wwPDB EM Validation Summary Report (i)

Mar 5, 2026 – 03:20 AM UTC

PDB ID	:	8UFB / pdb_00008ufb
EMDB ID	:	EMD-42190
Title	:	Eastern equine encephalitis virus (PE-6) VLP in complex with full-length VLDLR (asymmetric unit)
Authors	:	Adams, L.J.; Fremont, D.H.; Center for Structural Biology of Infectious Diseases (CSBID)
Deposited on	:	2023-10-04
Resolution	:	3.89 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:

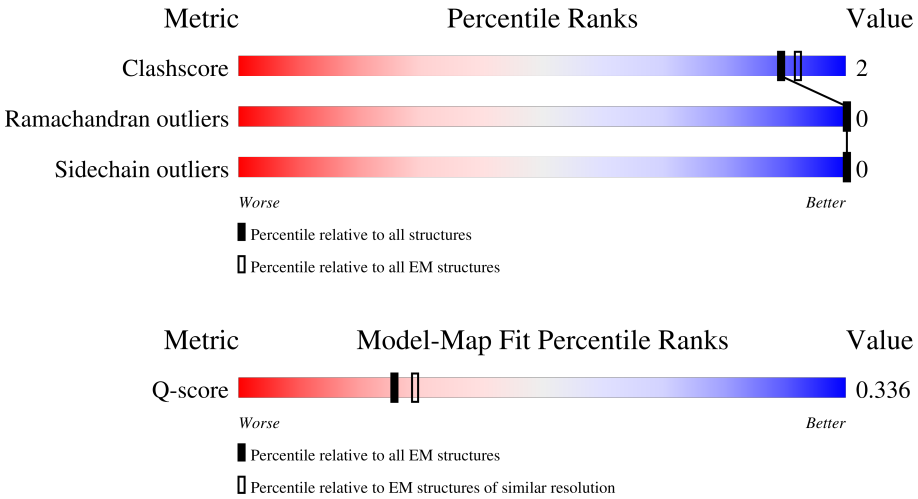
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.89 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8712 (3.39 - 4.39)

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	441	93% 7%
1	D	441	97% .
1	G	441	95% 5%
1	J	441	96% .

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Mol	Chain	Length	Quality of chain
2	B	414	96%
2	E	414	96%
2	H	414	94% 6%
2	K	414	98%
3	C	151	15% 87% 13%
3	F	151	15% 95% 5%
3	I	151	8% 95% 5%
3	L	151	97%
4	R	748	95%
4	S	748	95%
4	T	748	95%
4	U	748	95%
4	V	748	7% 10% 90%
4	W	748	9% 10% 90%
4	X	748	8% 9% 90%
4	Y	748	9% 10% 90%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 34656 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 E1 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	441	Total	C	N	O	S	0	0
			3370	2151	559	640	20		
1	D	441	Total	C	N	O	S	0	0
			3370	2151	559	640	20		
1	G	441	Total	C	N	O	S	0	0
			3370	2151	559	640	20		
1	J	441	Total	C	N	O	S	0	0
			3370	2151	559	640	20		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	89	TYR	TRP	conflict	UNP Q88678
A	392	ALA	PRO	conflict	UNP Q88678
D	89	TYR	TRP	conflict	UNP Q88678
D	392	ALA	PRO	conflict	UNP Q88678
G	89	TYR	TRP	conflict	UNP Q88678
G	392	ALA	PRO	conflict	UNP Q88678
J	89	TYR	TRP	conflict	UNP Q88678
J	392	ALA	PRO	conflict	UNP Q88678

- Molecule 2 is a protein called E2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	414	Total	C	N	O	S	0	0
			3253	2058	589	582	24		
2	E	414	Total	C	N	O	S	0	0
			3253	2058	589	582	24		
2	H	414	Total	C	N	O	S	0	0
			3253	2058	589	582	24		
2	K	414	Total	C	N	O	S	0	0
			3253	2058	589	582	24		

- Molecule 3 is a protein called Capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	151	Total	C	N	O	S	0	0
			1164	734	207	219	4		
3	F	151	Total	C	N	O	S	0	0
			1164	734	207	219	4		
3	I	151	Total	C	N	O	S	0	0
			1164	734	207	219	4		
3	L	151	Total	C	N	O	S	0	0
			1164	734	207	219	4		

- Molecule 4 is a protein called Isoform Short of Very low-density lipoprotein receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	V	78	Total	C	N	O	S	0	0
			588	345	100	131	12		
4	W	78	Total	C	N	O	S	0	0
			588	345	100	131	12		
4	X	78	Total	C	N	O	S	0	0
			588	345	100	131	12		
4	Y	78	Total	C	N	O	S	0	0
			588	345	100	131	12		
4	R	35	Total	C	N	O	S	0	0
			258	150	46	56	6		
4	S	35	Total	C	N	O	S	0	0
			258	150	46	56	6		
4	T	35	Total	C	N	O	S	0	0
			258	150	46	56	6		
4	U	35	Total	C	N	O	S	0	0
			258	150	46	56	6		

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	770	HIS	-	expression tag	UNP P98155
V	771	HIS	-	expression tag	UNP P98155
V	772	HIS	-	expression tag	UNP P98155
V	773	HIS	-	expression tag	UNP P98155
V	774	HIS	-	expression tag	UNP P98155
V	775	HIS	-	expression tag	UNP P98155
W	770	HIS	-	expression tag	UNP P98155
W	771	HIS	-	expression tag	UNP P98155
W	772	HIS	-	expression tag	UNP P98155
W	773	HIS	-	expression tag	UNP P98155
W	774	HIS	-	expression tag	UNP P98155

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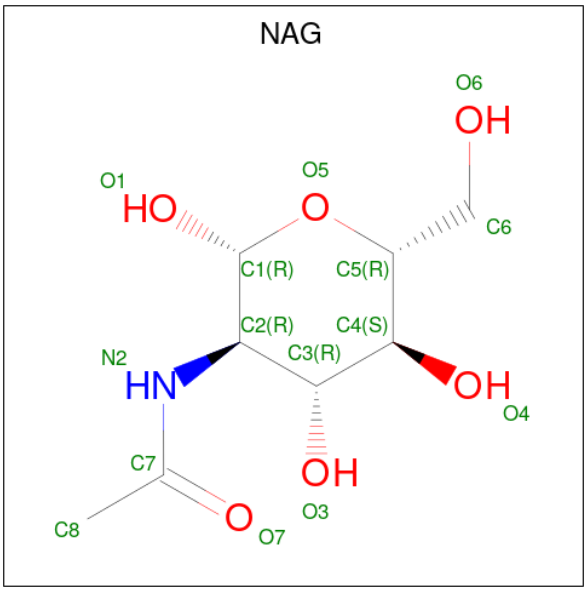
Chain	Residue	Modelled	Actual	Comment	Reference
W	775	HIS	-	expression tag	UNP P98155
X	770	HIS	-	expression tag	UNP P98155
X	771	HIS	-	expression tag	UNP P98155
X	772	HIS	-	expression tag	UNP P98155
X	773	HIS	-	expression tag	UNP P98155
X	774	HIS	-	expression tag	UNP P98155
X	775	HIS	-	expression tag	UNP P98155
Y	770	HIS	-	expression tag	UNP P98155
Y	771	HIS	-	expression tag	UNP P98155
Y	772	HIS	-	expression tag	UNP P98155
Y	773	HIS	-	expression tag	UNP P98155
Y	774	HIS	-	expression tag	UNP P98155
Y	775	HIS	-	expression tag	UNP P98155
R	770	HIS	-	expression tag	UNP P98155
R	771	HIS	-	expression tag	UNP P98155
R	772	HIS	-	expression tag	UNP P98155
R	773	HIS	-	expression tag	UNP P98155
R	774	HIS	-	expression tag	UNP P98155
R	775	HIS	-	expression tag	UNP P98155
S	770	HIS	-	expression tag	UNP P98155
S	771	HIS	-	expression tag	UNP P98155
S	772	HIS	-	expression tag	UNP P98155
S	773	HIS	-	expression tag	UNP P98155
S	774	HIS	-	expression tag	UNP P98155
S	775	HIS	-	expression tag	UNP P98155
T	770	HIS	-	expression tag	UNP P98155
T	771	HIS	-	expression tag	UNP P98155
T	772	HIS	-	expression tag	UNP P98155
T	773	HIS	-	expression tag	UNP P98155
T	774	HIS	-	expression tag	UNP P98155
T	775	HIS	-	expression tag	UNP P98155
U	770	HIS	-	expression tag	UNP P98155
U	771	HIS	-	expression tag	UNP P98155
U	772	HIS	-	expression tag	UNP P98155
U	773	HIS	-	expression tag	UNP P98155
U	774	HIS	-	expression tag	UNP P98155
U	775	HIS	-	expression tag	UNP P98155

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total C N O 14 8 1 5	0
5	B	1	Total C N O 14 8 1 5	0
5	D	1	Total C N O 14 8 1 5	0
5	E	1	Total C N O 14 8 1 5	0
5	G	1	Total C N O 14 8 1 5	0
5	H	1	Total C N O 14 8 1 5	0
5	J	1	Total C N O 14 8 1 5	0
5	K	1	Total C N O 14 8 1 5	0

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	AltConf
6	V	2	Total Ca 2 2	0
6	W	2	Total Ca 2 2	0
6	X	2	Total Ca 2 2	0
6	Y	2	Total Ca 2 2	0

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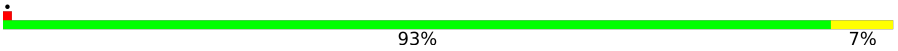
Mol	Chain	Residues	Atoms	AltConf
6	R	1	Total Ca 1 1	0
6	S	1	Total Ca 1 1	0
6	T	1	Total Ca 1 1	0
6	U	1	Total Ca 1 1	0

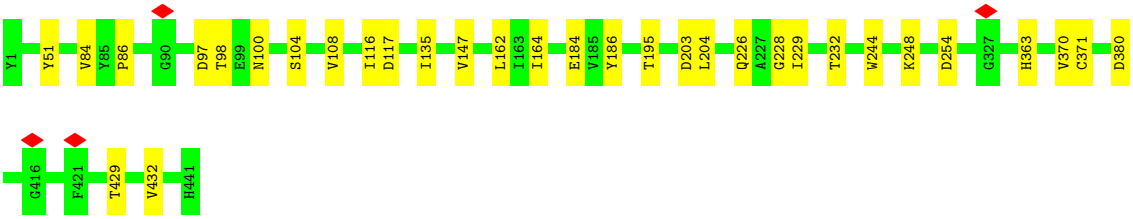
3 Residue-property plots (i)

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: E1 protein

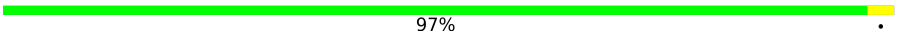
Chain A:

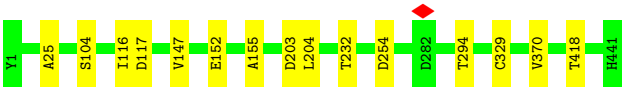




- Molecule 1: E1 protein

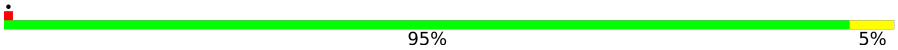
Chain D:

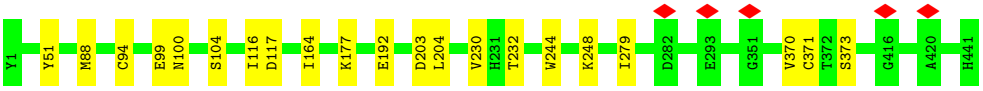




- Molecule 1: E1 protein

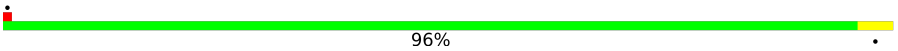
Chain G:

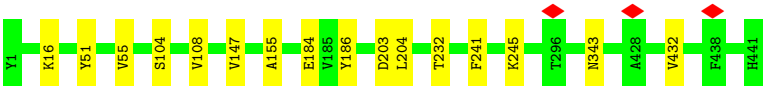




- Molecule 1: E1 protein

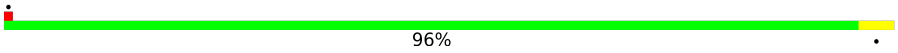
Chain J:

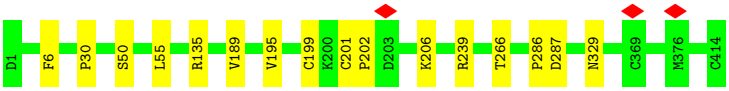




- Molecule 2: E2 protein

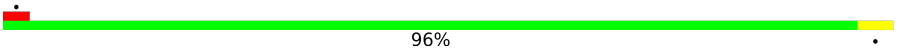
Chain B:





• Molecule 2: E2 protein

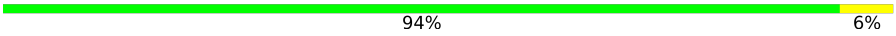
Chain E:





• Molecule 2: E2 protein

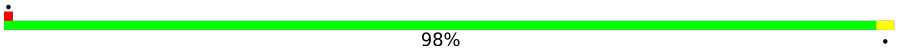
Chain H:

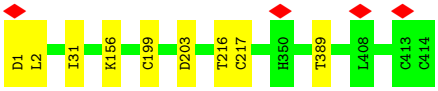




• Molecule 2: E2 protein

Chain K:

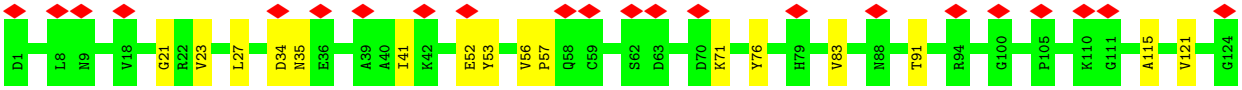


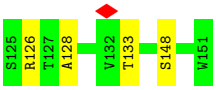


• Molecule 3: Capsid protein

Chain C:

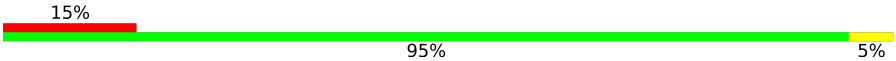


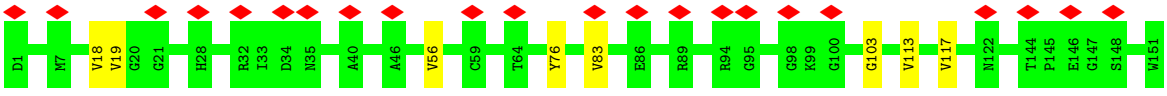




• Molecule 3: Capsid protein

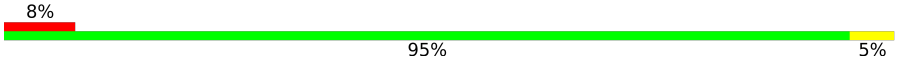
Chain F:

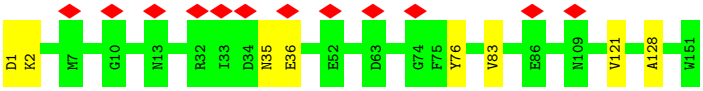




• Molecule 3: Capsid protein

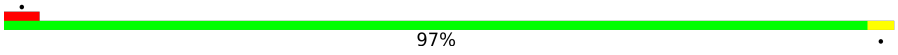
Chain I:

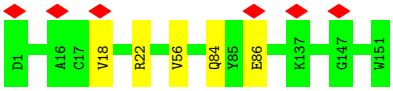




• Molecule 3: Capsid protein

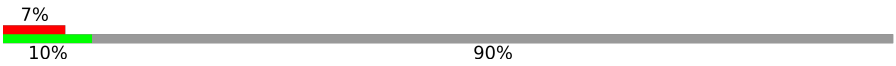
Chain L:

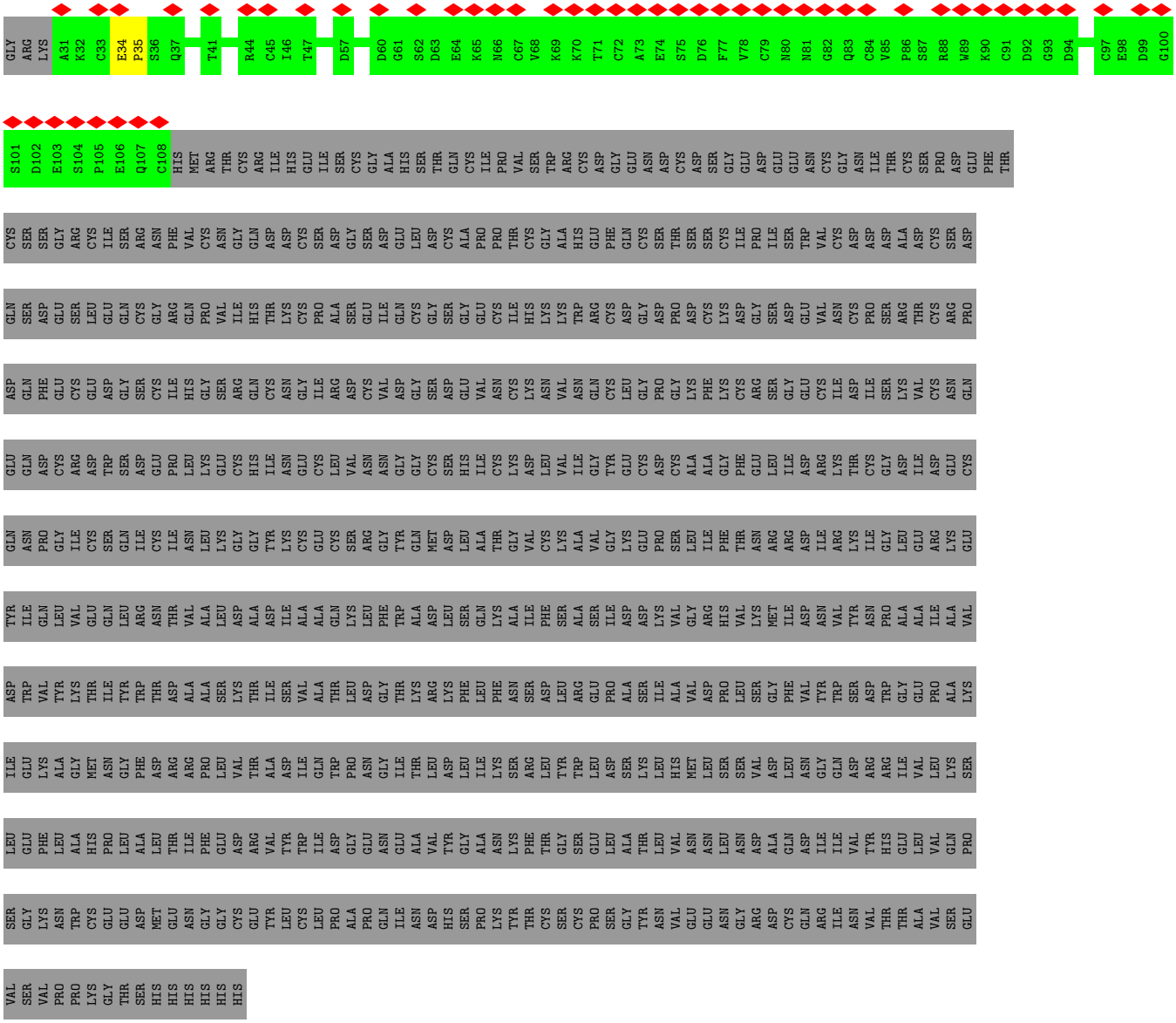




• Molecule 4: Isoform Short of Very low-density lipoprotein receptor

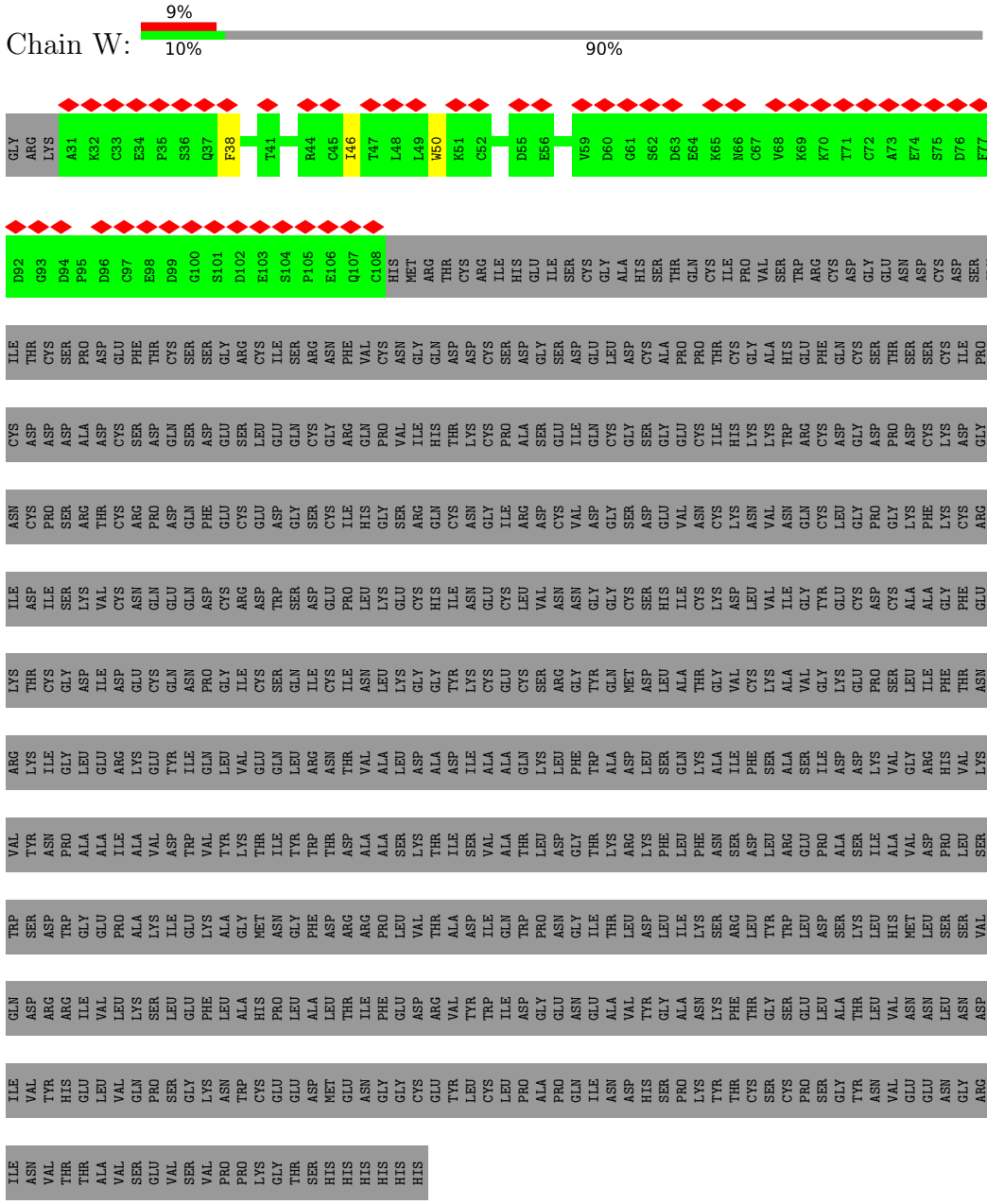
Chain V:





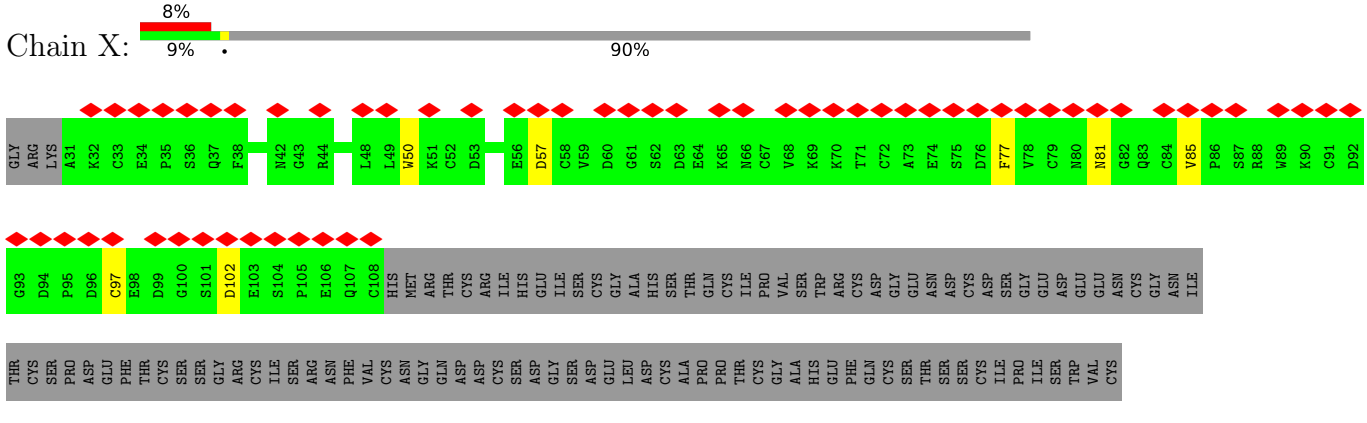
• Molecule 4: Isoform Short of Very low-density lipoprotein receptor

