



wwPDB EM Validation Summary Report ⓘ

Apr 5, 2026 – 04:28 PM UTC

PDB ID : 9HUY / pdb_00009huy
EMDB ID : EMD-52420
Title : CryoEM map of the large glutamate dehydrogenase composed of 180 kDa subunits from Mycobacterium smegmatis obtained in the presence of NAD⁺ and L-glutamate. Closed1 tetramer.
Authors : Lazaro, M.; Chamorro, N.; Lopez-Alonso, J.P.; Charro, D.; Rasia, R.M.; Jimenez-Oses, G.; Valle, M.; Lisa, M.N.
Deposited on : 2024-12-23
Resolution : 3.54 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 ⓘ 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 ⓘ](#)) 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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

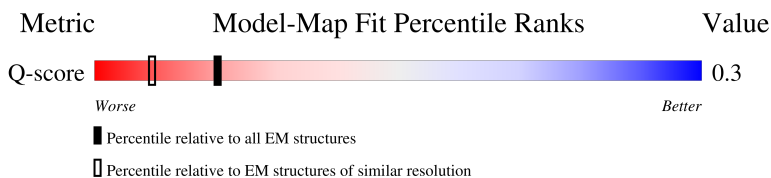
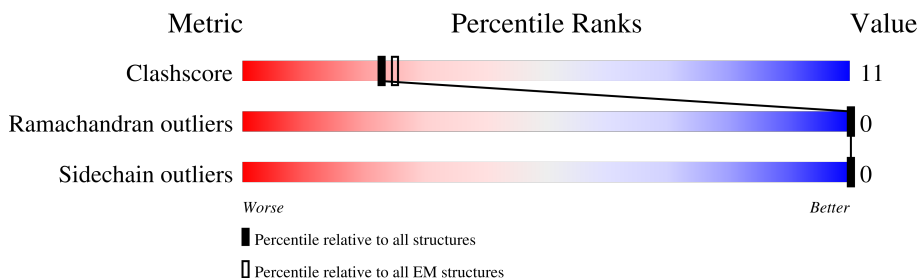
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.54 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	12891 (3.04 - 4.04)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1611	 50% 16% 33%
1	B	1611	 51% 16% 33%
1	C	1611	 51% 16% 33%

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Mol	Chain	Length	Quality of chain
1	D	1611	 51% 16% 33%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 33576 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
1	A	1075	Total	C	N	O	S	0	0
			8350	5240	1496	1594	20		
1	B	1075	Total	C	N	O	S	0	0
			8350	5240	1496	1594	20		
1	C	1075	Total	C	N	O	S	0	0
			8350	5240	1496	1594	20		
1	D	1075	Total	C	N	O	S	0	0
			8350	5240	1496	1594	20		

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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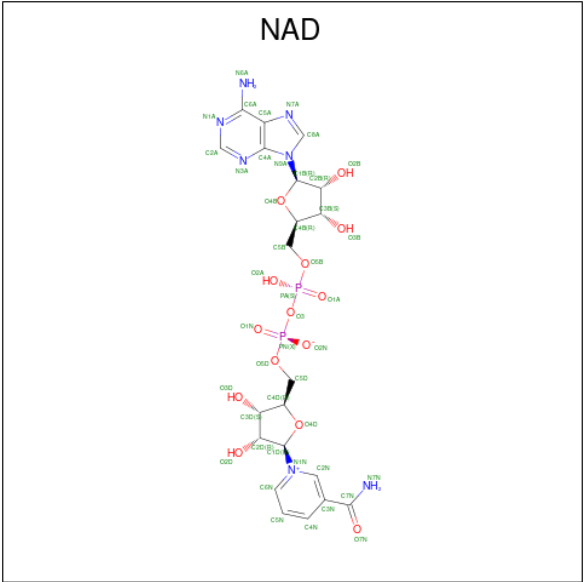
Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	HIS	-	expression tag	UNP A0R1C2
B	-10	HIS	-	expression tag	UNP A0R1C2
B	-9	GLU	-	expression tag	UNP A0R1C2
B	-8	ASN	-	expression tag	UNP A0R1C2
B	-7	LEU	-	expression tag	UNP A0R1C2
B	-6	TYR	-	expression tag	UNP A0R1C2
B	-5	PHE	-	expression tag	UNP 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

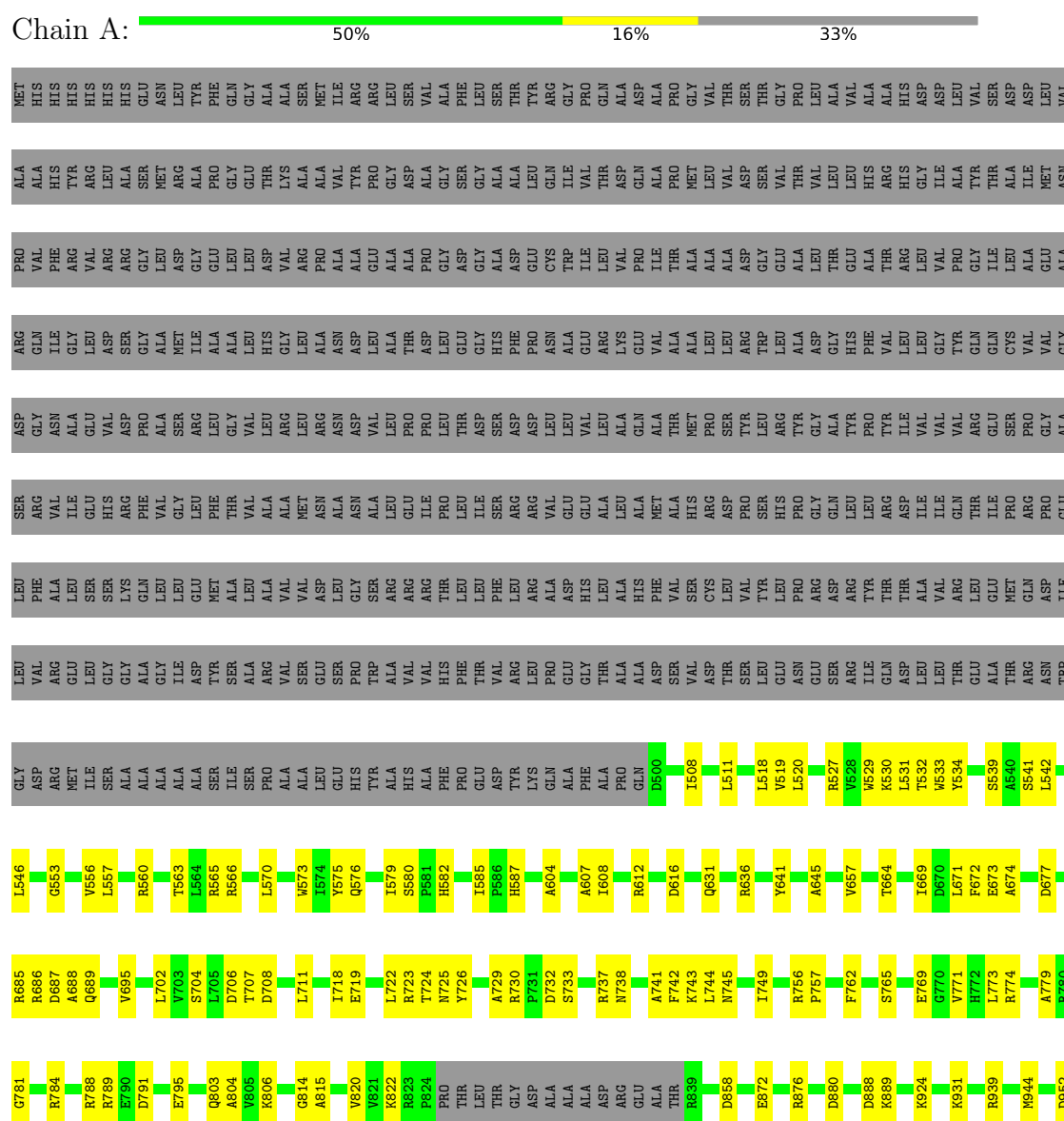
- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂) (labeled as "Ligand of Interest" by depositor).

