



## wwPDB EM Validation Summary Report ⓘ

Apr 5, 2026 – 05:17 PM UTC

PDB ID : 9HUZ / pdb\_00009huz  
EMDB ID : EMD-52421  
Title : CryoEM map of the large glutamate dehydrogenase composed of 180 kDa subunits from Mycobacterium smegmatis obtained in the presence of NAD<sup>+</sup> and L-glutamate. Closed2 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 : 3.57 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](mailto: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>.

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

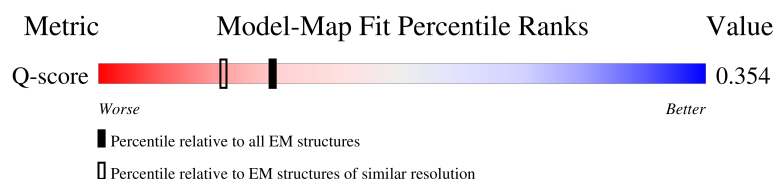
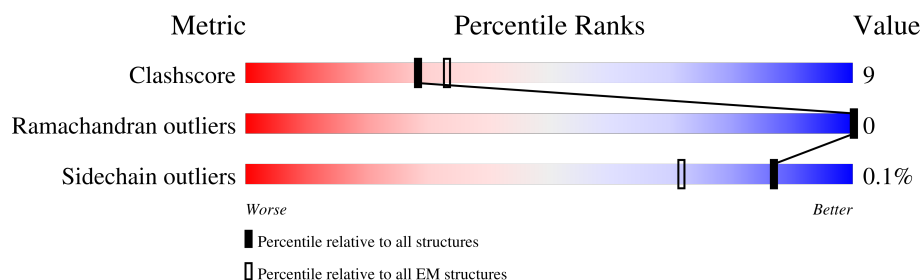
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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 3.57 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	12682 ( 3.07 - 4.07 )

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  $\geq 3$ , 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	
1	B	1611	
1	C	1611	

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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

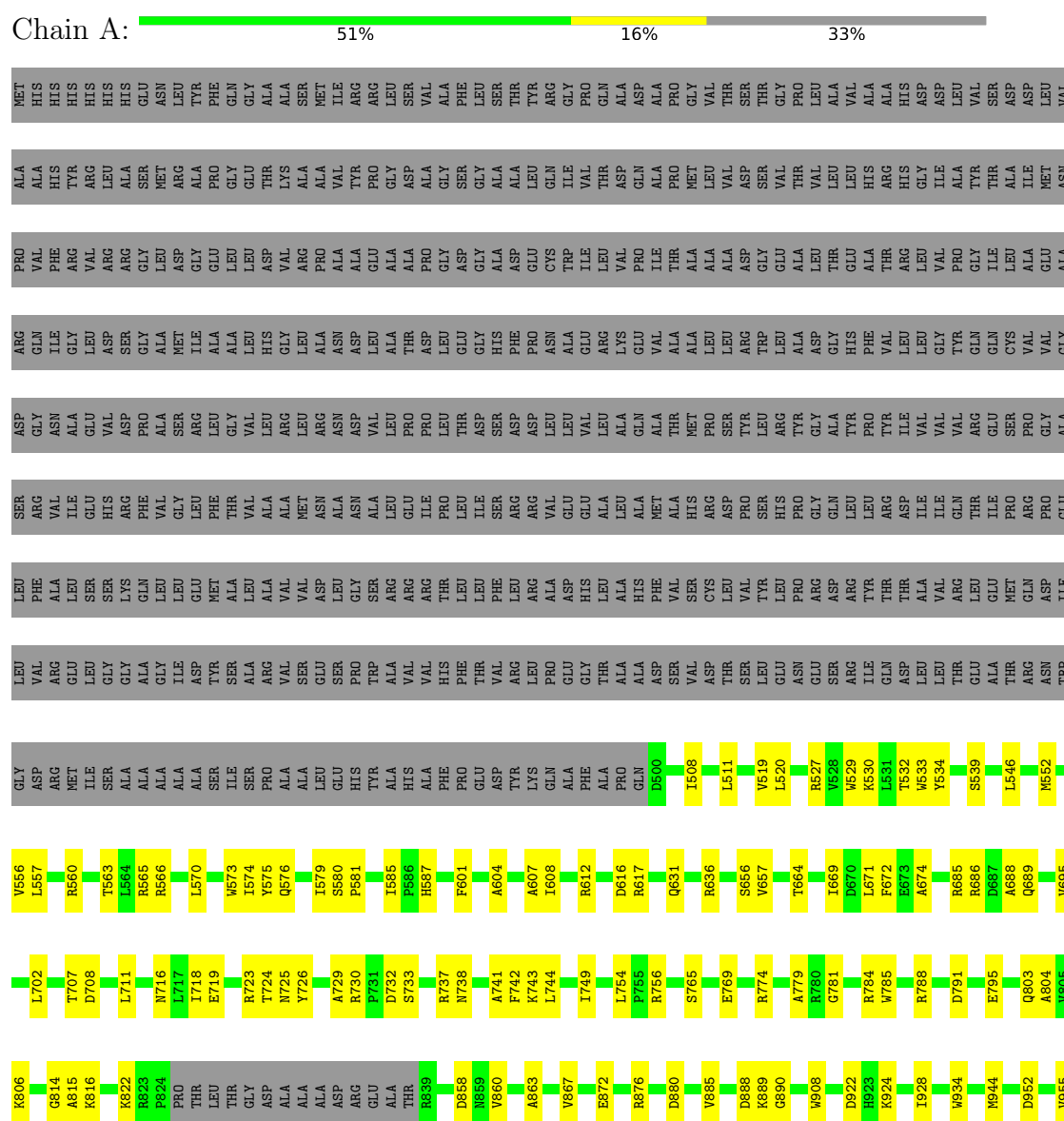
- # NAD

Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total 44	C 21	N 7	O 14	P 2	0
2	B	1	Total 44	C 21	N 7	O 14	P 2	0
2	C	1	Total 44	C 21	N 7	O 14	P 2	0
2	D	1	Total 44	C 21	N 7	O 14	P 2	0

### 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



V1553	L1390	V1219	L1070	V956
T1554	L1391	D1220		G957
R1555	L1392	N1221	M1073	F958
	R1393			G959
V1576	L1394	L1224	I1080	D960
			K1081	M961
R1579	A1399	E1227	D1092	D964
		L1228		V965
S1583	E1403			F966
M1584		P1232	M1095	G967
	G1408		D1096	N968
S1588		R1240	Q1097	
GLY	W1421		I1098	L972
THR	L1422	G1246	R1099	
GLY	R1423	L1247		
THR				
THR	P1443	E1251	R1106	H975
GLY			A1107	I976
	L1446	K1264	K1108	R977
			V1109	
I1450		Q1275	E1112	A981
	I1450	E1276	D983	F982
D1461		V1277	M1115	H984
		F1278		
	I1465		V1118	F988
		R1281		
D1474		L1282	A1137	N992
E1475				P993
		P1287	M1140	D994
D1478			S1141	
F1481		L1290	A1142	R997
A1482		L1294	G1143	
L1483			V1144	A1014
		E1297		
S1497			T1162	L1020
		H1301		
R1501			L1174	V1027
D1502		R1304	M1178	I1037
D1503			T1179	S1038
R1504		I1308	D1180	P1039
				Q1040
L1508		M1311	M1190	V1041
A1509		L1312		R1042
R1510		V1313	M1194	
			D1195	L1047
R1522		D1318	L1196	
A1523				
L1524		V1332	M1203	V1051
C1525				E1052
F1526		I1349	S1206	T1055
			L1207	P1056
E1536		I1359	L1208	P1057
			S1209	A1058
K1541		R1380	V1210	L1059
				I1060
T1547		V1383	M1214	
T1548				P1067
		R1388	D1217	V1068
P1550		H1390	T1216	D1069

- Molecule 1: NAD-specific glutamate dehydrogenase

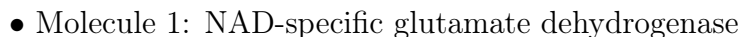
Chain B:  51% 15% 33%

[illegible]





