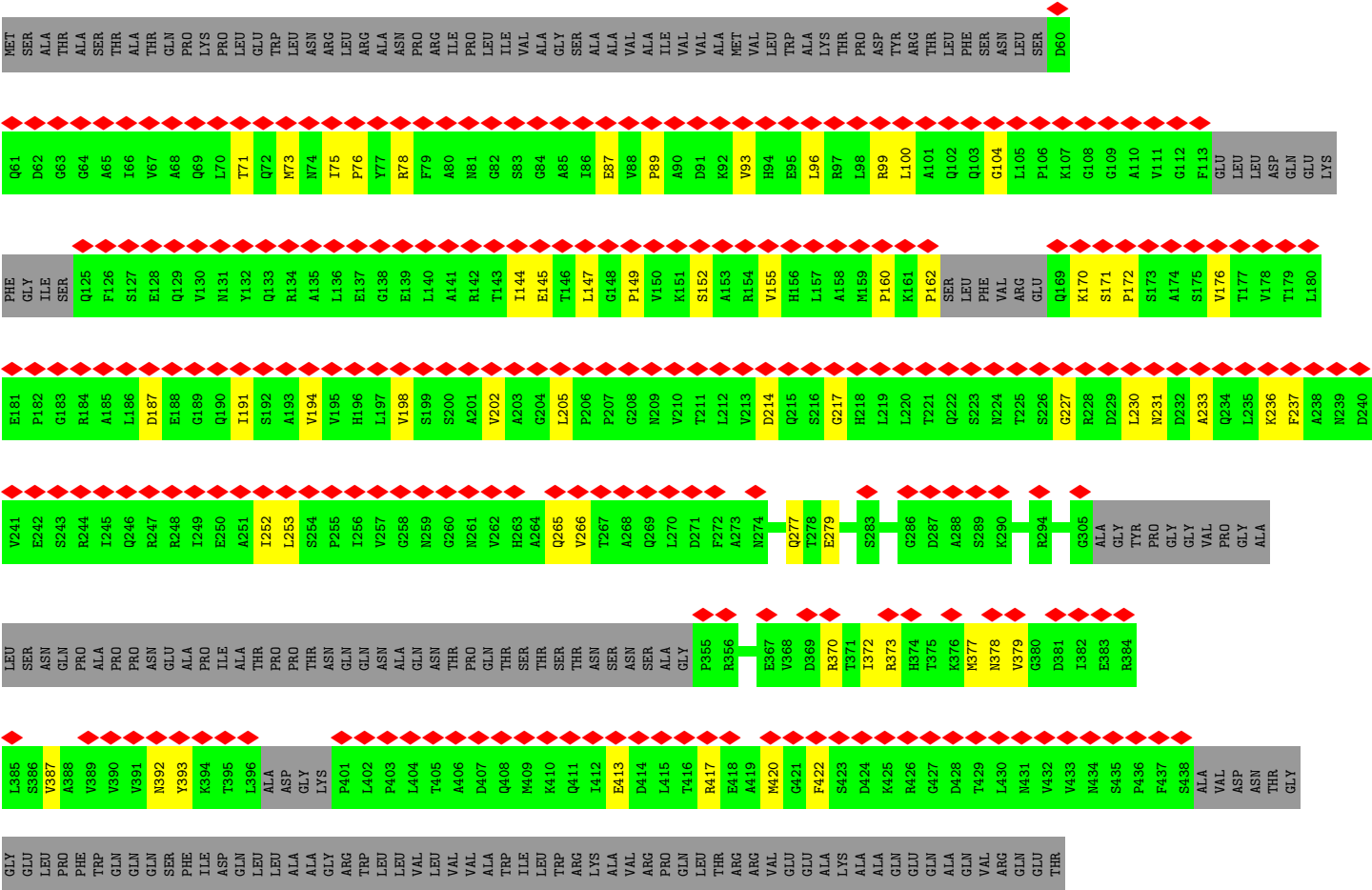
- Molecule 1: Flagellar M-ring protein



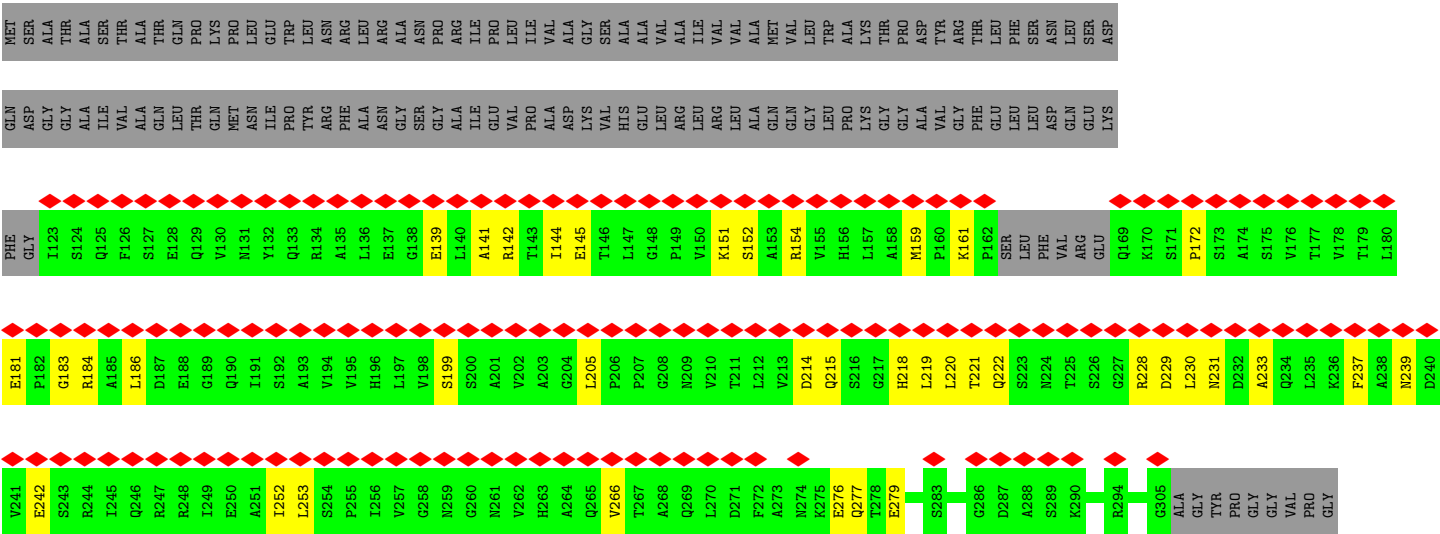
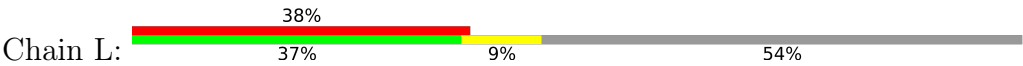


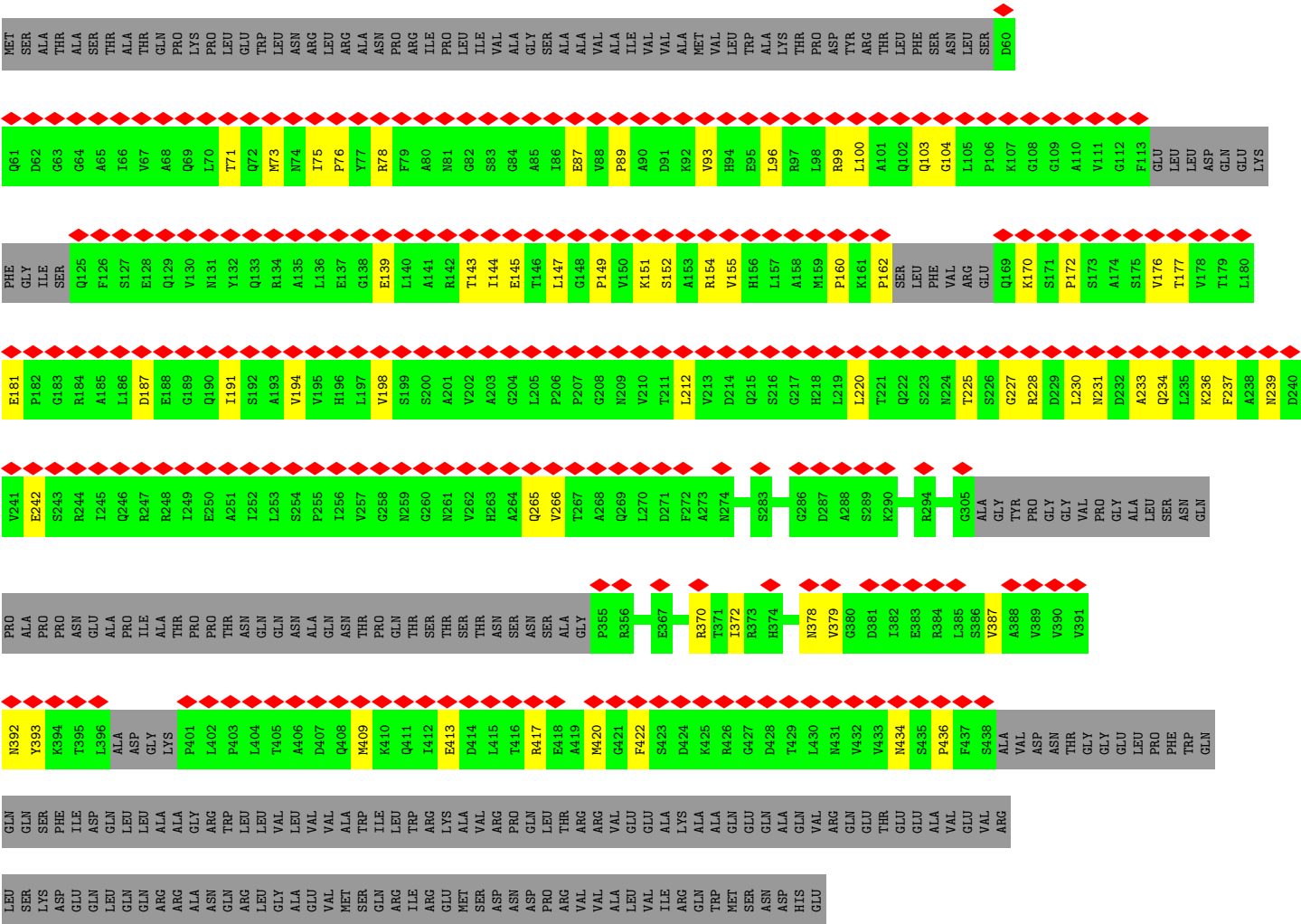
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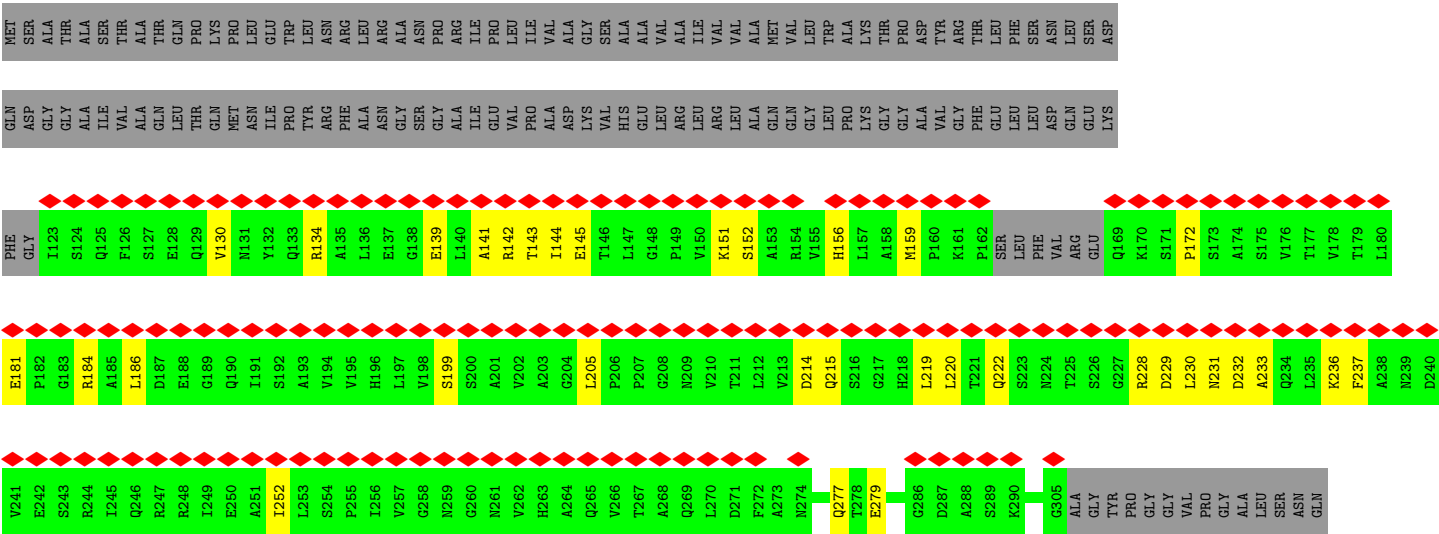
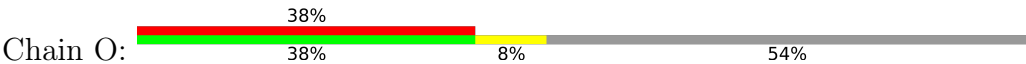


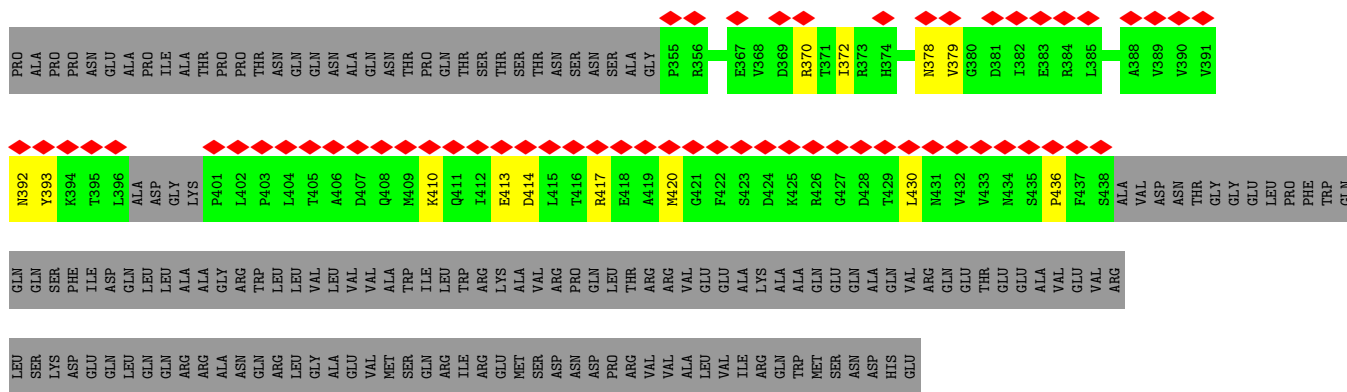
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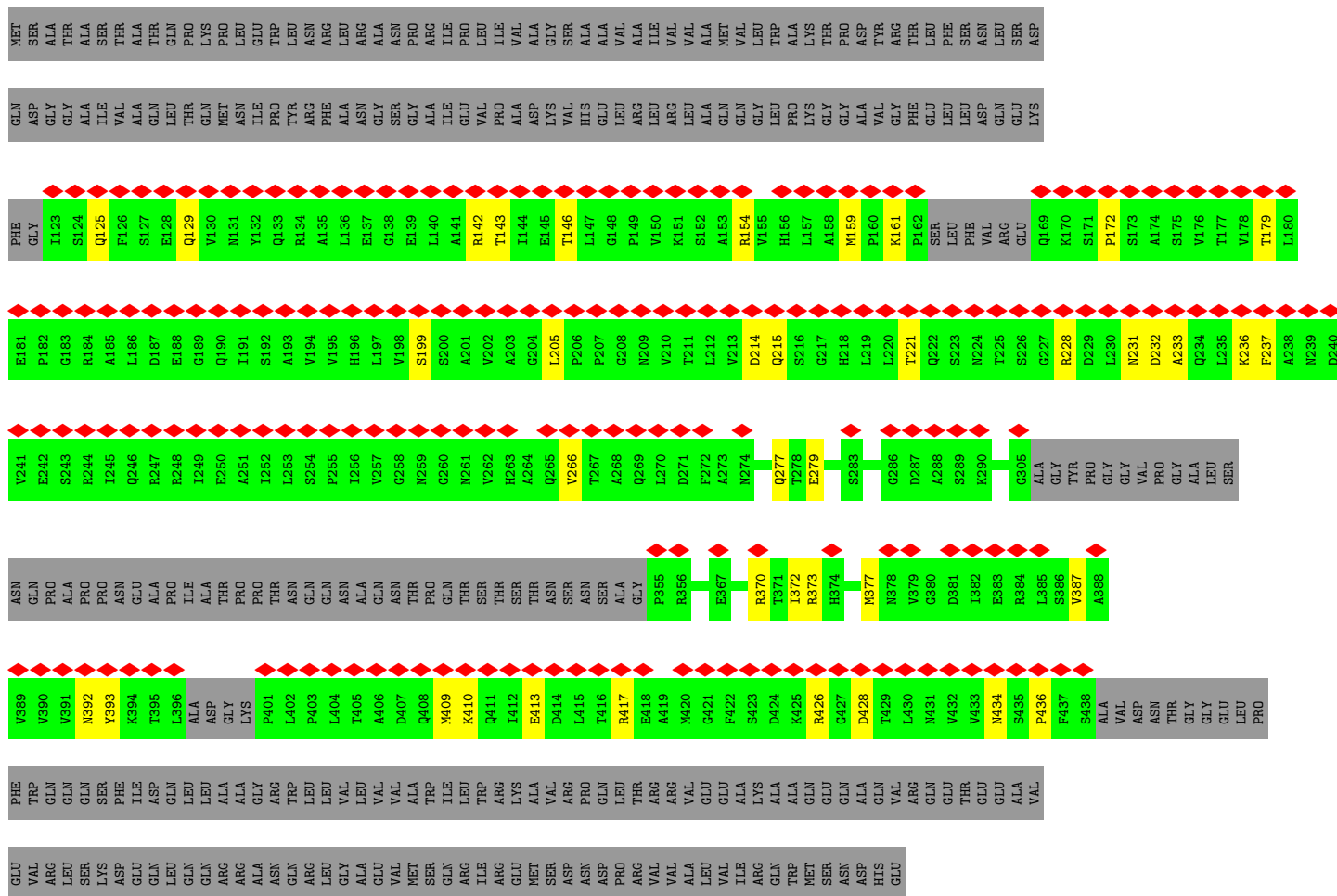
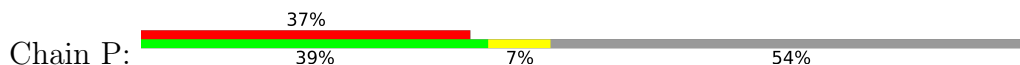


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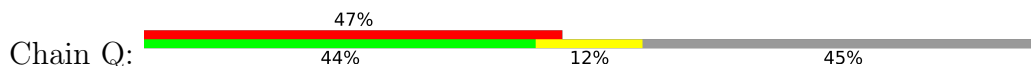


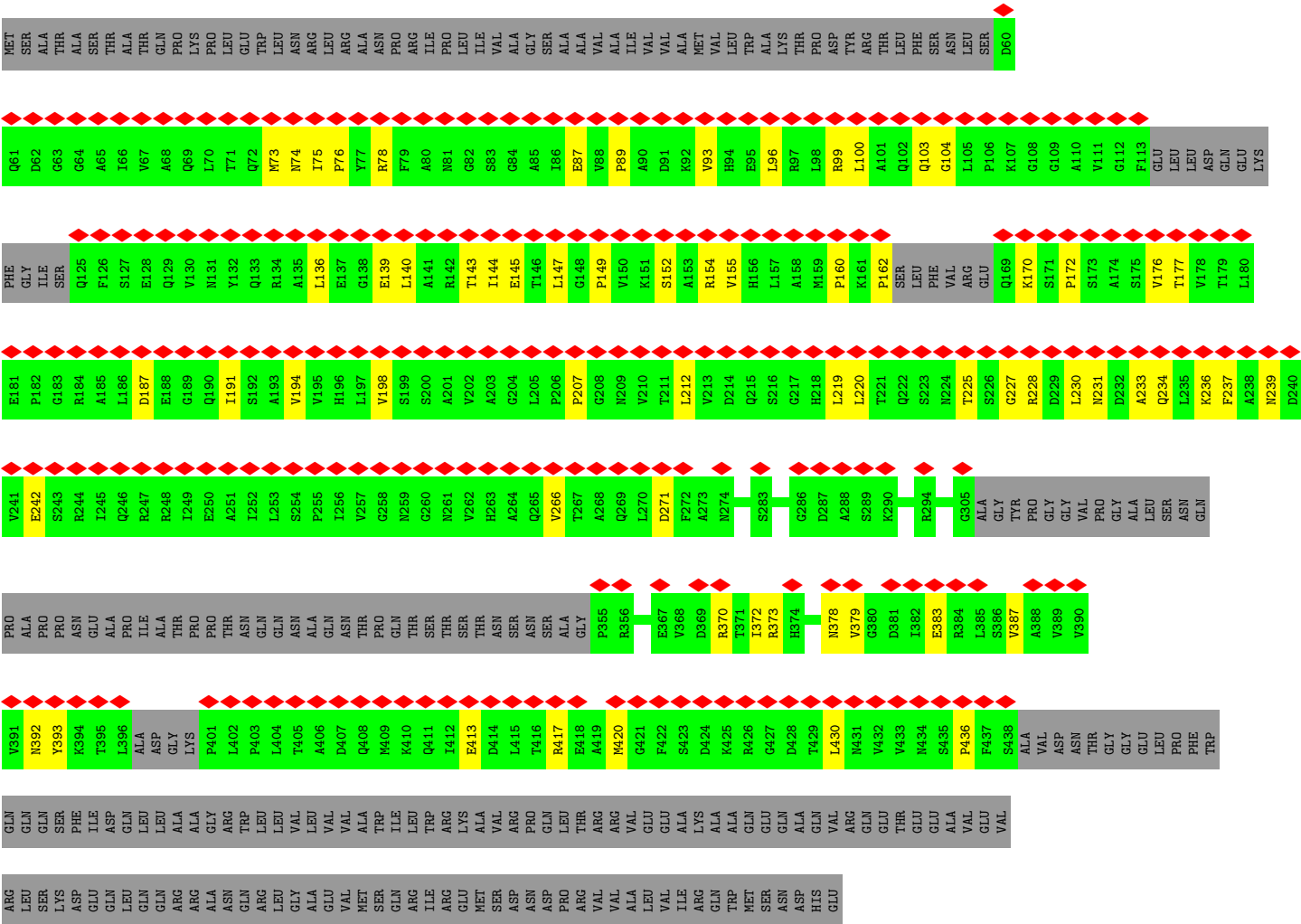


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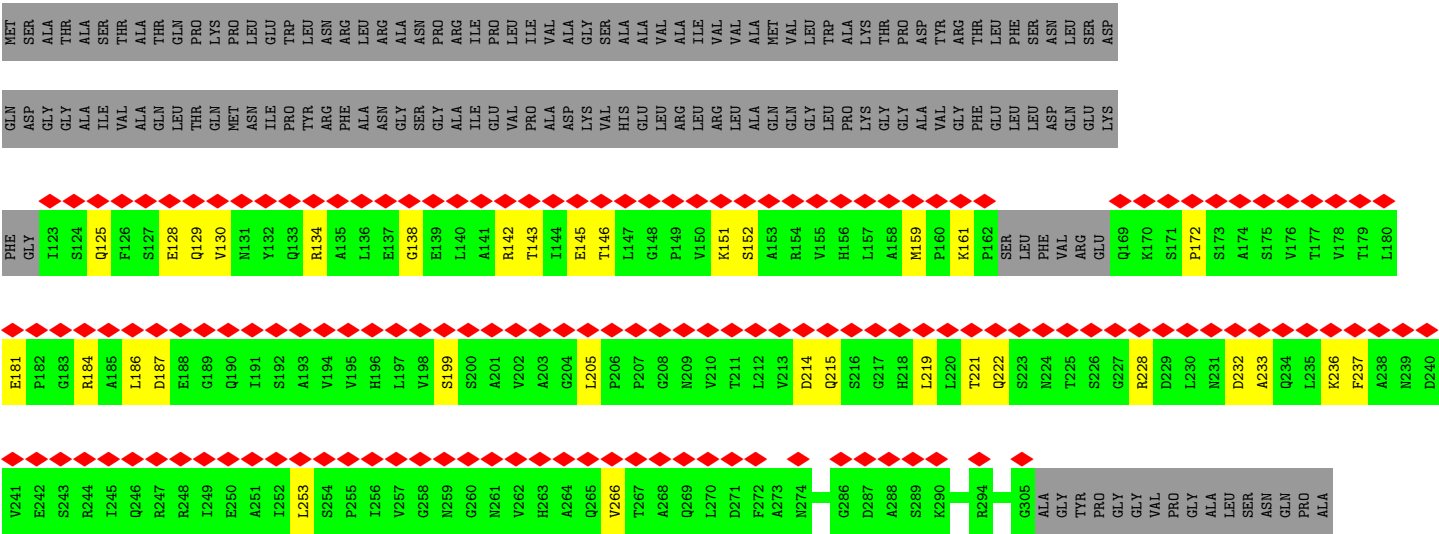
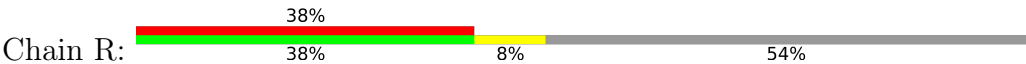


