



## Full wwPDB EM Validation Report ⓘ

Dec 11, 2022 – 01:54 pm GMT

PDB ID : 5AI7  
EMDB ID : EMD-2848  
Title : ParM doublet model  
Authors : Bharat, T.A.M.; Murshudov, G.N.; Sachse, C.; Lowe, J.  
Deposited on : 2015-02-12  
Resolution : Not provided

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

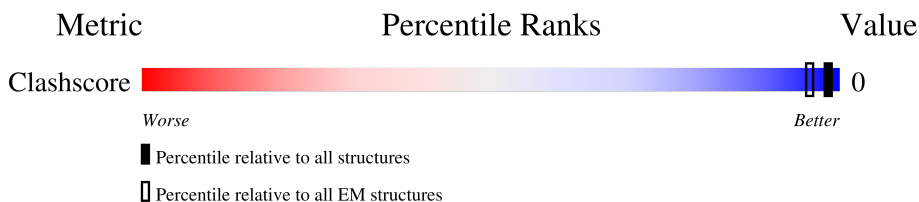
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is unknown.

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	158937	4297

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  $\geq 3$ , 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	318	100%
1	B	318	100%
1	C	318	100%
1	D	318	100%
1	E	318	100%
1	F	318	100%
1	G	318	100%
1	H	318	100%
1	I	318	100%
1	J	318	100%

*Continued on next page...*

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Mol	Chain	Length	Quality of chain
1	K	318	100%  100%
1	L	318	100%  100%
1	M	318	100%  100%
1	N	318	100%  100%

## 2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 4452 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.

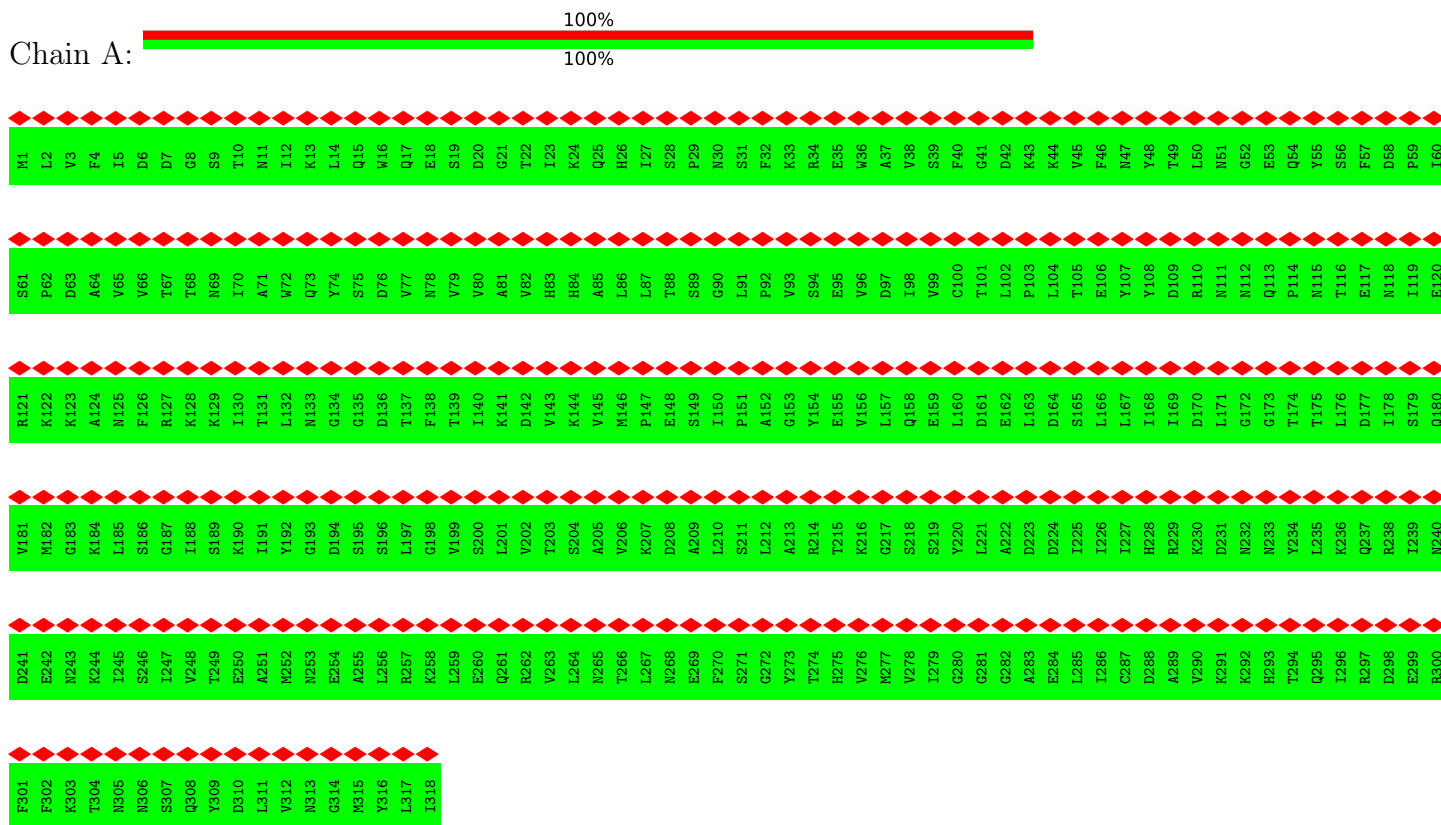
- Molecule 1 is a protein called PLASMID SEGREGATION PROTEIN PARM.

Mol	Chain	Residues	Atoms	AltConf	Trace
1	A	318	Total C 318 318	0	318
1	B	318	Total C 318 318	0	318
1	C	318	Total C 318 318	0	318
1	D	318	Total C 318 318	0	318
1	E	318	Total C 318 318	0	318
1	F	318	Total C 318 318	0	318
1	G	318	Total C 318 318	0	318
1	H	318	Total C 318 318	0	318
1	I	318	Total C 318 318	0	318
1	J	318	Total C 318 318	0	318
1	K	318	Total C 318 318	0	318
1	L	318	Total C 318 318	0	318
1	M	318	Total C 318 318	0	318
1	N	318	Total C 318 318	0	318