A	R560	GLY	LEU	LEU	SER	ASP	ARG	GLN	PRO	ALA	MET
	T563	ILE	GLY	PHE	ARG	GLY	ILE	GLN	VAL	ALA	HIS
	L564	GLY	LEU	ALA	ILE	ALA	GLY	GLY	ARG	TYR	HIS
	R565	SER	GLY	SER	HIS	VAL	ASP	ASP	VAL	LEU	HIS
	R566	ALA	GLY	LYS	ARG	ASP	SER	SER	ARG	ALA	HIS
	L570	ALA	ALA	GLN	PHE	PHO	GLY	GLY	GLY	SER	ASN
	W573	ALA	ASP	GLY	LEU	ARG	ILE	GLY	ALA	ALA	TYR
	I574	SER	TYR	MET	PHE	LEU	ALA	ALA	GLY	PRO	PHE
	Y575	ILE	SER	ALA	THR	GLY	LEU	ALA	LEU	GLY	GLN
	Q576	SER	ALA	VAL	THR	VAL	LEU	HIS	ASP	THR	GLY
B	I579	PRO	ARG	ALA	ALA	ARG	VAL	LEU	ASP	LYS	ALA
	S580	ALA	VAL	VAL	MET	LEU	ARG	GLY	ARG	ALA	SER
	P581	GLY	ASP	ASP	ASN	ARG	ALA	ASN	PRO	ALA	MET
	T585	LEU	SER	LEU	ALA	ASN	ALA	ASN	ALA	VAL	ILE
	P586	HIS	PRO	GLY	ASN	ASP	ASP	ASP	ALA	TYR	ARG
	H587	TYR	TRP	SER	ALA	VAL	LEU	LEU	GLY	PRO	ARG
	L588	ALA	ALA	ARG	LEU	ALA	ALA	ALA	ALA	GLY	LEU
	F601	HIS	VAL	ARG	GLY	PRO	THR	ASP	ALA	ASP	SER
	F602	ALA	VAL	ARG	ILE	PRO	PRO	ASP	PRO	ALA	VAL
	A604	PHE	HIS	THR	PRO	LEU	LEU	LEU	GLY	GLY	ALA
C	A607	PRO	PHE	LEU	ILE	THR	GLY	GLY	ASP	SER	PHE
	I608	GLY	THR	THR	SER	SER	HIS	GLY	ALA	ALA	SER
	L609	ASP	VAL	PHE	ARG	ASP	PHE	ASP	ASP	ALA	THR
	F612	LYS	LEU	ARG	ARG	ASP	PRO	ASN	GLY	LEU	TYR
	D616	GLN	GLU	VAL	VAL	LEU	ALA	GLN	CYS	GLN	ARG
	R617	ALA	GLY	HIS	GLY	VAL	ALA	ILE	THR	ILE	GLY
	L620	THR	THR	LEU	ALA	LEU	ARG	LEU	LEU	VAL	PRO
	Q631	ALA	ALA	HIS	LEU	ALA	LYS	VAL	VAL	ASP	ALA
	R636	ASP	ASP	PHE	MET	GLN	VAL	VAL	PRO	GLN	ASP
	S656	SER	VAL	VAL	ALA	THR	ALA	ILE	ALA	ALA	ALA
D	S657	VAL	VAL	SER	HIS	MET	ALA	ALA	THR	PRO	GLY
	V657	ASP	ASP	CYS	ARG	PRO	ALA	ALA	LEU	LEU	MET
	L511	THR	THR	LEU	ASP	SER	LEU	ALA	VAL	VAL	THR
	W519	SER	VAL	VAL	PRO	TYR	ARG	ASP	ASP	ASP	SER
	L520	LEU	LEU	THR	SER	LEU	TRP	TRP	GLY	SER	THR
	I669	GLY	GLY	THR	HIS	ARG	LEU	GLY	GLY	GLY	GLY
	D670	ASN	ASN	LEU	PRO	TYR	ASP	ALA	ALA	THR	PRO
	L671	GLU	GLU	ARG	GLY	GLY	ASP	GLY	LEU	VAL	LEU
	F672	SER	ARG	ASP	GLN	ALA	GLY	GLY	THR	LEU	ALA
	S673	ILE	ILE	TYR	LEU	TYR	PHE	HIS	GLY	VAL	VAL
E	A674	GLN	GLN	THR	ASP	PRO	THR	THR	GLY	HIS	ALA
	R695	ASP	THR	THR	ASN	ILE	LEU	LEU	ARG	ARG	HIS
	R686	LEU	LEU	ALA	ILE	VAL	GLY	GLY	GLY	GLY	ASP
	D687	LEU	VAL	VAL	ILE	VAL	GLY	VAL	VAL	ILE	ASP
	S539	THR	ARG	ARG	GLN	VAL	TYR	TYR	PRO	ALA	LEU
	Q689	GLY	GLY	LEU	THR	ARG	GLN	GLN	GLY	THR	VAL
	M552	ALA	ALA	GLU	ILE	GLU	GLN	ILE	THR	THR	SER
	V695	THR	ARG	GLU	PRO	SER	VAL	CYS	LEU	ALA	ASP
	L696	THR	ASN	GLN	ARG	PRO	VAL	VAL	ILE	ILE	ASP
	T703	ASP	THR	THR	PRO	GLY	GLY	GLY	GLY	MET	VAL



GLY	ASP	ARG	GLY	LEU	LEU	LEU	SER	ASP	ARG	PRO	VAL	ALA	MET
ASP	ARG	ARG	ALA	PHE	VAL	ALA	ARG	GLY	GLN	VAL	PHE	ALA	HIS
MET	GLU	LEU	LEU	SER	GLU	GLY	ILE	ALA	ILE	GLY	TYR	ARG	HIS
ILE	LEU	SER	GLY	SER	LEU	GLY	GLU	VAL	GLY	VAL	ARG	HIS	HIS
SER	GLY	LYS	HIS	ARG	HIS	ASP	ASP	ASP	ASP	ARG	LEU	HIS	HIS
ALA	ALA	GLN	PHE	GLN	PHE	ASP	ASP	GLY	SER	ARG	ALA	GLY	GLY
ALA	ALA	GLY	LEU	LEU	VAL	ALA	VAL	ALA	GLY	LEU	MET	ASN	ASN
ALA	ALA	ILE	GLY	LEU	GLY	GLY	GLY	SER	MET	ASP	LEU	ASP	ASN
ASP	ASP	ASP	GLY	GLY	GLY	GLY	LEU	LEU	ILE	GLY	ALA	TYR	TYR
SER	SER	TYR	PHE	MET	PHE	LEU	LEU	LEU	ALA	GLY	PRO	PHE	PHE
ILE	ILE	SER	ALA	ALA	ALA	THR	THR	GLY	ALA	LEU	GLY	GLN	GLN
SER	SER	ALA	ALA	LEU	VAL	ALA	ALA	VAL	HIS	LEU	THR	GLY	GLY
PRO	PRO	ALA	VAL	ALA	VAL	VAL	MET	ARG	ASN	PRO	ALA	LYS	ALA
ALA	ALA	VAL	SER	VAL	SER	ARG	MET	LEU	ALA	ALA	VAL	ALA	ALA
ALA	ALA	VAL	ARG	ARG	GLY	ILE	ASN	ARG	ALA	PRO	VAL	ALA	ALA
PHE	PHE	HIS	VAL	THR	THR	PRO	PRO	PRO	ASP	GLY	GLY	GLY	PHE
PRO	PRO	PHE	LEU	LEU	LEU	LEU	ILE	ASP	GLY	GLY	GLY	GLY	LEU
GLU	GLU	THR	LEU	PHE	LEU	LEU	ILE	ASP	HIS	ASP	ALA	ALA	SER
ASP	ASP	VAL	VAL	VAL	VAL	ARG	SER	ASP	PHE	ASP	ALA	ALA	THR
TYR	TYR	ARG	LEU	ARG	ARG	ARG	ARG	ASP	PRO	GLY	LEU	LEU	TYR
LYS	LYS	LEU	LEU	LEU	ALA	ALA	LEU	ASP	ASN	CYS	GLN	GLN	ARG
GLN	GLN	PRO	PRO	ALA	ALA	ASP	GLY	LEU	ALA	TRP	ILE	ILE	GLY
PHE	PHE	GLY	GLY	HIS	LEU	HIS	GLY	ILE	ALA	LEU	THR	THR	PRO
ALA	ALA	THR	ALA	LEU	ALA	ALA	ALA	VAL	LYS	PRO	ASP	ASP	ALA
PRO	PRO	ALA	ALA	ALA	LEU	LEU	ALA	GLN	GLY	VAL	GLN	GLN	ASP
GLN	GLN	ASP	PHE	PHE	ASP	ALA	MET	ALA	VAL	ILE	ALA	ALA	ASP
B500		SER	VAL	VAL	VAL	VAL	VAL	THR	THR	ALA	ALA	ALA	ALA
I508		VAL	SER	SER	SER	HIS	HIS	MET	ALA	ALA	ALA	ALA	ALA
L511		ASP	CYS	CYS	ASP	ASP	ASP	PRO	LEU	ALA	ALA	ALA	ALA
V519		THR	THR	VAL	PRO	PRO	PRO	TYR	ARG	ALA	VAL	VAL	THR
L520		LEU	LEU	LEU	SER	SER	SER	LEU	TRP	GLY	GLY	GLY	SER
A521		ASN	PRO	PRO	PRO	PRO	PRO	ARG	LEU	ALA	THR	THR	PRO
D522		GLU	ARG	ARG	GLY	GLY	GLY	GLY	ASP	LEU	VAL	VAL	ALA
		SER	ASP	ASP	GLN	GLN	GLN	ALA	GLY	THR	LEU	LEU	ALA
R527		ARG	ARG	ARG	LEU	LEU	LEU	TYR	PHE	GLY	LEU	LEU	VAL
V528		ILE	TYR	TYR	TYR	TYR	LEU	PRO	THR	GLY	GLY	GLY	ALA
W529		GLN	THR	THR	THR	THR	ASP	TYR	VAL	THR	THR	THR	VAL
K530		ASP	THR	THR	ASP	ASP	ASP	ILE	LEU	THR	ARG	HIS	HIS
L531		LEU	ALA	ALA	ILE	ILE	ILE	VAL	LEU	LEU	GLY	GLY	ASP
T532		LEU	VAL	VAL	ILE	ILE	ILE	VAL	GLY	VAL	ILE	ILE	ASP
W533		THR	ARG	ARG	GLN	GLN	GLN	VAL	TYR	PRO	ALA	ALA	LEU
F534		GLU	LEU	LEU	GLU	GLU	GLU	ARG	GLN	ILE	TYR	THR	VAL
		ALA	ALA	GLU	ILE	ILE	ILE	GLY	GLN	GLY	THR	THR	SER
S539		THR	MET	MET	PRO	PRO	PRO	SER	CYS	GLY	ILE	ILE	ASP
		ARG	GLN	GLN	ARG	ARG							

T1548	R1380	S1209	P1057	D952	K806	R686	V556
R1552	V1383	V1210	A1058	V955	G814	D687	L557
I1563		M1214	I1059	V956	A815	A688	R560
T1573	R1388	D1217	P1067	G957	K816	V695	T563
V1576	V1389	L1218	V1068	T568	K822	S704	L564
	L1390	V1219	D1069	G959	R823	S704	R565
R1579	L1391	D1220	L1070	M961	P824	D706	R566
	N1392	N1221	N1073		PRO	T707	L570
	Y1393	L1224		D964	THR		
S1583	R1394	E1227	I1080	V965	LEU	L711	W573
	G1408	L1228	K1081	F966	THR		I574
S1588	W1421	P1232	D1087	G967	GLY	I718	Y575
THR	L1422			N968	ASP	E719	Q576
GLY	R1423	R1240	D1092	L972	ALA		
THR	P1443	G1246	R1093	S973	ALA	R723	I579
THR	L1446	L1247	A1094	K974	ASP	T724	S580
GLY	I1450	E1251	N1095	H975	ARG	N725	P581
	D1461	K1264	D1096	I976	GLU	Y726	
	I1465	Q1275	Q1097	R977	ALA		I585
	D1474	V1277	I1098		THR	A729	P586
	E1475	F1278	R1099	A980	R839	R730	H587
	D1478	R1281		A981		P731	
F1481	L1282	L1282	R1106	F982	D858	D732	F601
L1483	P1287	P1287	A1107	D983	R859	S733	
	L1290		K1108	H984	V860		A604
S1497	L1294		V1109	F988	A863	R737	
R1501	E1297		E1112	N992	V867	A741	A607
D1502			M1115	P993	E872	F742	I608
D1503	H1301		V1118	D994	R876	K743	R612
R1504	R1304		A1137	R997	D880	L744	D616
L1508			M1140	S998	V885	L754	R617
A1509			S1141	W999		P755	Q631
R1510	I1308		A1142	A1014	S765	R756	V634
L1511	M1311		G1143	I1037			L635
A1512	L1312		V1144	S1038	D888	E769	R636
R1522	V1313		T1162	P1039	K889	R774	S856
A1523	D1318		D1180	Q1040	G890		V857
L1524			N1190	V1041	V901	A779	T664
E1536	V1332		M1194	R1042	S904	G781	I669
K1541			D1195	L1047	W908	R784	D670
			L1196	V1051	D922	W785	L671
			N1203	E1082	H923	R788	P672
			S1206	T1055	K924	D791	E673
			L1207	P1056	I928	E795	A674
			L1208		W934	A804	S679
					M944	V805	T662
							R685

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	32441	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	0.058	Depositor
Minimum map value	-0.021	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	0.09	0/8502	0.22	0/11541
1	B	0.09	0/8502	0.22	0/11541
1	C	0.09	0/8502	0.22	0/11541
1	D	0.09	0/8502	0.22	0/11541
All	All	0.09	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	165	0
1	B	8350	0	8301	155	0
1	C	8350	0	8301	158	0
1	D	8350	0	8301	163	0
2	A	44	0	26	4	0
2	B	44	0	26	4	0
2	C	44	0	26	4	0
2	D	44	0	26	4	0
All	All	33576	0	33308	633	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 9.

