wwPDB EM Validation Summary Report (i)

Jul 3, 2024 – 09:52 am BST

PDB ID	:	7A1D
EMDB ID	:	EMD-11606
Title	:	Cryo-EM map of the large glutamate dehydrogenase composed of 180 kDa subunits from Mycobacterium smegmatis (open conformation)
Authors	:	Lazaro, M.; Melero, R.; Huet, C.; Lopez-Alonso, J.P.; Delgado, S.; Dodu, A.; Bruch, E.M.; Abriata, L.A.; Alzari, P.M.; Valle, M.; Lisa, M.N.
Deposited on	:	2020-08-12
Resolution	:	4.19 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:

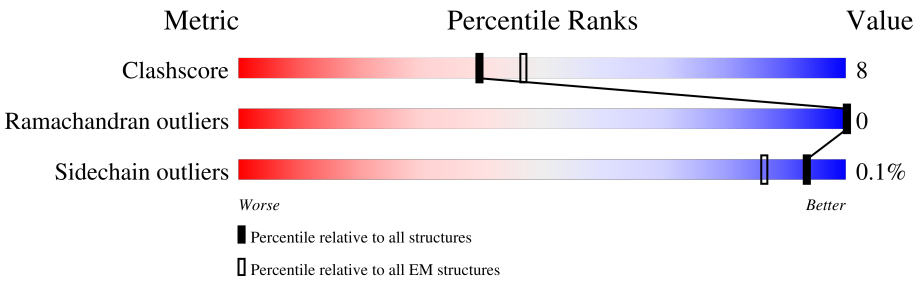
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 4.19 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
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	1611	5% 53% 13% 34%
1	B	1611	5% 53% 13% 34%
1	C	1611	5% 52% 14% 34%
1	D	1611	5% 52% 14% 34%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 33032 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 NAD-specific glutamate dehydrogenase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1063	8258	5186	1472	1581	19	0	0
1	B	1063	8258	5186	1472	1581	19	0	0
1	C	1063	8258	5186	1472	1581	19	0	0
1	D	1063	8258	5186	1472	1581	19	0	0

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	MET	-	initiating methionine	UNP A0R1C2
A	-15	HIS	-	expression tag	UNP A0R1C2
A	-14	HIS	-	expression tag	UNP A0R1C2
A	-13	HIS	-	expression tag	UNP A0R1C2
A	-12	HIS	-	expression tag	UNP A0R1C2
A	-11	HIS	-	expression tag	UNP A0R1C2
A	-10	HIS	-	expression tag	UNP A0R1C2
A	-9	GLU	-	expression tag	UNP A0R1C2
A	-8	ASN	-	expression tag	UNP A0R1C2
A	-7	LEU	-	expression tag	UNP A0R1C2
A	-6	TYR	-	expression tag	UNP A0R1C2
A	-5	PHE	-	expression tag	UNP A0R1C2
A	-4	GLN	-	expression tag	UNP A0R1C2
A	-3	GLY	-	expression tag	UNP A0R1C2
A	-2	ALA	-	expression tag	UNP A0R1C2
A	-1	ALA	-	expression tag	UNP A0R1C2
A	0	SER	-	expression tag	UNP A0R1C2
B	-16	MET	-	initiating methionine	UNP A0R1C2
B	-15	HIS	-	expression tag	UNP A0R1C2
B	-14	HIS	-	expression tag	UNP A0R1C2
B	-13	HIS	-	expression tag	UNP A0R1C2
B	-12	HIS	-	expression tag	UNP A0R1C2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	HIS	-	expression tag	UNP A0R1C2
B	-10	HIS	-	expression tag	UNP A0R1C2
B	-9	GLU	-	expression tag	UNP A0R1C2
B	-8	ASN	-	expression tag	UNP A0R1C2
B	-7	LEU	-	expression tag	UNP A0R1C2
B	-6	TYR	-	expression tag	UNP A0R1C2
B	-5	PHE	-	expression tag	UNP A0R1C2
B	-4	GLN	-	expression tag	UNP A0R1C2
B	-3	GLY	-	expression tag	UNP A0R1C2
B	-2	ALA	-	expression tag	UNP A0R1C2
B	-1	ALA	-	expression tag	UNP A0R1C2
B	0	SER	-	expression tag	UNP A0R1C2
C	-16	MET	-	initiating methionine	UNP A0R1C2
C	-15	HIS	-	expression tag	UNP A0R1C2
C	-14	HIS	-	expression tag	UNP A0R1C2
C	-13	HIS	-	expression tag	UNP A0R1C2
C	-12	HIS	-	expression tag	UNP A0R1C2
C	-11	HIS	-	expression tag	UNP A0R1C2
C	-10	HIS	-	expression tag	UNP A0R1C2
C	-9	GLU	-	expression tag	UNP A0R1C2
C	-8	ASN	-	expression tag	UNP A0R1C2
C	-7	LEU	-	expression tag	UNP A0R1C2
C	-6	TYR	-	expression tag	UNP A0R1C2
C	-5	PHE	-	expression tag	UNP A0R1C2
C	-4	GLN	-	expression tag	UNP A0R1C2
C	-3	GLY	-	expression tag	UNP A0R1C2
C	-2	ALA	-	expression tag	UNP A0R1C2
C	-1	ALA	-	expression tag	UNP A0R1C2
C	0	SER	-	expression tag	UNP A0R1C2
D	-16	MET	-	initiating methionine	UNP A0R1C2
D	-15	HIS	-	expression tag	UNP A0R1C2
D	-14	HIS	-	expression tag	UNP A0R1C2
D	-13	HIS	-	expression tag	UNP A0R1C2
D	-12	HIS	-	expression tag	UNP A0R1C2
D	-11	HIS	-	expression tag	UNP A0R1C2
D	-10	HIS	-	expression tag	UNP A0R1C2
D	-9	GLU	-	expression tag	UNP A0R1C2
D	-8	ASN	-	expression tag	UNP A0R1C2
D	-7	LEU	-	expression tag	UNP A0R1C2
D	-6	TYR	-	expression tag	UNP A0R1C2
D	-5	PHE	-	expression tag	UNP A0R1C2
D	-4	GLN	-	expression tag	UNP A0R1C2

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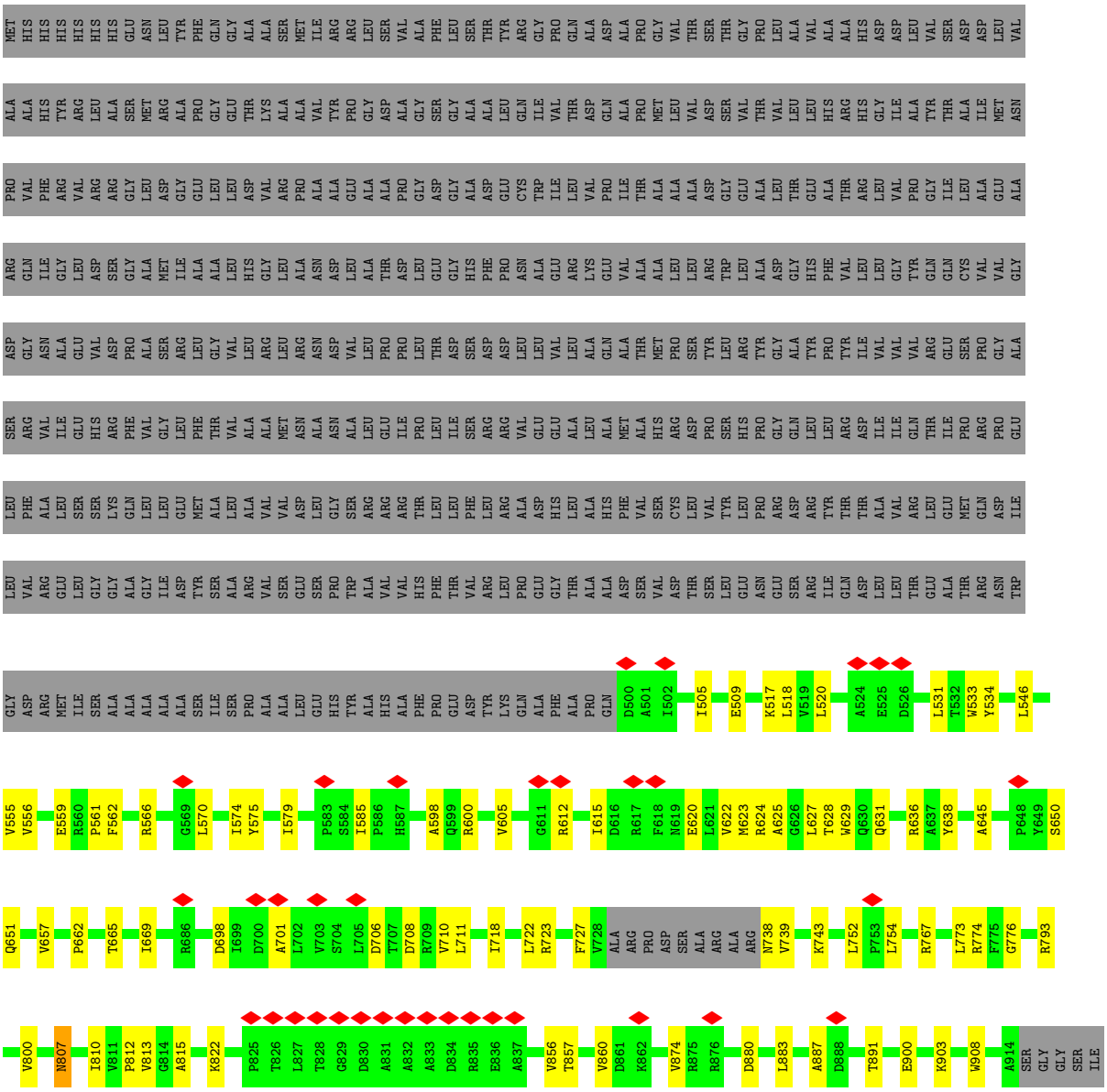
Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	GLY	-	expression tag	UNP A0R1C2
D	-2	ALA	-	expression tag	UNP A0R1C2
D	-1	ALA	-	expression tag	UNP A0R1C2
D	0	SER	-	expression tag	UNP A0R1C2