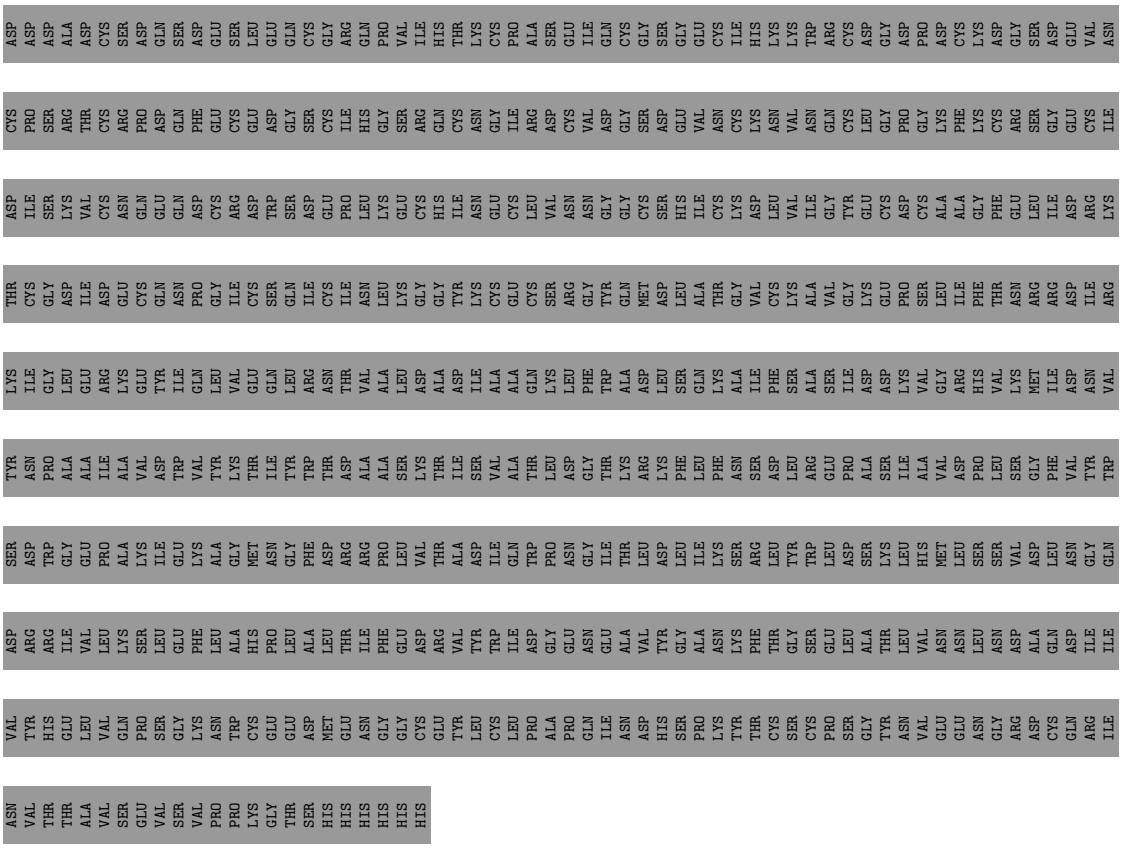
Chain W:



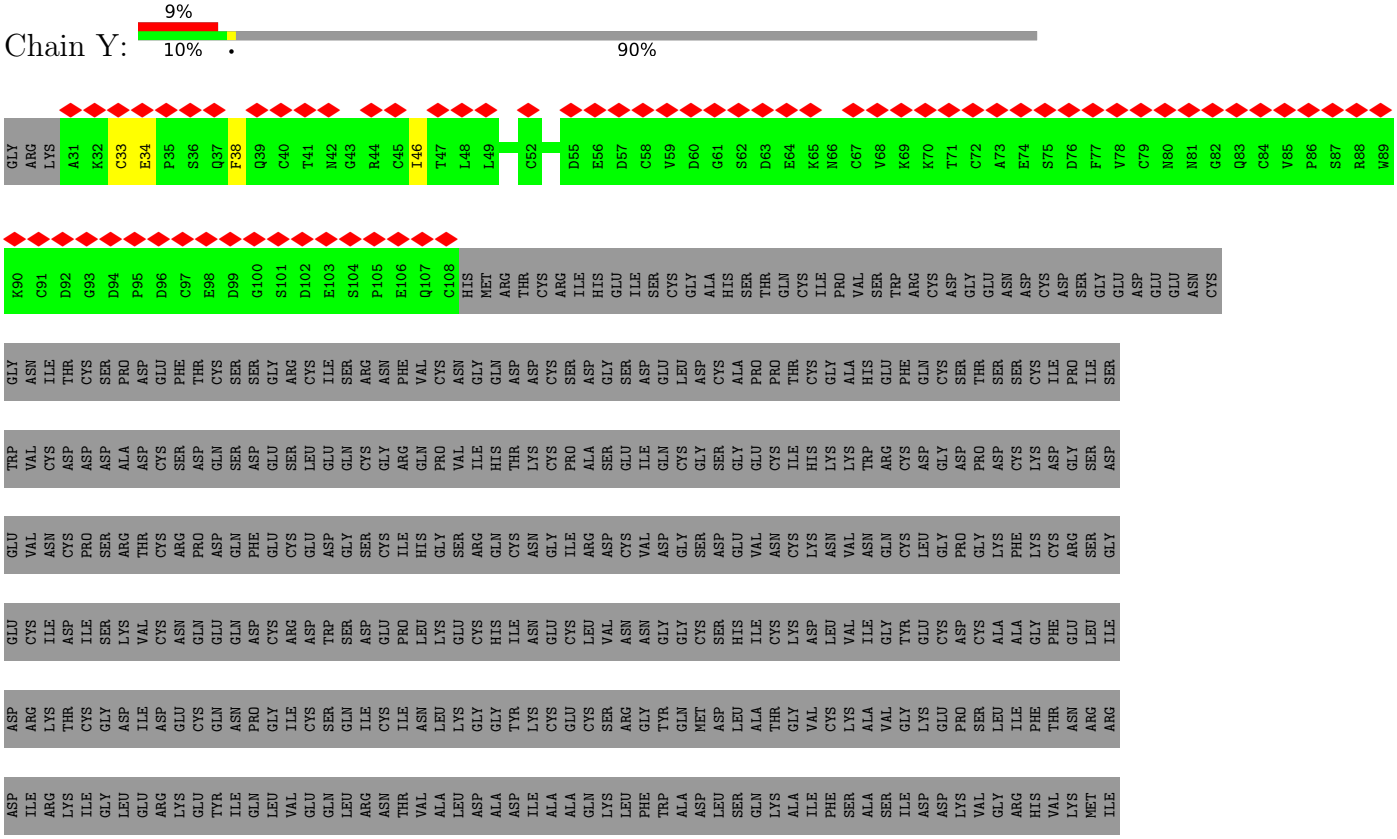
• Molecule 4: Isoform Short of Very low-density lipoprotein receptor

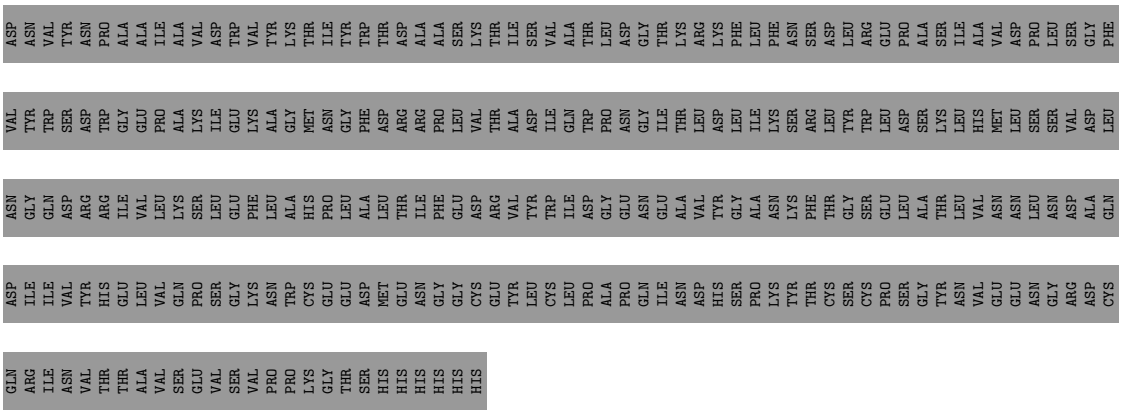
Chain X:





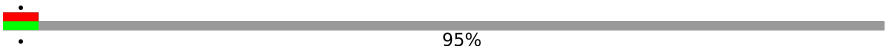
• Molecule 4: Isoform Short of Very low-density lipoprotein receptor

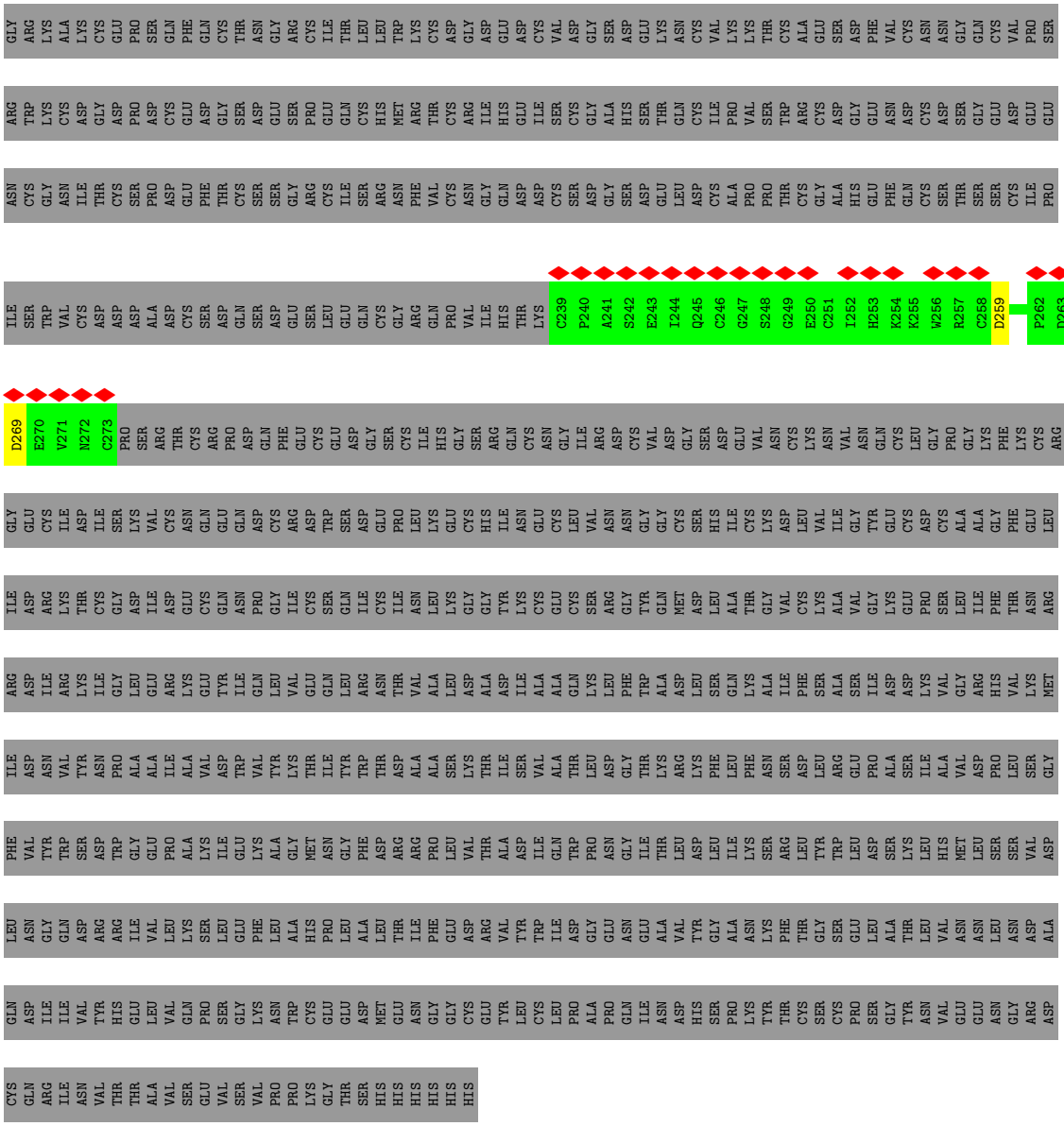




• Molecule 4: Isoform Short of Very low-density lipoprotein receptor

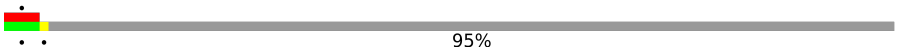
Chain R:

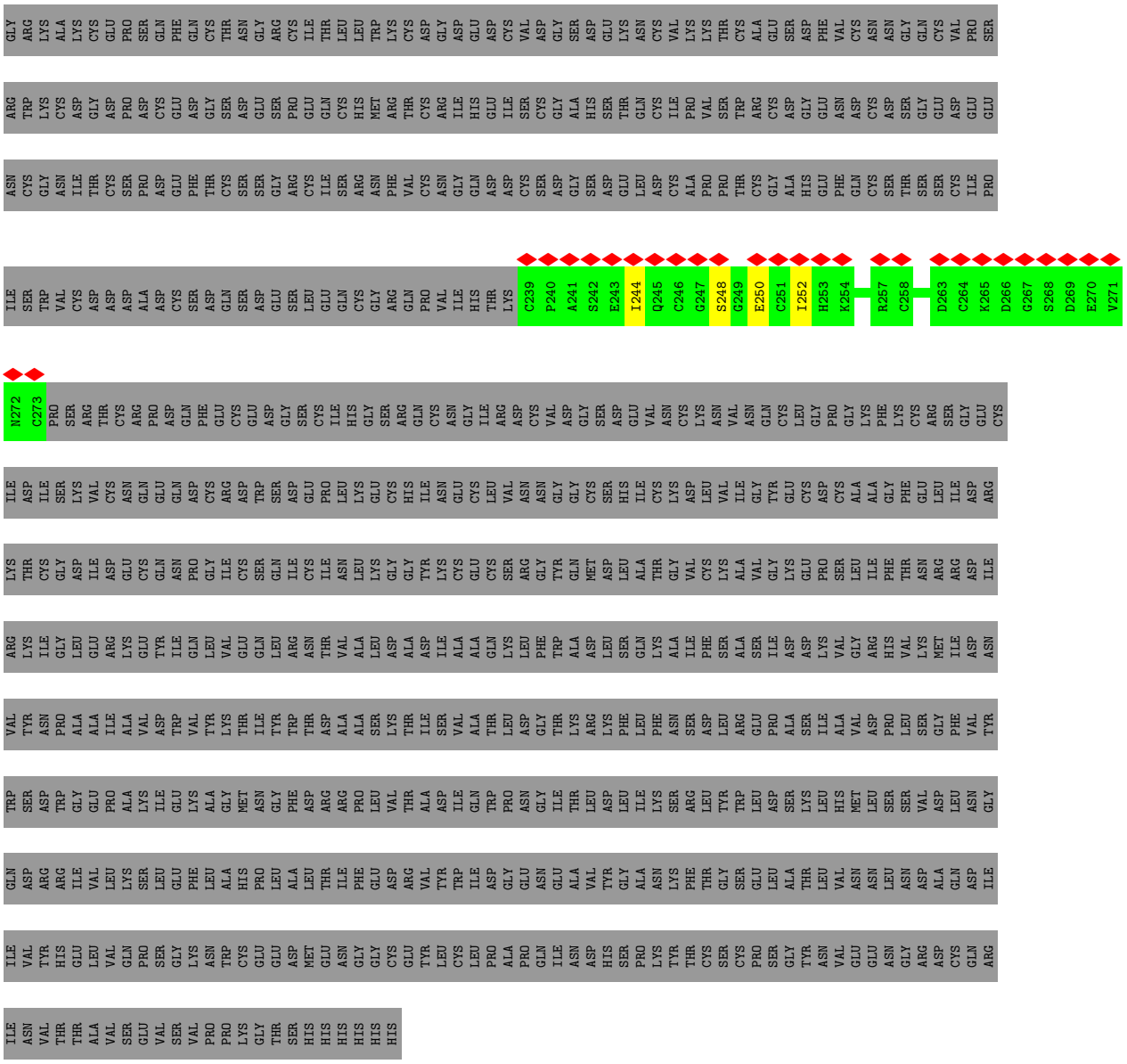




• Molecule 4: Isoform Short of Very low-density lipoprotein receptor

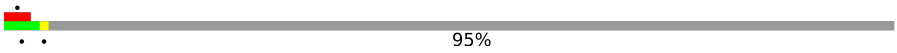
Chain S:

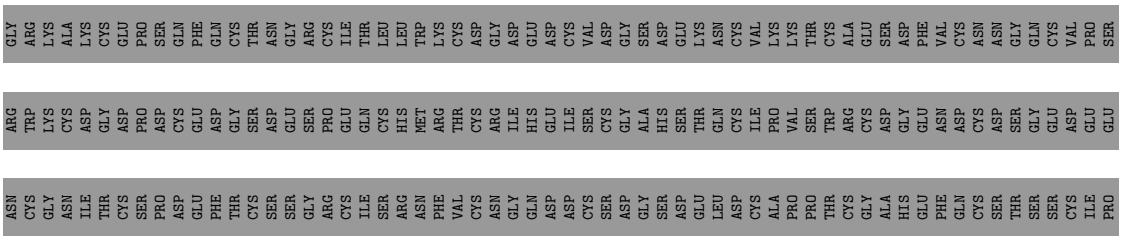


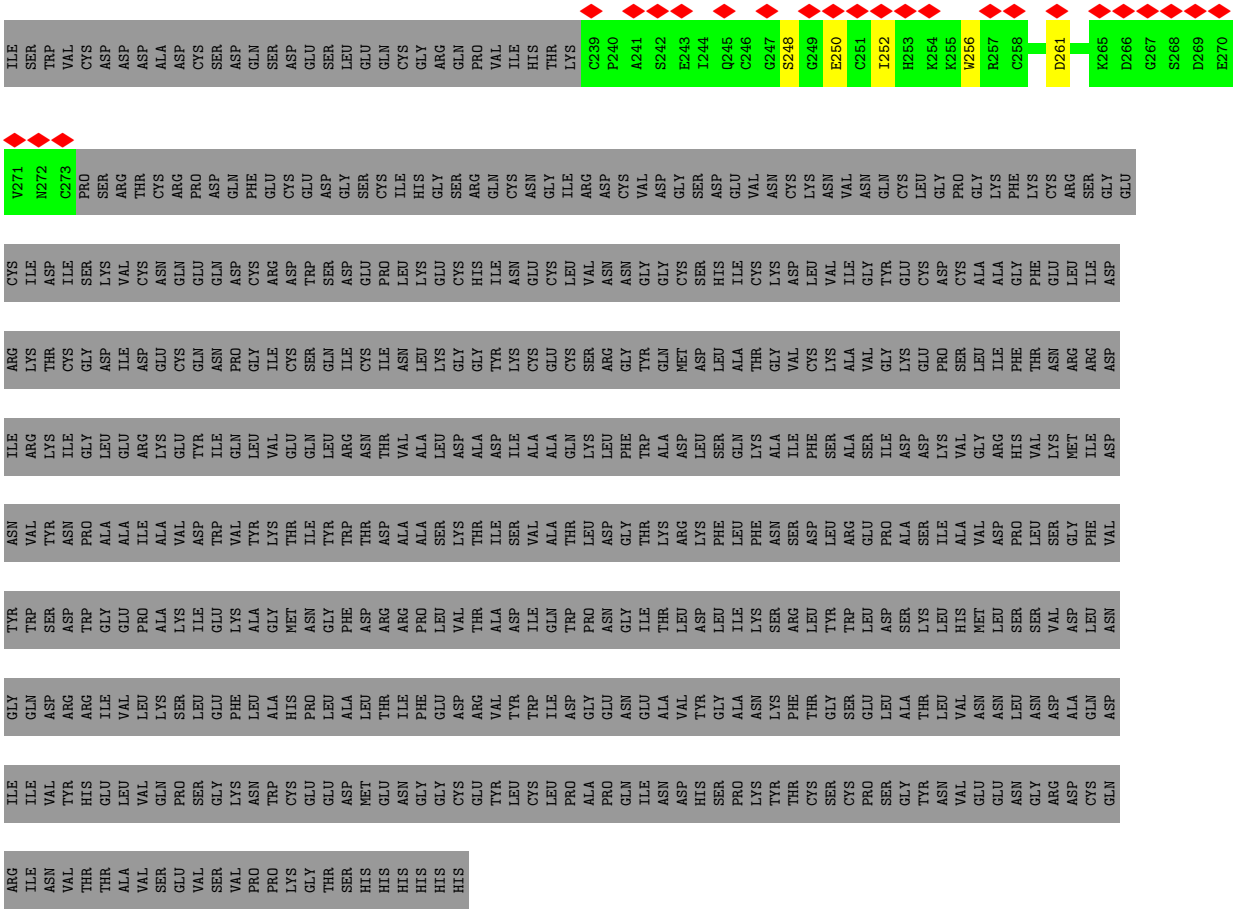


• Molecule 4: Isoform Short of Very low-density lipoprotein receptor

Chain T:

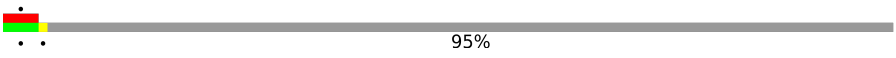


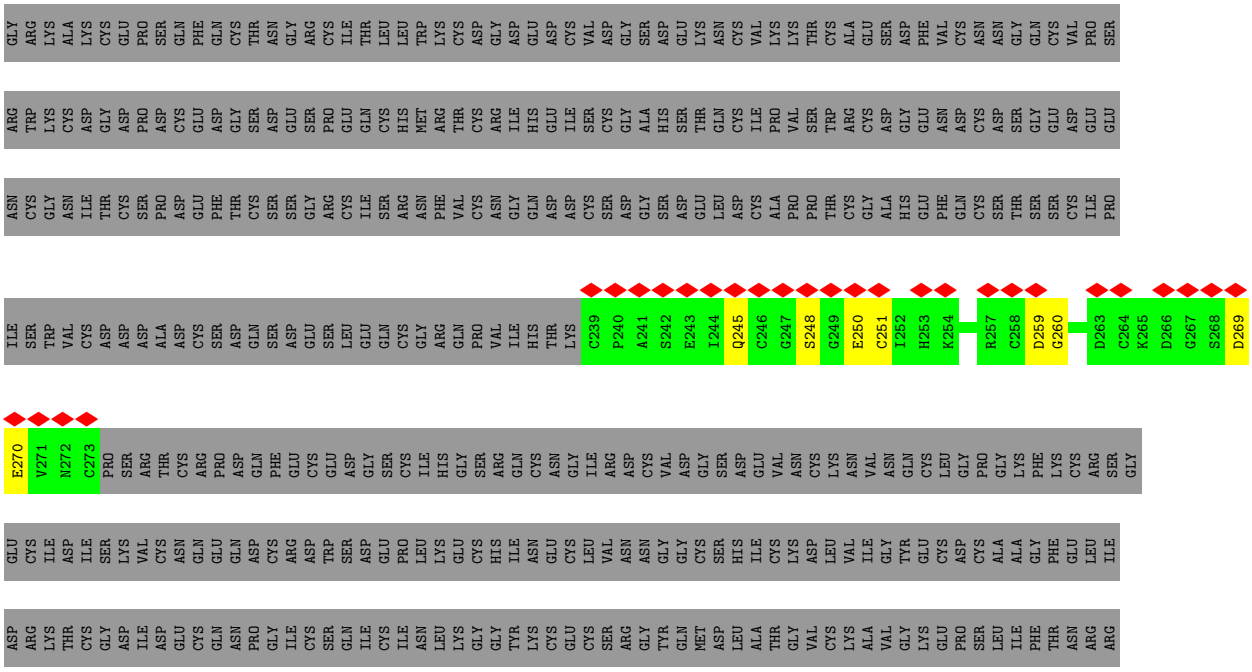




• Molecule 4: Isoform Short of Very low-density lipoprotein receptor

Chain U:





ASP ILE ARG LYS ILE GLY LEU GLU ARG LYS GLU TYR ILE GLN LEU VAL GLU GLN LEU ARG ASN THR VAL ALA LEU ASP ALA ASP ILE ALA ALA GLN LYS LEU PHE TRP ALA ASP LEU SER GLN LYS ALA ILE PHE SER ALA SER ILE ASP ASP LYS VAL GLY ARG HIS VAL LYS MET ILE

