



wwPDB EM Validation Summary Report ⓘ

Oct 5, 2024 – 04:54 PM EDT

PDB ID : 5WDA
EMDB ID : EMD-8812
Title : Structure of the PulG pseudopilus
Authors : Lopez-Castilla, A.; Thomassin, J.L.; Bardiaux, B.; Zheng, W.; Nivaskumar, M.; Yu, X.; Nilges, M.; Egelman, E.H.; Izadi-Pruneyre, N.; Francetic, O.
Deposited on : 2017-07-04
Resolution : 5.00 Å(reported)

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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.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

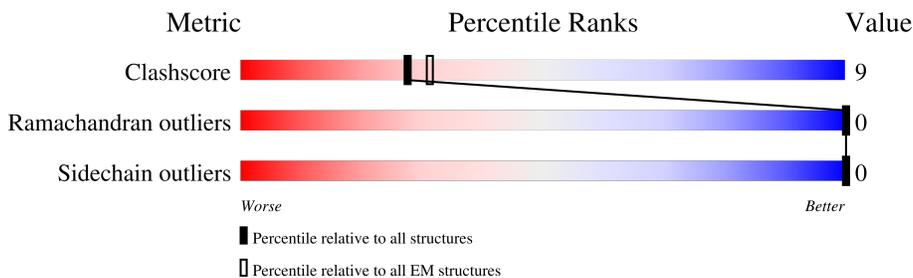
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.00 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	134	<div style="display: flex; justify-content: space-between;"> 33% 76% 21% </div>
1	B	134	<div style="display: flex; justify-content: space-between;"> 31% 74% 22% </div>
1	C	134	<div style="display: flex; justify-content: space-between;"> 32% 74% 22% </div>
1	D	134	<div style="display: flex; justify-content: space-between;"> 31% 73% 23% </div>
1	E	134	<div style="display: flex; justify-content: space-between;"> 30% 75% 22% </div>
1	F	134	<div style="display: flex; justify-content: space-between;"> 29% 73% 23% </div>
1	G	134	<div style="display: flex; justify-content: space-between;"> 29% 73% 23% </div>
1	H	134	<div style="display: flex; justify-content: space-between;"> 29% 74% 23% </div>

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Mol	Chain	Length	Quality of chain	
1	I	134	30%	72% 24% ..
1	J	134	25%	74% 23% .
1	K	134	28%	73% 23% ..
1	L	134	28%	74% 22% ..
1	M	134	28%	72% 24% ..
1	N	134	27%	73% 24% .
1	O	134	27%	73% 23% ..
1	P	134	28%	73% 23% ..
1	Q	134	25%	74% 23% .
1	R	134	25%	75% 22% .
1	S	134	25%	73% 23% ..
1	T	134	23%	73% 23% ..
1	U	134	22%	74% 23% .
1	V	134	24%	73% 23% ..
1	W	134	23%	75% 22% .
1	X	134	23%	73% 23% ..
1	Y	134	28%	76% 20% ..

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 49150 atoms, of which 24425 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 General secretion pathway protein G.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	130	1965	623	977	165	195	5	0	0
1	B	130	1965	623	977	165	195	5	0	0
1	C	130	1965	623	977	165	195	5	0	0
1	D	130	1965	623	977	165	195	5	0	0
1	E	130	1965	623	977	165	195	5	0	0
1	F	130	1965	623	977	165	195	5	0	0
1	G	130	1965	623	977	165	195	5	0	0
1	H	130	1965	623	977	165	195	5	0	0
1	I	130	1965	623	977	165	195	5	0	0
1	J	130	1965	623	977	165	195	5	0	0
1	K	130	1965	623	977	165	195	5	0	0
1	L	130	1965	623	977	165	195	5	0	0
1	M	130	1965	623	977	165	195	5	0	0
1	N	130	1965	623	977	165	195	5	0	0
1	O	130	1965	623	977	165	195	5	0	0
1	P	130	1965	623	977	165	195	5	0	0
1	Q	130	1965	623	977	165	195	5	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	R	130	1965	623	977	165	195	5	0	0
1	S	130	1965	623	977	165	195	5	0	0
1	T	130	1965	623	977	165	195	5	0	0
1	U	130	1965	623	977	165	195	5	0	0
1	V	130	1965	623	977	165	195	5	0	0
1	W	130	1965	623	977	165	195	5	0	0
1	X	130	1965	623	977	165	195	5	0	0
1	Y	130	1965	623	977	165	195	5	0	0

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	106	CYS	HIS	conflict	UNP A0A0G3SCW3
A	129	CYS	TRP	conflict	UNP A0A0G3SCW3
B	106	CYS	HIS	conflict	UNP A0A0G3SCW3
B	129	CYS	TRP	conflict	UNP A0A0G3SCW3
C	106	CYS	HIS	conflict	UNP A0A0G3SCW3
C	129	CYS	TRP	conflict	UNP A0A0G3SCW3
D	106	CYS	HIS	conflict	UNP A0A0G3SCW3
D	129	CYS	TRP	conflict	UNP A0A0G3SCW3
E	106	CYS	HIS	conflict	UNP A0A0G3SCW3
E	129	CYS	TRP	conflict	UNP A0A0G3SCW3
F	106	CYS	HIS	conflict	UNP A0A0G3SCW3
F	129	CYS	TRP	conflict	UNP A0A0G3SCW3
G	106	CYS	HIS	conflict	UNP A0A0G3SCW3
G	129	CYS	TRP	conflict	UNP A0A0G3SCW3
H	106	CYS	HIS	conflict	UNP A0A0G3SCW3
H	129	CYS	TRP	conflict	UNP A0A0G3SCW3
I	106	CYS	HIS	conflict	UNP A0A0G3SCW3
I	129	CYS	TRP	conflict	UNP A0A0G3SCW3
J	106	CYS	HIS	conflict	UNP A0A0G3SCW3
J	129	CYS	TRP	conflict	UNP A0A0G3SCW3
K	106	CYS	HIS	conflict	UNP A0A0G3SCW3
K	129	CYS	TRP	conflict	UNP A0A0G3SCW3
L	106	CYS	HIS	conflict	UNP A0A0G3SCW3

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Chain	Residue	Modelled	Actual	Comment	Reference
L	129	CYS	TRP	conflict	UNP A0A0G3SCW3
M	106	CYS	HIS	conflict	UNP A0A0G3SCW3
M	129	CYS	TRP	conflict	UNP A0A0G3SCW3
N	106	CYS	HIS	conflict	UNP A0A0G3SCW3
N	129	CYS	TRP	conflict	UNP A0A0G3SCW3
O	106	CYS	HIS	conflict	UNP A0A0G3SCW3
O	129	CYS	TRP	conflict	UNP A0A0G3SCW3
P	106	CYS	HIS	conflict	UNP A0A0G3SCW3
P	129	CYS	TRP	conflict	UNP A0A0G3SCW3
Q	106	CYS	HIS	conflict	UNP A0A0G3SCW3
Q	129	CYS	TRP	conflict	UNP A0A0G3SCW3
R	106	CYS	HIS	conflict	UNP A0A0G3SCW3
R	129	CYS	TRP	conflict	UNP A0A0G3SCW3
S	106	CYS	HIS	conflict	UNP A0A0G3SCW3
S	129	CYS	TRP	conflict	UNP A0A0G3SCW3
T	106	CYS	HIS	conflict	UNP A0A0G3SCW3
T	129	CYS	TRP	conflict	UNP A0A0G3SCW3
U	106	CYS	HIS	conflict	UNP A0A0G3SCW3
U	129	CYS	TRP	conflict	UNP A0A0G3SCW3
V	106	CYS	HIS	conflict	UNP A0A0G3SCW3
V	129	CYS	TRP	conflict	UNP A0A0G3SCW3
W	106	CYS	HIS	conflict	UNP A0A0G3SCW3
W	129	CYS	TRP	conflict	UNP A0A0G3SCW3
X	106	CYS	HIS	conflict	UNP A0A0G3SCW3
X	129	CYS	TRP	conflict	UNP A0A0G3SCW3
Y	106	CYS	HIS	conflict	UNP A0A0G3SCW3
Y	129	CYS	TRP	conflict	UNP A0A0G3SCW3

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	AltConf
2	A	1	Total Ca 1 1	0
2	B	1	Total Ca 1 1	0
2	C	1	Total Ca 1 1	0
2	D	1	Total Ca 1 1	0
2	E	1	Total Ca 1 1	0
2	F	1	Total Ca 1 1	0