- Molecule 1: Flagellar M-ring protein

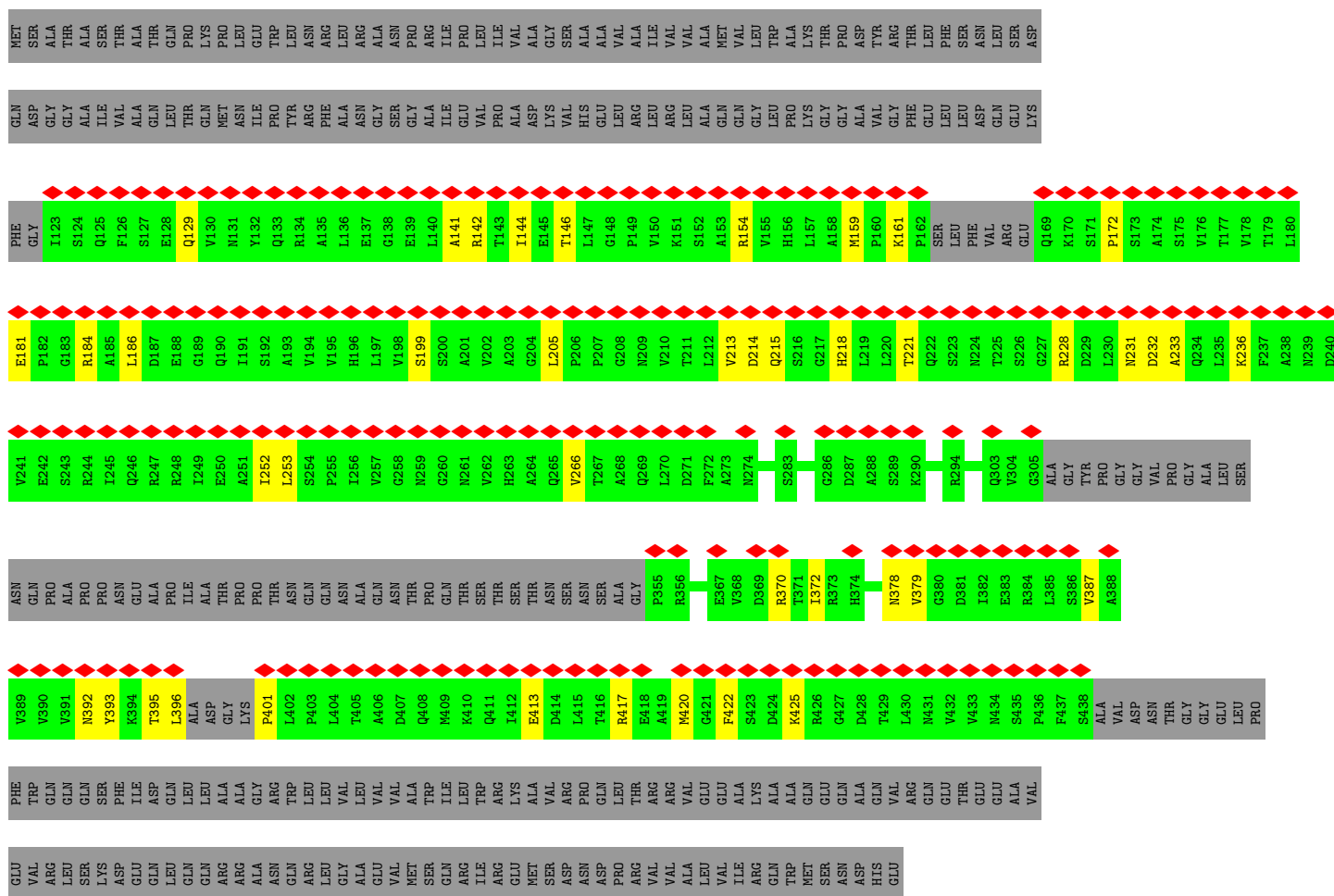
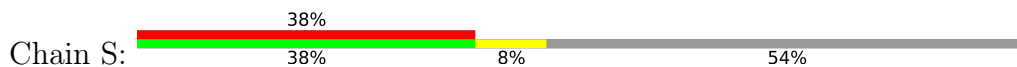




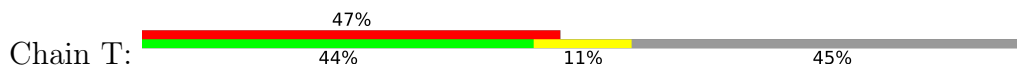
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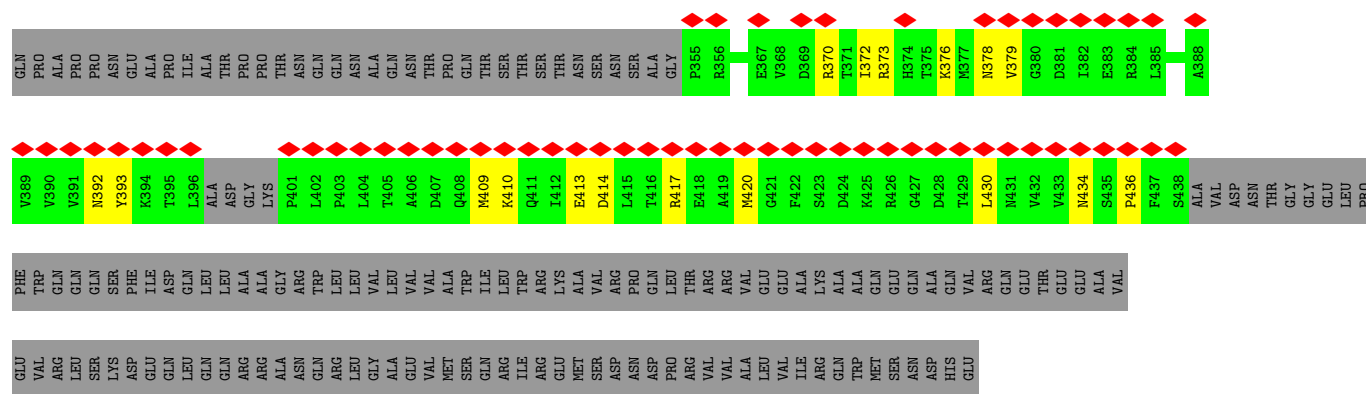


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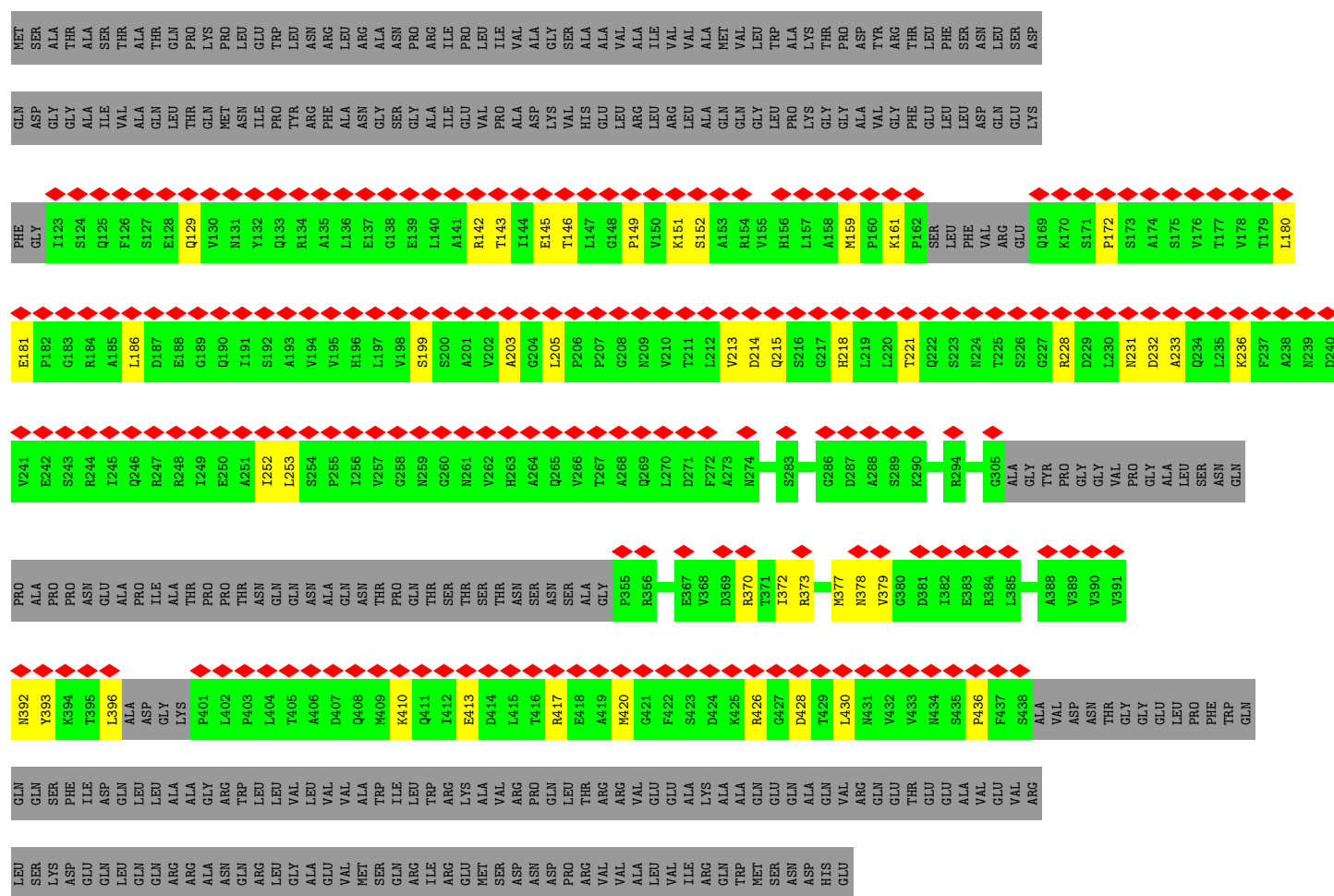
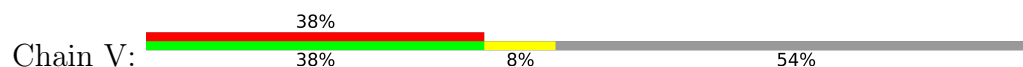


- Molecule 1: Flagellar M-ring protein



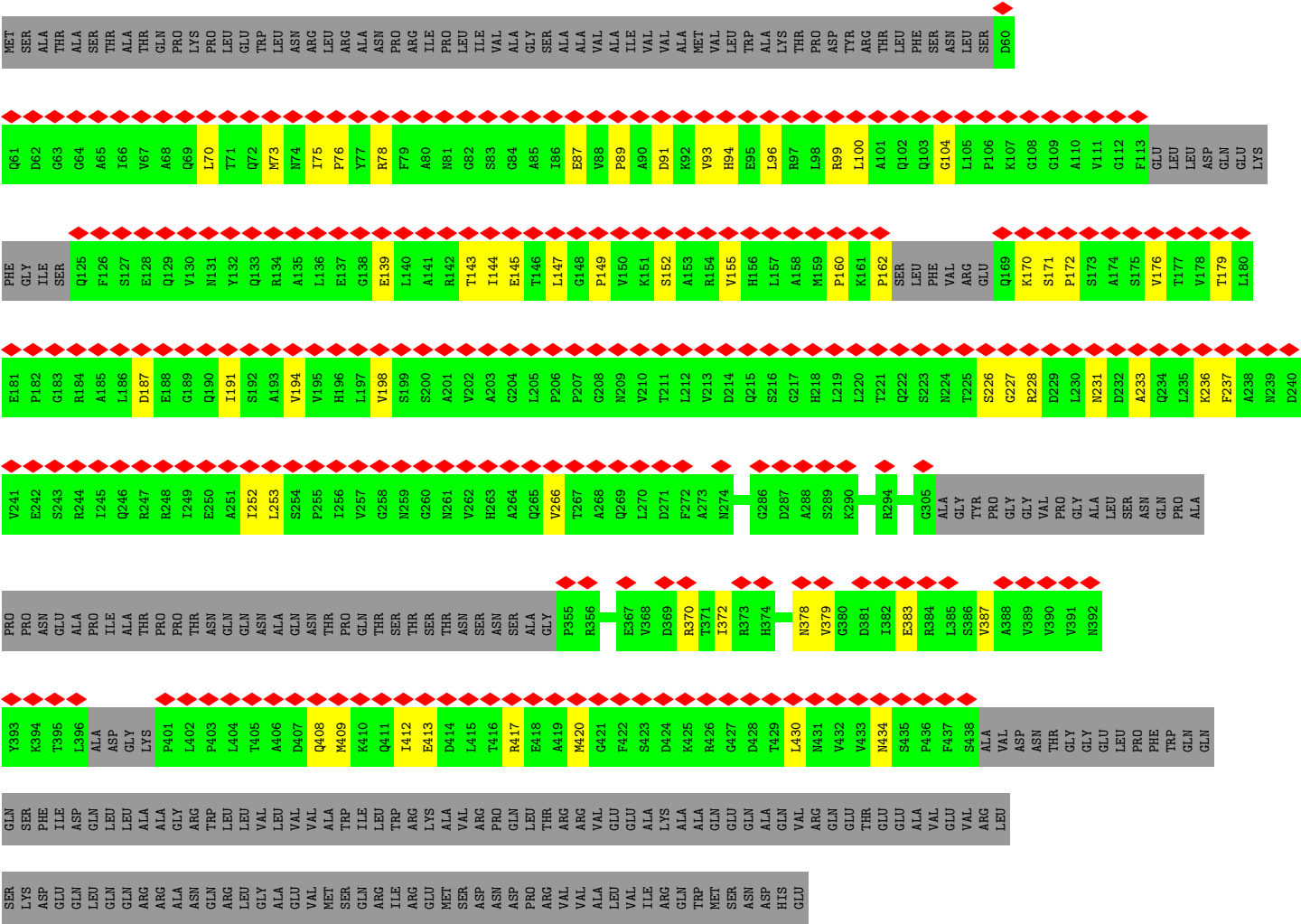


• Molecule 1: Flagellar M-ring protein

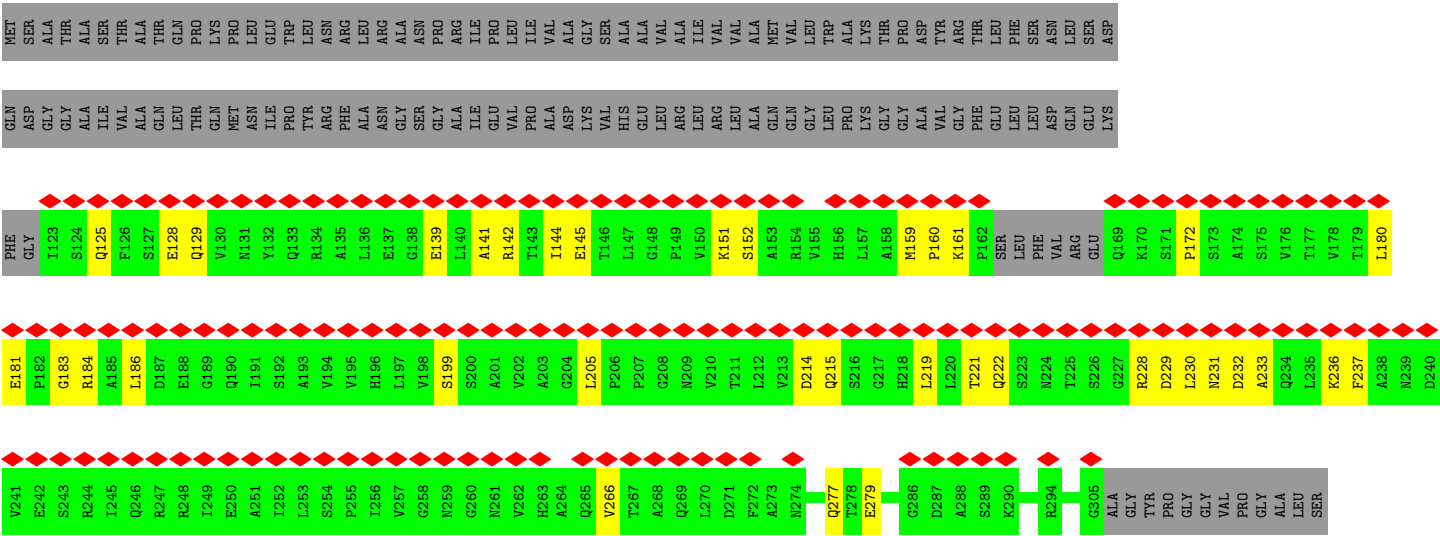
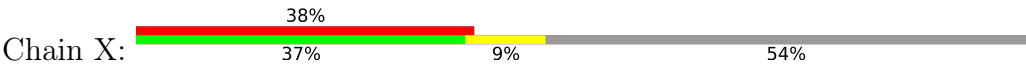


• Molecule 1: Flagellar M-ring protein



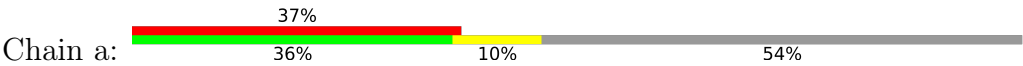


● Molecule 1: Flagellar M-ring protein



LEU	SER	LYS	ASP	GLU	GLN	LEU	LEU	GLN	ARG	ARG	ALA	GLY	ARG	TRP	LEU	GLY	GLU	GLU	VAL	VAL	MET	SER	GLN	ILE	TRP	ARG	LYS	ALA	VAL	VAL	GLY	PRO	ARG	THR	PRO	ILE	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL</
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● Molecule 1: Flagellar M-ring protein



V241	E242	S243	R244	T245	Q246	R247	R248	T249	E250	A251	T252	L253	S254	P255	T256	V257	G258	N259	G260	N261	V262	H263	A264	Q265	V266	T267	A268	Q269	L270	D271	F272	A273	N274	K275	E276	Q277	T278	E279	G286	D287	A288	S289	K290	G305	ALA	GLY	TYR	PRO	GLY	GLY	VAL	PRO	GLY	ALA	LEU	SER	ASN					
E181	P182	G183	R184	A185	L186	D187	E188	G189	Q190	I191	S192	A193	V194	V195	H196	L197	V198	S199	S200	A201	V202	A203	G204	L205	P206	P207	G208	N209	V210	T211	L212	V213	D214	Q215	S216	G217	H218	L219	L220	T221	Q222	S223	N224	T225	S226	Q227	R228	D229	L230	N231	D232	A233	Q234	L235	K236	F237	A238	N239	D240			
GLN	ASP	GLY	GLY	ALA	ILE	VAL	THR	GLN	LEU	THR	GLN	PRO	ASN	ASN	ARG	GLY	SER	ASN	GLY	ILE	ILE	GLU	VAL	PRO	ILE	VAL	GLY	VAL	ARG	LEU	K161	S152	A153	R154	V155	H156	L157	A158	M159	P160	K161	P162	SER	LEU	PHE	VAL	ARG	GLU	Q169	K170	S171	P172	S173	A174	S175	V176	T177	V178	T179	L180		
MET	SER	ALA	THR	ALA	SER	THR	ALA	THR	GLN	PRO	LYS	PRO	LEU	GLN	LYS	TRP	LEU	ASN	ARG	LEU	ARG	ALA	ASN	ARG	ALA	ILE	ILE	PRO	ARG	ALA	ILE	LEU	K151	S152	A153	R154	V155	H156	L157	A158	M159	P160	K161	P162	SER	LEU	PHE	VAL	ARG	GLU	Q169	K170	S171	P172	S173	A174	S175	V176	T177	V178	T179	L180
ASP	SER	THR	THR	SER	THR	ALA	GLN	THR	LEU	GLN	THR	PRO	ILE	ASN	LEU	GLY	ALA	ASN	ALA	PHE	ARG	LEU	GLY	VAL	LEU	ILE	PRO	VAL	GLU	HIS	VAL	VAL	LEU	S152	A153	R154	V155	H156	L157	A158	M159	P160	K161	P162	SER	LEU	PHE	VAL	ARG	GLU	Q169	K170	S171	P172	S173	A174	S175	V176	T177	V178	T179	L180
ASP	SER	THR	THR	SER	THR	ALA	GLN	THR	LEU	GLN	THR	PRO	ILE	ASN	LEU	GLY	ALA	ASN	ALA	PHE	ARG	LEU	GLY	VAL	LEU	ILE	PRO	VAL	GLU	HIS	VAL	VAL	LEU	S152	A153	R154	V155	H156	L157	A158	M159	P160	K161	P162	SER	LEU	PHE	VAL	ARG	GLU	Q169	K170	S171	P172	S173	A174	S175	V176	T177	V178	T179	L180

[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C11	Depositor
Number of particles used	70250	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	50000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.052	Depositor
Minimum map value	-0.013	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	400.0, 400.0, 400.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	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	0.19	0/2005	0.40	0/2713
1	B	0.18	0/2397	0.38	0/3242
1	C	0.20	0/2006	0.43	0/2715
1	D	0.19	0/2005	0.42	0/2713
1	E	0.18	0/2397	0.37	0/3242
1	F	0.20	0/2006	0.41	0/2715
1	G	0.19	0/2005	0.43	0/2713
1	H	0.19	0/2397	0.39	0/3242
1	I	0.19	0/2006	0.43	0/2715
1	J	0.19	0/2005	0.39	0/2713
1	K	0.18	0/2397	0.38	0/3242
1	L	0.20	0/2006	0.41	0/2715
1	M	0.19	0/2005	0.43	0/2713
1	N	0.19	0/2397	0.38	0/3242
1	O	0.19	0/2006	0.39	0/2715
1	P	0.20	0/2005	0.41	0/2713
1	Q	0.18	0/2397	0.39	0/3242
1	R	0.20	0/2006	0.40	0/2715
1	S	0.19	0/2005	0.40	0/2713
1	T	0.18	0/2397	0.38	0/3242
1	U	0.19	0/2006	0.41	0/2715
1	V	0.19	0/2005	0.43	0/2713
1	W	0.18	0/2397	0.38	0/3242
1	X	0.20	0/2006	0.42	0/2715
1	Y	0.20	0/2005	0.43	0/2713
1	Z	0.18	0/2397	0.38	0/3242
1	a	0.20	0/2006	0.42	0/2715
1	b	0.19	0/2005	0.40	0/2713
1	c	0.18	0/2397	0.39	0/3242
1	d	0.20	0/2006	0.41	0/2715
1	e	0.19	0/2005	0.39	0/2713
1	f	0.18	0/2397	0.38	0/3242
1	g	0.19	0/2006	0.41	0/2715
All	All	0.19	0/70488	0.40	0/95370

