wwPDB EM Validation Summary Report (i)

Dec 11, 2022 – 07:01 am GMT

PDB ID	:	6S1K
EMDB ID	:	EMD-10050
Title	:	E. coli Core Signaling Unit, carrying QQQQ receptor mutation
Authors	:	Cassidy, C.K.
Deposited on	:	2019-06-18
Resolution	:	8.38 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:

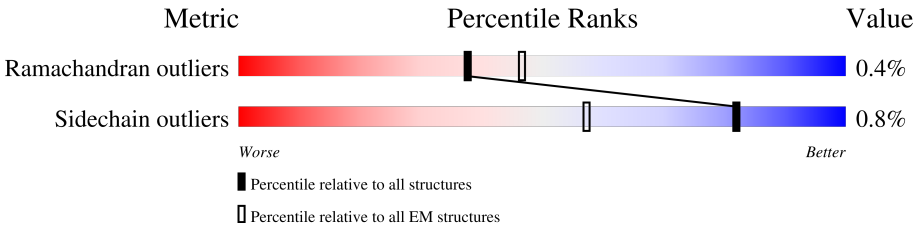
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 8.38 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	A	654	29% 57% · 41%
1	B	654	30% 57% · 41%
2	C	167	56% 82% 5% 13%
2	D	167	53% 83% · 13%
3	E	551	· 19% 81%
3	F	551	· 18% 81%
3	G	551	· 18% 81%
3	H	551	· 18% 81%
3	I	551	· 18% 81%

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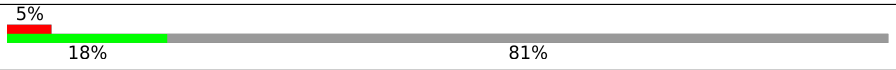
Mol	Chain	Length	Quality of chain
3	J	551	
3	K	551	
3	L	551	
3	M	551	
3	N	551	
3	O	551	
3	P	551	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 16884 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 Chemotaxis protein CheA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	383	Total	C	N	O	S	0	0
			2909	1818	519	559	13		
1	B	383	Total	C	N	O	S	0	0
			2909	1818	519	559	13		

- Molecule 2 is a protein called CheW.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	145	Total	C	N	O	S	0	0
			1117	715	183	217	2		
2	D	145	Total	C	N	O	S	0	0
			1117	715	183	217	2		

- Molecule 3 is a protein called Methyl-accepting chemotaxis protein I.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	102	Total	C	N	O	S	0	0
			736	449	134	152	1		
3	F	102	Total	C	N	O	S	0	0
			736	449	134	152	1		
3	G	102	Total	C	N	O	S	0	0
			736	449	134	152	1		
3	H	102	Total	C	N	O	S	0	0
			736	449	134	152	1		
3	I	102	Total	C	N	O	S	0	0
			736	449	134	152	1		
3	J	102	Total	C	N	O	S	0	0
			736	449	134	152	1		
3	K	102	Total	C	N	O	S	0	0
			736	449	134	152	1		
3	L	102	Total	C	N	O	S	0	0
			736	449	134	152	1		
3	M	102	Total	C	N	O	S	0	0
			736	449	134	152	1		

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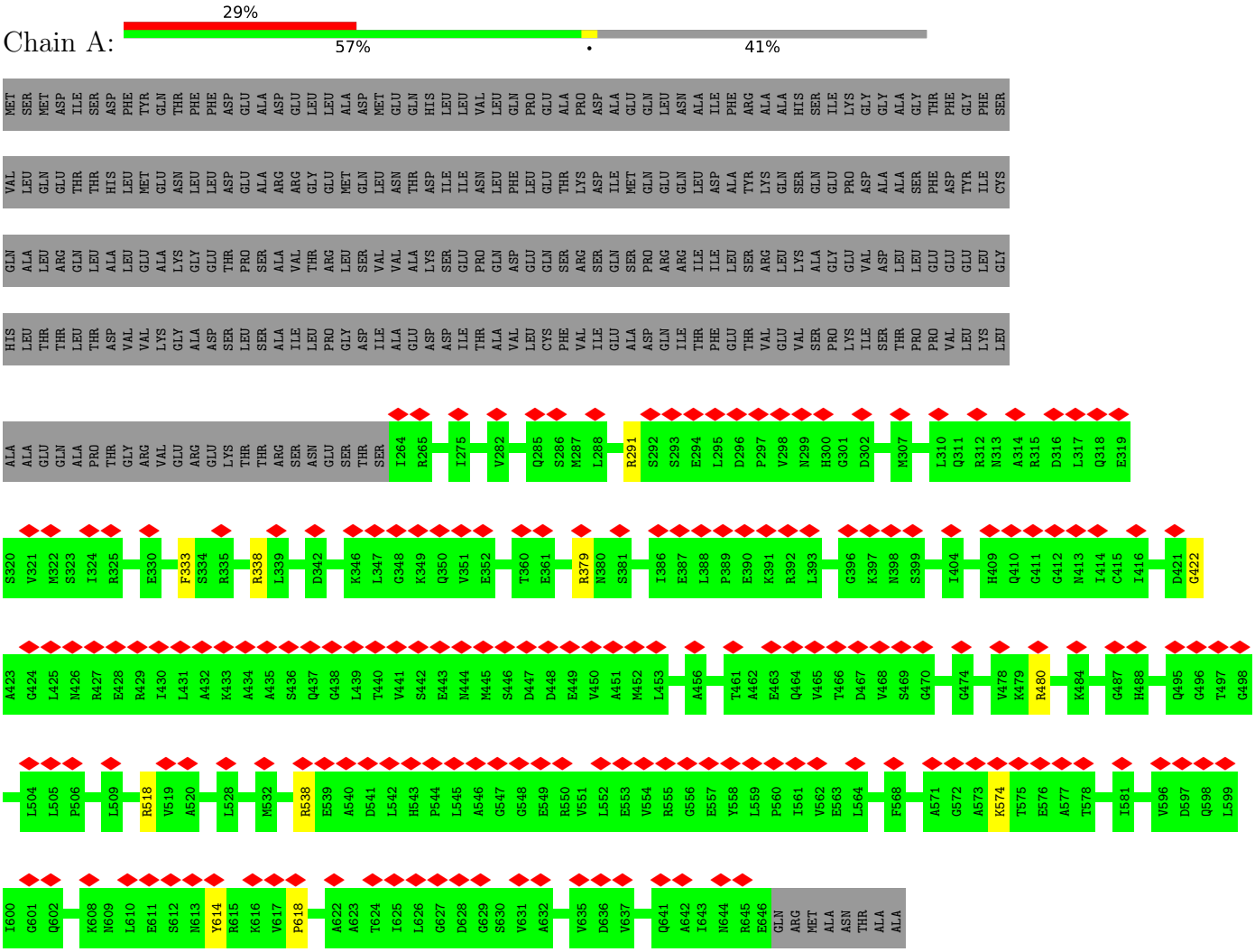
Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	102	Total	C	N	O	S	0	0
			736	449	134	152	1		
3	O	102	Total	C	N	O	S	0	0
			736	449	134	152	1		
3	P	102	Total	C	N	O	S	0	0
			736	449	134	152	1		

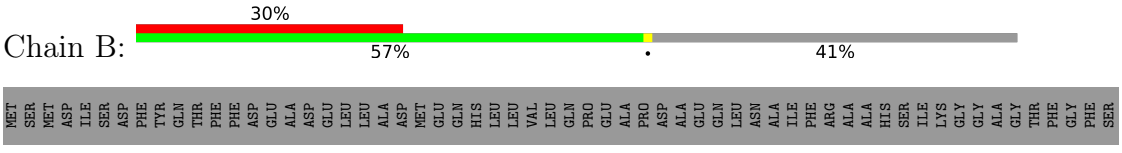
3 Residue-property plots (i)