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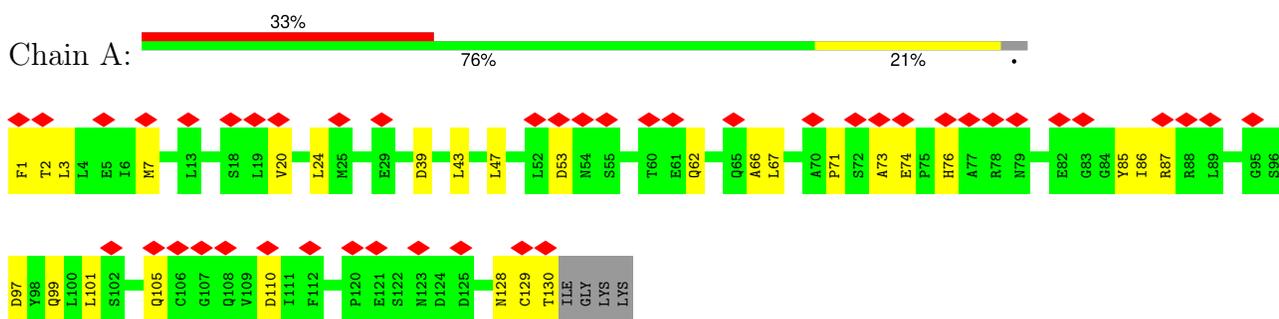
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Mol	Chain	Residues	Atoms		AltConf
2	G	1	Total 1	Ca 1	0
2	H	1	Total 1	Ca 1	0
2	I	1	Total 1	Ca 1	0
2	J	1	Total 1	Ca 1	0
2	K	1	Total 1	Ca 1	0
2	L	1	Total 1	Ca 1	0
2	M	1	Total 1	Ca 1	0
2	N	1	Total 1	Ca 1	0
2	O	1	Total 1	Ca 1	0
2	P	1	Total 1	Ca 1	0
2	Q	1	Total 1	Ca 1	0
2	R	1	Total 1	Ca 1	0
2	S	1	Total 1	Ca 1	0
2	T	1	Total 1	Ca 1	0
2	U	1	Total 1	Ca 1	0
2	V	1	Total 1	Ca 1	0
2	W	1	Total 1	Ca 1	0
2	X	1	Total 1	Ca 1	0
2	Y	1	Total 1	Ca 1	0

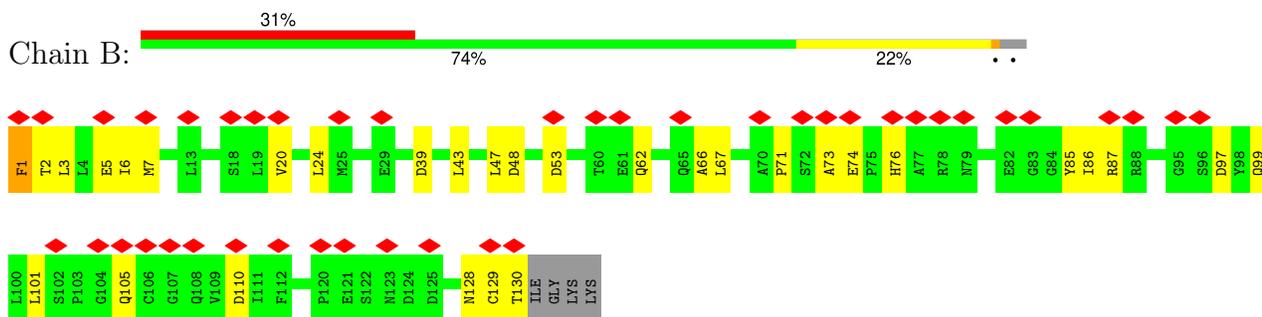
3 Residue-property plots [i](#)

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.

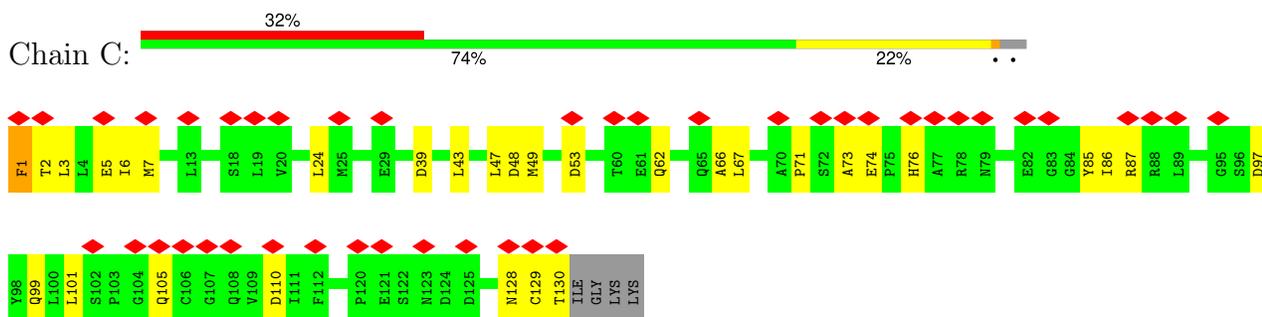
- Molecule 1: General secretion pathway protein G



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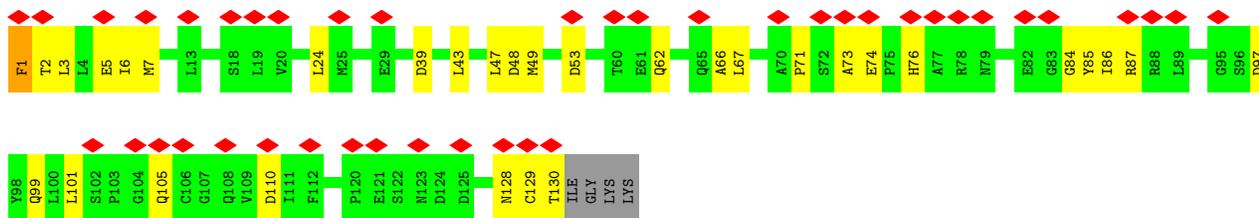


- Molecule 1: General secretion pathway protein G

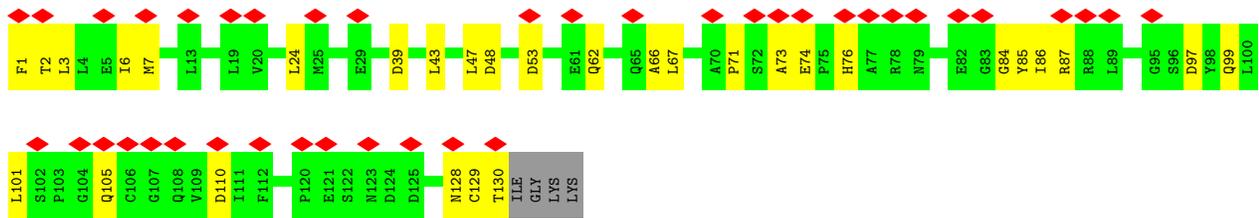
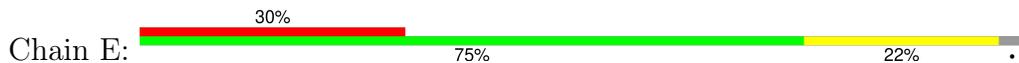


- Molecule 1: General secretion pathway protein G

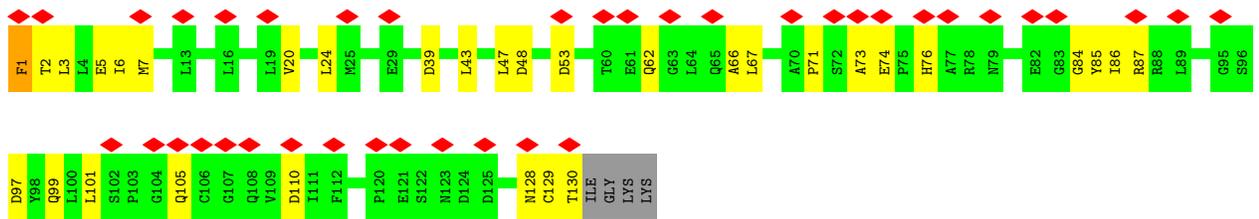




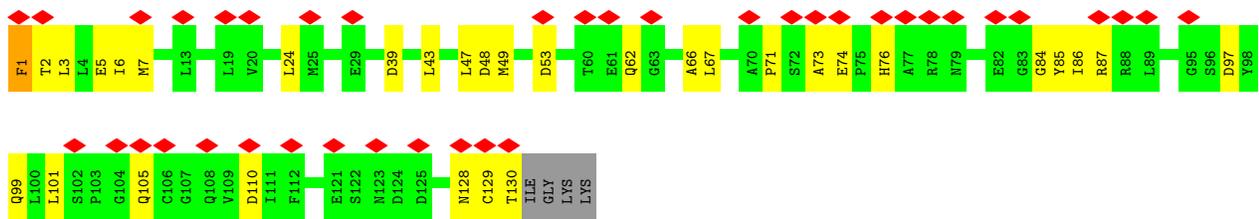
• Molecule 1: General secretion pathway protein G