ASP ASN VAL TYR ASN PRO ALA ALA ILE ALA VAL ASP TRP VAL TYR LYS THR ILE TYR TRP THR ASP ALA ALA SER LYS THR ILE SER VAL ALA THR LEU ASP GLY THR LYS ARG LYS PHE LEU PHE ASN SER ASP LEU ARG GLU PRO ALA SER ILE ALA VAL ASP PRO LEU SER GLY PHE

VAL TYR TRP SER ASP TRP GLY GLU PRO ALA LYS ILE GLU LYS ALA GLY MET ASN GLY PHE ASP ARG ARG PRO LEU VAL THR ALA ASP ILE GLN TRP PRO ASN GLY ILE THR LEU ASP LEU ILE LYS SER ARG LEU TYR TRP LEU ASP SER LYS LEU HIS MET LEU SER SER VAL ASP LEU

ASN GLY GLN ASP ARG ARG ILE VAL LEU LYS SER LEU GLU PHE LEU ALA HIS PRO LEU ALA LEU THR ILE PHE GLU ASP ARG VAL TRP ILE ASP GLY GLU ASN GLU ALA VAL TYR GLY ALA ASN LYS PHE THR GLY SER GLU LEU ALA THR LEU VAL ASN ASN LEU ASN ASP ALA GLN

ASP ILE ILE VAL TYR HIS GLU LEU VAL GLN PRO SER GLY LYS ASN TRP CYS GLU GLU ASP MET GLU ASN GLY GLY CYS GLU TYR LEU CYS LEU PRO ALA PRO GLN ILE ASN ASP HIS SER PRO LYS TYR THR CYS SER CYS PRO SER GLY TYR ASN VAL GLU GLU ASN GLY ARG ASP CYS

GLN ARG ILE ASN VAL THR THR ALA VAL SER GLU VAL SER VAL PRO PRO LYS GLY THR SER HIS HIS HIS HIS HIS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	391827	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 ($e^-/Å^2$)	37.90	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.072	Depositor
Minimum map value	-0.915	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.037	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	281.06, 281.06, 281.06	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.081, 1.081, 1.081	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, NAG

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	0.13	0/3462	0.36	0/4724
1	D	0.11	0/3462	0.31	0/4724
1	G	0.12	0/3462	0.32	0/4724
1	J	0.12	0/3462	0.32	0/4724
2	B	0.14	0/3347	0.39	0/4565
2	E	0.11	0/3347	0.32	0/4565
2	H	0.12	0/3347	0.32	0/4565
2	K	0.11	0/3347	0.31	0/4565
3	C	0.08	0/1191	0.27	0/1615
3	F	0.07	0/1191	0.26	0/1615
3	I	0.08	0/1191	0.29	0/1615
3	L	0.09	0/1191	0.31	0/1615
4	R	0.09	0/262	0.30	0/351
4	S	0.09	0/262	0.33	0/351
4	T	0.11	0/262	0.32	0/351
4	U	0.15	0/262	0.47	0/351
4	V	0.11	0/597	0.30	0/805
4	W	0.11	0/597	0.27	0/805
4	X	0.11	0/597	0.29	0/805
4	Y	0.13	0/597	0.36	0/805
All	All	0.11	0/35436	0.33	0/48240

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
2	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	239	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	3370	0	3277	19	0
1	D	3370	0	3277	9	0
1	G	3370	0	3277	12	0
1	J	3370	0	3277	10	0
2	B	3253	0	3211	9	0
2	E	3253	0	3211	10	0
2	H	3253	0	3211	14	0
2	K	3253	0	3211	6	0
3	C	1164	0	1149	12	0
3	F	1164	0	1149	4	0
3	I	1164	0	1149	4	0
3	L	1164	0	1149	3	0
4	R	258	0	221	2	0
4	S	258	0	221	2	0
4	T	258	0	221	3	0
4	U	258	0	221	5	0
4	V	588	0	507	1	0
4	W	588	0	507	2	0
4	X	588	0	507	4	0
4	Y	588	0	507	3	0
5	A	14	0	13	0	0
5	B	14	0	13	0	0
5	D	14	0	13	0	0
5	E	14	0	13	0	0
5	G	14	0	13	0	0
5	H	14	0	13	0	0
5	J	14	0	13	0	0
5	K	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	R	1	0	0	0	0
6	S	1	0	0	0	0
6	T	1	0	0	0	0
6	U	1	0	0	0	0
6	V	2	0	0	0	0
6	W	2	0	0	0	0
6	X	2	0	0	0	0
6	Y	2	0	0	0	0
All	All	34656	0	33564	124	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 2.

The worst 5 of 124 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)
2:H:398:LYS:O	3:L:22:ARG:NH1	2.26	0.68
1:A:254:ASP:OD2	2:B:135:ARG:NH2	2.28	0.66
1:A:203:ASP:OD1	1:A:204:LEU:N	2.29	0.65
3:L:84:GLN:NE2	3:L:86:GLU:OE2	2.31	0.63
3:I:76:TYR:O	3:I:83:VAL:N	2.26	0.62

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	439/441 (100%)	430 (98%)	9 (2%)	0	100	100
1	D	439/441 (100%)	433 (99%)	6 (1%)	0	100	100
1	G	439/441 (100%)	434 (99%)	5 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	439/441 (100%)	434 (99%)	5 (1%)	0	100	100
2	B	412/414 (100%)	397 (96%)	15 (4%)	0	100	100
2	E	412/414 (100%)	397 (96%)	15 (4%)	0	100	100
2	H	412/414 (100%)	392 (95%)	20 (5%)	0	100	100
2	K	412/414 (100%)	396 (96%)	16 (4%)	0	100	100
3	C	149/151 (99%)	147 (99%)	2 (1%)	0	100	100
3	F	149/151 (99%)	147 (99%)	2 (1%)	0	100	100
3	I	149/151 (99%)	147 (99%)	2 (1%)	0	100	100
3	L	149/151 (99%)	148 (99%)	1 (1%)	0	100	100
4	R	33/748 (4%)	30 (91%)	3 (9%)	0	100	100
4	S	33/748 (4%)	30 (91%)	3 (9%)	0	100	100
4	T	33/748 (4%)	31 (94%)	2 (6%)	0	100	100
4	U	33/748 (4%)	31 (94%)	2 (6%)	0	100	100
4	V	76/748 (10%)	73 (96%)	3 (4%)	0	100	100
4	W	76/748 (10%)	76 (100%)	0	0	100	100
4	X	76/748 (10%)	74 (97%)	2 (3%)	0	100	100
4	Y	76/748 (10%)	76 (100%)	0	0	100	100
All	All	4436/10008 (44%)	4323 (98%)	113 (2%)	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	A	370/370 (100%)	370 (100%)	0	100	100
1	D	370/370 (100%)	370 (100%)	0	100	100
1	G	370/370 (100%)	370 (100%)	0	100	100
1	J	370/370 (100%)	370 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	362/362 (100%)	362 (100%)	0	100	100
2	E	362/362 (100%)	362 (100%)	0	100	100
2	H	362/362 (100%)	362 (100%)	0	100	100
2	K	362/362 (100%)	362 (100%)	0	100	100
3	C	125/125 (100%)	125 (100%)	0	100	100
3	F	125/125 (100%)	125 (100%)	0	100	100
3	I	125/125 (100%)	125 (100%)	0	100	100
3	L	125/125 (100%)	125 (100%)	0	100	100
4	R	30/655 (5%)	30 (100%)	0	100	100
4	S	30/655 (5%)	30 (100%)	0	100	100
4	T	30/655 (5%)	30 (100%)	0	100	100
4	U	30/655 (5%)	30 (100%)	0	100	100
4	V	70/655 (11%)	70 (100%)	0	100	100
4	W	70/655 (11%)	70 (100%)	0	100	100
4	X	70/655 (11%)	70 (100%)	0	100	100
4	Y	70/655 (11%)	70 (100%)	0	100	100
All	All	3828/8668 (44%)	3828 (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. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	162	HIS
4	W	66	ASN
3	I	122	ASN
2	K	230	ASN
3	I	84	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 12 are monoatomic - leaving 8 for Mogul analysis.

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	$\#\|Z\| > 2$
5	NAG	D	501	1	14,14,15	0.32	0	17,19,21	0.59	0
5	NAG	B	501	2	14,14,15	0.16	0	17,19,21	0.44	0
5	NAG	E	501	2	14,14,15	0.18	0	17,19,21	0.57	0
5	NAG	J	501	1	14,14,15	0.28	0	17,19,21	0.82	1 (5%)
5	NAG	K	501	2	14,14,15	0.37	0	17,19,21	0.52	0
5	NAG	H	501	2	14,14,15	0.37	0	17,19,21	1.28	1 (5%)
5	NAG	G	501	1	14,14,15	0.24	0	17,19,21	0.46	0
5	NAG	A	501	1	14,14,15	0.22	0	17,19,21	0.67	1 (5%)

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
5	NAG	D	501	1	-	2/6/23/26	0/1/1/1
5	NAG	B	501	2	-	0/6/23/26	0/1/1/1
5	NAG	E	501	2	-	0/6/23/26	0/1/1/1
5	NAG	J	501	1	-	1/6/23/26	0/1/1/1
5	NAG	K	501	2	-	4/6/23/26	0/1/1/1
5	NAG	H	501	2	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	G	501	1	-	1/6/23/26	0/1/1/1
5	NAG	A	501	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	501	NAG	C1-O5-C5	4.77	118.57	112.19
5	J	501	NAG	C1-O5-C5	2.71	115.82	112.19
5	A	501	NAG	C1-O5-C5	2.14	115.06	112.19

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	K	501	NAG	O5-C5-C6-O6
5	K	501	NAG	C4-C5-C6-O6
5	A	501	NAG	O5-C5-C6-O6
5	A	501	NAG	C4-C5-C6-O6
5	D	501	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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.

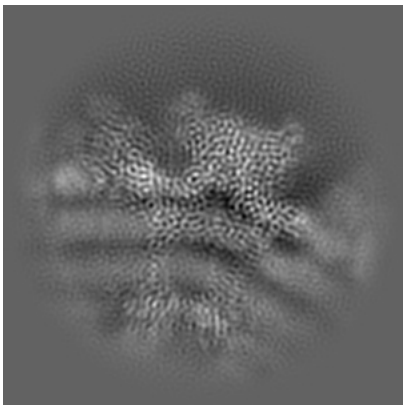
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-42190. These allow visual inspection of the internal detail of the map and identification of artifacts.

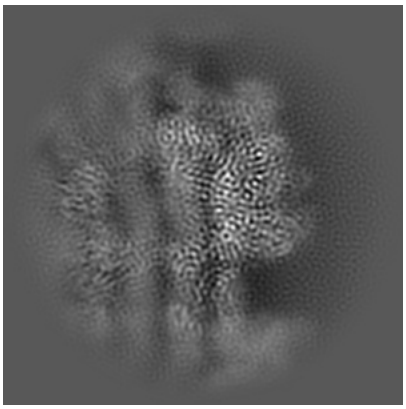
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

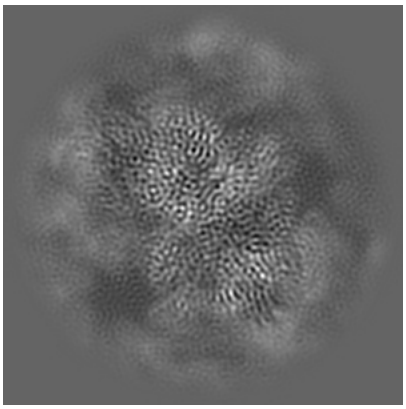
6.1.1 Primary map



X

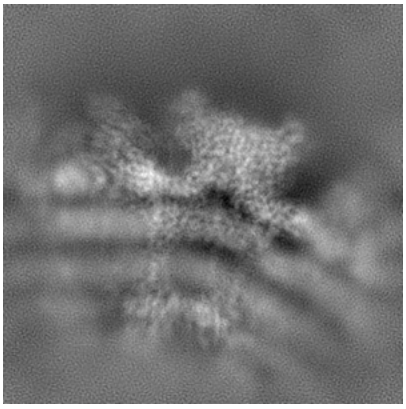


Y

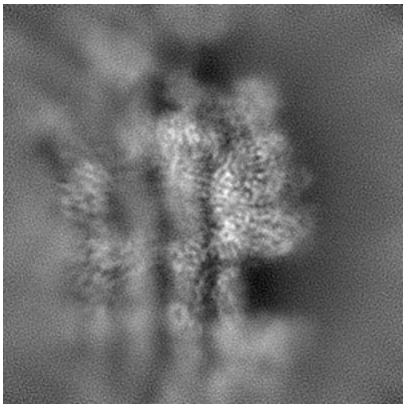


Z

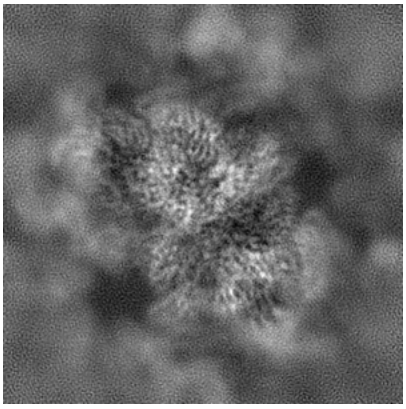
6.1.2 Raw map



X



Y

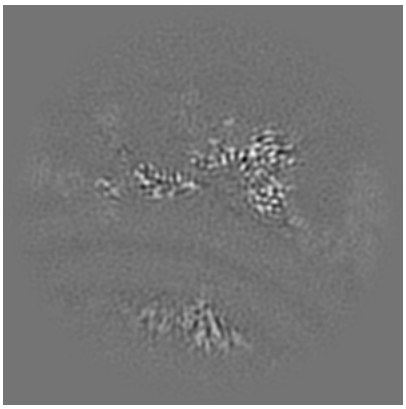


Z

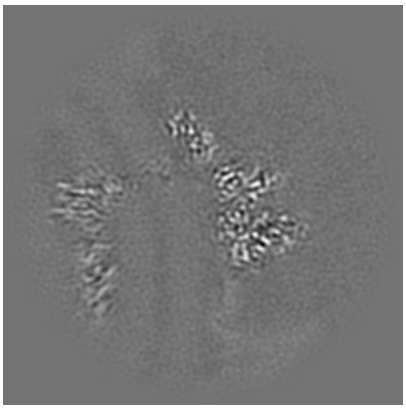
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