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

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	1977	0	1969	37	0
1	B	2363	0	2356	41	0
1	C	1978	0	1973	40	0
1	D	1977	0	1969	37	0
1	E	2363	0	2356	35	0
1	F	1978	0	1973	39	0
1	G	1977	0	1969	33	0
1	H	2363	0	2356	41	0
1	I	1978	0	1973	35	0
1	J	1977	0	1969	30	0
1	K	2363	0	2356	40	0
1	L	1978	0	1973	40	0
1	M	1977	0	1969	33	0
1	N	2363	0	2356	42	0
1	O	1978	0	1973	34	0
1	P	1977	0	1969	34	0
1	Q	2363	0	2356	44	0
1	R	1978	0	1973	33	0
1	S	1977	0	1969	26	0
1	T	2363	0	2356	42	0
1	U	1978	0	1973	38	0
1	V	1977	0	1969	35	0
1	W	2363	0	2356	37	0
1	X	1978	0	1973	37	0
1	Y	1977	0	1969	40	0
1	Z	2363	0	2356	39	0
1	a	1978	0	1973	40	0
1	b	1977	0	1969	34	0
1	c	2363	0	2356	36	0
1	d	1978	0	1973	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	e	1977	0	1969	34	0
1	f	2363	0	2356	47	0
1	g	1978	0	1973	44	0
All	All	69498	0	69278	1101	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 (1101) 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:M:151:LYS:HZ2	1:M:181:GLU:HA	1.38	0.88
1:a:151:LYS:HZ2	1:a:181:GLU:HA	1.42	0.83
1:d:154:ARG:HH22	1:e:143:THR:HA	1.44	0.83
1:X:151:LYS:HZ2	1:X:181:GLU:HA	1.45	0.82
1:I:151:LYS:HZ2	1:I:181:GLU:HA	1.43	0.82
1:D:151:LYS:HZ2	1:D:181:GLU:HA	1.46	0.80
1:G:151:LYS:HZ2	1:G:181:GLU:HA	1.46	0.79
1:H:145:GLU:HG3	1:H:152:SER:HA	1.65	0.78
1:U:151:LYS:HZ2	1:U:181:GLU:HA	1.48	0.78
1:e:154:ARG:HD3	1:g:142:ARG:HH12	1.47	0.77
1:Y:151:LYS:HZ2	1:Y:181:GLU:HA	1.50	0.76
1:V:151:LYS:HZ2	1:V:181:GLU:HA	1.51	0.76
1:d:151:LYS:HZ2	1:d:181:GLU:HA	1.51	0.76
1:f:227:GLY:HA2	1:g:233:ALA:HB1	1.68	0.76
1:Y:154:ARG:HD3	1:a:142:ARG:HH12	1.51	0.75
1:g:151:LYS:HZ2	1:g:181:GLU:HA	1.50	0.75
1:d:277:GLN:NE2	1:d:279:GLU:OE2	2.20	0.75
1:U:277:GLN:NE2	1:U:279:GLU:OE2	2.21	0.74
1:g:277:GLN:NE2	1:g:279:GLU:OE2	2.21	0.73
1:N:227:GLY:HA2	1:O:233:ALA:HB1	1.69	0.73
1:B:227:GLY:HA2	1:C:233:ALA:HB1	1.71	0.73
1:L:277:GLN:NE2	1:L:279:GLU:OE2	2.20	0.73
1:Y:213:VAL:HG22	1:Y:218:HIS:HB2	1.71	0.73
1:a:277:GLN:NE2	1:a:279:GLU:OE2	2.21	0.73
1:C:154:ARG:NH1	1:D:143:THR:OG1	2.22	0.73
1:P:409:MET:HE1	1:P:434:ASN:HB2	1.71	0.72
1:O:277:GLN:NE2	1:O:279:GLU:OE2	2.21	0.72
1:Z:227:GLY:HA2	1:a:233:ALA:HB1	1.70	0.72
1:Q:227:GLY:HA2	1:R:233:ALA:HB1	1.70	0.72
1:b:213:VAL:HG22	1:b:218:HIS:HB2	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:151:LYS:HZ3	1:L:181:GLU:HA	1.53	0.72
1:S:154:ARG:NH1	1:U:143:THR:OG1	2.22	0.72
1:S:213:VAL:HG22	1:S:218:HIS:HB2	1.72	0.71
1:K:227:GLY:HA2	1:L:233:ALA:HB1	1.72	0.71
1:L:181:GLU:OE1	1:L:184:ARG:NH2	2.21	0.71
1:L:154:ARG:NH1	1:M:143:THR:OG1	2.23	0.71
1:Y:277:GLN:NE2	1:Y:279:GLU:OE2	2.23	0.71
1:P:154:ARG:NH2	1:R:146:THR:OG1	2.24	0.70
1:C:151:LYS:HZ2	1:C:181:GLU:HA	1.55	0.70
1:P:277:GLN:NE2	1:P:279:GLU:OE2	2.23	0.70
1:I:420:MET:HE1	1:I:430:LEU:HD13	1.74	0.70
1:e:154:ARG:HD3	1:g:142:ARG:NH1	2.06	0.70
1:F:277:GLN:NE2	1:F:279:GLU:OE2	2.22	0.69
1:E:227:GLY:HA2	1:F:233:ALA:HB1	1.73	0.69
1:H:227:GLY:HA2	1:I:233:ALA:HB1	1.73	0.69
1:T:409:MET:HE1	1:T:434:ASN:HB2	1.75	0.69
1:X:277:GLN:NE2	1:X:279:GLU:OE2	2.21	0.69
1:R:409:MET:HE1	1:R:434:ASN:HB2	1.73	0.68
1:H:147:LEU:HG	1:H:149:PRO:HD2	1.75	0.68
1:K:277:GLN:NE2	1:K:279:GLU:OE2	2.24	0.68
1:W:147:LEU:HG	1:W:149:PRO:HD2	1.76	0.68
1:W:227:GLY:HA2	1:X:233:ALA:HB1	1.74	0.68
1:T:420:MET:HE1	1:T:430:LEU:HD13	1.76	0.68
1:I:154:ARG:NH1	1:J:143:THR:OG1	2.27	0.68
1:c:227:GLY:HA2	1:d:233:ALA:HB1	1.76	0.68
1:T:227:GLY:HA2	1:U:233:ALA:HB1	1.74	0.67
1:f:277:GLN:NE2	1:f:279:GLU:OE2	2.23	0.67
1:c:147:LEU:HG	1:c:149:PRO:HD2	1.77	0.67
1:H:94:HIS:CE1	1:H:146:THR:HB	2.30	0.67
1:U:420:MET:HE1	1:U:430:LEU:HD13	1.77	0.67
1:Y:154:ARG:HD3	1:a:142:ARG:NH1	2.10	0.67
1:F:181:GLU:OE1	1:F:184:ARG:NH2	2.25	0.67
1:C:277:GLN:NE2	1:C:279:GLU:OE2	2.24	0.66
1:B:147:LEU:HG	1:B:149:PRO:HD2	1.78	0.66
1:T:147:LEU:HG	1:T:149:PRO:HD2	1.78	0.66
1:A:143:THR:OG1	1:g:154:ARG:NH1	2.28	0.66
1:T:176:VAL:HG21	1:T:198:VAL:HG21	1.79	0.65
1:M:151:LYS:NZ	1:M:180:LEU:O	2.27	0.65
1:N:147:LEU:HG	1:N:149:PRO:HD2	1.78	0.65
1:Z:147:LEU:HG	1:Z:149:PRO:HD2	1.78	0.65
1:E:147:LEU:HG	1:E:149:PRO:HD2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:151:LYS:NZ	1:G:180:LEU:O	2.26	0.65
1:I:151:LYS:NZ	1:I:180:LEU:O	2.26	0.65
1:f:160:PRO:HD3	1:f:172:PRO:HB3	1.78	0.64
1:D:154:ARG:HH22	1:F:143:THR:HA	1.61	0.64
1:I:181:GLU:OE1	1:I:184:ARG:NH2	2.25	0.64
1:K:147:LEU:HG	1:K:149:PRO:HD2	1.78	0.64
1:f:147:LEU:HG	1:f:149:PRO:HD2	1.78	0.64
1:C:145:GLU:HG3	1:C:152:SER:HA	1.80	0.64
1:Q:147:LEU:HG	1:Q:149:PRO:HD2	1.79	0.64
1:d:181:GLU:OE1	1:d:184:ARG:NH2	2.24	0.64
1:U:154:ARG:NH1	1:V:143:THR:OG1	2.30	0.64
1:T:160:PRO:HD3	1:T:172:PRO:HB3	1.80	0.64
1:E:99:ARG:O	1:E:103:GLN:NE2	2.32	0.63
1:Q:73:MET:SD	1:Q:74:ASN:N	2.72	0.63
1:Z:100:LEU:O	1:Z:104:GLY:N	2.30	0.63
1:Z:160:PRO:HD3	1:Z:172:PRO:HB3	1.81	0.63
1:f:231:ASN:HB3	1:g:237:PHE:CE2	2.34	0.63
1:C:181:GLU:OE1	1:C:184:ARG:NH2	2.24	0.63
1:f:420:MET:HE1	1:f:430:LEU:HD13	1.80	0.63
1:K:231:ASN:HB3	1:L:237:PHE:CE2	2.33	0.63
1:F:151:LYS:HD2	1:F:181:GLU:HG2	1.81	0.63
1:a:154:ARG:NH1	1:b:143:THR:OG1	2.32	0.62
1:c:176:VAL:HG21	1:c:198:VAL:HG21	1.81	0.62
1:N:231:ASN:HB3	1:O:237:PHE:CE2	2.35	0.62
1:V:231:ASN:OD1	1:V:232:ASP:N	2.32	0.62
1:Z:231:ASN:HB3	1:a:237:PHE:CE2	2.34	0.62
1:B:99:ARG:O	1:B:103:GLN:NE2	2.32	0.62
1:P:154:ARG:CZ	1:R:143:THR:HA	2.30	0.62
1:W:176:VAL:HG21	1:W:198:VAL:HG21	1.82	0.62
1:Q:231:ASN:HB3	1:R:237:PHE:CE2	2.34	0.62
1:Q:100:LEU:O	1:Q:104:GLY:N	2.28	0.62
1:V:420:MET:HE1	1:V:430:LEU:HD13	1.80	0.62
1:Q:99:ARG:O	1:Q:103:GLN:NE2	2.32	0.62
1:H:99:ARG:O	1:H:103:GLN:NE2	2.33	0.62
1:N:99:ARG:O	1:N:103:GLN:NE2	2.32	0.62
1:c:160:PRO:HD3	1:c:172:PRO:HB3	1.82	0.62
1:E:160:PRO:HD3	1:E:172:PRO:HB3	1.82	0.62
1:T:99:ARG:O	1:T:103:GLN:NE2	2.33	0.62
1:U:221:THR:O	1:U:222:GLN:NE2	2.32	0.62
1:Z:99:ARG:O	1:Z:103:GLN:NE2	2.33	0.61
1:H:231:ASN:HB3	1:I:237:PHE:CE2	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:231:ASN:HB3	1:F:237:PHE:CE2	2.35	0.61
1:C:151:LYS:NZ	1:C:180:LEU:O	2.26	0.61
1:T:231:ASN:HB3	1:U:237:PHE:CE2	2.35	0.61
1:c:100:LEU:O	1:c:104:GLY:N	2.27	0.61
1:I:221:THR:O	1:I:222:GLN:NE2	2.34	0.60
1:E:145:GLU:HG3	1:E:152:SER:HA	1.82	0.60
1:K:145:GLU:HG3	1:K:152:SER:HA	1.82	0.60
1:f:100:LEU:O	1:f:104:GLY:N	2.28	0.60
1:H:176:VAL:HG21	1:H:198:VAL:HG21	1.82	0.60
1:d:221:THR:O	1:d:222:GLN:NE2	2.35	0.60
1:E:176:VAL:HG21	1:E:198:VAL:HG21	1.82	0.60
1:B:176:VAL:HG21	1:B:198:VAL:HG21	1.83	0.60
1:a:221:THR:O	1:a:222:GLN:NE2	2.35	0.60
1:c:145:GLU:HG3	1:c:152:SER:HA	1.82	0.60
1:H:100:LEU:O	1:H:104:GLY:N	2.31	0.60
1:X:151:LYS:NZ	1:X:181:GLU:HA	2.16	0.60
1:Z:155:VAL:HG22	1:Z:176:VAL:HG13	1.84	0.60
1:d:151:LYS:NZ	1:d:181:GLU:HA	2.16	0.60
1:N:160:PRO:HD3	1:N:172:PRO:HB3	1.84	0.60
1:R:221:THR:O	1:R:222:GLN:NE2	2.35	0.60
1:T:145:GLU:HG3	1:T:152:SER:HA	1.84	0.60
1:W:231:ASN:HB3	1:X:237:PHE:CE2	2.36	0.60
1:Z:145:GLU:HG3	1:Z:152:SER:HA	1.83	0.60
1:I:145:GLU:HG3	1:I:152:SER:HA	1.84	0.59
1:N:176:VAL:HG21	1:N:198:VAL:HG21	1.84	0.59
1:T:100:LEU:O	1:T:104:GLY:N	2.30	0.59
1:D:221:THR:O	1:D:228:ARG:NH2	2.35	0.59
1:W:160:PRO:HD3	1:W:172:PRO:HB3	1.84	0.59
1:B:100:LEU:O	1:B:104:GLY:N	2.31	0.59
1:B:160:PRO:HD3	1:B:172:PRO:HB3	1.84	0.59
1:D:151:LYS:NZ	1:D:181:GLU:HA	2.17	0.59
1:L:221:THR:O	1:L:222:GLN:NE2	2.35	0.59
1:X:221:THR:O	1:X:222:GLN:NE2	2.35	0.59
1:g:145:GLU:HG3	1:g:152:SER:HA	1.85	0.59
1:M:377:MET:HE3	1:M:377:MET:HA	1.84	0.59
1:F:221:THR:O	1:F:222:GLN:NE2	2.34	0.59
1:H:144:ILE:HD12	1:H:194:VAL:HG23	1.84	0.59
1:L:151:LYS:HD2	1:L:181:GLU:HG2	1.84	0.59
1:Q:176:VAL:HG21	1:Q:198:VAL:HG21	1.83	0.59
1:c:231:ASN:HB3	1:d:237:PHE:CE2	2.38	0.59
1:f:155:VAL:HG22	1:f:176:VAL:HG13	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:370:ARG:NH1	1:B:372:ILE:HD11	2.18	0.58
1:E:100:LEU:O	1:E:104:GLY:N	2.31	0.58
1:I:186:LEU:HD11	1:I:219:LEU:HD13	1.85	0.58
1:U:145:GLU:HG3	1:U:152:SER:HA	1.85	0.58
1:H:160:PRO:HD3	1:H:172:PRO:HB3	1.86	0.58
1:C:370:ARG:NH1	1:C:372:ILE:HD11	2.18	0.58
1:C:186:LEU:HD11	1:C:219:LEU:HD13	1.86	0.58
1:F:186:LEU:HD11	1:F:219:LEU:HD13	1.86	0.58
1:W:408:GLN:O	1:W:412:ILE:HG12	2.04	0.58
1:X:186:LEU:HD11	1:X:219:LEU:HD13	1.85	0.58
1:g:221:THR:O	1:g:222:GLN:NE2	2.35	0.58
1:O:139:GLU:HG2	1:O:142:ARG:HH22	1.68	0.58
1:g:370:ARG:NH1	1:g:372:ILE:HD11	2.19	0.58
1:F:370:ARG:NH1	1:F:372:ILE:HD11	2.19	0.58
1:W:145:GLU:HG3	1:W:152:SER:HA	1.84	0.58
1:Z:176:VAL:HG21	1:Z:198:VAL:HG21	1.85	0.58
1:f:370:ARG:NH1	1:f:372:ILE:HD11	2.19	0.58
1:Q:160:PRO:HD3	1:Q:172:PRO:HB3	1.86	0.58
1:P:377:MET:HE3	1:P:377:MET:HA	1.86	0.58
1:A:154:ARG:HH22	1:C:143:THR:HA	1.68	0.57
1:K:176:VAL:HG21	1:K:198:VAL:HG21	1.85	0.57
1:a:232:ASP:O	1:a:236:LYS:HG2	2.04	0.57
1:E:408:GLN:O	1:E:412:ILE:HG12	2.04	0.57
1:H:94:HIS:HE1	1:H:146:THR:HB	1.65	0.57
1:H:408:GLN:O	1:H:412:ILE:HG12	2.04	0.57
1:O:370:ARG:NH1	1:O:372:ILE:HD11	2.19	0.57
1:U:370:ARG:NH1	1:U:372:ILE:HD11	2.19	0.57
1:Y:151:LYS:NZ	1:Y:180:LEU:O	2.26	0.57
1:g:186:LEU:HD11	1:g:219:LEU:HD13	1.86	0.57
1:H:93:VAL:HA	1:H:96:LEU:HB3	1.85	0.57
1:N:100:LEU:O	1:N:104:GLY:N	2.29	0.57
1:F:231:ASN:HB3	1:G:237:PHE:CE2	2.39	0.57
1:L:228:ARG:HG3	1:M:233:ALA:HB1	1.86	0.57
1:O:231:ASN:HB3	1:P:237:PHE:CE2	2.40	0.57
1:X:370:ARG:NH1	1:X:372:ILE:HD11	2.19	0.57
1:G:370:ARG:NH1	1:G:372:ILE:HD11	2.20	0.57
1:K:370:ARG:NH1	1:K:372:ILE:HD11	2.19	0.57
1:Q:155:VAL:HG22	1:Q:176:VAL:HG13	1.86	0.57
1:R:370:ARG:NH1	1:R:372:ILE:HD11	2.19	0.57
1:I:370:ARG:NH1	1:I:372:ILE:HD11	2.19	0.57
1:N:155:VAL:HG22	1:N:176:VAL:HG13	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:151:LYS:HZ3	1:O:181:GLU:HG2	1.69	0.57
1:U:232:ASP:O	1:U:236:LYS:HG2	2.05	0.57
1:e:231:ASN:OD1	1:e:232:ASP:N	2.38	0.57
1:e:370:ARG:NH1	1:e:372:ILE:HD11	2.20	0.57
1:I:139:GLU:HG2	1:I:142:ARG:HH22	1.69	0.57
1:J:370:ARG:NH1	1:J:372:ILE:HD11	2.20	0.57
1:T:157:LEU:HD22	1:T:202:VAL:HG21	1.87	0.57
1:Y:370:ARG:NH1	1:Y:372:ILE:HD11	2.19	0.57
1:d:186:LEU:HD11	1:d:219:LEU:HD13	1.86	0.57
1:D:151:LYS:NZ	1:D:180:LEU:O	2.28	0.57
1:V:151:LYS:NZ	1:V:180:LEU:O	2.26	0.57
1:X:231:ASN:HB3	1:Y:237:PHE:CE2	2.39	0.57
1:H:370:ARG:NH1	1:H:372:ILE:HD11	2.19	0.57
1:Z:370:ARG:NH1	1:Z:372:ILE:HD11	2.19	0.56
1:a:231:ASN:HB3	1:b:237:PHE:CE2	2.40	0.56
1:b:231:ASN:OD1	1:b:232:ASP:N	2.38	0.56
1:b:370:ARG:NH1	1:b:372:ILE:HD11	2.20	0.56
1:A:377:MET:HE3	1:A:377:MET:HA	1.87	0.56
1:K:155:VAL:HG22	1:K:176:VAL:HG13	1.86	0.56
1:L:186:LEU:HD11	1:L:219:LEU:HD13	1.87	0.56
1:M:154:ARG:HH22	1:O:143:THR:HA	1.70	0.56
1:N:370:ARG:NH1	1:N:372:ILE:HD11	2.19	0.56
1:Q:145:GLU:HG3	1:Q:152:SER:HA	1.87	0.56
1:U:151:LYS:NZ	1:U:180:LEU:O	2.28	0.56
1:V:370:ARG:NH1	1:V:372:ILE:HD11	2.20	0.56
1:W:370:ARG:NH1	1:W:372:ILE:HD11	2.20	0.56
1:d:370:ARG:NH1	1:d:372:ILE:HD11	2.20	0.56
1:B:231:ASN:HB3	1:C:237:PHE:CE2	2.40	0.56
1:L:370:ARG:NH1	1:L:372:ILE:HD11	2.20	0.56
1:P:370:ARG:NH1	1:P:372:ILE:HD11	2.20	0.56
1:T:78:ARG:HB2	1:T:87:GLU:HB2	1.86	0.56
1:U:139:GLU:HG2	1:U:142:ARG:HH22	1.70	0.56
1:Y:231:ASN:OD1	1:Y:232:ASP:N	2.39	0.56
1:c:370:ARG:NH1	1:c:372:ILE:HD11	2.21	0.56
1:B:155:VAL:HG22	1:B:176:VAL:HG13	1.86	0.56
1:A:233:ALA:HB1	1:g:228:ARG:HG3	1.87	0.56
1:C:151:LYS:NZ	1:C:181:GLU:HA	2.19	0.56
1:G:413:GLU:OE2	1:G:417:ARG:NH2	2.39	0.56
1:M:221:THR:O	1:M:228:ARG:NH2	2.37	0.56
1:U:277:GLN:OE1	1:V:373:ARG:NH1	2.37	0.56
1:f:176:VAL:HG21	1:f:198:VAL:HG21	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:277:GLN:OE1	1:D:373:ARG:NH1	2.38	0.56
1:f:145:GLU:HG3	1:f:152:SER:HA	1.87	0.56
1:A:221:THR:O	1:A:228:ARG:NH2	2.38	0.56
1:K:100:LEU:O	1:K:104:GLY:N	2.29	0.56
1:M:370:ARG:NH1	1:M:372:ILE:HD11	2.20	0.56
1:Q:370:ARG:NH1	1:Q:372:ILE:HD11	2.20	0.56
1:T:73:MET:SD	1:T:99:ARG:NH1	2.79	0.56
1:g:232:ASP:O	1:g:236:LYS:HG2	2.06	0.56
1:A:237:PHE:CE2	1:g:231:ASN:HB3	2.40	0.56
1:E:370:ARG:NH1	1:E:372:ILE:HD11	2.21	0.56
1:d:232:ASP:O	1:d:236:LYS:HG2	2.06	0.56
1:A:373:ARG:NH1	1:g:277:GLN:OE1	2.39	0.56
1:G:231:ASN:OD1	1:G:232:ASP:N	2.38	0.56
1:G:275:LYS:HB2	1:G:377:MET:HE2	1.87	0.56
1:H:159:MET:HA	1:H:159:MET:HE3	1.88	0.56
1:R:232:ASP:O	1:R:236:LYS:HG2	2.06	0.56
1:A:370:ARG:NH1	1:A:372:ILE:HD11	2.21	0.55
1:I:232:ASP:O	1:I:236:LYS:HG2	2.06	0.55
1:T:133:GLN:HG3	1:T:157:LEU:HD11	1.88	0.55
1:T:370:ARG:NH1	1:T:372:ILE:HD11	2.21	0.55
1:d:277:GLN:OE1	1:e:373:ARG:NH1	2.38	0.55
1:C:231:ASN:HB3	1:D:237:PHE:CE2	2.41	0.55
1:J:231:ASN:OD1	1:J:232:ASP:N	2.39	0.55
1:U:410:LYS:HZ1	1:U:414:ASP:CG	2.14	0.55
1:L:231:ASN:HB3	1:M:237:PHE:CE2	2.42	0.55
1:T:155:VAL:HG13	1:T:176:VAL:HG22	1.88	0.55
1:F:277:GLN:OE1	1:G:373:ARG:NH1	2.38	0.55
1:H:155:VAL:HG22	1:H:176:VAL:HG13	1.87	0.55
1:P:231:ASN:OD1	1:P:232:ASP:N	2.39	0.55
1:Y:410:LYS:HZ1	1:Y:414:ASP:CG	2.14	0.55
1:a:370:ARG:NH1	1:a:372:ILE:HD11	2.20	0.55
1:d:228:ARG:HG3	1:e:233:ALA:HB1	1.88	0.55
1:d:231:ASN:HB3	1:e:237:PHE:CE2	2.42	0.55
1:X:139:GLU:HG2	1:X:142:ARG:HH22	1.71	0.55
1:a:145:GLU:HG3	1:a:152:SER:HA	1.88	0.55
1:L:145:GLU:HG3	1:L:152:SER:HA	1.88	0.55
1:L:377:MET:HE2	1:L:377:MET:N	2.22	0.55
1:N:145:GLU:HG3	1:N:152:SER:HA	1.89	0.55
1:S:231:ASN:OD1	1:S:232:ASP:N	2.39	0.55