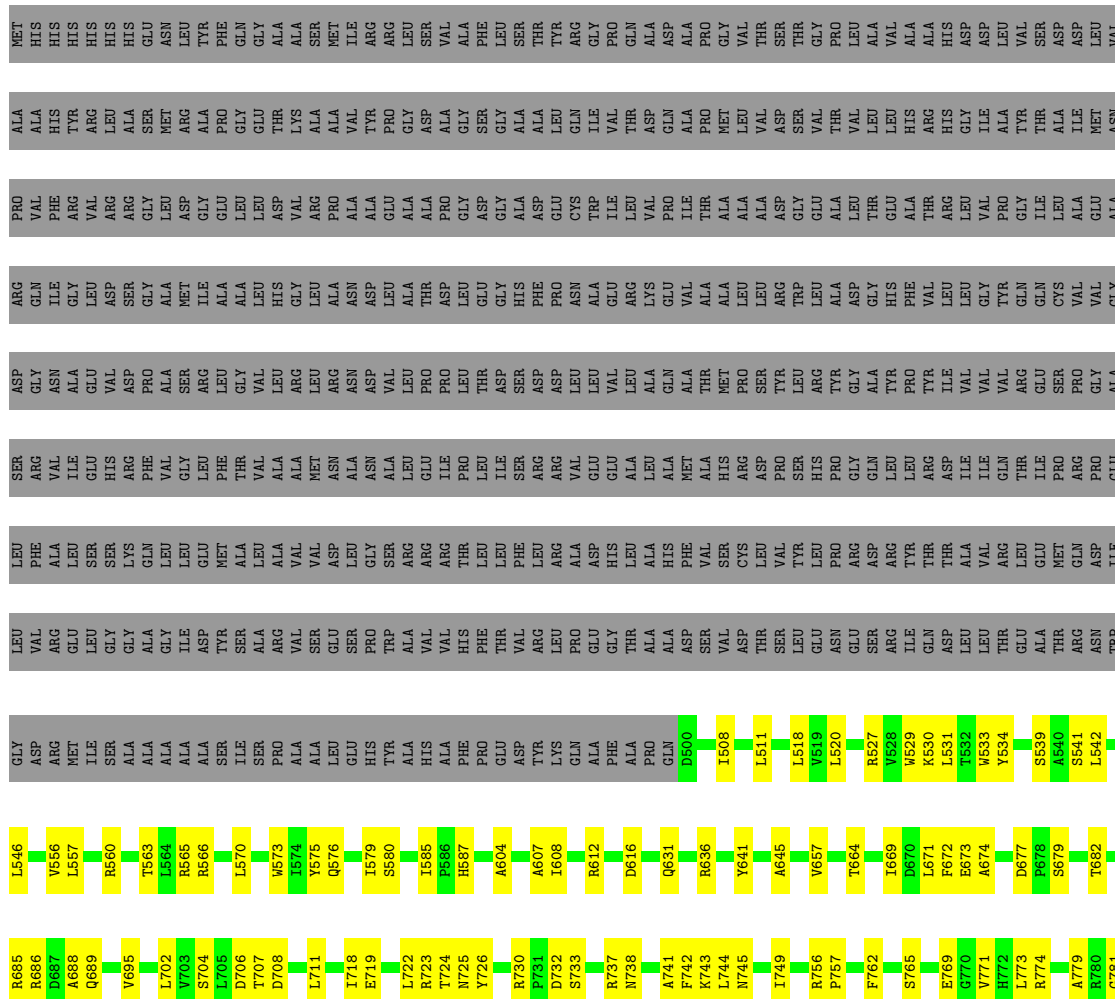


3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: NAD-specific glutamate dehydrogenase

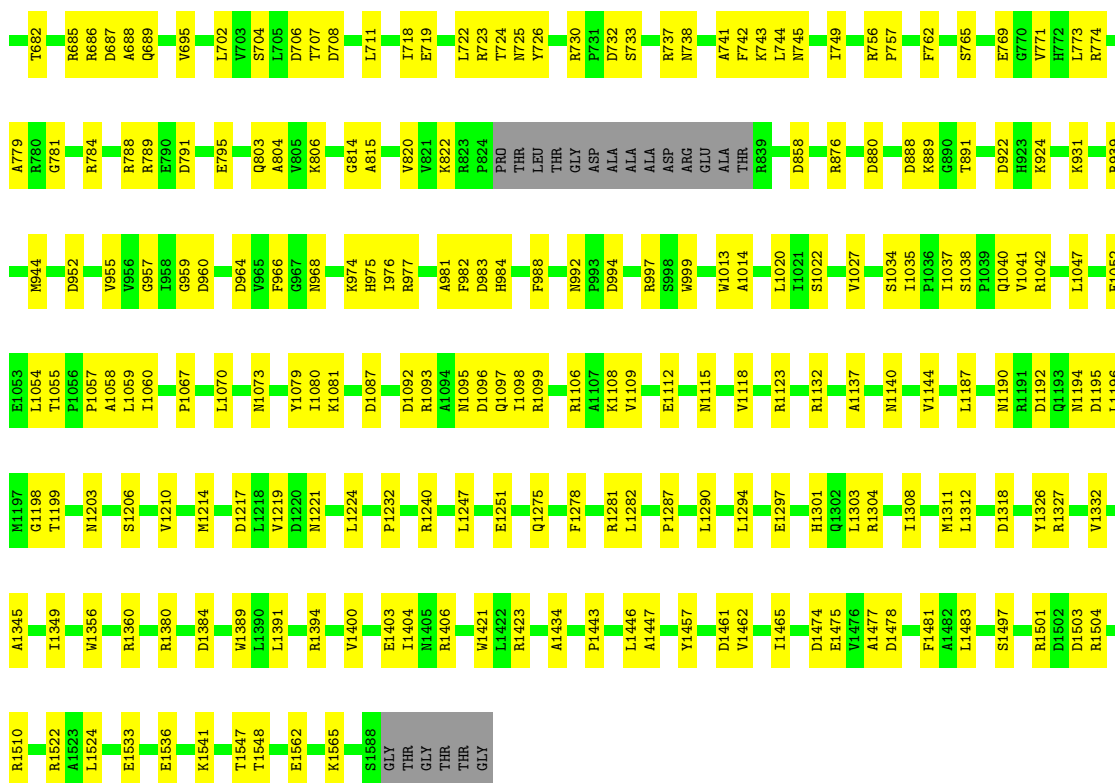




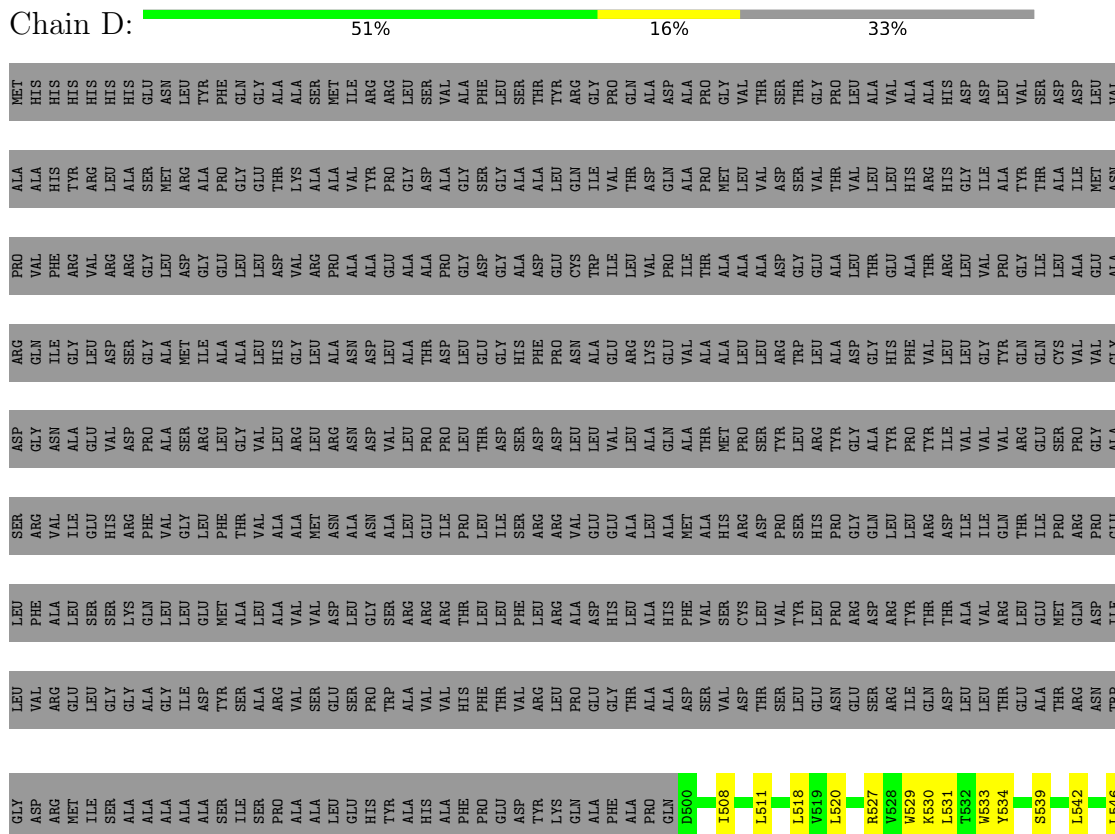


Response	Percentage
U.S. is responsible	51%
U.S. is not responsible	16%
U.S. is not responsible	33%





- Molecule 1: NAD-specific glutamate dehydrogenase



I1349	S1206	P1067	I988	R784	R886	V556
W1356	V1210	L1070	D960	R788	D687	L557
R1360	M1214	N1073	D964	R789	Q689	R560
G1363	D1217	N1073	P965	D791	V695	T563
V1367	L1218	Y1079	G967	E796	L702	L564
R1380	V1219	I1080	N968	Q803	V703	R565
E1336	D1220	K1081	K974	A804	L705	R566
W1389	M1221	D1087	H975	R805	D706	L570
L1390	L1224	D1092	R977	R796	D708	W573
T1391	M1225	R1093	A981	G814	L711	L574
T1547	R1226	A1094	F982	A815		W575
T1548	E1227	N1095	D983			Q576
R1394	L1228		H984			
V1400	P1232	I1098	F988	V820	I718	I579
A1403	R1240	R1106	N992	V821	E719	S580
I1404	L1247	A1107	P992	R823	L722	
N1405	L1247	K1108	P993	P824	R723	I585
R1406	E1251	V1109	D994	THR	T724	P586
W1421	Q1275	E1112	R997	THR	N725	H587
L1422	L1422		S998	GLY	I726	A604
R1423	F1278	N1115	W999	ASP	R730	A607
A1434	R1281	V1118	A1014	ALA	D732	I608
P1443	L1282	R1123	L1020	ARG	N738	R612
L1446	P1287	R1132	I1021	GLU	A741	Q631
A1447	L1290	A1137	S1022	THR	F742	R636
D1461	L1294	N1140	V1027		L744	
V1462	E1297	V1144	S1034	D858	N745	Y641
I1465	H1301	K1165	I1035	R876	I749	A645
D1474	Q1302	L1303	P1038	D880	R756	V657
E1475	R1304	D1180	Q1040	D888	P757	T664
A1477	I1308	L1187	V1041	K889	F762	Q669
D1478	M1311	N1190	R1042	G890	S765	L669
F1481	L1312	D1192	L1047	K924	L671	D670
A1482	D1318	Q1193	E1052	K931	E769	F672
L1483	Y1326	D1195	L1054	W644	G770	E673
M1484	V1332	L1196	T1055	D952	V771	A674
S1497	G1333	T1199	P1056	R774	H772	D677
R1501	A1345	N1203	P1057		L773	P678
D1502			A1058	D952	R774	S679
D1503			L1059	V955	A779	R780
R1504			T1060	R782	R780	T682
P1510				G781		P685

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	45998	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.053	Depositor
Minimum map value	-0.019	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	439.41602, 439.41602, 439.41602	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2924, 1.2924, 1.2924	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAD

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	0.08	0/8502	0.22	0/11541
1	B	0.08	0/8502	0.22	0/11541
1	C	0.08	0/8502	0.22	0/11541
1	D	0.08	0/8502	0.22	0/11541
All	All	0.08	0/34008	0.22	0/46164

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	8350	0	8301	193	0
1	B	8350	0	8301	189	0
1	C	8350	0	8301	186	0
1	D	8350	0	8301	189	0
2	A	44	0	26	11	0
2	B	44	0	26	11	0
2	C	44	0	26	11	0
2	D	44	0	26	11	0
All	All	33576	0	33308	750	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 11.