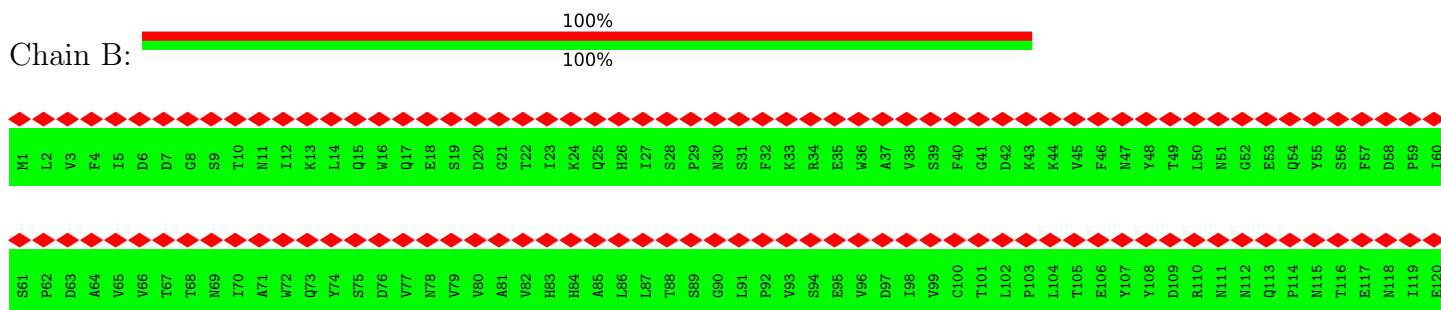
### 3 Residue-property plots

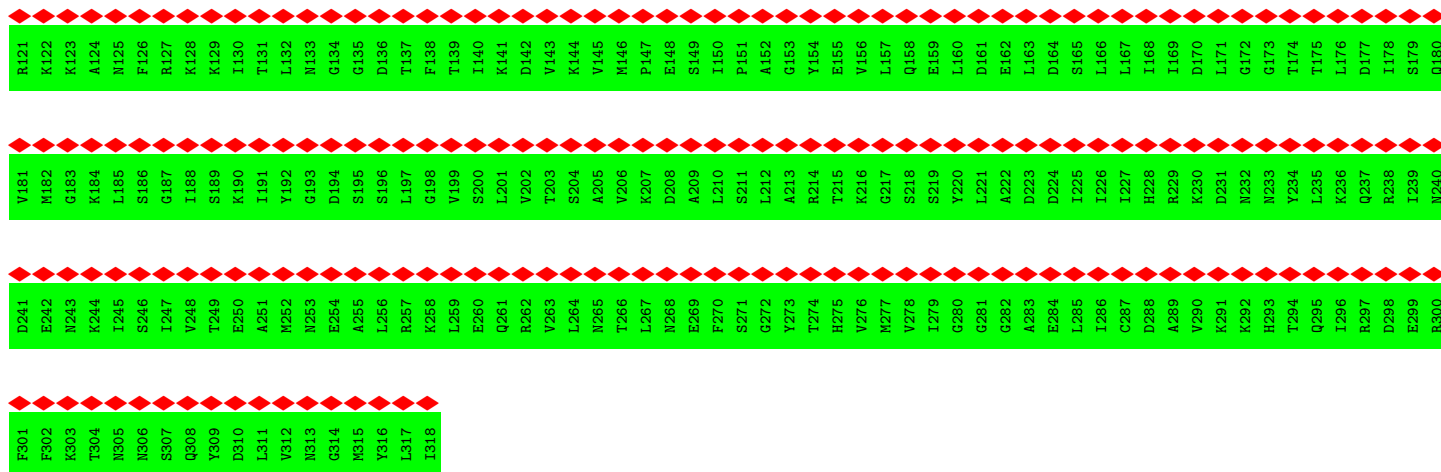
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: PLASMID SEGREGATION PROTEIN PARM