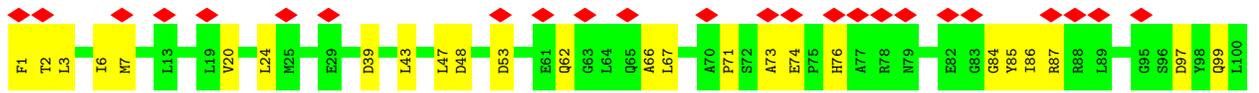
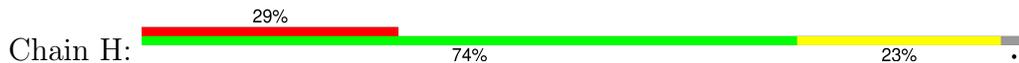
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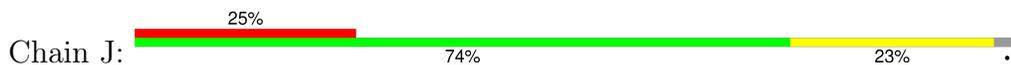




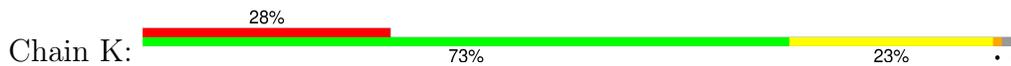
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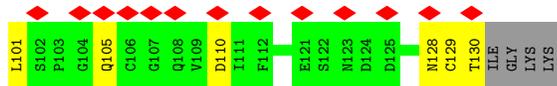
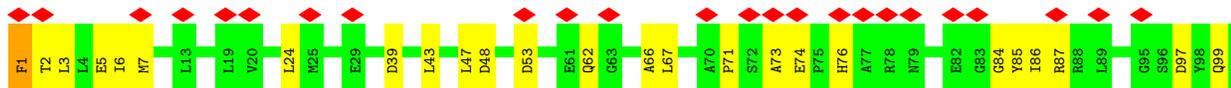
• Molecule 1: General secretion pathway protein G



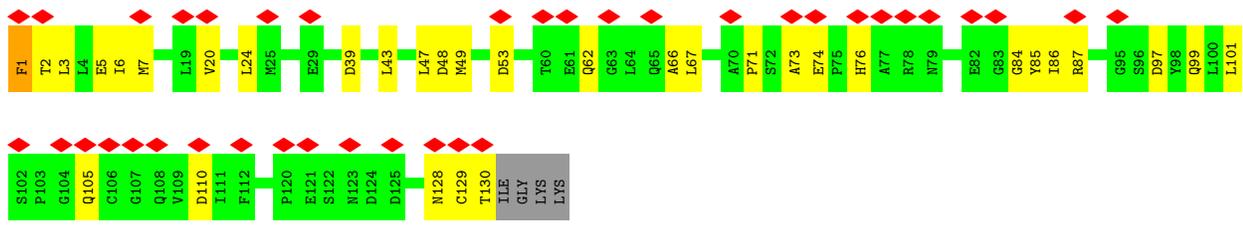
• Molecule 1: General secretion pathway protein G



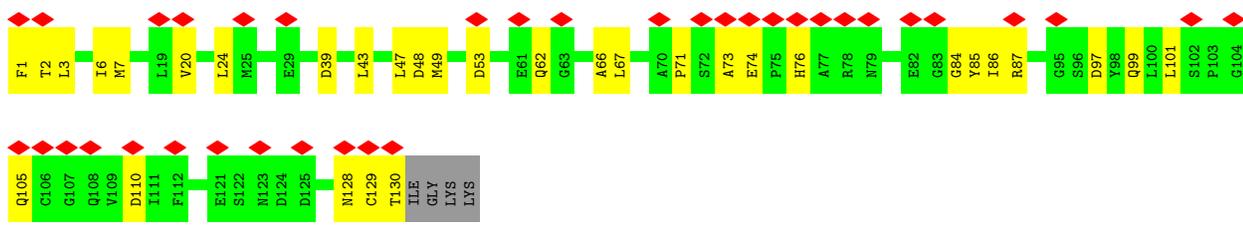
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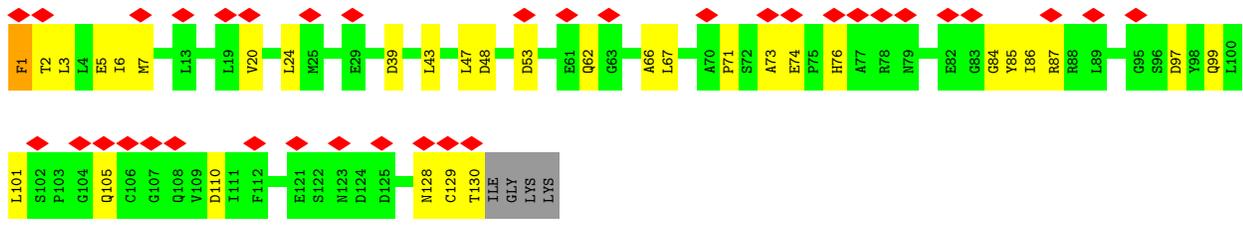
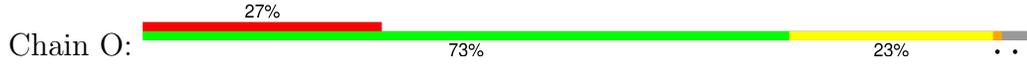
• Molecule 1: General secretion pathway protein G



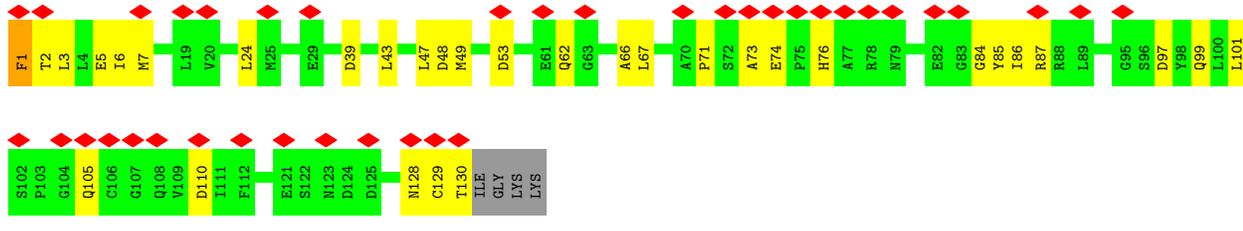
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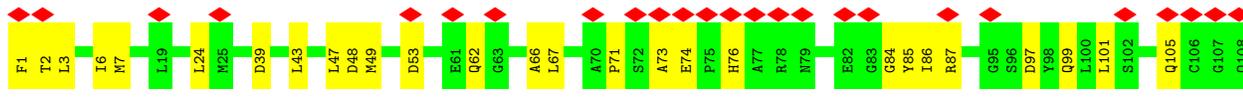
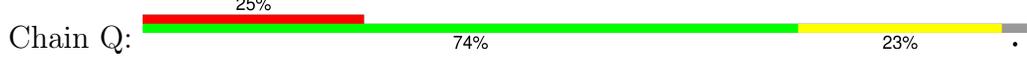
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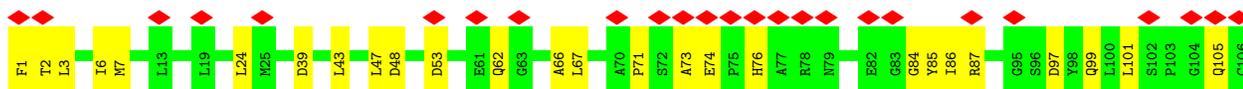
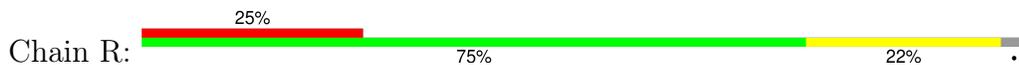