The worst 5 of 750 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:A:960:ASP:HB2	1:A:983:ASP:OD2	1.42	1.20
1:B:960:ASP:HB2	1:B:983:ASP:OD2	1.42	1.20
1:D:960:ASP:HB2	1:D:983:ASP:OD2	1.42	1.20
1:C:960:ASP:HB2	1:C:983:ASP:OD2	1.42	1.20
1:B:960:ASP:CB	1:B:983:ASP:OD2	2.24	0.86

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	1071/1611 (66%)	1047 (98%)	24 (2%)	0	100	100
1	B	1071/1611 (66%)	1047 (98%)	24 (2%)	0	100	100
1	C	1071/1611 (66%)	1046 (98%)	25 (2%)	0	100	100
1	D	1071/1611 (66%)	1048 (98%)	23 (2%)	0	100	100
All	All	4284/6444 (66%)	4188 (98%)	96 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	877/1294 (68%)	877 (100%)	0	100	100
1	B	877/1294 (68%)	877 (100%)	0	100	100
1	C	877/1294 (68%)	877 (100%)	0	100	100
1	D	877/1294 (68%)	877 (100%)	0	100	100
All	All	3508/5176 (68%)	3508 (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 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	1115	ASN
1	D	1225	ASN
1	D	1449	HIS
1	B	1225	ASN
1	B	1115	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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	$\# Z > 2$
2	NAD	A	1601	-	46,48,48	0.63	1 (2%)	64,73,73	0.59	1 (1%)
2	NAD	D	1601	-	46,48,48	0.63	1 (2%)	64,73,73	0.58	0
2	NAD	C	1601	-	46,48,48	0.64	1 (2%)	64,73,73	0.58	0
2	NAD	B	1601	-	46,48,48	0.63	1 (2%)	64,73,73	0.59	1 (1%)

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
2	NAD	A	1601	-	-	1/30/62/62	0/5/5/5
2	NAD	D	1601	-	-	1/30/62/62	0/5/5/5
2	NAD	C	1601	-	-	1/30/62/62	0/5/5/5
2	NAD	B	1601	-	-	1/30/62/62	0/5/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1601	NAD	C2N-N1N	2.79	1.38	1.35
2	C	1601	NAD	C2N-N1N	2.79	1.38	1.35
2	A	1601	NAD	C2N-N1N	2.78	1.38	1.35
2	D	1601	NAD	C2N-N1N	2.67	1.37	1.35

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1601	NAD	C6N-N1N-C2N	-2.03	120.15	121.88
2	B	1601	NAD	C6N-N1N-C2N	-2.01	120.17	121.88

There are no chirality outliers.

All (4) torsion outliers are listed below:

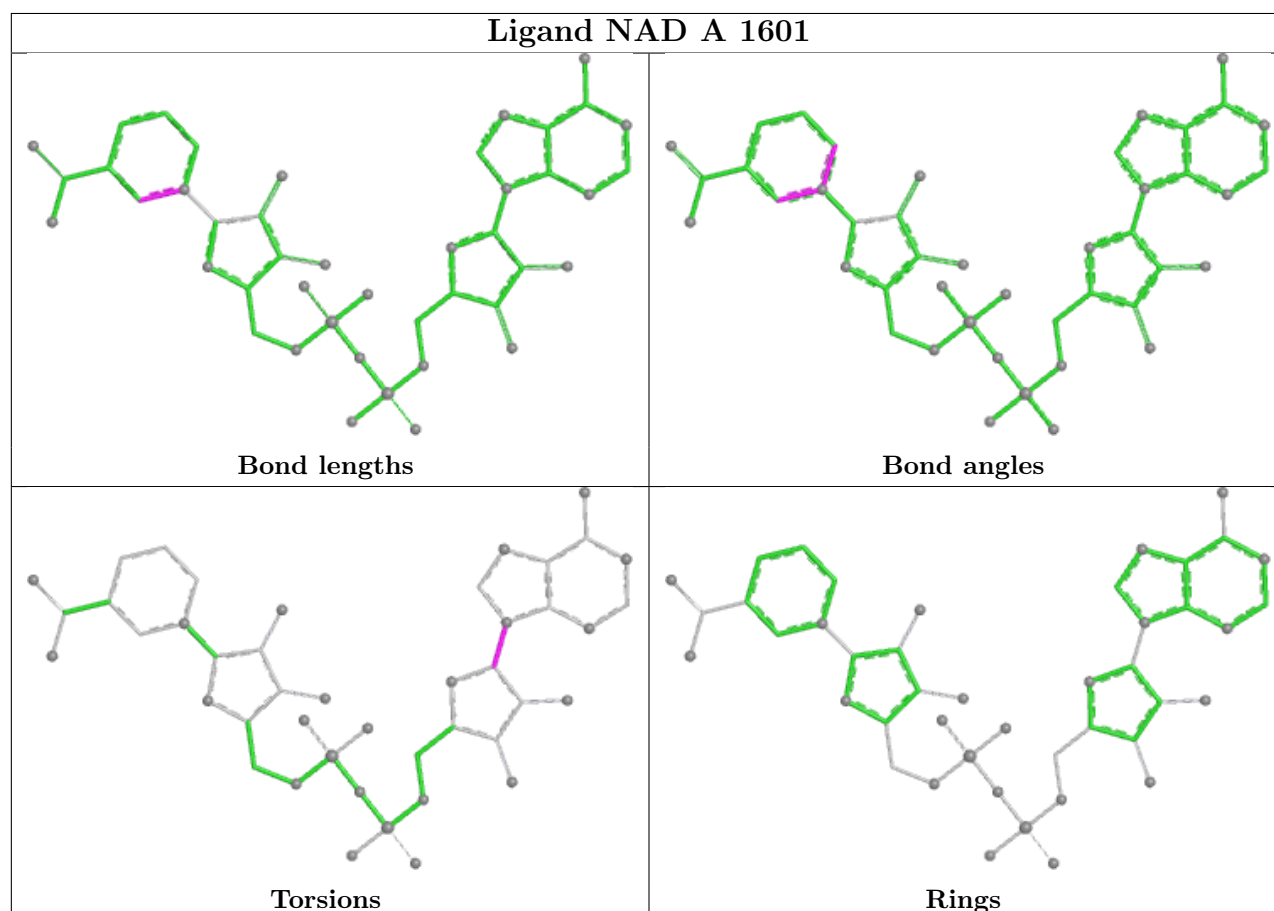
Mol	Chain	Res	Type	Atoms
2	A	1601	NAD	C2B-C1B-N9A-C8A
2	B	1601	NAD	C2B-C1B-N9A-C8A
2	C	1601	NAD	C2B-C1B-N9A-C8A
2	D	1601	NAD	C2B-C1B-N9A-C8A

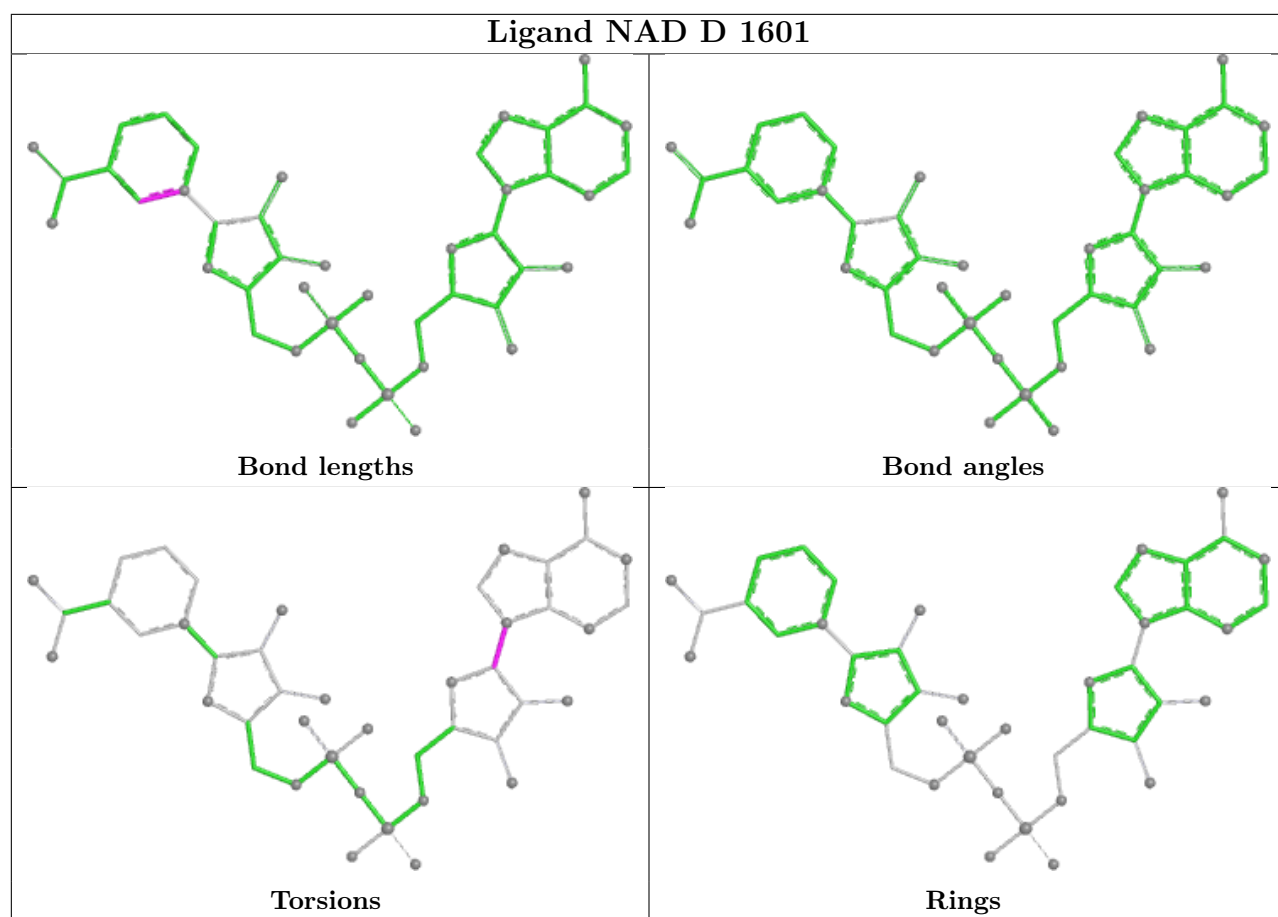
There are no ring outliers.