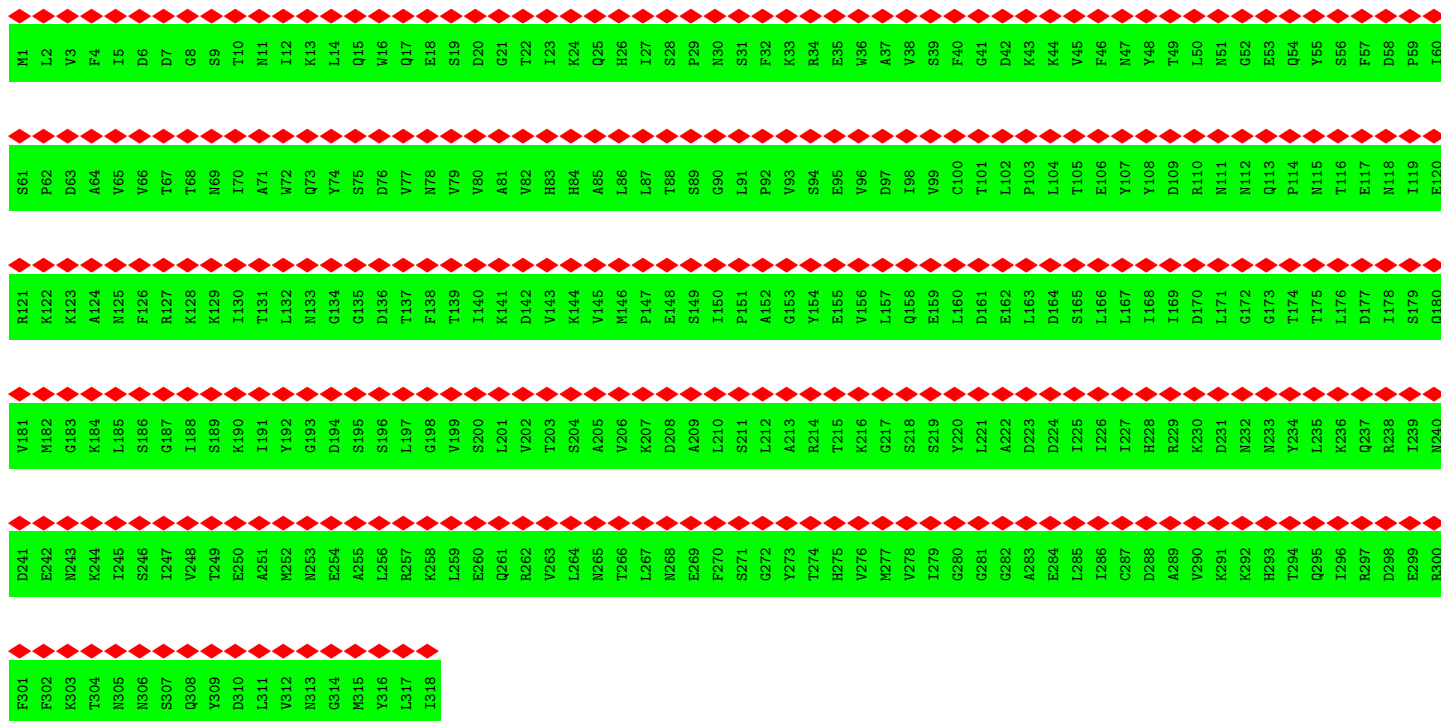


- Molecule 1: PLASMID SEGREGATION PROTEIN PARM



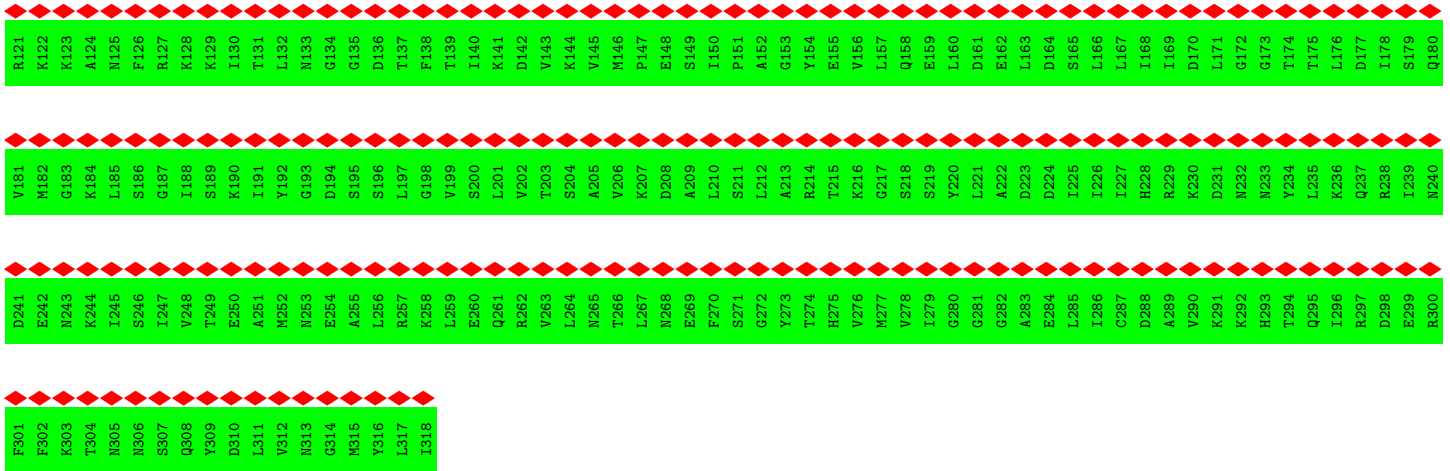


• Molecule 1: PLASMID SEGREGATION PROTEIN PARM

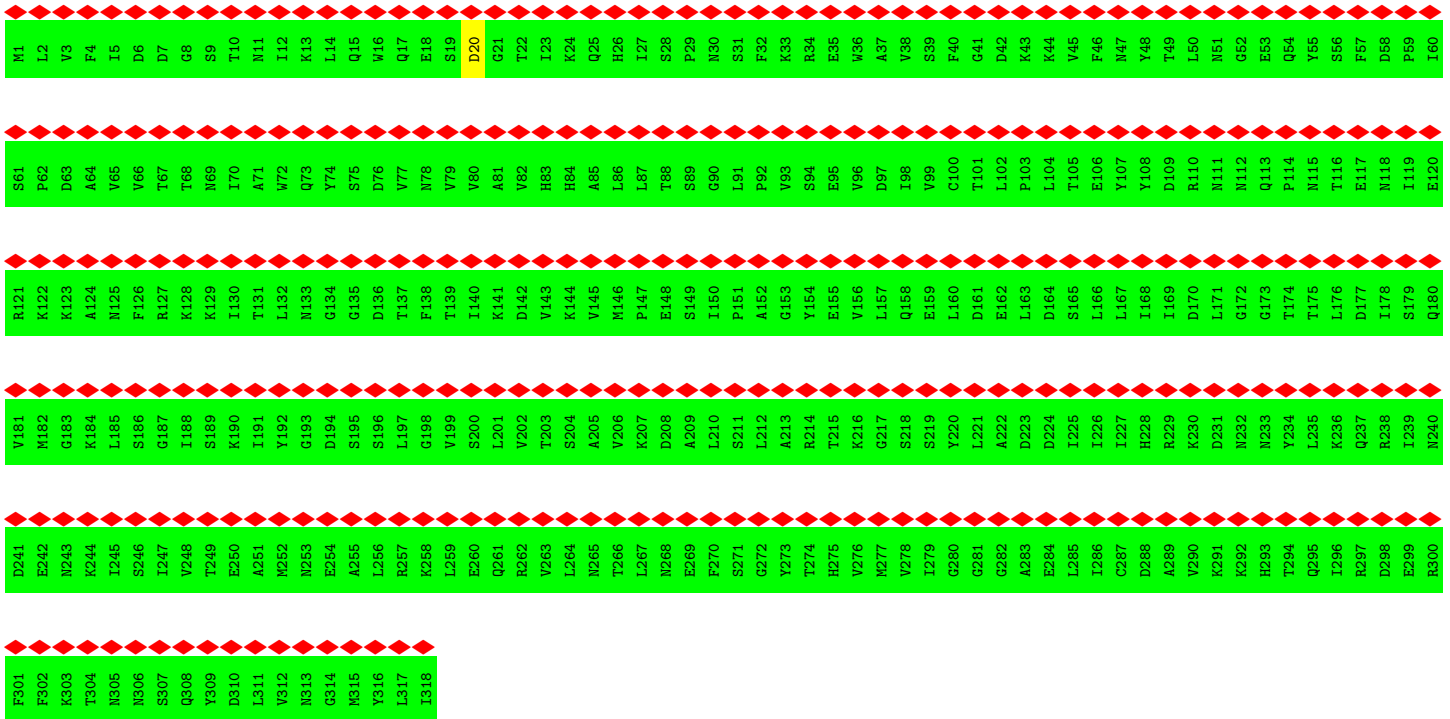


• Molecule 1: PLASMID SEGREGATION PROTEIN PARM