• Molecule 1: General secretion pathway protein G





• Molecule 1: General secretion pathway protein G



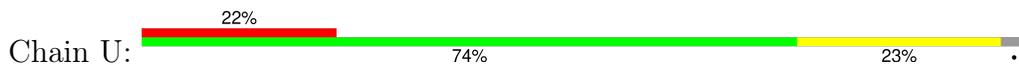
• Molecule 1: General secretion pathway protein G



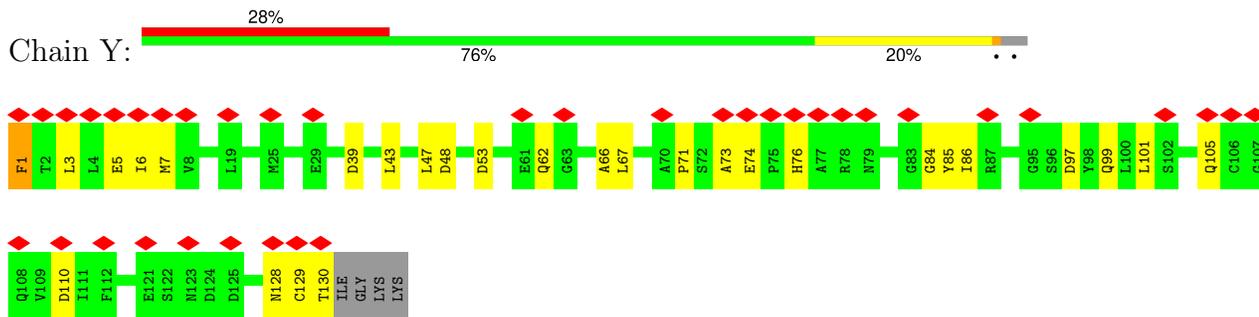
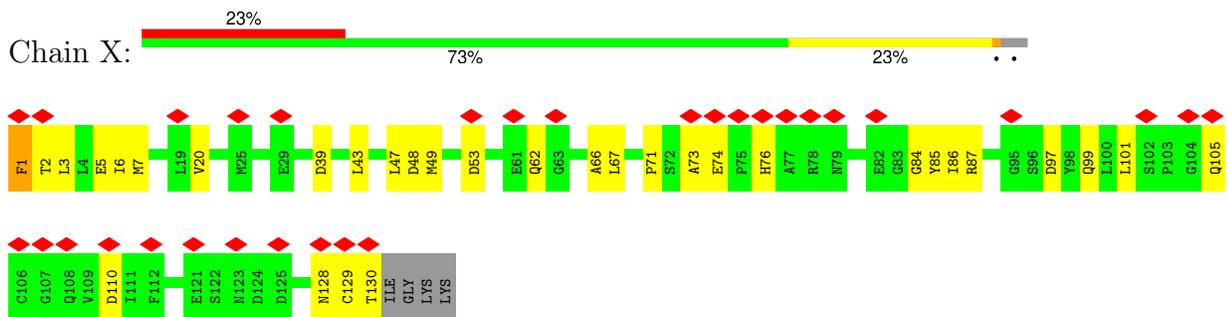
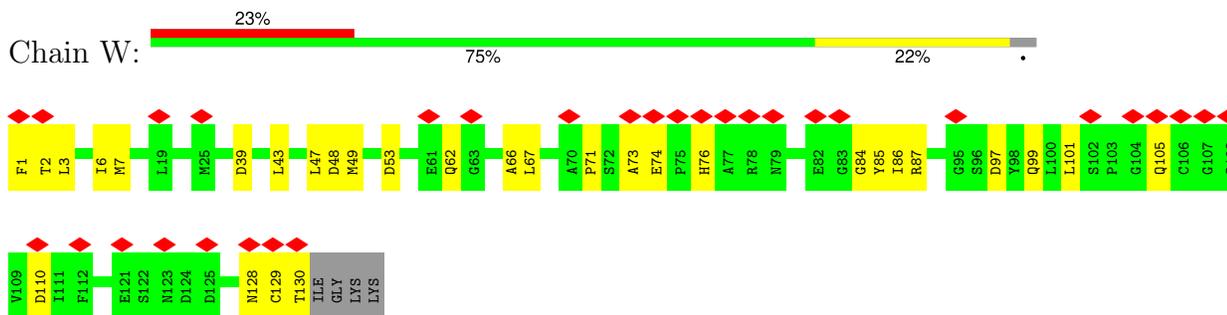
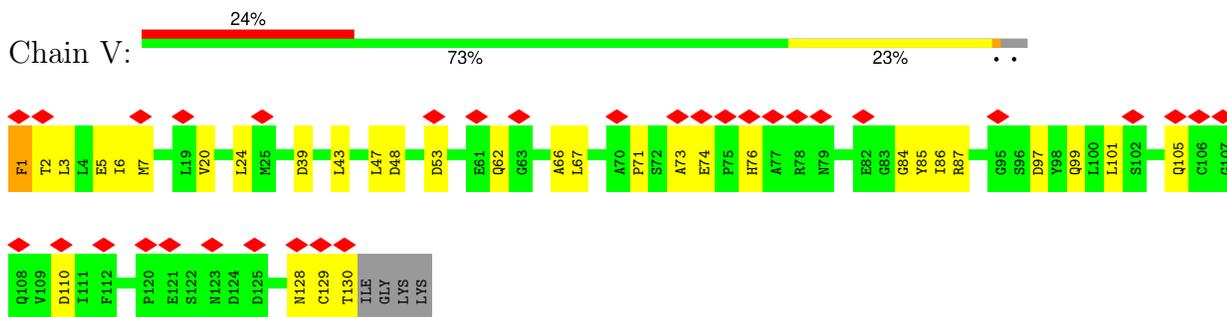
• Molecule 1: General secretion pathway protein G



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• Molecule 1: General secretion pathway protein G



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=83.2°, rise=10.2 Å, axial sym=C1	Depositor
Number of segments used	85619	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	20	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.113	Depositor
Minimum map value	-0.044	Depositor
Average map value	0.012	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.056	Depositor
Map size (Å)	88.2, 88.2, 315.0	wwPDB
Map dimensions	84, 84, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.60	0/994	0.64	0/1355
1	B	0.61	0/994	0.64	0/1355
1	C	0.60	0/994	0.64	0/1355
1	D	0.61	0/994	0.64	0/1355
1	E	0.60	0/994	0.64	0/1355
1	F	0.61	0/994	0.64	0/1355
1	G	0.60	0/994	0.64	0/1355
1	H	0.60	0/994	0.64	0/1355
1	I	0.60	0/994	0.64	0/1355
1	J	0.60	0/994	0.64	0/1355
1	K	0.61	0/994	0.64	0/1355
1	L	0.60	0/994	0.64	0/1355
1	M	0.60	0/994	0.64	0/1355
1	N	0.60	0/994	0.64	0/1355
1	O	0.60	0/994	0.64	0/1355
1	P	0.60	0/994	0.64	0/1355
1	Q	0.60	0/994	0.64	0/1355
1	R	0.61	0/994	0.64	0/1355
1	S	0.60	0/994	0.64	0/1355
1	T	0.60	0/994	0.64	0/1355
1	U	0.61	0/994	0.64	0/1355
1	V	0.60	0/994	0.64	0/1355
1	W	0.60	0/994	0.64	0/1355
1	X	0.60	0/994	0.64	0/1355
1	Y	0.60	0/994	0.64	0/1355
All	All	0.60	0/24850	0.64	0/33875

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	988	977	977	18	0
1	B	988	977	977	22	0
1	C	988	977	977	21	0
1	D	988	977	977	22	0
1	E	988	977	977	20	0
1	F	988	977	977	22	0
1	G	988	977	977	22	0
1	H	988	977	977	21	0
1	I	988	977	977	23	0
1	J	988	977	977	21	0
1	K	988	977	977	23	0
1	L	988	977	977	21	0
1	M	988	977	977	24	0
1	N	988	977	977	22	0
1	O	988	977	977	23	0
1	P	988	977	977	22	0
1	Q	988	977	977	21	0
1	R	988	977	977	20	0
1	S	988	977	977	22	0
1	T	988	977	977	22	0
1	U	988	977	977	21	0
1	V	988	977	977	22	0
1	W	988	977	977	20	0
1	X	988	977	977	22	0
1	Y	988	977	977	18	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
2	O	1	0	0	0	0
2	P	1	0	0	0	0
2	Q	1	0	0	0	0
2	R	1	0	0	0	0
2	S	1	0	0	0	0
2	T	1	0	0	0	0
2	U	1	0	0	0	0
2	V	1	0	0	0	0
2	W	1	0	0	0	0
2	X	1	0	0	0	0
2	Y	1	0	0	0	0
All	All	24725	24425	24425	465	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.