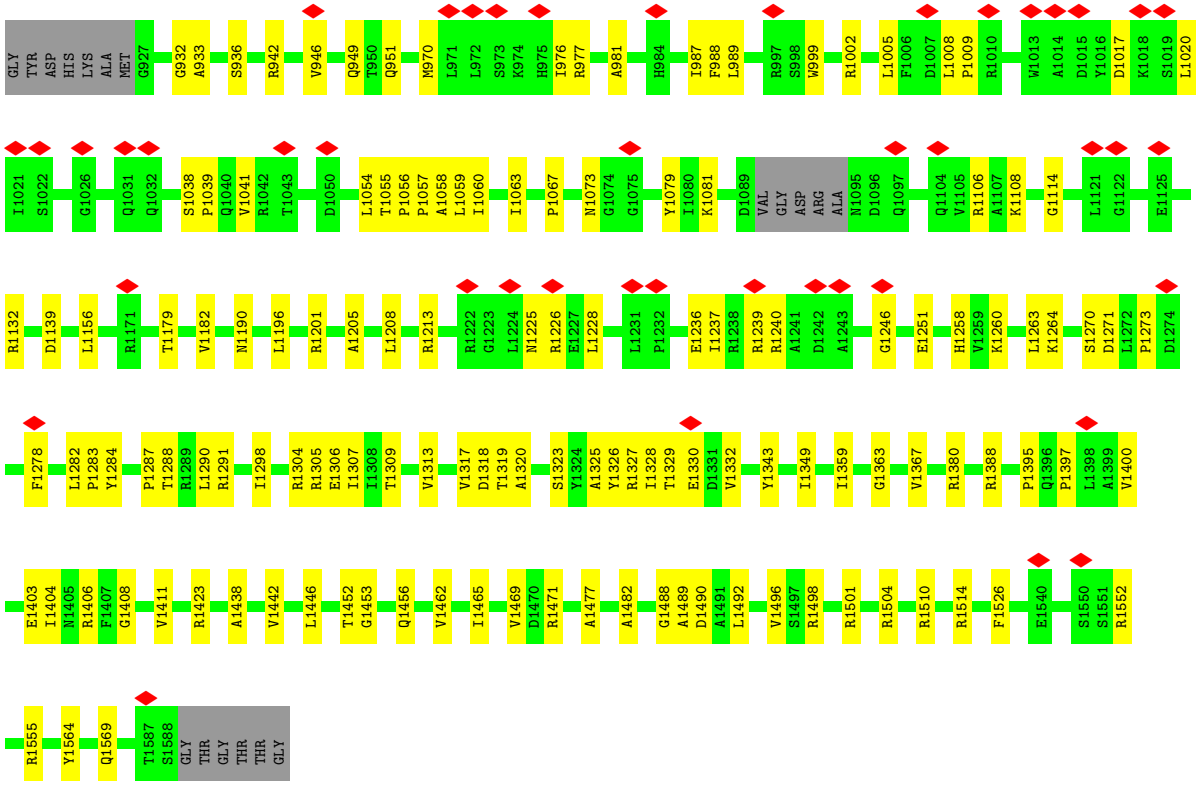
3 Residue-property plots (i)

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: NAD-specific glutamate dehydrogenase

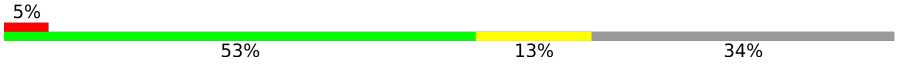
Chain A: 5% 53% 13% 34%

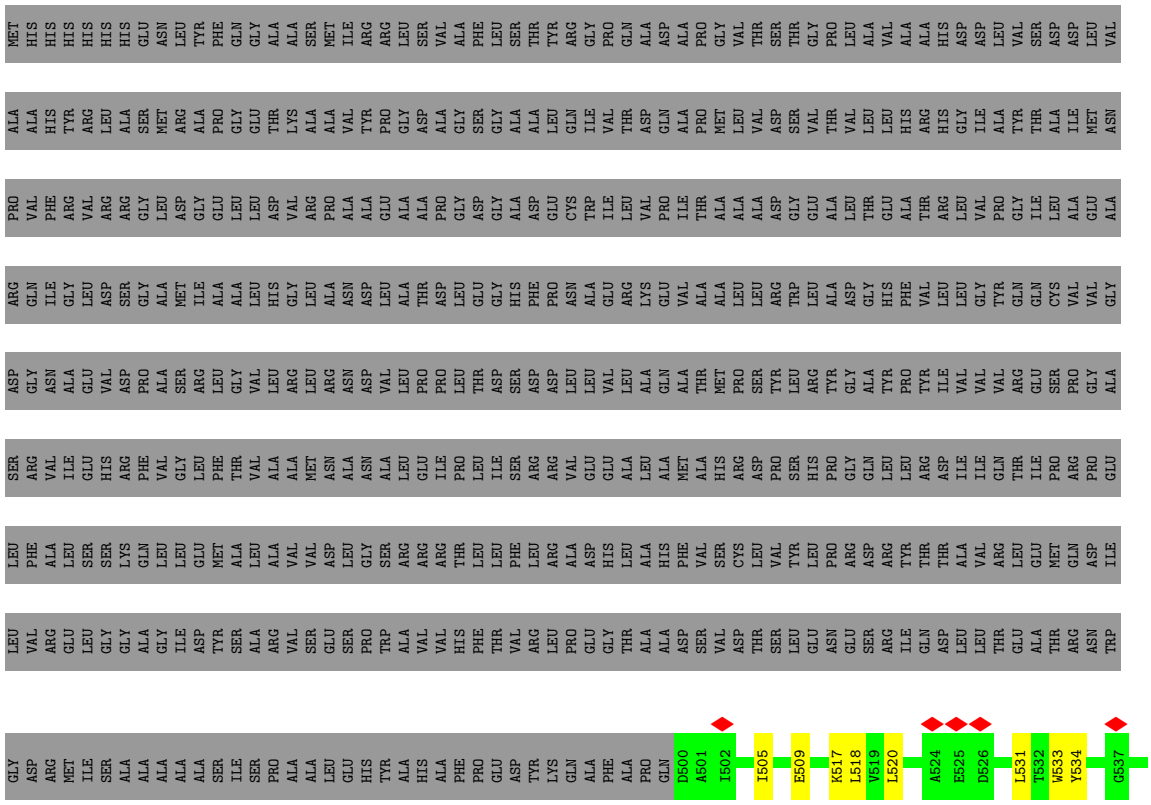


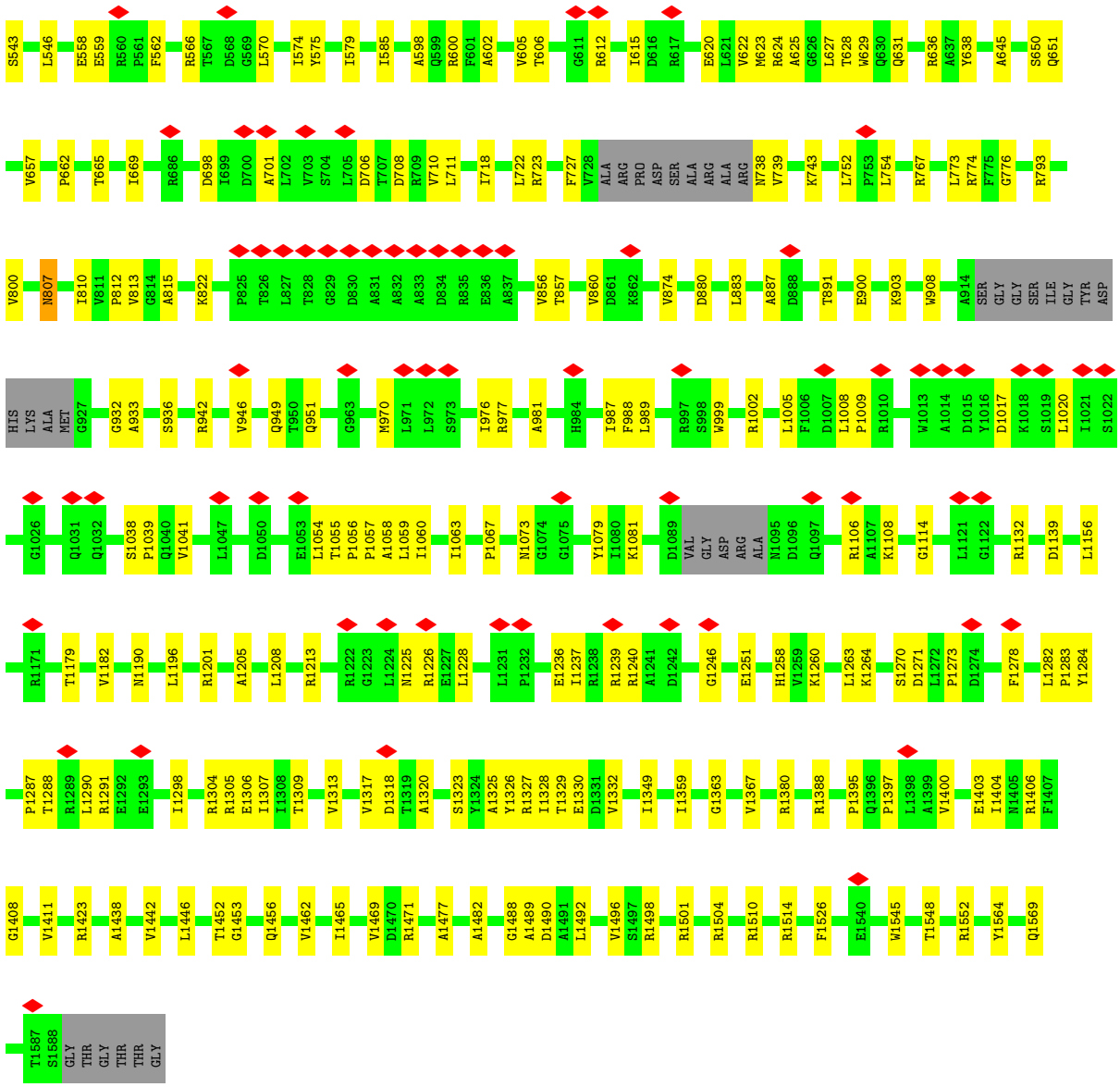


- Molecule 1: NAD-specific glutamate dehydrogenase

Chain B:

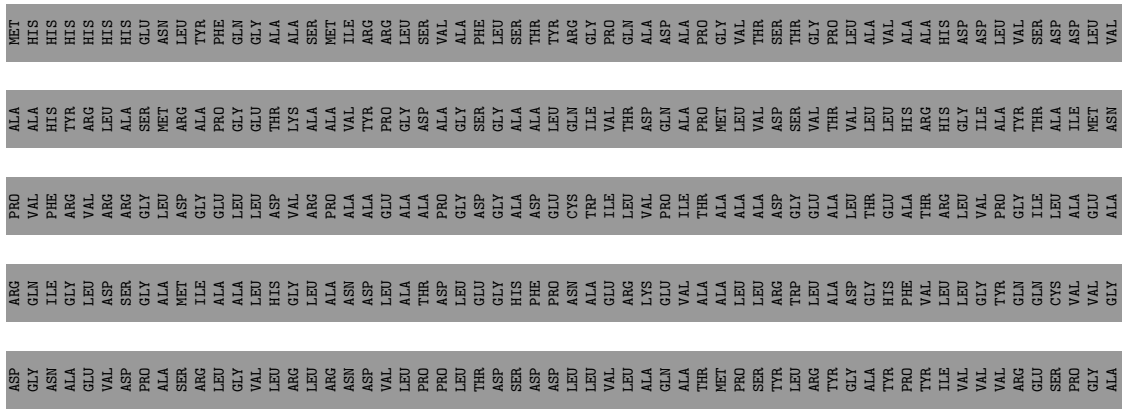


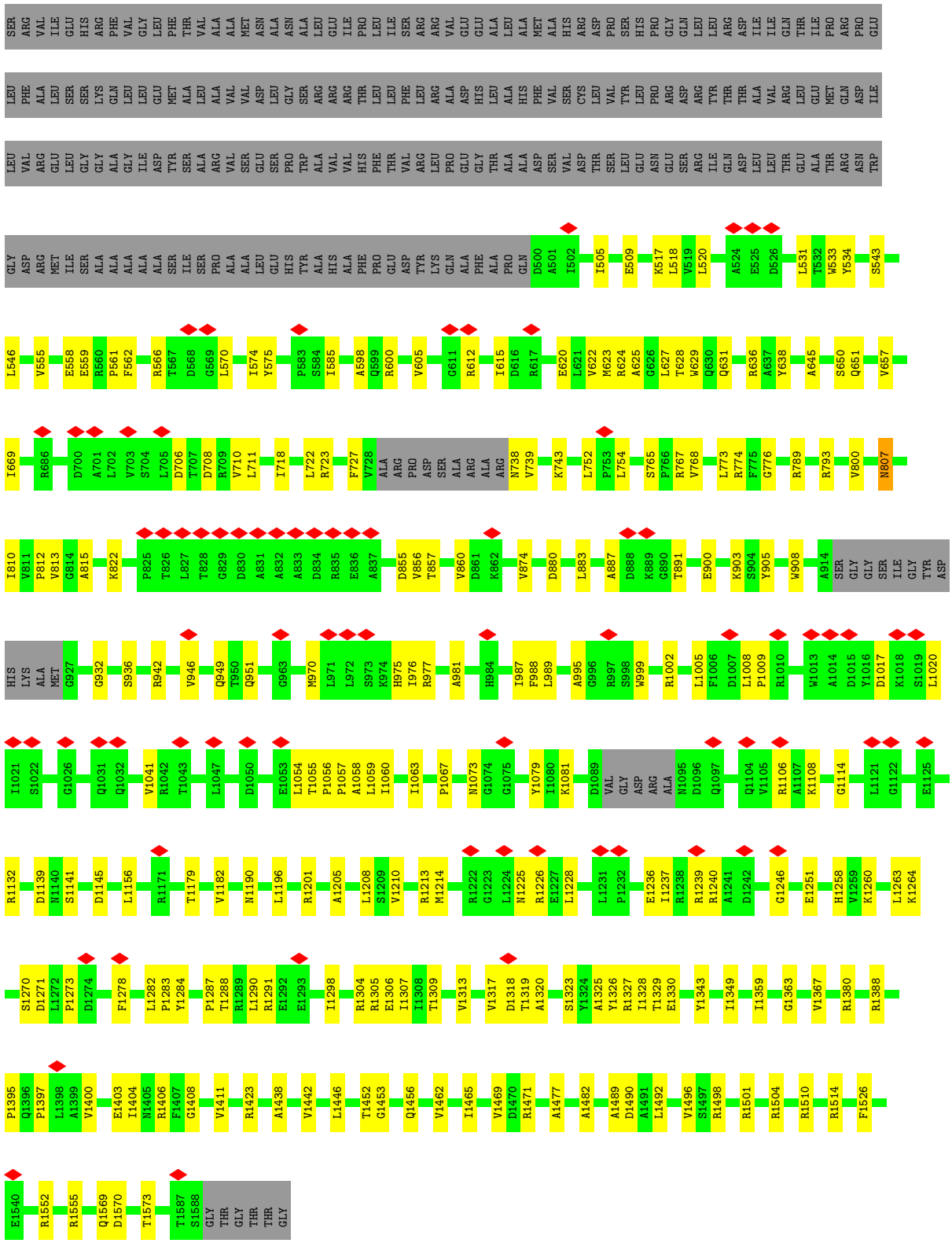




- Molecule 1: NAD-specific glutamate dehydrogenase

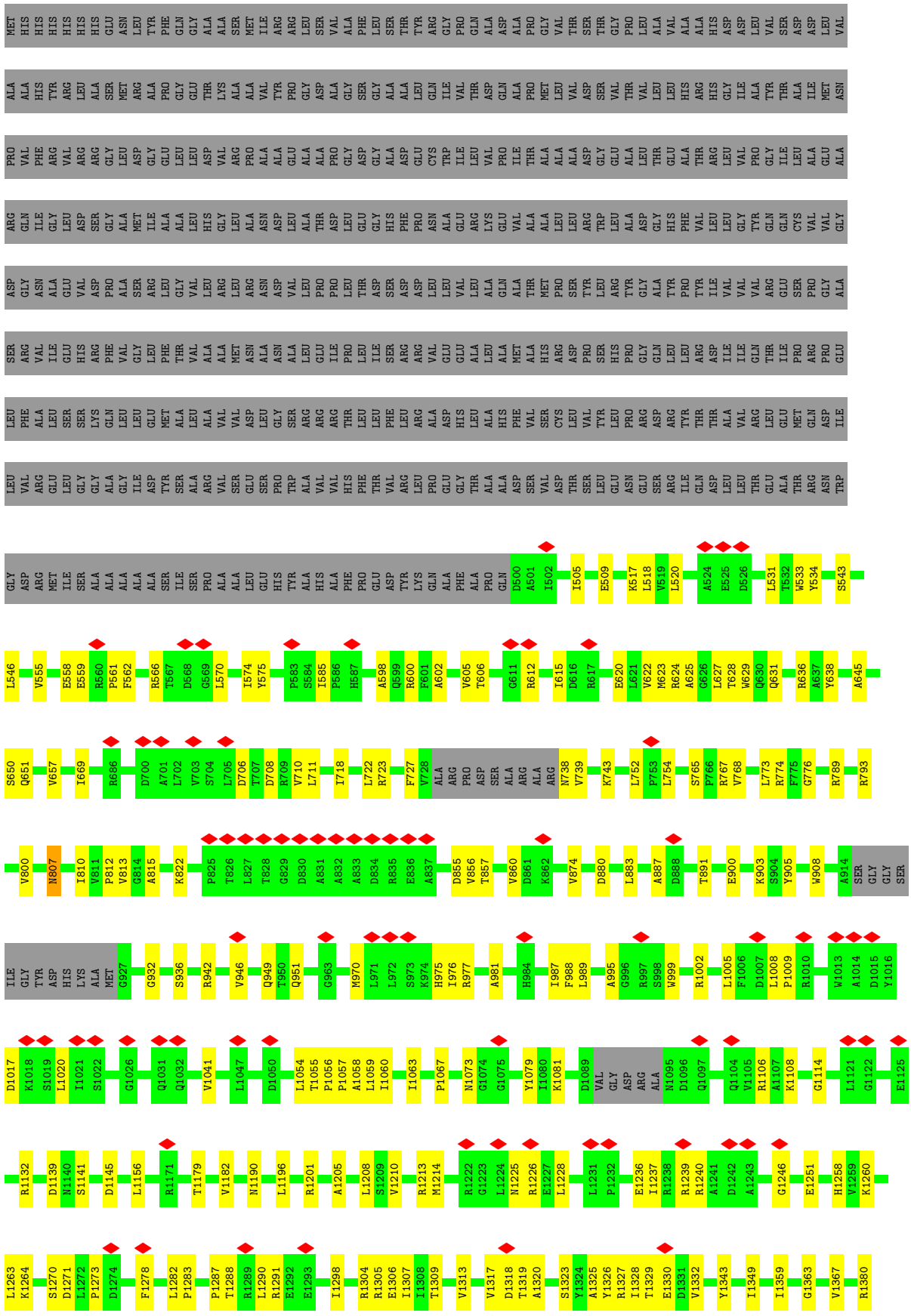
Chain C:

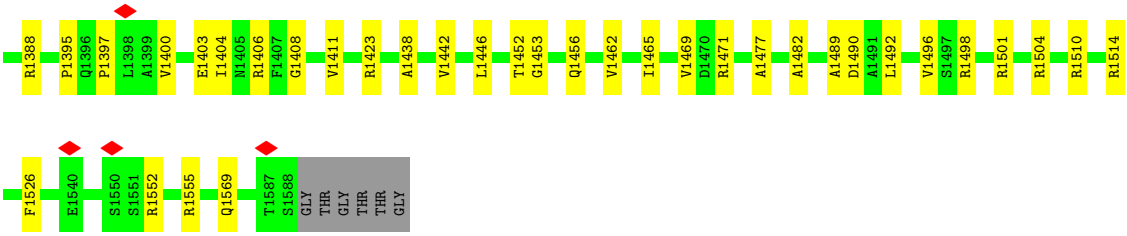




- Molecule 1: NAD-specific glutamate dehydrogenase

Chain D:


MET HIS HIS HIS HIS HIS HIS GLU ASN LEU TYR PHE GLN GLY ALA ALA SER MET ILE ARG ARG LEU SER VAL ALA PHE LEU SER THR TYR ARG GLY PRO GLN ALA ASP ALA PRO GLY VAL THR SER THR GLY PRO LEU ALA VAL ALA ALA HIS ASP ASP LEU VAL SER ASP ASP LEU VAL
ALA ALA HIS TYR ARG LEU ALA PRO GLY GLU THR LYS ALA ALA VAL TYR PRO GLY ASP ALA GLY SER GLY ALA ALA LEU GLN ILE VAL THR ASP GLN ALA PRO MET LEU VAL ASP SER VAL THR GLU ALA THR ARG HIS GLY ILE ALA TYR THR ALA LEU LEU HIS ARG HIS ILE ALA MET ASN
PRO VAL PHE ARG VAL ARG ARG GLY LEU ASP GLY GLU LEU LEU ASP VAL ARG PRO ALA ALA GLU ALA ALA PRO GLY ASP GLY ALA ASP GLU CYS TRP ILE LEU VAL PRO ILE THR ALA ALA ALA ASP GLY GLU ALA LEU THR GLY LEU LEU VAL VAL PRO GLY ILE LEU ALA GLU GLU ALA
ARG GLN ILE GLY LEU ASP SER GLY ALA MET ILE ALA ALA LEU HIS GLY LEU ALA ASN ASP LEU ALA THR ASP LEU GLU GLY HIS PHE PRO ASN ALA GLU ARG LYS GLU VAL ALA ALA LEU LEU ARG TRP LEU ALA ARG ASP GLY TYR GLN GLN CYS VAL VAL GLY
ASP GLY ASN ALA GLU VAL ASP PRO ALA SER ARG LEU GLY VAL LEU ARG LEU ARG ASN ASP VAL LEU PRO PRO LEU THR ASP SER ASP ASP LEU LEU VAL LEU ALA GLN ALA THR MET PRO SER TYR LEU ARG TYR GLY ALA TYR PRO TYR ILE VAL VAL VAL ARG GLU SER PRO GLY ALA
SER ARG VAL ILE GLU HIS ARG PHE VAL GLY LEU PHE THR VAL ALA ALA MET ASN ALA ASN ALA LEU LEU ILE PRO LEU ILE SER ALA LEU GLU ILE PRO LEU GLU GLU ALA MET ALA HIS ARG ASP PRO SER HIS PRO GLY ALA ILE ILE GLN THR ILE PRO ARG PRO GLU
LEU PHE ALA LEU SER SER LYS GLN LEU LEU GLU MET ALA LEU ALA VAL VAL ASP LEU GLY SER ARG ARG ARG THR LEU PHE LEU ARG ALA ASP HIS LEU ALA HIS PHE VAL SER CYS LEU VAL TYR LEU PRO ARG ASP ARG TYR THR THR ALA ALA LEU GLU LEU ALA ILE
LEU VAL ARG GLU LEU GLY GLY ALA GLY ILE ASP TYR SER ALA ARG VAL SER GLU SER PRO TRP ALA VAL VAL HIS PHE THR VAL ARG LEU PRO GLU GLY THR ALA ALA ASP SER VAL ASP THR SER LEU GLU ASN GLU SER ARG ILE GLN ASP LEU LEU THR GLU ALA THR ARG ASN TRP
GLY ASP ARG MET ILE SER ALA ALA ALA ALA SER ILE SER PRO ALA ALA LEU GLU HIS TYR ALA HIS ALA PHE PRO GLU ASP TYR LYS GLN ALA PHE ALA PRO GLN D500 A501 I502 I505 E509 K517 L518 V519 L520 A524 E525 D526 L531 T532 W533 Y534 S543
L546 V555 E558 E559 R560 P561 F562 R566 T567 D568 G569 L570 I574 Y575 P583 S584 I585 P586 H587 A598 Q599 R600 F601 A602 V605 T606 G611 R612 I615 D616 R617 E620 L621 V622 M623 R624 A625 G626 L627 T628 W629 Q630 Q631 R636 A637 Y638 A645
S650 Q651 V657 I669 R686 D700 A701 L702 V703 S704 L705 D706 T707 D708 R709 V710 L711 I718 L722 R723 F727 V728 ALA ARG PRO ASP SER ALA ARG ALA ARG N738 V739 K743 L752 P753 L754 S765 P766 R767 V768 L773 R774 F775 G776 R789 R793
V800 N807 I810 V811 P812 V813 G814 A815 K822 P825 T826 L827 T828 G829 D830 A831 A832 A833 D834 R835 E836 A837 D855 V856 T857 V860 D861 K862 V874 D880 L883 A887 D888 T891 E900 K903 S904 Y905 W908 A914 SER GLY GLY SER
ILE GLY TYR ASP HIS LYS ALA MET G927 G932 S936 R942 V946 Q949 T950 Q951 G963 M970 L971 L972 S973 K974 H975 I976 R977 A981 H984 I987 F988 L989 A995 G996 R997 S998 W999 R1002 L1005 F1006 D1007 L1008 P1009 R1010 W1013 A1014 D1015 Y1016
D1017 K1018 S1019 L1020 I1021 S1022 G1026 Q1031 Q1032 V1041 L1047 D1050 L1054 T1055 P1056 P1057 A1058 L1059 I1060 I1063 P1067 N1073 G1074 G1075 Y1079 I1080 K1081 D1089 VAL GLY ASP ARG ALA N1095 D1096 Q1097 Q1104 V1105 R1106 A1107 K1108 G1114 L1121 G1122 E1125
R1132 D1139 N1140 S1141 D1145 L1156 R1171 T1179 V1182 N1190 L1196 R1201 A1205 L1208 S1209 V1210 R1213 M1214 R1222 G1223 L1224 N1225 R1226 E1227 L1228 L1231 P1232 E1236 I1237 R1238 R1239 R1240 A1241 D1242 A1243 G1246 E1251 H1258 V1259 K1260
L1263 K1264 S1270 D1271 L1272 P1273 D1274 F1278 L1282 P1283 P1287 T1288 R1289 L1290 R1291 E1292 E1293 I1298 R1304 R1305 E1306 I1307 I1308 T1309 V1313 V1317 D1318 T1319 A1320 S1323 Y1324 A1325 Y1326 R1327 I1328 T1329 E1330 D1331 V1332 Y1343 I1349 I1359 G1363 V1367 R1380


R1388
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Q1396
P1397
L1398
A1399
V1400
E1403
I1404
N1405
R1406
F1407
G1408
V1411
R1423
A1438
V1442
L1446
T1452
G1453
Q1456
V1462
I1465
V1469
D1470
R1471
A1477
A1482
A1489
D1490
A1491
L1492
V1496
S1497
R1498
R1501
R1504
R1510
R1514
F1526
E1540
S1550
S1551
R1552
R1555
Q1569
T1587
S1588
GLY
THR
GLY
THR
THR
GLY

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D2	Depositor
Number of particles used	63715	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	670	Depositor
Maximum defocus (nm)	3260	Depositor
Magnification	47170	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.050	Depositor
Minimum map value	-0.024	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0104	Depositor
Map size (Å)	402.8, 402.8, 402.8	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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	A	0.33	0/8406	0.60	0/11414
1	B	0.33	0/8406	0.60	0/11414
1	C	0.33	0/8406	0.60	0/11414
1	D	0.33	0/8406	0.60	0/11414
All	All	0.33	0/33624	0.60	0/45656

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8258	0	8207	133	0
1	B	8258	0	8207	132	0
1	C	8258	0	8207	133	0
1	D	8258	0	8207	133	0
All	All	33032	0	32828	510	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 8.

The worst 5 of 510 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:546:LEU:HD13	1:D:546:LEU:HD13	1.74	0.69
1:B:1306:GLU:O	1:B:1309:THR:HB	1.93	0.69
1:A:1306:GLU:O	1:A:1309:THR:HB	1.93	0.69
1:D:1306:GLU:O	1:D:1309:THR:HB	1.93	0.68
1:C:1306:GLU:O	1:C:1309:THR:HB	1.93	0.68

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	1055/1611 (66%)	967 (92%)	88 (8%)	0	100	100
1	B	1055/1611 (66%)	967 (92%)	88 (8%)	0	100	100
1	C	1055/1611 (66%)	966 (92%)	89 (8%)	0	100	100
1	D	1055/1611 (66%)	967 (92%)	88 (8%)	0	100	100
All	All	4220/6444 (66%)	3867 (92%)	353 (8%)	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	869/1294 (67%)	868 (100%)	1 (0%)	93	97
1	B	869/1294 (67%)	868 (100%)	1 (0%)	93	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	869/1294 (67%)	868 (100%)	1 (0%)	93	97
1	D	869/1294 (67%)	868 (100%)	1 (0%)	93	97
All	All	3476/5176 (67%)	3472 (100%)	4 (0%)	93	97

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	807	ASN
1	B	807	ASN
1	C	807	ASN
1	D	807	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	1097	GLN
1	D	807	ASN
1	C	807	ASN
1	B	1097	GLN
1	C	1097	GLN

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.

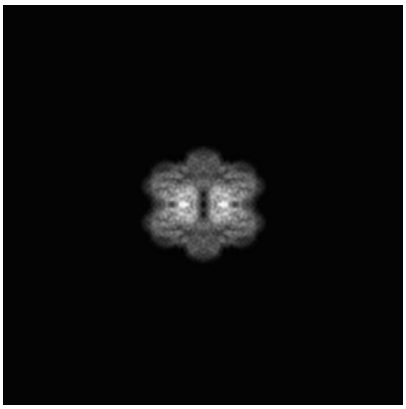
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-11606. These allow visual inspection of the internal detail of the map and identification of artifacts.

