wwPDB EM Validation Summary Report (i)

Nov 28, 2022 – 11:53 AM EST

PDB ID	:	7SPK
EMDB ID	:	EMD-24773
Title	:	Models for C16 reconstruction of Outer Membrane Core Complex (OMCC) of Type IV Secretion System (T4SS) encoded by a plasmid overproducing TraV, TraK and TraB of pED208
Authors	:	Liu, X.; Khara, P.; Baker, M.L.; Christie, P.J.; Hu, B.
Deposited on	:	2021-11-02
Resolution	:	3.90 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

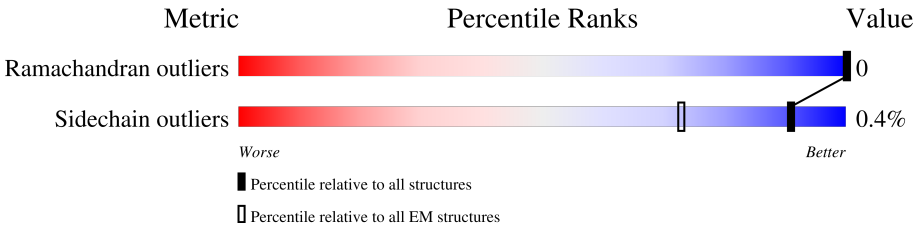
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.90 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	AB1	204	18% 82%
1	AB10	204	18% 82%
1	AB11	204	18% 82%
1	AB12	204	18% 82%
1	AB13	204	18% 82%
1	AB14	204	18% 82%
1	AB15	204	18% 82%
1	AB16	204	18% 82%
1	AB2	204	18% 82%

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Mol	Chain	Length	Quality of chain
1	AB3	204	18% 82%
1	AB4	204	18% 82%
1	AB5	204	18% 82%
1	AB6	204	18% 82%
1	AB7	204	18% 82%
1	AB8	204	18% 82%
1	AB9	204	18% 82%
2	EF1	453	43% 57%
2	EF10	453	43% 57%
2	EF11	453	43% 57%
2	EF12	453	43% 57%
2	EF13	453	43% 57%
2	EF14	453	43% 57%
2	EF15	453	43% 57%
2	EF16	453	43% 57%
2	EF2	453	43% 57%
2	EF3	453	43% 57%
2	EF4	453	43% 57%
2	EF5	453	43% 57%
2	EF6	453	43% 57%
2	EF7	453	43% 57%
2	EF8	453	43% 57%
2	EF9	453	43% 57%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 27968 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 TraV.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AB1	37	Total	C	N	O	S	0	0
			261	153	47	56	5		
1	AB2	37	Total	C	N	O	S	0	0
			261	153	47	56	5		
1	AB3	37	Total	C	N	O	S	0	0
			261	153	47	56	5		
1	AB4	37	Total	C	N	O	S	0	0
			261	153	47	56	5		
1	AB5	37	Total	C	N	O	S	0	0
			261	153	47	56	5		
1	AB6	37	Total	C	N	O	S	0	0
			261	153	47	56	5		
1	AB7	37	Total	C	N	O	S	0	0
			261	153	47	56	5		
1	AB8	37	Total	C	N	O	S	0	0
			261	153	47	56	5		
1	AB9	37	Total	C	N	O	S	0	0
			261	153	47	56	5		
1	AB10	37	Total	C	N	O	S	0	0
			261	153	47	56	5		
1	AB11	37	Total	C	N	O	S	0	0
			261	153	47	56	5		
1	AB12	37	Total	C	N	O	S	0	0
			261	153	47	56	5		
1	AB13	37	Total	C	N	O	S	0	0
			261	153	47	56	5		
1	AB14	37	Total	C	N	O	S	0	0
			261	153	47	56	5		
1	AB15	37	Total	C	N	O	S	0	0
			261	153	47	56	5		
1	AB16	37	Total	C	N	O	S	0	0
			261	153	47	56	5		

- Molecule 2 is a protein called TraB.

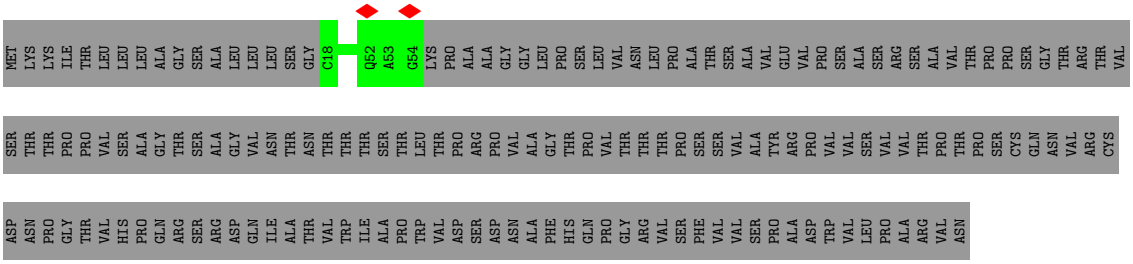
Mol	Chain	Residues	Atoms					AltConf	Trace
2	EF1	197	Total	C	N	O	S	0	0
			1487	930	260	291	6		
2	EF2	197	Total	C	N	O	S	0	0
			1487	930	260	291	6		
2	EF3	197	Total	C	N	O	S	0	0
			1487	930	260	291	6		
2	EF4	197	Total	C	N	O	S	0	0
			1487	930	260	291	6		
2	EF5	197	Total	C	N	O	S	0	0
			1487	930	260	291	6		
2	EF6	197	Total	C	N	O	S	0	0
			1487	930	260	291	6		
2	EF7	197	Total	C	N	O	S	0	0
			1487	930	260	291	6		
2	EF8	197	Total	C	N	O	S	0	0
			1487	930	260	291	6		
2	EF9	197	Total	C	N	O	S	0	0
			1487	930	260	291	6		
2	EF10	197	Total	C	N	O	S	0	0
			1487	930	260	291	6		
2	EF11	197	Total	C	N	O	S	0	0
			1487	930	260	291	6		
2	EF12	197	Total	C	N	O	S	0	0
			1487	930	260	291	6		
2	EF13	197	Total	C	N	O	S	0	0
			1487	930	260	291	6		
2	EF14	197	Total	C	N	O	S	0	0
			1487	930	260	291	6		
2	EF15	197	Total	C	N	O	S	0	0
			1487	930	260	291	6		
2	EF16	197	Total	C	N	O	S	0	0
			1487	930	260	291	6		

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.

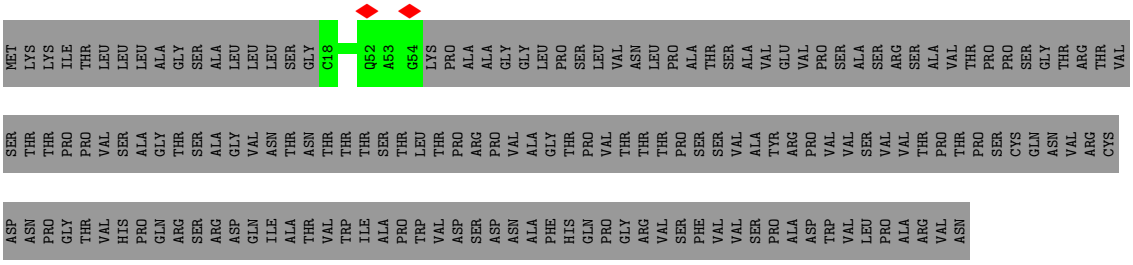
• Molecule 1: TraV

Chain AB1:



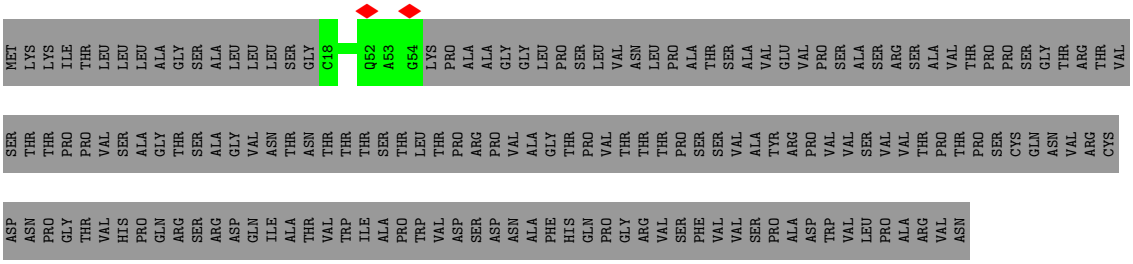
• Molecule 1: TraV

Chain AB2:



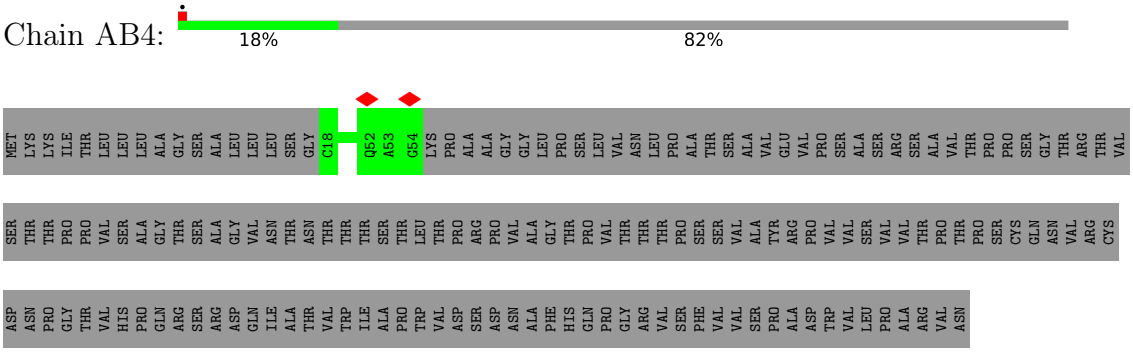
• Molecule 1: TraV

Chain AB3:



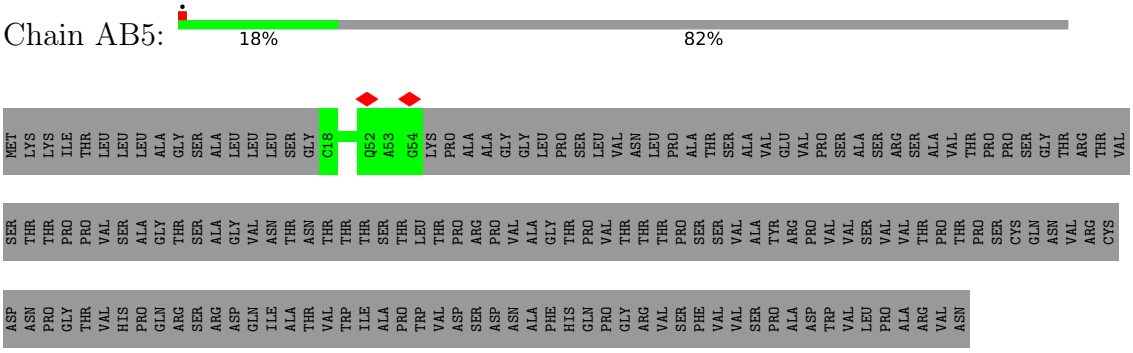
• Molecule 1: TraV

Chain AB4:



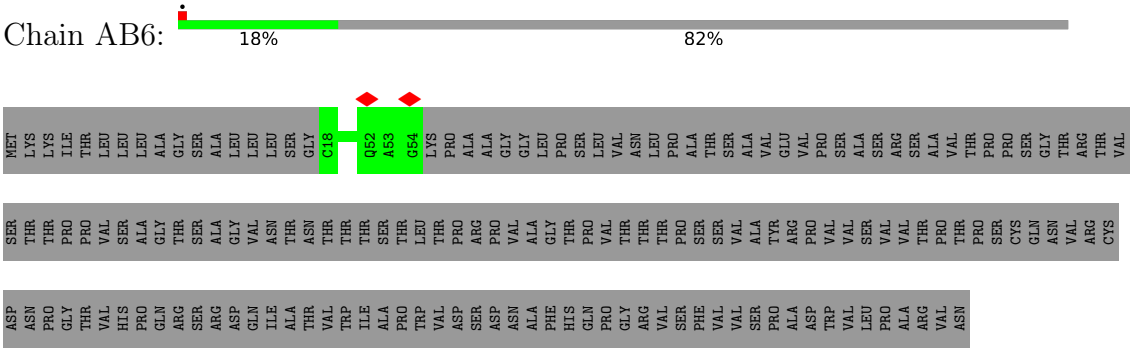
• Molecule 1: TraV

Chain AB5:



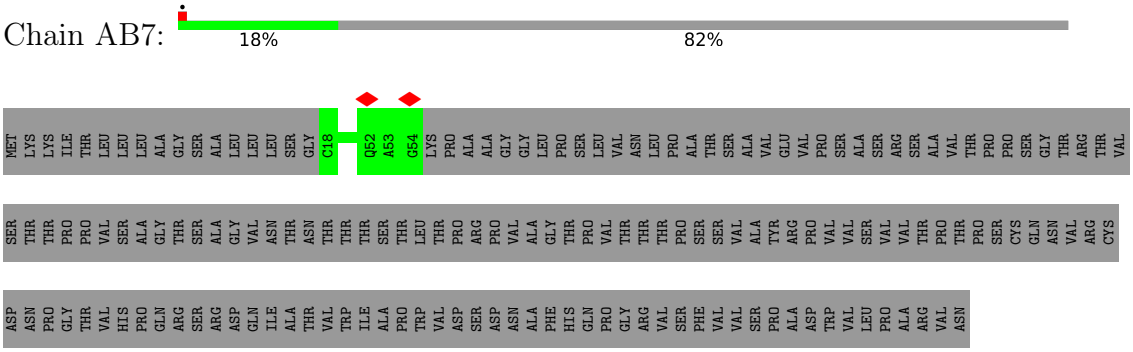
• Molecule 1: TraV

Chain AB6:



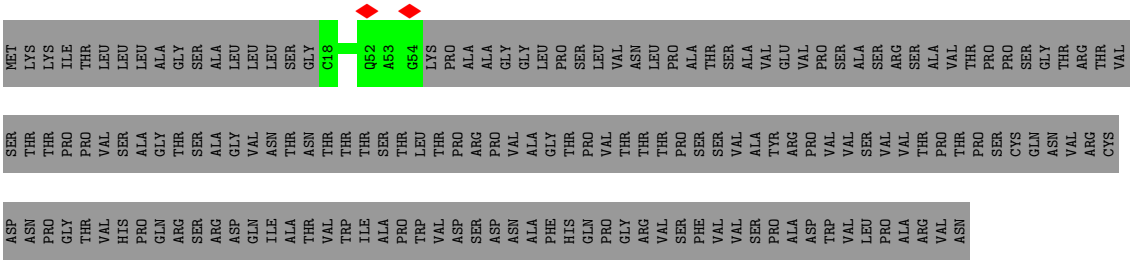
• Molecule 1: TraV

Chain AB7:



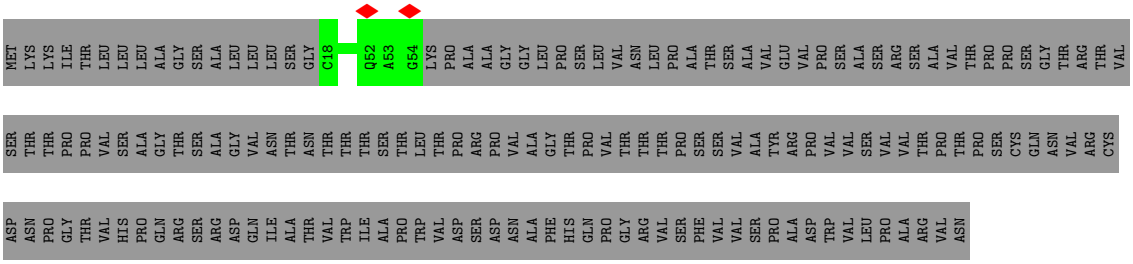
• Molecule 1: TraV

Chain AB8:



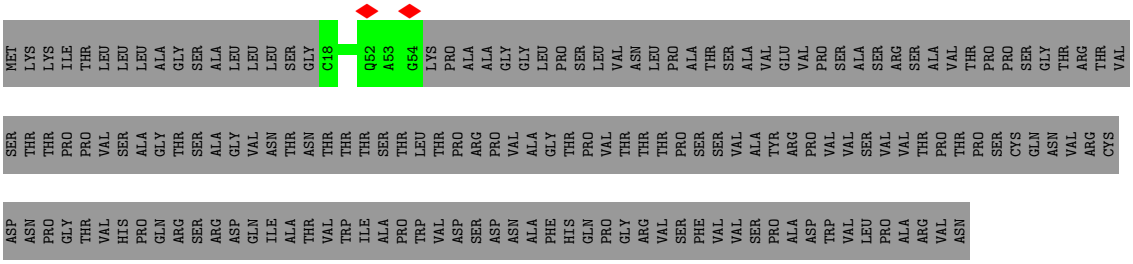
• Molecule 1: TraV

Chain AB9:



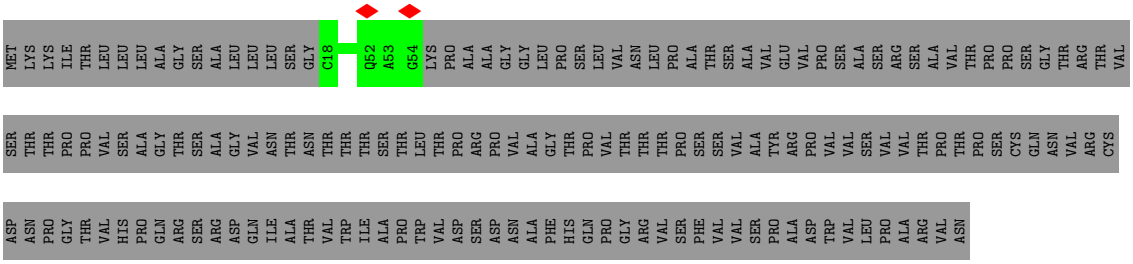
• Molecule 1: TraV

Chain AB10:



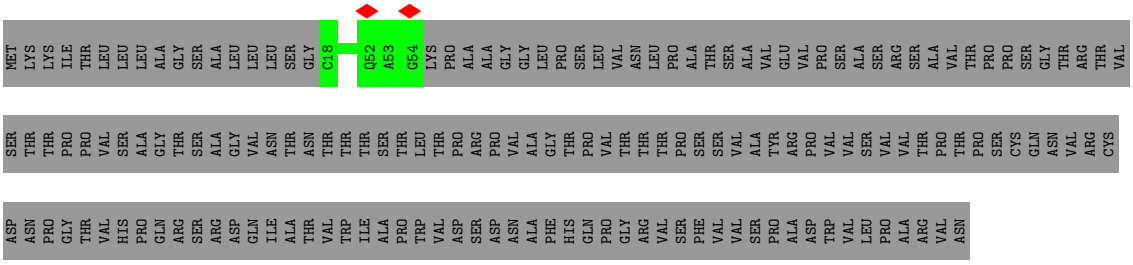
• Molecule 1: TraV

Chain AB11:



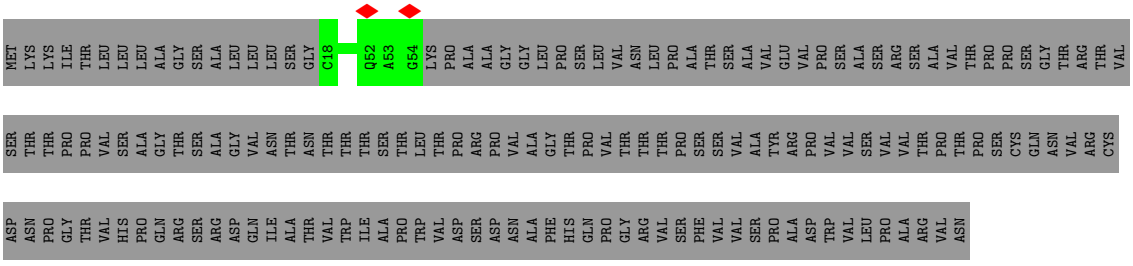
• Molecule 1: TraV

Chain AB12:



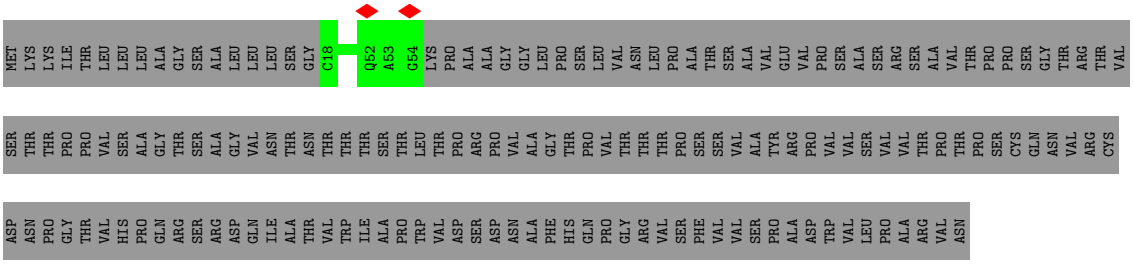
• Molecule 1: TraV

Chain AB13:



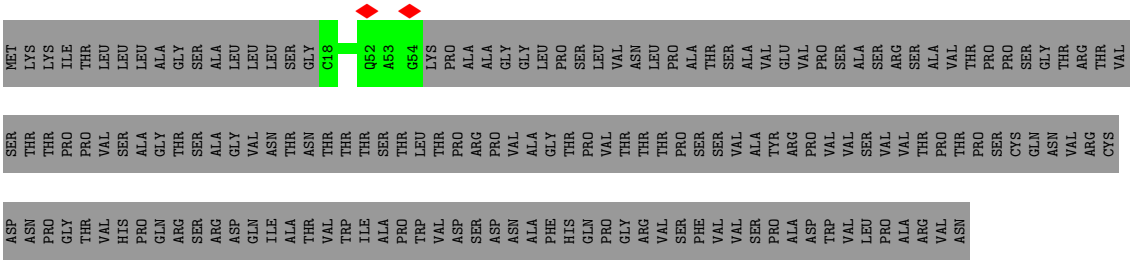
• Molecule 1: TraV

Chain AB14:



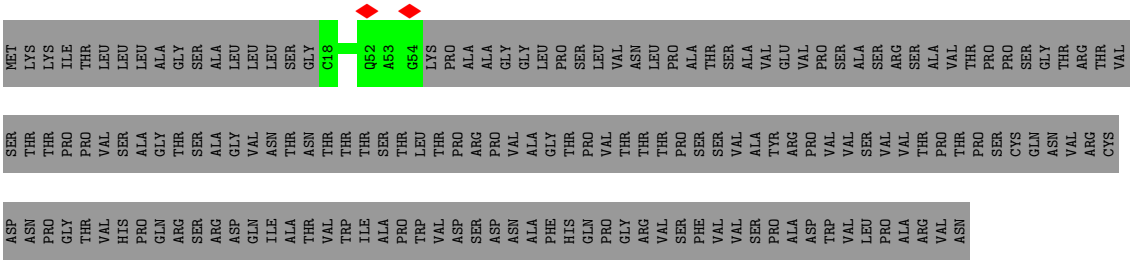
• Molecule 1: TraV

Chain AB15:



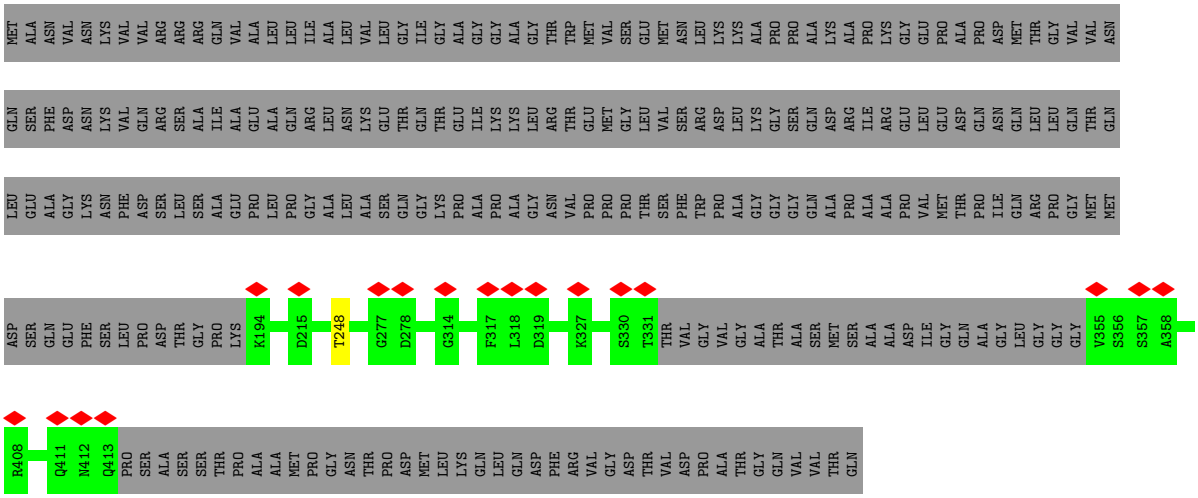
• Molecule 1: TraV

Chain AB16:



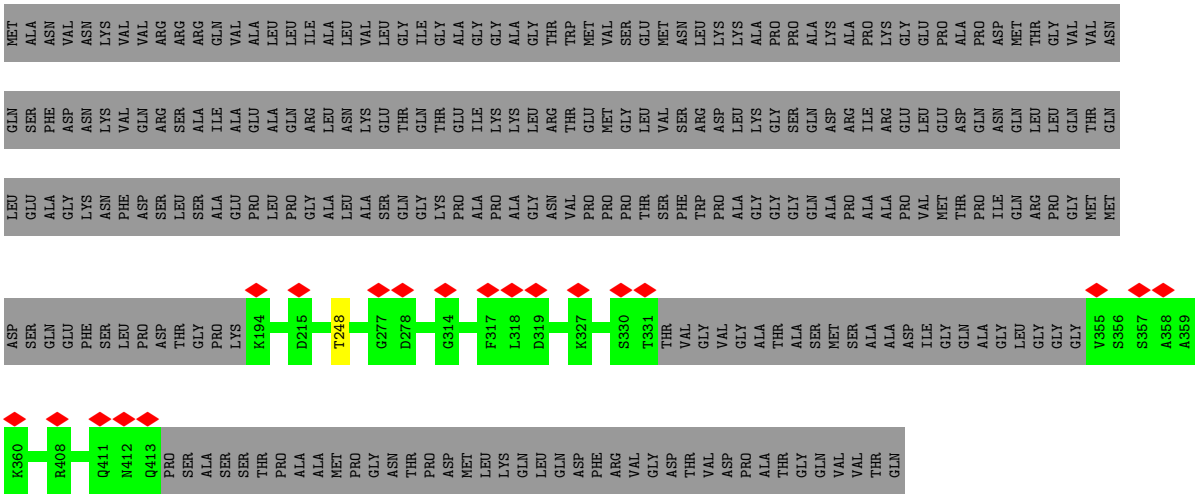
• Molecule 2: TraB

Chain EF1:



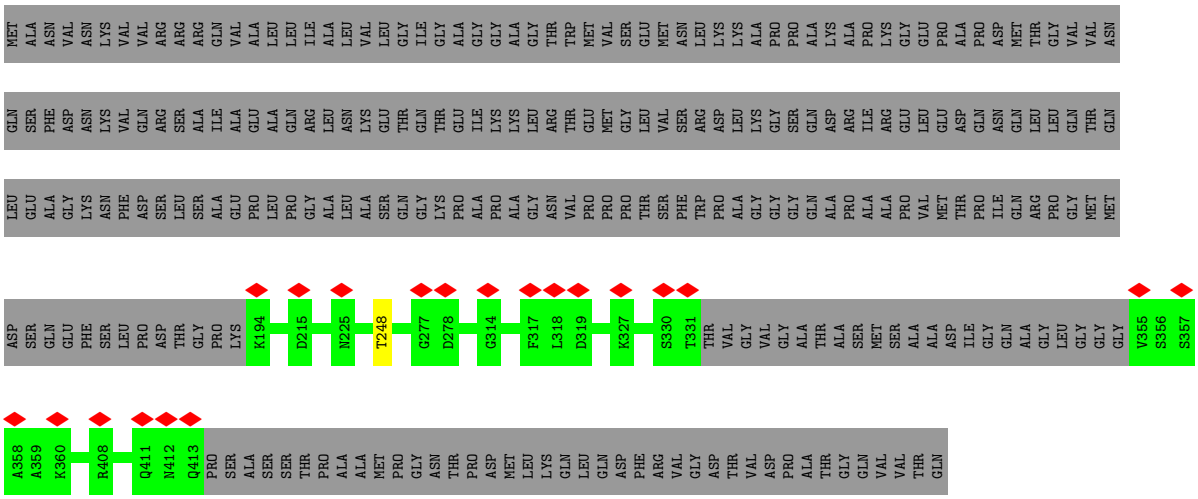
• Molecule 2: TraB

Chain EF2:



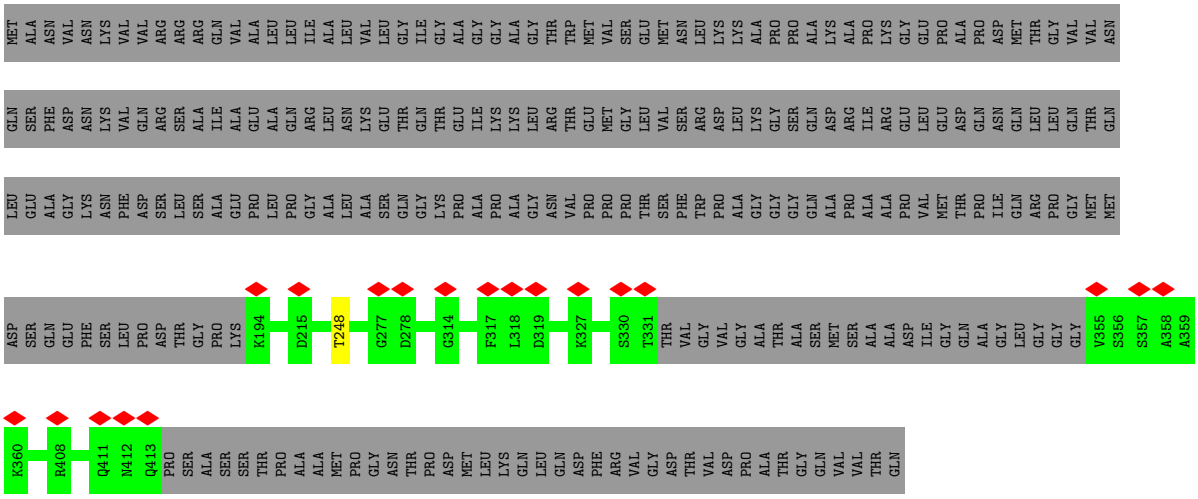
• Molecule 2: TraB

Chain EF3:



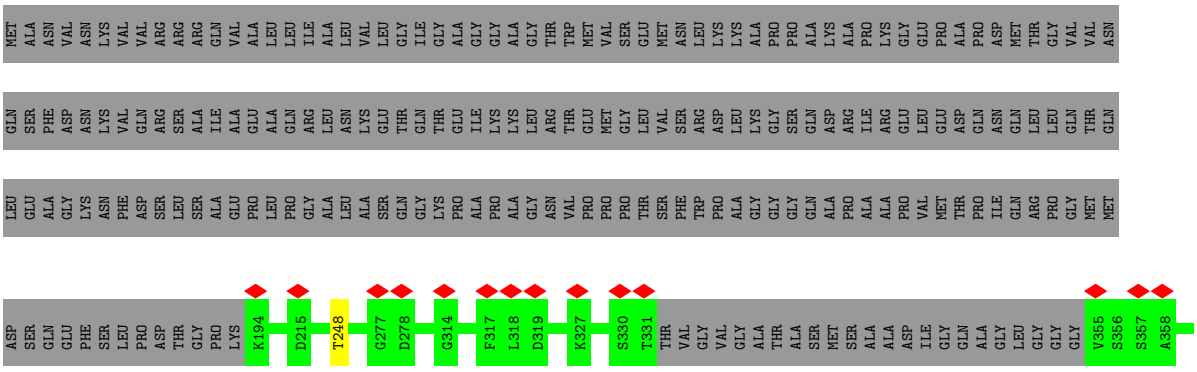
• Molecule 2: TraB

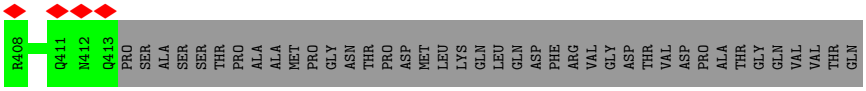
Chain EF4:



• Molecule 2: TraB

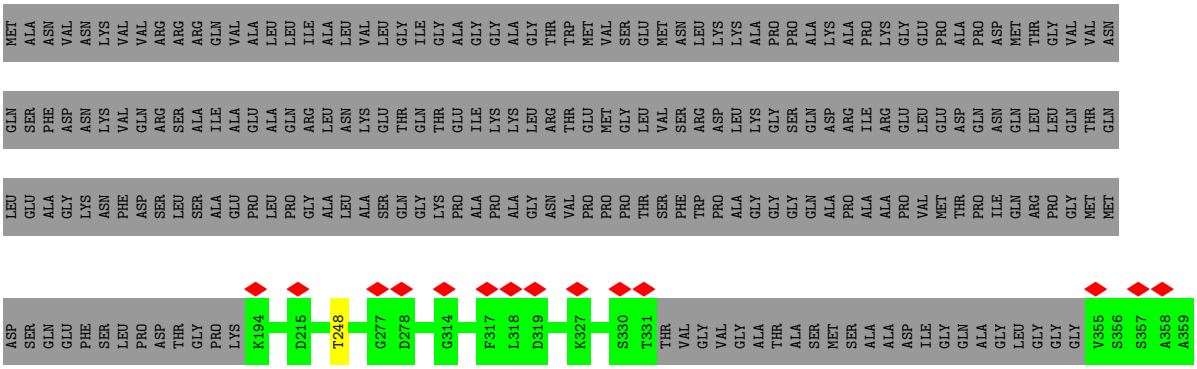
Chain EF5:





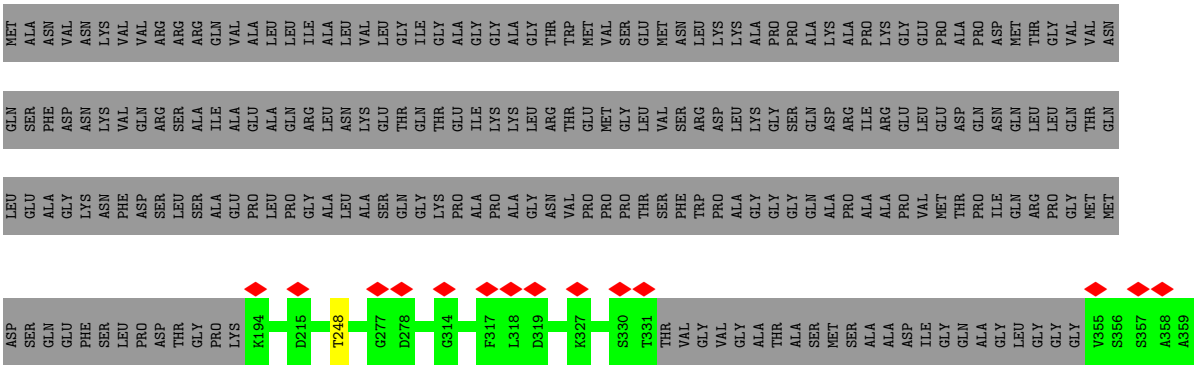
• Molecule 2: TraB

Chain EF6:



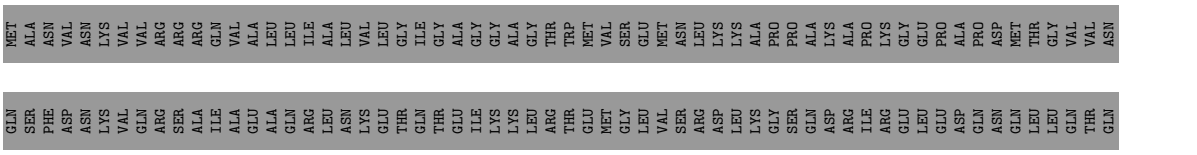
• Molecule 2: TraB

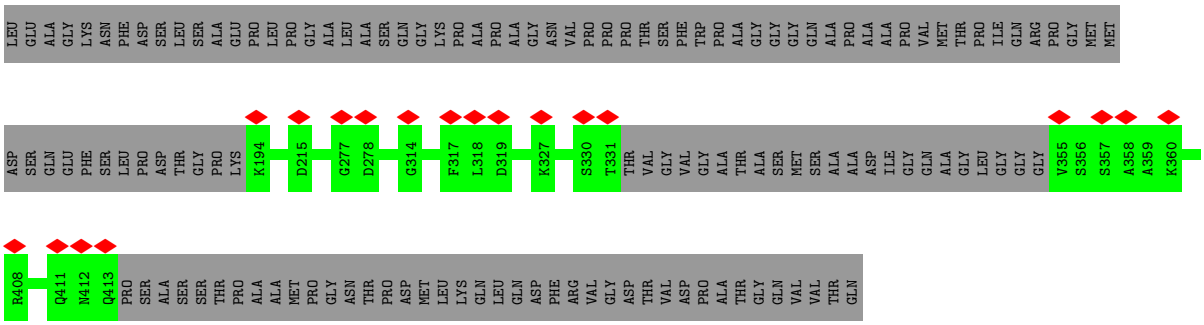
Chain EF7:



• Molecule 2: TraB

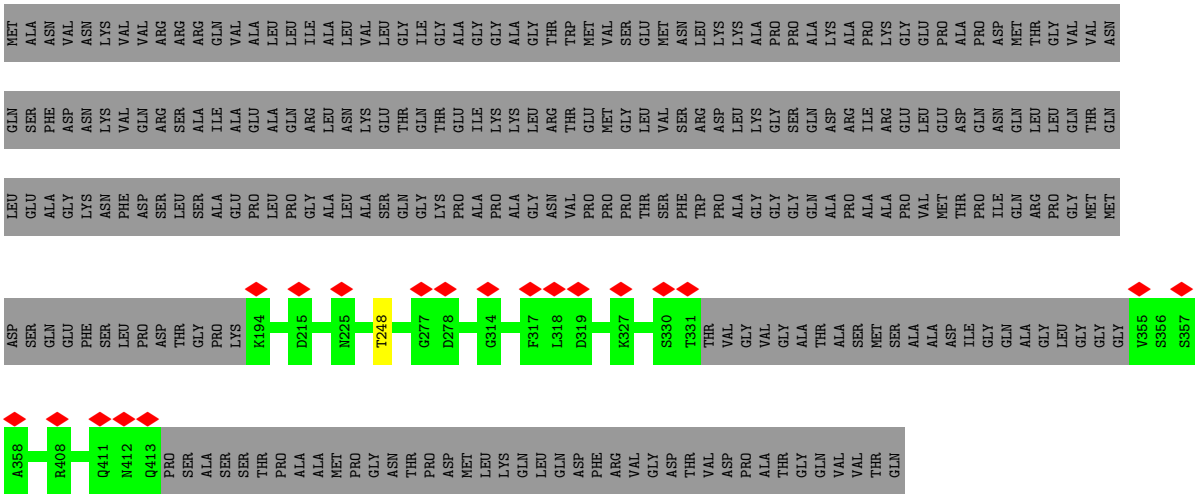
Chain EF8:





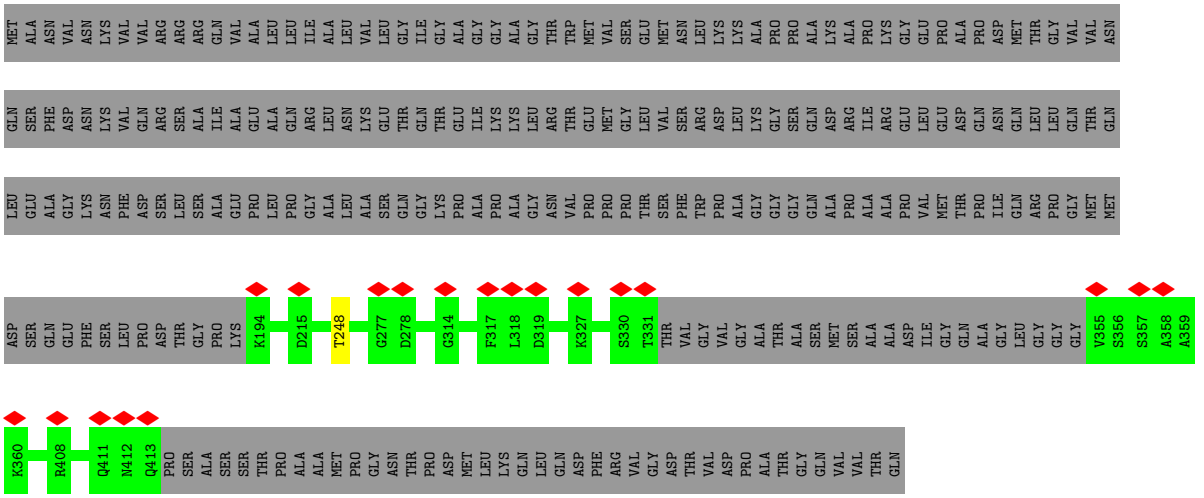
• Molecule 2: TraB

Chain EF9:



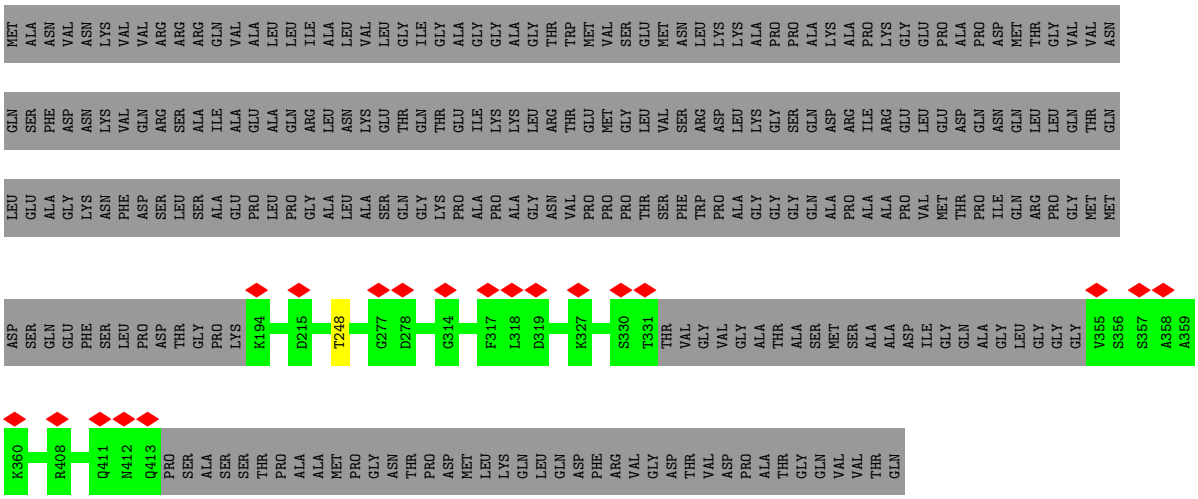
• Molecule 2: TraB

Chain EF10:



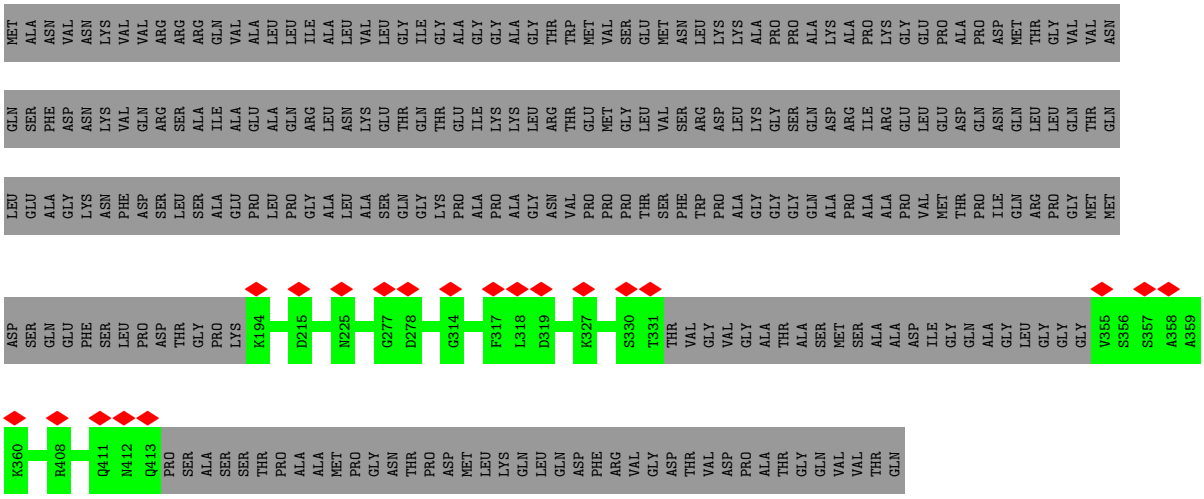
• Molecule 2: TraB

Chain EF11:



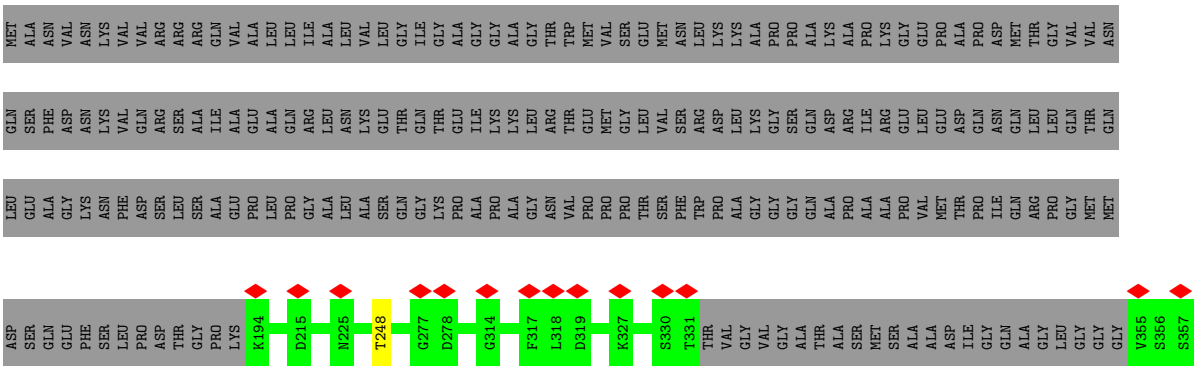
• Molecule 2: TraB

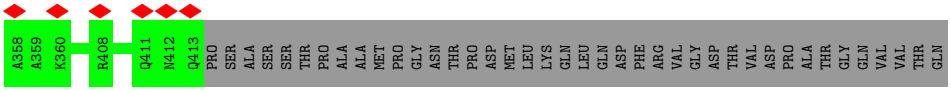
Chain EF12:



• Molecule 2: TraB

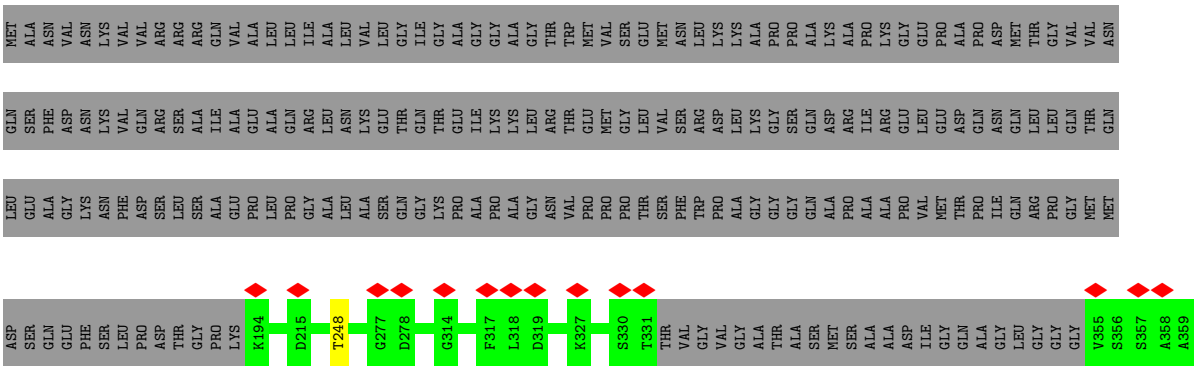
Chain EF13:

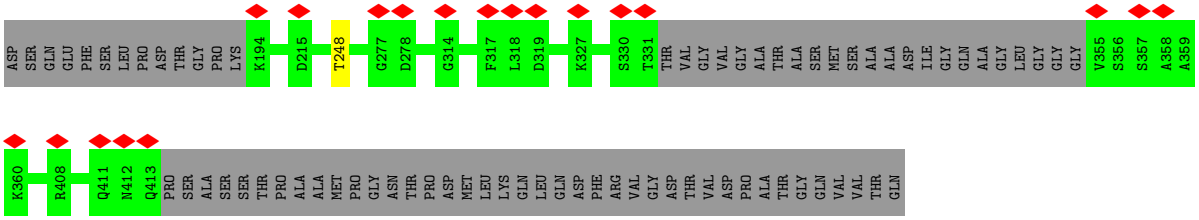




• Molecule 2: TraB

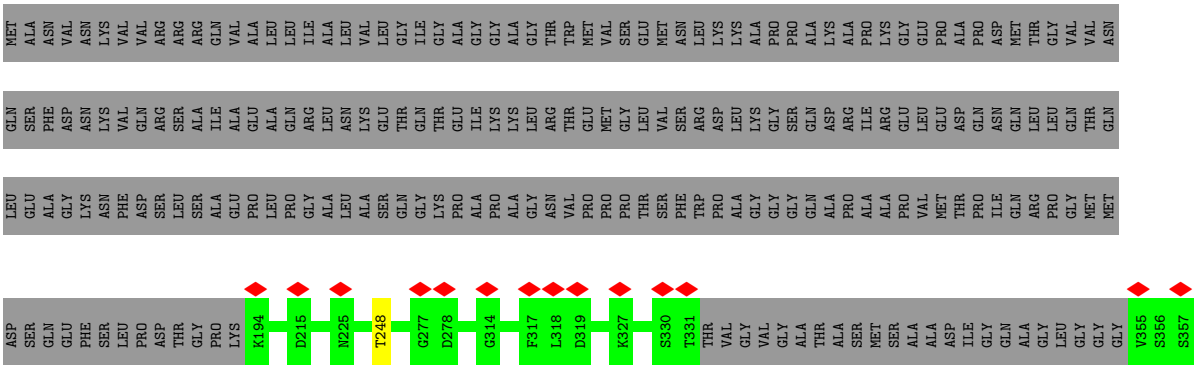
Chain EF14:

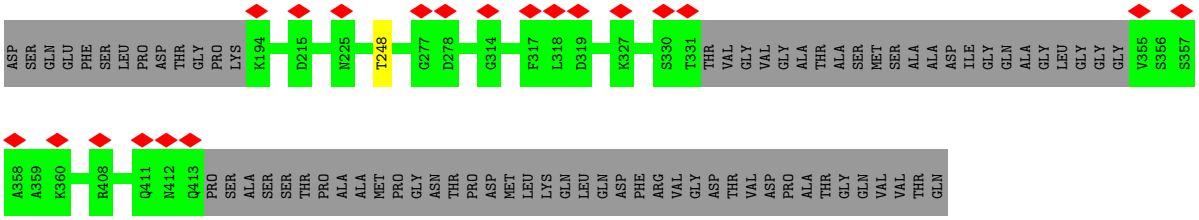




• Molecule 2: TraB

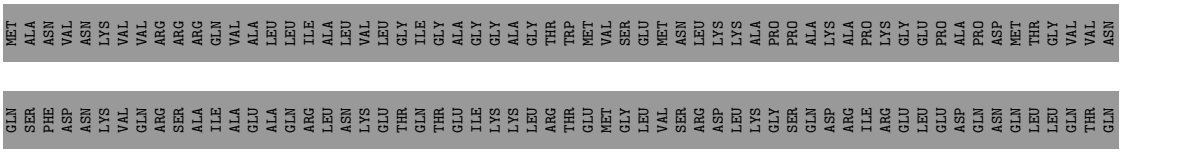
Chain EF15:

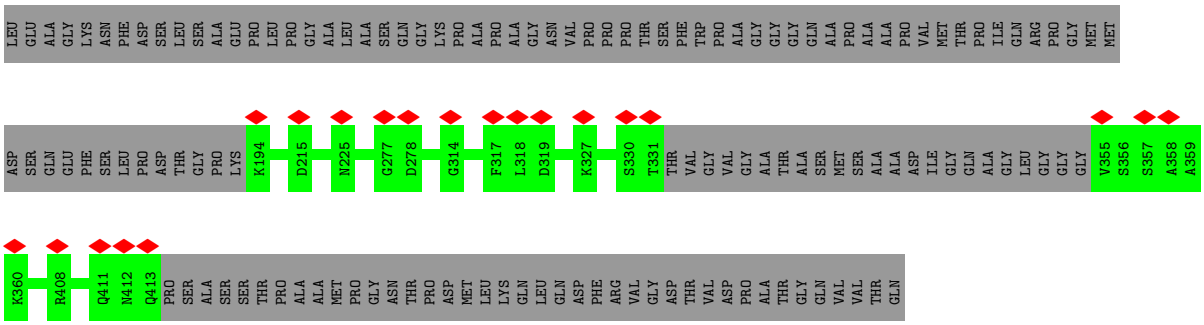




• Molecule 2: TraB

Chain EF16:




LEU GLU ALA GLY LYS ASN PHE ASP SER LEU SER ALA GLU PRO LEU PRO GLY ALA LEU ALA SER GLN GLY LYS PRO ALA PRO ALA GLY ASN VAL PRO PRO PRO THR SER PHE TRP PRO ALA GLY GLY GLY GLN ALA PRO ALA ALA PRO VAL MET THR PRO ILE GLN ARG PRO GLY MET MET
ASP SER GLN GLU PHE SER LEU PRO ASP THR GLY PRO LYS K194 D215 N225 G277 D278 G314 F317 L318 D319 K327 S330 T331 THR VAL GLY VAL GLY ALA THR ALA SER MET SER ALA ALA ASP ILE GLY GLN ALA GLY LEU GLY GLY GLY V355 S356 S357 A358 A359
K360 R408 Q411 N412 Q413 PRO SER ALA SER SER THR PRO ALA ALA MET PRO GLY ASN THR PRO ASP MET LEU LYS GLN LEU GLN ASP PHE ARG VAL GLY ASP THR VAL ASP PRO ALA THR GLY GLN VAL VAL THR GLN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	22000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.328	Depositor
Minimum map value	-0.752	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.053	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	426.08, 426.08, 426.08	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0652, 1.0652, 1.0652	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	AB1	0.24	0/261	0.51	0/348
1	AB10	0.24	0/261	0.51	0/348
1	AB11	0.24	0/261	0.51	0/348
1	AB12	0.24	0/261	0.51	0/348
1	AB13	0.24	0/261	0.51	0/348
1	AB14	0.24	0/261	0.51	0/348
1	AB15	0.24	0/261	0.51	0/348
1	AB16	0.34	0/261	0.59	0/348
1	AB2	0.24	0/261	0.51	0/348
1	AB3	0.24	0/261	0.51	0/348
1	AB4	0.24	0/261	0.51	0/348
1	AB5	0.24	0/261	0.51	0/348
1	AB6	0.24	0/261	0.51	0/348
1	AB7	0.24	0/261	0.51	0/348
1	AB8	0.24	0/261	0.51	0/348
1	AB9	0.24	0/261	0.50	0/348
2	EF1	0.31	0/1509	0.54	0/2031
2	EF10	0.31	0/1509	0.54	0/2031
2	EF11	0.31	0/1509	0.54	0/2031
2	EF12	0.31	0/1509	0.55	0/2031
2	EF13	0.31	0/1509	0.54	0/2031
2	EF14	0.31	0/1509	0.54	0/2031
2	EF15	0.31	0/1509	0.54	0/2031
2	EF16	0.31	0/1509	0.54	0/2031
2	EF2	0.31	0/1509	0.54	0/2031
2	EF3	0.31	0/1509	0.54	0/2031
2	EF4	0.31	0/1509	0.54	0/2031
2	EF5	0.32	0/1509	0.54	0/2031
2	EF6	0.31	0/1509	0.54	0/2031
2	EF7	0.31	0/1509	0.54	0/2031
2	EF8	0.31	0/1509	0.54	0/2031
2	EF9	0.31	0/1509	0.54	0/2031
All	All	0.30	0/28320	0.54	0/38064