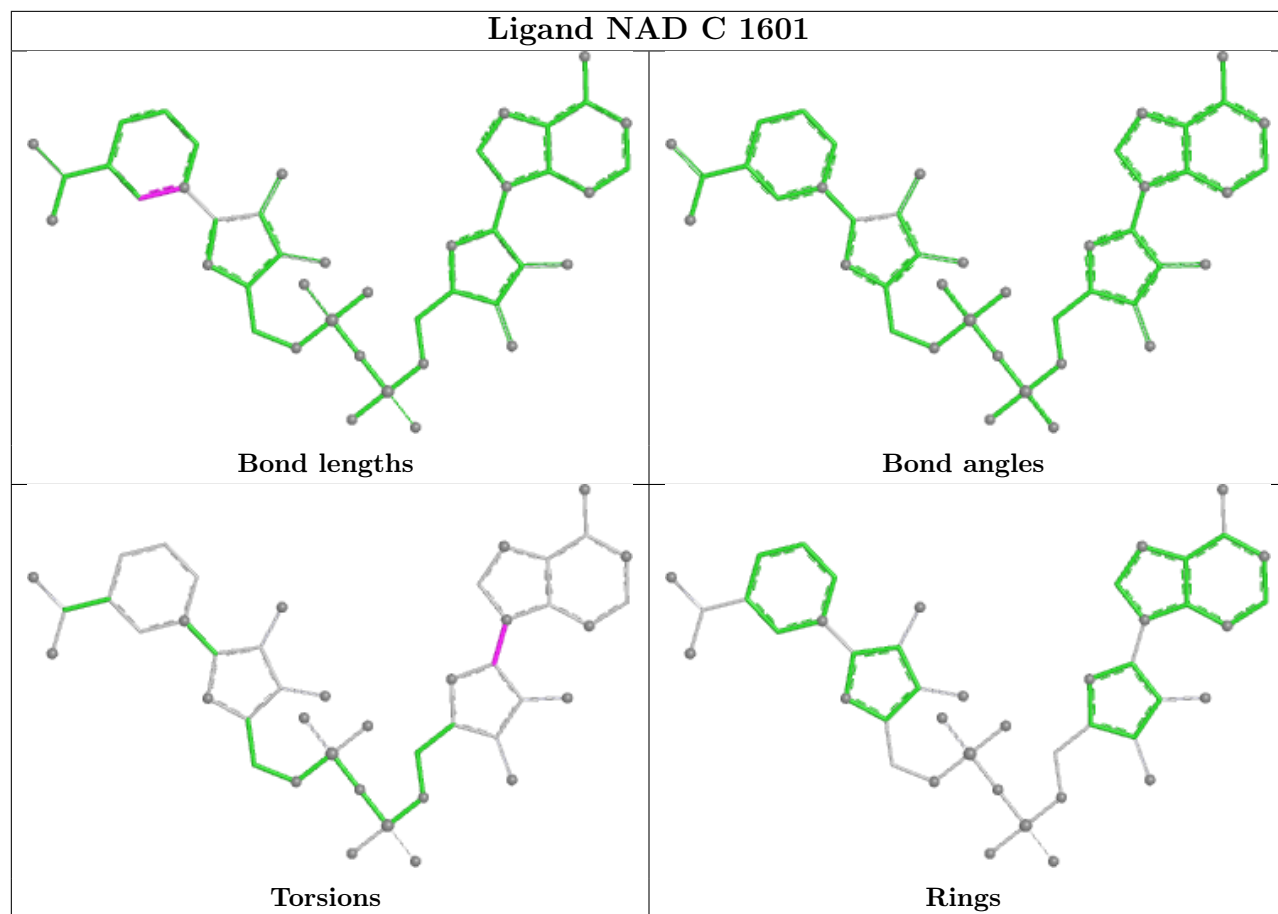
4 monomers are involved in 44 short contacts:

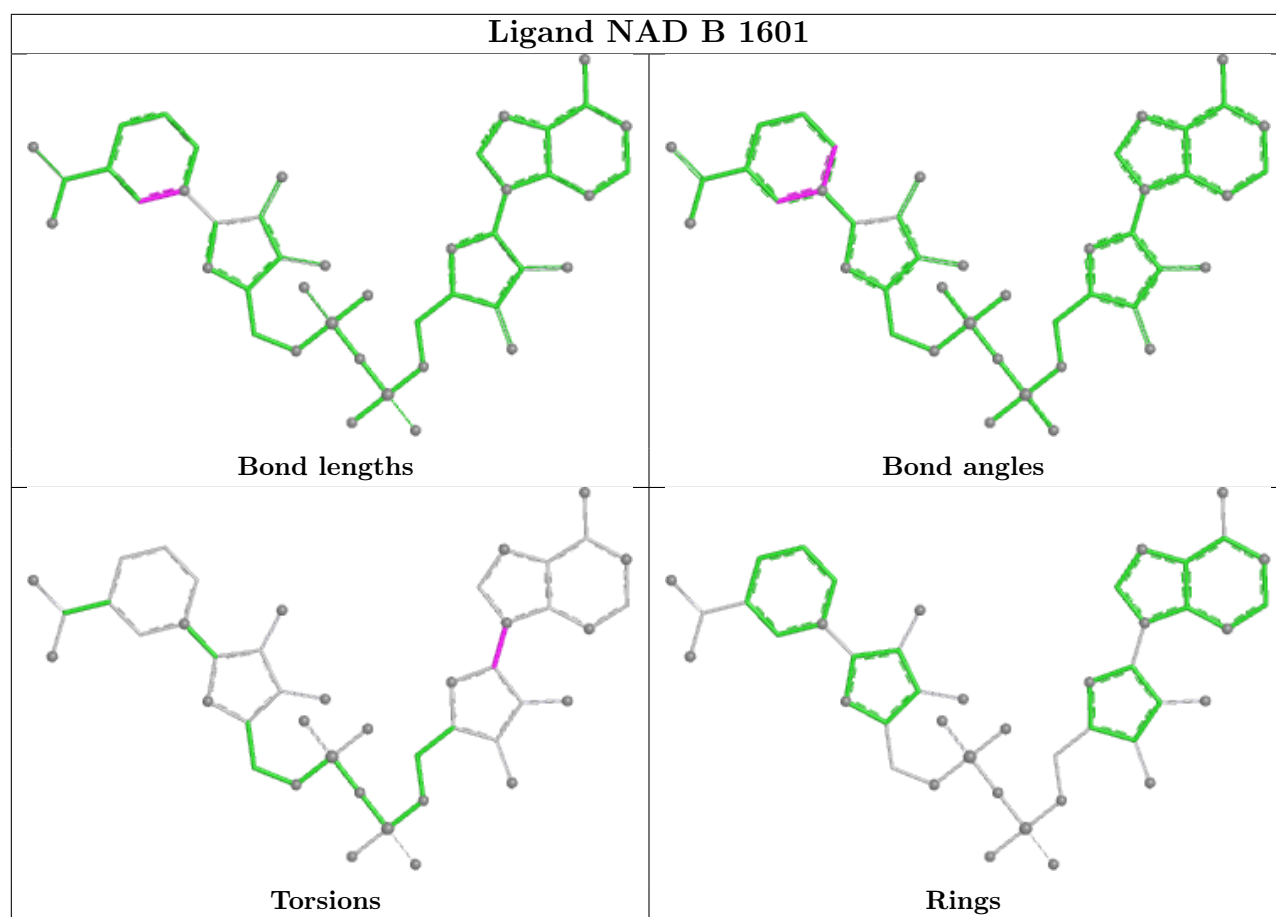
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1601	NAD	11	0
2	D	1601	NAD	11	0
2	C	1601	NAD	11	0
2	B	1601	NAD	11	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









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.

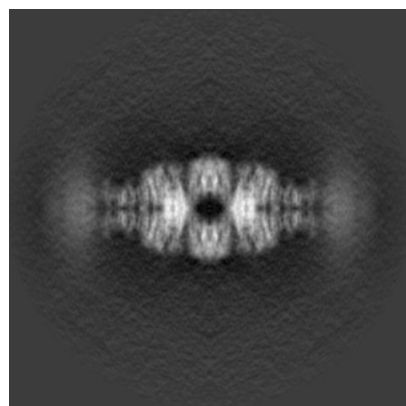
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52420. These allow visual inspection of the internal detail of the map and identification of artifacts.