1:C:228:ARG:HD2	1:D:233:ALA:HB1	1.88	0.55
1:D:370:ARG:NH1	1:D:372:ILE:HD11	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:125:GLN:O	1:R:128:GLU:HG2	2.06	0.55
1:a:186:LEU:HD11	1:a:219:LEU:HD13	1.88	0.55
1:B:73:MET:SD	1:B:99:ARG:NH1	2.79	0.55
1:L:277:GLN:OE1	1:M:373:ARG:NH1	2.39	0.55
1:X:228:ARG:HG3	1:Y:233:ALA:HB1	1.87	0.55
1:a:181:GLU:OE1	1:a:184:ARG:NH2	2.26	0.55
1:A:231:ASN:OD1	1:A:232:ASP:N	2.40	0.55
1:D:231:ASN:OD1	1:D:232:ASP:N	2.40	0.55
1:g:151:LYS:NZ	1:g:181:GLU:HA	2.20	0.55
1:D:420:MET:HE1	1:D:430:LEU:HD13	1.89	0.55
1:E:144:ILE:HD12	1:E:194:VAL:HG23	1.88	0.55
1:V:231:ASN:HB2	1:W:237:PHE:CE2	2.42	0.55
1:e:159:MET:HG3	1:e:172:PRO:HB3	1.89	0.55
1:E:155:VAL:HG22	1:E:176:VAL:HG13	1.88	0.54
1:I:377:MET:N	1:I:377:MET:HE2	2.22	0.54
1:M:159:MET:HG3	1:M:172:PRO:HB3	1.88	0.54
1:O:228:ARG:HD2	1:P:233:ALA:HB1	1.88	0.54
1:O:370:ARG:HH12	1:O:372:ILE:HD11	1.72	0.54
1:X:181:GLU:OE1	1:X:184:ARG:NH2	2.25	0.54
1:U:186:LEU:HD11	1:U:219:LEU:HD13	1.88	0.54
1:c:73:MET:SD	1:c:99:ARG:NH1	2.80	0.54
1:E:71:THR:HA	1:E:75:ILE:HG12	1.89	0.54
1:F:228:ARG:HG3	1:G:233:ALA:HB1	1.89	0.54
1:O:145:GLU:HG3	1:O:152:SER:HA	1.89	0.54
1:a:277:GLN:OE1	1:b:373:ARG:NH1	2.40	0.54
1:L:159:MET:HG3	1:L:172:PRO:HB3	1.89	0.54
1:Z:370:ARG:HH12	1:Z:372:ILE:HD11	1.73	0.54
1:g:370:ARG:HH12	1:g:372:ILE:HD11	1.73	0.54
1:C:228:ARG:HG3	1:D:233:ALA:HB1	1.90	0.54
1:C:370:ARG:HH12	1:C:372:ILE:HD11	1.73	0.54
1:U:125:GLN:O	1:U:128:GLU:HG2	2.07	0.54
1:X:277:GLN:OE1	1:Y:373:ARG:NH1	2.40	0.54
1:c:144:ILE:HD12	1:c:194:VAL:HG23	1.90	0.54
1:O:228:ARG:HG3	1:P:233:ALA:HB1	1.90	0.54
1:B:145:GLU:HG3	1:B:152:SER:HA	1.88	0.54
1:b:231:ASN:HB2	1:c:237:PHE:CE2	2.43	0.54
1:M:231:ASN:OD1	1:M:232:ASP:N	2.40	0.54
1:S:231:ASN:HB2	1:T:237:PHE:CE2	2.43	0.54
1:a:151:LYS:NZ	1:a:180:LEU:O	2.33	0.54
1:c:78:ARG:HB2	1:c:87:GLU:HB2	1.89	0.54
1:V:151:LYS:NZ	1:V:181:GLU:HA	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:266:VAL:HG22	1:C:387:VAL:HG22	1.89	0.53
1:a:151:LYS:NZ	1:a:181:GLU:HA	2.17	0.53
1:C:159:MET:HG3	1:C:172:PRO:HB3	1.90	0.53
1:F:409:MET:HE2	1:F:434:ASN:HB2	1.90	0.53
1:H:78:ARG:HB2	1:H:87:GLU:HB2	1.89	0.53
1:S:370:ARG:NH1	1:S:372:ILE:HD11	2.22	0.53
1:F:266:VAL:HG22	1:F:387:VAL:HG22	1.91	0.53
1:L:370:ARG:HH12	1:L:372:ILE:HD11	1.74	0.53
1:R:186:LEU:HD11	1:R:219:LEU:HD13	1.90	0.53
1:W:100:LEU:O	1:W:104:GLY:N	2.26	0.53
1:F:228:ARG:HD2	1:G:233:ALA:HB1	1.91	0.53
1:J:221:THR:O	1:J:228:ARG:NH2	2.40	0.53
1:K:277:GLN:OE1	1:L:373:ARG:NH1	2.40	0.53
1:U:151:LYS:NZ	1:U:181:GLU:HA	2.20	0.53
1:b:159:MET:HG3	1:b:172:PRO:HB3	1.90	0.53
1:b:413:GLU:OE2	1:b:417:ARG:NH2	2.41	0.53
1:O:420:MET:HE1	1:O:430:LEU:HD13	1.91	0.53
1:R:159:MET:HG3	1:R:172:PRO:HB3	1.89	0.53
1:c:370:ARG:HH12	1:c:372:ILE:HD11	1.74	0.53
1:W:409:MET:HE3	1:W:434:ASN:HB2	1.91	0.53
1:g:181:GLU:OE1	1:g:184:ARG:NH2	2.28	0.53
1:B:144:ILE:HD12	1:B:194:VAL:HG23	1.91	0.53
1:L:409:MET:CE	1:L:434:ASN:HB2	2.39	0.53
1:d:159:MET:HG3	1:d:172:PRO:HB3	1.91	0.53
1:d:228:ARG:HD2	1:e:233:ALA:HB1	1.90	0.53
1:K:266:VAL:HG22	1:K:387:VAL:HG22	1.91	0.53
1:N:266:VAL:HG22	1:N:387:VAL:HG22	1.91	0.53
1:Y:151:LYS:NZ	1:Y:181:GLU:HA	2.21	0.53
1:X:370:ARG:HH12	1:X:372:ILE:HD11	1.73	0.53
1:Z:73:MET:SD	1:Z:99:ARG:NH1	2.82	0.53
1:Z:377:MET:N	1:Z:377:MET:HE2	2.24	0.53
1:G:151:LYS:NZ	1:G:181:GLU:HA	2.21	0.53
1:N:73:MET:SD	1:N:99:ARG:NH1	2.82	0.53
1:S:413:GLU:OE2	1:S:417:ARG:NH2	2.42	0.53
1:T:413:GLU:OE2	1:T:417:ARG:NH2	2.42	0.53
1:U:181:GLU:OE1	1:U:184:ARG:NH2	2.24	0.53
1:W:73:MET:SD	1:W:99:ARG:NH1	2.81	0.52
1:f:158:ALA:C	1:f:159:MET:HE2	2.34	0.52
1:L:139:GLU:HG2	1:L:142:ARG:HH22	1.74	0.52
1:E:93:VAL:HA	1:E:96:LEU:HB3	1.91	0.52
1:F:370:ARG:HH12	1:F:372:ILE:HD11	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:413:GLU:OE2	1:P:417:ARG:NH2	2.42	0.52
1:W:413:GLU:OE2	1:W:417:ARG:NH2	2.42	0.52
1:f:228:ARG:HG3	1:f:228:ARG:HH11	1.74	0.52
1:C:221:THR:O	1:C:222:GLN:NE2	2.42	0.52
1:G:231:ASN:HB2	1:H:237:PHE:CE2	2.45	0.52
1:A:159:MET:HG3	1:A:172:PRO:HB3	1.91	0.52
1:A:233:ALA:HB1	1:g:228:ARG:HD2	1.90	0.52
1:J:410:LYS:NZ	1:J:413:GLU:OE1	2.43	0.52
1:K:160:PRO:HD3	1:K:172:PRO:HB3	1.92	0.52
1:Q:78:ARG:HB2	1:Q:87:GLU:HB2	1.90	0.52
1:X:228:ARG:HD2	1:Y:233:ALA:HB1	1.90	0.52
1:C:151:LYS:HD3	1:C:181:GLU:HG2	1.90	0.52
1:J:159:MET:HG3	1:J:172:PRO:HB3	1.91	0.52
1:Z:71:THR:HA	1:Z:75:ILE:HG12	1.91	0.52
1:O:159:MET:HG3	1:O:172:PRO:HB3	1.92	0.52
1:W:155:VAL:HG22	1:W:176:VAL:HG13	1.91	0.52
1:e:221:THR:O	1:e:228:ARG:NH2	2.42	0.52
1:g:151:LYS:NZ	1:g:180:LEU:O	2.29	0.52
1:O:277:GLN:OE1	1:P:373:ARG:NH1	2.43	0.52
1:U:156:HIS:NE2	1:V:143:THR:OG1	2.37	0.52
1:Z:93:VAL:HA	1:Z:96:LEU:HB3	1.92	0.52
1:e:231:ASN:HB2	1:f:237:PHE:CE2	2.44	0.52
1:F:229:ASP:OD1	1:F:230:LEU:N	2.43	0.52
1:A:277:GLN:OE1	1:B:373:ARG:NH1	2.43	0.52
1:M:231:ASN:HB2	1:N:237:PHE:CE2	2.45	0.52
1:Y:231:ASN:HB2	1:Z:237:PHE:CE2	2.45	0.52
1:d:154:ARG:NH2	1:e:143:THR:HA	2.20	0.52
1:A:413:GLU:OE2	1:A:417:ARG:NH2	2.42	0.51
1:B:78:ARG:HB2	1:B:87:GLU:HB2	1.91	0.51
1:K:413:GLU:OE2	1:K:417:ARG:NH2	2.42	0.51
1:D:410:LYS:NZ	1:D:413:GLU:OE1	2.43	0.51
1:H:142:ARG:HH11	1:H:146:THR:HG21	1.75	0.51
1:O:181:GLU:OE1	1:O:184:ARG:NH2	2.29	0.51
1:P:231:ASN:HB2	1:Q:237:PHE:CE2	2.45	0.51
1:S:159:MET:HG3	1:S:172:PRO:HB3	1.90	0.51
1:V:413:GLU:OE2	1:V:417:ARG:NH2	2.43	0.51
1:T:144:ILE:HD12	1:T:194:VAL:HG23	1.91	0.51
1:X:145:GLU:HG3	1:X:152:SER:HA	1.92	0.51
1:N:413:GLU:OE2	1:N:417:ARG:NH2	2.43	0.51
1:R:370:ARG:HH12	1:R:372:ILE:HD11	1.74	0.51
1:W:160:PRO:HB3	1:W:170:LYS:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:151:LYS:NZ	1:I:181:GLU:HA	2.20	0.51
1:N:78:ARG:HB2	1:N:87:GLU:HB2	1.91	0.51
1:O:229:ASP:OD1	1:O:230:LEU:N	2.44	0.51
1:U:370:ARG:HH12	1:U:372:ILE:HD11	1.76	0.51
1:V:221:THR:O	1:V:228:ARG:NH2	2.42	0.51
1:Q:413:GLU:OE2	1:Q:417:ARG:NH2	2.42	0.51
1:g:159:MET:HG3	1:g:172:PRO:HB3	1.93	0.51
1:A:221:THR:HB	1:A:228:ARG:HH21	1.76	0.51
1:L:228:ARG:HD2	1:M:233:ALA:HB1	1.92	0.51
1:T:160:PRO:HB3	1:T:170:LYS:HB2	1.93	0.51
1:a:239:ASN:HA	1:a:242:GLU:HG2	1.93	0.51
1:c:279:GLU:N	1:c:279:GLU:OE1	2.43	0.51
1:g:266:VAL:HG22	1:g:387:VAL:HG22	1.92	0.51
1:H:228:ARG:HG3	1:H:228:ARG:HH11	1.75	0.51
1:K:162:PRO:HD2	1:K:170:LYS:HG3	1.93	0.51
1:L:413:GLU:OE2	1:L:417:ARG:NH2	2.44	0.51
1:M:413:GLU:OE2	1:M:417:ARG:NH2	2.42	0.51
1:d:370:ARG:HH12	1:d:372:ILE:HD11	1.74	0.51
1:E:370:ARG:HH12	1:E:372:ILE:HD11	1.77	0.51
1:U:413:GLU:OE2	1:U:417:ARG:NH2	2.44	0.51
1:X:229:ASP:OD1	1:X:230:LEU:N	2.44	0.51
1:a:159:MET:HG3	1:a:172:PRO:HB3	1.92	0.51
1:G:159:MET:HG3	1:G:172:PRO:HB3	1.92	0.50
1:J:231:ASN:HB2	1:K:237:PHE:CE2	2.46	0.50
1:K:93:VAL:HA	1:K:96:LEU:HB3	1.92	0.50
1:N:228:ARG:HH11	1:N:228:ARG:HG3	1.76	0.50
1:E:73:MET:SD	1:E:99:ARG:NH1	2.85	0.50
1:Q:228:ARG:HG3	1:Q:228:ARG:HH11	1.75	0.50
1:W:370:ARG:HH12	1:W:372:ILE:HD11	1.76	0.50
1:e:413:GLU:OE2	1:e:417:ARG:NH2	2.43	0.50
1:W:93:VAL:HA	1:W:96:LEU:HB3	1.93	0.50
1:W:144:ILE:HD12	1:W:194:VAL:HG23	1.93	0.50
1:W:266:VAL:HG22	1:W:387:VAL:HG22	1.92	0.50
1:X:266:VAL:HG22	1:X:387:VAL:HG22	1.92	0.50
1:W:155:VAL:HG13	1:W:176:VAL:HG22	1.94	0.50
1:d:229:ASP:OD1	1:d:230:LEU:N	2.44	0.50
1:g:409:MET:HE2	1:g:434:ASN:HB2	1.93	0.50
1:K:144:ILE:HD12	1:K:194:VAL:HG23	1.93	0.50
1:N:144:ILE:HD12	1:N:194:VAL:HG23	1.93	0.50
1:b:393:TYR:CZ	1:b:436:PRO:HD3	2.47	0.50
1:g:229:ASP:OD1	1:g:230:LEU:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:231:ASN:HB2	1:E:237:PHE:CE2	2.46	0.50
1:Y:413:GLU:OE2	1:Y:417:ARG:NH2	2.43	0.50
1:a:266:VAL:HG22	1:a:387:VAL:HG22	1.93	0.50
1:C:229:ASP:OD1	1:C:230:LEU:N	2.45	0.50
1:H:370:ARG:HH12	1:H:372:ILE:HD11	1.75	0.50
1:W:226:SER:HB3	1:X:236:LYS:HD2	1.94	0.50
1:Y:277:GLN:OE1	1:Z:373:ARG:NH1	2.45	0.50
1:c:155:VAL:HG22	1:c:176:VAL:HG13	1.93	0.50
1:I:159:MET:HG3	1:I:172:PRO:HB3	1.93	0.50
1:W:228:ARG:HG3	1:W:228:ARG:HH11	1.76	0.50
1:f:370:ARG:HH12	1:f:372:ILE:HD11	1.77	0.50
1:L:229:ASP:OD1	1:L:230:LEU:N	2.45	0.50
1:M:393:TYR:CZ	1:M:436:PRO:HD3	2.46	0.50
1:a:276:GLU:HG2	1:a:376:LYS:HG2	1.94	0.50
1:a:413:GLU:OE2	1:a:417:ARG:NH2	2.45	0.50
1:I:370:ARG:HH12	1:I:372:ILE:HD11	1.77	0.49
1:O:151:LYS:NZ	1:O:181:GLU:HG2	2.26	0.49
1:Q:266:VAL:HG22	1:Q:387:VAL:HG22	1.93	0.49
1:R:266:VAL:HG22	1:R:387:VAL:HG22	1.93	0.49
1:d:145:GLU:HG3	1:d:152:SER:HA	1.95	0.49
1:d:151:LYS:HZ3	1:d:180:LEU:C	2.17	0.49
1:A:231:ASN:HB2	1:B:237:PHE:CE2	2.47	0.49
1:C:151:LYS:HZ3	1:C:180:LEU:C	2.14	0.49
1:F:159:MET:HG3	1:F:172:PRO:HB3	1.94	0.49
1:K:370:ARG:HH12	1:K:372:ILE:HD11	1.76	0.49
1:Q:144:ILE:HD12	1:Q:194:VAL:HG23	1.94	0.49
1:W:75:ILE:N	1:W:76:PRO:HD3	2.27	0.49
1:e:409:MET:HE2	1:e:434:ASN:HB2	1.94	0.49
1:B:160:PRO:HB3	1:B:170:LYS:HB2	1.94	0.49
1:c:225:THR:HG23	1:c:227:GLY:H	1.75	0.49
1:f:73:MET:SD	1:f:99:ARG:NH1	2.86	0.49
1:D:231:ASN:HB2	1:E:237:PHE:CD2	2.47	0.49
1:Q:370:ARG:HH12	1:Q:372:ILE:HD11	1.76	0.49
1:X:159:MET:HG3	1:X:172:PRO:HB3	1.93	0.49
1:X:232:ASP:C	1:X:236:LYS:HZ2	2.20	0.49
1:b:129:GLN:HG3	1:b:161:LYS:NZ	2.27	0.49
1:g:410:LYS:HZ1	1:g:414:ASP:CG	2.21	0.49
1:G:129:GLN:HG3	1:G:161:LYS:NZ	2.27	0.49
1:P:179:THR:OG1	1:P:215:GLN:OE1	2.22	0.49
1:D:221:THR:HB	1:D:228:ARG:HH21	1.77	0.49
1:R:228:ARG:HD2	1:S:233:ALA:HB1	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:75:ILE:N	1:T:76:PRO:HD3	2.28	0.49
1:I:409:MET:HE2	1:I:434:ASN:HB2	1.94	0.49
1:T:225:THR:HG23	1:T:227:GLY:H	1.77	0.49
1:Z:413:GLU:OE2	1:Z:417:ARG:NH2	2.44	0.49
1:c:413:GLU:OE2	1:c:417:ARG:NH2	2.44	0.49
1:e:410:LYS:HZ1	1:e:414:ASP:CG	2.21	0.49
1:A:410:LYS:HZ1	1:A:414:ASP:CG	2.20	0.49
1:B:370:ARG:HH12	1:B:372:ILE:HD11	1.76	0.49
1:H:162:PRO:HD2	1:H:170:LYS:HG3	1.94	0.49
1:J:413:GLU:OE2	1:J:417:ARG:NH2	2.43	0.49
1:Q:75:ILE:N	1:Q:76:PRO:HD3	2.28	0.49
1:Z:78:ARG:HB2	1:Z:87:GLU:HB2	1.94	0.49
1:Z:101:ALA:O	1:Z:196:HIS:CE1	2.66	0.49
1:f:277:GLN:OE1	1:g:373:ARG:NH1	2.46	0.49
1:A:231:ASN:HB2	1:B:237:PHE:CD2	2.47	0.48
1:K:75:ILE:N	1:K:76:PRO:HD3	2.28	0.48
1:S:233:ALA:O	1:S:236:LYS:HG3	2.13	0.48
1:T:155:VAL:HG22	1:T:176:VAL:HG13	1.95	0.48
1:U:228:ARG:HG3	1:V:233:ALA:HB1	1.94	0.48
1:W:78:ARG:HB2	1:W:87:GLU:HB2	1.94	0.48
1:Y:159:MET:HG3	1:Y:172:PRO:HB3	1.94	0.48
1:B:93:VAL:HA	1:B:96:LEU:HB3	1.95	0.48
1:B:413:GLU:OE2	1:B:417:ARG:NH2	2.44	0.48
1:S:129:GLN:HG3	1:S:161:LYS:NZ	2.29	0.48
1:Z:426:ARG:NH2	1:Z:428:ASP:OD2	2.46	0.48
1:c:160:PRO:HB3	1:c:170:LYS:HB2	1.94	0.48
1:X:393:TYR:CZ	1:X:436:PRO:HD3	2.49	0.48
1:Y:129:GLN:HG3	1:Y:161:LYS:NZ	2.28	0.48
1:f:413:GLU:OE2	1:f:417:ARG:NH2	2.44	0.48
1:N:160:PRO:HB3	1:N:170:LYS:HB2	1.95	0.48
1:N:370:ARG:HH12	1:N:372:ILE:HD11	1.77	0.48
1:V:159:MET:HG3	1:V:172:PRO:HB3	1.95	0.48
1:f:93:VAL:HA	1:f:96:LEU:HB3	1.95	0.48
1:A:129:GLN:HG3	1:A:161:LYS:NZ	2.29	0.48
1:X:151:LYS:NZ	1:X:180:LEU:O	2.33	0.48
1:c:75:ILE:N	1:c:76:PRO:HD3	2.28	0.48
1:f:162:PRO:HD2	1:f:170:LYS:HG3	1.95	0.48
1:H:73:MET:SD	1:H:99:ARG:NH1	2.86	0.48
1:M:151:LYS:NZ	1:M:181:GLU:HA	2.17	0.48
1:N:75:ILE:N	1:N:76:PRO:HD3	2.29	0.48
1:X:413:GLU:OE2	1:X:417:ARG:NH2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:393:TYR:CZ	1:d:436:PRO:HD3	2.49	0.48
1:D:233:ALA:O	1:D:236:LYS:HG3	2.14	0.48
1:D:413:GLU:OE2	1:D:417:ARG:NH2	2.43	0.48
1:M:231:ASN:HB2	1:N:237:PHE:CD2	2.49	0.48
1:a:370:ARG:HH12	1:a:372:ILE:HD11	1.78	0.48
1:I:413:GLU:OE2	1:I:417:ARG:NH2	2.47	0.48
1:K:420:MET:SD	1:K:422:PHE:HD2	2.36	0.48
1:T:162:PRO:HD2	1:T:170:LYS:HG3	1.95	0.48
1:a:393:TYR:CZ	1:a:436:PRO:HD3	2.49	0.48
1:B:75:ILE:N	1:B:76:PRO:HD3	2.28	0.48
1:B:426:ARG:NH2	1:B:428:ASP:OD2	2.47	0.48
1:G:370:ARG:HH12	1:G:372:ILE:HD11	1.79	0.48
1:H:75:ILE:N	1:H:76:PRO:HD3	2.29	0.48
1:I:393:TYR:CZ	1:I:436:PRO:HD3	2.48	0.48
1:J:179:THR:OG1	1:J:215:GLN:OE1	2.23	0.48
1:Y:393:TYR:CZ	1:Y:436:PRO:HD3	2.49	0.48
1:a:420:MET:SD	1:a:422:PHE:HD2	2.37	0.48
1:g:413:GLU:OE2	1:g:417:ARG:NH2	2.47	0.48
1:B:101:ALA:O	1:B:196:HIS:CE1	2.67	0.47
1:G:233:ALA:O	1:G:236:LYS:HG3	2.14	0.47
1:d:413:GLU:OE2	1:d:417:ARG:NH2	2.47	0.47
1:e:370:ARG:HH12	1:e:372:ILE:HD11	1.79	0.47
1:E:78:ARG:HB2	1:E:87:GLU:HB2	1.96	0.47
1:E:413:GLU:OE2	1:E:417:ARG:NH2	2.45	0.47
1:I:151:LYS:HD3	1:I:181:GLU:HG2	1.96	0.47
1:J:233:ALA:O	1:J:236:LYS:HG3	2.14	0.47
1:N:93:VAL:HA	1:N:96:LEU:HB3	1.95	0.47
1:P:159:MET:HG3	1:P:172:PRO:HB3	1.95	0.47
1:P:231:ASN:HB2	1:Q:237:PHE:CD2	2.49	0.47
1:P:233:ALA:O	1:P:236:LYS:HG3	2.14	0.47
1:a:145:GLU:CG	1:a:152:SER:HA	2.43	0.47
1:A:142:ARG:O	1:A:146:THR:HG23	2.14	0.47
1:E:160:PRO:HB3	1:E:170:LYS:HB2	1.96	0.47
1:g:145:GLU:CG	1:g:152:SER:HA	2.44	0.47
1:Q:93:VAL:HA	1:Q:96:LEU:HB3	1.95	0.47
1:V:233:ALA:O	1:V:236:LYS:HG3	2.14	0.47
1:Y:233:ALA:O	1:Y:236:LYS:HG3	2.14	0.47
1:f:78:ARG:HB2	1:f:87:GLU:HB2	1.95	0.47
1:K:78:ARG:HB2	1:K:87:GLU:HB2	1.95	0.47
1:O:232:ASP:O	1:O:236:LYS:HG2	2.15	0.47
1:Q:160:PRO:HB3	1:Q:170:LYS:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:420:MET:SD	1:X:422:PHE:HD2	2.38	0.47
1:Y:370:ARG:HH12	1:Y:372:ILE:HD11	1.79	0.47
1:e:129:GLN:HG3	1:e:161:LYS:NZ	2.29	0.47
1:J:275:LYS:HD2	1:K:373:ARG:HH21	1.80	0.47
1:L:239:ASN:HA	1:L:242:GLU:HG2	1.96	0.47
1:M:233:ALA:O	1:M:236:LYS:HG3	2.14	0.47
1:V:214:ASP:CG	1:V:215:GLN:H	2.22	0.47