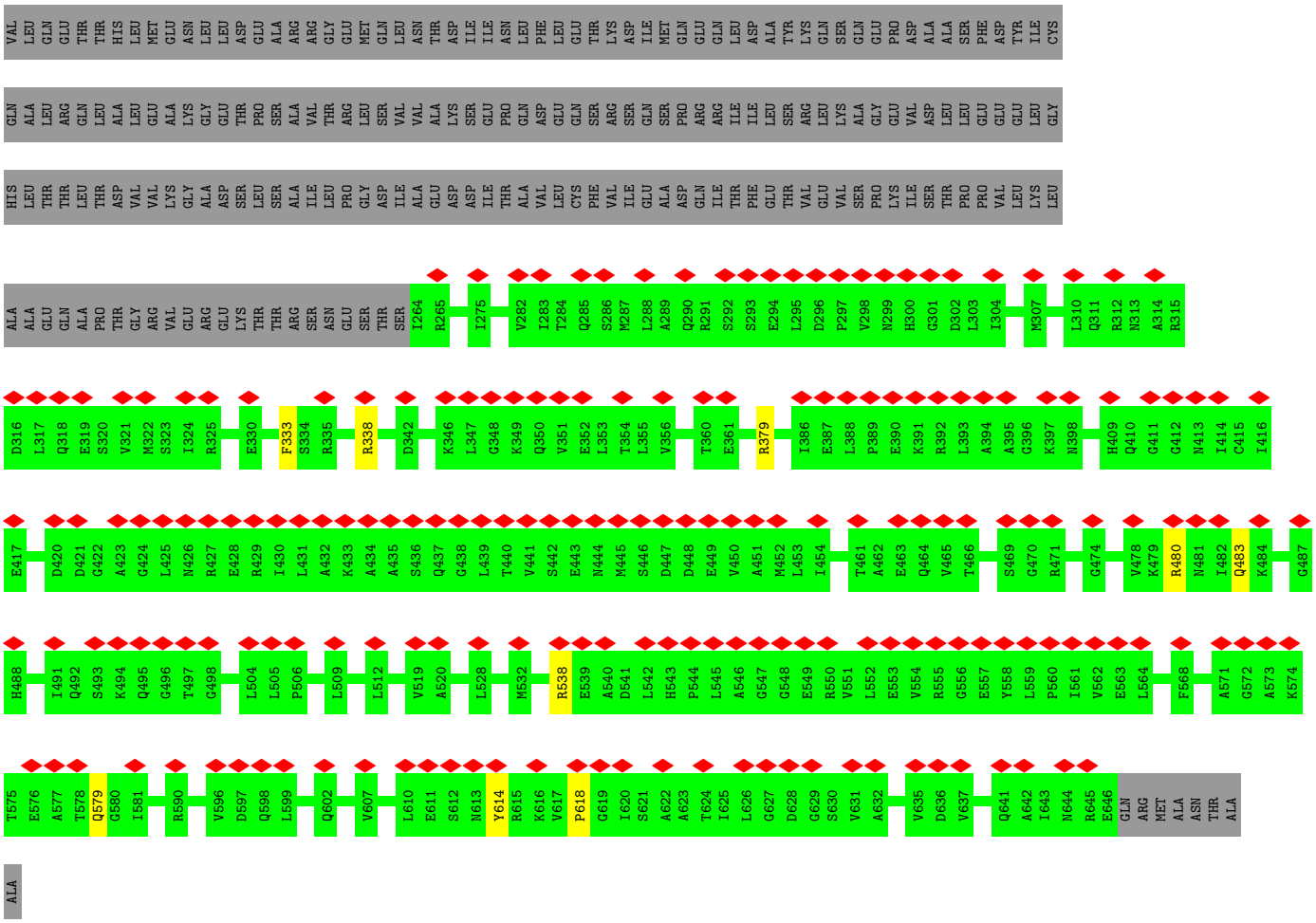
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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



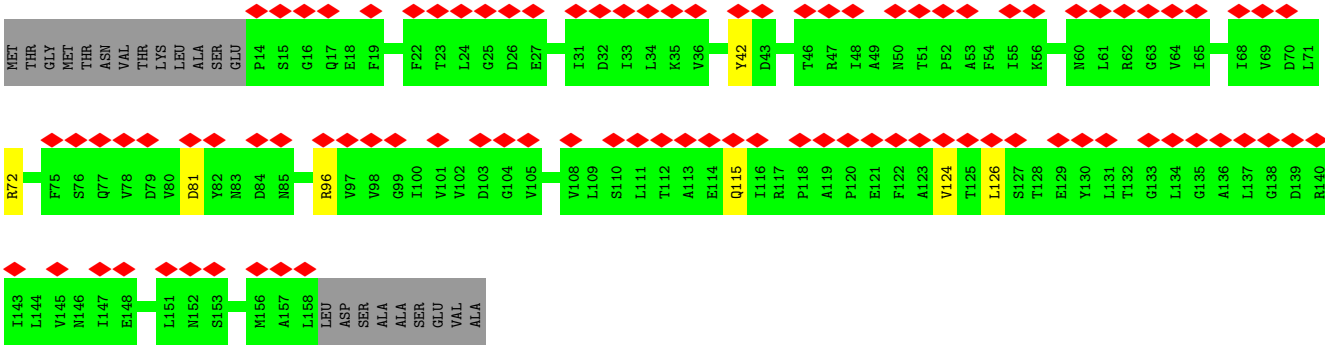
• Molecule 1: Chemotaxis protein CheA





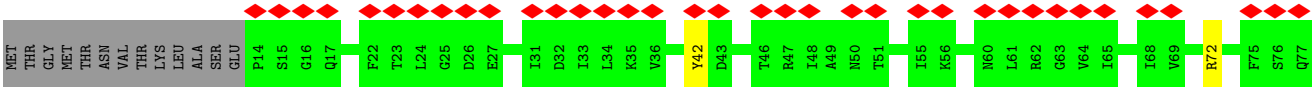
• Molecule 2: CheW

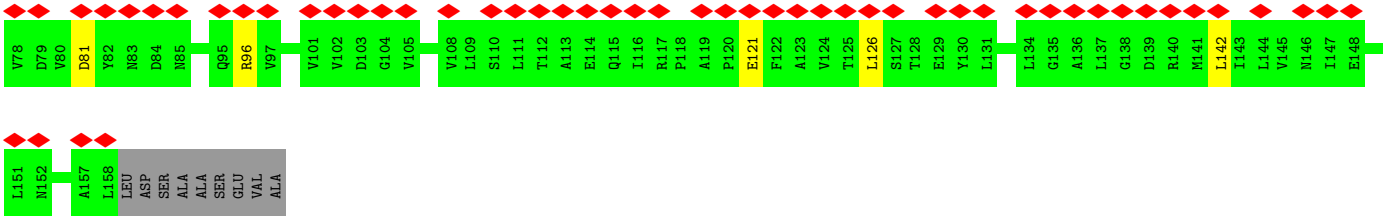
Chain C:



• Molecule 2: CheW

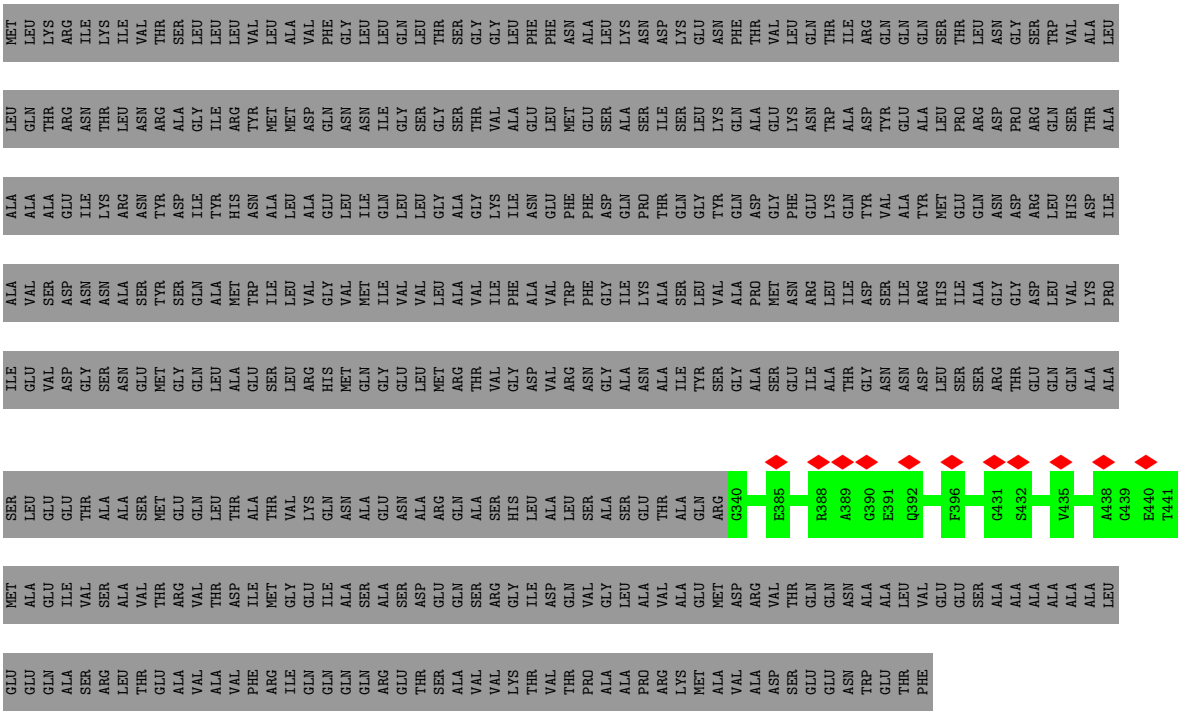
Chain D:





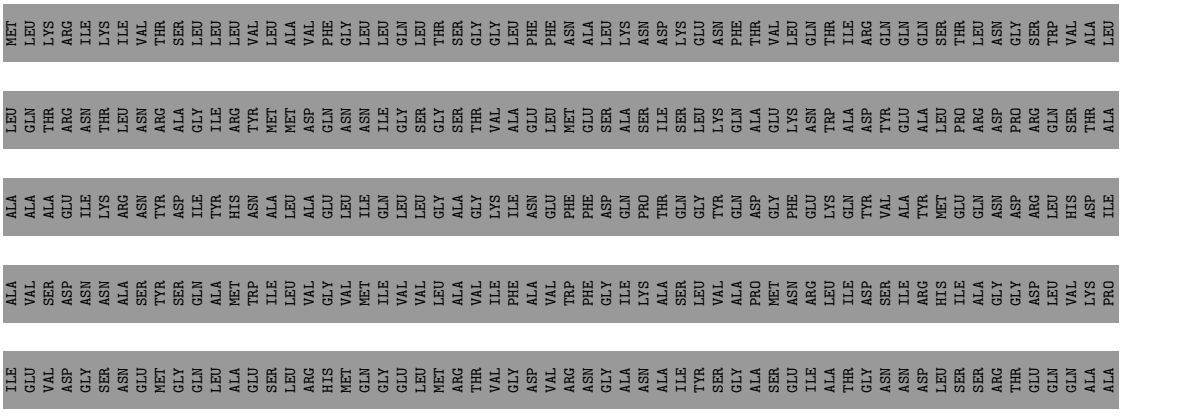
• Molecule 3: Methyl-accepting chemotaxis protein I