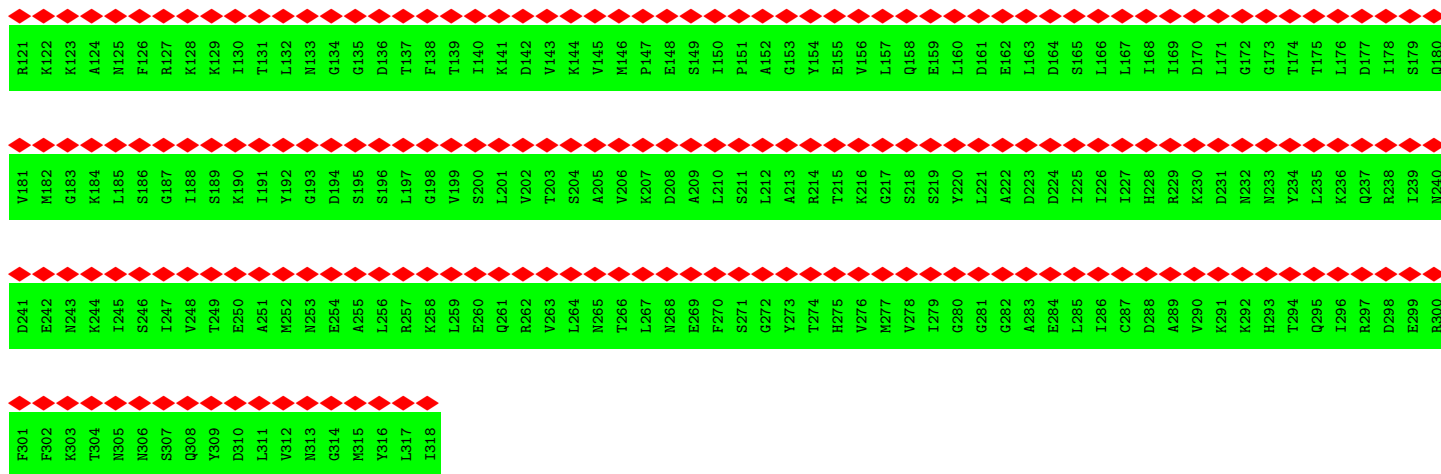


• Molecule 1: PLASMID SEGREGATION PROTEIN PARM

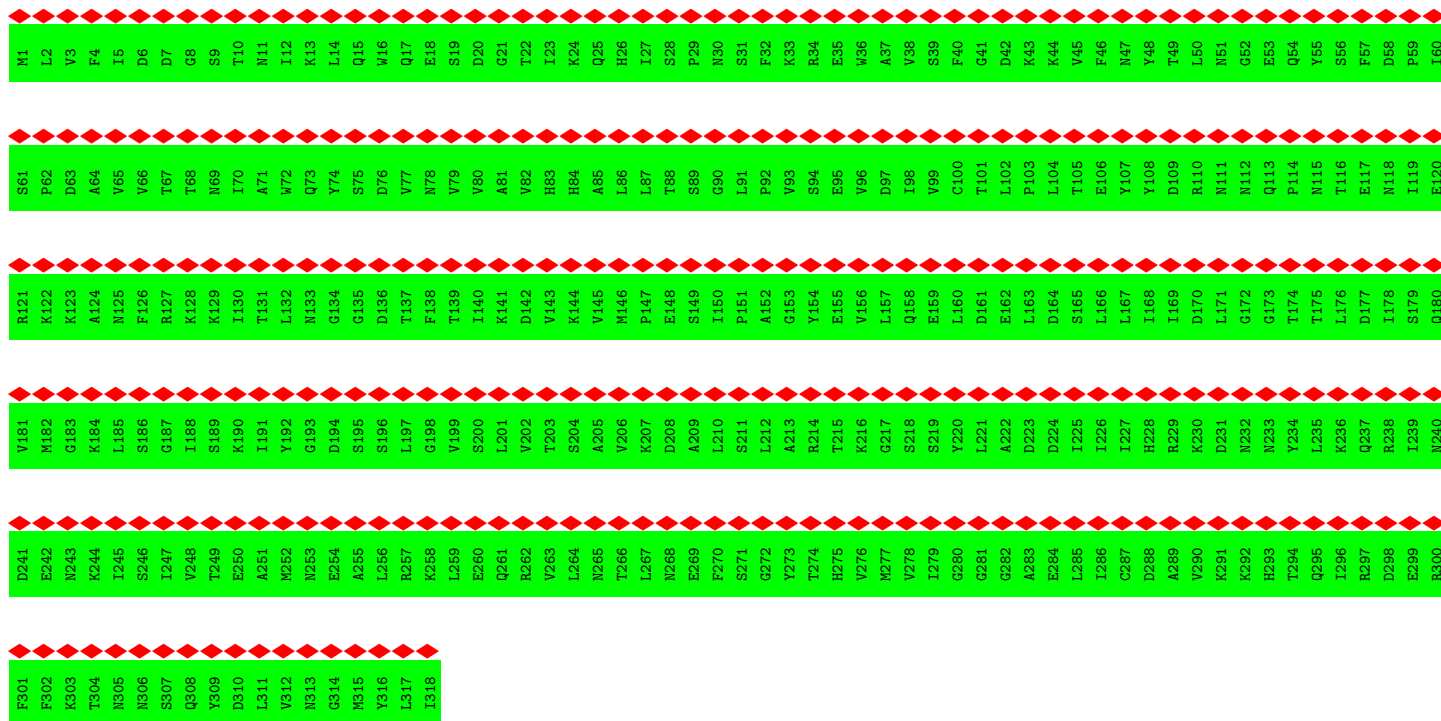


• Molecule 1: PLASMID SEGREGATION PROTEIN PARM





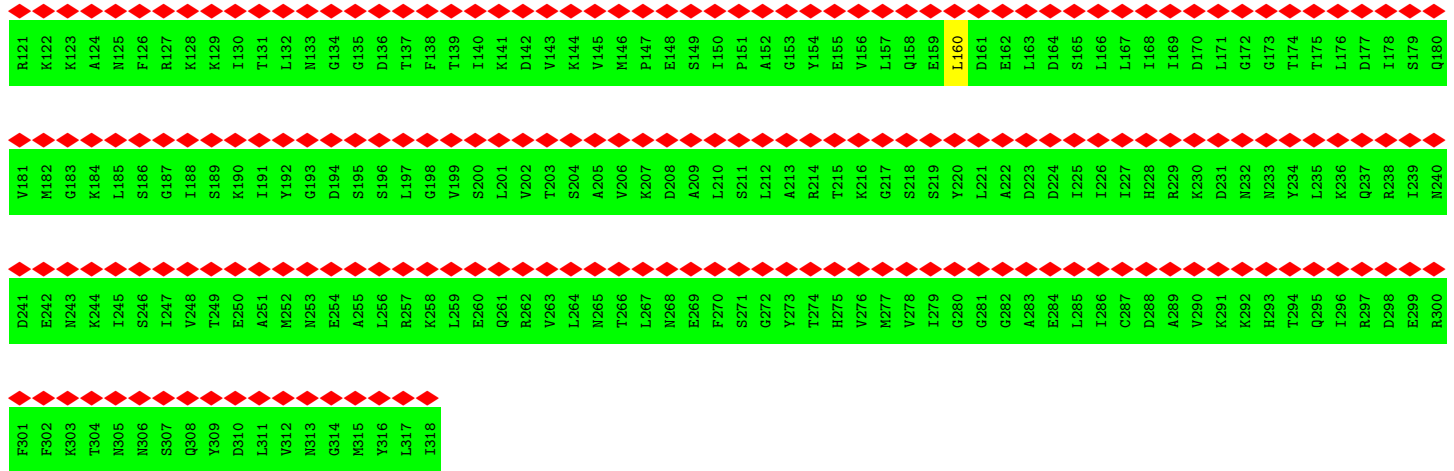
• Molecule 1: PLASMID SEGREGATION PROTEIN PARM



