



## wwPDB EM Validation Summary Report ⓘ

May 10, 2025 – 12:29 PM EDT

PDB ID : 8VF7 / pdb\_00008vf7  
EMDB ID : EMD-43187  
Title : Modifying portion of human FASN with NADPH and the ACP at the ER domain  
Authors : Schultz, K.; Marmorstein, R.  
Deposited on : 2023-12-21  
Resolution : 3.20 Å (reported)  
Based on initial models : ., 2CG5

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.dev118  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

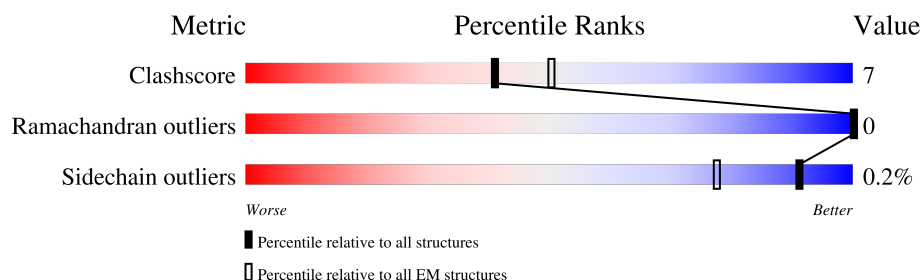
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.20 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	2553	
2	B	2553	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 38890 atoms, of which 19416 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 Fatty acid synthase.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1216	Total	C	H	N	O	S	0	0
			18703	5928	9357	1644	1735	39		

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-31	MET	-	initiating methionine	UNP P49327
A	-30	SER	-	expression tag	UNP P49327
A	-29	TYR	-	expression tag	UNP P49327
A	-28	TYR	-	expression tag	UNP P49327
A	-27	ASP	-	expression tag	UNP P49327
A	-26	TYR	-	expression tag	UNP P49327
A	-25	LYS	-	expression tag	UNP P49327
A	-24	ASP	-	expression tag	UNP P49327
A	-23	ASP	-	expression tag	UNP P49327
A	-22	ASP	-	expression tag	UNP P49327
A	-21	ASP	-	expression tag	UNP P49327
A	-20	LYS	-	expression tag	UNP P49327
A	-19	ASP	-	expression tag	UNP P49327
A	-18	TYR	-	expression tag	UNP P49327
A	-17	ASP	-	expression tag	UNP P49327
A	-16	ILE	-	expression tag	UNP P49327
A	-15	PRO	-	expression tag	UNP P49327
A	-14	THR	-	expression tag	UNP P49327
A	-13	THR	-	expression tag	UNP P49327
A	-12	GLU	-	expression tag	UNP P49327
A	-11	ASN	-	expression tag	UNP P49327
A	-10	LEU	-	expression tag	UNP P49327
A	-9	TYR	-	expression tag	UNP P49327
A	-8	PHE	-	expression tag	UNP P49327
A	-7	GLN	-	expression tag	UNP P49327
A	-6	GLY	-	expression tag	UNP P49327
A	-5	ALA	-	expression tag	UNP P49327
A	-4	MET	-	expression tag	UNP P49327

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP P49327
A	-2	SER	-	expression tag	UNP P49327
A	-1	GLY	-	expression tag	UNP P49327
A	0	ILE	-	expression tag	UNP P49327
A	1	PRO	-	expression tag	UNP P49327
A	1151	THR	LYS	conflict	UNP P49327
A	2512	LEU	-	expression tag	UNP P49327
A	2513	GLU	-	expression tag	UNP P49327
A	2514	HIS	-	expression tag	UNP P49327
A	2515	HIS	-	expression tag	UNP P49327
A	2516	HIS	-	expression tag	UNP P49327
A	2517	HIS	-	expression tag	UNP P49327
A	2518	HIS	-	expression tag	UNP P49327
A	2519	HIS	-	expression tag	UNP P49327
A	2520	HIS	-	expression tag	UNP P49327
A	2521	HIS	-	expression tag	UNP P49327

- Molecule 2 is a protein called Fatty acid synthase.