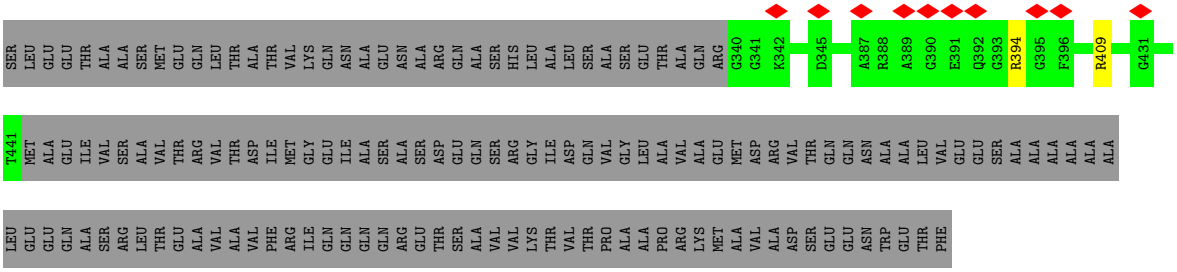
Chain E:



• Molecule 3: Methyl-accepting chemotaxis protein I

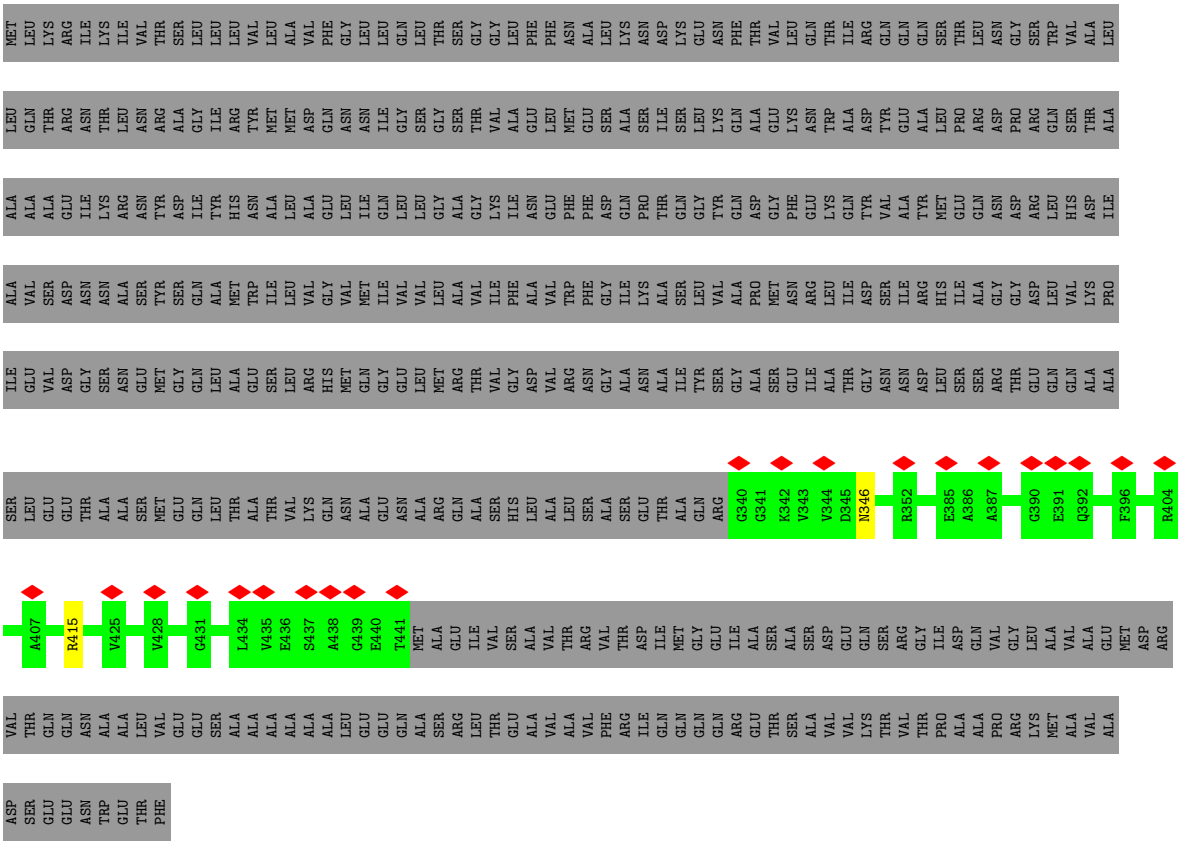
Chain F:





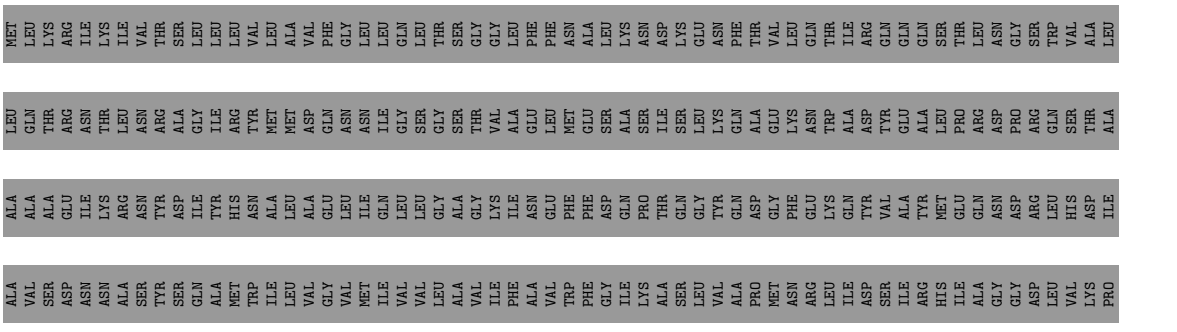
• Molecule 3: Methyl-accepting chemotaxis protein I

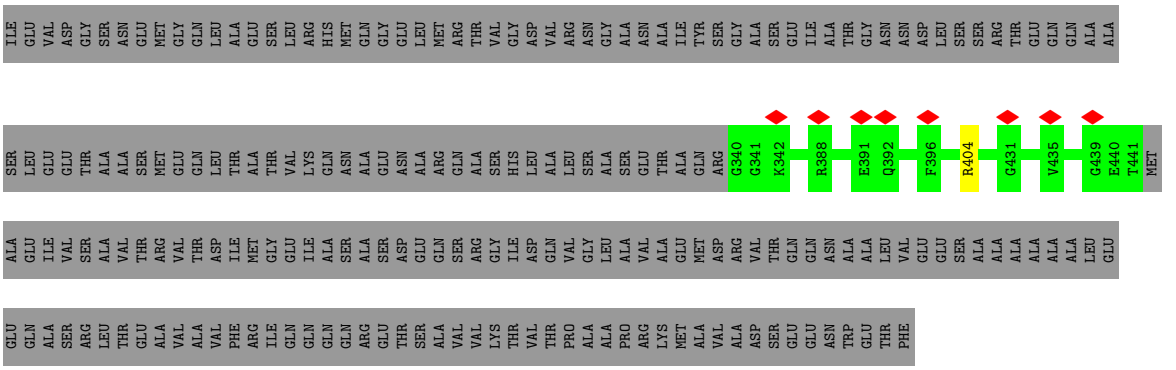
Chain G:



• Molecule 3: Methyl-accepting chemotaxis protein I

Chain H:



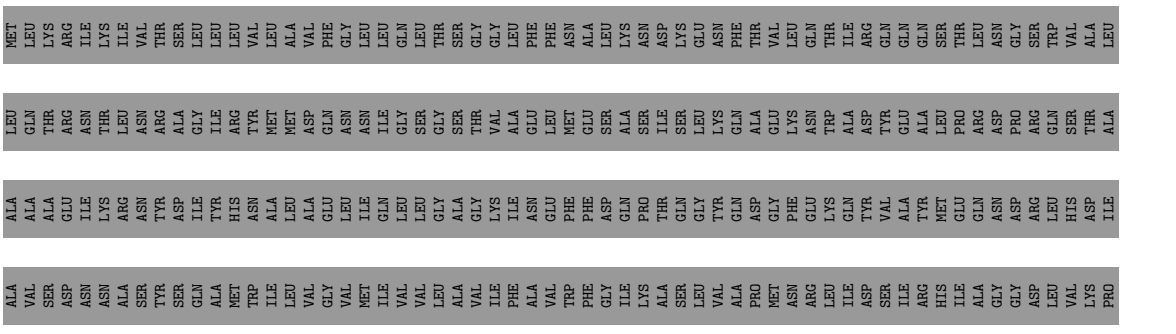


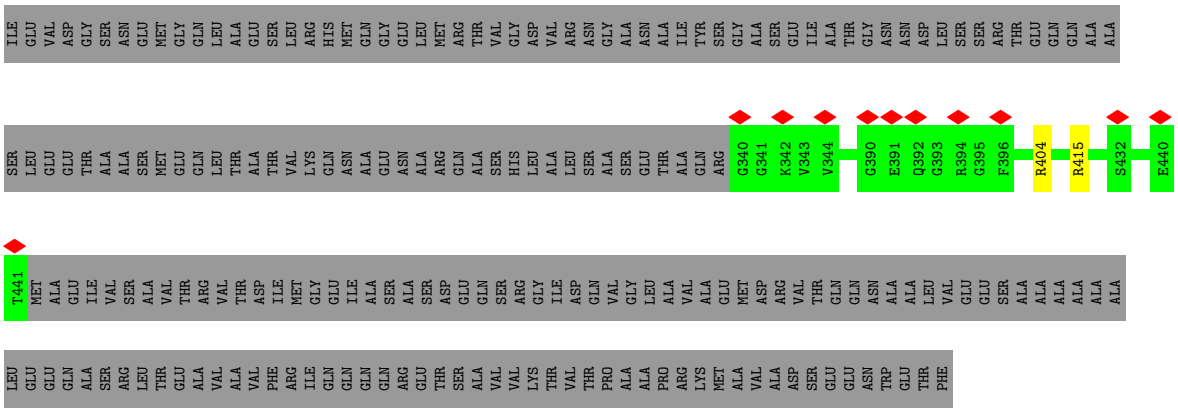
• Molecule 3: Methyl-accepting chemotaxis protein I