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)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	AB1	35/204 (17%)	35 (100%)	0	0	100	100
1	AB10	35/204 (17%)	35 (100%)	0	0	100	100
1	AB11	35/204 (17%)	35 (100%)	0	0	100	100
1	AB12	35/204 (17%)	35 (100%)	0	0	100	100
1	AB13	35/204 (17%)	35 (100%)	0	0	100	100
1	AB14	35/204 (17%)	35 (100%)	0	0	100	100
1	AB15	35/204 (17%)	35 (100%)	0	0	100	100
1	AB16	35/204 (17%)	35 (100%)	0	0	100	100
1	AB2	35/204 (17%)	35 (100%)	0	0	100	100
1	AB3	35/204 (17%)	35 (100%)	0	0	100	100
1	AB4	35/204 (17%)	35 (100%)	0	0	100	100
1	AB5	35/204 (17%)	35 (100%)	0	0	100	100
1	AB6	35/204 (17%)	35 (100%)	0	0	100	100
1	AB7	35/204 (17%)	35 (100%)	0	0	100	100
1	AB8	35/204 (17%)	35 (100%)	0	0	100	100
1	AB9	35/204 (17%)	35 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	EF1	193/453 (43%)	183 (95%)	10 (5%)	0	100	100
2	EF10	193/453 (43%)	184 (95%)	9 (5%)	0	100	100
2	EF11	193/453 (43%)	183 (95%)	10 (5%)	0	100	100
2	EF12	193/453 (43%)	184 (95%)	9 (5%)	0	100	100
2	EF13	193/453 (43%)	183 (95%)	10 (5%)	0	100	100
2	EF14	193/453 (43%)	183 (95%)	10 (5%)	0	100	100
2	EF15	193/453 (43%)	183 (95%)	10 (5%)	0	100	100
2	EF16	193/453 (43%)	184 (95%)	9 (5%)	0	100	100
2	EF2	193/453 (43%)	183 (95%)	10 (5%)	0	100	100
2	EF3	193/453 (43%)	183 (95%)	10 (5%)	0	100	100
2	EF4	193/453 (43%)	184 (95%)	9 (5%)	0	100	100
2	EF5	193/453 (43%)	183 (95%)	10 (5%)	0	100	100
2	EF6	193/453 (43%)	183 (95%)	10 (5%)	0	100	100
2	EF7	193/453 (43%)	183 (95%)	10 (5%)	0	100	100
2	EF8	193/453 (43%)	184 (95%)	9 (5%)	0	100	100
2	EF9	193/453 (43%)	183 (95%)	10 (5%)	0	100	100
All	All	3648/10512 (35%)	3493 (96%)	155 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AB1	28/168 (17%)	28 (100%)	0	100	100
1	AB10	28/168 (17%)	28 (100%)	0	100	100
1	AB11	28/168 (17%)	28 (100%)	0	100	100
1	AB12	28/168 (17%)	28 (100%)	0	100	100
1	AB13	28/168 (17%)	28 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AB14	28/168 (17%)	28 (100%)	0	100	100
1	AB15	28/168 (17%)	28 (100%)	0	100	100
1	AB16	28/168 (17%)	28 (100%)	0	100	100
1	AB2	28/168 (17%)	28 (100%)	0	100	100
1	AB3	28/168 (17%)	28 (100%)	0	100	100
1	AB4	28/168 (17%)	28 (100%)	0	100	100
1	AB5	28/168 (17%)	28 (100%)	0	100	100
1	AB6	28/168 (17%)	28 (100%)	0	100	100
1	AB7	28/168 (17%)	28 (100%)	0	100	100
1	AB8	28/168 (17%)	28 (100%)	0	100	100
1	AB9	28/168 (17%)	28 (100%)	0	100	100
2	EF1	156/353 (44%)	155 (99%)	1 (1%)	86	91
2	EF10	156/353 (44%)	155 (99%)	1 (1%)	86	91
2	EF11	156/353 (44%)	155 (99%)	1 (1%)	86	91
2	EF12	156/353 (44%)	156 (100%)	0	100	100
2	EF13	156/353 (44%)	155 (99%)	1 (1%)	86	91
2	EF14	156/353 (44%)	155 (99%)	1 (1%)	86	91
2	EF15	156/353 (44%)	155 (99%)	1 (1%)	86	91
2	EF16	156/353 (44%)	156 (100%)	0	100	100
2	EF2	156/353 (44%)	155 (99%)	1 (1%)	86	91
2	EF3	156/353 (44%)	155 (99%)	1 (1%)	86	91
2	EF4	156/353 (44%)	155 (99%)	1 (1%)	86	91
2	EF5	156/353 (44%)	155 (99%)	1 (1%)	86	91
2	EF6	156/353 (44%)	155 (99%)	1 (1%)	86	91
2	EF7	156/353 (44%)	155 (99%)	1 (1%)	86	91
2	EF8	156/353 (44%)	156 (100%)	0	100	100
2	EF9	156/353 (44%)	155 (99%)	1 (1%)	86	91
All	All	2944/8336 (35%)	2931 (100%)	13 (0%)	91	94

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	EF9	248	THR

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Mol	Chain	Res	Type
2	EF10	248	THR
2	EF15	248	THR
2	EF13	248	THR
2	EF14	248	THR

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)

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 (i)

There are no chain breaks in this entry.

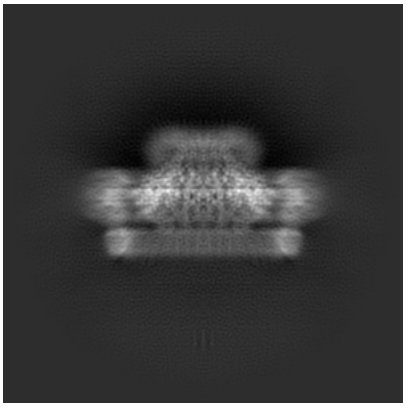
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-24773. These allow visual inspection of the internal detail of the map and identification of artifacts.

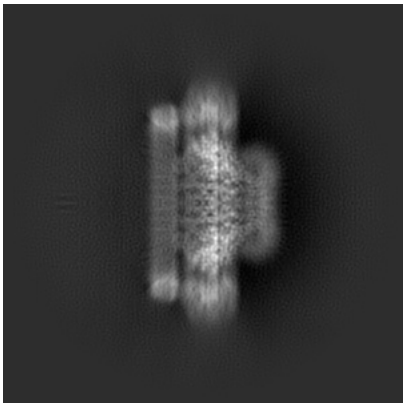
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

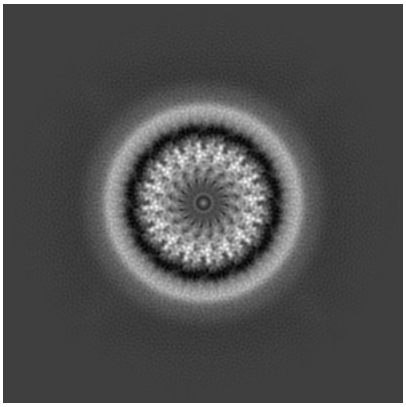
6.1.1 Primary map



X



Y

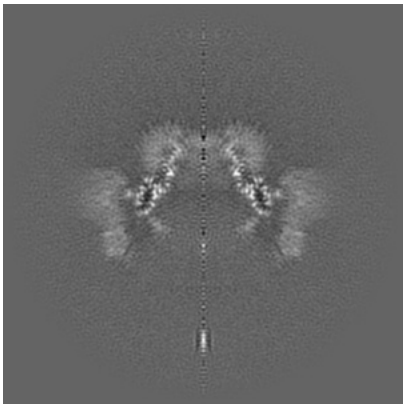


Z

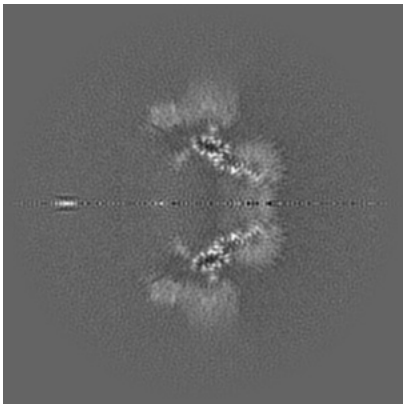
The images above show the map projected in three orthogonal directions.

6.2 Central slices

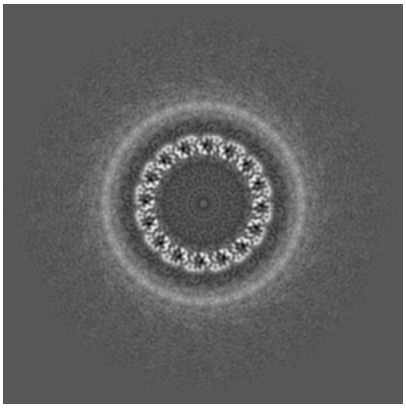
6.2.1 Primary map



X Index: 200



Y Index: 200

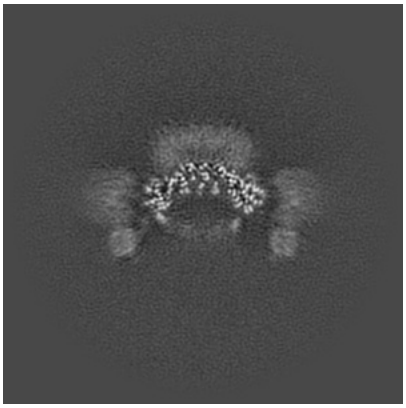


Z Index: 200

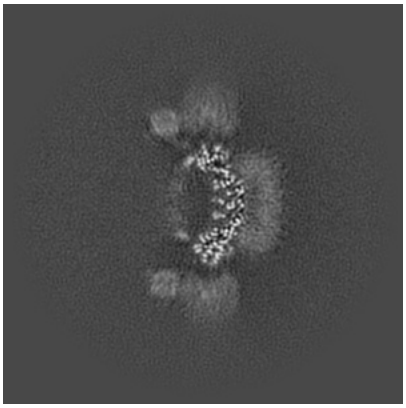
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