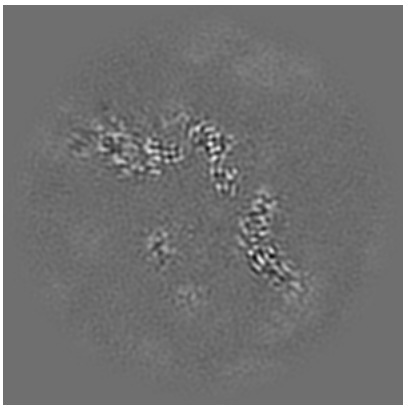
6.2.1 Primary map



X Index: 130

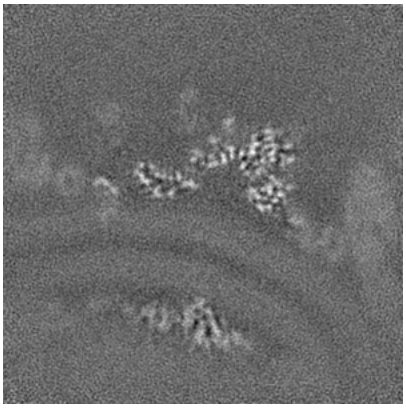


Y Index: 130

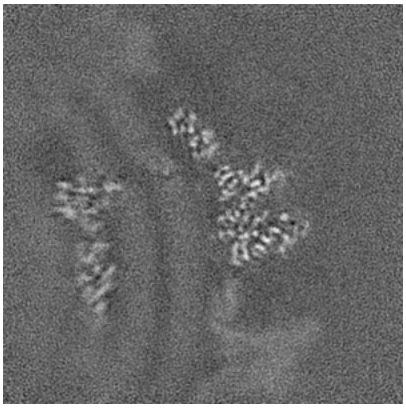


Z Index: 130

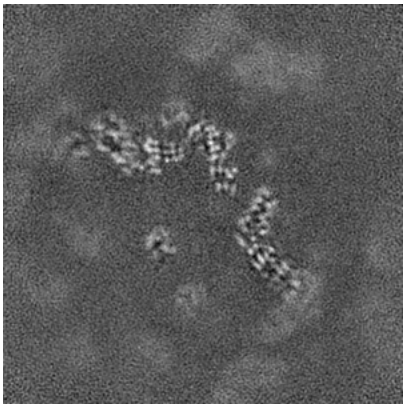
6.2.2 Raw map



X Index: 130



Y Index: 130

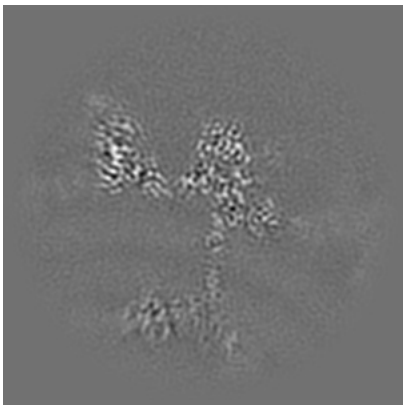


Z Index: 130

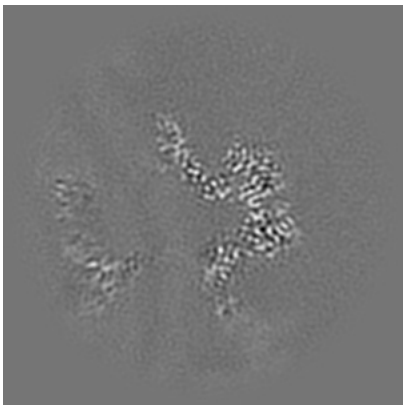
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

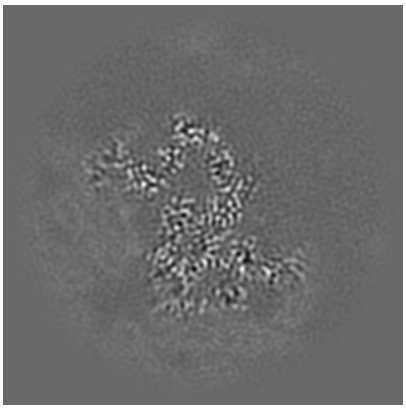
6.3.1 Primary map



X Index: 148

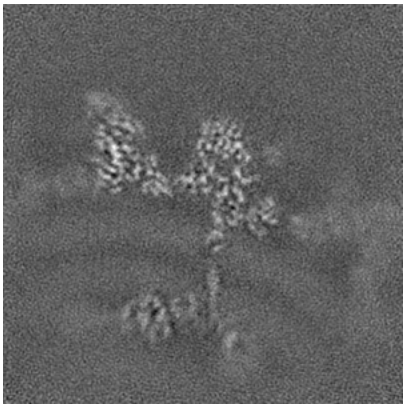


Y Index: 148

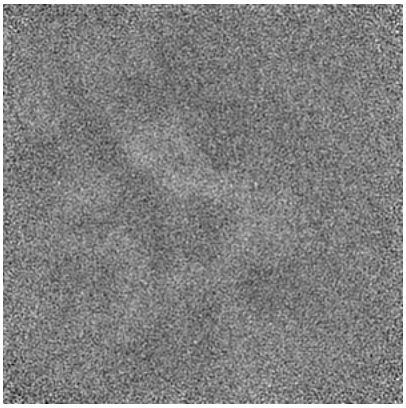


Z Index: 144

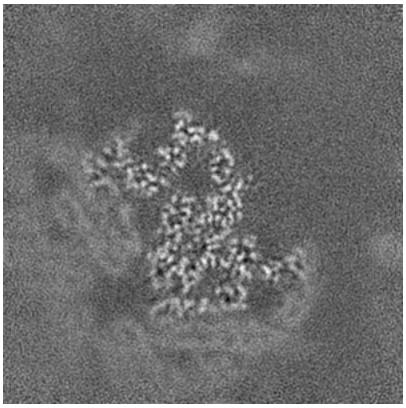
6.3.2 Raw map



X Index: 148



Y Index: 0

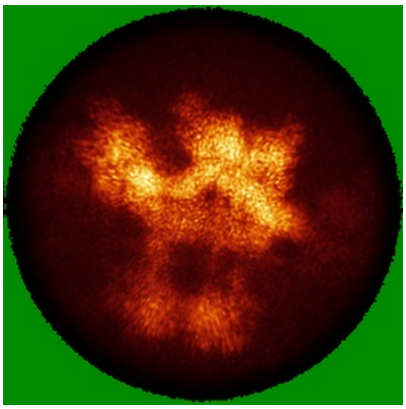


Z Index: 144

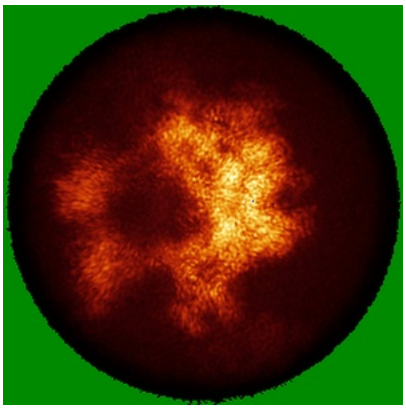
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

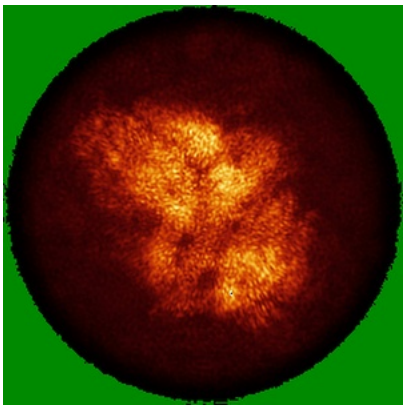
6.4.1 Primary map



X

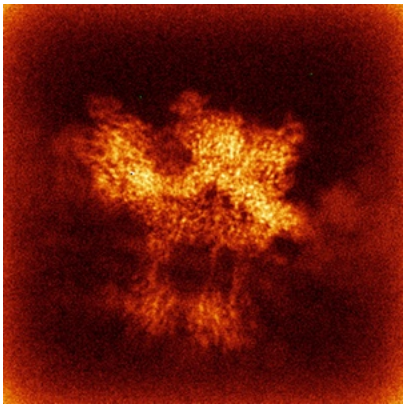


Y

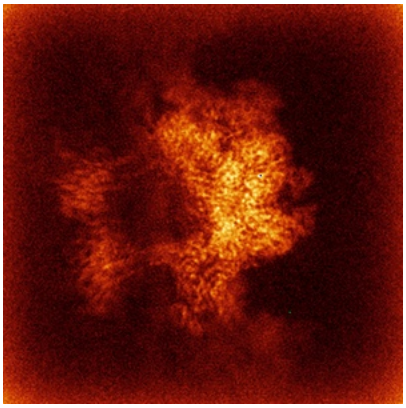


Z

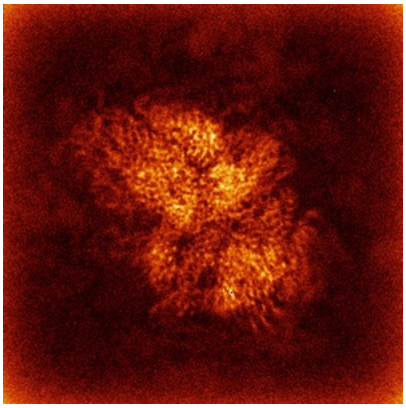
6.4.2 Raw map



X



Y

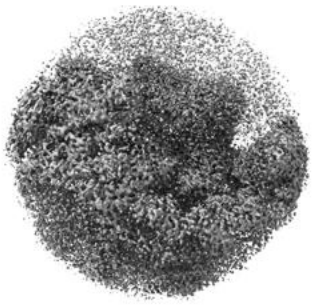


Z

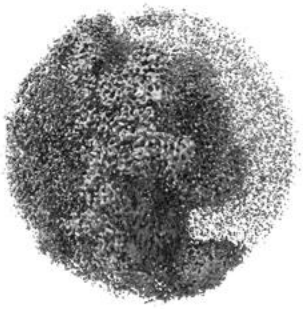
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X



Y



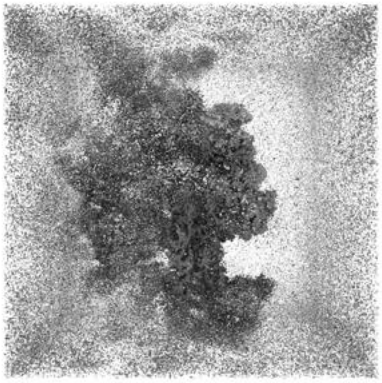
Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

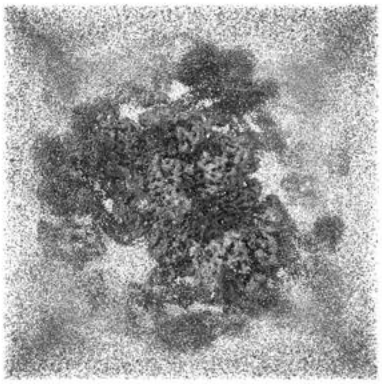
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