Chain I:

• Molecule 3: Methyl-accepting chemotaxis protein I

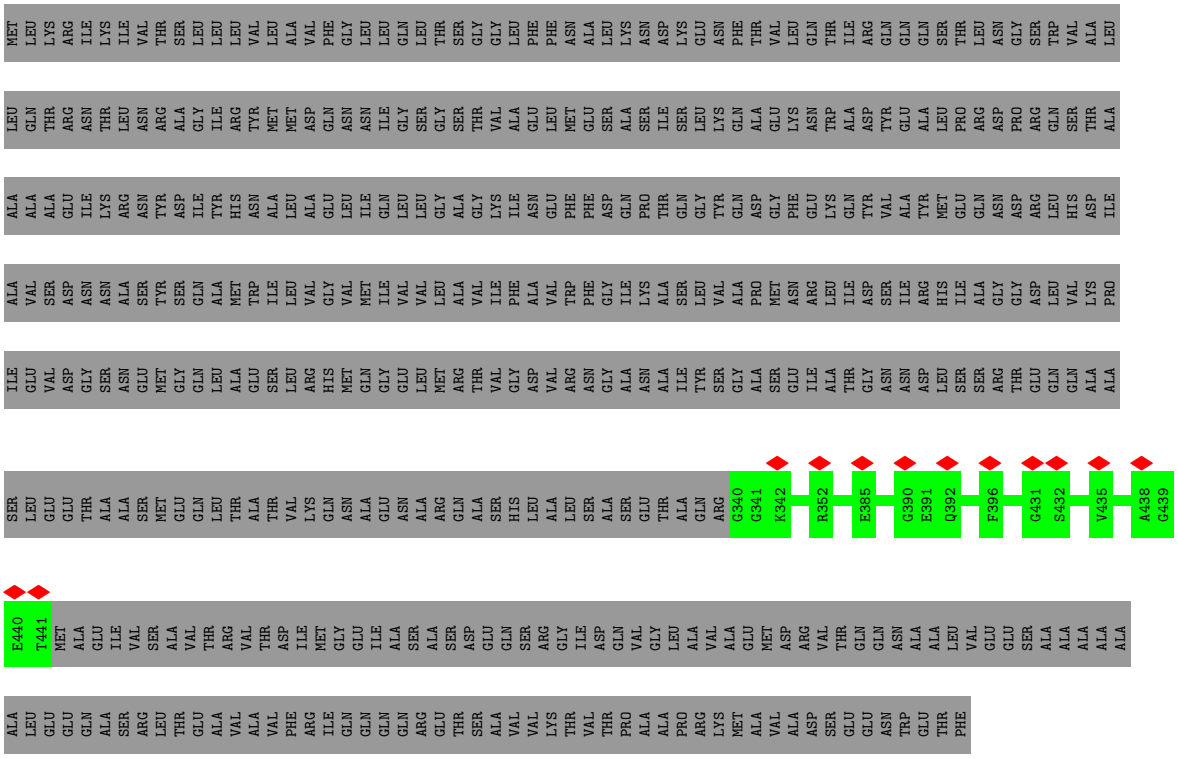
Chain J:





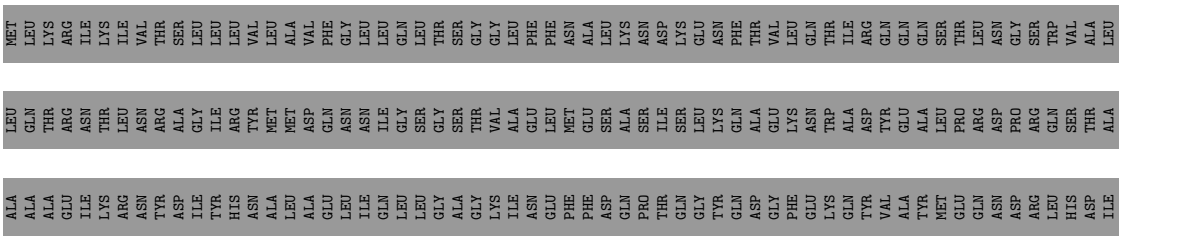
• Molecule 3: Methyl-accepting chemotaxis protein I

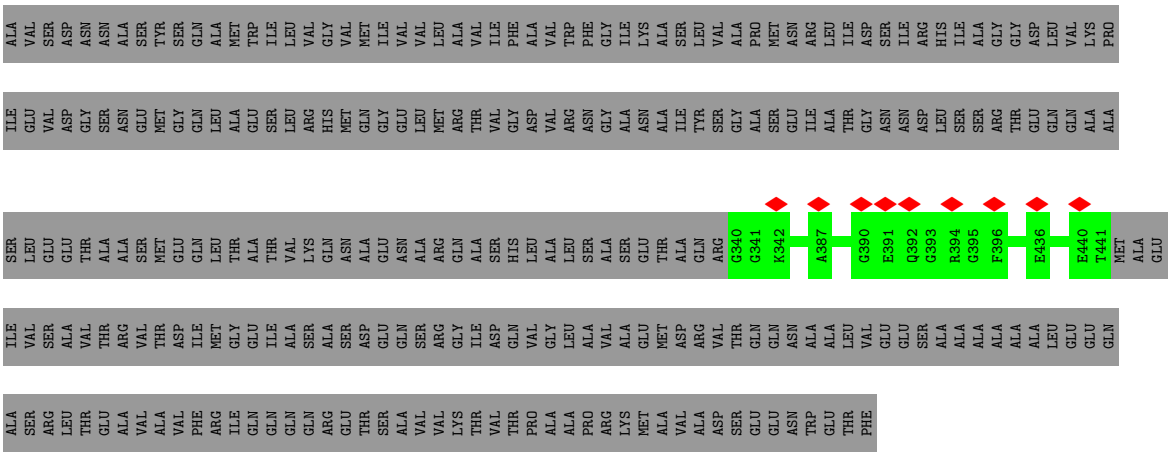
Chain K:



• Molecule 3: Methyl-accepting chemotaxis protein I

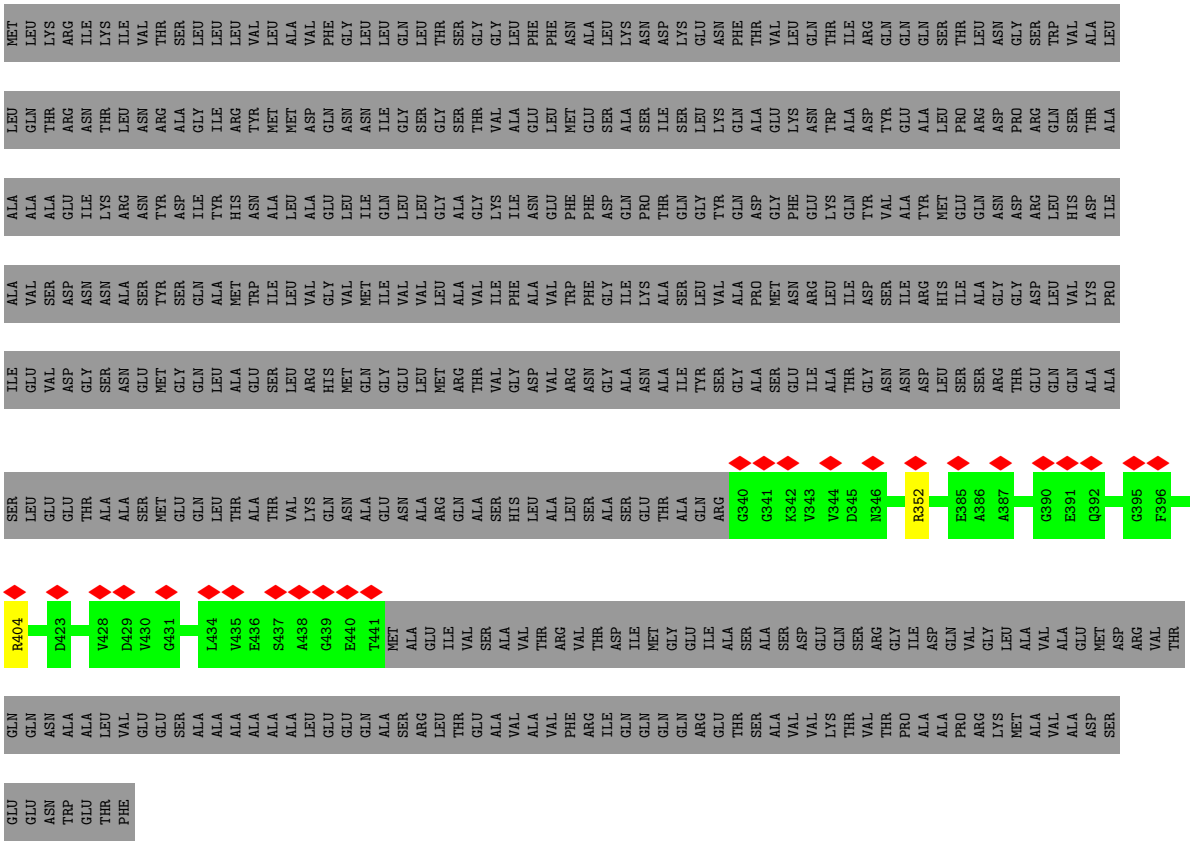
Chain L:





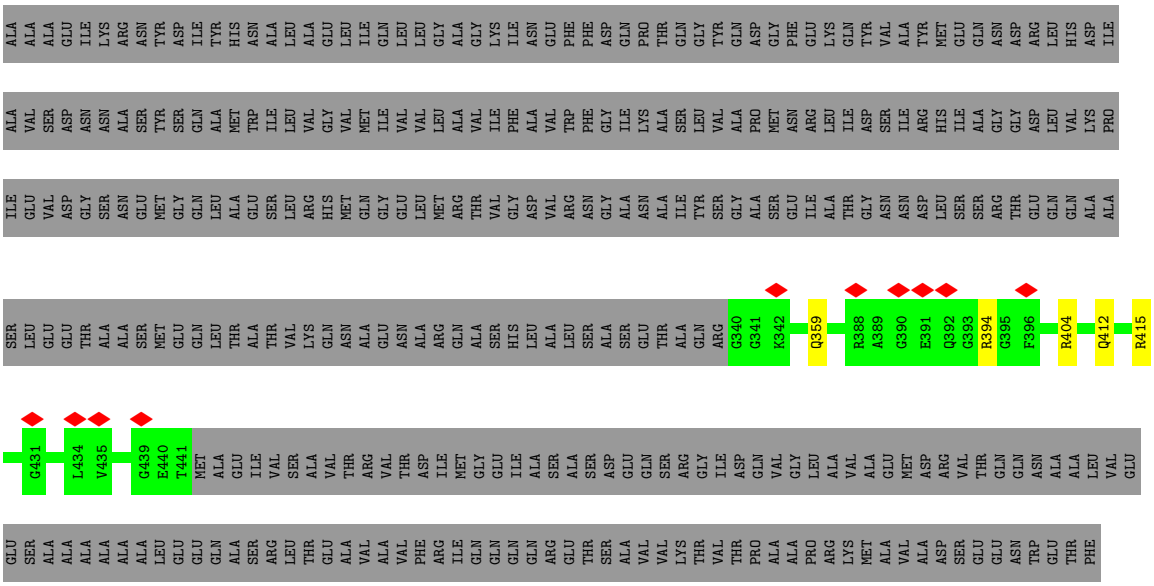
• Molecule 3: Methyl-accepting chemotaxis protein I

Chain M:



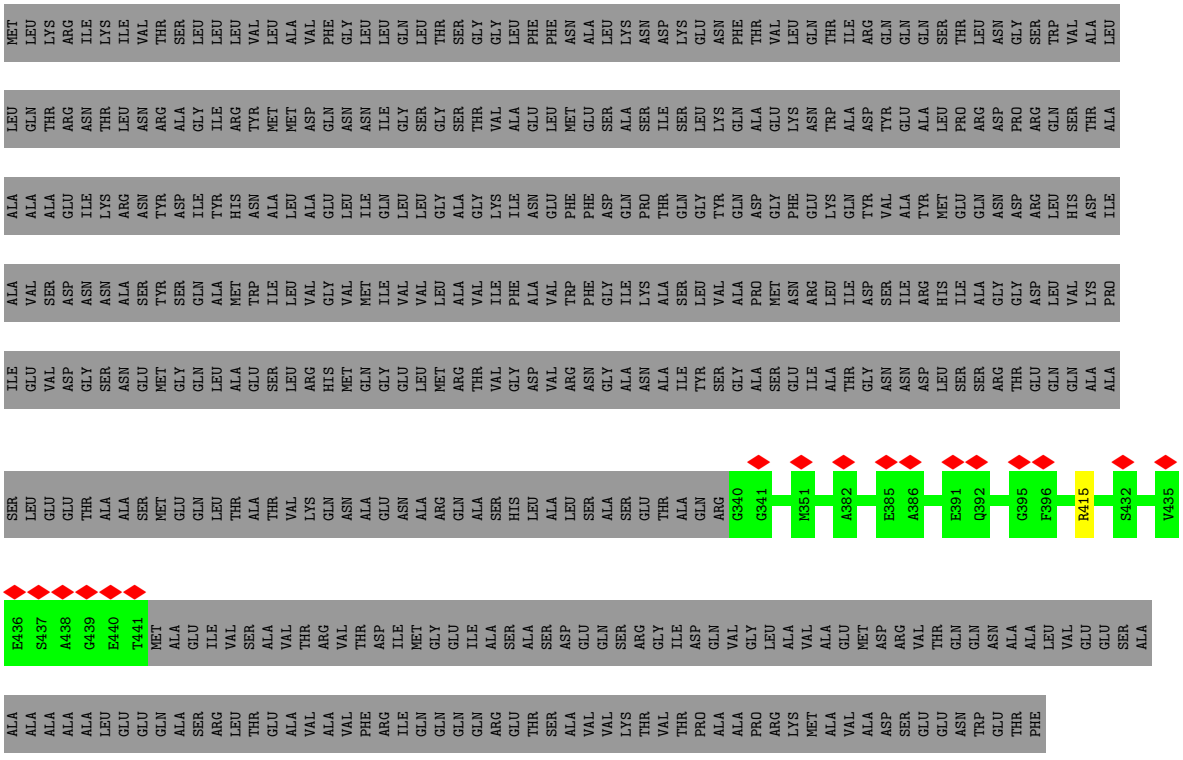
• Molecule 3: Methyl-accepting chemotaxis protein I

Chain N:



• Molecule 3: Methyl-accepting chemotaxis protein I

Chain O:



• Molecule 3: Methyl-accepting chemotaxis protein I

Chain P:


LEU GLN THR ARG ASN THR LEU ASN ARG ALA GLY ILE ARG TYR MET MET ASP GLN ASN ASN ILE GLY SER GLY SER THR VAL ALA GLU LEU MET GLU SER ALA SER ILE SER LEU LYS GLN ALA GLU LYS ASN TRP ALA ASP TYR GLU ALA LEU PRO ARG ASP PRO ARG GLN SER THR ALA
ALA ALA ALA GLU ILE LYS ARG ASN TYR ASP ILE TYR HIS ASN ALA LEU ALA GLU LEU ILE GLN LEU LEU GLY ALA GLY LYS ILE ASN GLU PHE PHE ASP GLN PRO THR GLN GLY TYR GLN ASP GLY PHE GLU LYS GLN TYR VAL ALA TYR MET GLU GLN ASN ASP ARG LEU HIS ASP ILE
ALA VAL SER ASP ASN ASN ALA SER TYR SER GLN ALA MET TRP ILE LEU VAL GLY VAL MET ILE VAL VAL LEU ALA VAL ILE PHE ALA VAL TRP PHE GLY ILE LYS ALA SER LEU VAL ALA PRO MET ASN ARG LEU ILE ASP SER ILE ARG HIS ILE ALA GLY GLY ASP LEU VAL LYS PRO
ILE GLU VAL ASP GLY SER ASN GLU MET GLY GLN LEU ALA GLU SER LEU ARG HIS MET GLN GLY GLU LEU MET ARG THR VAL GLY ASP VAL ARG ASN GLY ALA GLY ASP ALA ILE TYR SER GLY ALA SER GLU ILE ALA THR GLY ASN ASN ASP LEU SER SER ARG THR GLU GLN GLN ALA ALA
SER LEU GLU VAL ALA ARG GLN ALA SER HIS LEU ALA LEU SER ALA SER GLU THR ALA GLN ARG G340 G341 K342 V343 V344 R388 E391 Q392 G393 R394 G395 F396 R409 S432 T441 MET
ALA GLU ILE VAL SER ALA VAL THR ARG VAL THR ASP ILE MET GLY GLU ILE ALA SER ALA SER ASP GLU GLN SER ARG GLY ILE ASP GLN VAL GLY LEU ALA VAL ALA GLU MET ASP ARG VAL THR GLN GLN ASN ALA ALA LEU VAL GLU GLU SER ALA ALA ALA ALA ALA ALA LEU GLU
GLU GLN ALA SER ARG LEU THR GLU ALA VAL ALA VAL PHE ARG ILE GLN GLN GLN GLN ARG GLU THR SER ALA VAL VAL LYS THR VAL THR PRO ALA ALA PRO ARG LYS MET ALA VAL ALA ASP SER GLU GLU ASN TRP GLU THR PHE

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of subtomograms used	91636	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.3	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor
Maximum map value	14.403	Depositor
Minimum map value	-7.622	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.175	Depositor
Recommended contour level	2.15	Depositor
Map size (Å)	627.50397, 627.50397, 627.50397	wwPDB
Map dimensions	204, 204, 204	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	3.0759997, 3.0759997, 3.0759997	Depositor

5 Model quality

5.1 Standard geometry

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	0.70	0/2939	0.91	2/3975 (0.1%)
1	B	0.70	0/2939	0.90	2/3975 (0.1%)
2	C	0.73	0/1130	0.94	1/1537 (0.1%)
2	D	0.72	0/1130	0.94	1/1537 (0.1%)
3	E	0.72	0/737	0.92	0/994
3	F	0.72	0/737	0.91	0/994
3	G	0.71	0/737	0.91	0/994
3	H	0.72	0/737	0.90	0/994
3	I	0.72	0/737	0.90	0/994
3	J	0.73	0/737	0.90	0/994
3	K	0.71	0/737	0.91	0/994
3	L	0.72	0/737	0.92	0/994
3	M	0.73	0/737	0.91	0/994
3	N	0.72	0/737	0.94	0/994
3	O	0.72	0/737	0.92	0/994
3	P	0.73	0/737	0.92	0/994
All	All	0.72	0/16982	0.91	6/22952 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	B	0	5
3	F	0	2
3	G	0	1
3	H	0	1
3	I	0	1
3	J	0	2
3	M	0	2
3	N	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	O	0	1
3	P	0	1
All	All	0	25

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	333	PHE	CB-CG-CD1	5.58	124.70	120.80
1	A	333	PHE	CB-CG-CD1	5.45	124.62	120.80
1	B	333	PHE	CB-CG-CD2	-5.32	117.07	120.80
2	D	42	TYR	CB-CG-CD2	-5.29	117.83	121.00
2	C	42	TYR	CB-CG-CD2	-5.21	117.87	121.00

There are no chirality outliers.