• Molecule 1: PLASMID SEGREGATION PROTEIN PARM





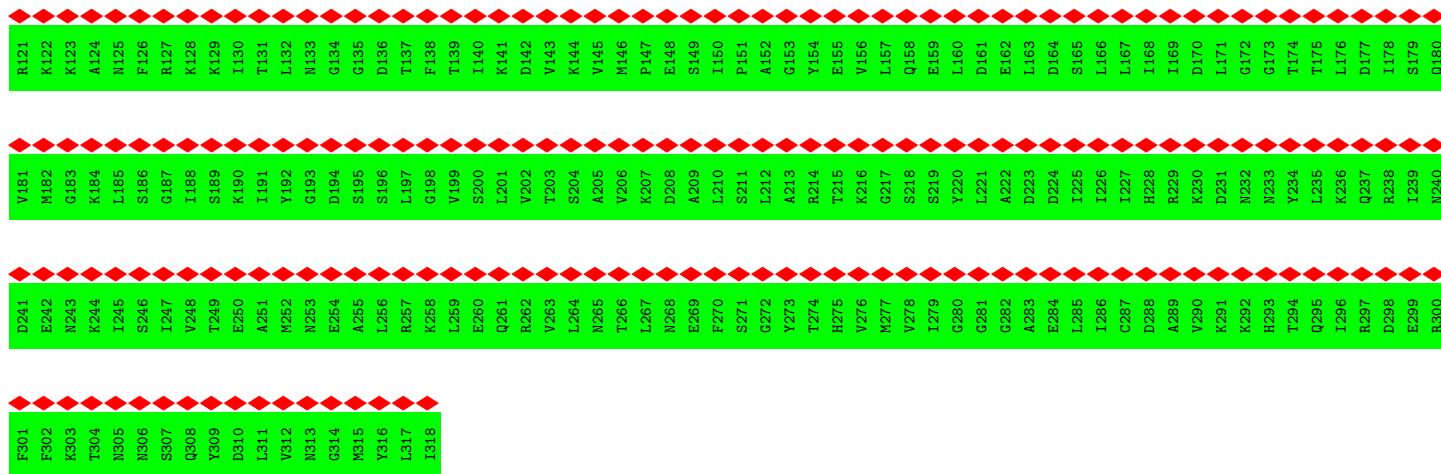


• Molecule 1: PLASMID SEGREGATION PROTEIN PARM

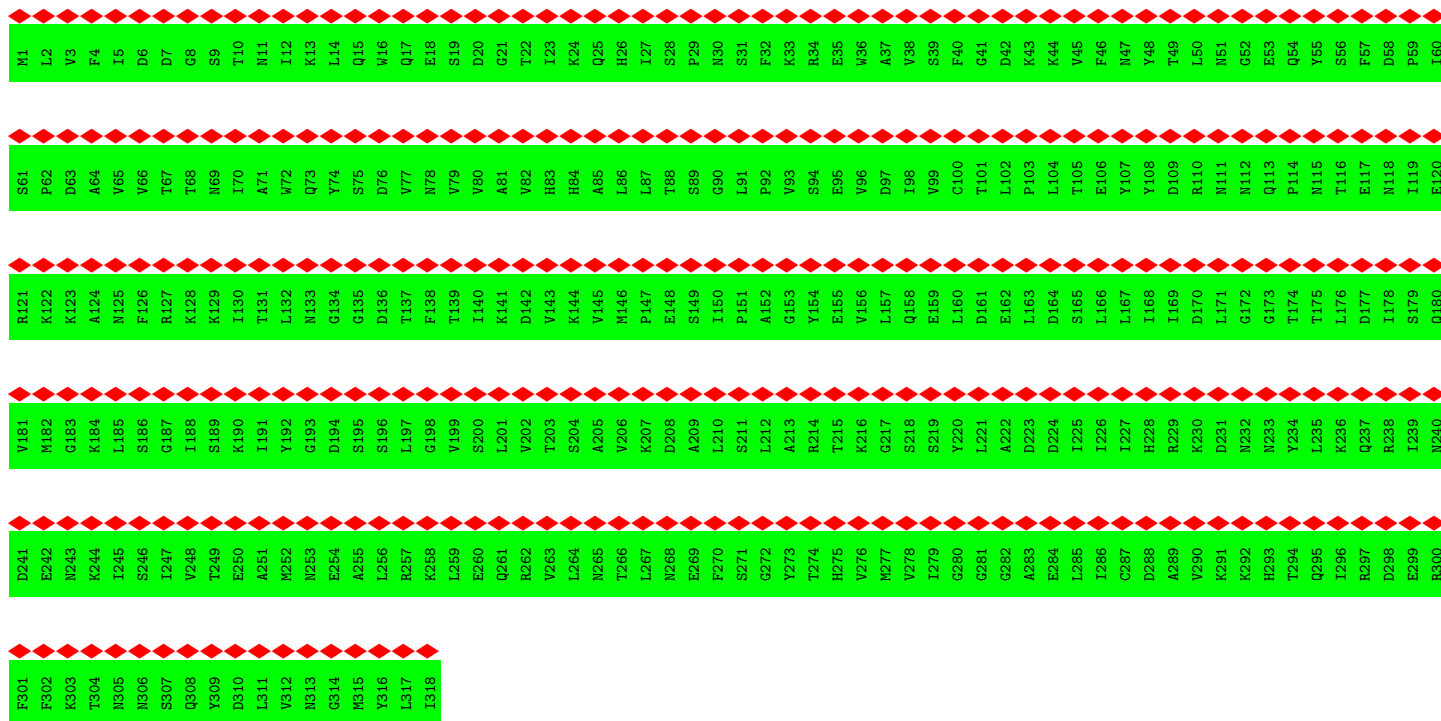


• Molecule 1: PLASMID SEGREGATION PROTEIN PARM



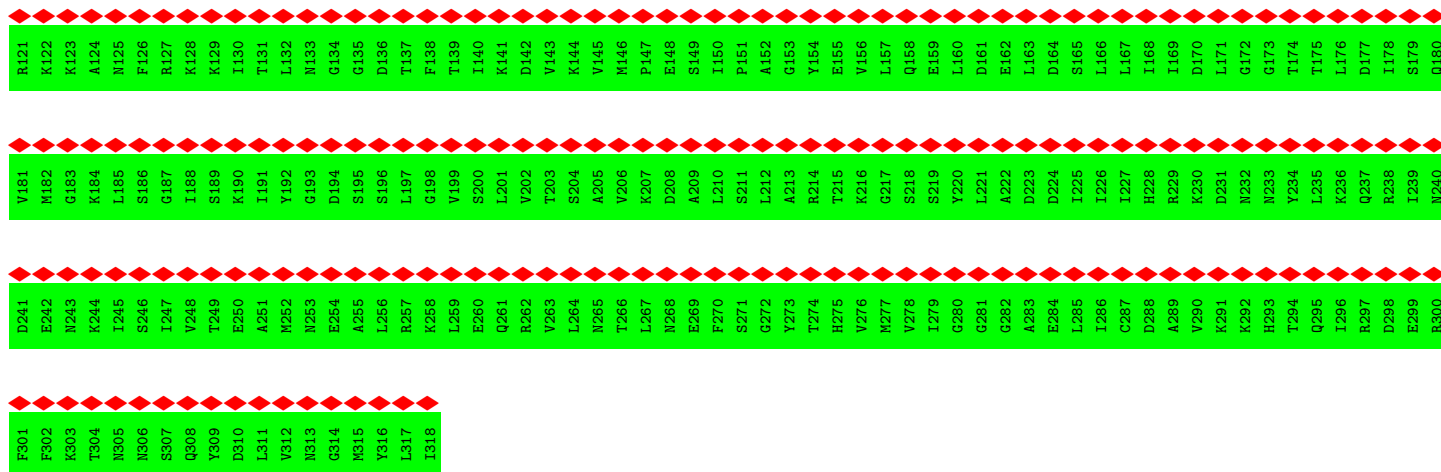


• Molecule 1: PLASMID SEGREGATION PROTEIN PARM

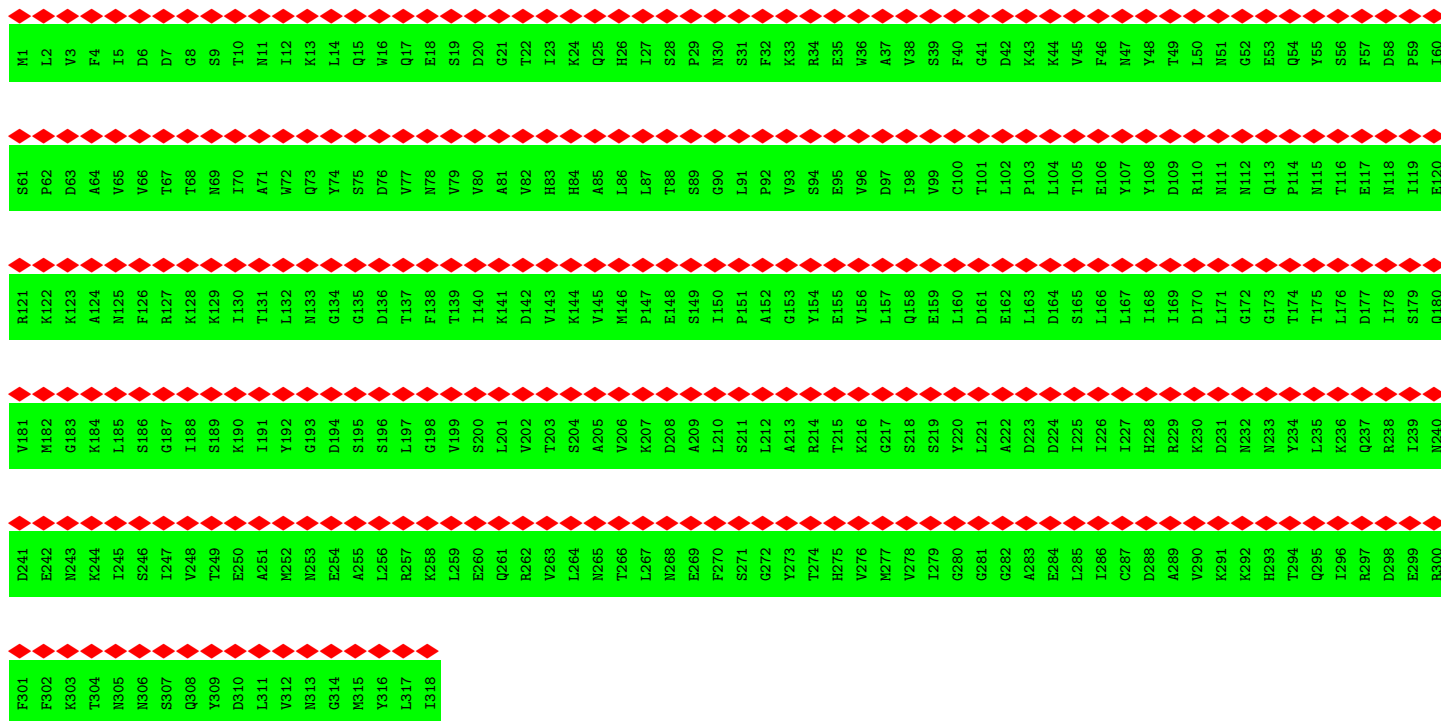


• Molecule 1: PLASMID SEGREGATION PROTEIN PARM





• Molecule 1: PLASMID SEGREGATION PROTEIN PARM



• Molecule 1: PLASMID SEGREGATION PROTEIN PARM



R121	K122	K123	A124	N125	F126	R127	K128	K129	I130	T131	L132	N133	G134	G135	D136	T137	F138	T139	I140	K141	D142	V143	K144	V145	M146	P147	E148	S149	I150	P151	A152	G153	Y154	E155	V156	L157	Q158	E159	L160	D161	E162	L163	D164	S165	L166	L167	I168	I169	D170	L171	G172	G173	T174	T175	L176	D177	I178	S179	Q180
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V181	M182	G183	K184	L185	S186	G187	I188	S189	K190	I191	Y192	G193	D194	S195	S196	L197	G198	V199	S200	L201	V202	T203	S204	A205	V206	K207	D208	A209	L210	S211	L212	A213	R214	T215	K216	G217	S218	S219	Y220	L221	A222	D223	D224	I225	I226	I227	H228	R229	K230	D231	N232	N233	Y234	L235	K236	Q237	R238	I239	N240
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D241	E242	N243	K244	I245	S246	I247	V248	T249	E250	A251	M252	N253	E254	A255	L256	R257	K258	L259	E260	Q261	R262	V263	L264	N265	T266	L267	N268	E269	F270	S271	G272	Y273	T274	H275	V276	M277	V278	I279	G280	G281	A282	A283	E284	L285	I286	C287	D288	A289	V290	K291	K292	H293	T294	Q295	I296	R297	D298	E299	R300
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F301	F302	K303	T304	N305	N306	S307	Q308	Y309	D310	L311	V312	N313	G314	M315	Y316	L317	I318