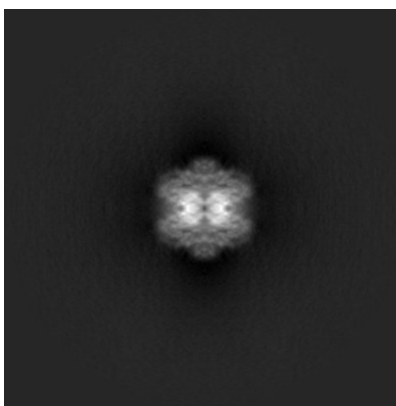
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

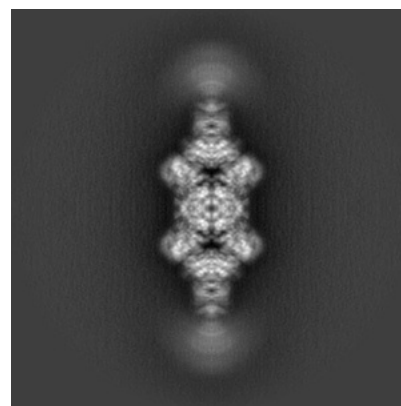
6.1.1 Primary map



X

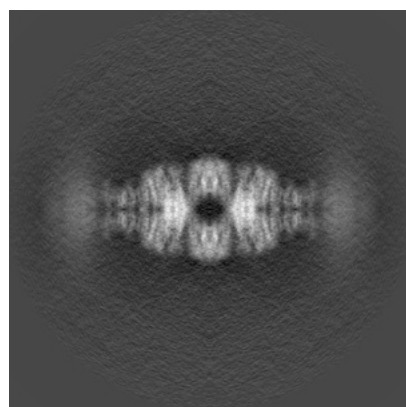


Y

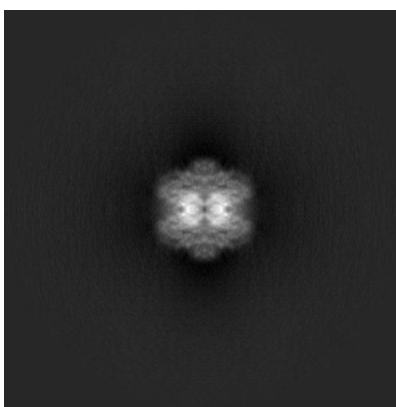


Z

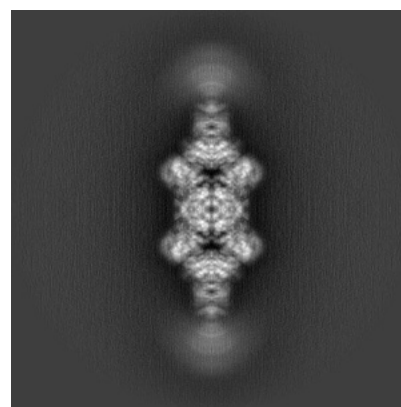
6.1.2 Raw map



X



Y

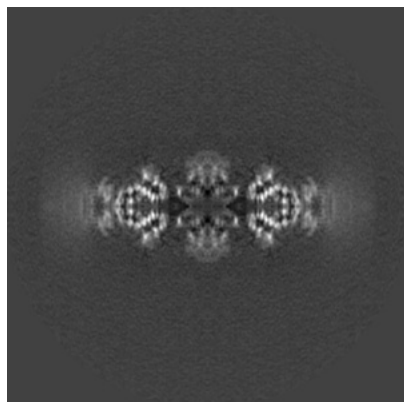


Z

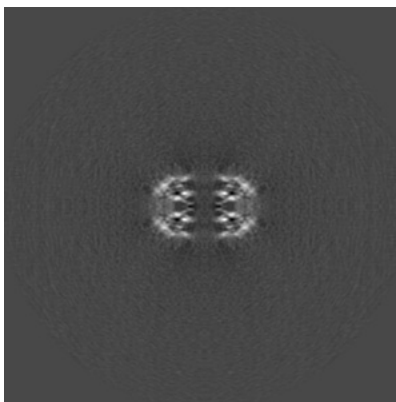
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

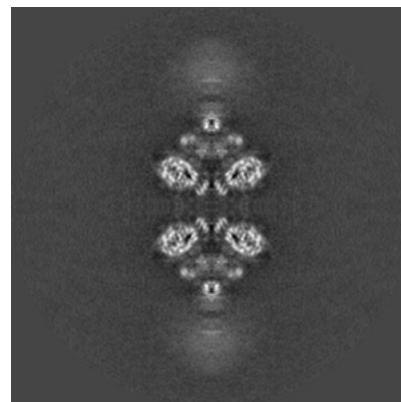
6.2.1 Primary map



X Index: 170

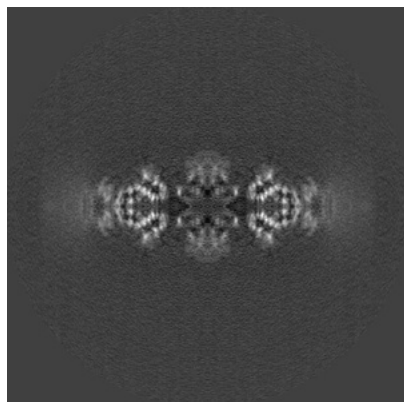


Y Index: 170

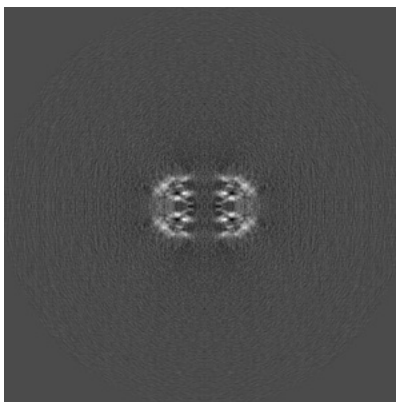


Z Index: 170

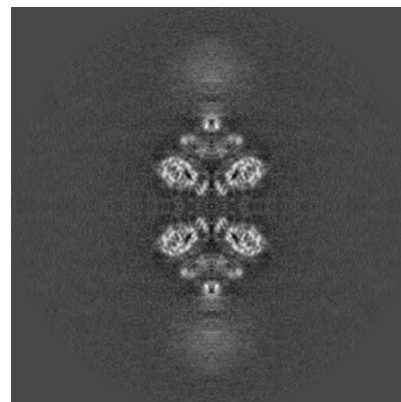
6.2.2 Raw map



X Index: 170



Y Index: 170

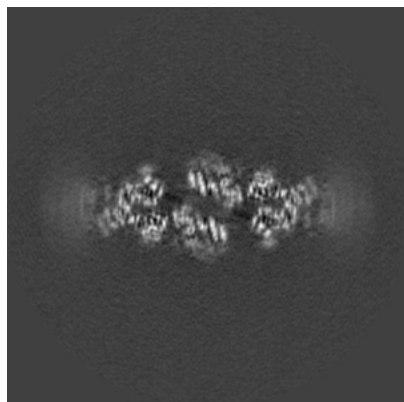


Z Index: 170

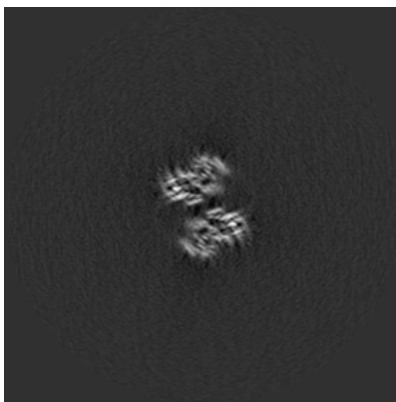
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

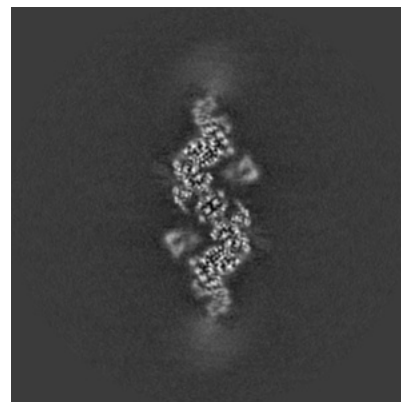
6.3.1 Primary map



X Index: 174

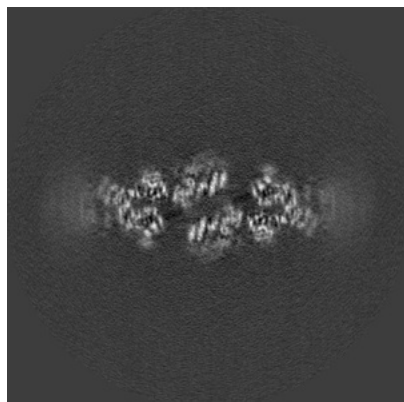


Y Index: 143

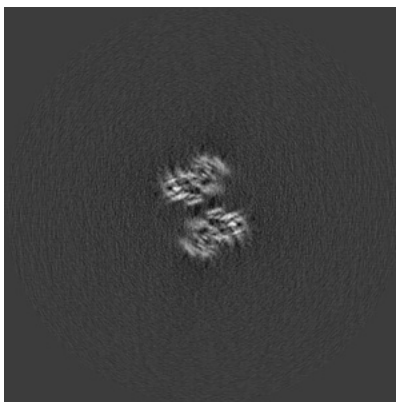


Z Index: 157

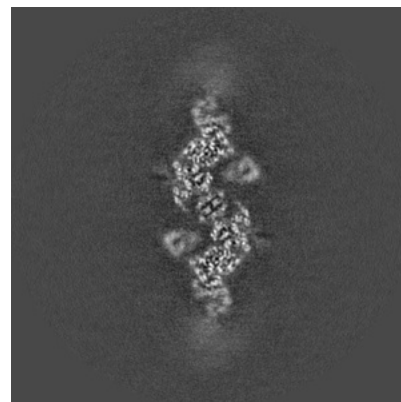
6.3.2 Raw map



X Index: 166



Y Index: 143

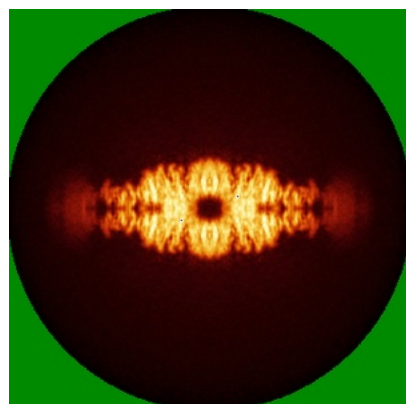


Z Index: 158

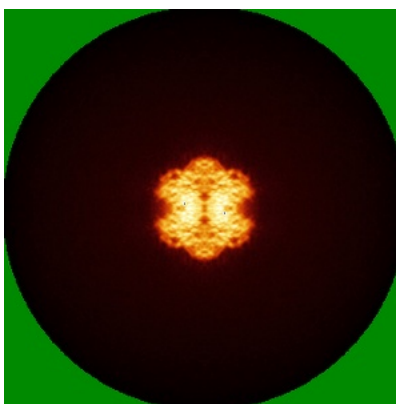
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