5 of 25 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	338	ARG	Sidechain
1	A	379	ARG	Sidechain
1	A	480	ARG	Sidechain
1	A	518	ARG	Sidechain
1	A	538	ARG	Sidechain

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	2909	0	3009	0	0
1	B	2909	0	3009	0	0
2	C	1117	0	1152	0	0
2	D	1117	0	1152	0	0
3	E	736	0	750	0	0
3	F	736	0	750	0	0
3	G	736	0	750	0	0
3	H	736	0	750	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	736	0	750	0	0
3	J	736	0	750	0	0
3	K	736	0	750	0	0
3	L	736	0	750	0	0
3	M	736	0	750	0	0
3	N	736	0	750	0	0
3	O	736	0	750	0	0
3	P	736	0	750	0	0
All	All	16884	0	17322	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

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	381/654 (58%)	368 (97%)	10 (3%)	3 (1%)	19	60
1	B	381/654 (58%)	372 (98%)	7 (2%)	2 (0%)	29	69
2	C	143/167 (86%)	135 (94%)	6 (4%)	2 (1%)	11	46
2	D	143/167 (86%)	135 (94%)	6 (4%)	2 (1%)	11	46
3	E	100/551 (18%)	100 (100%)	0	0	100	100
3	F	100/551 (18%)	100 (100%)	0	0	100	100
3	G	100/551 (18%)	100 (100%)	0	0	100	100
3	H	100/551 (18%)	100 (100%)	0	0	100	100
3	I	100/551 (18%)	100 (100%)	0	0	100	100
3	J	100/551 (18%)	100 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	K	100/551 (18%)	100 (100%)	0	0	100	100
3	L	100/551 (18%)	100 (100%)	0	0	100	100
3	M	100/551 (18%)	100 (100%)	0	0	100	100
3	N	100/551 (18%)	100 (100%)	0	0	100	100
3	O	100/551 (18%)	100 (100%)	0	0	100	100
3	P	100/551 (18%)	100 (100%)	0	0	100	100
All	All	2248/8254 (27%)	2210 (98%)	29 (1%)	9 (0%)	38	72

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	81	ASP
2	D	81	ASP
1	A	618	PRO
1	B	579	GLN
1	B	618	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	321/552 (58%)	320 (100%)	1 (0%)	92	95
1	B	321/552 (58%)	320 (100%)	1 (0%)	92	95
2	C	126/143 (88%)	121 (96%)	5 (4%)	31	55
2	D	126/143 (88%)	122 (97%)	4 (3%)	39	61
3	E	77/438 (18%)	77 (100%)	0	100	100
3	F	77/438 (18%)	77 (100%)	0	100	100
3	G	77/438 (18%)	76 (99%)	1 (1%)	69	81
3	H	77/438 (18%)	77 (100%)	0	100	100
3	I	77/438 (18%)	77 (100%)	0	100	100
3	J	77/438 (18%)	77 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	K	77/438 (18%)	77 (100%)	0	100 100
3	L	77/438 (18%)	77 (100%)	0	100 100
3	M	77/438 (18%)	77 (100%)	0	100 100
3	N	77/438 (18%)	75 (97%)	2 (3%)	46 66
3	O	77/438 (18%)	77 (100%)	0	100 100
3	P	77/438 (18%)	77 (100%)	0	100 100
All	All	1818/6646 (27%)	1804 (99%)	14 (1%)	82 89

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	72	ARG
2	D	96	ARG
3	N	412	GLN
3	G	346	ASN
3	N	359	GLN

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-10050. 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

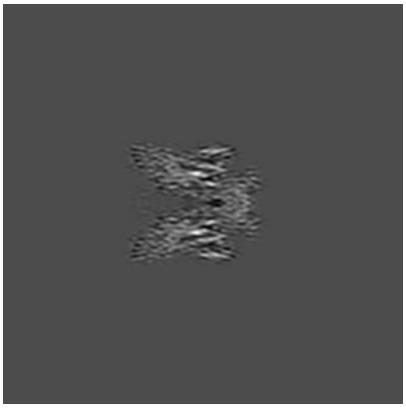
Z

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

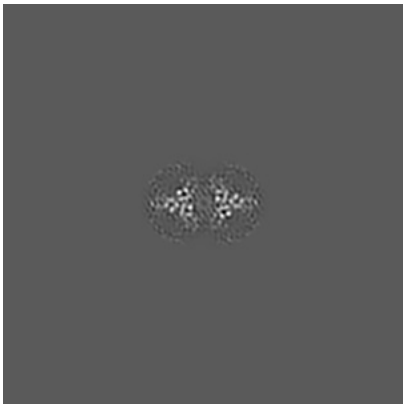
6.2 Central slices

6.2.1 Primary map

X Index: 102



Y Index: 102

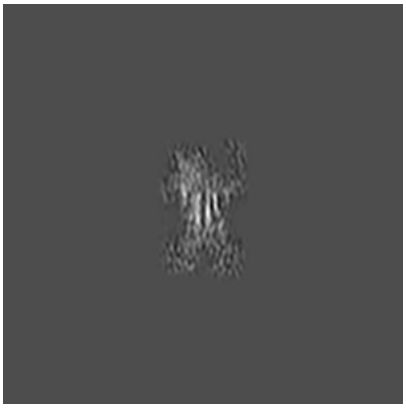


Z Index: 102

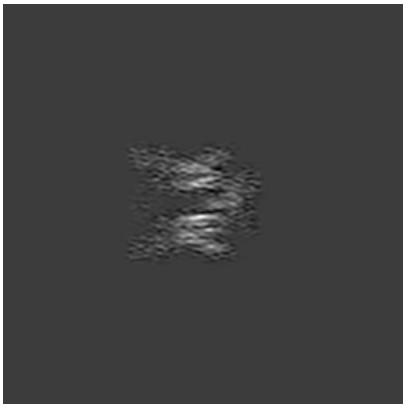
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

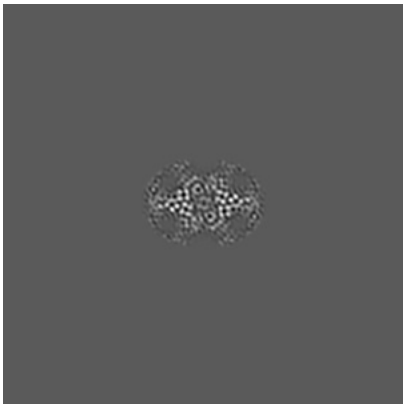
6.3.1 Primary map



X Index: 110



Y Index: 100



Z Index: 105

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

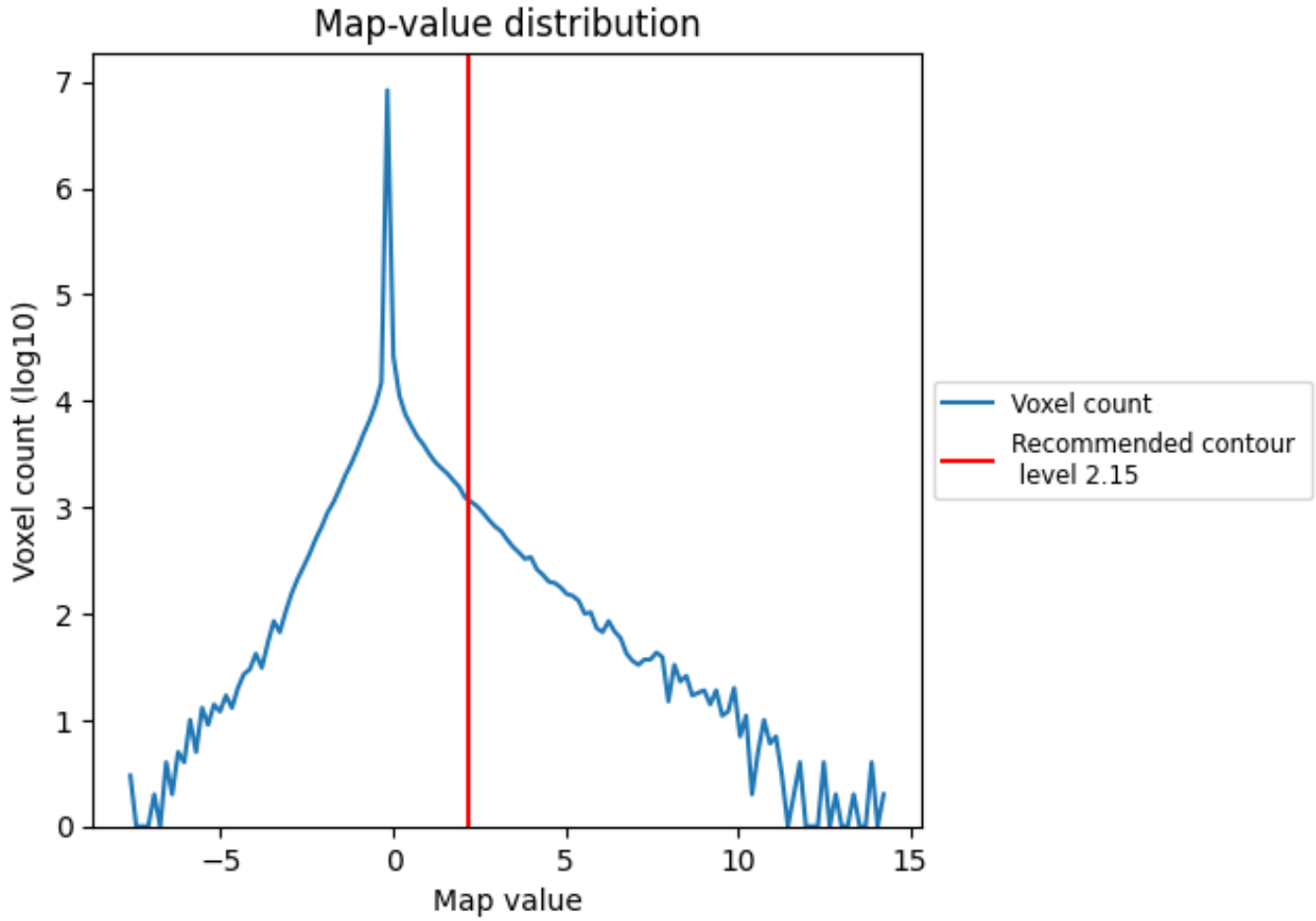
6.5 Mask visualisation (i)