Mol	Chain	Residues	Atoms							AltConf	Trace
2	B	1289	Total	C	H	N	O	P	S	0	0
			19891	6290	9955	1750	1854	1	41		

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-31	MET	-	initiating methionine	UNP P49327
B	-30	SER	-	expression tag	UNP P49327
B	-29	TYR	-	expression tag	UNP P49327
B	-28	TYR	-	expression tag	UNP P49327
B	-27	ASP	-	expression tag	UNP P49327
B	-26	TYR	-	expression tag	UNP P49327
B	-25	LYS	-	expression tag	UNP P49327
B	-24	ASP	-	expression tag	UNP P49327
B	-23	ASP	-	expression tag	UNP P49327
B	-22	ASP	-	expression tag	UNP P49327
B	-21	ASP	-	expression tag	UNP P49327
B	-20	LYS	-	expression tag	UNP P49327
B	-19	ASP	-	expression tag	UNP P49327
B	-18	TYR	-	expression tag	UNP P49327
B	-17	ASP	-	expression tag	UNP P49327
B	-16	ILE	-	expression tag	UNP P49327

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	PRO	-	expression tag	UNP P49327
B	-14	THR	-	expression tag	UNP P49327
B	-13	THR	-	expression tag	UNP P49327
B	-12	GLU	-	expression tag	UNP P49327
B	-11	ASN	-	expression tag	UNP P49327
B	-10	LEU	-	expression tag	UNP P49327
B	-9	TYR	-	expression tag	UNP P49327
B	-8	PHE	-	expression tag	UNP P49327
B	-7	GLN	-	expression tag	UNP P49327
B	-6	GLY	-	expression tag	UNP P49327
B	-5	ALA	-	expression tag	UNP P49327
B	-4	MET	-	expression tag	UNP P49327
B	-3	GLY	-	expression tag	UNP P49327
B	-2	SER	-	expression tag	UNP P49327
B	-1	GLY	-	expression tag	UNP P49327
B	0	ILE	-	expression tag	UNP P49327
B	1	PRO	-	expression tag	UNP P49327
B	1151	THR	LYS	conflict	UNP P49327
B	2512	LEU	-	expression tag	UNP P49327
B	2513	GLU	-	expression tag	UNP P49327
B	2514	HIS	-	expression tag	UNP P49327
B	2515	HIS	-	expression tag	UNP P49327
B	2516	HIS	-	expression tag	UNP P49327
B	2517	HIS	-	expression tag	UNP P49327
B	2518	HIS	-	expression tag	UNP P49327
B	2519	HIS	-	expression tag	UNP P49327
B	2520	HIS	-	expression tag	UNP P49327
B	2521	HIS	-	expression tag	UNP P49327

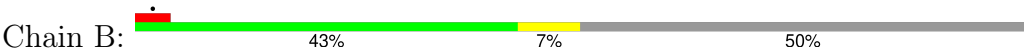
- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula:  $C_{21}H_{30}N_7O_{17}P_3$ ) (labeled as "Ligand of Interest" by depositor).