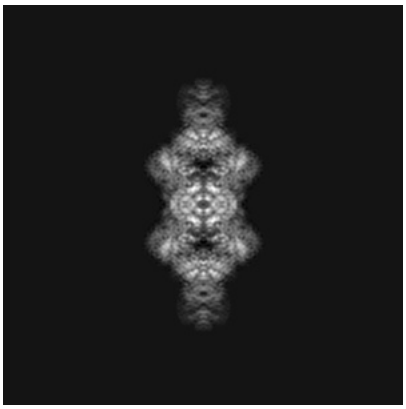
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

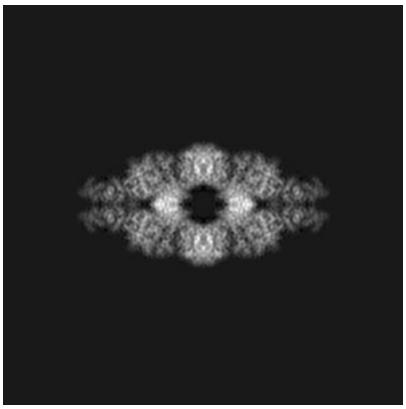
6.1.1 Primary map



X

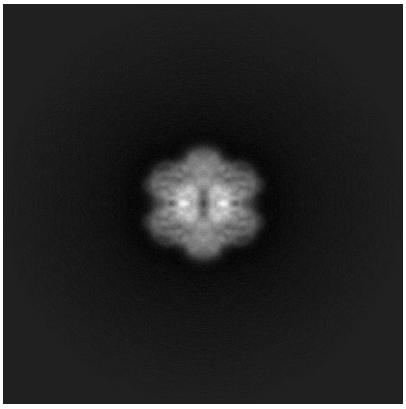


Y

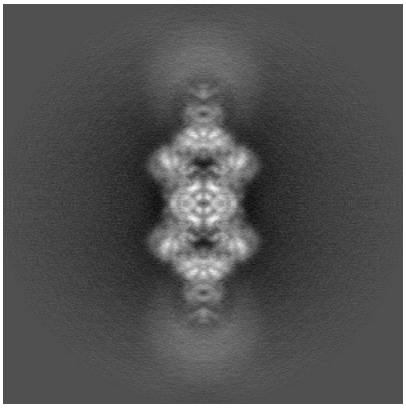


Z

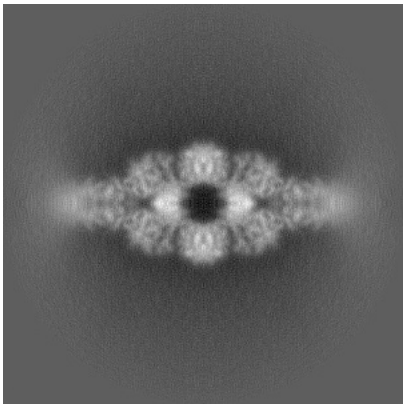
6.1.2 Raw map



X



Y

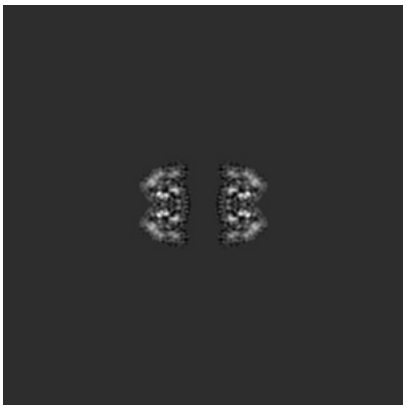


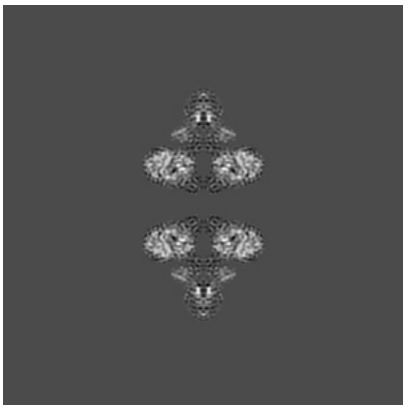
Z

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

6.2 Central slices (i)

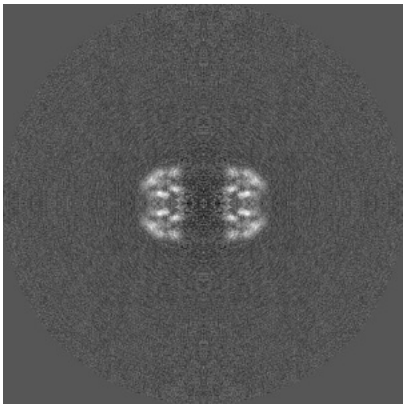
6.2.1 Primary map

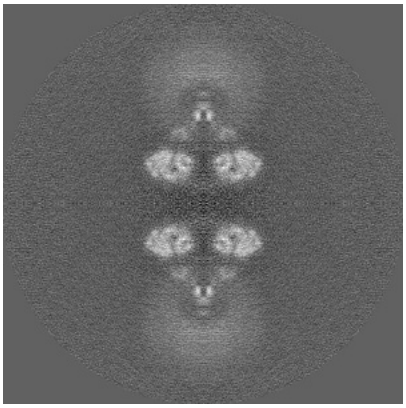

X Index: 190

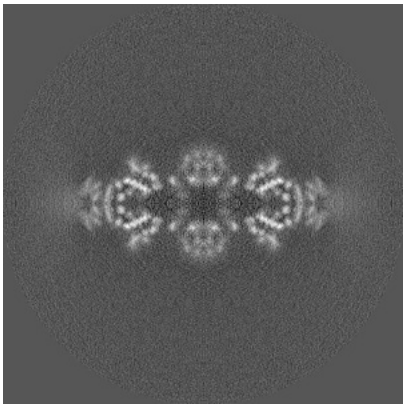

Y Index: 190

Z Index: 190

6.2.2 Raw map


X Index: 190


Y Index: 190

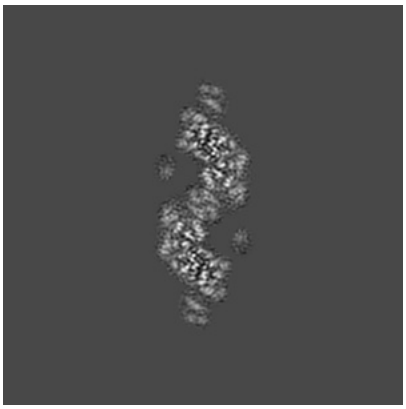

Z Index: 190

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

6.3 Largest variance slices (i)

6.3.1 Primary map

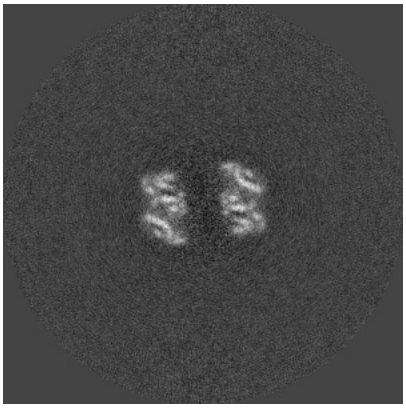
X Index: 185



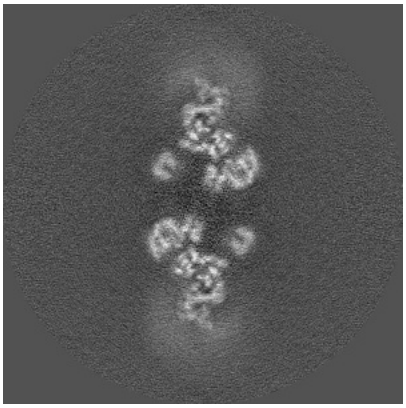
Y Index: 210

Z Index: 200

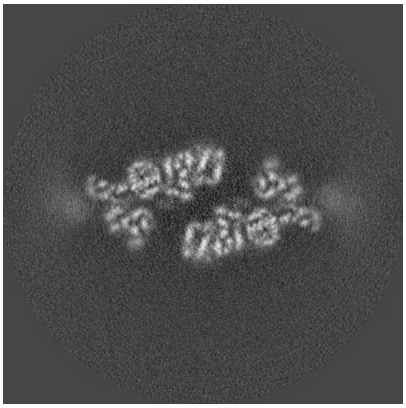
6.3.2 Raw map



X Index: 196



Y Index: 201

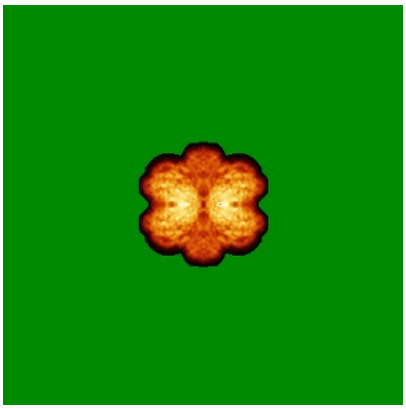


Z Index: 181

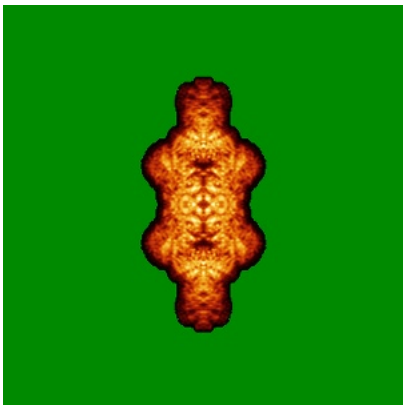
The images above show the largest variance slices of the map in three orthogonal directions.