The worst 5 of 633 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:546:LEU:HD22	1:B:546:LEU:HD22	1.54	0.87
1:D:1037:ILE:HB	1:D:1052:GLU:HA	1.69	0.74
1:B:1037:ILE:HB	1:B:1052:GLU:HA	1.69	0.74
1:C:1037:ILE:HB	1:C:1052:GLU:HA	1.69	0.73
1:A:1037:ILE:HB	1:A:1052:GLU:HA	1.69	0.72

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	1071/1611 (66%)	1055 (98%)	16 (2%)	0	100	100
1	B	1071/1611 (66%)	1056 (99%)	15 (1%)	0	100	100
1	C	1071/1611 (66%)	1056 (99%)	15 (1%)	0	100	100
1	D	1071/1611 (66%)	1055 (98%)	16 (2%)	0	100	100
All	All	4284/6444 (66%)	4222 (99%)	62 (1%)	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	877/1294 (68%)	876 (100%)	1 (0%)	88	87
1	B	877/1294 (68%)	876 (100%)	1 (0%)	88	87
1	C	877/1294 (68%)	876 (100%)	1 (0%)	88	87
1	D	877/1294 (68%)	876 (100%)	1 (0%)	88	87
All	All	3508/5176 (68%)	3504 (100%)	4 (0%)	87	87

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

Mol	Chain	Res	Type
1	A	1051	VAL
1	B	1051	VAL
1	C	1051	VAL
1	D	1051	VAL

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	949	GLN
1	D	984	HIS
1	D	1225	ASN
1	B	984	HIS
1	B	949	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 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	D	1601	-	46,48,48	0.65	1 (2%)	64,73,73	0.60	1 (1%)
2	NAD	A	1601	-	46,48,48	0.64	1 (2%)	64,73,73	0.60	1 (1%)
2	NAD	B	1601	-	46,48,48	0.64	1 (2%)	64,73,73	0.59	1 (1%)
2	NAD	C	1601	-	46,48,48	0.64	1 (2%)	64,73,73	0.59	0

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1601	NAD	C2N-N1N	2.85	1.38	1.35
2	A	1601	NAD	C2N-N1N	2.81	1.38	1.35
2	B	1601	NAD	C2N-N1N	2.81	1.38	1.35
2	C	1601	NAD	C2N-N1N	2.81	1.38	1.35

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1601	NAD	C6N-N1N-C2N	-2.06	120.12	121.88
2	B	1601	NAD	C6N-N1N-C2N	-2.03	120.15	121.88
2	A	1601	NAD	C6N-N1N-C2N	-2.00	120.17	121.88

There are no chirality outliers.



5 of 8 torsion outliers are listed below:

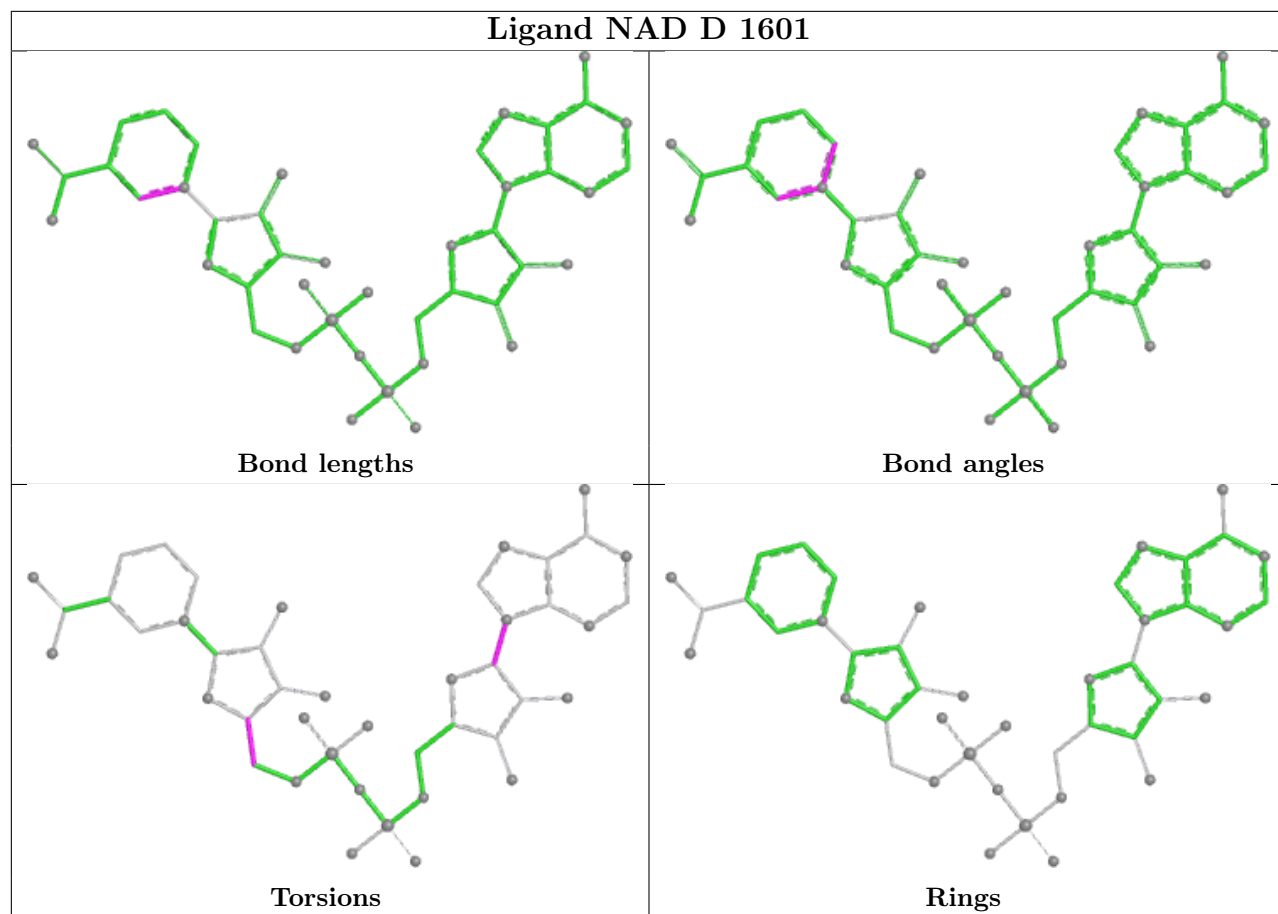
Mol	Chain	Res	Type	Atoms
2	A	1601	NAD	C2B-C1B-N9A-C8A
2	B	1601	NAD	C2B-C1B-N9A-C8A
2	C	1601	NAD	C2B-C1B-N9A-C8A
2	D	1601	NAD	C2B-C1B-N9A-C8A
2	A	1601	NAD	O4D-C4D-C5D-O5D

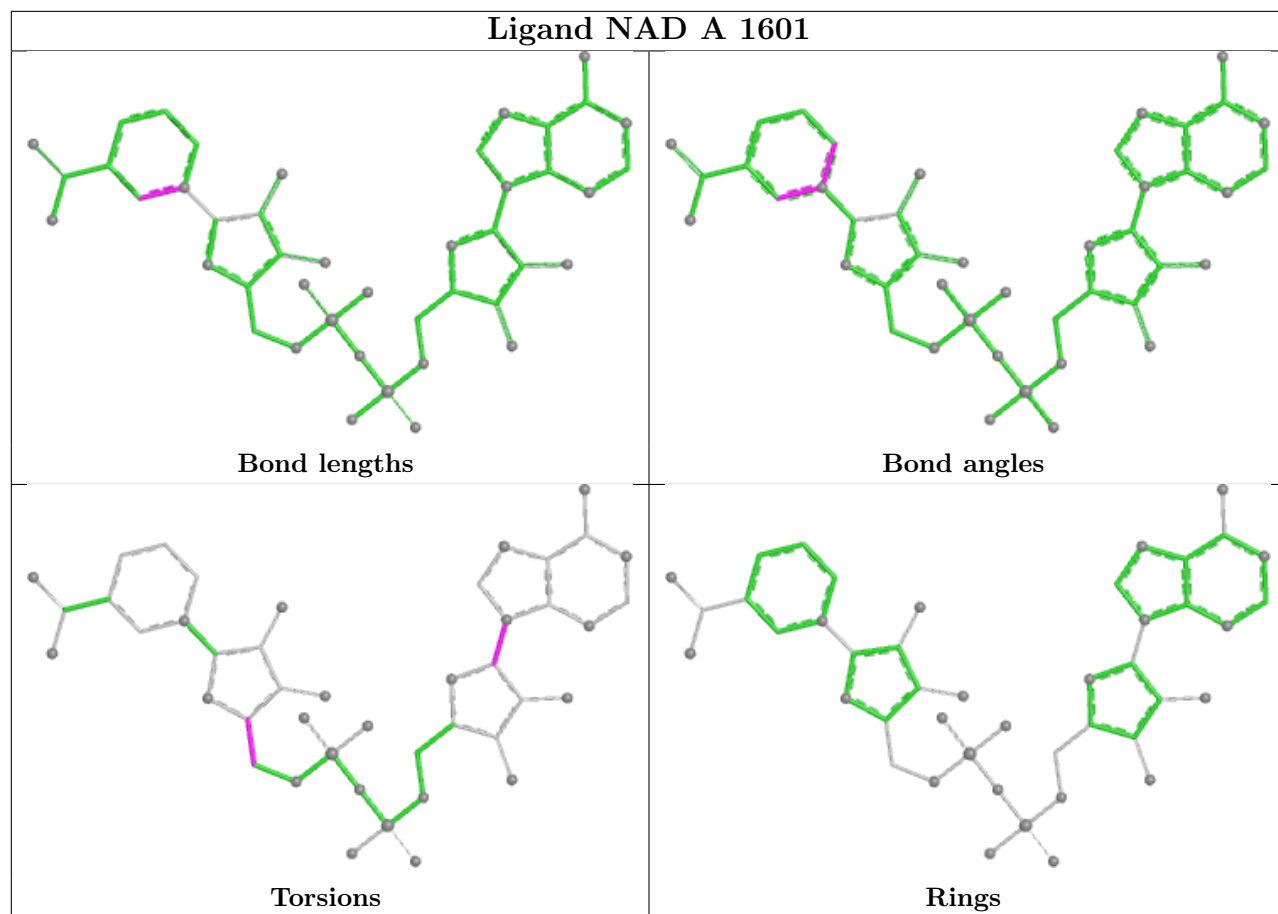
There are no ring outliers.