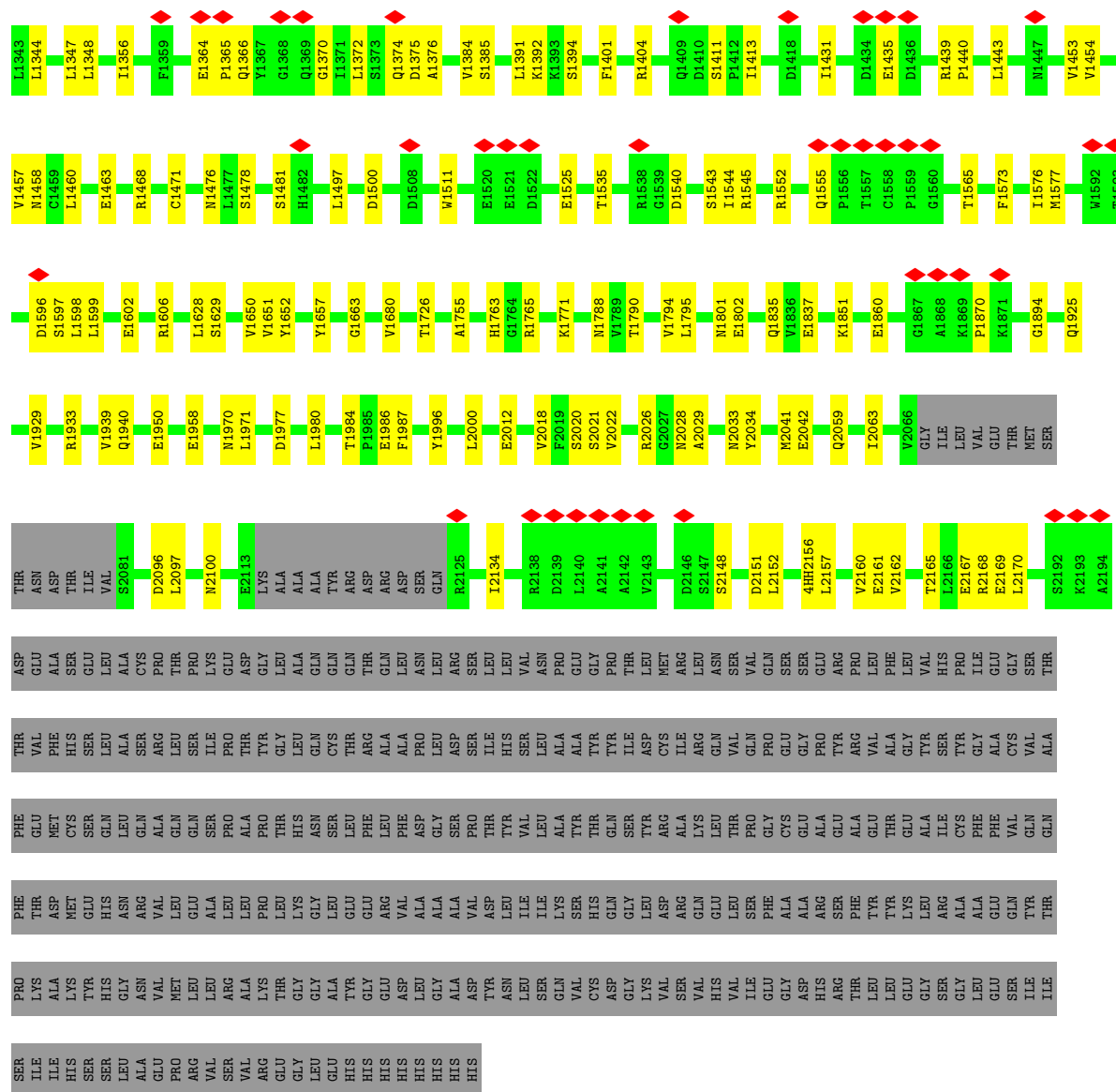
THR	LEU	THR	ALA	ARG	PRO	THR	SER	R1933	S1723	L1493	E1388	A1199	R1104	D877	ASP
LEU	THR	THR	GLU	ARG	LEU	LEU	GLN	V1939	T1726	L1497	L1343	Q1200	R1105	L899	ALA
GLY	LEU	GLY	VAL	ASP	LEU	LEU	ASP	Q1940	Q1730	D1500	R1349	V1201	Q1106	L905	ASN
VAL	GLN	VAL	THR	LEU	GLU	GLU	VAL	E1958	H1751	L1501	R1356	L1202	Q1107	L905	ASN
PRO	PRO	PRO	PRO	GLY	PRO	PRO	ALA	L1971	V1732	V1502	I1356	Q1204	E1108	E934	LEU
ILE	ALA	ILE	ILE	ALA	ILE	ILE	ALA	A1972	V1733	M1503	T1361	E1205	P1121	E939	PHE
THR	THR	THR	THR	THR	THR	THR	HIS	V1973	T1736	E1521	S1362	R1206	L1144	E945	PRO
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ILE	G1737	G1738	R1545	T1363	P1207	V1145	E945	VAL
GLU	GLU	GLU	GLU	GLU	GLU	GLU	LEU	G1738	E1760	Q1555	L1148	K1208	L1148	V958	PHE
VAL	VAL	VAL	VAL	VAL	VAL	VAL	GLY	E1760	L1753	P1556	GLN	P1210	THR	PRO	PRO
ALA	ALA	ALA	ALA	ALA	ALA	ALA	ILE	L1753	Q1555	P1556	THR	P1210	THR	ALA	ALA
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	Q1754	T1557	P1556	THR	D1220	THR	ARG	ARG
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	A1755	C1558	P1557	THR	M1235	VAL	GLY	GLY
ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	R1765	P1559	C1558	THR	L1238	THR	THR	THR
ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	G1765	G1560	P1559	THR	M1240	GLN	PRO	PRO
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	I1769	S1570	S1570	THR	K1239	GLN	LEU	LEU
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	V1794	S1570	S1570	THR	M1240	GLY	SER	SER
THR	THR	THR	THR	THR	THR	THR	THR	E1802	S1594	S1594	THR	E1244	LEU	PRO	PRO
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	S1803	Q1595	Q1595	THR	V1245	LEU	LEU	LEU
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	S1803	D1596	D1596	THR	V1246	VAL	ILE	ILE
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	F1831	S1597	S1597	THR	L1246	PRO	TRP	TRP
GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	G1832	E1502	E1502	THR	S1261	GLY	ASP	ASP
THR	THR	THR	THR	THR	THR	THR	THR	G1833	D1507	D1507	THR	P1262	LEU	HIS	HIS
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	V1836	D1507	D1507	THR	L1265	ASP	SER	SER
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	I1849	K1611	K1611	THR	L1270	GLY	LEU	LEU
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	G1850	V1617	V1617	THR	F1273	ALA	ALA	ALA
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	K1851	L1622	L1622	THR	E1281	GLN	TRP	TRP
THR	THR	THR	THR	THR	THR	THR	THR	V1854	L1622	L1622	THR	A1173	ASP	PRO	PRO
ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	Q1855	V1626	V1626	THR	S1174	ALA	ALA	ALA
VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	E1860	L1627	L1627	THR	Q1175	GLU	GLU	GLU
ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	L1628	L1628	L1628	THR	Q1176	PHE	PHE	PHE
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	E1867	F1632	F1632	THR	E1177	PRO	PRO	PRO
GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	A1868	L1633	L1633	THR	R1180	ASN	ASN	ASN
THR	THR	THR	THR	THR	THR	THR	THR	K1869	A1846	A1846	THR	L1181	GLY	GLY	GLY
ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	I1876	V1650	V1650	THR	A1184	SER	SER	SER
ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	L1893	V1651	V1651	THR	A1185	PRO	PRO	PRO
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	L1914	Y1652	Y1652	THR	C1186	SER	SER	SER
VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	T1915	R1662	R1662	THR	R1187	ALA	ALA	ALA
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	R1917	E1669	E1669	THR	L1188	VAL	VAL	VAL
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	Q1928	S1916	S1916	THR	Q1189	GLY	GLY	GLY
THR	THR	THR	THR	THR	THR	THR	THR	R1931	R1917	R1917	THR	L1190	THR	THR	THR
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	W1932	L1671	L1671	THR	N1191	GLY	GLY	GLY
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	Q1928	L1671	L1671	THR	G1192	ALA	ALA	ALA
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	W1932	Y1707	Y1707	THR	N1193	PRO	PRO	PRO
THR	THR	THR	THR	THR	THR	THR	THR	Q1714	Q1714	Q1714	THR	L1194	SER	SER	SER
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	Q1714	Q1714	Q1714	THR	Q1195	THR	THR	THR
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	Q1714	Q1714	Q1714	THR	L1196	GLY	GLY	GLY
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	Q1714	Q1714	Q1714	THR	E1197	ALA	ALA	ALA
THR	THR	THR	THR	THR	THR	THR	THR	Q1714	Q1714	Q1714	THR	L1198	SER	SER	SER