The worst 5 of 465 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:O:97:ASP:OD1	1:O:99:GLN:NE2	2.17	0.78
1:B:97:ASP:OD1	1:B:99:GLN:NE2	2.17	0.78
1:W:97:ASP:OD1	1:W:99:GLN:NE2	2.17	0.78
1:K:97:ASP:OD1	1:K:99:GLN:NE2	2.17	0.78
1:G:97:ASP:OD1	1:G:99:GLN:NE2	2.17	0.78

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	128/134 (96%)	111 (87%)	17 (13%)	0	100	100
1	B	128/134 (96%)	111 (87%)	17 (13%)	0	100	100
1	C	128/134 (96%)	111 (87%)	17 (13%)	0	100	100
1	D	128/134 (96%)	111 (87%)	17 (13%)	0	100	100
1	E	128/134 (96%)	111 (87%)	17 (13%)	0	100	100
1	F	128/134 (96%)	112 (88%)	16 (12%)	0	100	100
1	G	128/134 (96%)	111 (87%)	17 (13%)	0	100	100
1	H	128/134 (96%)	111 (87%)	17 (13%)	0	100	100
1	I	128/134 (96%)	111 (87%)	17 (13%)	0	100	100
1	J	128/134 (96%)	111 (87%)	17 (13%)	0	100	100
1	K	128/134 (96%)	111 (87%)	17 (13%)	0	100	100
1	L	128/134 (96%)	111 (87%)	17 (13%)	0	100	100
1	M	128/134 (96%)	111 (87%)	17 (13%)	0	100	100
1	N	128/134 (96%)	111 (87%)	17 (13%)	0	100	100
1	O	128/134 (96%)	111 (87%)	17 (13%)	0	100	100
1	P	128/134 (96%)	111 (87%)	17 (13%)	0	100	100
1	Q	128/134 (96%)	111 (87%)	17 (13%)	0	100	100
1	R	128/134 (96%)	111 (87%)	17 (13%)	0	100	100
1	S	128/134 (96%)	112 (88%)	16 (12%)	0	100	100
1	T	128/134 (96%)	111 (87%)	17 (13%)	0	100	100
1	U	128/134 (96%)	111 (87%)	17 (13%)	0	100	100
1	V	128/134 (96%)	111 (87%)	17 (13%)	0	100	100
1	W	128/134 (96%)	111 (87%)	17 (13%)	0	100	100
1	X	128/134 (96%)	111 (87%)	17 (13%)	0	100	100
1	Y	128/134 (96%)	111 (87%)	17 (13%)	0	100	100
All	All	3200/3350 (96%)	2777 (87%)	423 (13%)	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	109/112 (97%)	109 (100%)	0	100	100
1	B	109/112 (97%)	109 (100%)	0	100	100
1	C	109/112 (97%)	109 (100%)	0	100	100
1	D	109/112 (97%)	109 (100%)	0	100	100
1	E	109/112 (97%)	109 (100%)	0	100	100
1	F	109/112 (97%)	109 (100%)	0	100	100
1	G	109/112 (97%)	109 (100%)	0	100	100
1	H	109/112 (97%)	109 (100%)	0	100	100
1	I	109/112 (97%)	109 (100%)	0	100	100
1	J	109/112 (97%)	109 (100%)	0	100	100
1	K	109/112 (97%)	109 (100%)	0	100	100
1	L	109/112 (97%)	109 (100%)	0	100	100
1	M	109/112 (97%)	109 (100%)	0	100	100
1	N	109/112 (97%)	109 (100%)	0	100	100
1	O	109/112 (97%)	109 (100%)	0	100	100
1	P	109/112 (97%)	109 (100%)	0	100	100
1	Q	109/112 (97%)	109 (100%)	0	100	100
1	R	109/112 (97%)	109 (100%)	0	100	100
1	S	109/112 (97%)	109 (100%)	0	100	100
1	T	109/112 (97%)	109 (100%)	0	100	100
1	U	109/112 (97%)	109 (100%)	0	100	100
1	V	109/112 (97%)	109 (100%)	0	100	100
1	W	109/112 (97%)	109 (100%)	0	100	100
1	X	109/112 (97%)	109 (100%)	0	100	100
1	Y	109/112 (97%)	109 (100%)	0	100	100
All	All	2725/2800 (97%)	2725 (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. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

25 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MEA	E	1	1	11,12,13	0.67	0	13,14,16	1.10	1 (7%)
1	MEA	T	1	1	11,12,13	0.67	0	13,14,16	1.10	1 (7%)
1	MEA	C	1	1	11,12,13	0.67	0	13,14,16	1.10	1 (7%)
1	MEA	O	1	1	11,12,13	0.67	0	13,14,16	1.10	1 (7%)
1	MEA	B	1	1	11,12,13	0.68	0	13,14,16	1.09	1 (7%)
1	MEA	Y	1	1	11,12,13	0.67	0	13,14,16	1.09	1 (7%)
1	MEA	S	1	1	11,12,13	0.67	0	13,14,16	1.09	1 (7%)
1	MEA	J	1	1	11,12,13	0.67	0	13,14,16	1.09	1 (7%)
1	MEA	H	1	1	11,12,13	0.67	0	13,14,16	1.09	1 (7%)
1	MEA	V	1	1	11,12,13	0.67	0	13,14,16	1.09	1 (7%)
1	MEA	L	1	1	11,12,13	0.67	0	13,14,16	1.10	1 (7%)
1	MEA	Q	1	1	11,12,13	0.67	0	13,14,16	1.09	1 (7%)
1	MEA	P	1	1	11,12,13	0.67	0	13,14,16	1.09	1 (7%)
1	MEA	U	1	1	11,12,13	0.68	0	13,14,16	1.09	1 (7%)
1	MEA	A	1	1	11,12,13	0.67	0	13,14,16	1.10	1 (7%)
1	MEA	D	1	1	11,12,13	0.67	0	13,14,16	1.09	1 (7%)
1	MEA	W	1	1	11,12,13	0.66	0	13,14,16	1.10	1 (7%)
1	MEA	R	1	1	11,12,13	0.68	0	13,14,16	1.09	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MEA	M	1	1	11,12,13	0.67	0	13,14,16	1.09	1 (7%)
1	MEA	N	1	1	11,12,13	0.67	0	13,14,16	1.10	1 (7%)
1	MEA	I	1	1	11,12,13	0.67	0	13,14,16	1.10	1 (7%)
1	MEA	K	1	1	11,12,13	0.67	0	13,14,16	1.10	1 (7%)
1	MEA	X	1	1	11,12,13	0.67	0	13,14,16	1.09	1 (7%)
1	MEA	G	1	1	11,12,13	0.67	0	13,14,16	1.10	1 (7%)
1	MEA	F	1	1	11,12,13	0.67	0	13,14,16	1.10	1 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MEA	E	1	1	-	0/5/8/10	0/1/1/1
1	MEA	T	1	1	-	0/5/8/10	0/1/1/1
1	MEA	C	1	1	-	0/5/8/10	0/1/1/1
1	MEA	O	1	1	-	0/5/8/10	0/1/1/1
1	MEA	B	1	1	-	0/5/8/10	0/1/1/1
1	MEA	Y	1	1	-	0/5/8/10	0/1/1/1
1	MEA	S	1	1	-	0/5/8/10	0/1/1/1
1	MEA	J	1	1	-	0/5/8/10	0/1/1/1
1	MEA	H	1	1	-	0/5/8/10	0/1/1/1
1	MEA	V	1	1	-	0/5/8/10	0/1/1/1
1	MEA	L	1	1	-	0/5/8/10	0/1/1/1
1	MEA	Q	1	1	-	0/5/8/10	0/1/1/1
1	MEA	P	1	1	-	0/5/8/10	0/1/1/1
1	MEA	U	1	1	-	0/5/8/10	0/1/1/1
1	MEA	A	1	1	-	0/5/8/10	0/1/1/1
1	MEA	D	1	1	-	0/5/8/10	0/1/1/1
1	MEA	W	1	1	-	0/5/8/10	0/1/1/1
1	MEA	R	1	1	-	0/5/8/10	0/1/1/1
1	MEA	M	1	1	-	0/5/8/10	0/1/1/1
1	MEA	N	1	1	-	0/5/8/10	0/1/1/1
1	MEA	I	1	1	-	0/5/8/10	0/1/1/1
1	MEA	K	1	1	-	0/5/8/10	0/1/1/1
1	MEA	X	1	1	-	0/5/8/10	0/1/1/1
1	MEA	G	1	1	-	0/5/8/10	0/1/1/1
1	MEA	F	1	1	-	0/5/8/10	0/1/1/1

There are no bond length outliers.