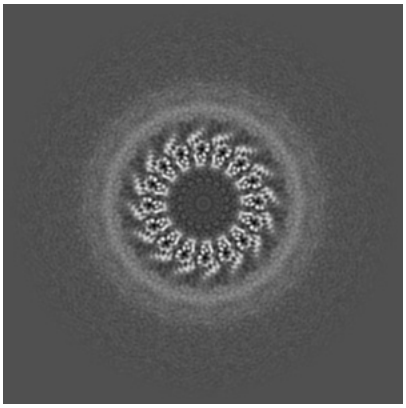
6.3.1 Primary map



X Index: 164



Y Index: 164

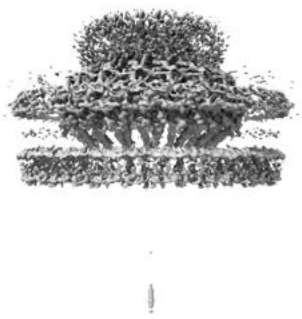


Z Index: 212

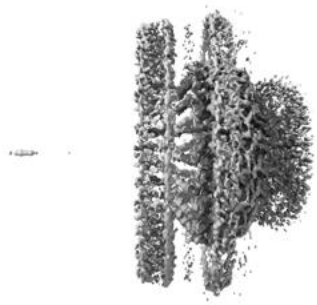
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

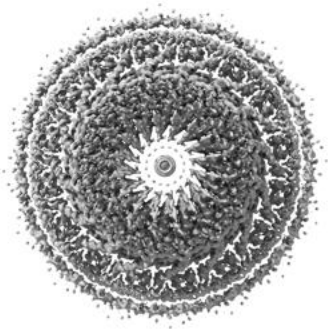
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.35. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

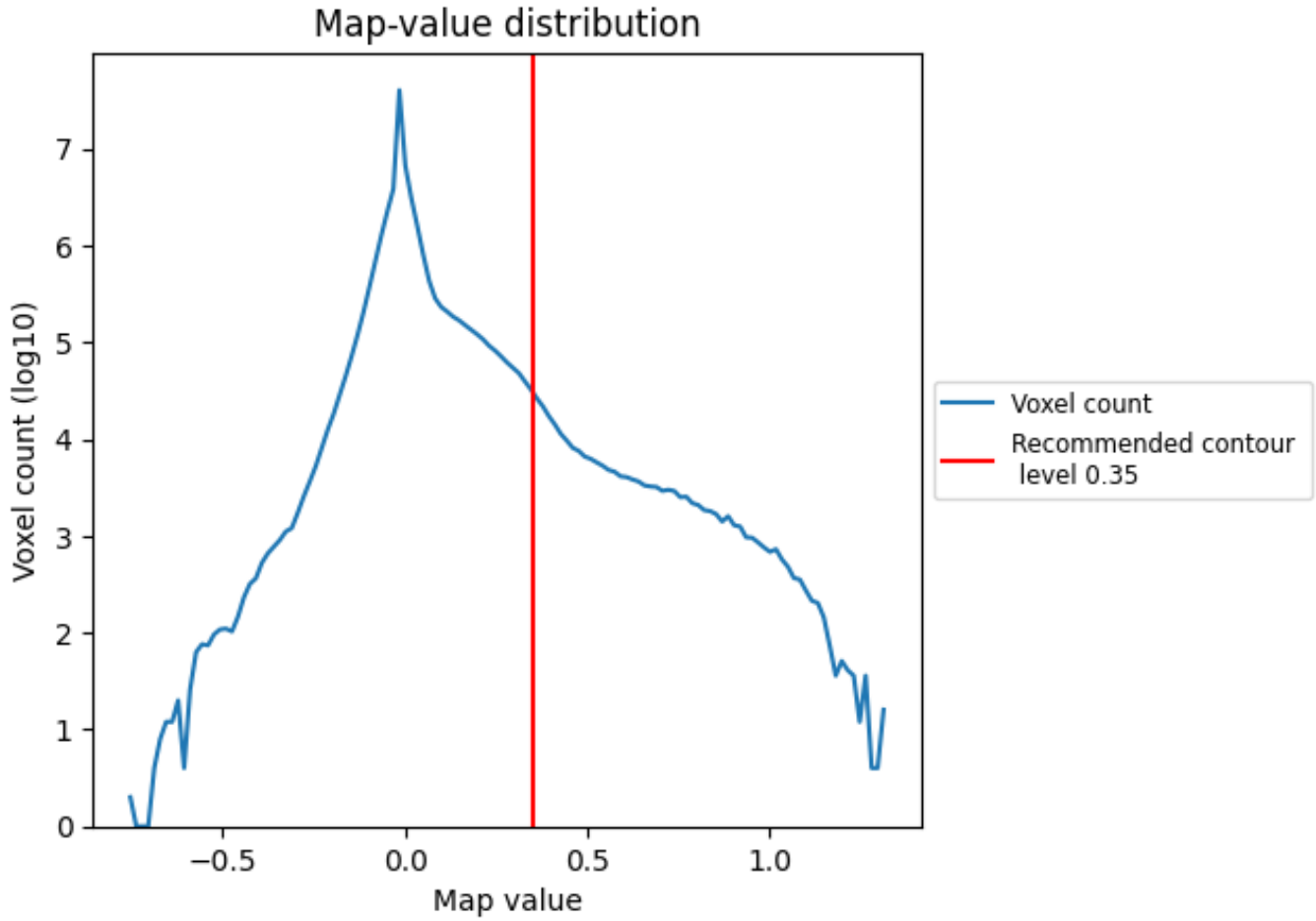
6.5 Mask visualisation (i)

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

7 Map analysis

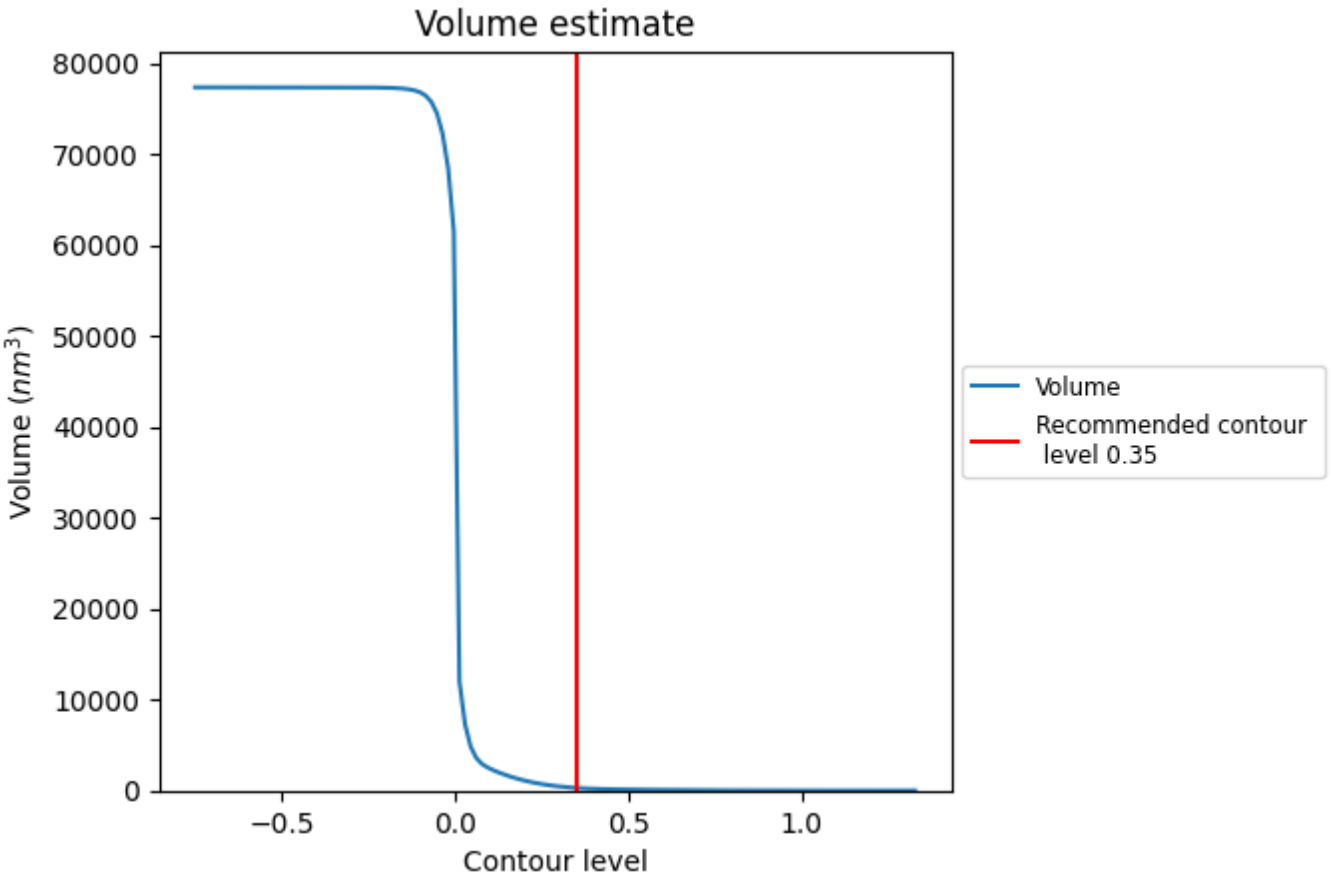
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

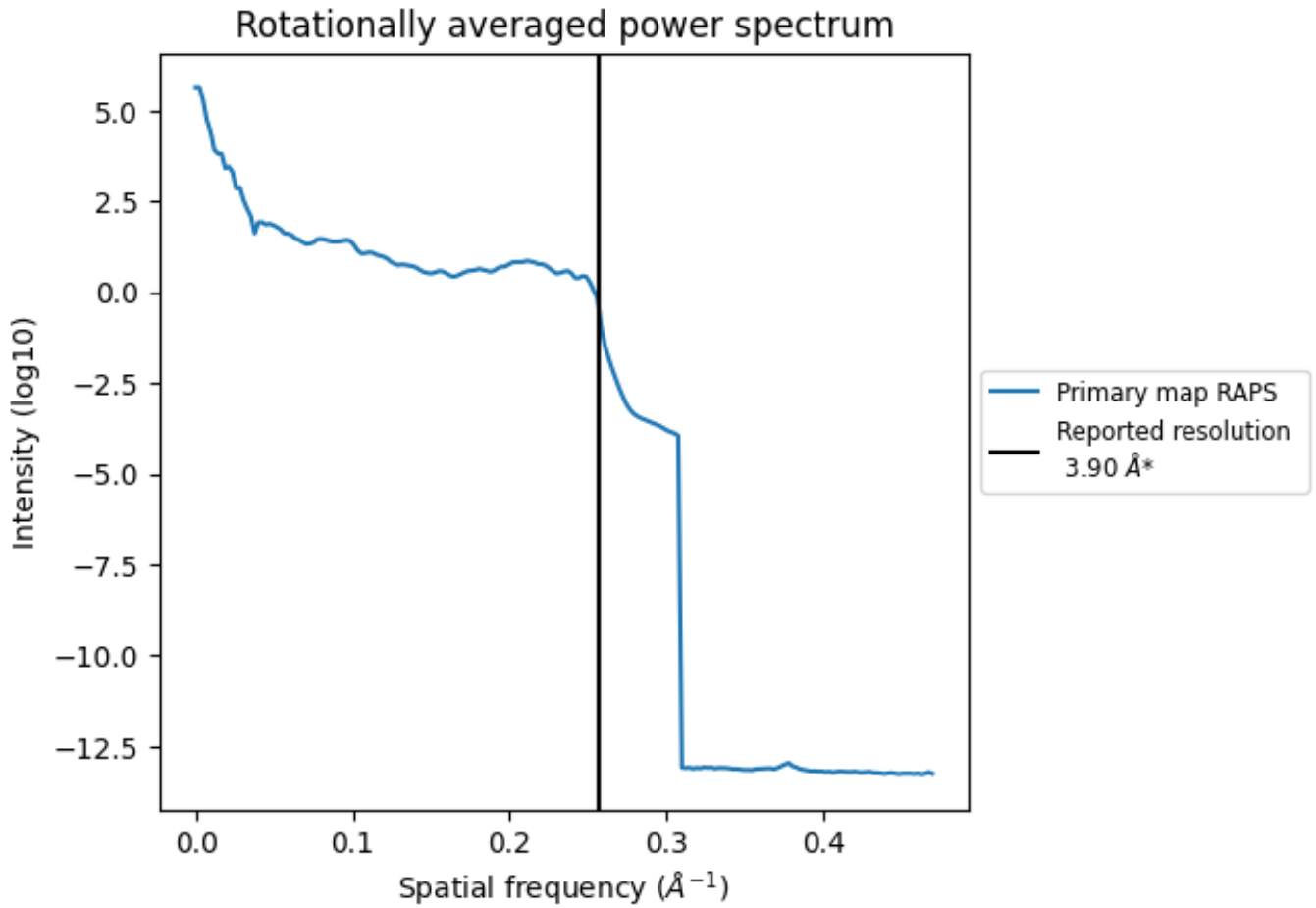
7.2 Volume estimate (i)