● Molecule 2: Fatty acid synthase









## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	103038	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 ( $e^-/\text{\AA}^2$ )	52.4	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.795	Depositor
Minimum map value	-0.239	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.221	Depositor
Map size ( $\text{\AA}$ )	384.84, 384.84, 384.84	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.069, 1.069, 1.069	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: NDP, 4HH

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	0.11	0/9552	0.24	0/12985
2	B	0.11	0/10114	0.25	0/13741
All	All	0.11	0/19666	0.24	0/26726

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	9346	9357	9351	122	0
2	B	9936	9955	9971	143	0
3	A	96	52	52	7	0
3	B	96	52	52	11	0
All	All	19474	19416	19426	262	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 7.

The worst 5 of 262 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2156:4HH:HT3	3:B:2601:NDP:H2D	1.56	0.88
2:B:1577:MET:HE1	2:B:2156:4HH:HO2	1.57	0.84
2:B:1552:ARG:O	2:B:1555:GLN:NE2	2.14	0.81
1:A:1994:PRO:HB3	3:A:2602:NDP:N6A	1.99	0.77
2:B:1241:LYS:NZ	2:B:1307:LEU:O	2.19	0.76

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	1210/2553 (47%)	1182 (98%)	28 (2%)	0	100	100
2	B	1280/2553 (50%)	1250 (98%)	30 (2%)	0	100	100
All	All	2490/5106 (49%)	2432 (98%)	58 (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	1009/2117 (48%)	1006 (100%)	3 (0%)	91	96
2	B	1073/2116 (51%)	1072 (100%)	1 (0%)	92	98
All	All	2082/4233 (49%)	2078 (100%)	4 (0%)	91	97

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

Mol	Chain	Res	Type
1	A	985	LEU
1	A	1602	GLU
1	A	1854	VAL
2	B	1463	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	1107	GLN
2	B	1351	HIS
2	B	1251	HIS
2	B	1482	HIS
1	A	1845	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	4HH	B	2156	2	22,26,27	0.43	0	27,35,37	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	4HH	B	2156	2	-	20/33/35/37	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2156	4HH	C-CA-CB-OG
2	B	2156	4HH	CB-OG-P-O2P
2	B	2156	4HH	CB-OG-P-O3P
2	B	2156	4HH	O3P-CJ-CK-CL1
2	B	2156	4HH	O3P-CJ-CK-CL2

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2156	4HH	7	0

## 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	$\# Z  > 2$
3	NDP	B	2601	-	47,52,52	0.64	0	61,80,80	0.87	2 (3%)
3	NDP	A	2602	-	47,52,52	0.66	0	61,80,80	0.80	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NDP	A	2601	-	47,52,52	0.64	0	61,80,80	0.87	2 (3%)
3	NDP	B	2602	-	47,52,52	0.63	0	61,80,80	0.84	3 (4%)