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	MEA	CB-CA-N	3.03	114.94	110.48
1	F	1	MEA	CB-CA-N	3.03	114.94	110.48
1	O	1	MEA	CB-CA-N	3.03	114.94	110.48
1	K	1	MEA	CB-CA-N	3.02	114.93	110.48
1	E	1	MEA	CB-CA-N	3.02	114.93	110.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	T	1	MEA	1	0
1	C	1	MEA	1	0
1	O	1	MEA	2	0
1	B	1	MEA	2	0
1	Y	1	MEA	1	0
1	S	1	MEA	1	0
1	V	1	MEA	1	0
1	L	1	MEA	1	0
1	P	1	MEA	1	0
1	D	1	MEA	1	0
1	M	1	MEA	2	0
1	I	1	MEA	1	0
1	K	1	MEA	2	0
1	X	1	MEA	1	0
1	G	1	MEA	1	0
1	F	1	MEA	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 25 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8812. These allow visual inspection of the internal detail of the map and identification of artifacts.

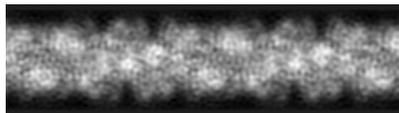
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

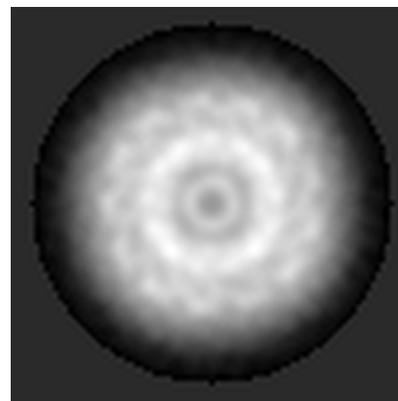
6.1.1 Primary map



X



Y



Z

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

6.2 Central slices [i](#)

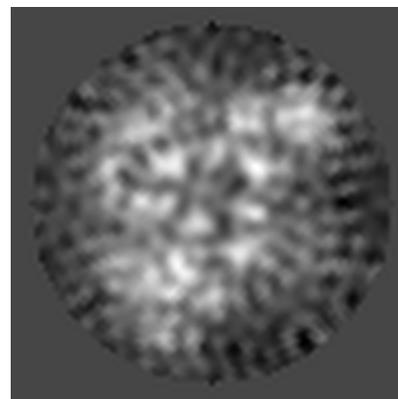
6.2.1 Primary map



X Index:
42



Y Index: 42



Z Index: 150

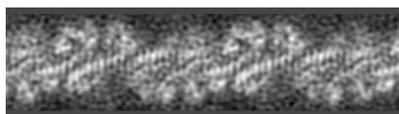
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