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

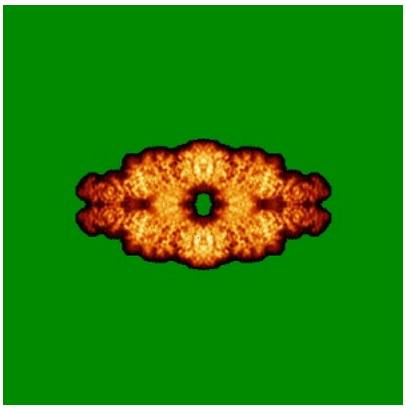
6.4.1 Primary map



X

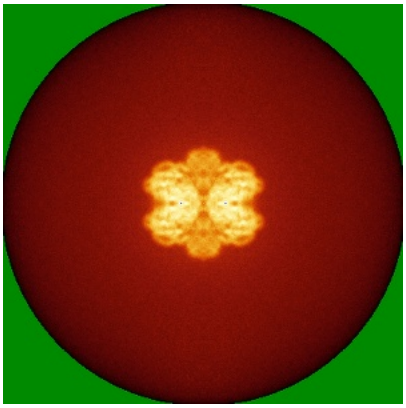


Y

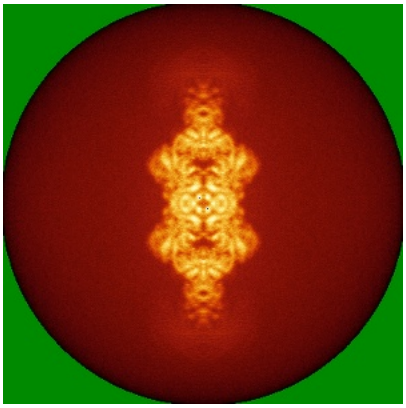


Z

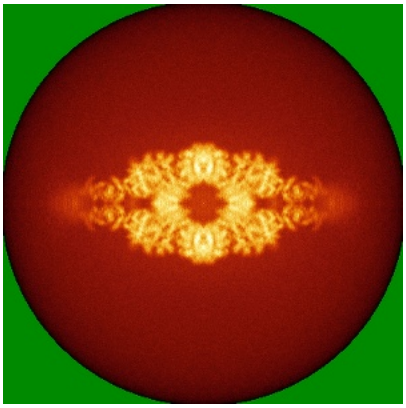
6.4.2 Raw map



X



Y

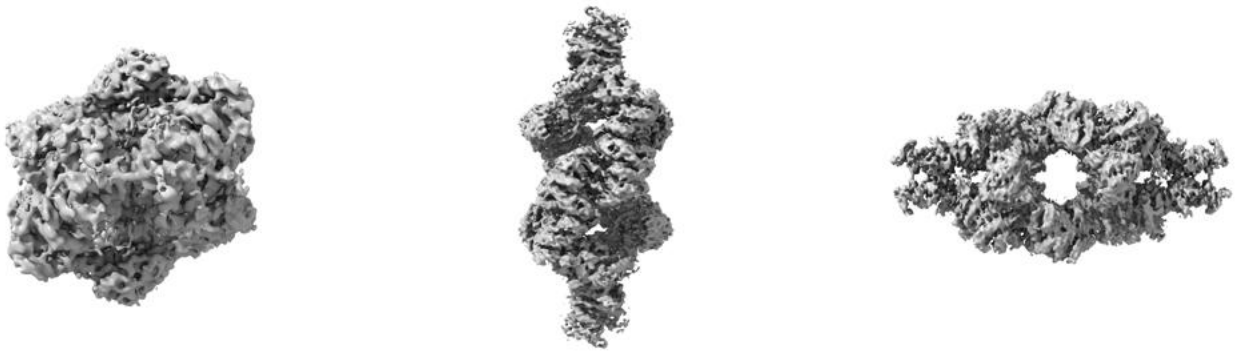


Z

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 0.0104. 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.

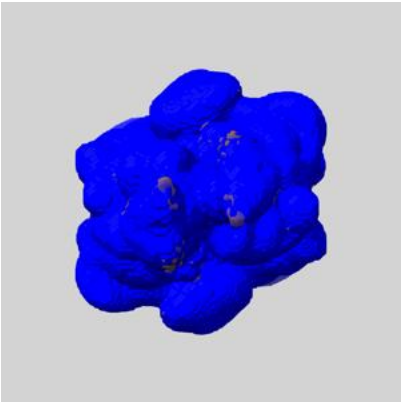
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

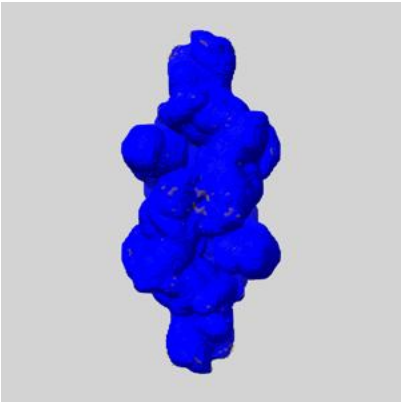
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

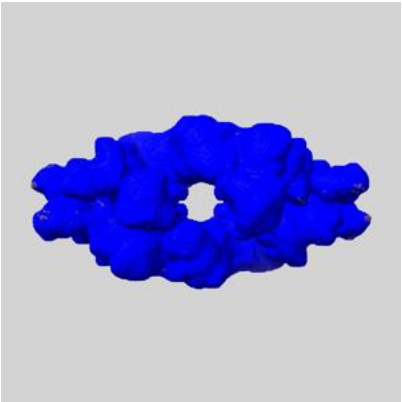
6.6.1 emd_11606_msk_1.map (i)