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## 4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=Not provided°, rise=Not provided Å, axial sym=Not provided	Depositor
Number of segments used	Not provided	
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{Å}^2$ )	0.3	Depositor
Minimum defocus (nm)	3000	Depositor
Maximum defocus (nm)	6000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	5.497	Depositor
Minimum map value	-2.327	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1.3	Depositor
Map size (Å)	104.0, 104.0, 312.0	wwPDB
Map dimensions	40, 40, 120	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.6, 2.6, 2.6	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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	318	0	0	0	0
1	B	318	0	0	0	0
1	C	318	0	0	0	0
1	D	318	0	0	0	0
1	E	318	0	0	1	0
1	F	318	0	0	0	0
1	G	318	0	0	0	0
1	H	318	0	0	1	0
1	I	318	0	0	0	0
1	J	318	0	0	0	0
1	K	318	0	0	0	0
1	L	318	0	0	0	0
1	M	318	0	0	0	0
1	N	318	0	0	0	0
All	All	4452	0	0	1	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 0.

All (1) 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:E:20:ASP:CA	1:H:160:LEU:CA	2.15	1.23

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

### 5.3.2 Protein sidechains [i](#)

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

### 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 monosaccharides 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

There are no chain breaks in this entry.



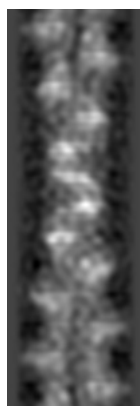
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2848. 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](#)