The volume at the recommended contour level is 284 nm^3; this corresponds to an approximate mass of 257 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.256 $Å^{-1}$

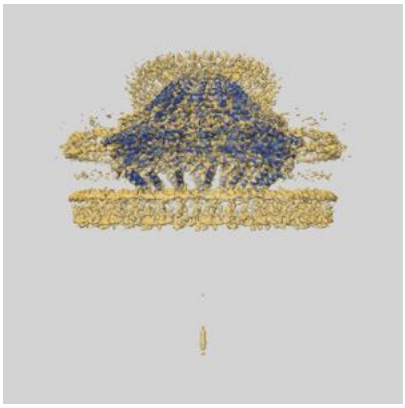
8 Fourier-Shell correlation

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

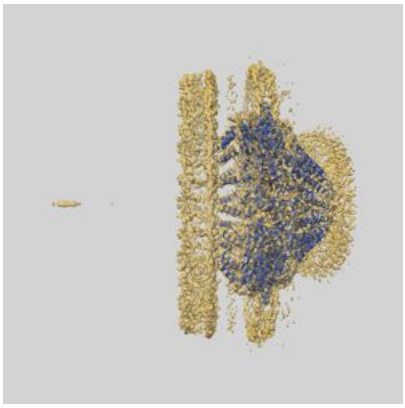
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-24773 and PDB model 7SPK. Per-residue inclusion information can be found in section 3 on page 6.

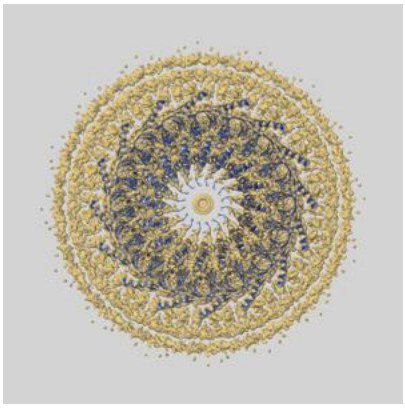
9.1 Map-model overlay



X



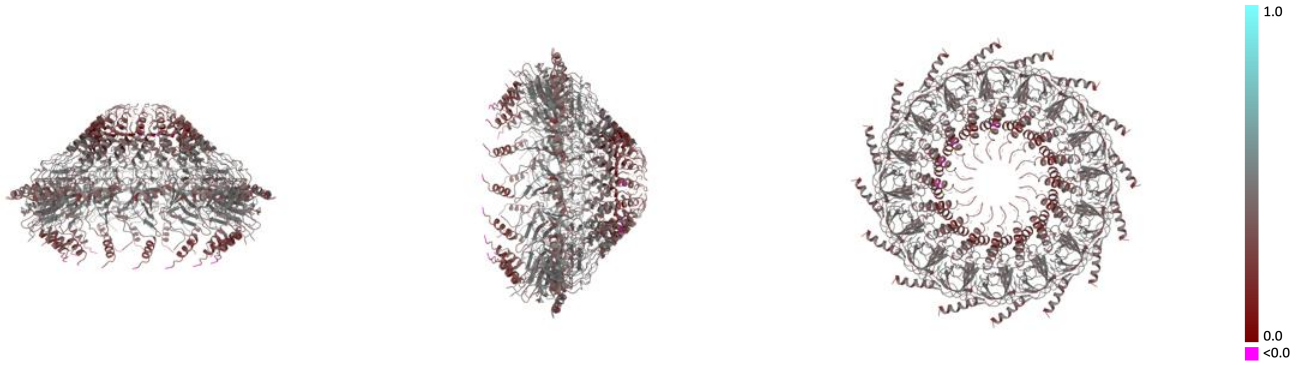
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.35 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.

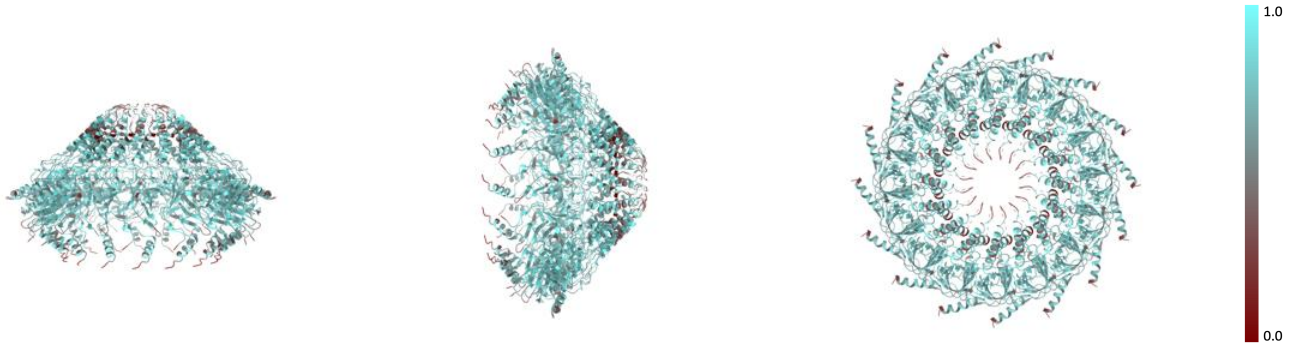
9.2 Q-score mapped to coordinate model



X Y Z

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

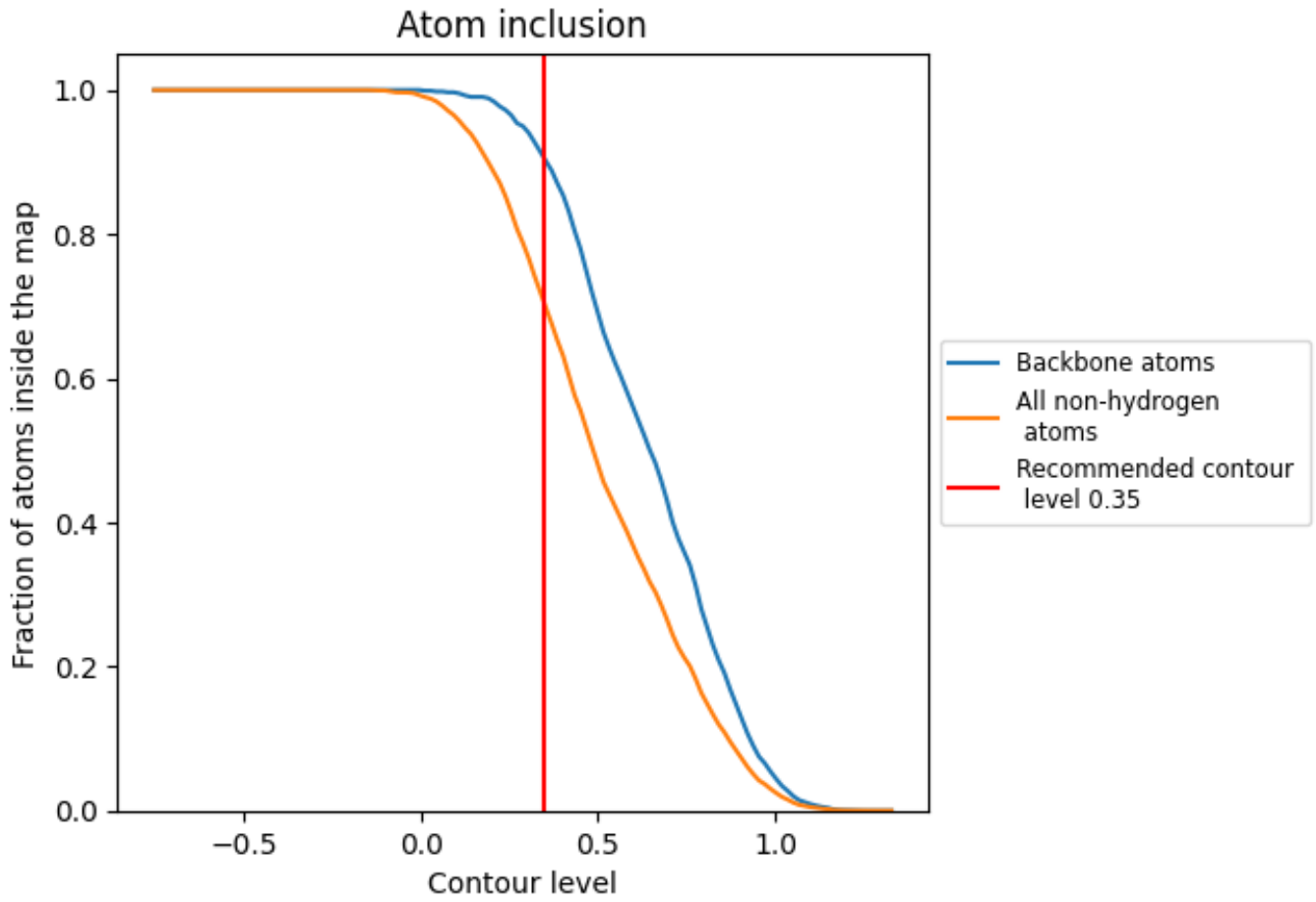
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.35).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 70% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7029	0.3980
AB1	0.6680	0.3920
AB10	0.6718	0.3920
AB11	0.6641	0.3910
AB12	0.6680	0.3940
AB13	0.6680	0.3920
AB14	0.6718	0.3960
AB15	0.6641	0.3910
AB16	0.6718	0.3950
AB2	0.6718	0.3950
AB3	0.6641	0.3890
AB4	0.6680	0.3910
AB5	0.6680	0.3930
AB6	0.6718	0.3910
AB7	0.6641	0.3890
AB8	0.6680	0.3890
AB9	0.6680	0.3910
EF1	0.7129	0.3990
EF10	0.7095	0.4000
EF11	0.7081	0.3990
EF12	0.7081	0.4000
EF13	0.7054	0.3990
EF14	0.7081	0.3990
EF15	0.7068	0.3990
EF16	0.7095	0.4000
EF2	0.7102	0.3990
EF3	0.7054	0.4000
EF4	0.7109	0.4010
EF5	0.7143	0.4000
EF6	0.7088	0.4000
EF7	0.7075	0.4000
EF8	0.7122	0.4000
EF9	0.7061	0.4000