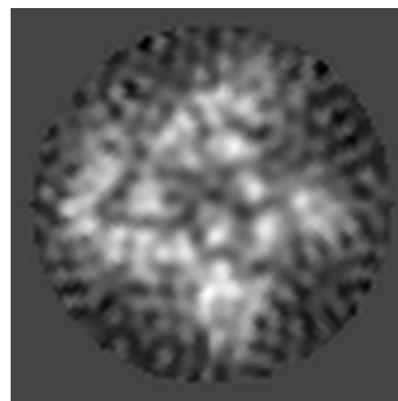
6.3.1 Primary map



X Index:
53



Y Index: 53

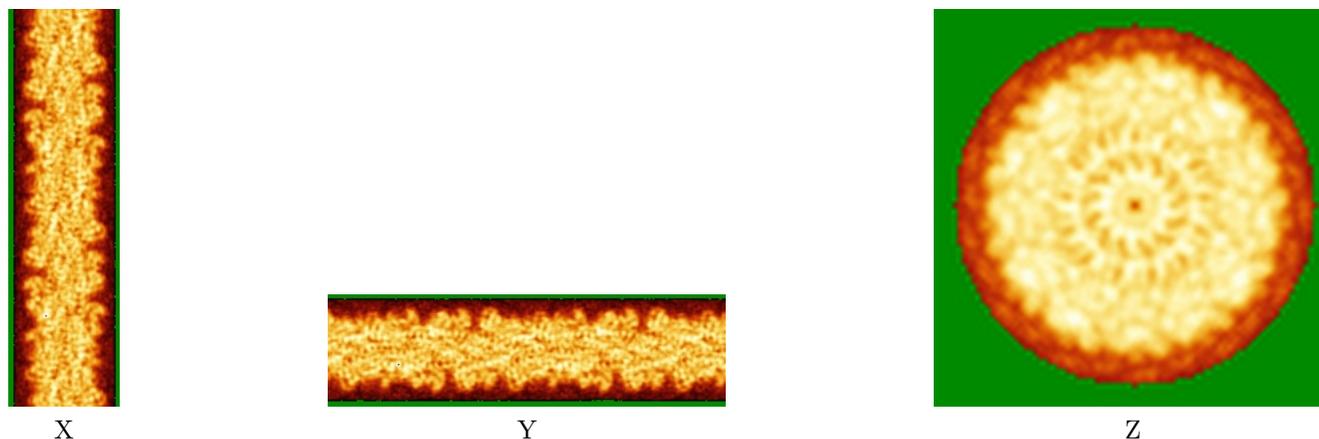


Z Index: 233

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

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

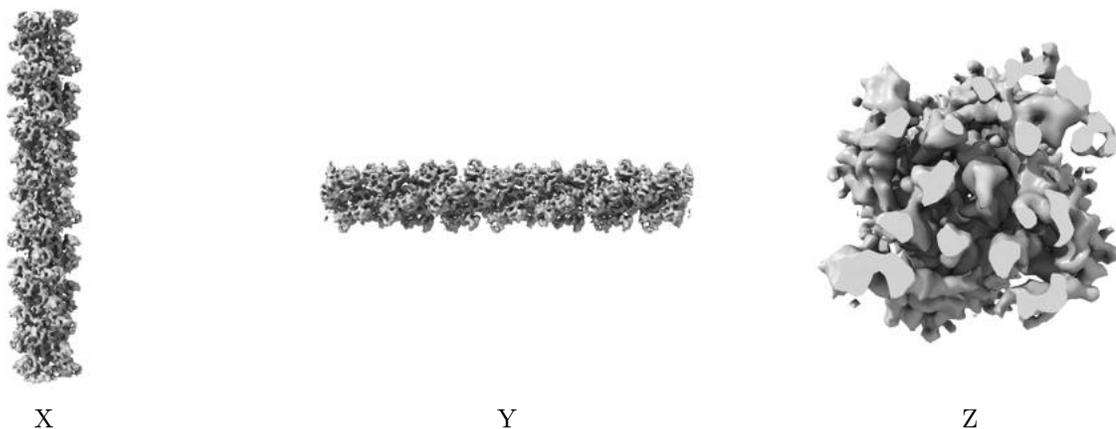
6.4.1 Primary map



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

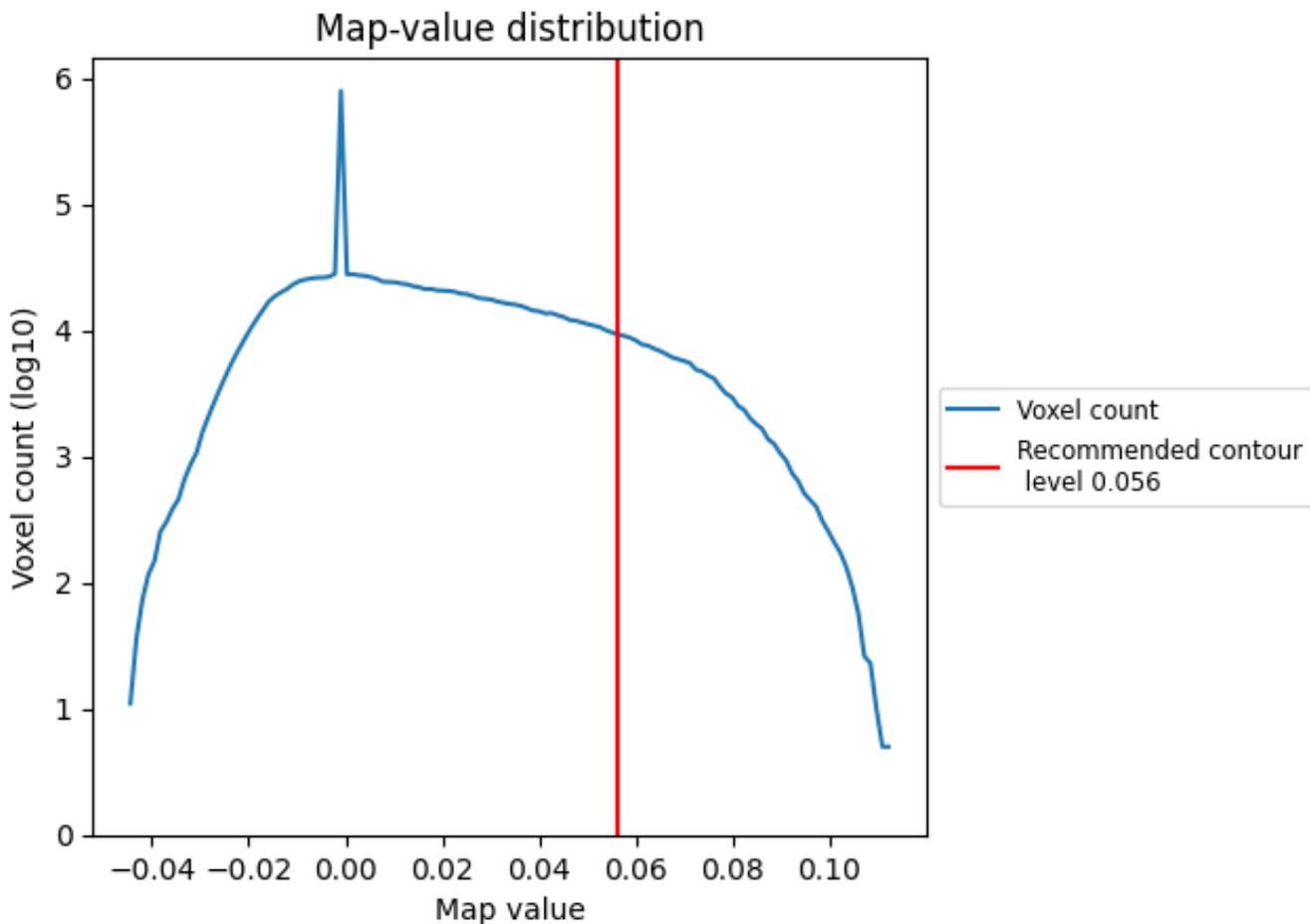
6.6 Mask visualisation

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

7 Map analysis [i](#)

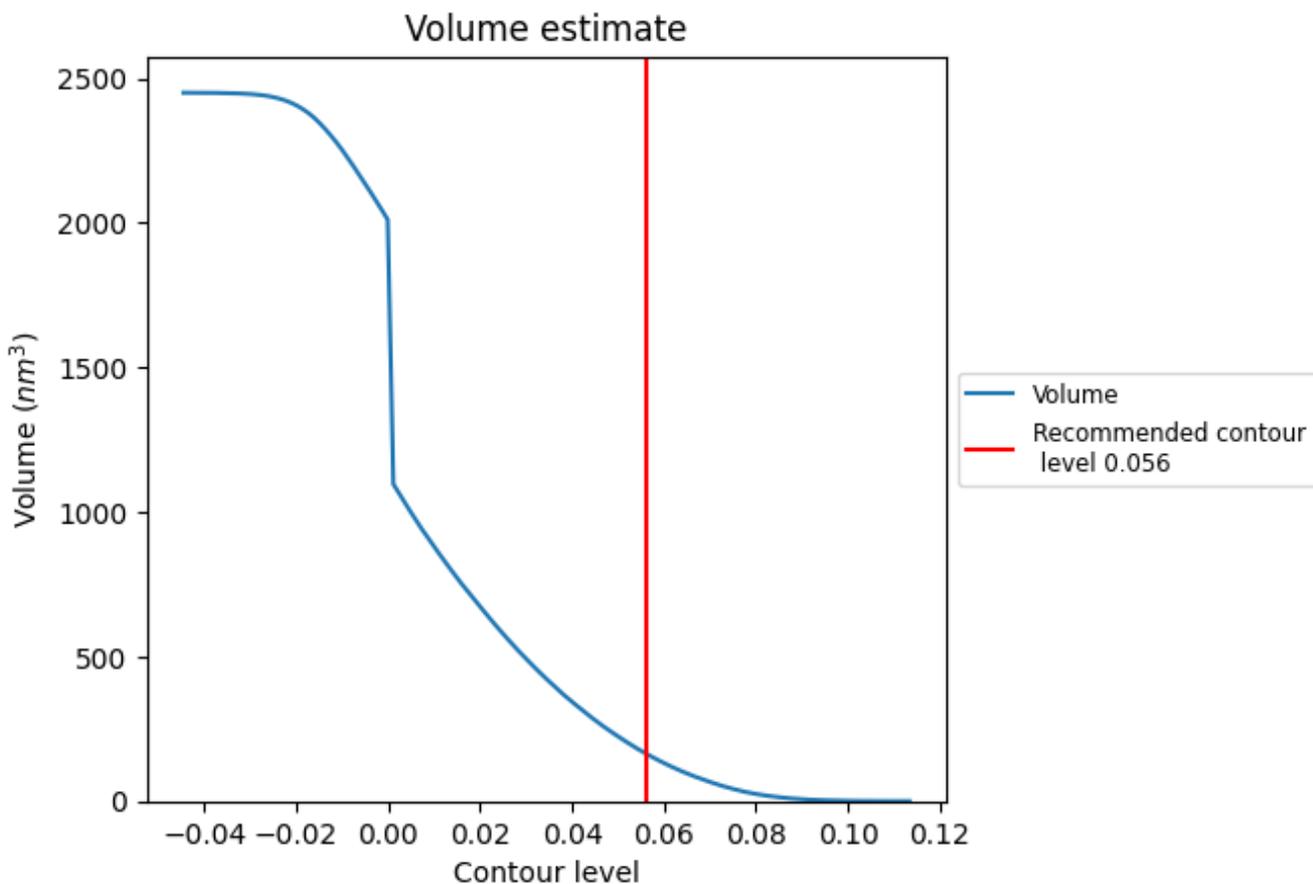
This section contains the results of statistical analysis of the map.

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 165 nm³; this corresponds to an approximate mass of 149 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](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

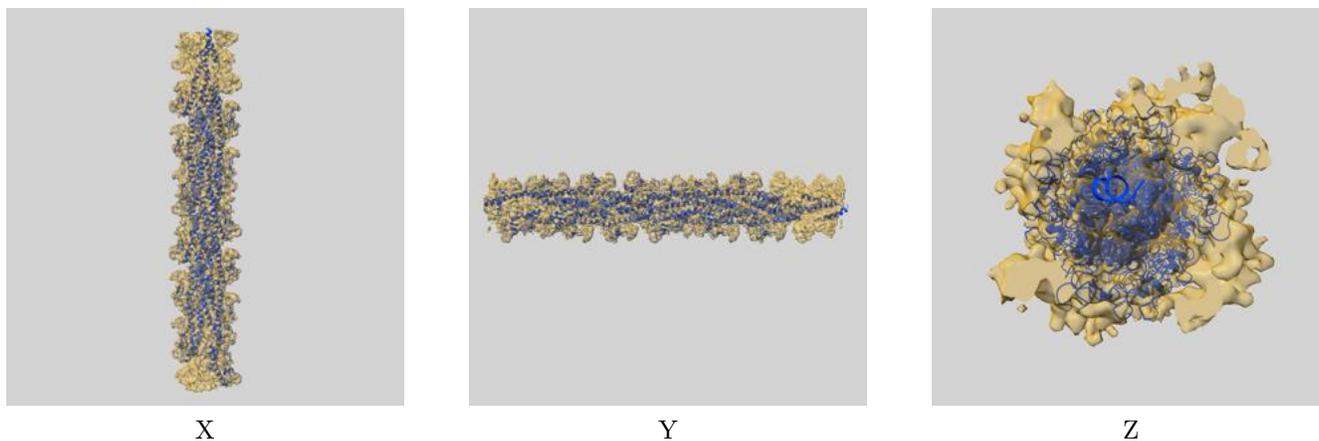
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