1:Z:75:ILE:N	1:Z:76:PRO:HD3	2.30	0.47
1:A:233:ALA:O	1:A:236:LYS:HG3	2.14	0.47
1:D:154:ARG:NH2	1:F:143:THR:HA	2.30	0.47
1:D:199:SER:HA	1:D:205:LEU:HD22	1.97	0.47
1:F:276:GLU:HG2	1:F:376:LYS:HG2	1.96	0.47
1:H:413:GLU:OE2	1:H:417:ARG:NH2	2.46	0.47
1:K:73:MET:SD	1:K:99:ARG:NH1	2.88	0.47
1:M:199:SER:HA	1:M:205:LEU:HD22	1.97	0.47
1:P:154:ARG:HH11	1:R:142:ARG:NH2	2.13	0.47
1:V:370:ARG:HH12	1:V:372:ILE:HD11	1.78	0.47
1:b:220:LEU:HG	1:b:222:GLN:HB2	1.96	0.47
1:e:410:LYS:NZ	1:e:413:GLU:OE1	2.46	0.47
1:f:71:THR:HA	1:f:75:ILE:HG12	1.96	0.47
1:g:420:MET:SD	1:g:422:PHE:HD2	2.38	0.47
1:L:276:GLU:HG2	1:L:376:LYS:HG2	1.96	0.47
1:Y:392:ASN:OD1	1:Y:393:TYR:N	2.48	0.47
1:c:378:ASN:OD1	1:c:379:VAL:N	2.48	0.47
1:g:393:TYR:CZ	1:g:436:PRO:HD3	2.49	0.47
1:E:75:ILE:N	1:E:76:PRO:HD3	2.30	0.47
1:M:145:GLU:HG3	1:M:152:SER:HA	1.97	0.47
1:Y:199:SER:HA	1:Y:205:LEU:HD22	1.97	0.47
1:Y:231:ASN:HB2	1:Z:237:PHE:CD2	2.49	0.47
1:f:378:ASN:OD1	1:f:379:VAL:N	2.48	0.47
1:g:218:HIS:ND1	1:g:220:LEU:O	2.46	0.47
1:S:420:MET:SD	1:S:422:PHE:HD2	2.38	0.47
1:V:199:SER:HA	1:V:205:LEU:HD22	1.97	0.47
1:V:410:LYS:NZ	1:V:413:GLU:OE1	2.45	0.47
1:e:393:TYR:CZ	1:e:436:PRO:HD3	2.50	0.47
1:G:231:ASN:HB2	1:H:237:PHE:CD2	2.50	0.46
1:O:393:TYR:CZ	1:O:436:PRO:HD3	2.50	0.46
1:S:266:VAL:HG22	1:S:387:VAL:HG22	1.97	0.46
1:f:75:ILE:N	1:f:76:PRO:HD3	2.29	0.46
1:C:413:GLU:OE2	1:C:417:ARG:NH2	2.47	0.46
1:G:404:LEU:HB2	1:G:409:MET:HE2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:71:THR:HA	1:N:75:ILE:HG12	1.97	0.46
1:P:410:LYS:HD2	1:P:410:LYS:HA	1.76	0.46
1:Q:378:ASN:OD1	1:Q:379:VAL:N	2.48	0.46
1:U:393:TYR:CZ	1:U:436:PRO:HD3	2.50	0.46
1:b:142:ARG:O	1:b:146:THR:HG23	2.15	0.46
1:d:410:LYS:HZ1	1:d:414:ASP:CG	2.22	0.46
1:e:233:ALA:O	1:e:236:LYS:HG3	2.14	0.46
1:S:392:ASN:OD1	1:S:393:TYR:N	2.49	0.46
1:W:378:ASN:OD1	1:W:379:VAL:N	2.49	0.46
1:e:231:ASN:HB2	1:f:237:PHE:CD2	2.50	0.46
1:A:393:TYR:CZ	1:A:436:PRO:HD3	2.49	0.46
1:D:125:GLN:O	1:D:129:GLN:HG2	2.15	0.46
1:O:186:LEU:HD11	1:O:219:LEU:HD13	1.97	0.46
1:P:129:GLN:HG3	1:P:161:LYS:NZ	2.30	0.46
1:Q:136:LEU:O	1:Q:140:LEU:HD12	2.15	0.46
1:Z:89:PRO:O	1:Z:93:VAL:HG23	2.16	0.46
1:b:199:SER:HA	1:b:205:LEU:HD22	1.98	0.46
1:C:378:ASN:OD1	1:C:379:VAL:N	2.48	0.46
1:E:426:ARG:NH2	1:E:428:ASP:OD2	2.49	0.46
1:K:89:PRO:O	1:K:93:VAL:HG23	2.15	0.46
1:a:160:PRO:HG3	1:b:203:ALA:HB1	1.97	0.46
1:a:409:MET:HE2	1:a:434:ASN:HB2	1.97	0.46
1:A:370:ARG:HH12	1:A:372:ILE:HD11	1.80	0.46
1:H:225:THR:HG23	1:H:227:GLY:H	1.81	0.46
1:H:378:ASN:OD1	1:H:379:VAL:N	2.49	0.46
1:J:370:ARG:HH12	1:J:372:ILE:HD11	1.80	0.46
1:P:370:ARG:HH12	1:P:372:ILE:HD11	1.79	0.46
1:D:370:ARG:HH12	1:D:372:ILE:HD11	1.80	0.46
1:E:89:PRO:O	1:E:93:VAL:HG23	2.16	0.46
1:K:71:THR:HA	1:K:75:ILE:HG12	1.98	0.46
1:P:277:GLN:OE1	1:Q:373:ARG:NH1	2.48	0.46
1:V:393:TYR:CZ	1:V:436:PRO:HD3	2.51	0.46
1:e:409:MET:CE	1:e:434:ASN:HB2	2.46	0.46
1:J:393:TYR:CZ	1:J:436:PRO:HD3	2.50	0.46
1:L:161:LYS:HD3	1:L:161:LYS:C	2.41	0.46
1:N:409:MET:CE	1:N:434:ASN:HB2	2.45	0.46
1:S:214:ASP:CG	1:S:215:GLN:H	2.24	0.46
1:e:199:SER:HA	1:e:205:LEU:HD22	1.98	0.46
1:G:221:THR:O	1:G:228:ARG:NH2	2.46	0.46
1:M:214:ASP:CG	1:M:215:GLN:H	2.24	0.46
1:N:420:MET:SD	1:N:422:PHE:HD2	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:377:MET:HE3	1:b:377:MET:HA	1.98	0.46
1:f:159:MET:HE2	1:f:159:MET:N	2.31	0.46
1:D:214:ASP:CG	1:D:215:GLN:H	2.23	0.46
1:H:426:ARG:NH2	1:H:428:ASP:OD2	2.49	0.46
1:E:226:SER:HB3	1:F:236:LYS:HD2	1.99	0.45
1:P:199:SER:HA	1:P:205:LEU:HD22	1.99	0.45
1:R:181:GLU:OE1	1:R:184:ARG:NH2	2.32	0.45
1:b:370:ARG:HH12	1:b:372:ILE:HD11	1.80	0.45
1:F:145:GLU:HG3	1:F:152:SER:HA	1.98	0.45
1:G:214:ASP:CG	1:G:215:GLN:H	2.24	0.45
1:P:125:GLN:O	1:P:129:GLN:HG2	2.16	0.45
1:P:214:ASP:CG	1:P:215:GLN:H	2.24	0.45
1:S:370:ARG:HH12	1:S:372:ILE:HD11	1.80	0.45
1:T:233:ALA:O	1:T:236:LYS:HG3	2.16	0.45
1:A:154:ARG:NH2	1:C:143:THR:HA	2.31	0.45
1:B:265:GLN:HG3	1:C:252:ILE:HB	1.99	0.45
1:D:392:ASN:OD1	1:D:393:TYR:N	2.49	0.45
1:R:161:LYS:HD3	1:R:161:LYS:C	2.40	0.45
1:W:89:PRO:O	1:W:93:VAL:HG23	2.17	0.45
1:Z:160:PRO:HB3	1:Z:170:LYS:HB2	1.98	0.45
1:T:370:ARG:HH12	1:T:372:ILE:HD11	1.79	0.45
1:Z:233:ALA:O	1:Z:236:LYS:HG3	2.16	0.45
1:a:161:LYS:HD3	1:a:161:LYS:C	2.41	0.45
1:d:161:LYS:HD3	1:d:161:LYS:C	2.41	0.45
1:D:145:GLU:HG3	1:D:152:SER:HA	1.98	0.45
1:F:393:TYR:CZ	1:F:436:PRO:HD3	2.51	0.45
1:R:145:GLU:HG3	1:R:152:SER:HA	1.99	0.45
1:V:145:GLU:HG3	1:V:152:SER:HA	1.97	0.45
1:f:101:ALA:O	1:f:196:HIS:NE2	2.48	0.45
1:F:153:ALA:HB2	1:F:178:VAL:HG22	1.97	0.45
1:F:420:MET:SD	1:F:422:PHE:HD2	2.40	0.45
1:B:162:PRO:HD2	1:B:170:LYS:HG3	1.98	0.45
1:J:199:SER:HA	1:J:205:LEU:HD22	1.98	0.45
1:J:214:ASP:CG	1:J:215:GLN:H	2.24	0.45
1:P:142:ARG:O	1:P:146:THR:HG23	2.15	0.45
1:R:413:GLU:OE2	1:R:417:ARG:NH2	2.46	0.45
1:V:142:ARG:O	1:V:146:THR:HG23	2.16	0.45
1:g:151:LYS:HD3	1:g:181:GLU:HG2	1.97	0.45
1:G:142:ARG:O	1:G:146:THR:HG23	2.17	0.45
1:H:233:ALA:O	1:H:236:LYS:HG3	2.17	0.45
1:K:160:PRO:HB3	1:K:170:LYS:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:378:ASN:OD1	1:K:379:VAL:N	2.49	0.45
1:R:151:LYS:NZ	1:R:181:GLU:HG2	2.32	0.45
1:X:161:LYS:C	1:X:161:LYS:HD3	2.41	0.45
1:c:93:VAL:HA	1:c:96:LEU:HB3	1.99	0.45
1:c:233:ALA:O	1:c:236:LYS:HG3	2.16	0.45
1:e:214:ASP:CG	1:e:215:GLN:H	2.24	0.45
1:A:129:GLN:HG3	1:A:161:LYS:HZ1	1.80	0.45
1:A:410:LYS:NZ	1:A:413:GLU:OE1	2.38	0.45
1:B:378:ASN:OD1	1:B:379:VAL:N	2.50	0.45
1:G:199:SER:HA	1:G:205:LEU:HD22	1.99	0.45
1:P:393:TYR:CZ	1:P:436:PRO:HD3	2.52	0.45
1:T:93:VAL:HA	1:T:96:LEU:HB3	1.98	0.45
1:Y:214:ASP:CG	1:Y:215:GLN:H	2.25	0.45
1:b:154:ARG:NH2	1:d:142:ARG:O	2.50	0.45
1:d:199:SER:HA	1:d:205:LEU:HD22	1.99	0.45
1:C:236:LYS:NZ	1:D:244:ARG:HH22	2.15	0.45
1:E:252:ILE:HG23	1:E:253:LEU:HD22	1.98	0.45
1:F:232:ASP:O	1:F:236:LYS:HG2	2.17	0.45
1:F:413:GLU:OE2	1:F:417:ARG:NH2	2.49	0.45
1:M:213:VAL:HA	1:M:218:HIS:HA	1.99	0.45
1:W:162:PRO:HD2	1:W:170:LYS:HG3	1.98	0.45
1:c:155:VAL:HG13	1:c:176:VAL:HG22	1.99	0.45
1:A:199:SER:HA	1:A:205:LEU:HD22	1.99	0.44
1:J:392:ASN:OD1	1:J:393:TYR:N	2.50	0.44
1:M:392:ASN:OD1	1:M:393:TYR:N	2.49	0.44
1:P:266:VAL:HG22	1:P:387:VAL:HG22	1.98	0.44
1:Q:225:THR:HG23	1:Q:227:GLY:H	1.80	0.44
1:S:425:LYS:HE3	1:S:425:LYS:HB3	1.88	0.44
1:U:199:SER:HA	1:U:205:LEU:HD22	1.99	0.44
1:f:160:PRO:HB3	1:f:170:LYS:HB2	1.98	0.44
1:f:228:ARG:HG3	1:f:228:ARG:NH1	2.32	0.44
1:F:151:LYS:HZ3	1:F:181:GLU:HA	1.82	0.44
1:F:410:LYS:HZ1	1:F:414:ASP:CG	2.25	0.44
1:I:161:LYS:HD3	1:I:161:LYS:C	2.41	0.44
1:I:426:ARG:NH2	1:I:428:ASP:OD2	2.50	0.44
1:K:233:ALA:O	1:K:236:LYS:HG3	2.17	0.44
1:L:218:HIS:ND1	1:L:220:LEU:O	2.48	0.44
1:Q:162:PRO:HD2	1:Q:170:LYS:HG3	1.99	0.44
1:Q:187:ASP:O	1:Q:191:ILE:HG12	2.17	0.44
1:S:199:SER:HA	1:S:205:LEU:HD22	1.99	0.44
1:Y:221:THR:O	1:Y:228:ARG:NH2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:214:ASP:CG	1:b:215:GLN:H	2.25	0.44
1:G:378:ASN:OD1	1:G:379:VAL:N	2.50	0.44
1:Z:187:ASP:O	1:Z:191:ILE:HG12	2.17	0.44
1:a:218:HIS:ND1	1:a:220:LEU:O	2.48	0.44
1:b:233:ALA:O	1:b:236:LYS:HG3	2.17	0.44
1:d:151:LYS:NZ	1:d:180:LEU:O	2.34	0.44
1:A:392:ASN:OD1	1:A:393:TYR:N	2.50	0.44
1:D:253:LEU:HD23	1:D:253:LEU:HA	1.88	0.44
1:O:410:LYS:HZ1	1:O:414:ASP:CG	2.24	0.44
1:T:187:ASP:O	1:T:191:ILE:HG12	2.17	0.44
1:b:410:LYS:NZ	1:b:413:GLU:OE1	2.47	0.44
1:A:214:ASP:CG	1:A:215:GLN:H	2.24	0.44
1:A:396:LEU:HD23	1:A:396:LEU:H	1.82	0.44
1:B:233:ALA:O	1:B:236:LYS:HG3	2.17	0.44
1:N:225:THR:HG23	1:N:227:GLY:H	1.82	0.44
1:O:413:GLU:OE2	1:O:417:ARG:NH2	2.48	0.44
1:P:392:ASN:OD1	1:P:393:TYR:N	2.50	0.44
1:Y:220:LEU:HG	1:Y:222:GLN:HB2	1.99	0.44
1:K:202:VAL:HB	1:K:205:LEU:HD12	2.00	0.44
1:M:141:ALA:O	1:M:144:ILE:N	2.51	0.44
1:N:233:ALA:O	1:N:236:LYS:HG3	2.17	0.44
1:T:212:LEU:O	1:T:220:LEU:HD11	2.17	0.44
1:F:392:ASN:OD1	1:F:393:TYR:N	2.51	0.44
1:K:187:ASP:O	1:K:191:ILE:HG12	2.18	0.44
1:N:187:ASP:O	1:N:191:ILE:HG12	2.18	0.44
1:X:378:ASN:OD1	1:X:379:VAL:N	2.50	0.44
1:Y:425:LYS:HE3	1:Y:425:LYS:HB3	1.89	0.44
1:b:392:ASN:OD1	1:b:393:TYR:N	2.51	0.44
1:c:195:VAL:HG23	1:c:210:VAL:HB	1.98	0.44
1:f:187:ASP:O	1:f:191:ILE:HG12	2.18	0.44
1:C:409:MET:CE	1:C:434:ASN:HB2	2.47	0.44
1:C:409:MET:HE1	1:C:434:ASN:HB2	2.00	0.44
1:D:141:ALA:O	1:D:144:ILE:N	2.51	0.44
1:F:253:LEU:HD23	1:F:253:LEU:HA	1.87	0.44
1:M:149:PRO:O	1:M:180:LEU:HD12	2.18	0.44
1:Y:181:GLU:OE1	1:Y:184:ARG:NH2	2.39	0.44
1:b:179:THR:OG1	1:b:215:GLN:OE1	2.23	0.44
1:C:169:GLN:C	1:C:170:LYS:HD3	2.43	0.44
1:C:199:SER:HA	1:C:205:LEU:HD22	2.00	0.44
1:G:145:GLU:HG3	1:G:152:SER:HA	1.99	0.44
1:Q:233:ALA:O	1:Q:236:LYS:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:393:TYR:CZ	1:R:436:PRO:HD3	2.53	0.44
1:T:78:ARG:N	1:T:87:GLU:O	2.48	0.44
1:a:228:ARG:CG	1:b:233:ALA:HB1	2.48	0.44
1:E:212:LEU:O	1:E:220:LEU:HD11	2.18	0.43
1:F:125:GLN:O	1:F:129:GLN:HG2	2.18	0.43
1:F:183:GLY:C	1:F:184:ARG:HD3	2.43	0.43
1:H:195:VAL:HG23	1:H:210:VAL:HB	2.00	0.43
1:N:265:GLN:HG3	1:O:252:ILE:HB	2.00	0.43
1:U:159:MET:HG3	1:U:172:PRO:HB3	2.00	0.43
1:X:125:GLN:O	1:X:129:GLN:HG2	2.18	0.43
1:a:149:PRO:O	1:a:180:LEU:HD12	2.18	0.43
1:e:141:ALA:O	1:e:144:ILE:N	2.51	0.43
1:G:393:TYR:CZ	1:G:436:PRO:HD3	2.53	0.43
1:O:214:ASP:CG	1:O:215:GLN:H	2.27	0.43
1:Q:393:TYR:CE2	1:Q:436:PRO:HD3	2.53	0.43
1:R:125:GLN:O	1:R:129:GLN:HG2	2.18	0.43
1:R:378:ASN:OD1	1:R:379:VAL:N	2.52	0.43
1:W:383:GLU:N	1:W:383:GLU:OE1	2.52	0.43
1:Y:142:ARG:O	1:Y:146:THR:HG23	2.17	0.43
1:Z:393:TYR:CZ	1:Z:436:PRO:HD3	2.53	0.43
1:G:396:LEU:H	1:G:396:LEU:HD23	1.84	0.43
1:L:410:LYS:HD2	1:L:410:LYS:HA	1.77	0.43
1:c:187:ASP:O	1:c:191:ILE:HG12	2.18	0.43
1:f:225:THR:HG23	1:f:227:GLY:H	1.82	0.43
1:H:154:ARG:O	1:H:177:THR:N	2.50	0.43
1:H:187:ASP:O	1:H:191:ILE:HG12	2.18	0.43
1:K:155:VAL:HG13	1:K:176:VAL:HG22	2.00	0.43
1:N:154:ARG:O	1:N:177:THR:N	2.51	0.43
1:Q:207:PRO:HD2	1:R:187:ASP:OD1	2.18	0.43
1:W:187:ASP:O	1:W:191:ILE:HG12	2.19	0.43
1:Z:212:LEU:O	1:Z:220:LEU:HD11	2.19	0.43
1:f:233:ALA:O	1:f:236:LYS:HG3	2.17	0.43
1:E:187:ASP:O	1:E:191:ILE:HG12	2.18	0.43
1:J:231:ASN:HB2	1:K:237:PHE:CD2	2.53	0.43
1:V:392:ASN:OD1	1:V:393:TYR:N	2.51	0.43
1:f:89:PRO:O	1:f:93:VAL:HG23	2.18	0.43
1:f:393:TYR:CZ	1:f:436:PRO:HD3	2.54	0.43
1:L:253:LEU:HD23	1:L:253:LEU:HA	1.88	0.43
1:N:378:ASN:OD1	1:N:379:VAL:N	2.51	0.43
1:O:199:SER:HA	1:O:205:LEU:HD22	2.01	0.43
1:U:125:GLN:O	1:U:129:GLN:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:233:ALA:O	1:W:236:LYS:HG3	2.18	0.43
1:d:154:ARG:HH21	1:e:146:THR:HG21	1.83	0.43
1:A:233:ALA:HB1	1:g:228:ARG:CG	2.49	0.43
1:C:393:TYR:CZ	1:C:436:PRO:HD3	2.54	0.43
1:F:228:ARG:CG	1:G:233:ALA:HB1	2.48	0.43
1:K:377:MET:HE3	1:K:377:MET:HB3	1.87	0.43
1:L:266:VAL:HG22	1:L:387:VAL:HG22	2.01	0.43
1:N:239:ASN:HA	1:N:242:GLU:HG2	2.01	0.43
1:R:420:MET:SD	1:R:422:PHE:HD2	2.42	0.43
1:T:378:ASN:OD1	1:T:379:VAL:N	2.52	0.43
1:a:199:SER:HA	1:a:205:LEU:HD22	2.01	0.43
1:b:231:ASN:HB2	1:c:237:PHE:CD2	2.53	0.43
1:b:266:VAL:HG22	1:b:387:VAL:HG22	2.00	0.43
1:b:378:ASN:OD1	1:b:379:VAL:N	2.52	0.43
1:f:202:VAL:HB	1:f:205:LEU:HD12	2.01	0.43
1:g:125:GLN:O	1:g:129:GLN:HG2	2.18	0.43
1:A:266:VAL:HG22	1:A:387:VAL:HG22	2.00	0.43
1:B:225:THR:HG23	1:B:227:GLY:H	1.83	0.43
1:G:125:GLN:O	1:G:129:GLN:HG2	2.19	0.43
1:L:392:ASN:OD1	1:L:393:TYR:N	2.52	0.43
1:N:162:PRO:HD2	1:N:170:LYS:HG3	1.99	0.43
1:f:190:GLN:O	1:f:194:VAL:HG12	2.19	0.43
1:g:214:ASP:CG	1:g:215:GLN:H	2.27	0.43
1:B:89:PRO:O	1:B:93:VAL:HG23	2.19	0.43
1:B:187:ASP:O	1:B:191:ILE:HG12	2.18	0.43
1:B:212:LEU:O	1:B:220:LEU:HD11	2.18	0.43
1:D:139:GLU:HA	1:D:142:ARG:NH1	2.34	0.43
1:E:233:ALA:O	1:E:236:LYS:HG3	2.18	0.43
1:X:228:ARG:CG	1:Y:233:ALA:HB1	2.49	0.43
1:b:271:ASP:OD2	1:b:275:LYS:NZ	2.48	0.43
1:c:78:ARG:N	1:c:87:GLU:O	2.48	0.43
1:e:266:VAL:HG22	1:e:387:VAL:HG22	2.00	0.43
1:f:212:LEU:O	1:f:220:LEU:HD11	2.19	0.43
1:B:155:VAL:HG13	1:B:176:VAL:HG22	2.01	0.43
1:I:199:SER:HA	1:I:205:LEU:HD22	2.00	0.43
1:K:252:ILE:HG23	1:K:253:LEU:HD22	2.00	0.43
1:Q:393:TYR:CZ	1:Q:436:PRO:HD3	2.54	0.43
1:R:138:GLY:O	1:R:142:ARG:HG2	2.18	0.43
1:d:228:ARG:CG	1:e:233:ALA:HB1	2.49	0.43
1:g:141:ALA:O	1:g:144:ILE:N	2.52	0.43
1:g:426:ARG:NH2	1:g:428:ASP:OD2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:394:LYS:NZ	1:D:403:PRO:O	2.52	0.42
1:E:162:PRO:HD2	1:E:170:LYS:HG3	2.01	0.42
1:G:392:ASN:OD1	1:G:393:TYR:N	2.51	0.42
1:J:396:LEU:HD23	1:J:396:LEU:H	1.84	0.42
1:N:89:PRO:O	1:N:93:VAL:HG23	2.19	0.42
1:N:409:MET:HE1	1:N:434:ASN:HB2	2.01	0.42
1:S:142:ARG:O	1:S:146:THR:HG23	2.19	0.42
1:S:231:ASN:HB2	1:T:237:PHE:CD2	2.53	0.42
1:Y:149:PRO:O	1:Y:180:LEU:HD12	2.19	0.42
1:Y:426:ARG:NH2	1:Y:428:ASP:OD2	2.52	0.42
1:c:162:PRO:HD2	1:c:170:LYS:HG3	2.01	0.42
1:d:145:GLU:CG	1:d:152:SER:HA	2.49	0.42
1:C:214:ASP:CG	1:C:215:GLN:H	2.27	0.42
1:F:214:ASP:CG	1:F:215:GLN:H	2.27	0.42
1:L:214:ASP:CG	1:L:215:GLN:H	2.27	0.42
1:O:220:LEU:HD11	1:O:222:GLN:HE22	1.83	0.42
1:Q:271:ASP:HB2	1:Q:383:GLU:OE2	2.19	0.42
1:U:151:LYS:HZ3	1:U:180:LEU:C	2.19	0.42
1:V:129:GLN:HG3	1:V:161:LYS:NZ	2.34	0.42
1:a:141:ALA:O	1:a:144:ILE:N	2.52	0.42
1:d:125:GLN:O	1:d:129:GLN:HG2	2.19	0.42
1:B:393:TYR:CE2	1:B:436:PRO:HD3	2.55	0.42