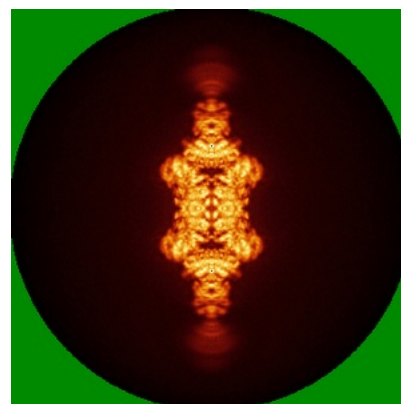
6.4.1 Primary map



X

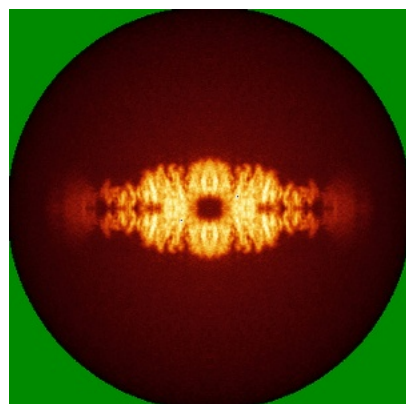


Y

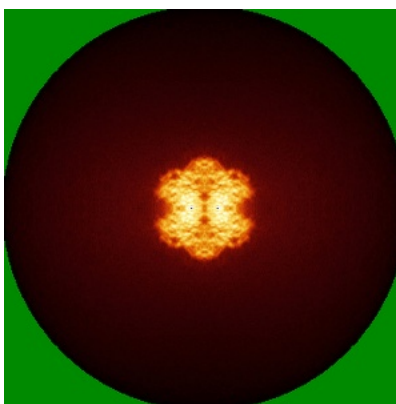


Z

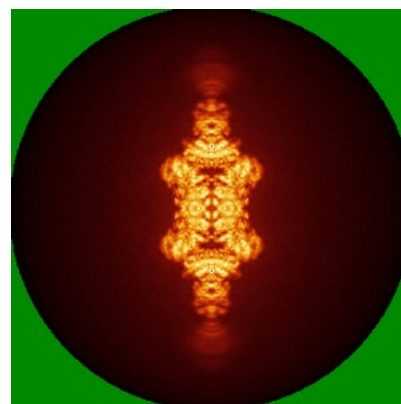
6.4.2 Raw map



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.

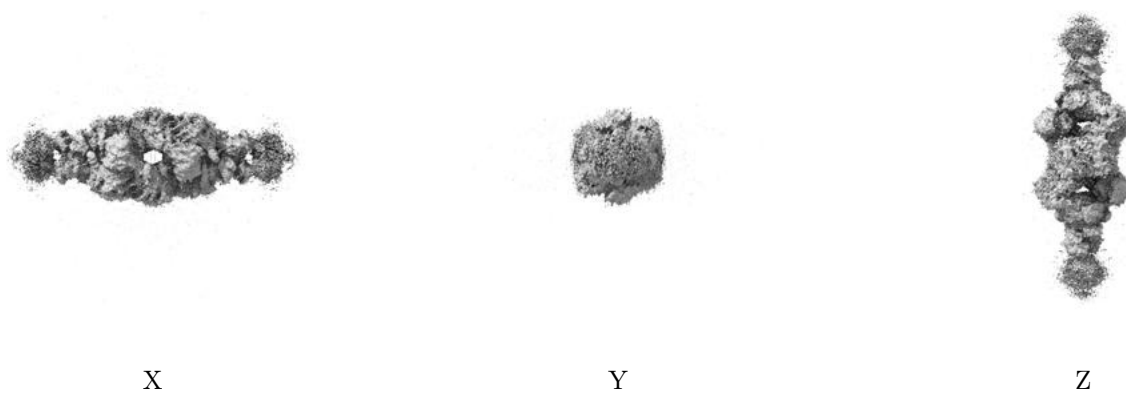
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.005. 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



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

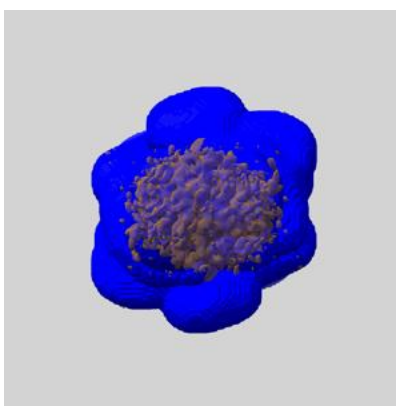
A mask typically either:

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

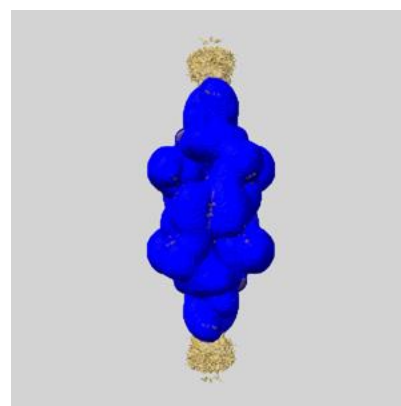
6.6.1 emd_52420_msk_1.map [i](#)