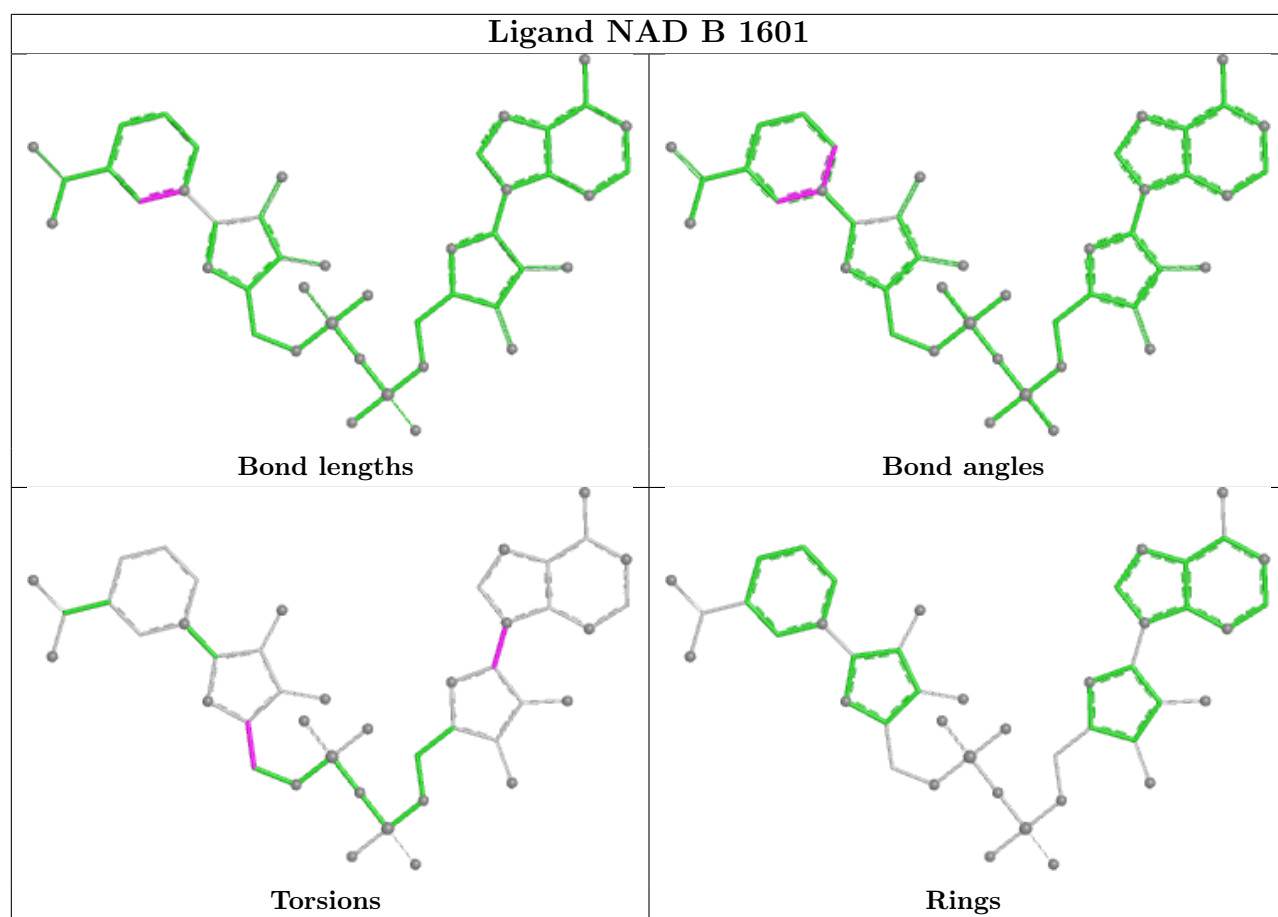
4 monomers are involved in 16 short contacts:

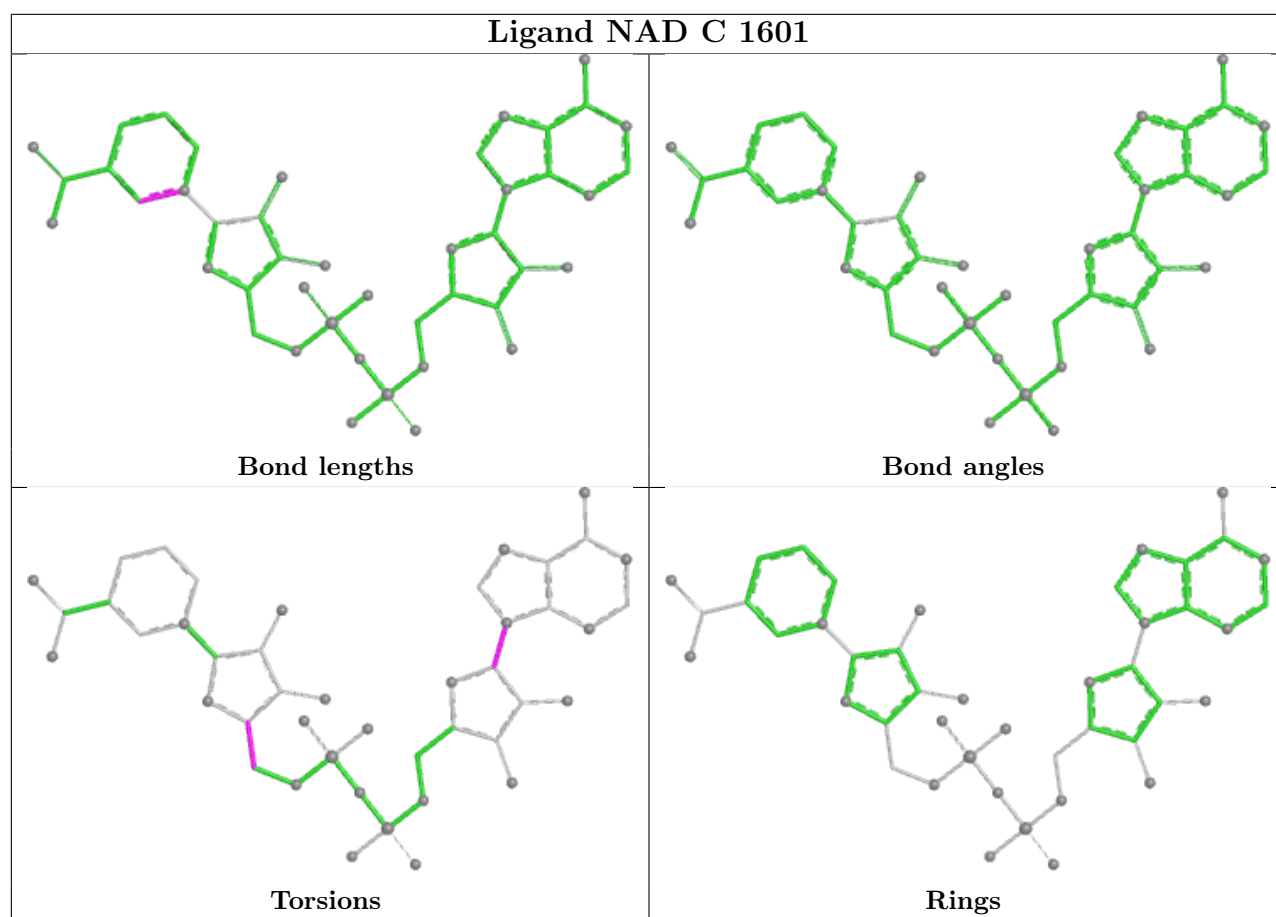
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1601	NAD	4	0
2	A	1601	NAD	4	0
2	B	1601	NAD	4	0
2	C	1601	NAD	4	0

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.

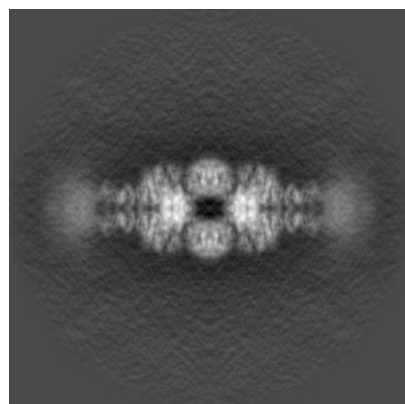
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52421. These allow visual inspection of the internal detail of the map and identification of artifacts.