1:I:228:ARG:CG	1:J:233:ALA:HB1	2.48	0.42
1:I:392:ASN:OD1	1:I:393:TYR:N	2.52	0.42
1:N:392:ASN:OD1	1:N:393:TYR:N	2.53	0.42
1:Q:239:ASN:HA	1:Q:242:GLU:HG2	2.01	0.42
1:R:199:SER:HA	1:R:205:LEU:HD22	2.01	0.42
1:X:183:GLY:C	1:X:184:ARG:HD3	2.44	0.42
1:Y:253:LEU:HD23	1:Y:253:LEU:HA	1.80	0.42
1:b:221:THR:O	1:b:228:ARG:NH2	2.52	0.42
1:A:239:ASN:HA	1:A:242:GLU:HG2	2.01	0.42
1:B:70:LEU:HD21	1:B:76:PRO:O	2.20	0.42
1:C:183:GLY:C	1:C:184:ARG:HD3	2.45	0.42
1:E:378:ASN:OD1	1:E:379:VAL:N	2.52	0.42
1:I:183:GLY:C	1:I:184:ARG:HD3	2.45	0.42
1:L:199:SER:HA	1:L:205:LEU:HD22	2.01	0.42
1:N:151:LYS:HE3	1:N:181:GLU:HA	2.00	0.42
1:Z:225:THR:HG23	1:Z:227:GLY:H	1.83	0.42
1:b:420:MET:HE1	1:b:430:LEU:HD13	2.00	0.42
1:A:181:GLU:OE1	1:A:184:ARG:NH2	2.31	0.42
1:Q:89:PRO:O	1:Q:93:VAL:HG23	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:154:ARG:O	1:Q:177:THR:N	2.51	0.42
1:V:396:LEU:H	1:V:396:LEU:HD23	1.84	0.42
1:X:160:PRO:HG3	1:Y:203:ALA:HB1	2.01	0.42
1:Z:392:ASN:OD1	1:Z:393:TYR:N	2.52	0.42
1:Z:393:TYR:CE2	1:Z:436:PRO:HD3	2.55	0.42
1:c:139:GLU:O	1:c:143:THR:HG23	2.19	0.42
1:f:252:ILE:HG23	1:f:253:LEU:HD22	2.00	0.42
1:B:393:TYR:CZ	1:B:436:PRO:HD3	2.55	0.42
1:Q:212:LEU:O	1:Q:220:LEU:HD11	2.19	0.42
1:S:141:ALA:O	1:S:144:ILE:N	2.52	0.42
1:X:199:SER:HA	1:X:205:LEU:HD22	2.02	0.42
1:a:230:LEU:O	1:a:234:GLN:HG3	2.19	0.42
1:d:220:LEU:HD12	1:d:220:LEU:HA	1.87	0.42
1:D:151:LYS:HZ3	1:D:180:LEU:C	2.21	0.42
1:H:155:VAL:HG13	1:H:176:VAL:HG22	2.01	0.42
1:T:89:PRO:O	1:T:93:VAL:HG23	2.20	0.42
1:X:141:ALA:O	1:X:144:ILE:N	2.53	0.42
1:g:392:ASN:OD1	1:g:393:TYR:N	2.52	0.42
1:H:252:ILE:HG23	1:H:253:LEU:HD22	2.00	0.42
1:Q:392:ASN:OD1	1:Q:393:TYR:N	2.53	0.42
1:T:70:LEU:HD21	1:T:76:PRO:O	2.20	0.42
1:B:392:ASN:OD1	1:B:393:TYR:N	2.53	0.42
1:O:378:ASN:OD1	1:O:379:VAL:N	2.53	0.42
1:V:426:ARG:NH2	1:V:428:ASP:OD2	2.53	0.42
1:X:214:ASP:CG	1:X:215:GLN:H	2.27	0.42
1:c:265:GLN:HG3	1:d:252:ILE:HB	2.02	0.42
1:f:392:ASN:OD1	1:f:393:TYR:N	2.53	0.42
1:g:199:SER:HA	1:g:205:LEU:HD22	2.02	0.42
1:F:378:ASN:OD1	1:F:379:VAL:N	2.53	0.42
1:L:151:LYS:NZ	1:L:181:GLU:HG2	2.34	0.42
1:N:78:ARG:N	1:N:87:GLU:O	2.51	0.42
1:S:396:LEU:H	1:S:396:LEU:HD23	1.85	0.42
1:U:141:ALA:O	1:U:144:ILE:N	2.52	0.42
1:U:392:ASN:OD1	1:U:393:TYR:N	2.53	0.42
1:a:214:ASP:CG	1:a:215:GLN:H	2.27	0.42
1:e:221:THR:C	1:e:228:ARG:HH21	2.27	0.42
1:F:125:GLN:O	1:F:128:GLU:HG2	2.20	0.41
1:H:393:TYR:CE2	1:H:436:PRO:HD3	2.55	0.41
1:I:214:ASP:CG	1:I:215:GLN:H	2.27	0.41
1:K:392:ASN:OD1	1:K:393:TYR:N	2.53	0.41
1:L:228:ARG:CG	1:M:233:ALA:HB1	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:221:THR:C	1:P:228:ARG:HH21	2.28	0.41
1:R:130:VAL:O	1:R:134:ARG:HG2	2.19	0.41
1:R:214:ASP:CG	1:R:215:GLN:H	2.27	0.41
1:S:181:GLU:OE1	1:S:184:ARG:NH2	2.33	0.41
1:U:228:ARG:CG	1:V:233:ALA:HB1	2.49	0.41
1:Z:378:ASN:OD1	1:Z:379:VAL:N	2.53	0.41
1:C:170:LYS:HD3	1:C:170:LYS:N	2.34	0.41
1:I:141:ALA:O	1:I:144:ILE:N	2.53	0.41
1:V:149:PRO:O	1:V:180:LEU:HD12	2.21	0.41
1:W:91:ASP:HA	1:W:94:HIS:HD2	1.86	0.41
1:Y:396:LEU:HD23	1:Y:396:LEU:H	1.85	0.41
1:Z:155:VAL:HG13	1:Z:176:VAL:HG22	2.01	0.41
1:d:183:GLY:C	1:d:184:ARG:HD3	2.45	0.41
1:e:392:ASN:OD1	1:e:393:TYR:N	2.51	0.41
1:f:393:TYR:CE2	1:f:436:PRO:HD3	2.55	0.41
1:B:154:ARG:O	1:B:177:THR:N	2.50	0.41
1:D:159:MET:HG3	1:D:172:PRO:HB3	2.02	0.41
1:H:393:TYR:CZ	1:H:436:PRO:HD3	2.55	0.41
1:R:392:ASN:OD1	1:R:393:TYR:N	2.53	0.41
1:T:139:GLU:O	1:T:143:THR:HG23	2.19	0.41
1:T:409:MET:CE	1:T:434:ASN:HB2	2.47	0.41
1:U:214:ASP:CG	1:U:215:GLN:H	2.28	0.41
1:V:213:VAL:HG22	1:V:218:HIS:HB3	2.01	0.41
1:Y:125:GLN:O	1:Y:129:GLN:HG2	2.20	0.41
1:a:130:VAL:O	1:a:134:ARG:HG2	2.21	0.41
1:a:392:ASN:OD1	1:a:393:TYR:N	2.53	0.41
1:c:89:PRO:O	1:c:93:VAL:HG23	2.20	0.41
1:d:214:ASP:CG	1:d:215:GLN:H	2.27	0.41
1:G:221:THR:C	1:G:228:ARG:HH21	2.28	0.41
1:H:279:GLU:N	1:H:279:GLU:OE1	2.54	0.41
1:J:141:ALA:O	1:J:144:ILE:N	2.53	0.41
1:J:213:VAL:HA	1:J:218:HIS:HA	2.03	0.41
1:L:393:TYR:CZ	1:L:436:PRO:HD3	2.54	0.41
1:M:213:VAL:HG22	1:M:218:HIS:HB3	2.03	0.41
1:M:370:ARG:HH12	1:M:372:ILE:HD11	1.81	0.41
1:M:396:LEU:HD23	1:M:396:LEU:H	1.85	0.41
1:Q:194:VAL:O	1:Q:198:VAL:HG23	2.19	0.41
1:S:221:THR:C	1:S:228:ARG:HH21	2.29	0.41
1:S:378:ASN:OD1	1:S:379:VAL:N	2.54	0.41
1:T:154:ARG:HB3	1:T:177:THR:OG1	2.20	0.41
1:T:195:VAL:HG23	1:T:210:VAL:HB	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:145:GLU:CG	1:X:152:SER:HA	2.50	0.41
1:Y:130:VAL:O	1:Y:134:ARG:HG2	2.20	0.41
1:c:70:LEU:HD21	1:c:76:PRO:O	2.20	0.41
1:H:152:SER:OG	1:H:179:THR:OG1	2.33	0.41
1:I:230:LEU:O	1:I:234:GLN:HG3	2.20	0.41
1:J:142:ARG:O	1:J:146:THR:HG23	2.19	0.41
1:J:181:GLU:OE1	1:J:184:ARG:NH2	2.33	0.41
1:J:221:THR:C	1:J:228:ARG:HH21	2.28	0.41
1:J:266:VAL:HG22	1:J:387:VAL:HG22	2.01	0.41
1:M:154:ARG:NH2	1:O:143:THR:HA	2.34	0.41
1:M:161:LYS:N	1:M:161:LYS:HD3	2.35	0.41
1:O:392:ASN:OD1	1:O:393:TYR:N	2.54	0.41
1:U:160:PRO:HG3	1:V:203:ALA:HB1	2.01	0.41
1:U:230:LEU:O	1:U:234:GLN:HG3	2.21	0.41
1:C:130:VAL:O	1:C:134:ARG:HG2	2.20	0.41
1:E:154:ARG:O	1:E:177:THR:N	2.52	0.41
1:E:265:GLN:HG3	1:F:252:ILE:HB	2.02	0.41
1:K:214:ASP:HB2	1:K:217:GLY:O	2.21	0.41
1:L:141:ALA:O	1:L:144:ILE:N	2.53	0.41
1:T:277:GLN:OE1	1:U:373:ARG:NH1	2.53	0.41
1:V:213:VAL:HG22	1:V:218:HIS:CB	2.51	0.41
1:X:125:GLN:O	1:X:128:GLU:HG2	2.21	0.41
1:X:392:ASN:OD1	1:X:393:TYR:N	2.53	0.41
1:Y:221:THR:C	1:Y:228:ARG:HH21	2.28	0.41
1:Z:91:ASP:HA	1:Z:94:HIS:HD2	1.86	0.41
1:b:175:SER:HB3	1:d:200:SER:OG	2.20	0.41
1:e:377:MET:N	1:e:377:MET:HE2	2.35	0.41
1:B:74:ASN:C	1:B:76:PRO:HD3	2.46	0.41
1:B:132:TYR:HA	1:B:135:ALA:HB3	2.03	0.41
1:I:160:PRO:HG3	1:J:203:ALA:HB1	2.01	0.41
1:O:141:ALA:O	1:O:144:ILE:N	2.54	0.41
1:O:228:ARG:CG	1:P:233:ALA:HB1	2.50	0.41
1:P:426:ARG:NH2	1:P:428:ASP:OD2	2.53	0.41
1:R:142:ARG:HA	1:R:145:GLU:OE1	2.20	0.41
1:W:70:LEU:HD21	1:W:76:PRO:O	2.20	0.41
1:f:144:ILE:HD12	1:f:194:VAL:HG23	2.02	0.41
1:A:125:GLN:O	1:A:129:GLN:HG2	2.20	0.41
1:B:230:LEU:O	1:B:234:GLN:HG3	2.21	0.41
1:C:149:PRO:O	1:C:180:LEU:HD12	2.20	0.41
1:L:220:LEU:HD12	1:L:220:LEU:HA	1.87	0.41
1:M:252:ILE:HG23	1:M:253:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:156:HIS:NE2	1:P:143:THR:OG1	2.42	0.41
1:T:230:LEU:O	1:T:234:GLN:HG3	2.21	0.41
1:T:392:ASN:OD1	1:T:393:TYR:N	2.53	0.41
1:Z:144:ILE:HD12	1:Z:194:VAL:HG23	2.02	0.41
1:b:125:GLN:O	1:b:129:GLN:HG2	2.21	0.41
1:b:396:LEU:H	1:b:396:LEU:HD23	1.85	0.41
1:c:392:ASN:OD1	1:c:393:TYR:N	2.53	0.41
1:d:378:ASN:OD1	1:d:379:VAL:N	2.54	0.41
1:f:139:GLU:O	1:f:143:THR:HG23	2.21	0.41
1:A:130:VAL:O	1:A:134:ARG:HG2	2.21	0.41
1:A:132:TYR:CD2	1:g:126:PHE:HZ	2.39	0.41
1:E:392:ASN:OD1	1:E:393:TYR:N	2.54	0.41
1:I:149:PRO:O	1:I:180:LEU:HD12	2.21	0.41
1:I:228:ARG:NH1	1:I:231:ASN:HD22	2.18	0.41
1:K:171:SER:HA	1:K:172:PRO:HD3	1.98	0.41
1:K:265:GLN:HG3	1:L:252:ILE:HB	2.03	0.41
1:N:139:GLU:O	1:N:143:THR:HG23	2.20	0.41
1:N:393:TYR:CE2	1:N:436:PRO:HD3	2.56	0.41
1:Q:155:VAL:HG13	1:Q:176:VAL:HG22	2.03	0.41
1:Q:219:LEU:C	1:Q:220:LEU:HD12	2.46	0.41
1:Q:420:MET:HE1	1:Q:430:LEU:HD13	2.02	0.41
1:R:253:LEU:HD23	1:R:253:LEU:HA	1.80	0.41
1:T:219:LEU:C	1:T:220:LEU:HD12	2.46	0.41
1:V:252:ILE:HG23	1:V:253:LEU:HD22	2.02	0.41
1:V:378:ASN:OD1	1:V:379:VAL:N	2.54	0.41
1:W:252:ILE:HG23	1:W:253:LEU:HD22	2.02	0.41
1:W:420:MET:HE1	1:W:430:LEU:HD13	2.03	0.41
1:Z:162:PRO:HD2	1:Z:170:LYS:HG3	2.02	0.41
1:a:410:LYS:HZ1	1:a:414:ASP:CG	2.29	0.41
1:b:221:THR:C	1:b:228:ARG:HH21	2.28	0.41
1:c:230:LEU:O	1:c:234:GLN:HG3	2.21	0.41
1:d:392:ASN:OD1	1:d:393:TYR:N	2.54	0.41
1:f:230:LEU:O	1:f:234:GLN:HG3	2.21	0.41
1:f:426:ARG:NH2	1:f:428:ASP:OD2	2.53	0.41
1:g:130:VAL:O	1:g:134:ARG:HG2	2.21	0.41
1:D:151:LYS:HD3	1:D:181:GLU:HG2	2.02	0.41
1:F:199:SER:HA	1:F:205:LEU:HD22	2.03	0.41
1:G:420:MET:HE2	1:G:422:PHE:CD2	2.56	0.41
1:J:224:ASN:HD22	1:K:230:LEU:HA	1.86	0.41
1:Q:230:LEU:O	1:Q:234:GLN:HG3	2.21	0.41
1:W:152:SER:OG	1:W:179:THR:OG1	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:230:LEU:O	1:Z:234:GLN:HG3	2.21	0.41
1:d:125:GLN:O	1:d:128:GLU:HG2	2.21	0.41
1:e:125:GLN:O	1:e:129:GLN:HG2	2.21	0.41
1:f:78:ARG:N	1:f:87:GLU:O	2.53	0.41
1:f:154:ARG:O	1:f:177:THR:N	2.50	0.41
1:g:125:GLN:O	1:g:128:GLU:HG2	2.21	0.41
1:C:392:ASN:OD1	1:C:393:TYR:N	2.53	0.40
1:D:149:PRO:O	1:D:180:LEU:HD12	2.21	0.40
1:H:219:LEU:C	1:H:220:LEU:HD12	2.47	0.40
1:I:378:ASN:OD1	1:I:379:VAL:N	2.54	0.40
1:U:378:ASN:OD1	1:U:379:VAL:N	2.54	0.40
1:U:409:MET:HE2	1:U:434:ASN:HB2	2.02	0.40
1:W:171:SER:HA	1:W:172:PRO:HD3	1.98	0.40
1:B:139:GLU:O	1:B:143:THR:HG23	2.20	0.40
1:D:378:ASN:OD1	1:D:379:VAL:N	2.55	0.40
1:H:392:ASN:OD1	1:H:393:TYR:N	2.54	0.40
1:J:378:ASN:OD1	1:J:379:VAL:N	2.54	0.40
1:V:221:THR:C	1:V:228:ARG:HH21	2.29	0.40
1:V:377:MET:HA	1:V:377:MET:HE3	2.03	0.40
1:c:202:VAL:HB	1:c:205:LEU:HD12	2.04	0.40
1:g:220:LEU:HD12	1:g:220:LEU:HA	1.88	0.40
1:A:213:VAL:HA	1:A:218:HIS:HA	2.02	0.40
1:G:213:VAL:HA	1:G:218:HIS:HA	2.03	0.40
1:I:130:VAL:O	1:I:134:ARG:HG2	2.20	0.40
1:J:426:ARG:NH2	1:J:428:ASP:OD2	2.54	0.40
1:L:183:GLY:C	1:L:184:ARG:HD3	2.46	0.40
1:N:230:LEU:O	1:N:234:GLN:HG3	2.20	0.40
1:S:252:ILE:HG23	1:S:253:LEU:HD22	2.03	0.40
1:S:395:THR:HG22	1:S:401:PRO:N	2.37	0.40
1:U:276:GLU:HG2	1:U:376:LYS:HG2	2.02	0.40
1:Z:266:VAL:HG22	1:Z:387:VAL:HG22	2.03	0.40
1:g:183:GLY:C	1:g:184:ARG:HD3	2.45	0.40
1:N:212:LEU:O	1:N:220:LEU:HD11	2.20	0.40
1:O:130:VAL:O	1:O:134:ARG:HG2	2.21	0.40
1:Q:139:GLU:O	1:Q:143:THR:HG23	2.22	0.40
1:W:139:GLU:O	1:W:143:THR:HG23	2.22	0.40
1:a:183:GLY:C	1:a:184:ARG:HD3	2.46	0.40
1:c:212:LEU:O	1:c:220:LEU:HD11	2.22	0.40
1:e:378:ASN:OD1	1:e:379:VAL:N	2.55	0.40
1:f:219:LEU:C	1:f:220:LEU:HD12	2.46	0.40
1:C:152:SER:OG	1:C:153:ALA:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:213:VAL:HA	1:D:218:HIS:HA	2.02	0.40
1:E:219:LEU:C	1:E:220:LEU:HD12	2.47	0.40
1:G:149:PRO:O	1:G:180:LEU:HD12	2.21	0.40
1:J:224:ASN:HD21	1:K:230:LEU:HD13	1.86	0.40
1:P:154:ARG:NH1	1:R:143:THR:HA	2.36	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	250/560 (45%)	240 (96%)	10 (4%)	0	100	100
1	B	300/560 (54%)	284 (95%)	16 (5%)	0	100	100
1	C	250/560 (45%)	241 (96%)	9 (4%)	0	100	100
1	D	250/560 (45%)	239 (96%)	11 (4%)	0	100	100
1	E	300/560 (54%)	284 (95%)	16 (5%)	0	100	100
1	F	250/560 (45%)	240 (96%)	10 (4%)	0	100	100
1	G	250/560 (45%)	239 (96%)	11 (4%)	0	100	100
1	H	300/560 (54%)	285 (95%)	15 (5%)	0	100	100
1	I	250/560 (45%)	239 (96%)	11 (4%)	0	100	100
1	J	250/560 (45%)	238 (95%)	12 (5%)	0	100	100
1	K	300/560 (54%)	282 (94%)	18 (6%)	0	100	100
1	L	250/560 (45%)	240 (96%)	10 (4%)	0	100	100
1	M	250/560 (45%)	235 (94%)	15 (6%)	0	100	100
1	N	300/560 (54%)	283 (94%)	17 (6%)	0	100	100
1	O	250/560 (45%)	241 (96%)	9 (4%)	0	100	100
1	P	250/560 (45%)	241 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	300/560 (54%)	284 (95%)	16 (5%)	0	100	100
1	R	250/560 (45%)	240 (96%)	10 (4%)	0	100	100
1	S	250/560 (45%)	241 (96%)	9 (4%)	0	100	100
1	T	300/560 (54%)	285 (95%)	15 (5%)	0	100	100
1	U	250/560 (45%)	241 (96%)	9 (4%)	0	100	100
1	V	250/560 (45%)	240 (96%)	10 (4%)	0	100	100
1	W	300/560 (54%)	285 (95%)	15 (5%)	0	100	100
1	X	250/560 (45%)	240 (96%)	10 (4%)	0	100	100
1	Y	250/560 (45%)	239 (96%)	11 (4%)	0	100	100
1	Z	300/560 (54%)	285 (95%)	15 (5%)	0	100	100
1	a	250/560 (45%)	240 (96%)	10 (4%)	0	100	100
1	b	250/560 (45%)	239 (96%)	11 (4%)	0	100	100
1	c	300/560 (54%)	286 (95%)	14 (5%)	0	100	100
1	d	250/560 (45%)	242 (97%)	8 (3%)	0	100	100
1	e	250/560 (45%)	241 (96%)	9 (4%)	0	100	100
1	f	300/560 (54%)	284 (95%)	16 (5%)	0	100	100
1	g	250/560 (45%)	239 (96%)	11 (4%)	0	100	100
All	All	8800/18480 (48%)	8402 (96%)	398 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	A	223/467 (48%)	222 (100%)	1 (0%)	84	86
1	B	260/467 (56%)	260 (100%)	0	100	100
1	C	223/467 (48%)	223 (100%)	0	100	100
1	D	223/467 (48%)	222 (100%)	1 (0%)	84	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	260/467 (56%)	260 (100%)	0	100	100
1	F	223/467 (48%)	223 (100%)	0	100	100
1	G	222/467 (48%)	222 (100%)	0	100	100
1	H	260/467 (56%)	260 (100%)	0	100	100
1	I	223/467 (48%)	223 (100%)	0	100	100
1	J	223/467 (48%)	222 (100%)	1 (0%)	84	86
1	K	260/467 (56%)	260 (100%)	0	100	100
1	L	223/467 (48%)	223 (100%)	0	100	100
1	M	223/467 (48%)	222 (100%)	1 (0%)	84	86
1	N	260/467 (56%)	260 (100%)	0	100	100
1	O	223/467 (48%)	223 (100%)	0	100	100
1	P	222/467 (48%)	222 (100%)	0	100	100
1	Q	260/467 (56%)	260 (100%)	0	100	100
1	R	223/467 (48%)	223 (100%)	0	100	100
1	S	223/467 (48%)	222 (100%)	1 (0%)	84	86
1	T	260/467 (56%)	260 (100%)	0	100	100
1	U	223/467 (48%)	223 (100%)	0	100	100
1	V	223/467 (48%)	222 (100%)	1 (0%)	84	86
1	W	260/467 (56%)	260 (100%)	0	100	100
1	X	223/467 (48%)	223 (100%)	0	100	100
1	Y	223/467 (48%)	222 (100%)	1 (0%)	84	86
1	Z	260/467 (56%)	260 (100%)	0	100	100
1	a	223/467 (48%)	223 (100%)	0	100	100
1	b	223/467 (48%)	222 (100%)	1 (0%)	84	86
1	c	260/467 (56%)	260 (100%)	0	100	100
1	d	223/467 (48%)	223 (100%)	0	100	100
1	e	223/467 (48%)	222 (100%)	1 (0%)	84	86
1	f	260/467 (56%)	260 (100%)	0	100	100
1	g	223/467 (48%)	223 (100%)	0	100	100
All	All	7764/15411 (50%)	7755 (100%)	9 (0%)	87	90