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

7 Map analysis

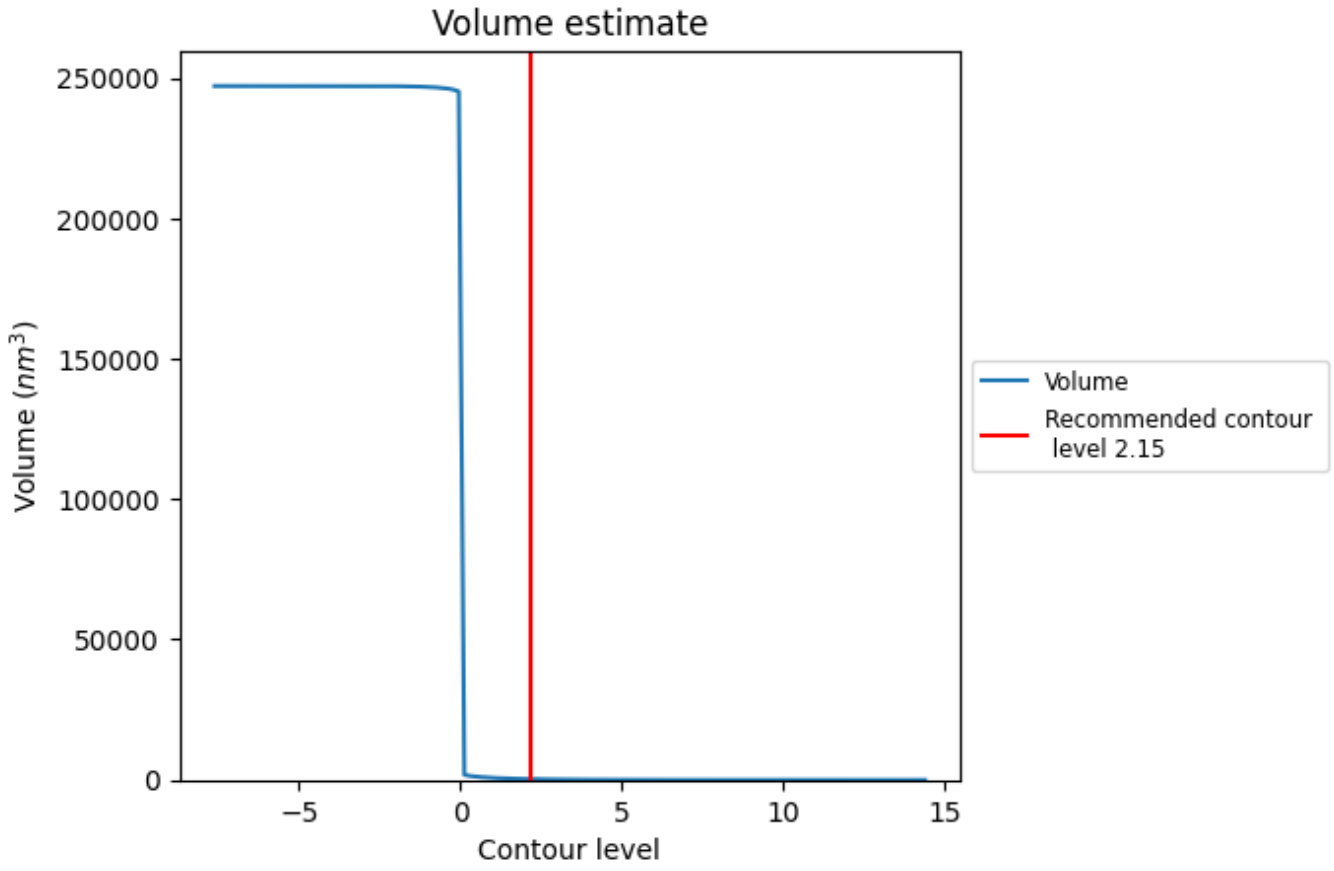
This section contains the results of statistical analysis of the map.

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.

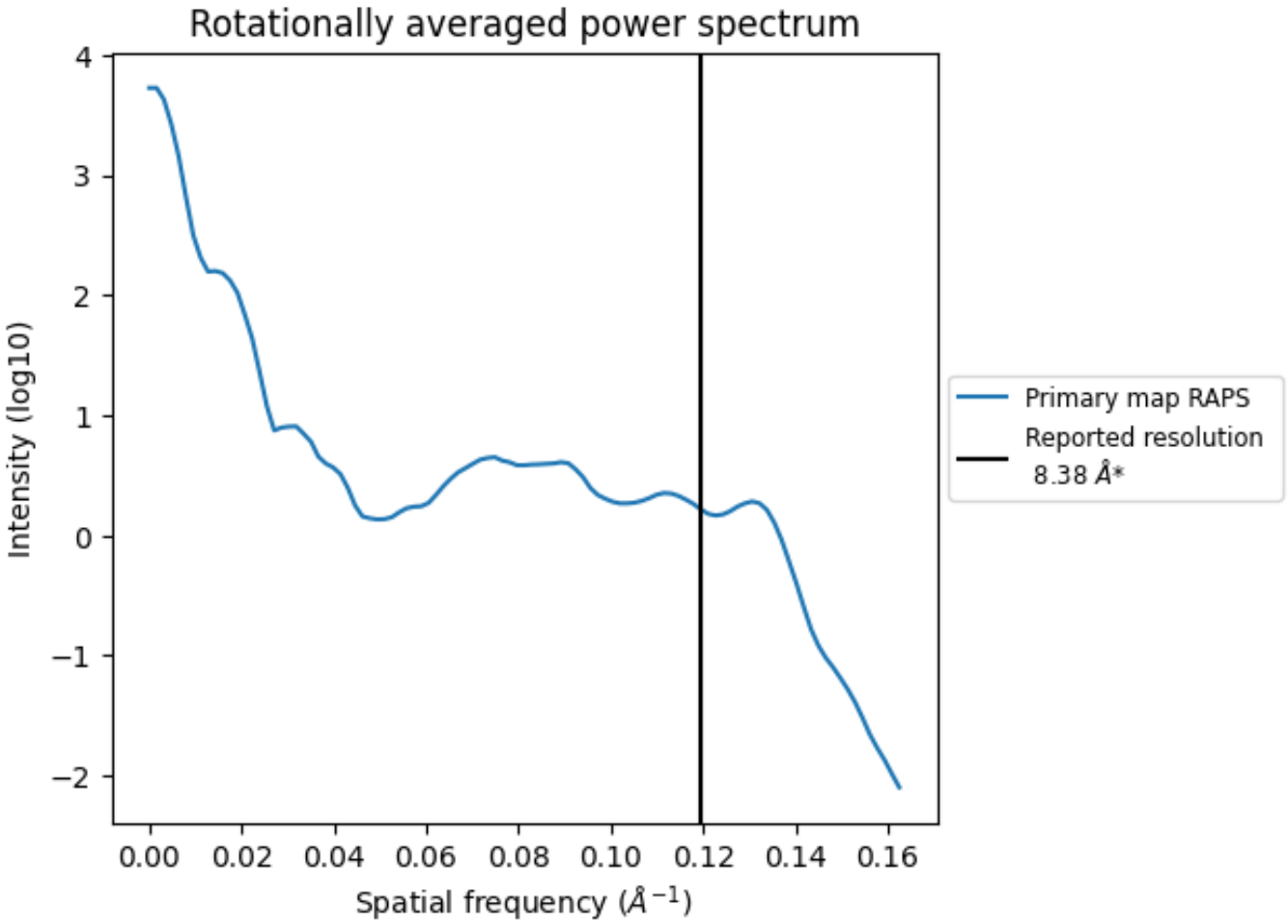
7.2 Volume estimate (i)



The volume at the recommended contour level is 305 nm^3; this corresponds to an approximate mass of 275 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 0.119 $Å^{-1}$

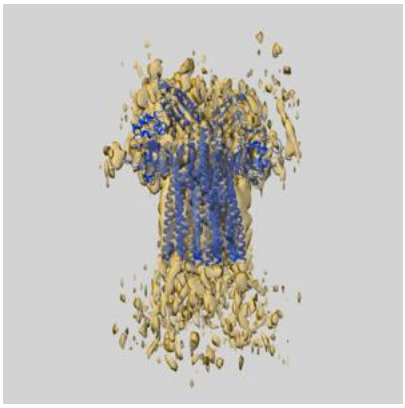
8 Fourier-Shell correlation (i)

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

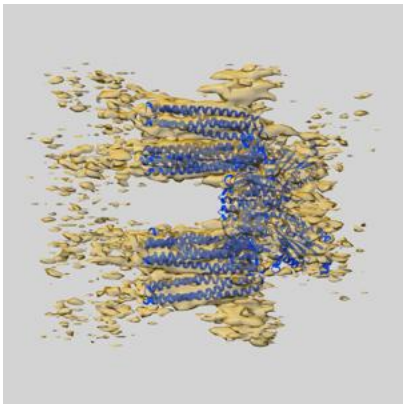
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10050 and PDB model 6S1K. Per-residue inclusion information can be found in section 3 on page 6.