X



Y

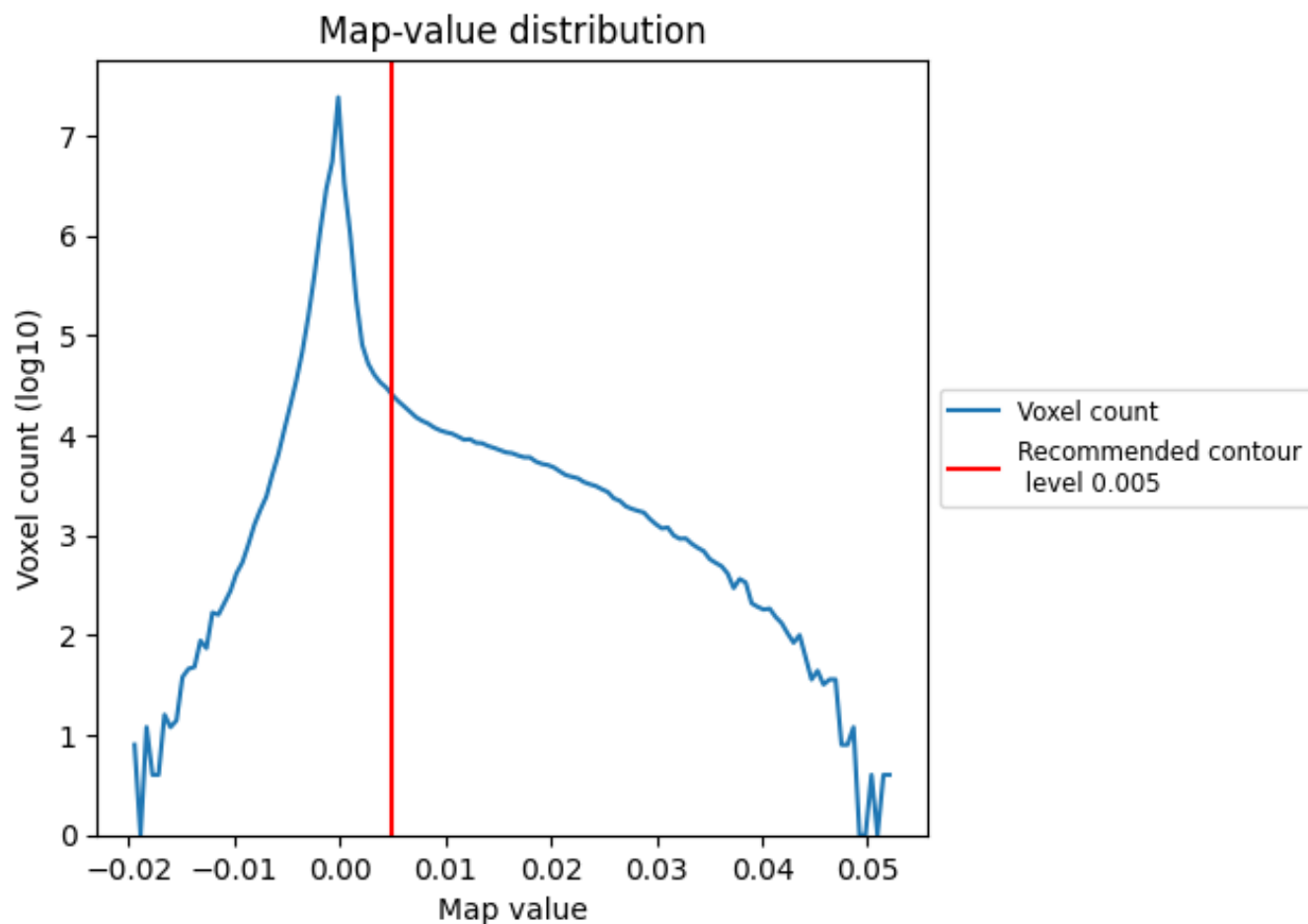


Z

7 Map analysis [i](#)

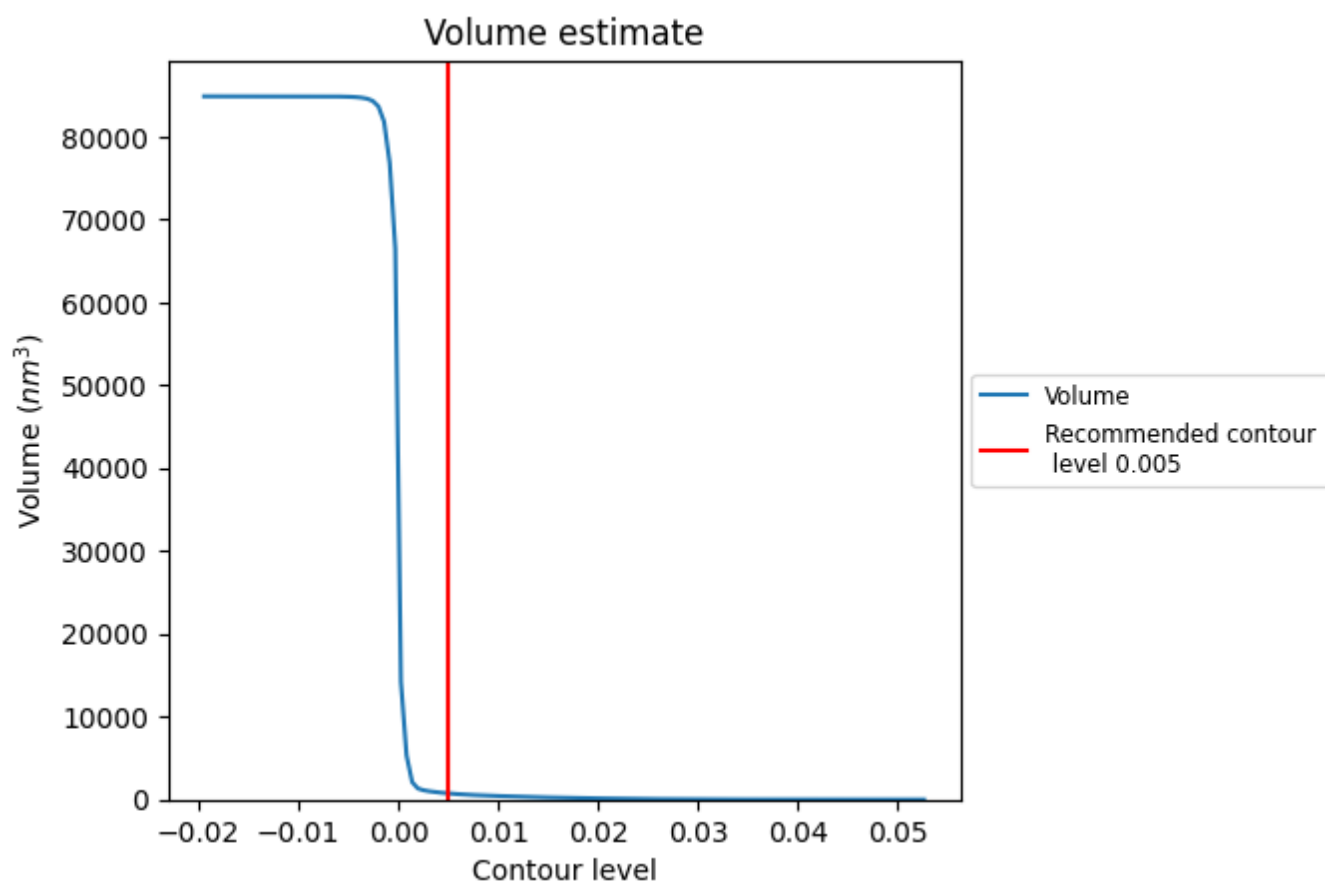
This section contains the results of statistical analysis of the map.

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.

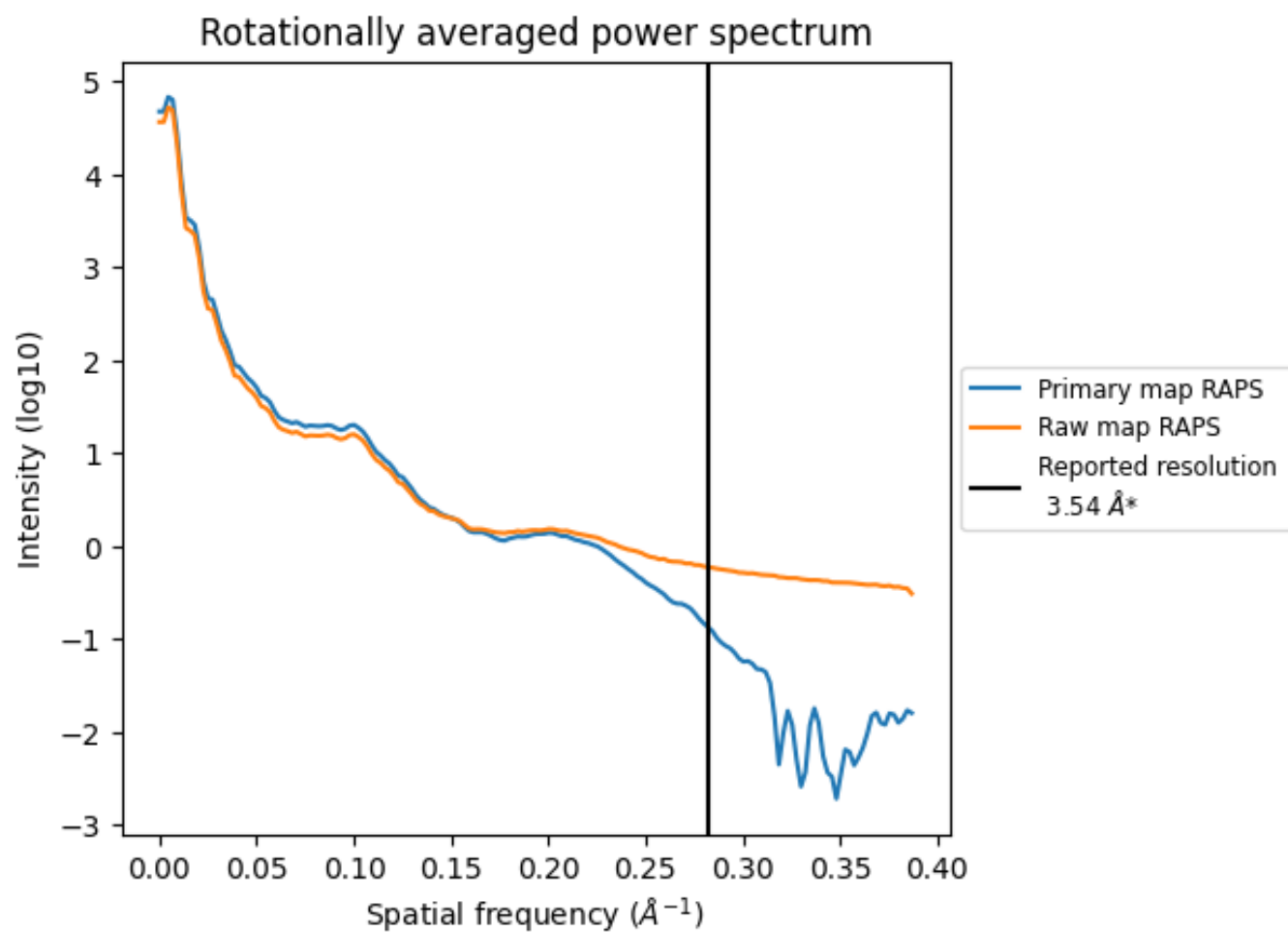
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 747 nm^3 ; this corresponds to an approximate mass of 675 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 ⓘ

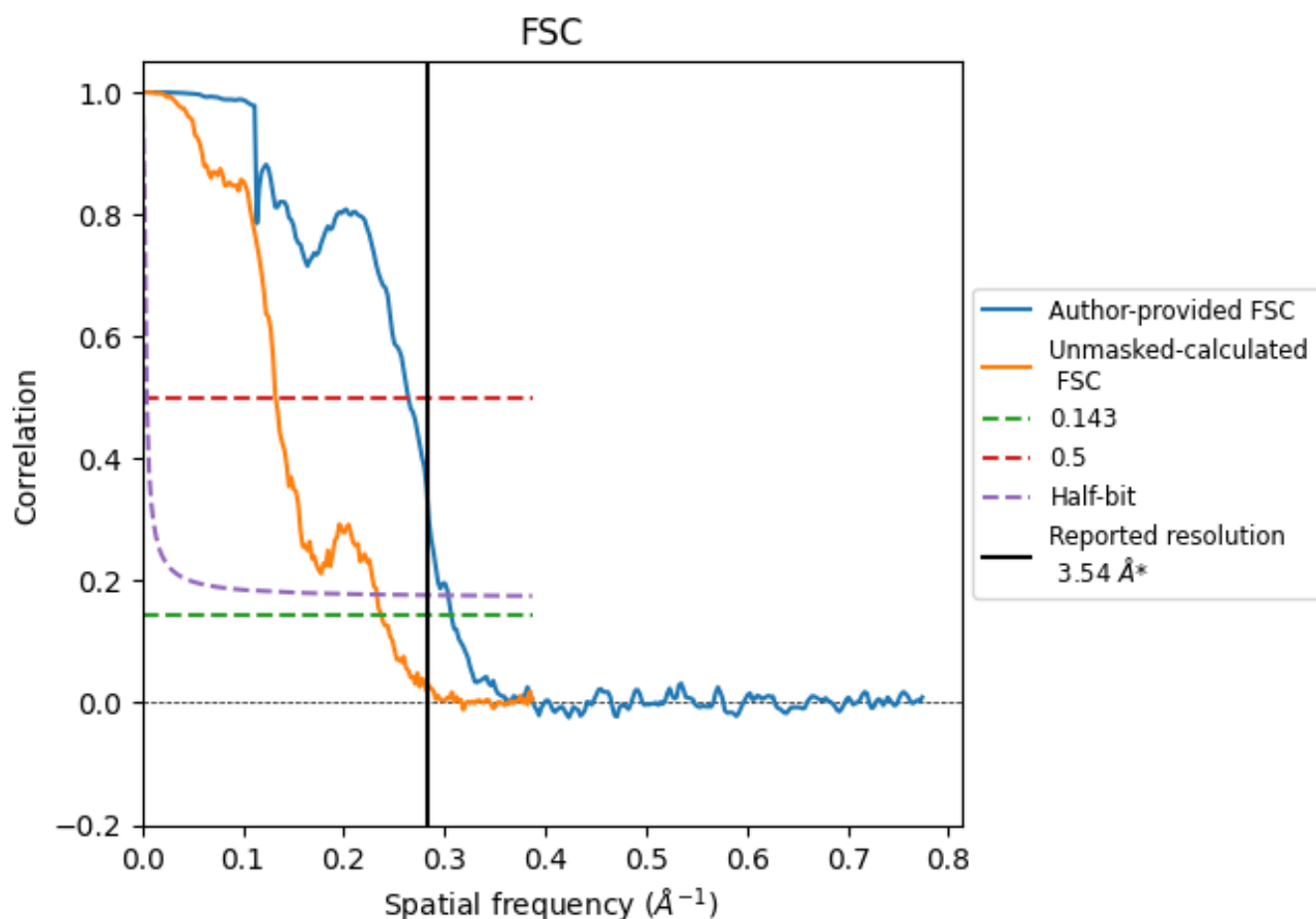


*Reported resolution corresponds to spatial frequency of 0.282 Å⁻¹

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 0.282 Å⁻¹

8.2 Resolution estimates [i](#)

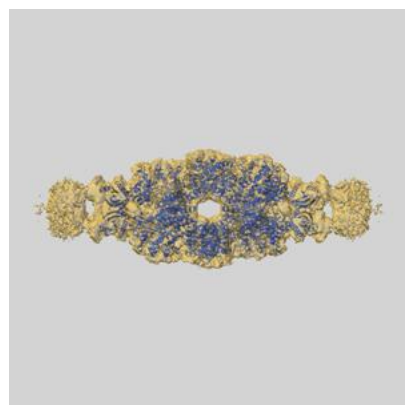
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.54	-	-
Author-provided FSC curve	3.26	3.79	3.29
Unmasked-calculated*	4.21	7.56	4.30