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	186	LEU
1	D	186	LEU
1	J	186	LEU
1	M	186	LEU
1	S	186	LEU
1	V	186	LEU
1	Y	186	LEU
1	b	186	LEU
1	e	186	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	431	ASN
1	B	103	GLN
1	B	196	HIS
1	B	431	ASN
1	C	215	GLN
1	D	434	ASN
1	E	103	GLN
1	E	196	HIS
1	G	133	GLN
1	H	94	HIS
1	H	103	GLN
1	H	196	HIS
1	H	431	ASN
1	I	215	GLN
1	I	231	ASN
1	J	224	ASN
1	J	431	ASN
1	K	196	HIS
1	L	133	GLN
1	L	215	GLN
1	L	431	ASN
1	M	133	GLN
1	M	224	ASN
1	M	431	ASN
1	N	103	GLN
1	P	133	GLN
1	P	224	ASN
1	P	431	ASN
1	Q	103	GLN
1	Q	431	ASN

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Mol	Chain	Res	Type
1	R	133	GLN
1	R	231	ASN
1	R	431	ASN
1	S	133	GLN
1	T	103	GLN
1	T	156	HIS
1	T	431	ASN
1	U	431	ASN
1	V	431	ASN
1	W	411	GLN
1	W	431	ASN
1	Y	431	ASN
1	Z	103	GLN
1	Z	196	HIS
1	b	133	GLN
1	b	259	ASN
1	b	431	ASN
1	e	133	GLN
1	e	431	ASN
1	g	215	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.

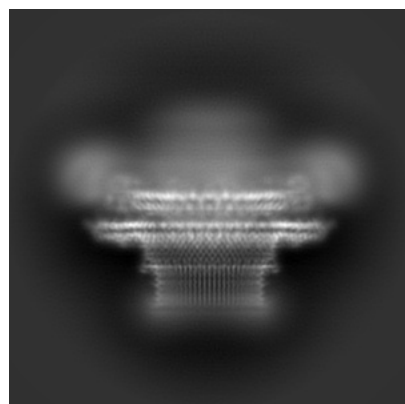
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60007. These allow visual inspection of the internal detail of the map and identification of artifacts.

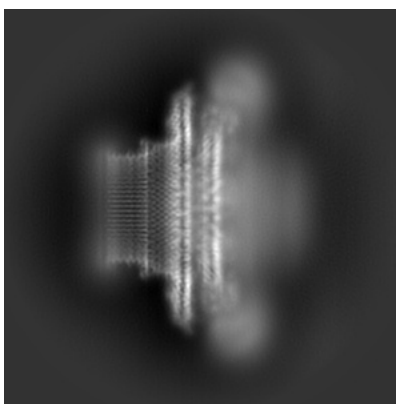
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

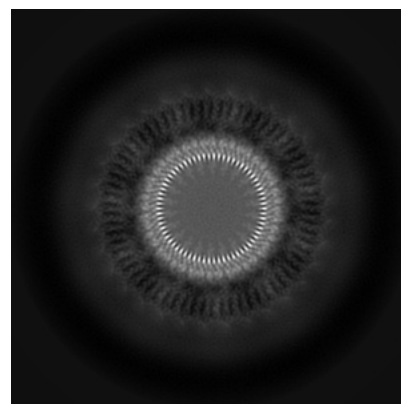
6.1.1 Primary map



X

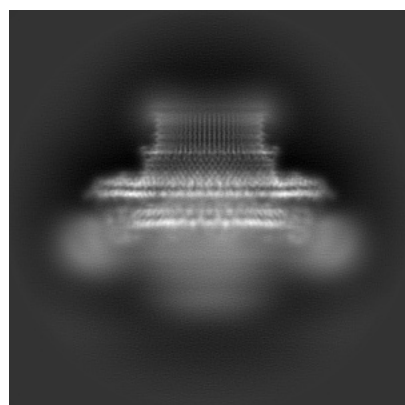


Y

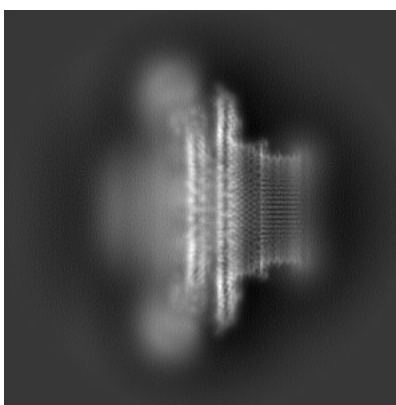


Z

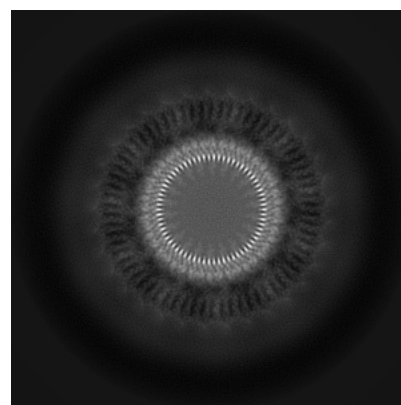
6.1.2 Raw map



X



Y

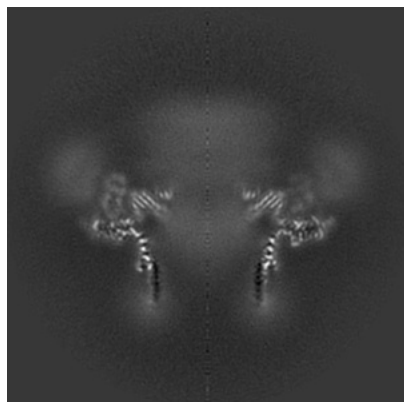


Z

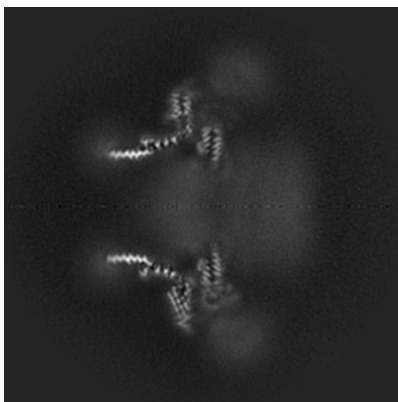
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

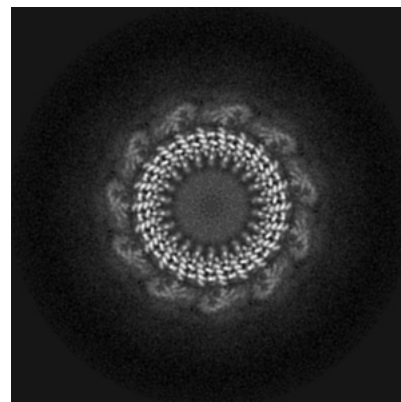
6.2.1 Primary map



X Index: 200

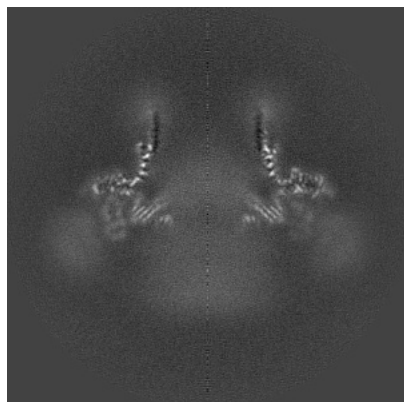


Y Index: 200

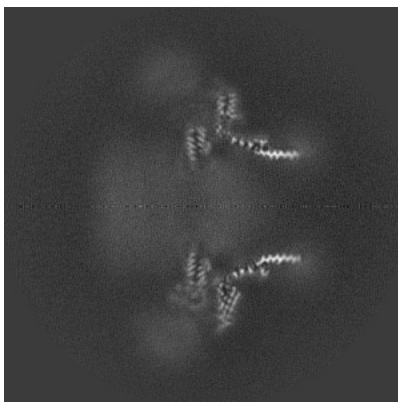


Z Index: 200

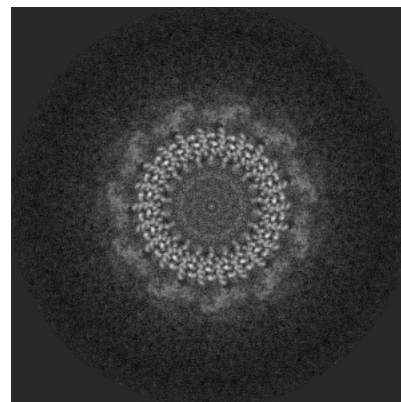
6.2.2 Raw map



X Index: 200



Y Index: 200

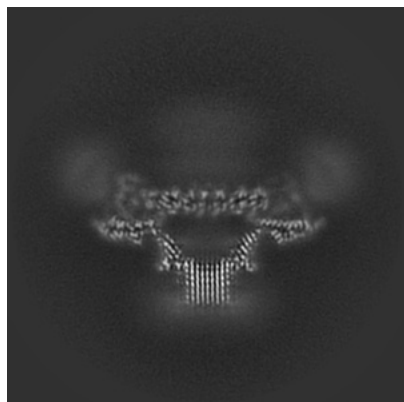


Z Index: 200

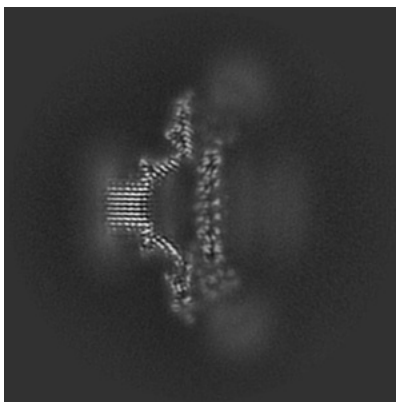
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

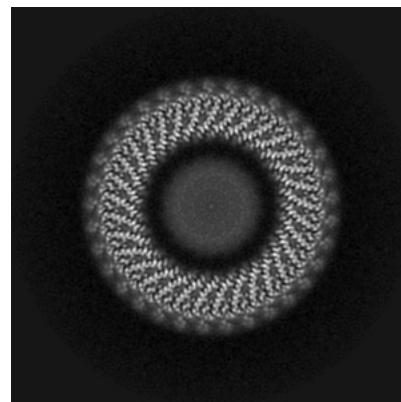
6.3.1 Primary map



X Index: 149

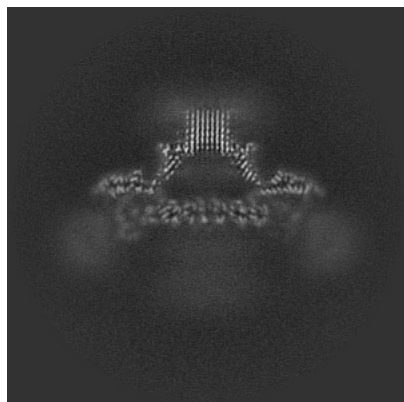


Y Index: 251

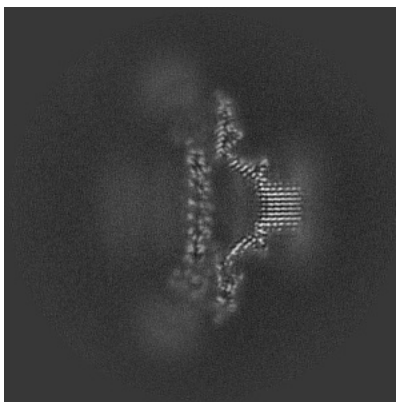


Z Index: 183

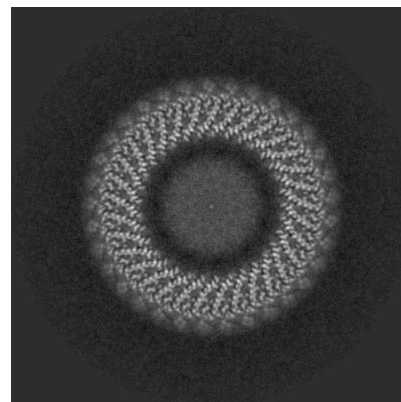
6.3.2 Raw map



X Index: 149



Y Index: 251

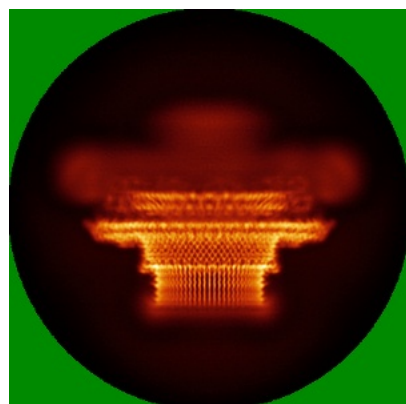


Z Index: 216

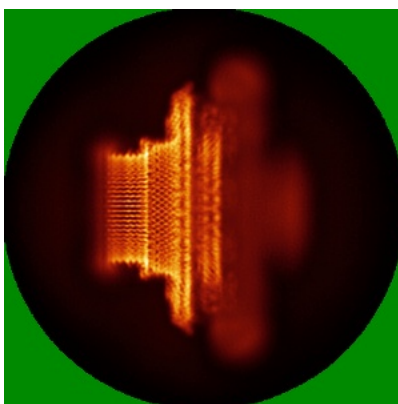
The images above show the largest variance slices of the map in three orthogonal directions.

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

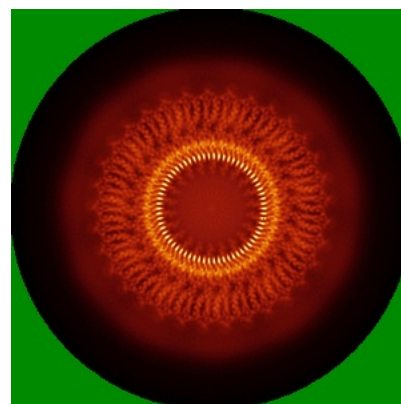
6.4.1 Primary map



X

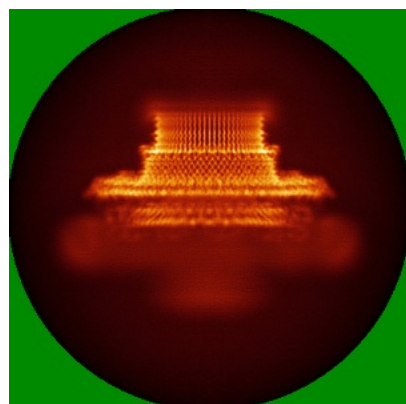


Y

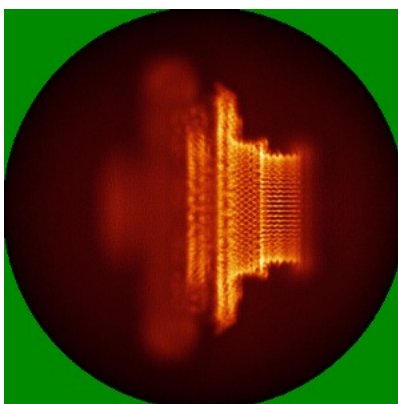


Z

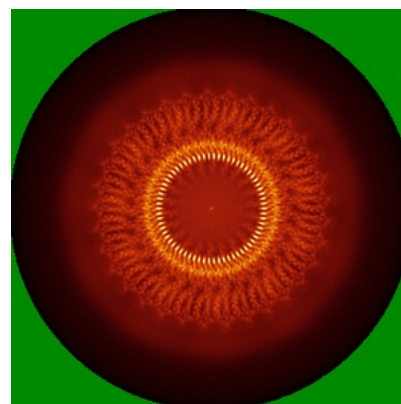
6.4.2 Raw map



X



Y

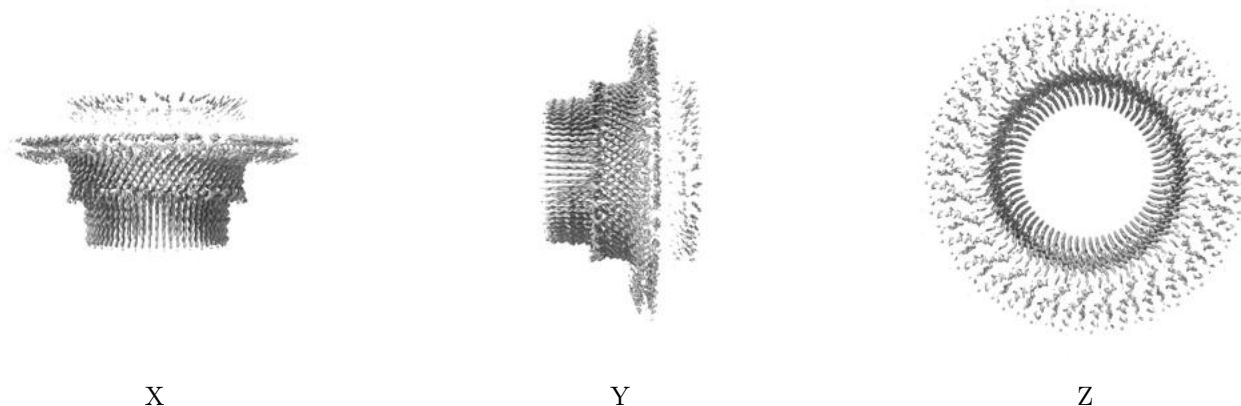


Z

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 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