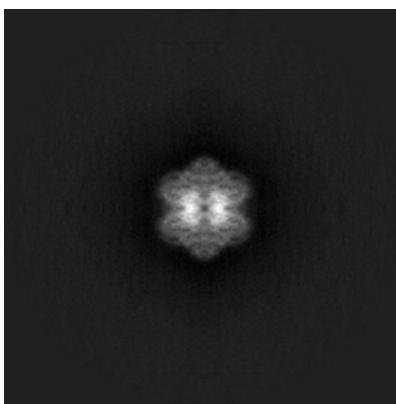
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

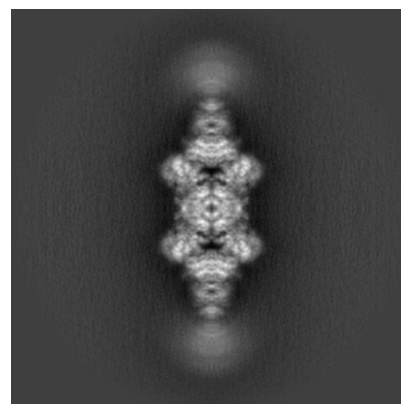
#### 6.1.1 Primary map



X

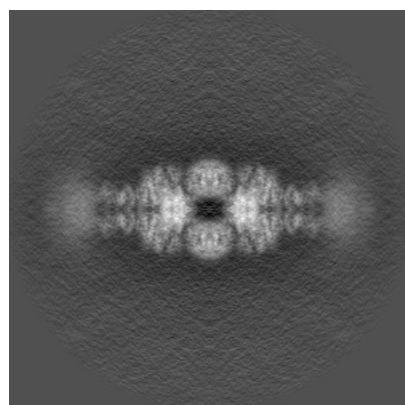


Y

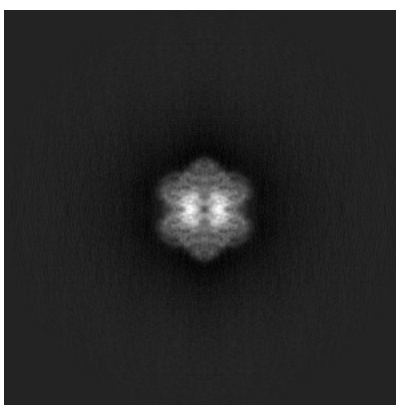


Z

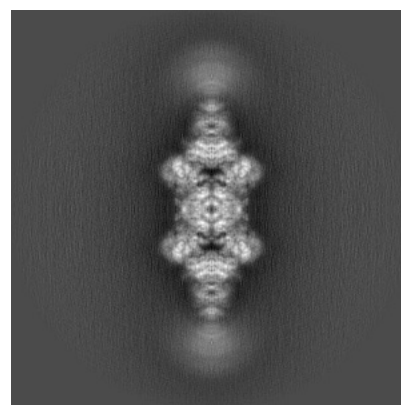
#### 6.1.2 Raw map



X



Y

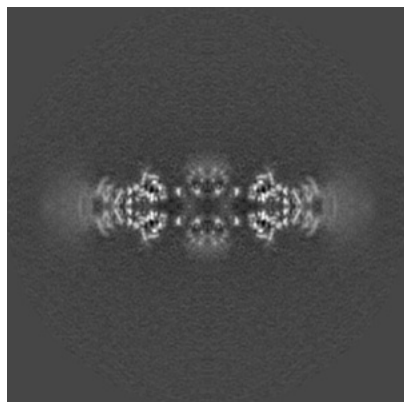


Z

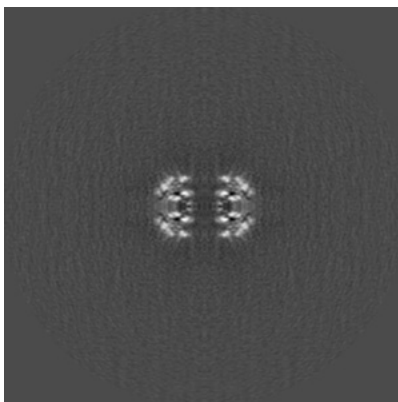
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

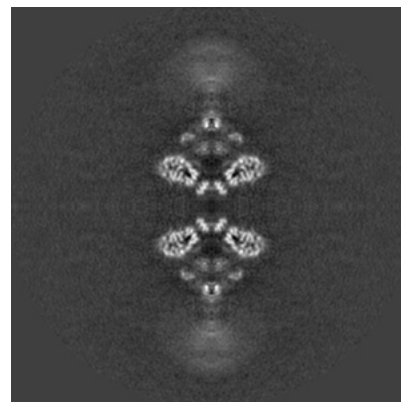
### 6.2.1 Primary map



X Index: 170

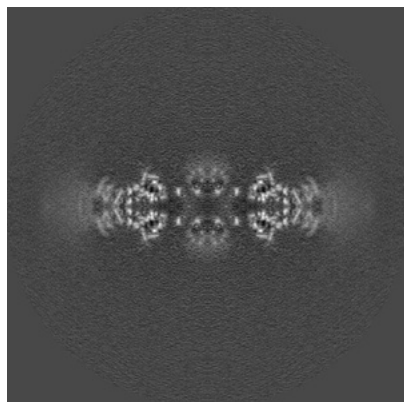


Y Index: 170

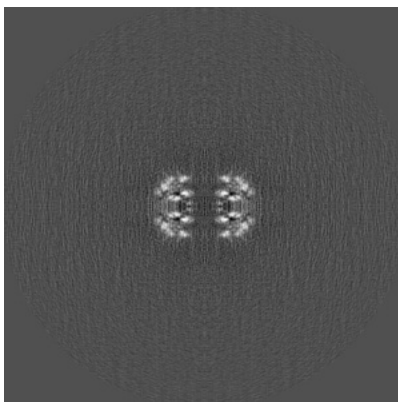


Z Index: 170

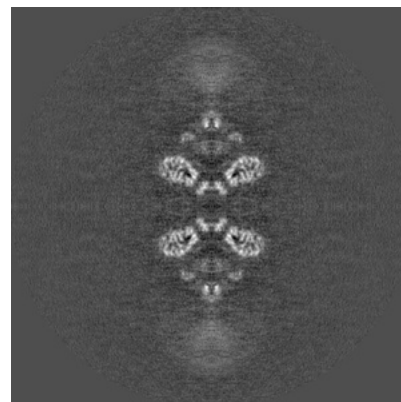
### 6.2.2 Raw map



X Index: 170



Y Index: 170

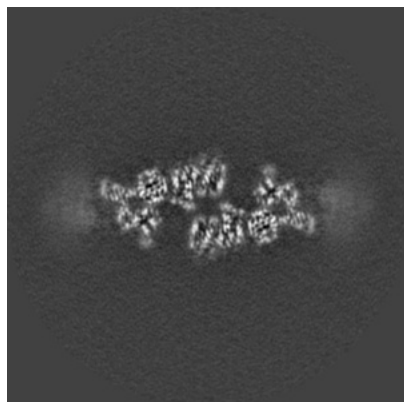


Z Index: 170

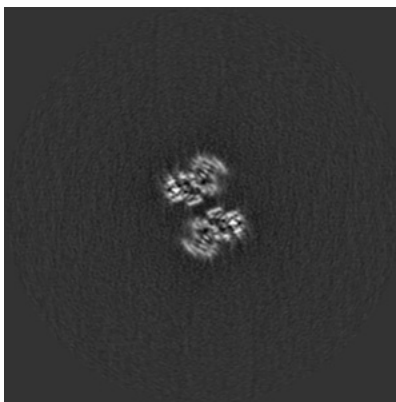
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