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
3	NDP	B	2601	-	-	14/30/77/77	0/5/5/5
3	NDP	A	2602	-	-	8/30/77/77	0/5/5/5
3	NDP	A	2601	-	-	9/30/77/77	0/5/5/5
3	NDP	B	2602	-	-	9/30/77/77	0/5/5/5

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2601	NDP	P2B-O2B-C2B	-4.50	111.42	123.43
3	A	2602	NDP	P2B-O2B-C2B	-4.28	111.99	123.43
3	B	2601	NDP	P2B-O2B-C2B	-4.01	112.72	123.43
3	B	2602	NDP	P2B-O2B-C2B	-3.43	114.27	123.43
3	B	2602	NDP	C5A-C6A-N6A	2.24	123.72	120.31

There are no chirality outliers.

5 of 40 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2601	NDP	C5B-O5B-PA-O3
3	A	2601	NDP	C2N-C3N-C7N-N7N
3	A	2602	NDP	O4B-C4B-C5B-O5B
3	A	2602	NDP	C3B-C4B-C5B-O5B
3	A	2602	NDP	C5D-O5D-PN-O3

There are no ring outliers.

4 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2601	NDP	8	0

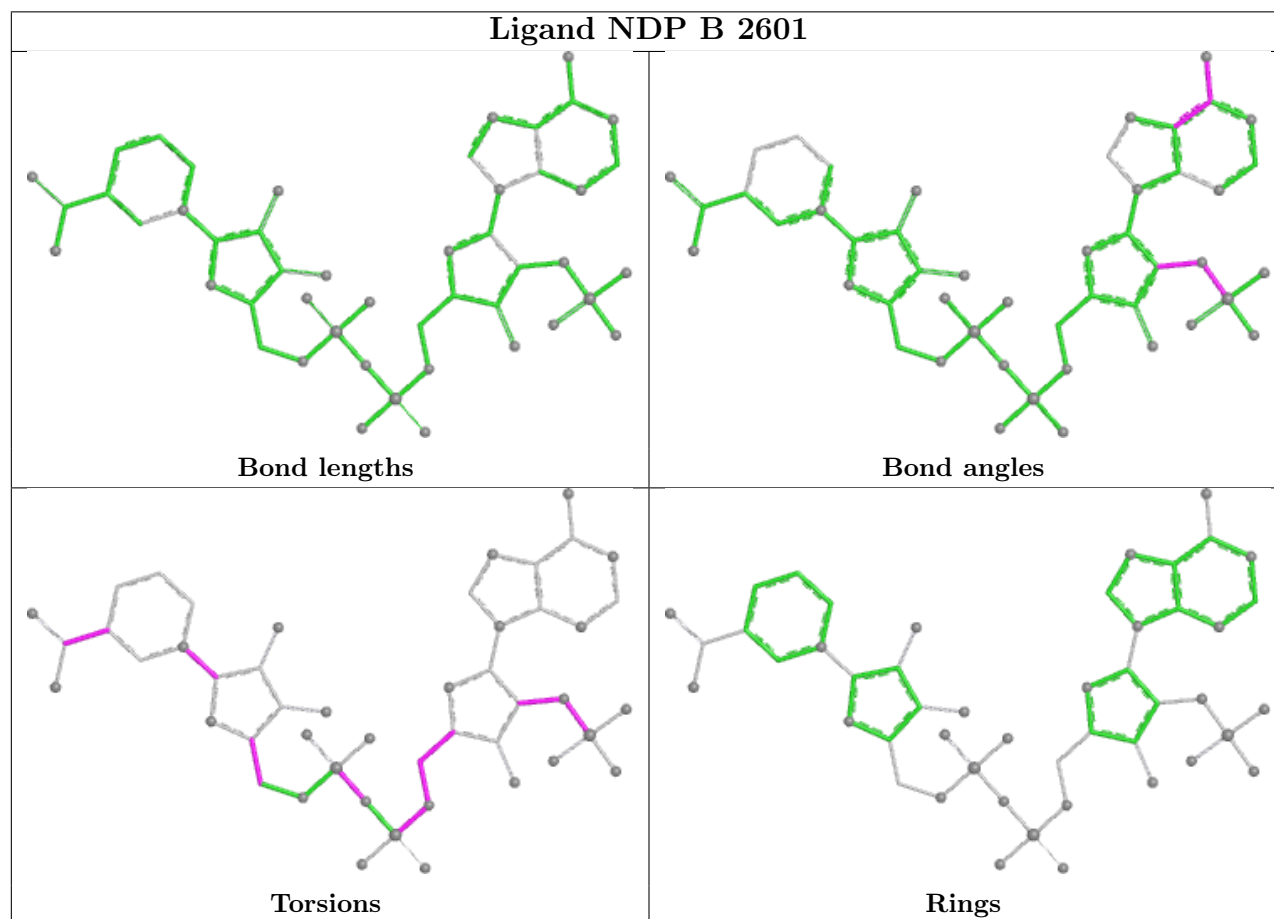
*Continued on next page...*

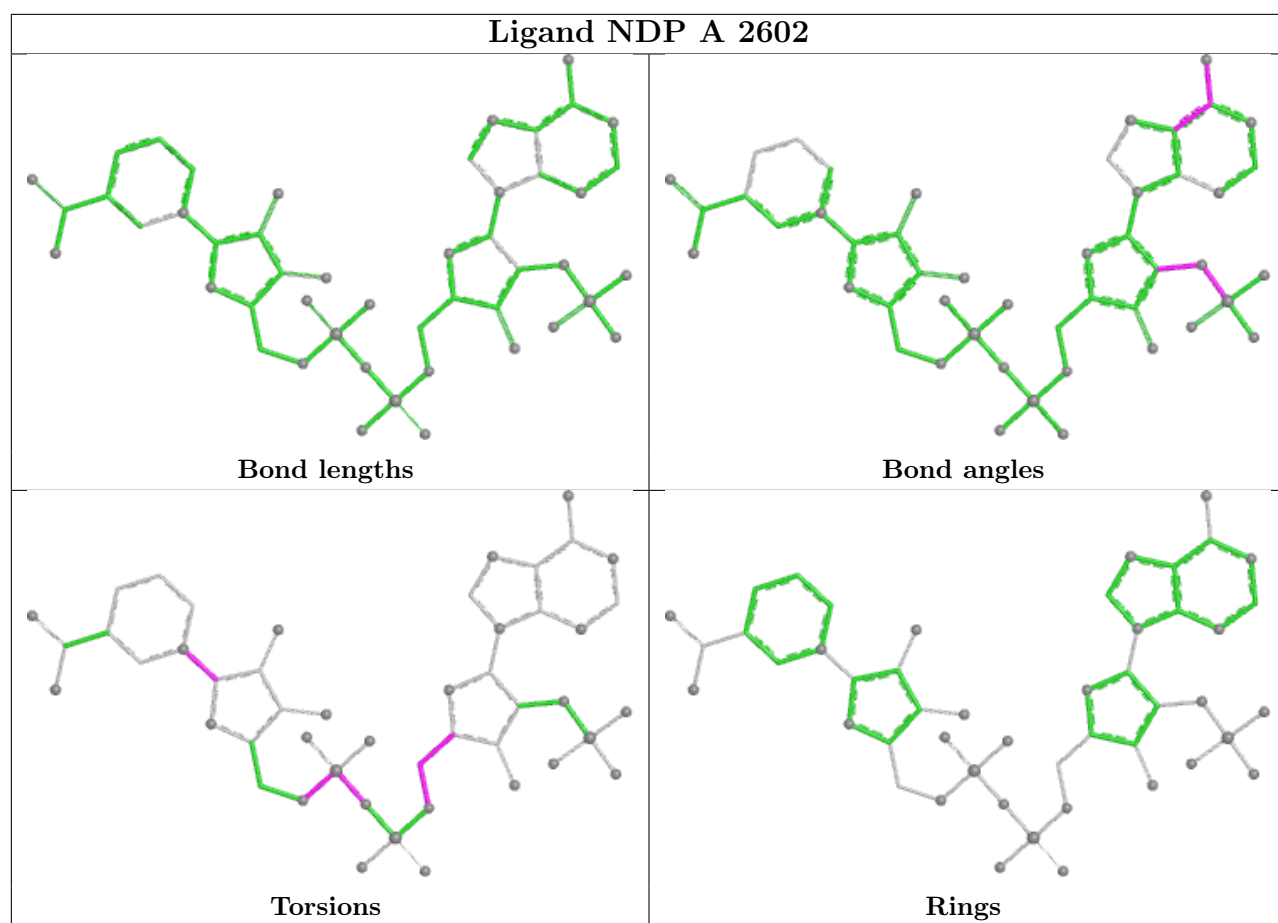


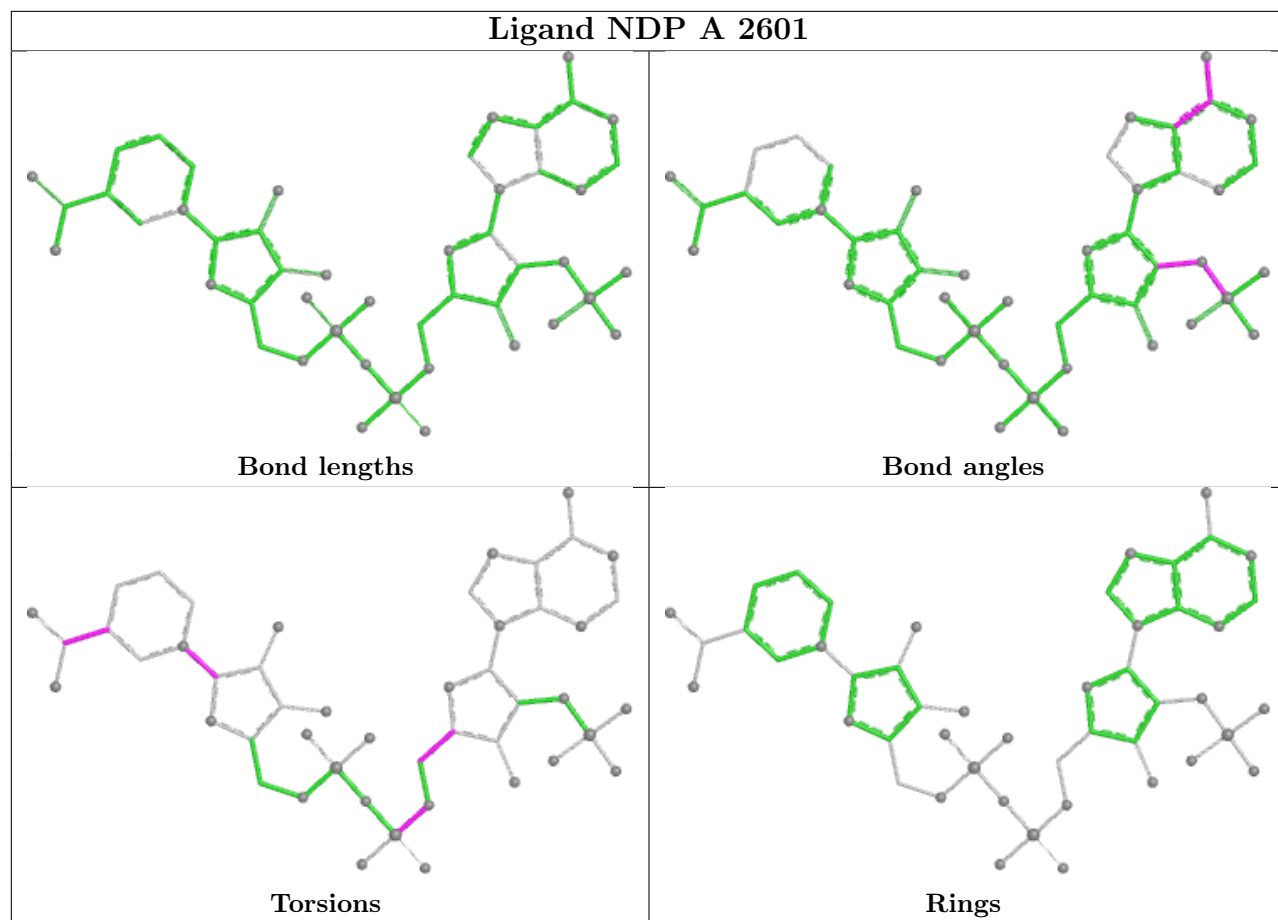
*Continued from previous page...*

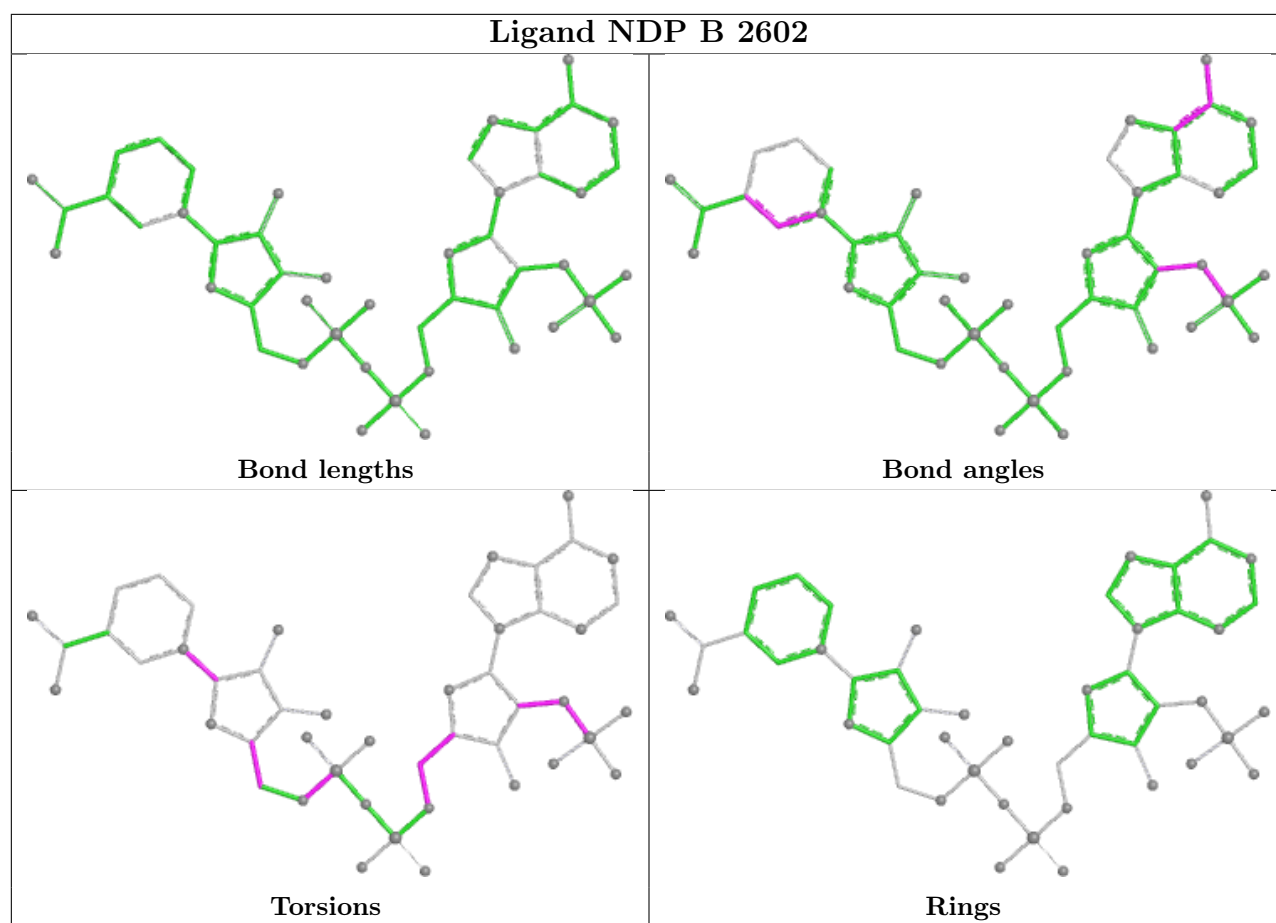
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2602	NDP	5	0
3	A	2601	NDP	2	0
3	B	2602	NDP	3	0

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.