X



Y

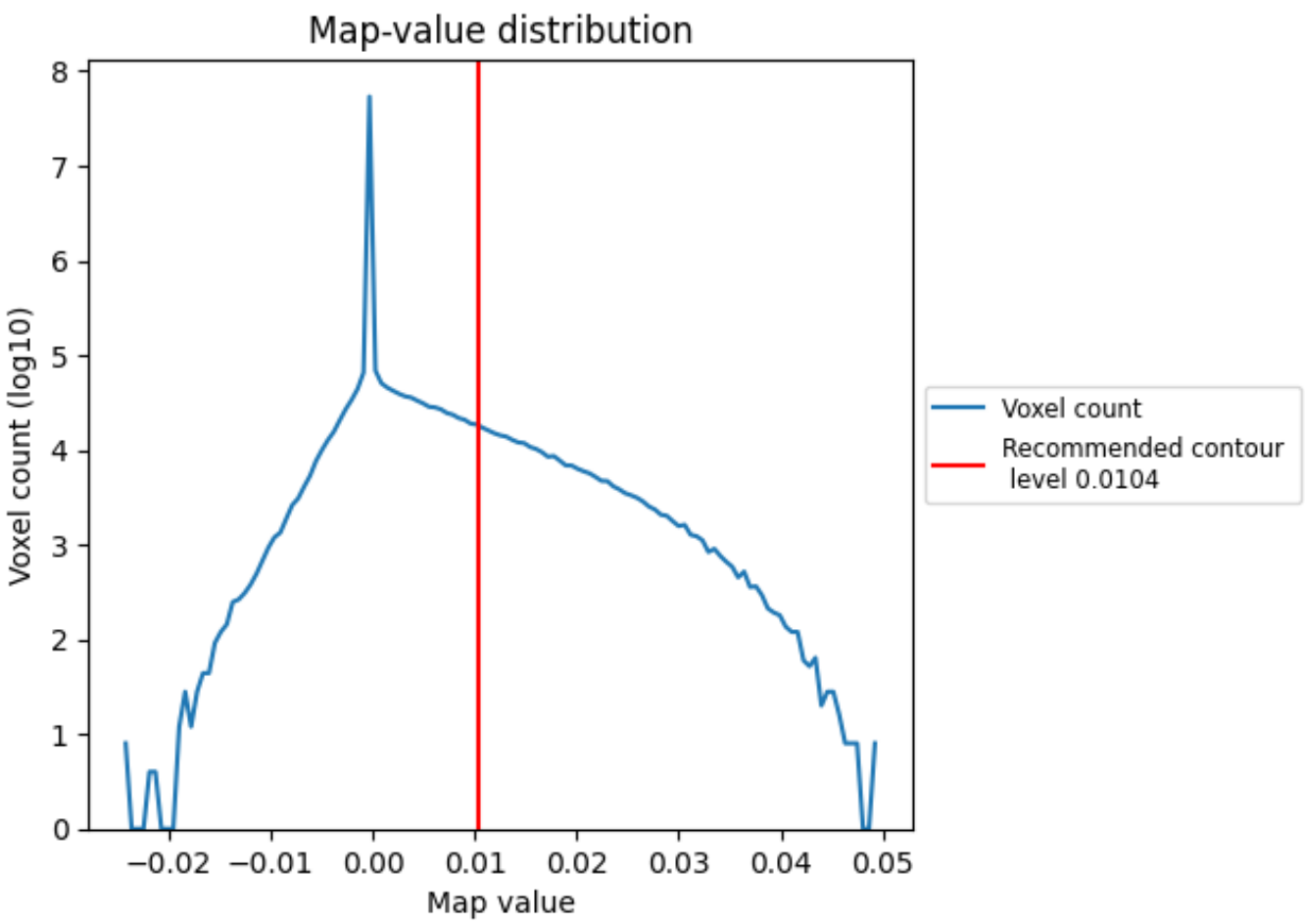


Z

7 Map analysis (i)

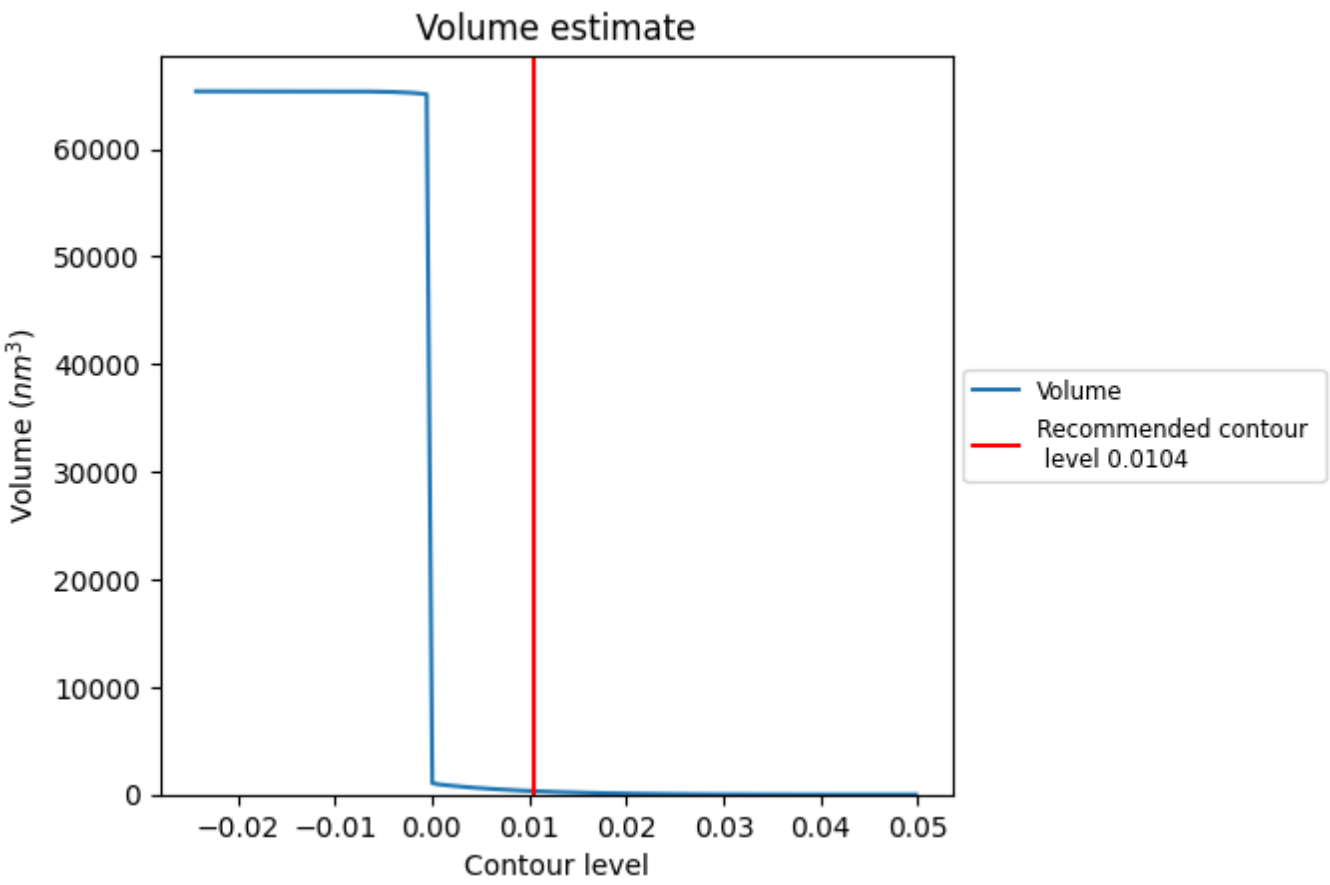
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

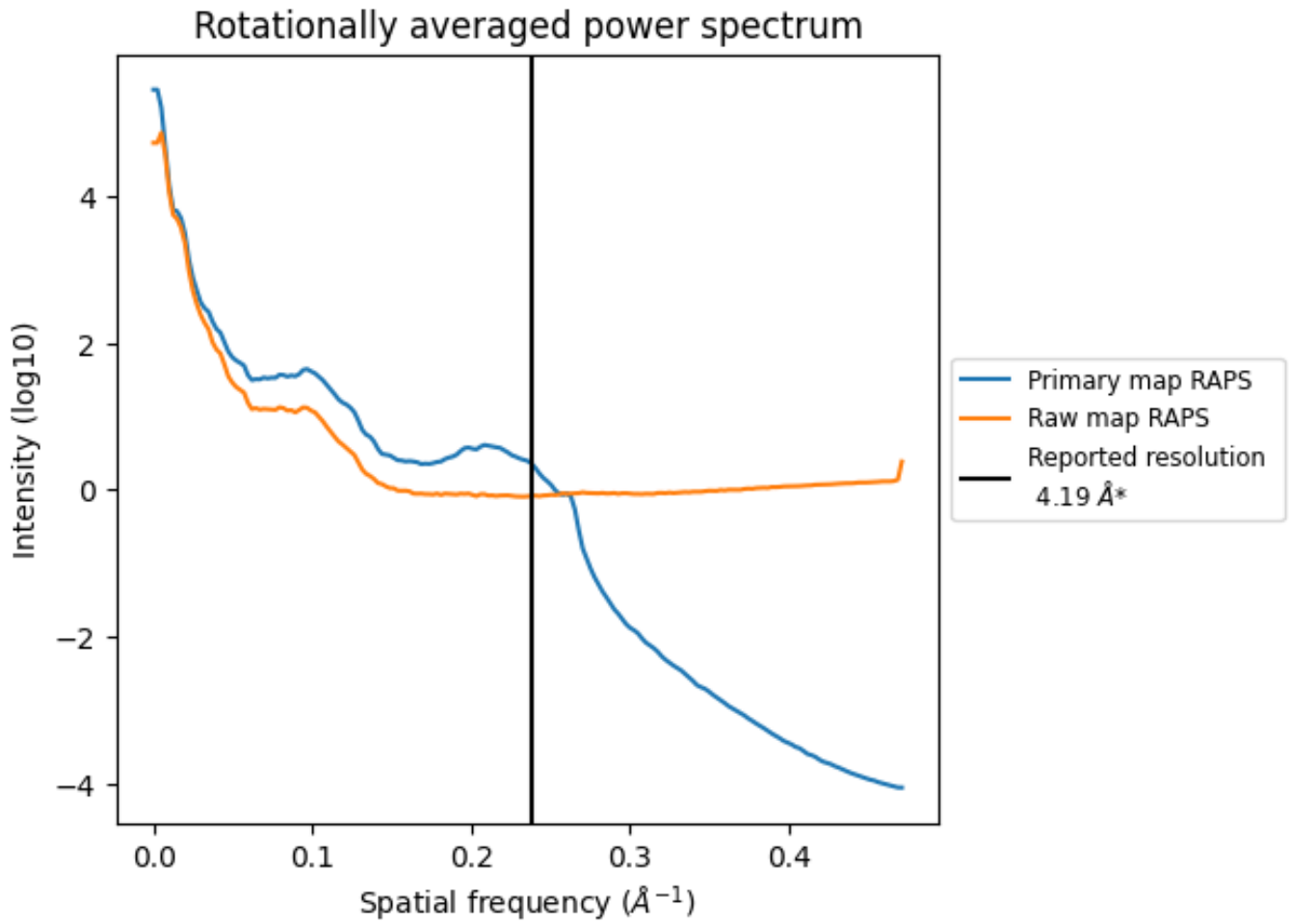
7.2 Volume estimate (i)



The volume at the recommended contour level is 322 nm^3; this corresponds to an approximate mass of 291 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)

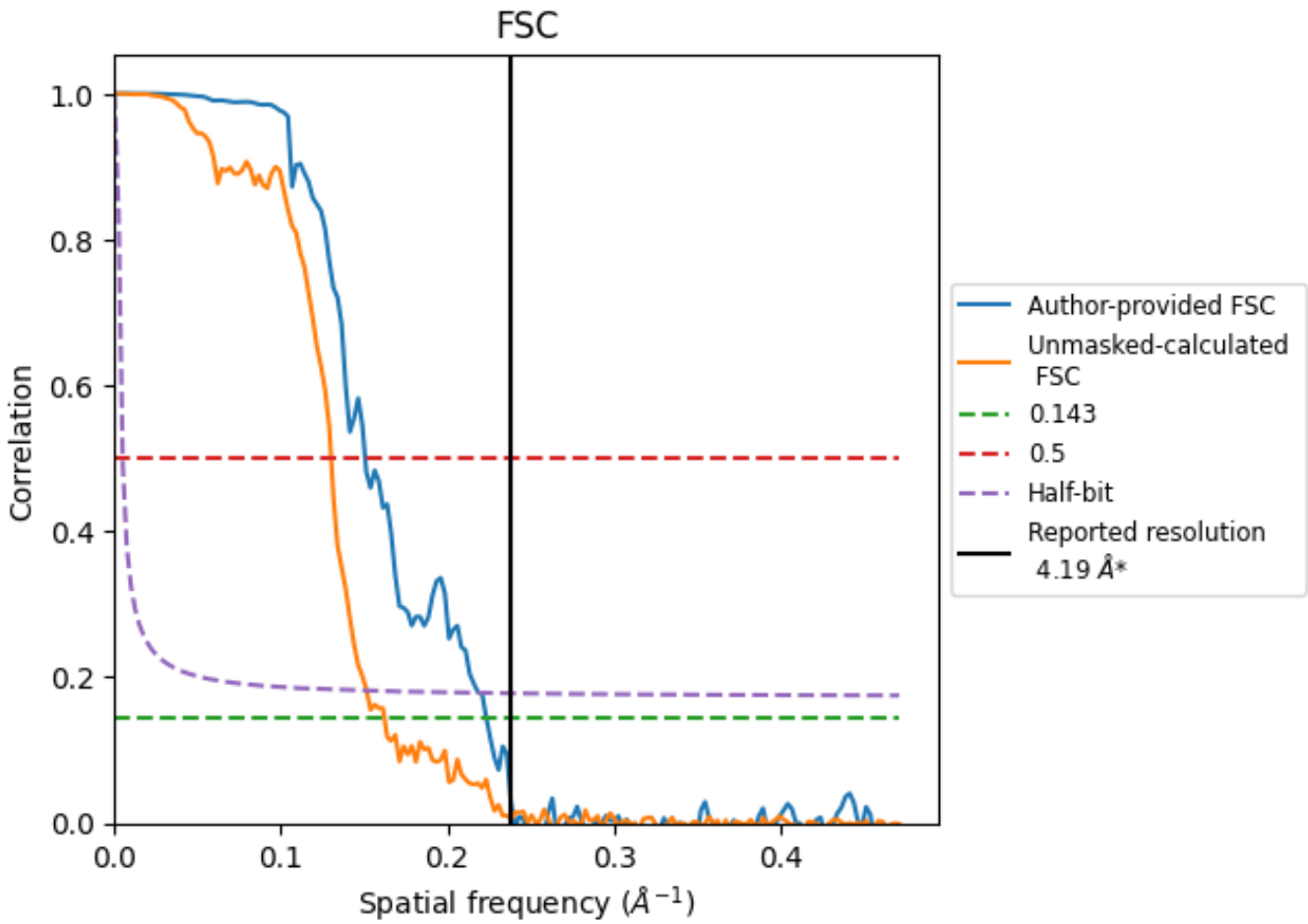


*Reported resolution corresponds to spatial frequency of 0.239 Å^{-1}

8 Fourier-Shell correlation (i)

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 (i)