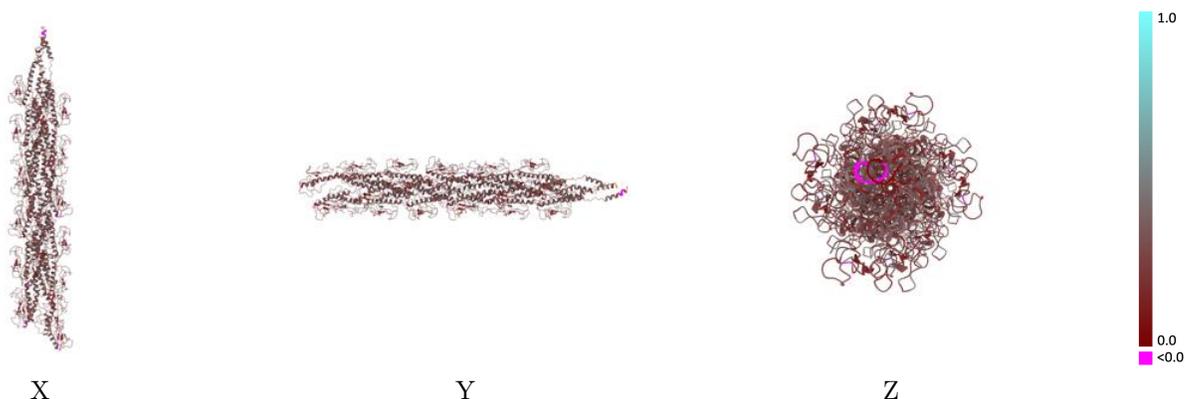
This section contains information regarding the fit between EMDB map EMD-8812 and PDB model 5WDA. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



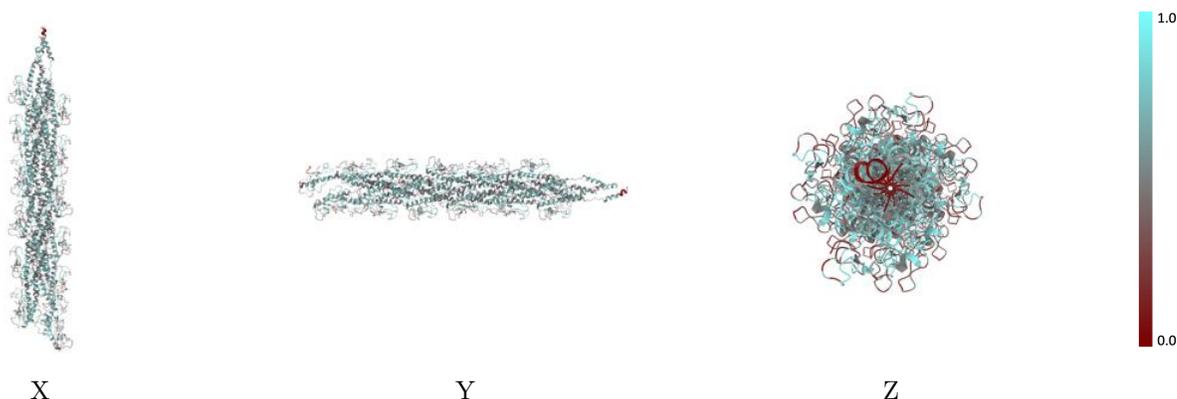
The images above show the 3D surface view of the map at the recommended contour level 0.056 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



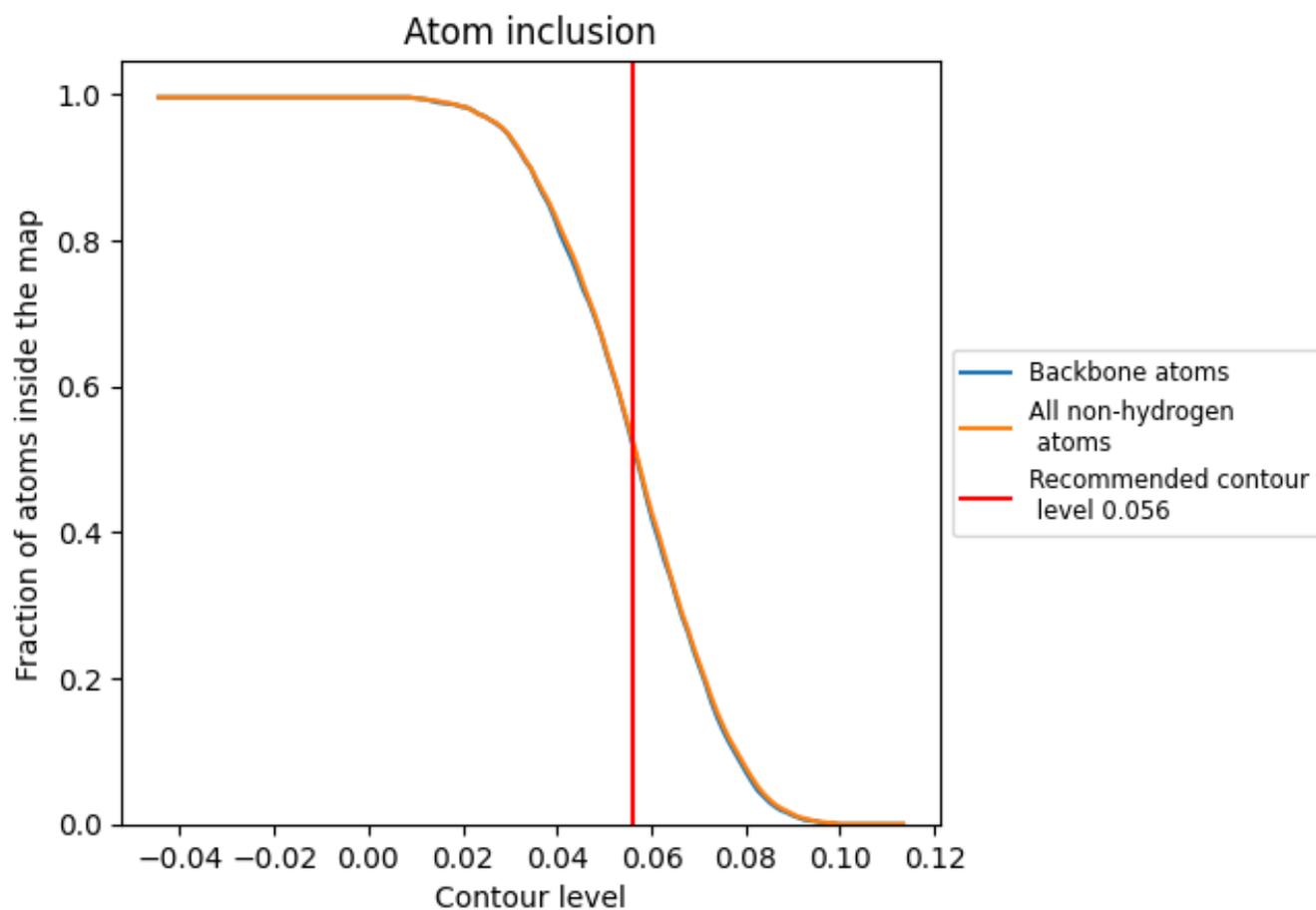
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.056).

9.4 Atom inclusion [i](#)



At the recommended contour level, 52% of all backbone atoms, 53% 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 (0.056) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5260	 0.2810
A	 0.5030	 0.2710
B	 0.5220	 0.2830
C	 0.5260	 0.2850
D	 0.5270	 0.2870
E	 0.5260	 0.2830
F	 0.5260	 0.2820
G	 0.5270	 0.2850
H	 0.5300	 0.2860
I	 0.5320	 0.2860
J	 0.5300	 0.2830
K	 0.5280	 0.2830
L	 0.5330	 0.2880
M	 0.5240	 0.2830
N	 0.5310	 0.2820
O	 0.5350	 0.2840
P	 0.5330	 0.2860
Q	 0.5360	 0.2840
R	 0.5360	 0.2790
S	 0.5380	 0.2780
T	 0.5400	 0.2800
U	 0.5410	 0.2840
V	 0.5430	 0.2810
W	 0.5350	 0.2760
X	 0.5430	 0.2760
Y	 0.5100	 0.2600