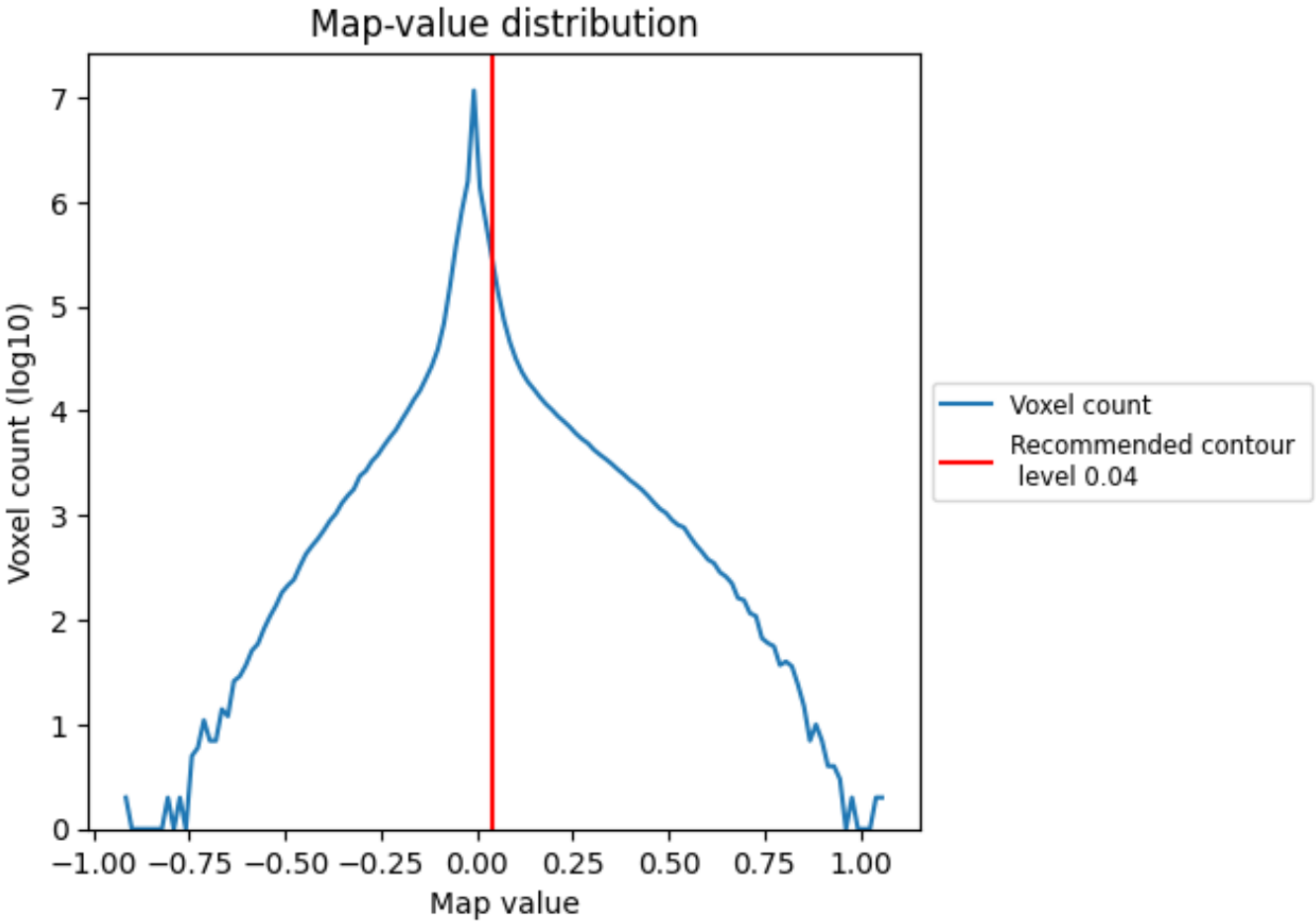
6.6 Mask visualisation (i)

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

7 Map analysis

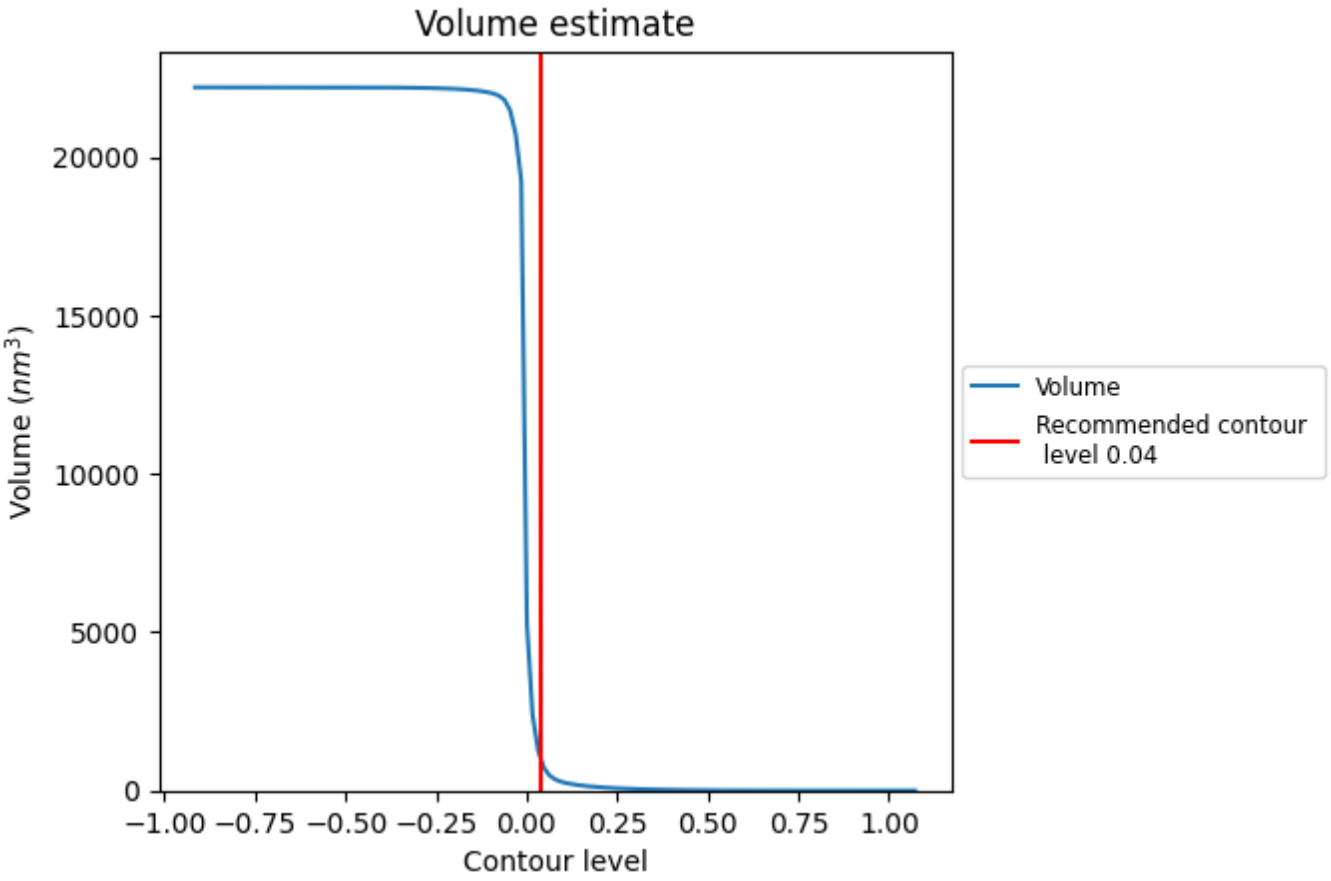
This section contains the results of statistical analysis of the map.

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.

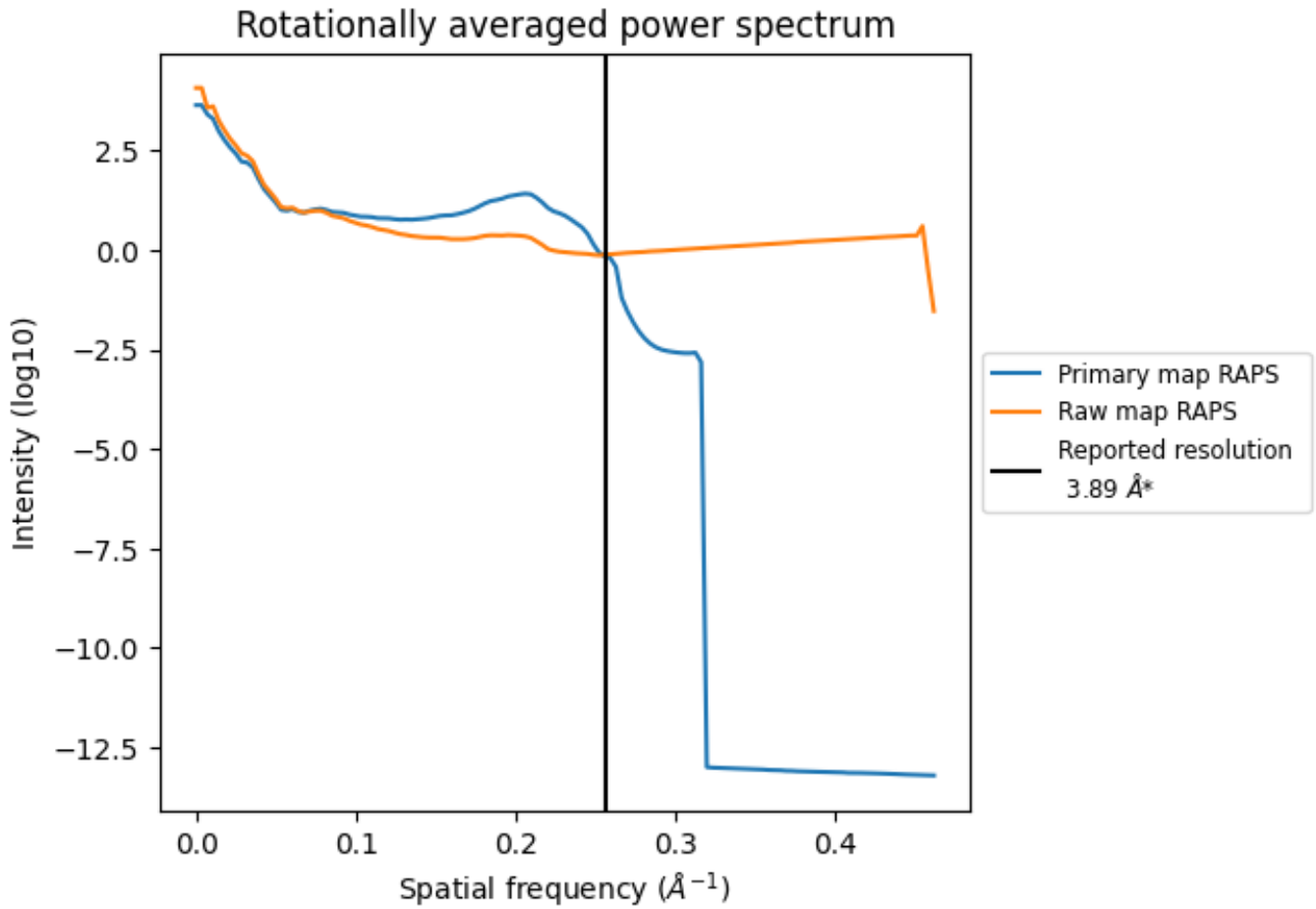
7.2 Volume estimate (i)



The volume at the recommended contour level is 978 nm^3; this corresponds to an approximate mass of 883 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)