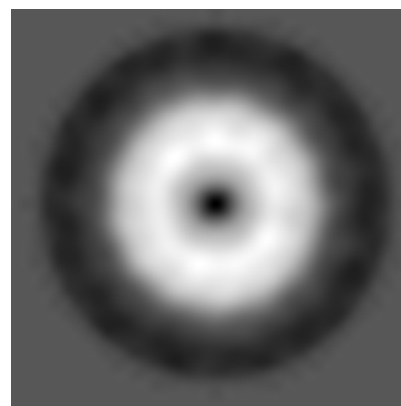
#### 6.1.1 Primary map



X



Y



Z

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

## 6.2 Central slices [i](#)

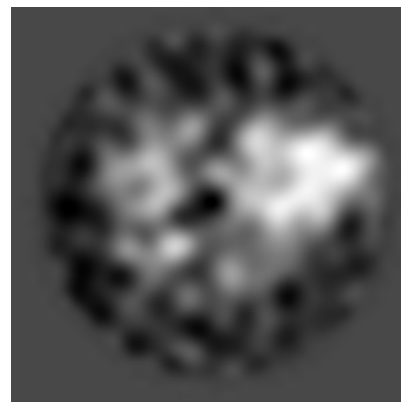
### 6.2.1 Primary map



X Index:  
20



Y Index: 20



Z Index: 60

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

## 6.3 Largest variance slices [i](#)

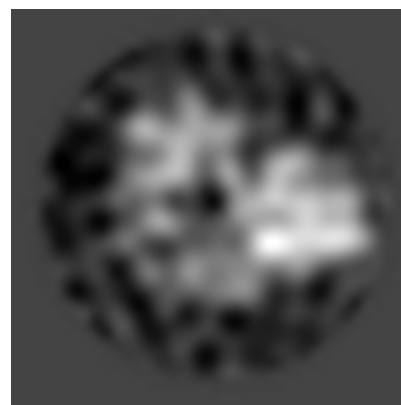
### 6.3.1 Primary map



X Index:  
15



Y Index: 14

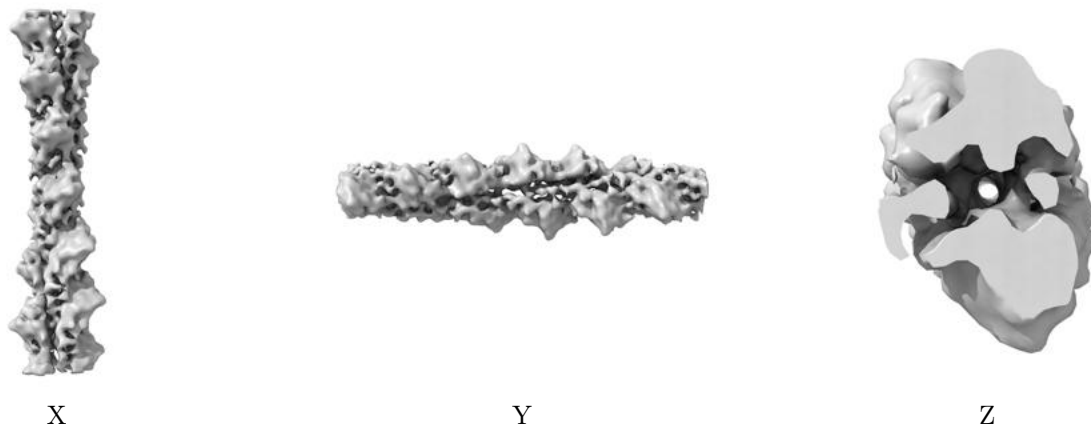


Z Index: 79

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

## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

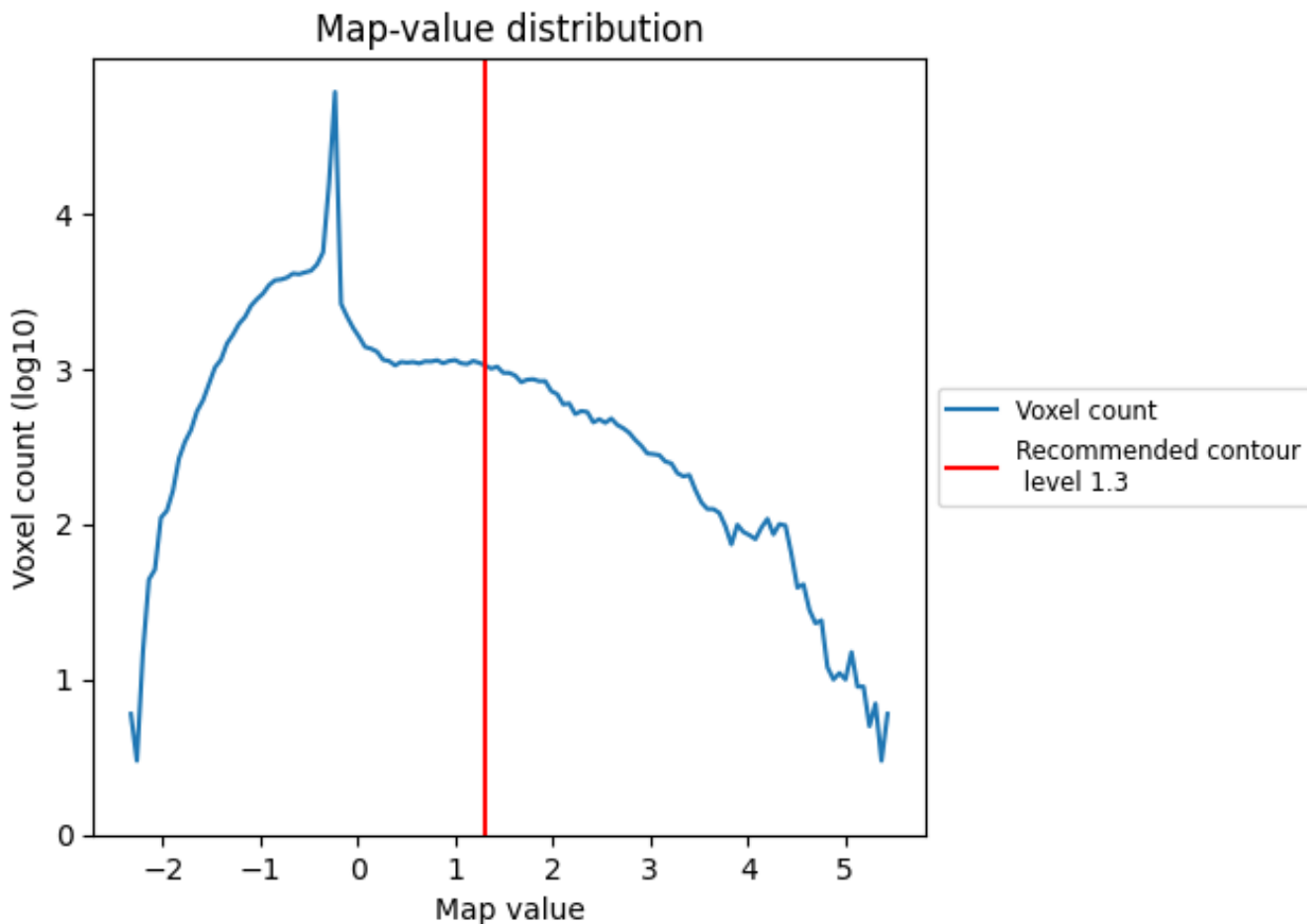
## 6.5 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

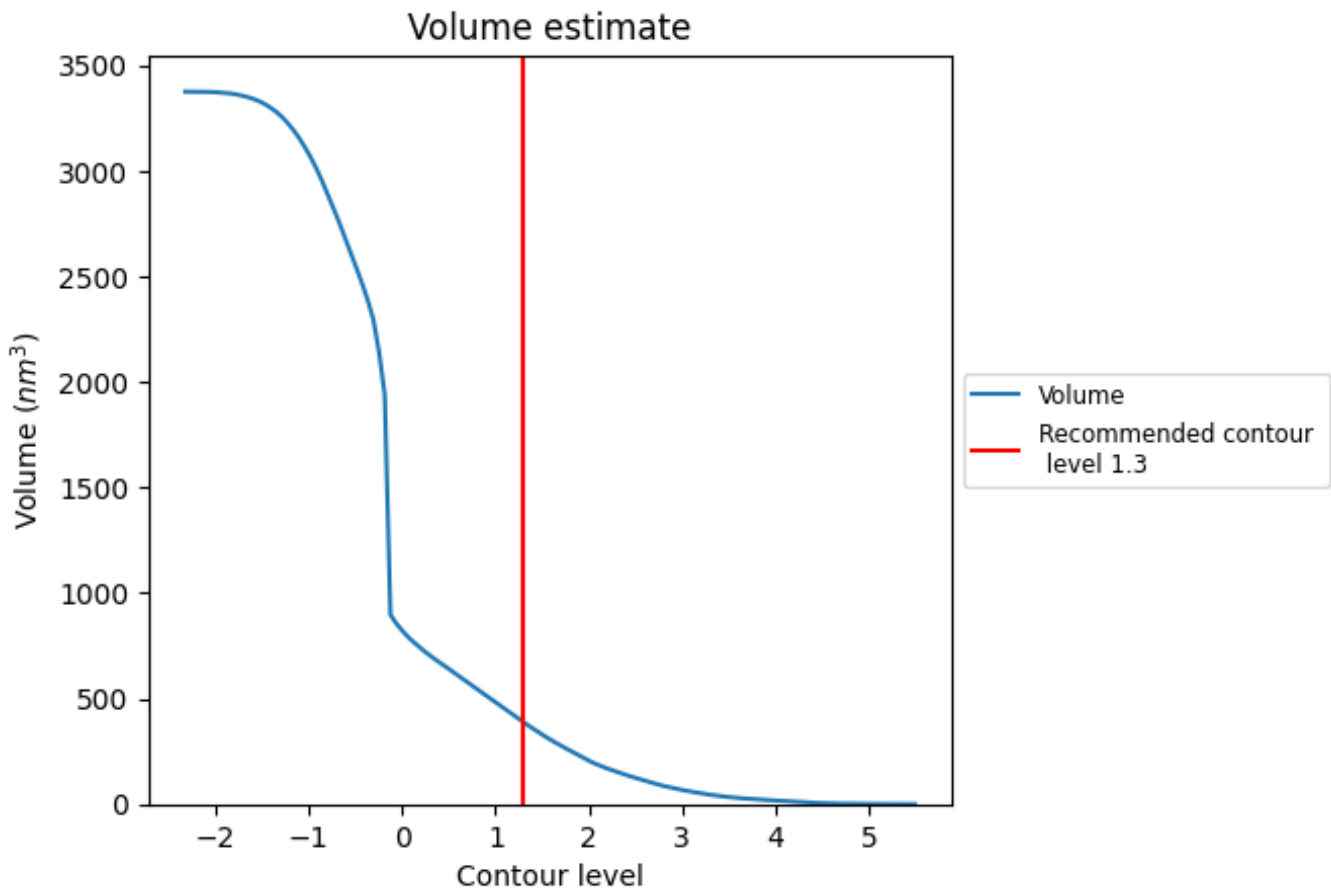
This section contains the results of statistical analysis of the map.

### 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 388 nm<sup>3</sup>; this corresponds to an approximate mass of 351 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.

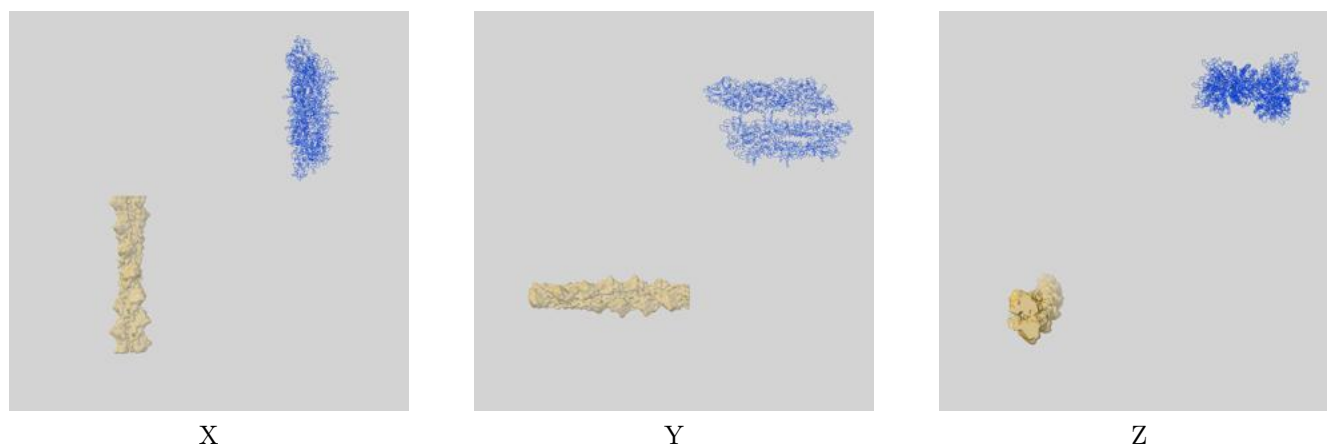
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