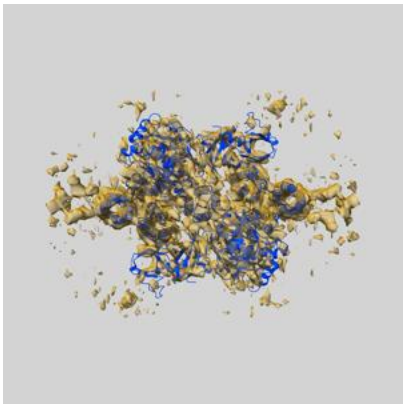
9.1 Map-model overlay



X



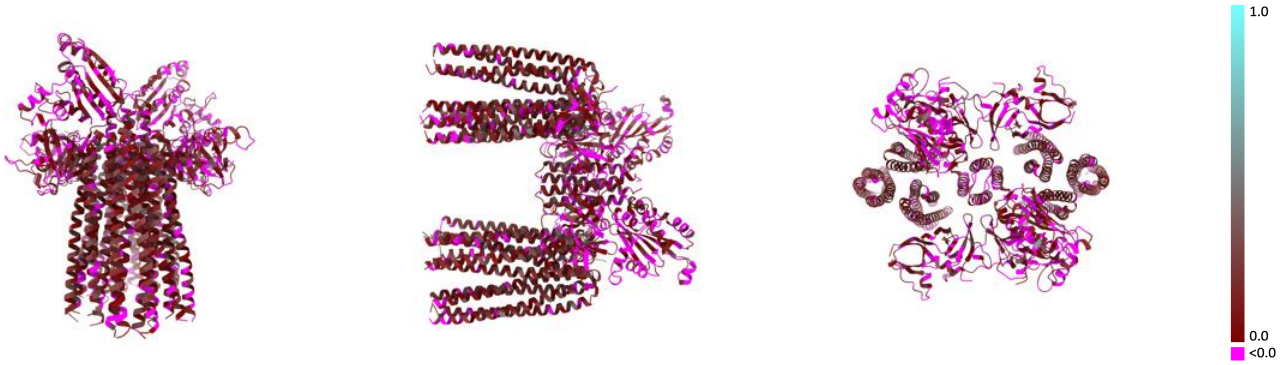
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

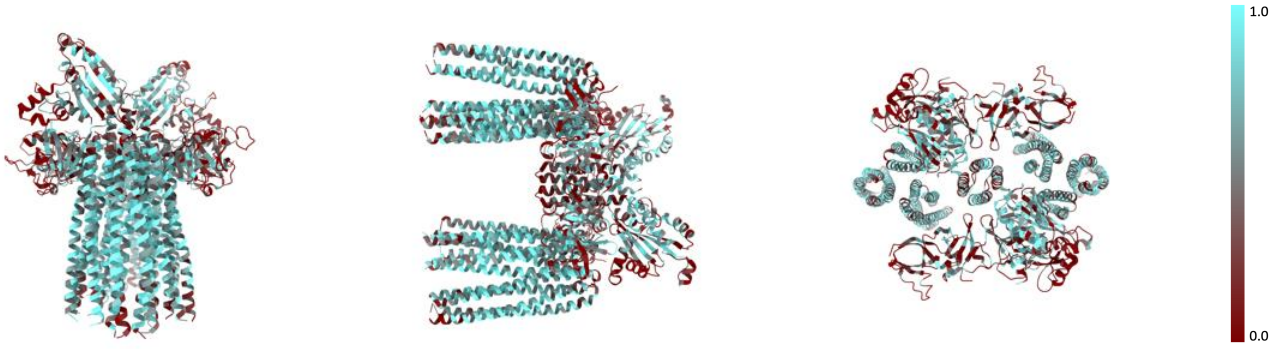
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

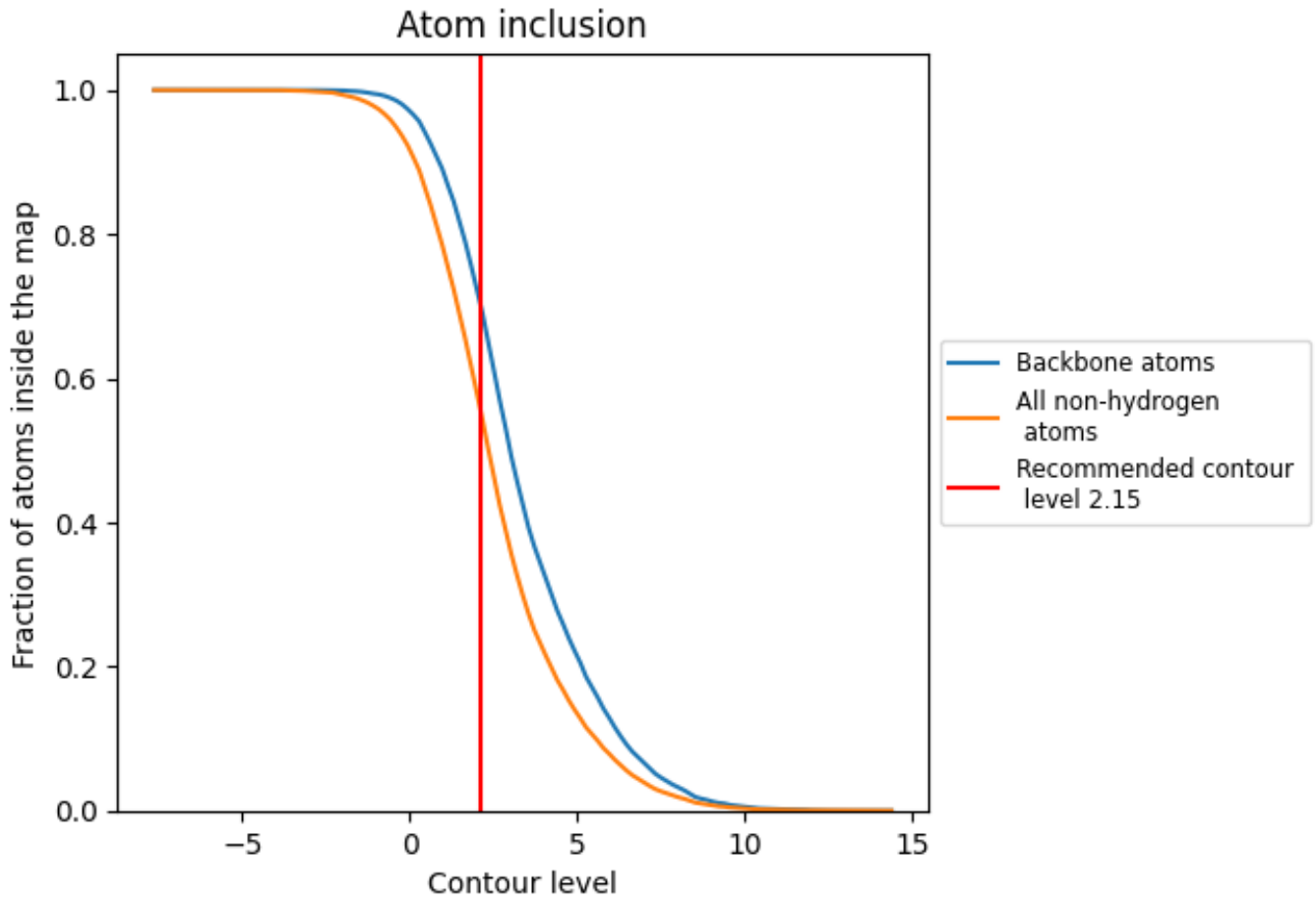
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2.15).

9.4 Atom inclusion (i)



At the recommended contour level, 70% of all backbone atoms, 55% 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 (2.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5501	0.0880
A	0.4196	0.0390
B	0.4140	0.0380
C	0.3039	0.0660
D	0.3048	0.0480
E	0.6878	0.1330
F	0.7569	0.1300
G	0.6326	0.1230
H	0.7666	0.1270
I	0.6630	0.1200
J	0.7113	0.1200
K	0.6796	0.1340
L	0.7680	0.1470
M	0.6133	0.1220
N	0.7459	0.1350
O	0.6602	0.1160
P	0.7141	0.1240