*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 4.21 differs from the reported value 3.54 by more than 10 %

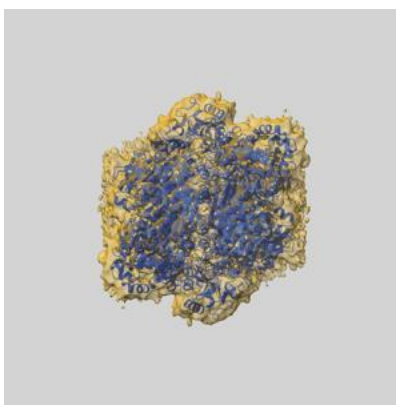
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-52420 and PDB model 9HUY. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

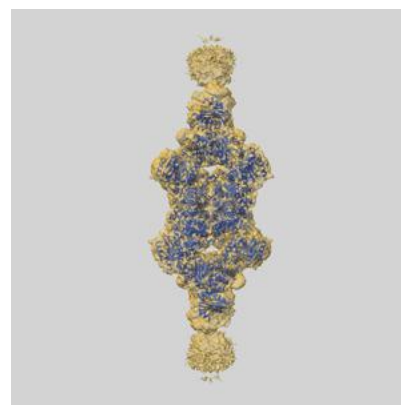
9.1 Map-model overlay [i](#)



X



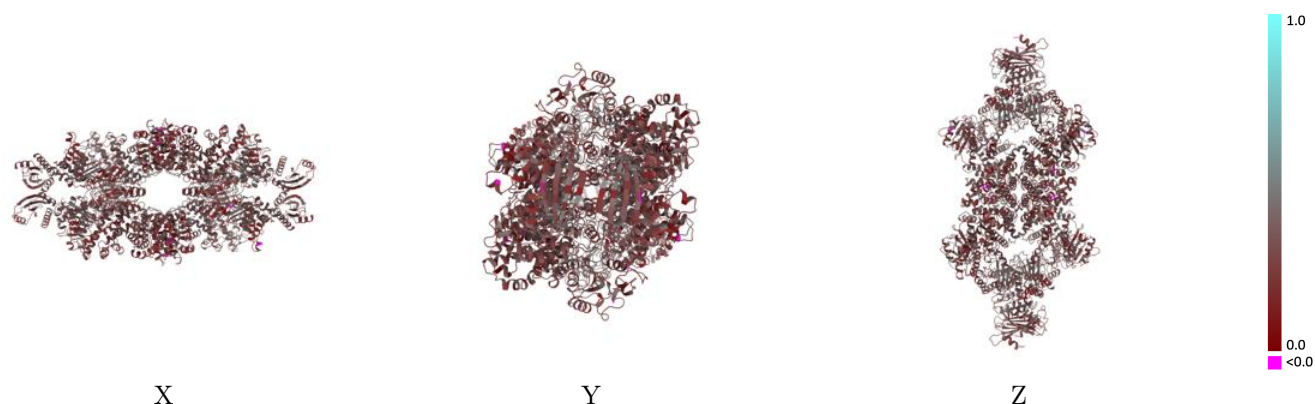
Y



Z

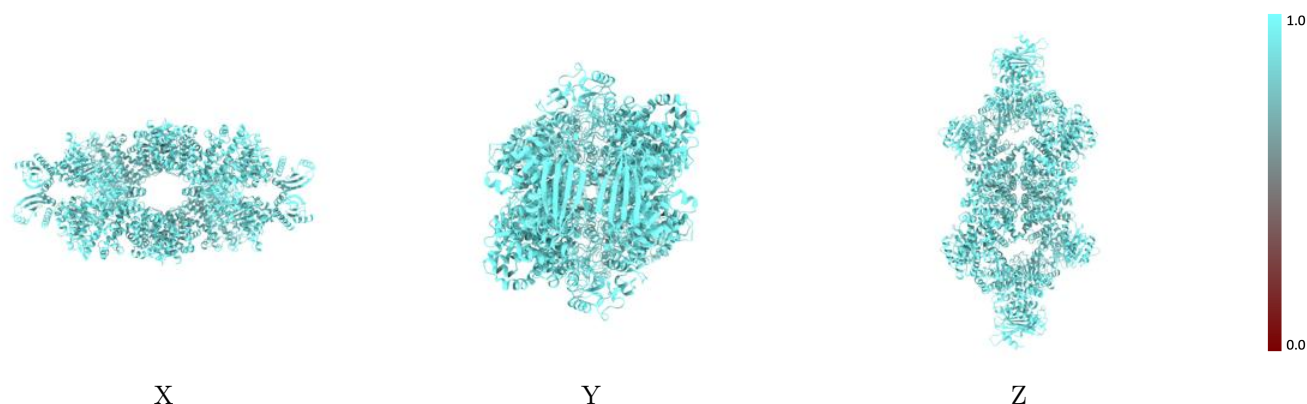
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



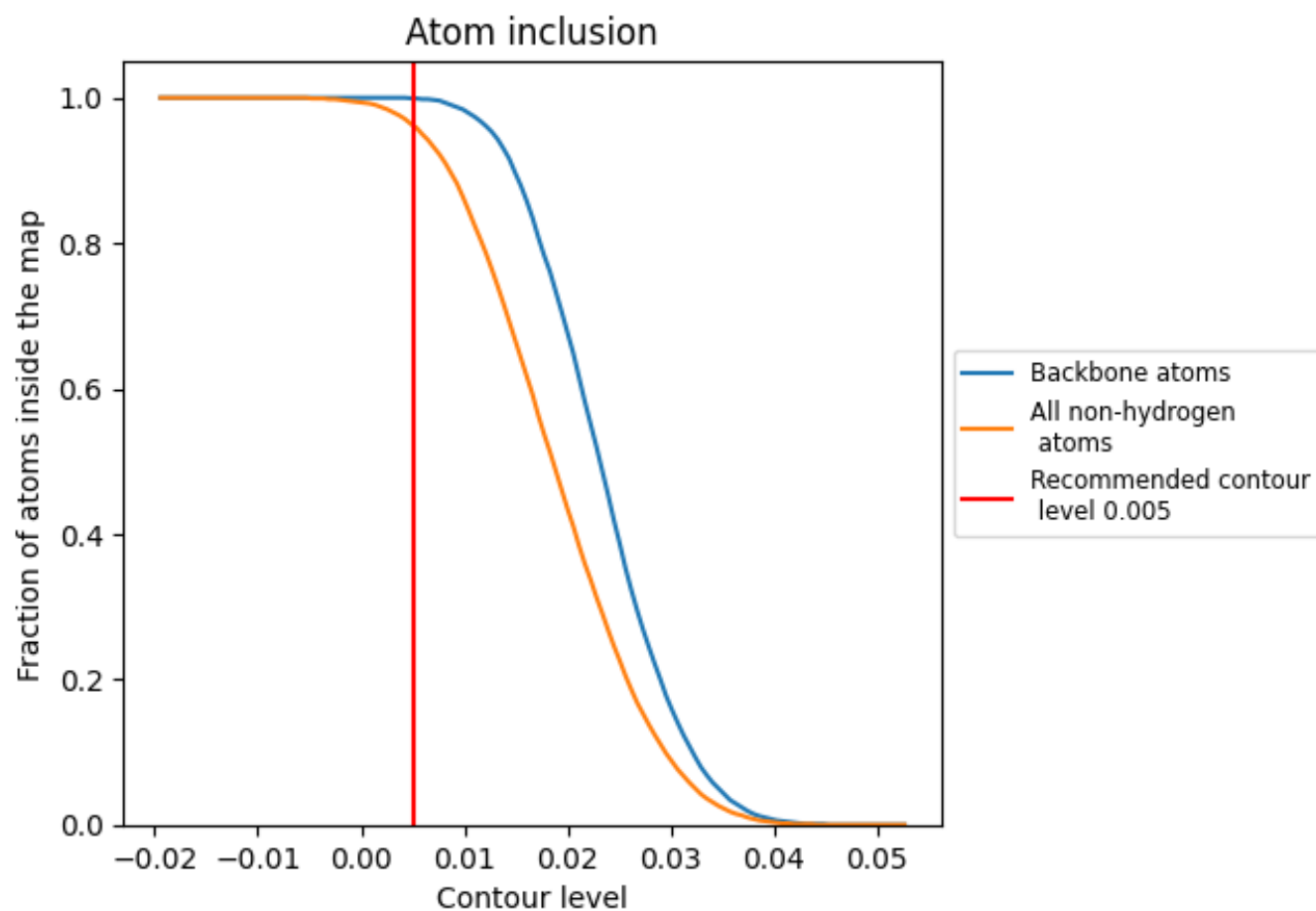
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.005).

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 96% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9620	<div></div> 0.3000
A	<div></div> 0.9610	<div></div> 0.3020
B	<div></div> 0.9640	<div></div> 0.3030
C	<div></div> 0.9620	<div></div> 0.3000
D	<div></div> 0.9630	<div></div> 0.2960