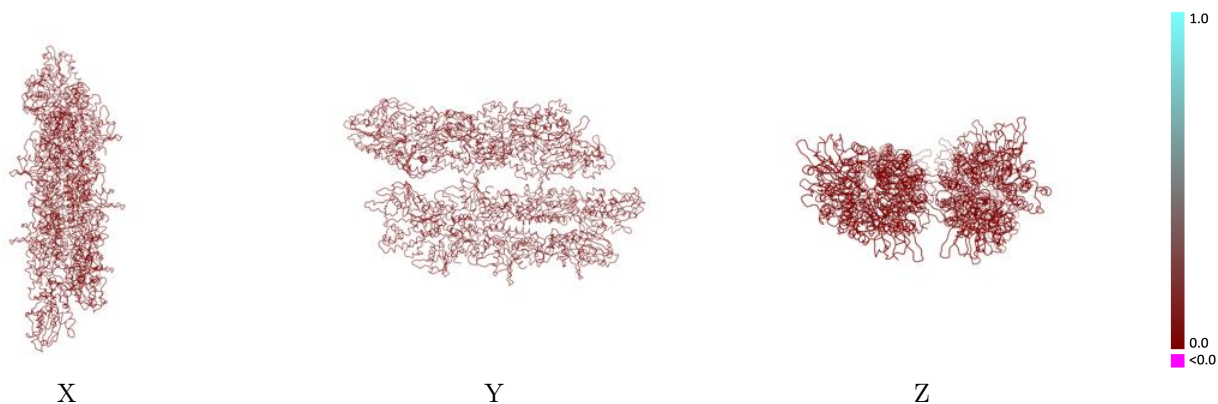
This section contains information regarding the fit between EMDB map EMD-2848 and PDB model 5AI7. Per-residue inclusion information can be found in section 3 on page 5.

### 9.1 Map-model overlay [i](#)



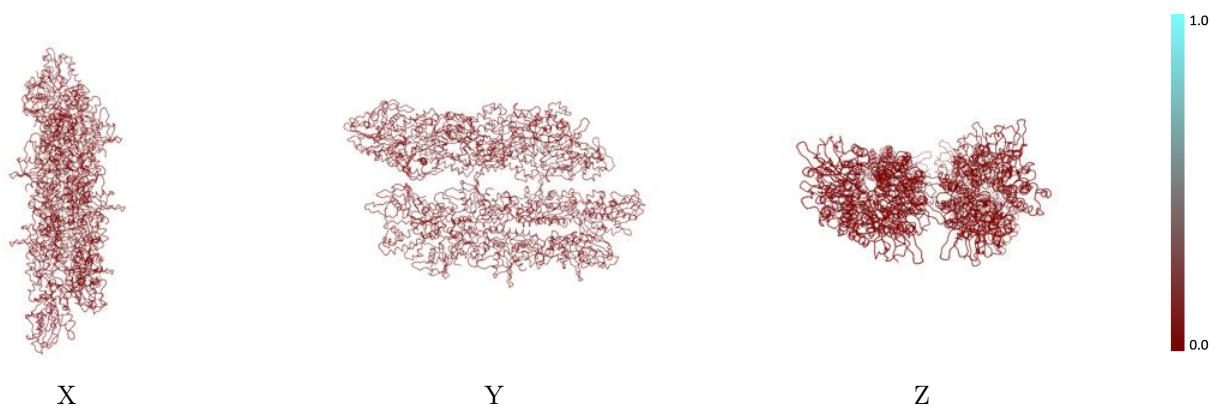
The images above show the 3D surface view of the map at the recommended contour level 1.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



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

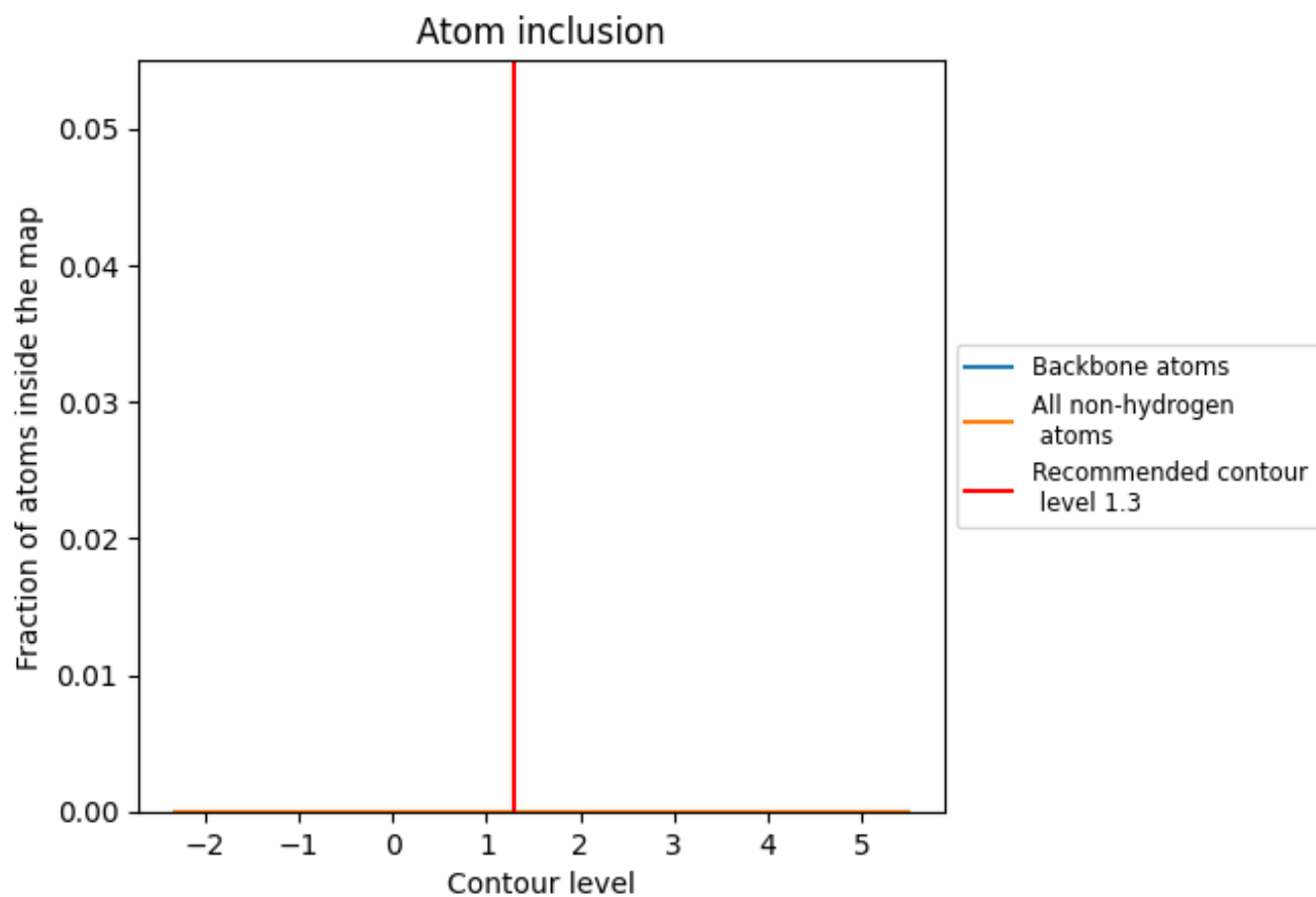
## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.3).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 0% of all backbone atoms, 0% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (1.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.0000	0.0000
A	0.0000	0.0000
B	0.0000	0.0000
C	0.0000	0.0000
D	0.0000	0.0000
E	0.0000	0.0000
F	0.0000	0.0000
G	0.0000	0.0000
H	0.0000	0.0000
I	0.0000	0.0000
J	0.0000	0.0000
K	0.0000	0.0000
L	0.0000	0.0000
M	0.0000	0.0000
N	0.0000	0.0000