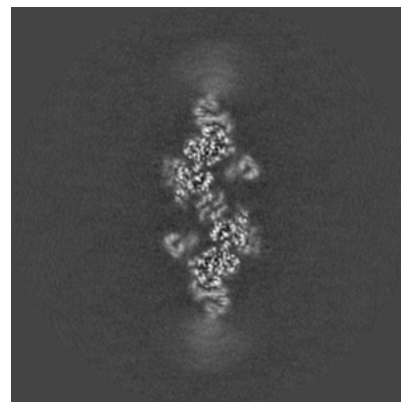
### 6.3.1 Primary map



X Index: 163

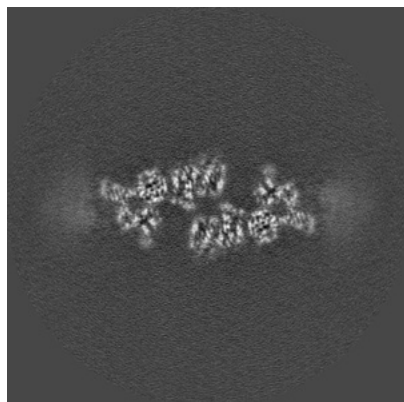


Y Index: 142

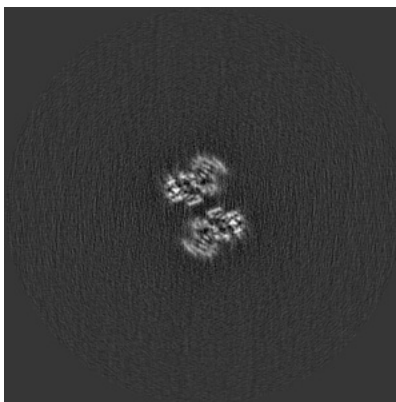


Z Index: 159

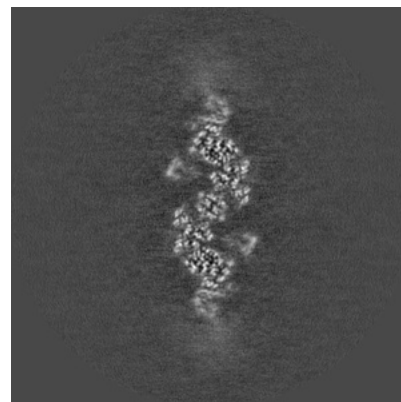
### 6.3.2 Raw map



X Index: 163



Y Index: 142



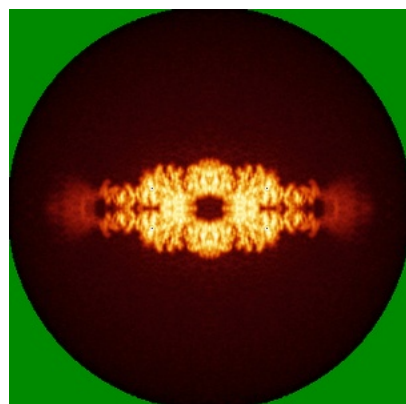
Z Index: 183

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

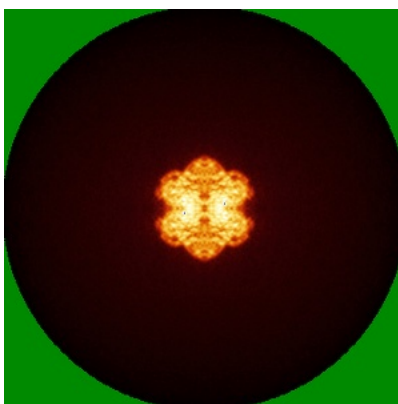


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

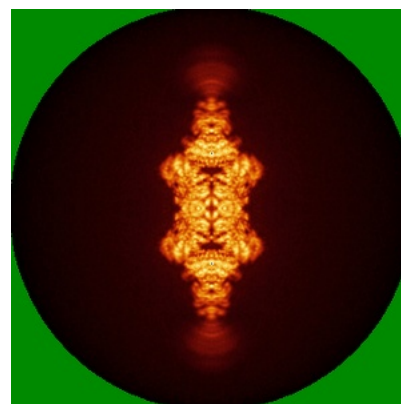
### 6.4.1 Primary map



X

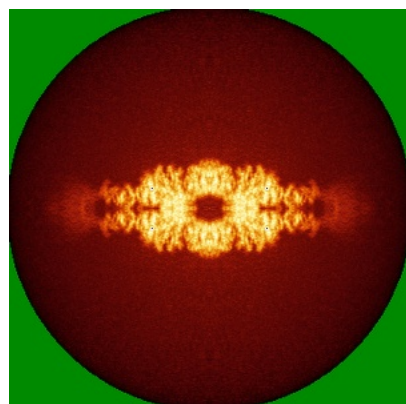


Y

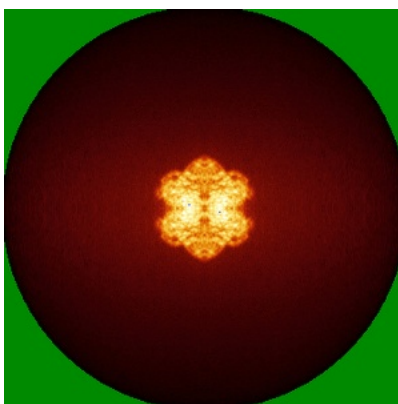


Z

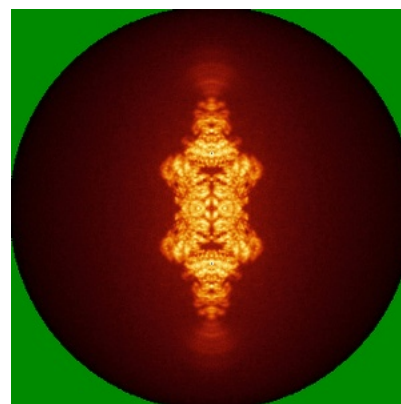
### 6.4.2 Raw map



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.

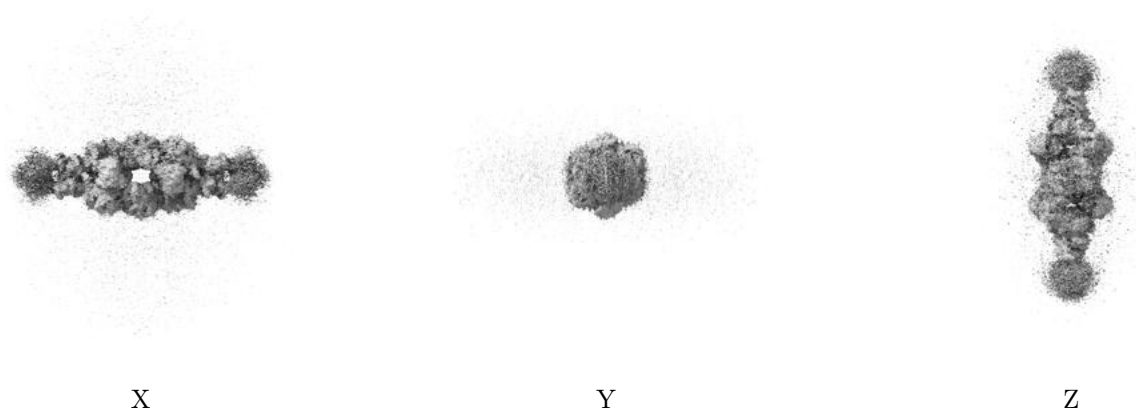
## 6.5 Orthogonal surface views [i](#)

### 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.

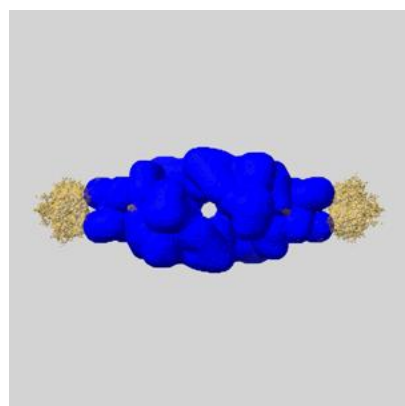
## 6.6 Mask visualisation [i](#)

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

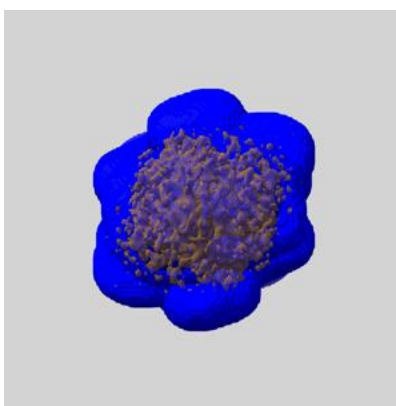
A mask typically either:

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

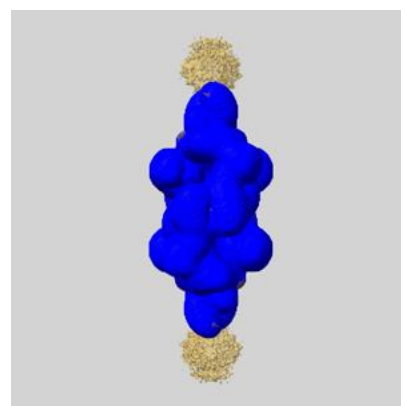
### 6.6.1 emd\_52421\_msk\_1.map [i](#)