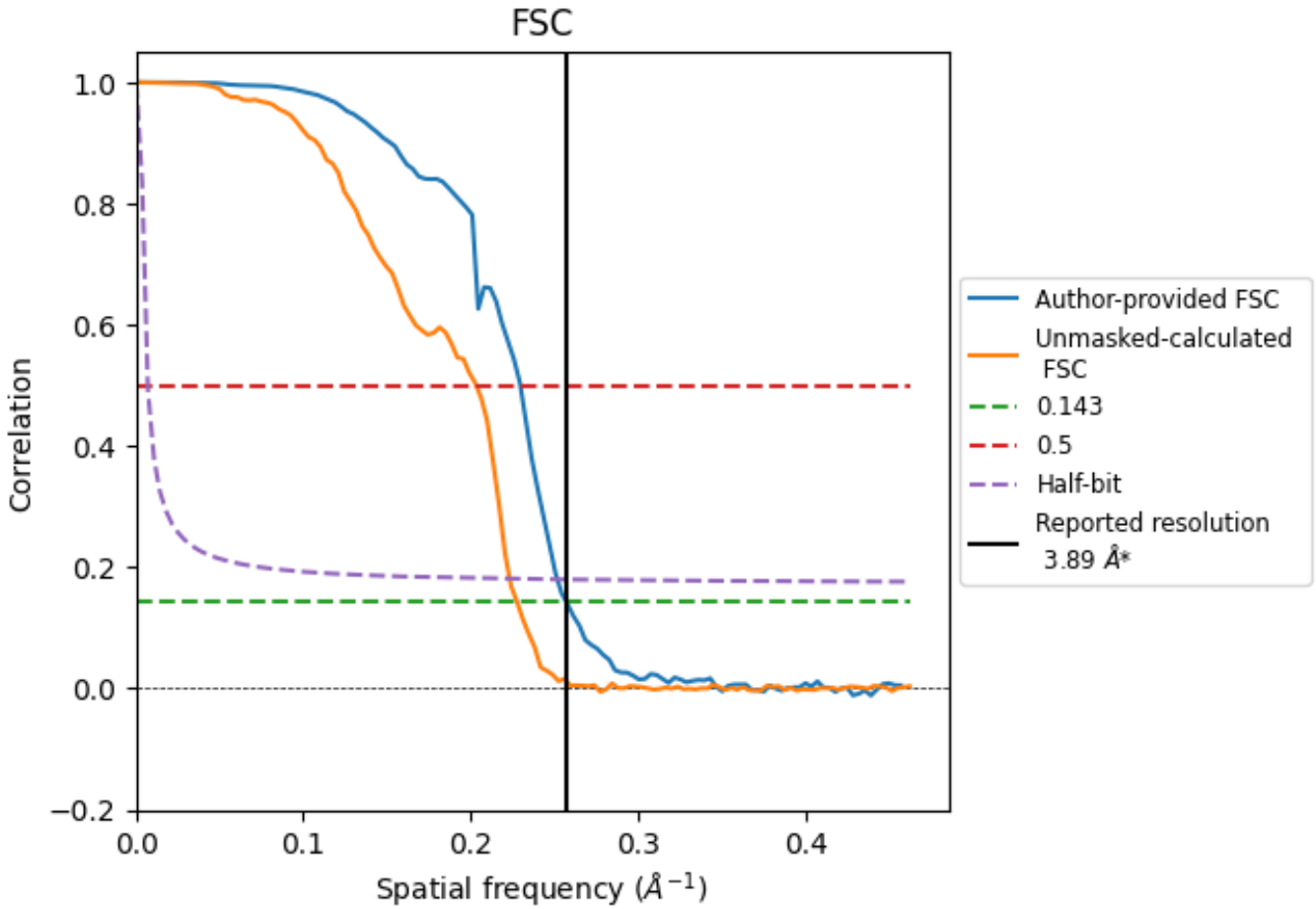


*Reported resolution corresponds to spatial frequency of 0.257 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.257 Å^{-1}

8.2 Resolution estimates (i)

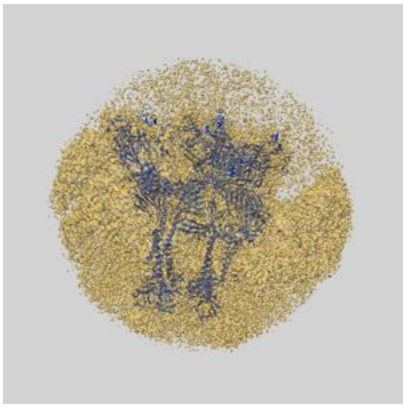
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.89	-	-
Author-provided FSC curve	3.89	4.35	3.97
Unmasked-calculated*	4.39	4.92	4.48

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.39 differs from the reported value 3.89 by more than 10 %

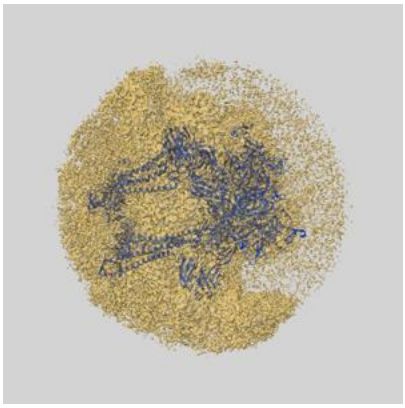
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-42190 and PDB model 8UFB. Per-residue inclusion information can be found in section 3 on page 9.

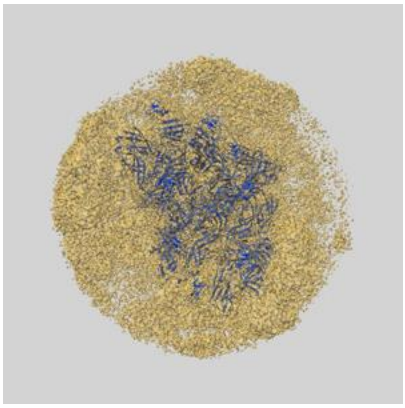
9.1 Map-model overlay



X



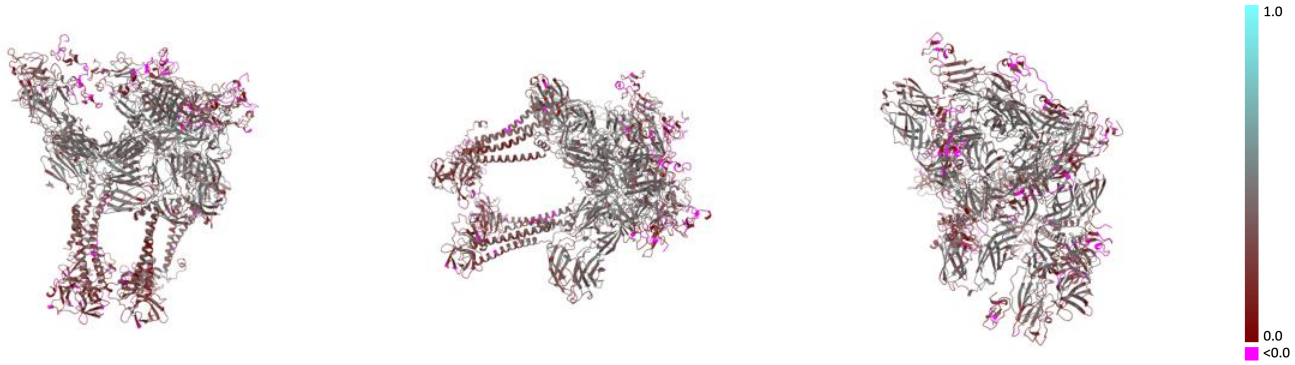
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 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.

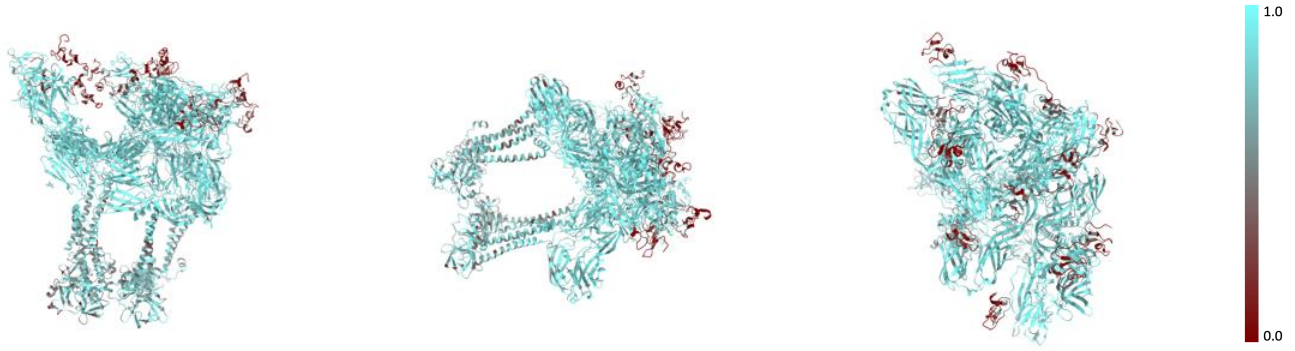
9.2 Q-score mapped to coordinate model (i)



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.

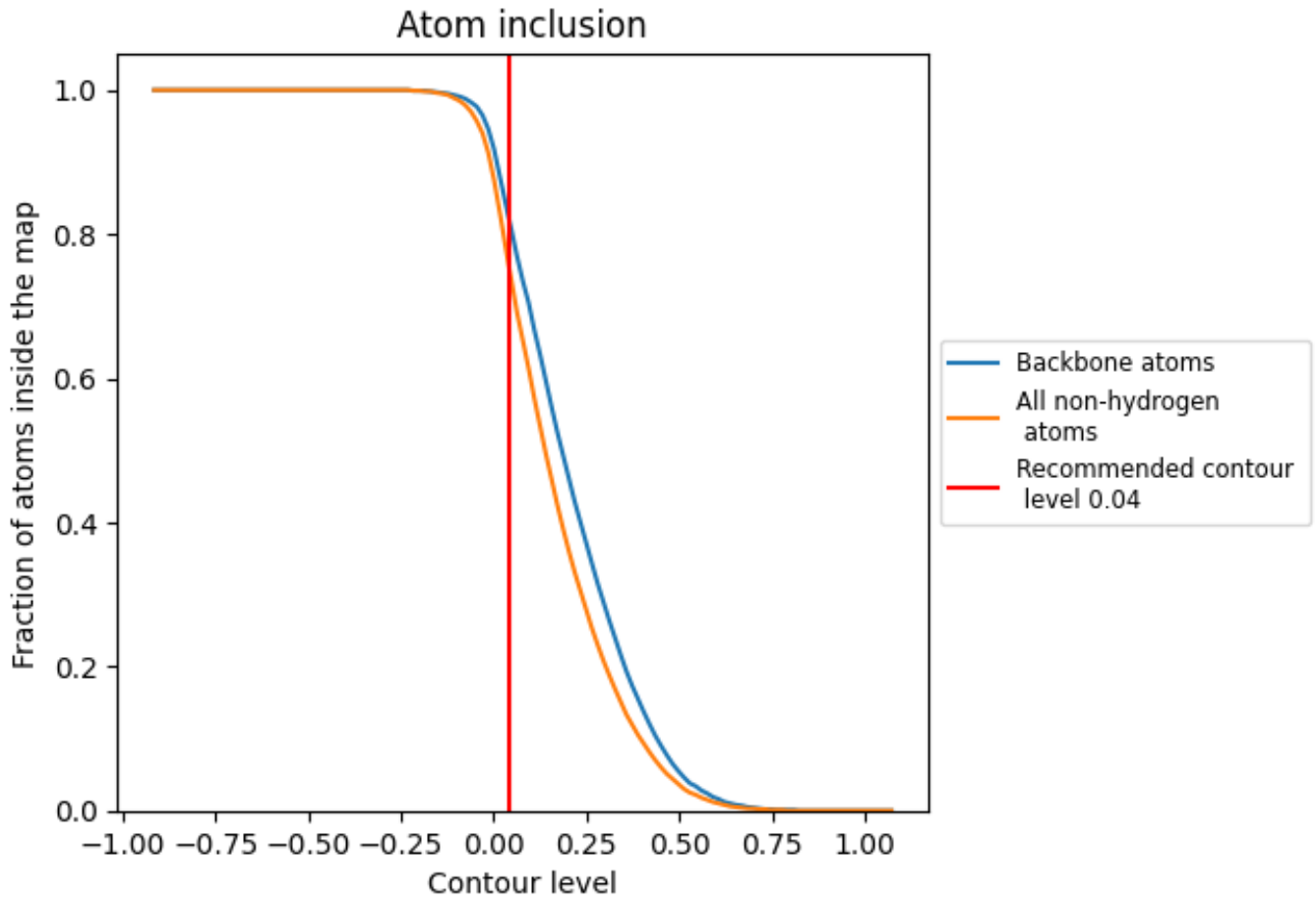
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.04).

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 76% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7570	0.3360
A	0.8370	0.3910
B	0.8210	0.3580
C	0.6440	0.1830
D	0.8520	0.4060
E	0.8360	0.3840
F	0.6570	0.2060
G	0.8380	0.3810
H	0.8440	0.3850
I	0.7140	0.2370
J	0.8370	0.3920
K	0.8460	0.3950
L	0.7240	0.2360
R	0.1640	0.1160
S	0.2150	0.1610
T	0.2970	0.1220
U	0.2380	0.1640
V	0.3130	0.1270
W	0.2120	0.0640
X	0.1950	0.1060
Y	0.1300	0.0630