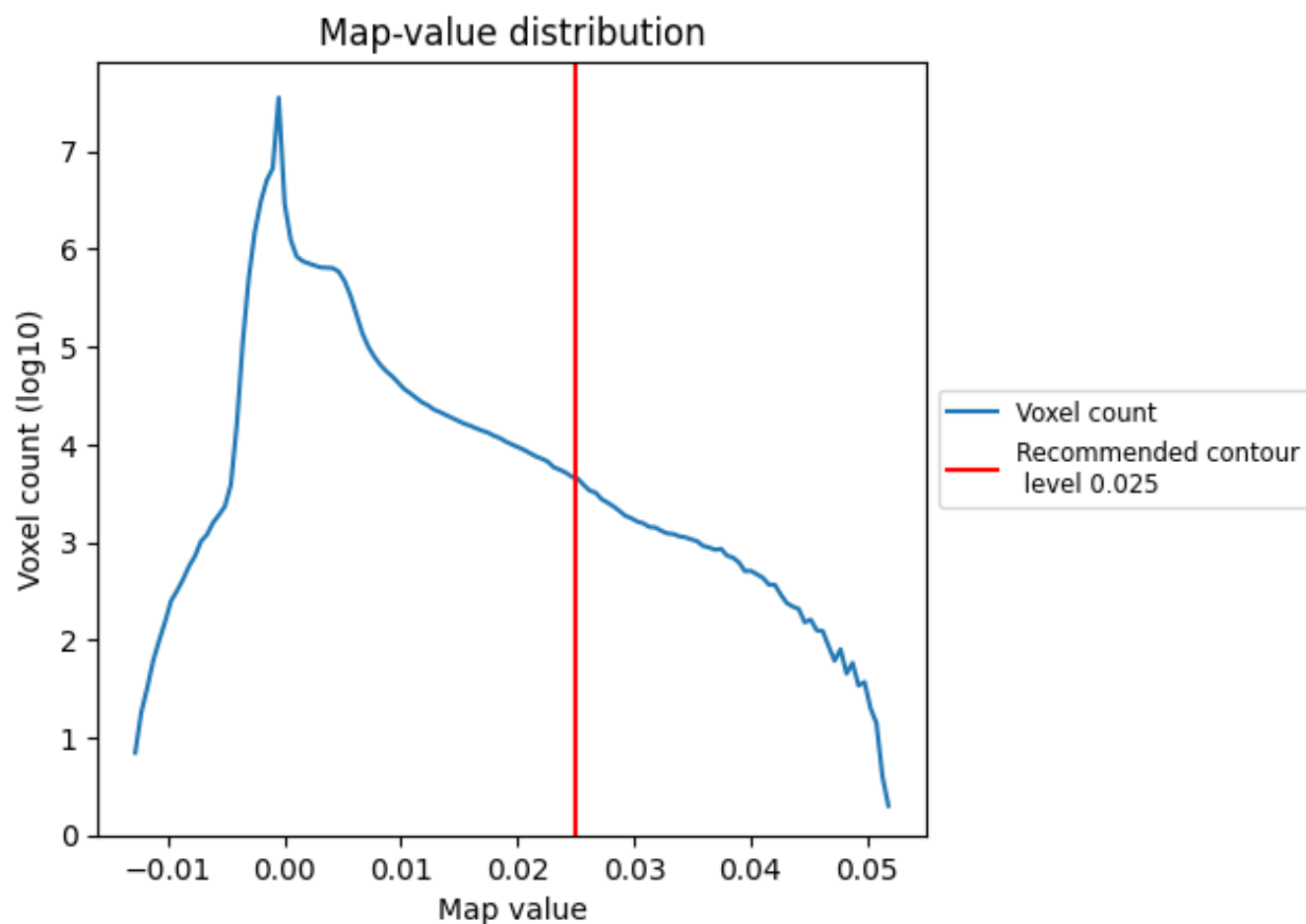
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

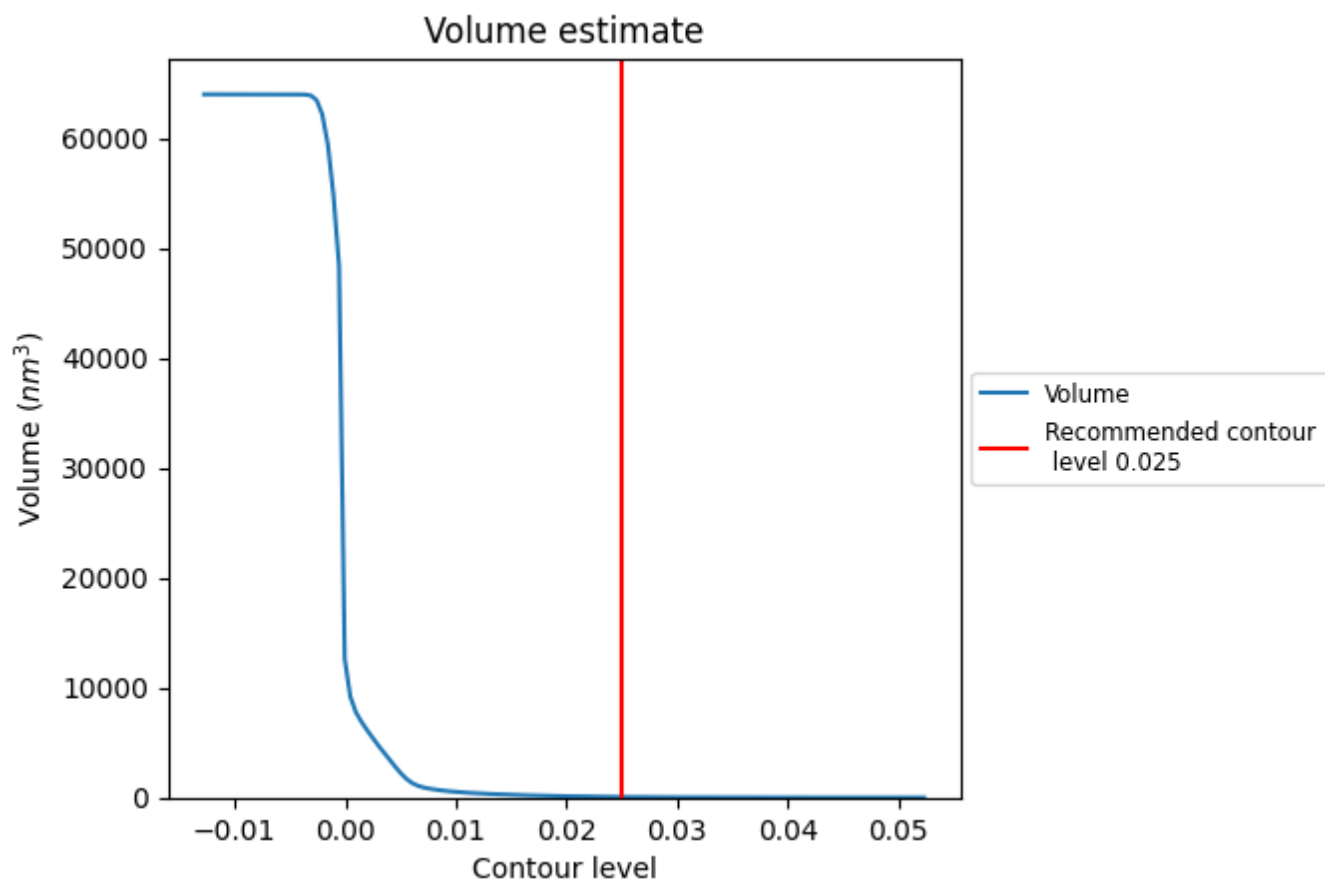
This section contains the results of statistical analysis of the map.

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.

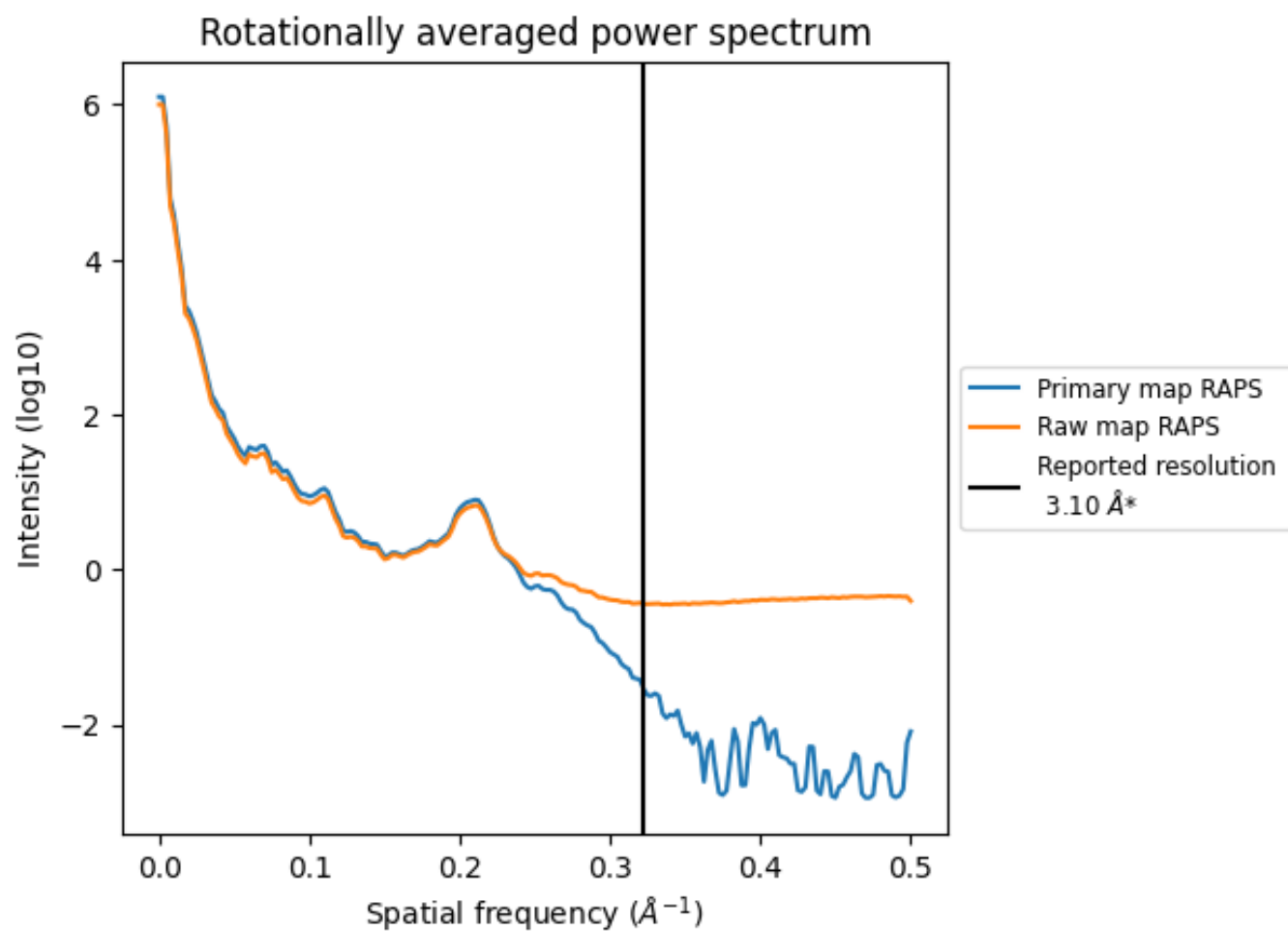
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 54 nm³; this corresponds to an approximate mass of 49 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 ⓘ

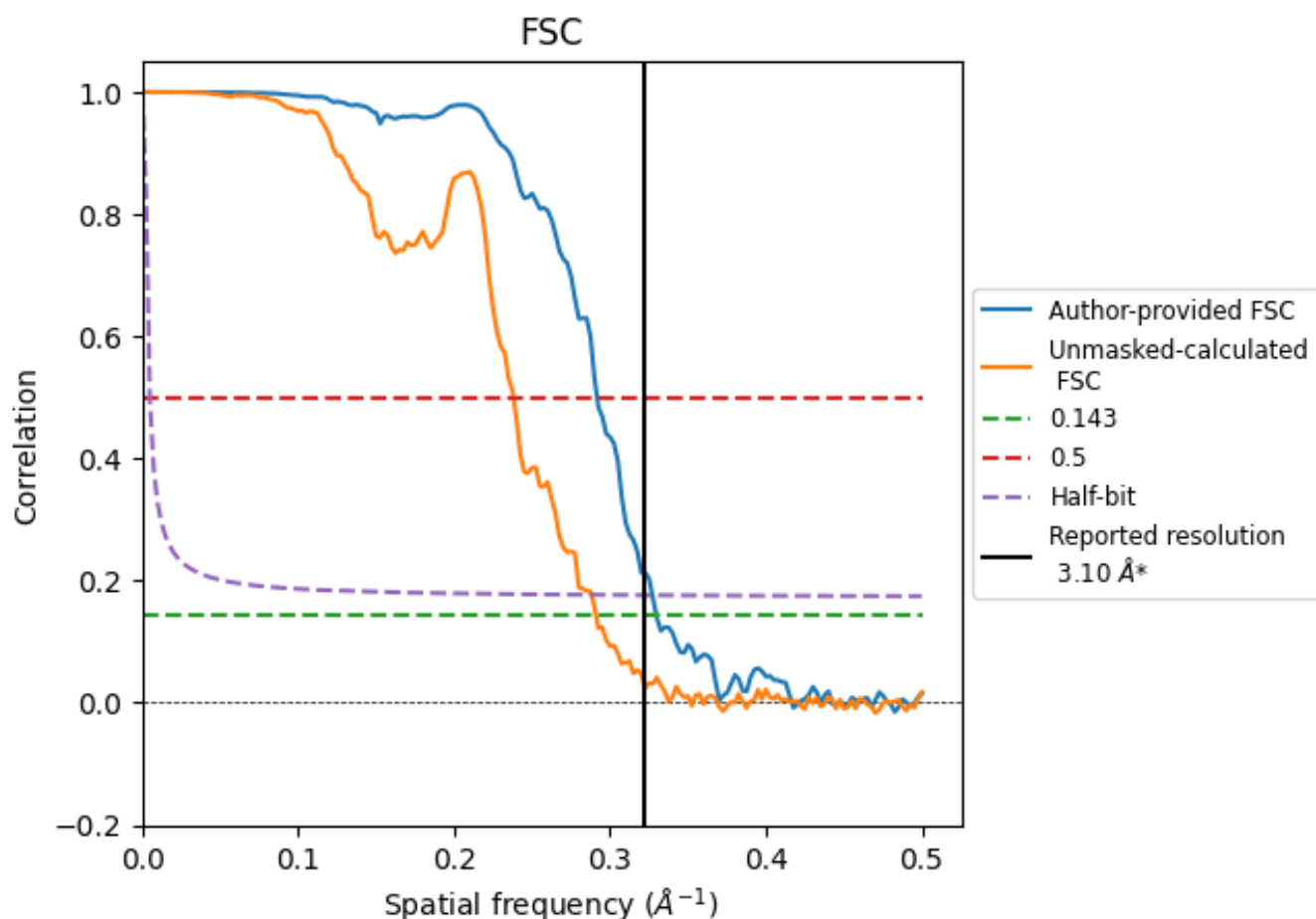


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 0.323 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

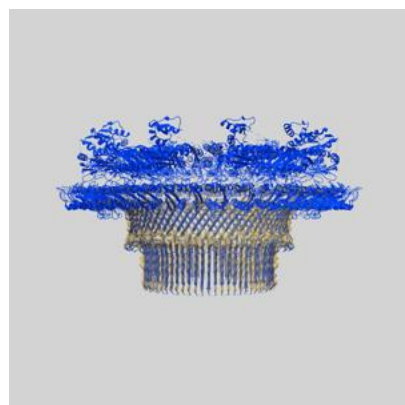
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.03	3.43	3.06
Unmasked-calculated*	3.44	4.20	3.47

*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 3.44 differs from the reported value 3.1 by more than 10 %

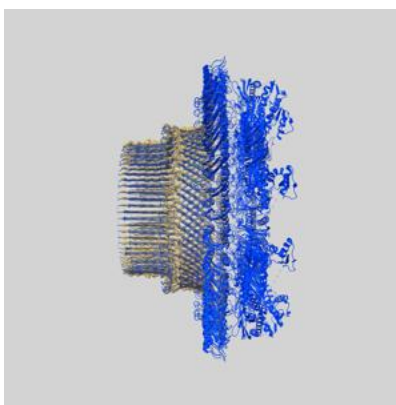
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-60007 and PDB model 8ZDS. Per-residue inclusion information can be found in section [3](#) on page [7](#).

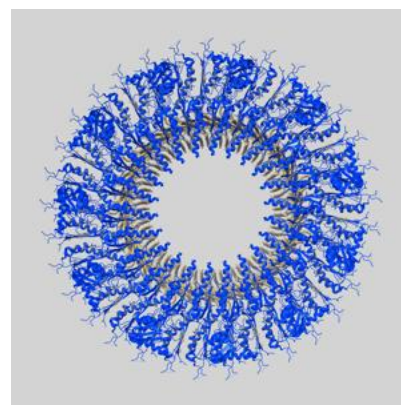
9.1 Map-model overlay [i](#)



X



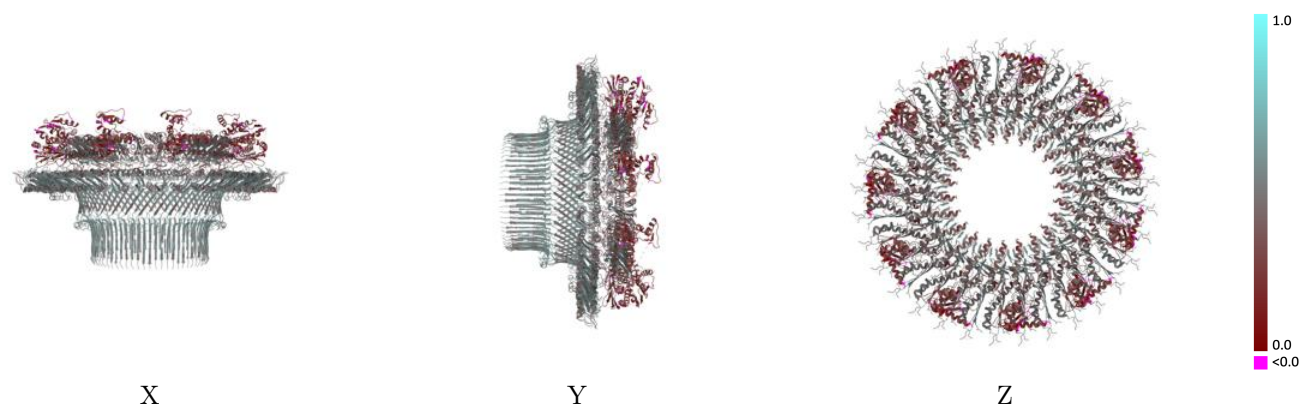
Y



Z

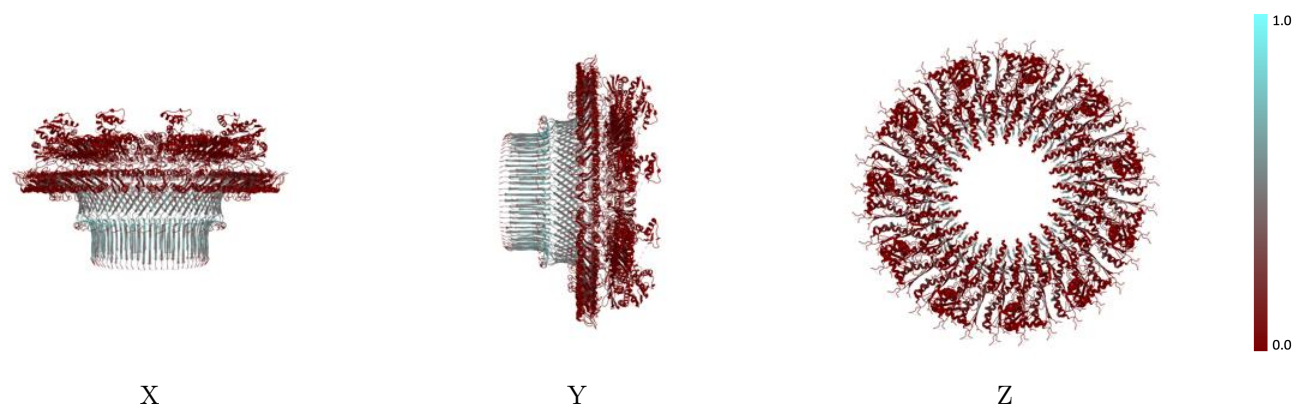
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



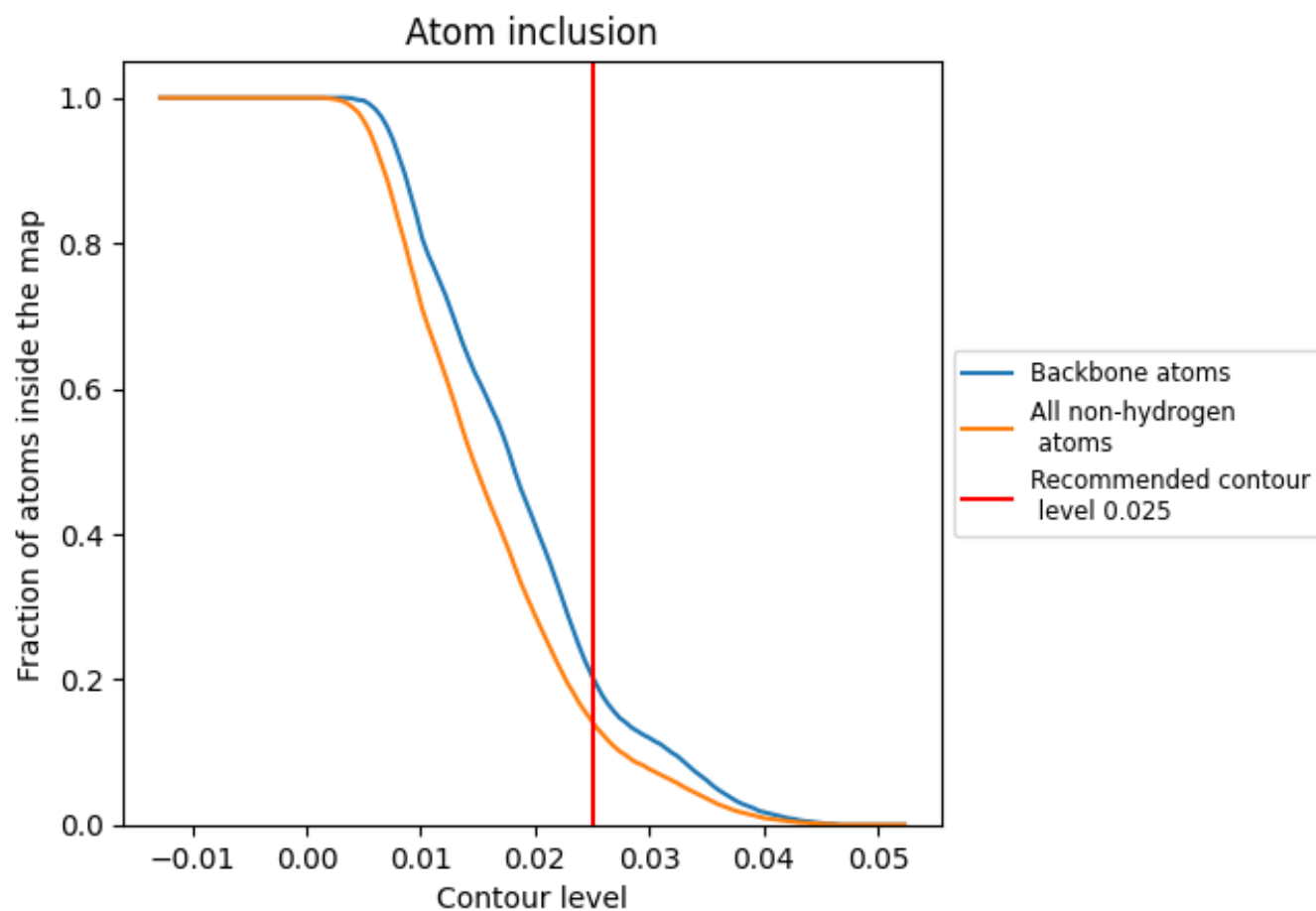
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 20% of all backbone atoms, 14% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.1420	 0.4300
A	 0.1580	 0.4660
B	 0.1260	 0.3720
C	 0.1510	 0.4630
D	 0.1510	 0.4650
E	 0.1260	 0.3710
F	 0.1500	 0.4640
G	 0.1500	 0.4650
H	 0.1260	 0.3720
I	 0.1540	 0.4610
J	 0.1570	 0.4670
K	 0.1270	 0.3710
L	 0.1520	 0.4620
M	 0.1510	 0.4630
N	 0.1260	 0.3720
O	 0.1530	 0.4620
P	 0.1540	 0.4660
Q	 0.1240	 0.3750
R	 0.1510	 0.4640
S	 0.1490	 0.4670
T	 0.1230	 0.3760
U	 0.1460	 0.4630
V	 0.1490	 0.4660
W	 0.1240	 0.3780
X	 0.1500	 0.4650
Y	 0.1490	 0.4660
Z	 0.1240	 0.3730
a	 0.1520	 0.4630
b	 0.1530	 0.4670
c	 0.1260	 0.3750
d	 0.1530	 0.4640
e	 0.1520	 0.4650
f	 0.1240	 0.3720
g	 0.1540	 0.4640