X



Y

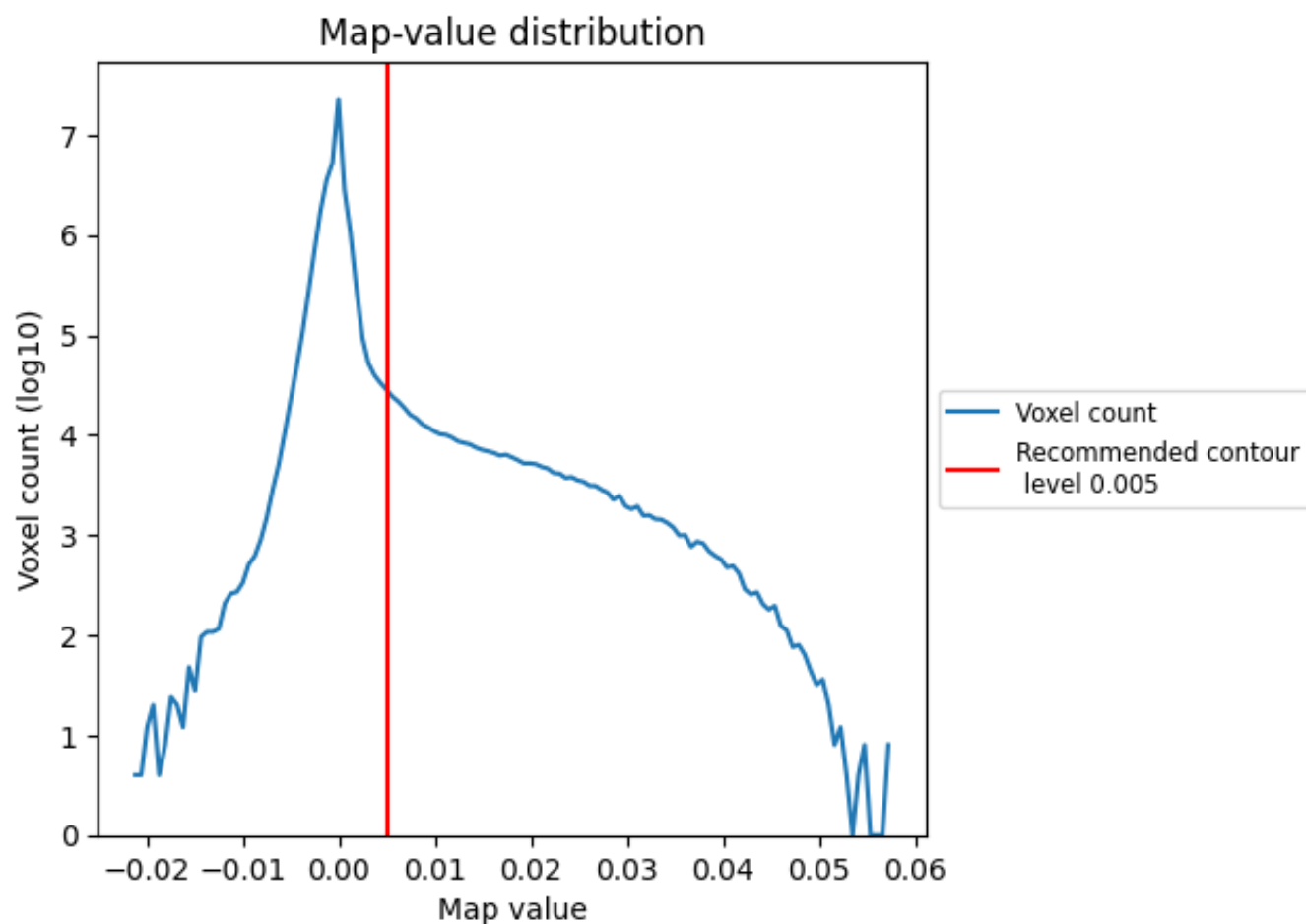


Z

## 7 Map analysis [i](#)

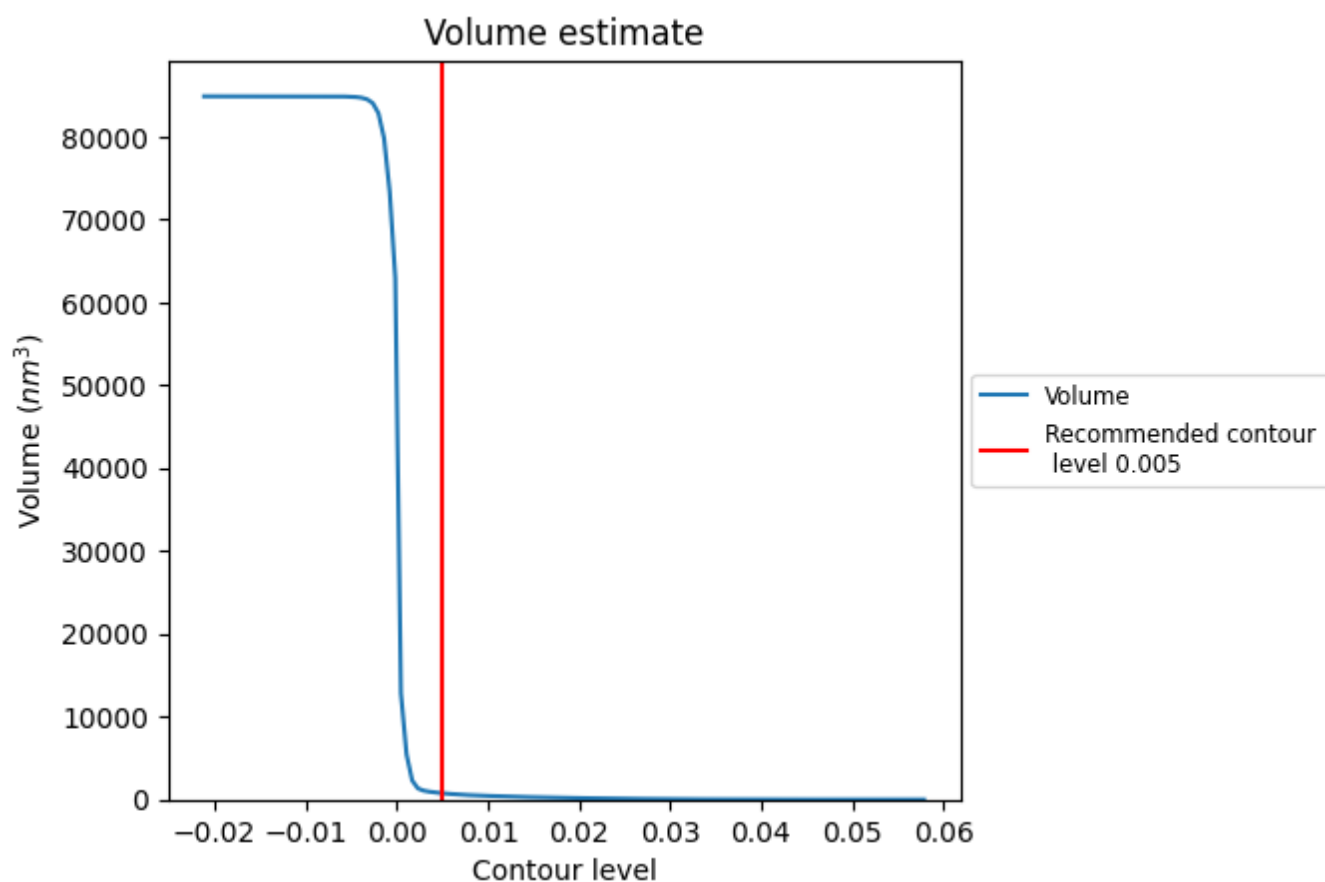
This section contains the results of statistical analysis of the map.

### 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.

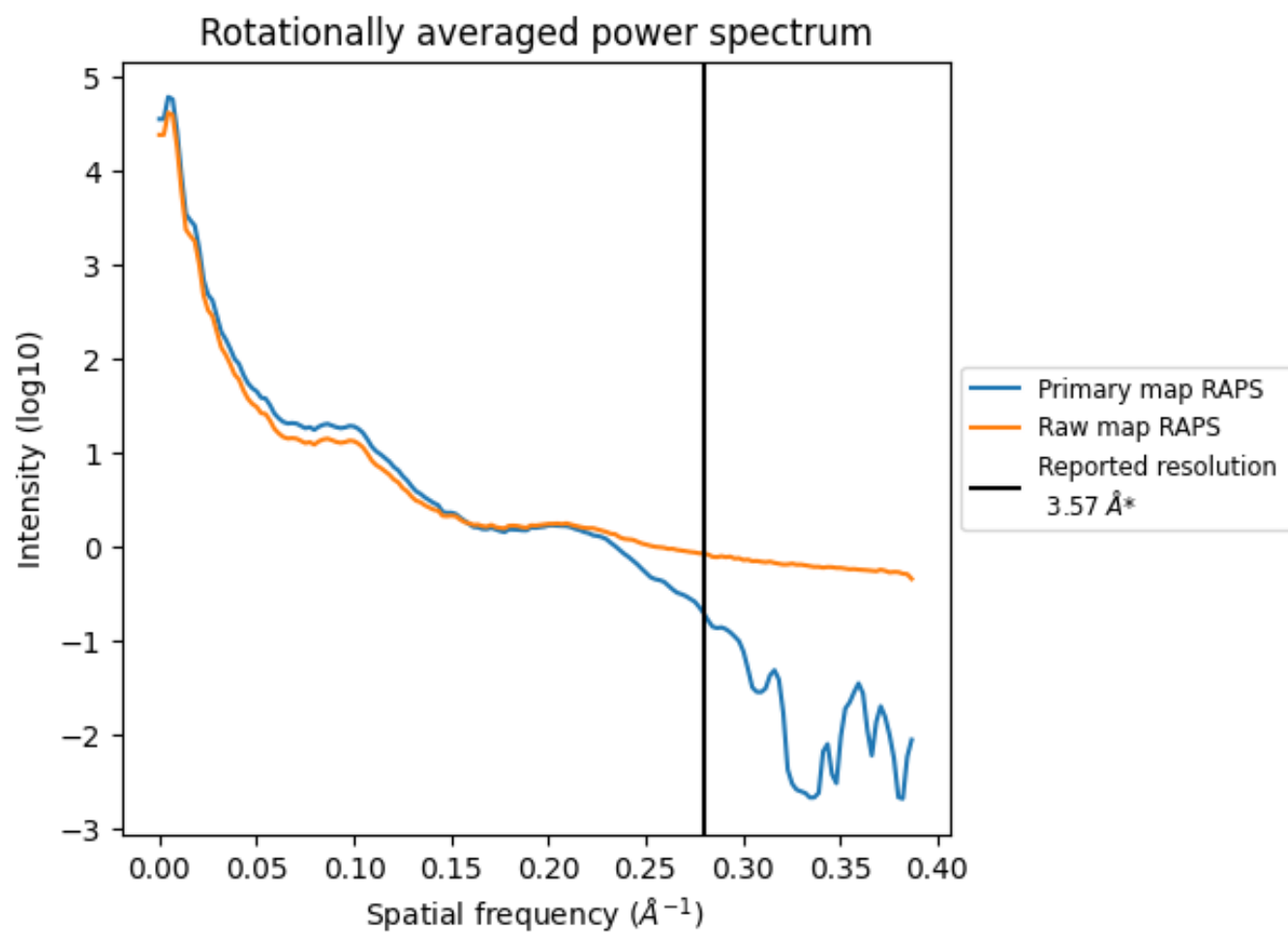
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 764  $\text{nm}^3$ ; this corresponds to an approximate mass of 690 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 ⓘ

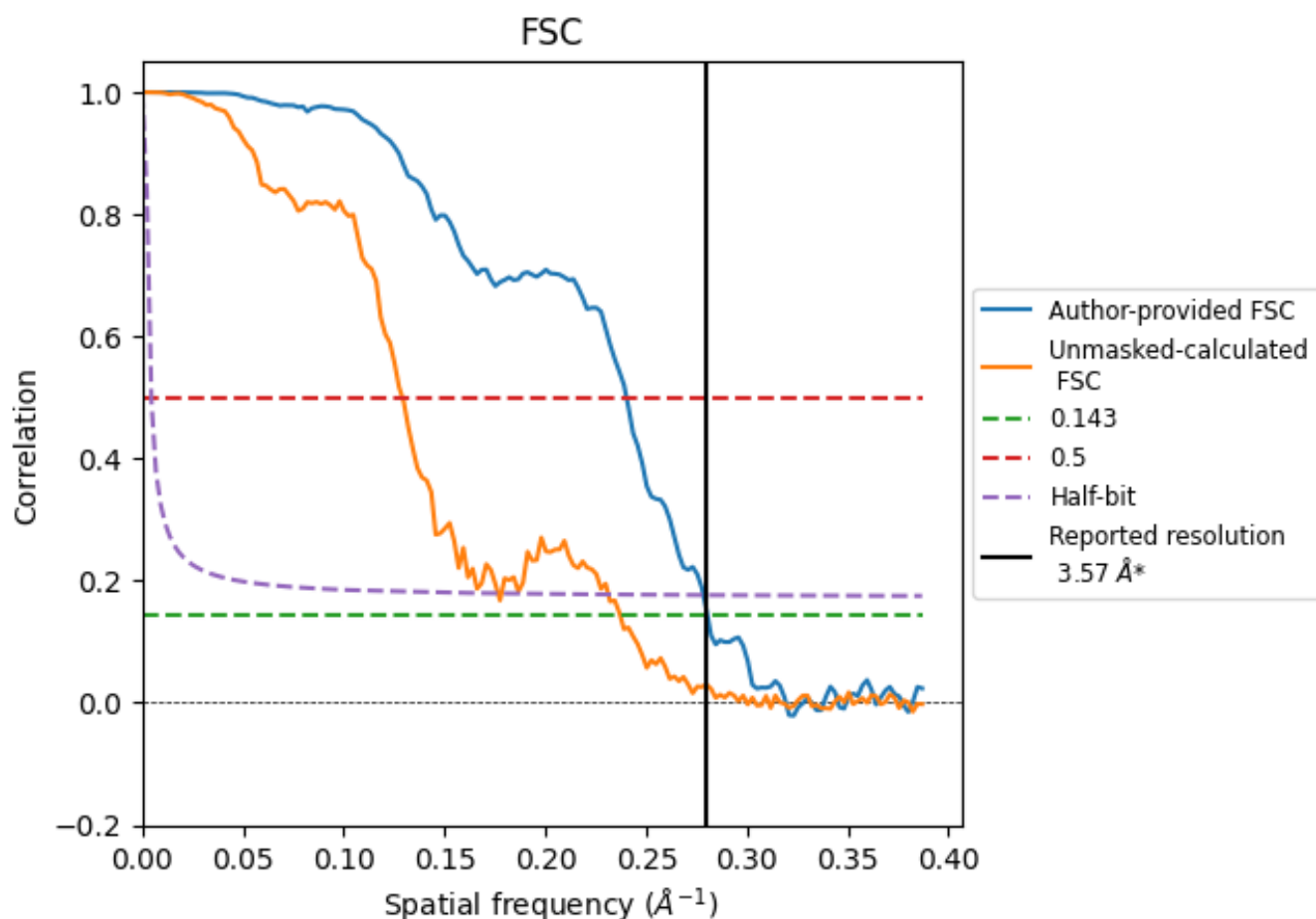


\*Reported resolution corresponds to spatial frequency of 0.280 Å<sup>-1</sup>

## 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 0.280  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.57	-	-
Author-provided FSC curve	3.57	4.16	3.59
Unmasked-calculated*	4.22	7.75	5.67