*Reported resolution corresponds to spatial frequency of 0.239 Å^{-1}

8.2 Resolution estimates (i)

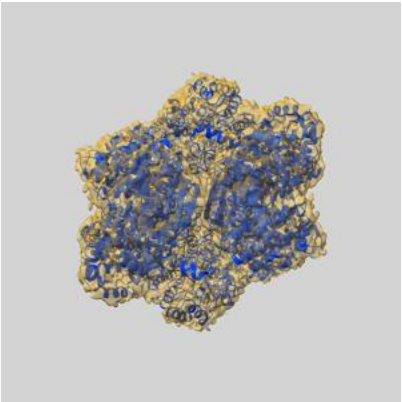
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.19	-	-
Author-provided FSC curve	4.47	6.64	4.56
Unmasked-calculated*	6.16	7.68	6.60

*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 6.16 differs from the reported value 4.19 by more than 10 %

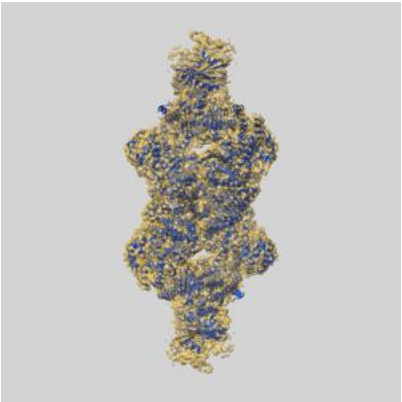
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-11606 and PDB model 7A1D. Per-residue inclusion information can be found in section 3 on page 6.

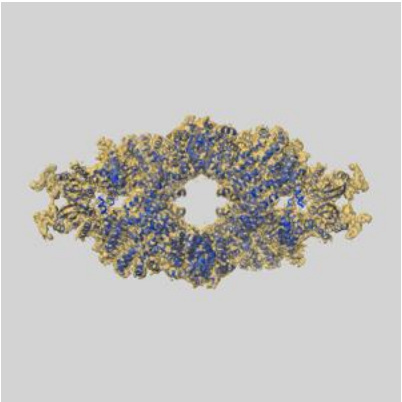
9.1 Map-model overlay (i)



X



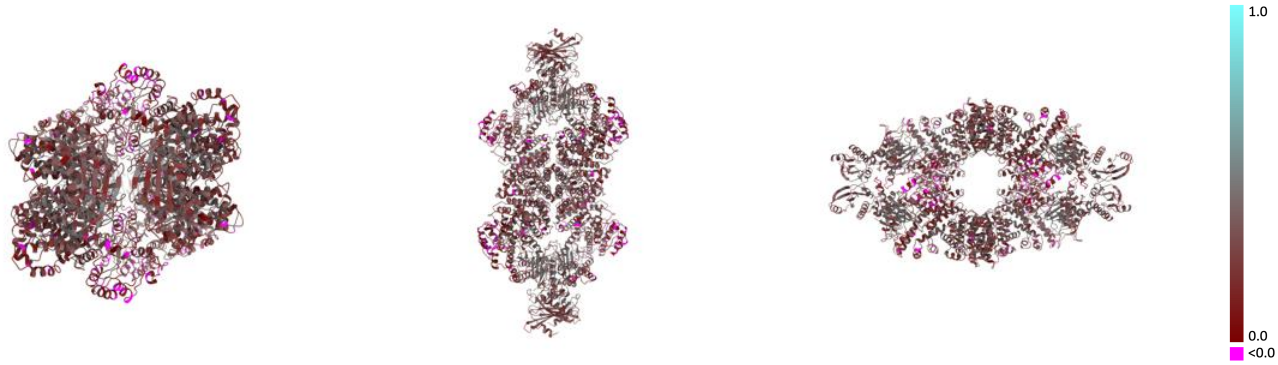
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0104 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.

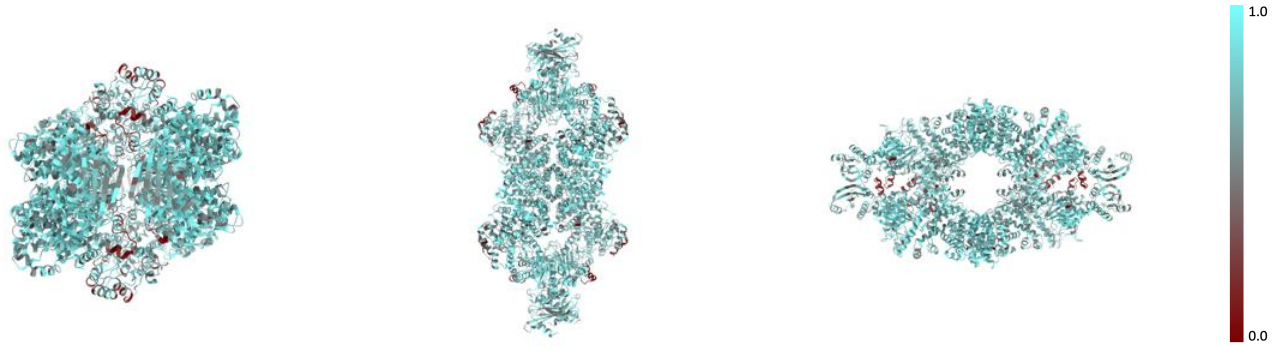
9.2 Q-score mapped to coordinate model (i)



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.

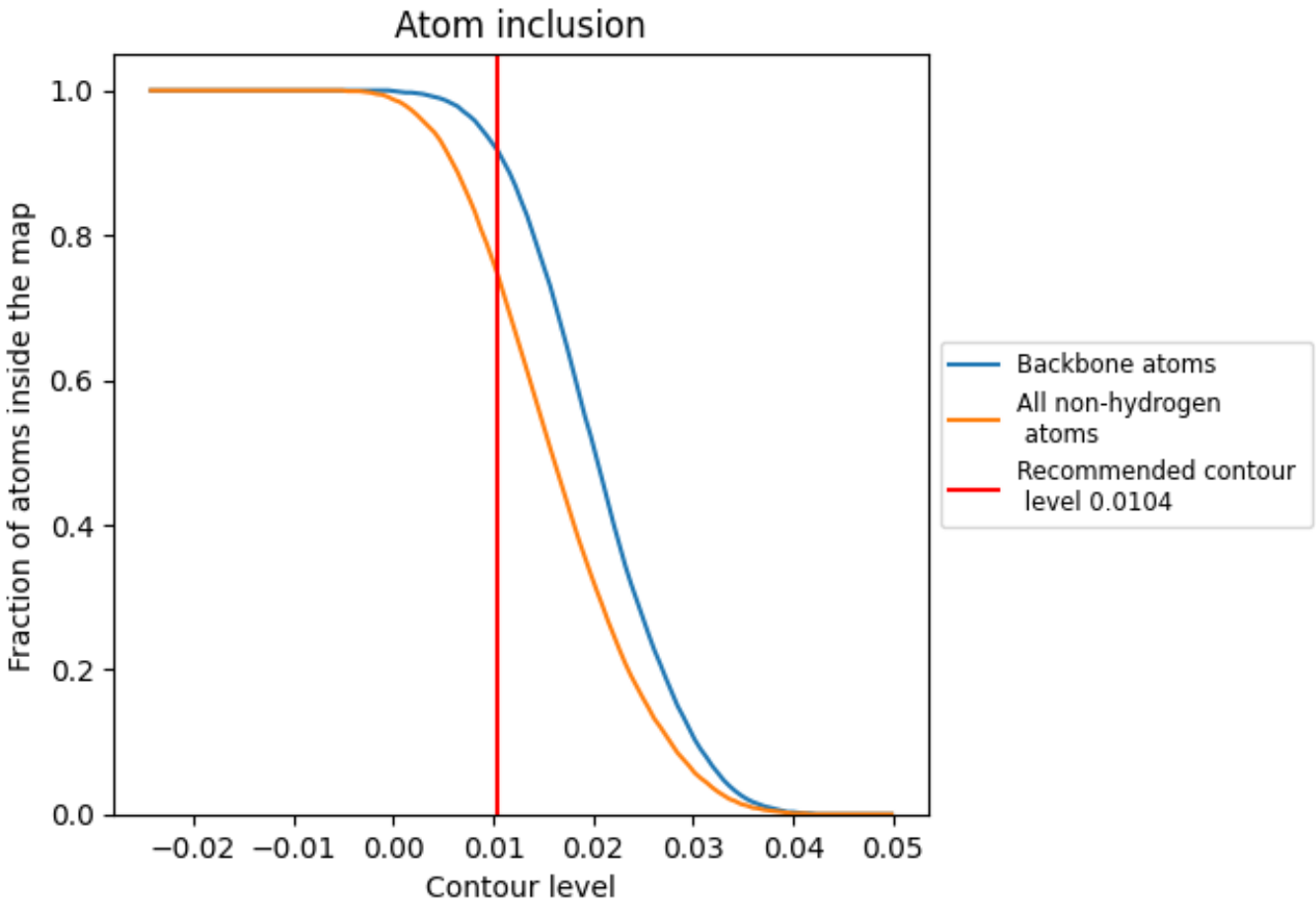
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0104).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0104) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7470	0.2810
A	0.7460	0.2810
B	0.7480	0.2790
C	0.7480	0.2810
D	0.7460	0.2820