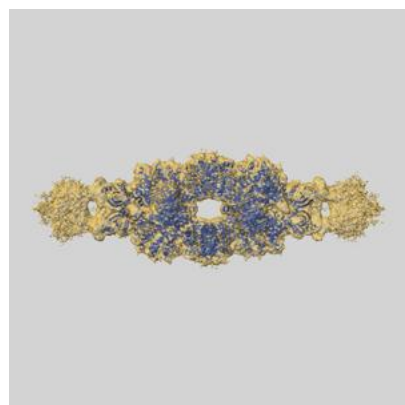
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.22 differs from the reported value 3.57 by more than 10 %



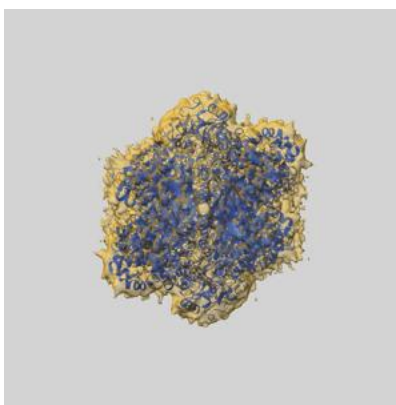
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-52421 and PDB model 9HUZ. Per-residue inclusion information can be found in section [3](#) on page [7](#).

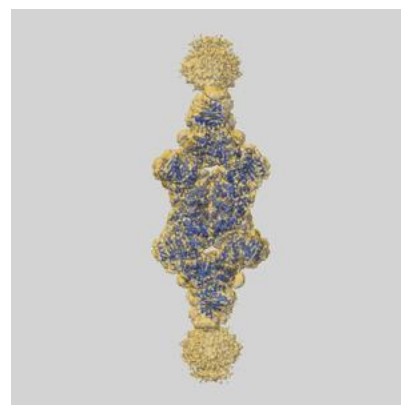
### 9.1 Map-model overlay [i](#)



X



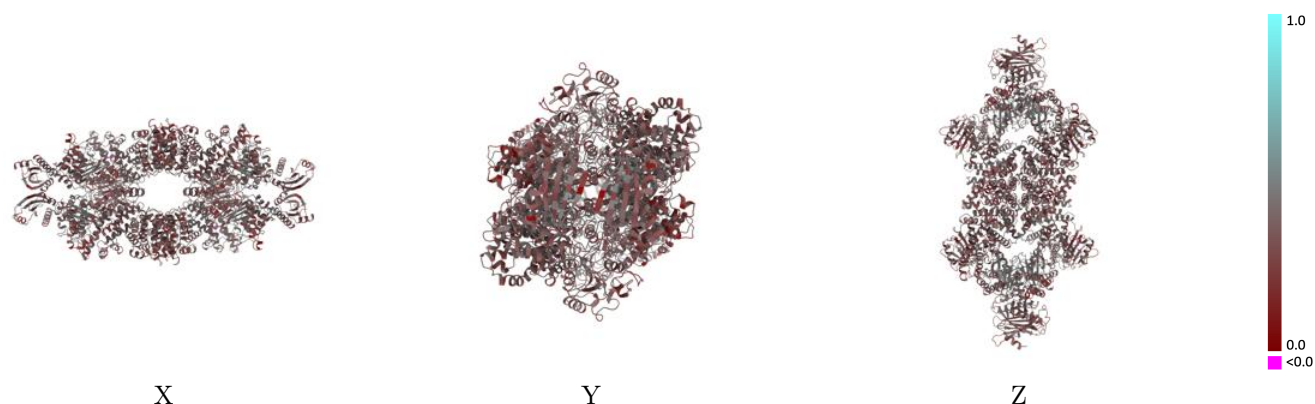
Y



Z

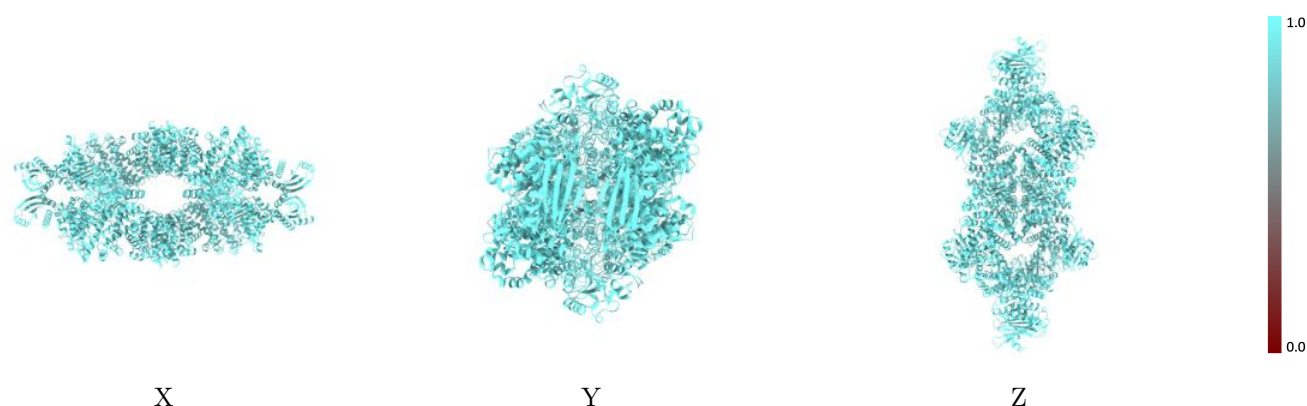
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



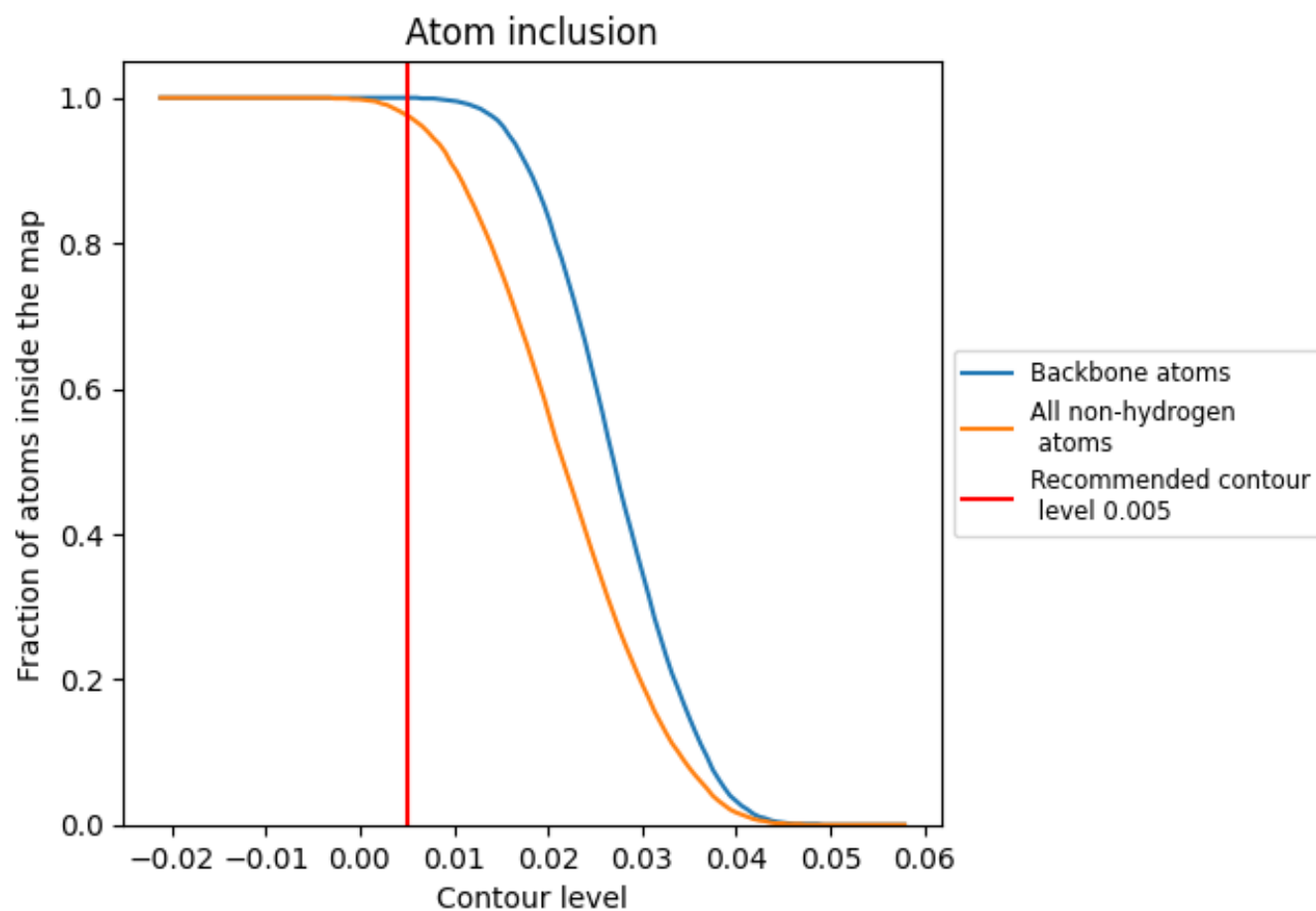
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 98% 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> 0.9760	<div></div> 0.3540
A	<div></div> 0.9760	<div></div> 0.3550
B	<div></div> 0.9760	<div></div> 0.3540
C	<div></div> 0.9760	<div></div> 0.3520
D	<div></div> 0.9760	<div></div> 0.3550