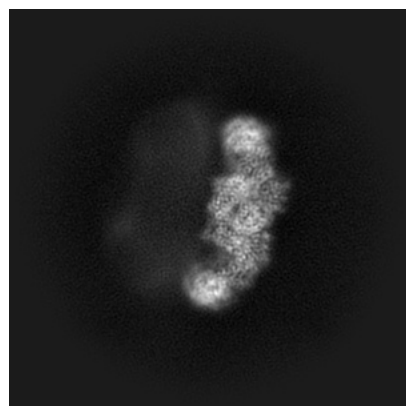
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43187. These allow visual inspection of the internal detail of the map and identification of artifacts.

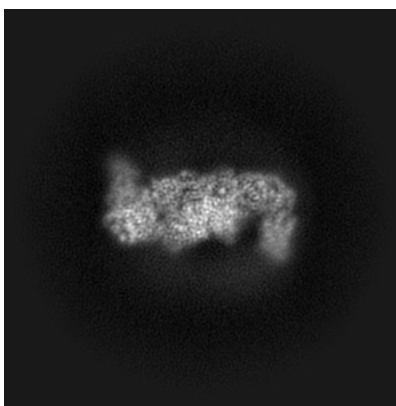
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

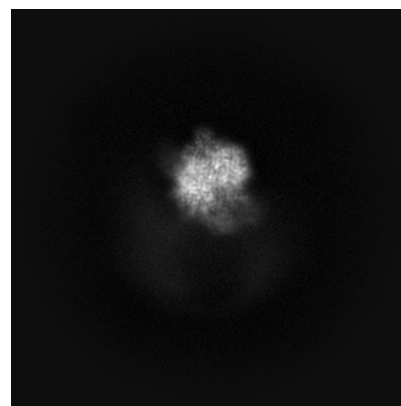
#### 6.1.1 Primary map



X

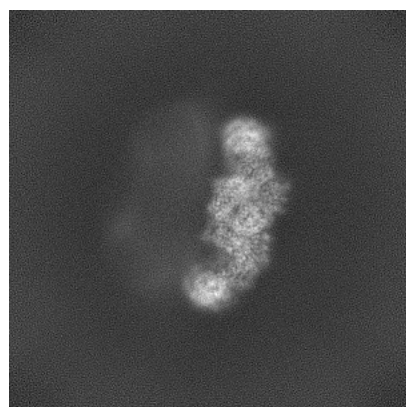


Y

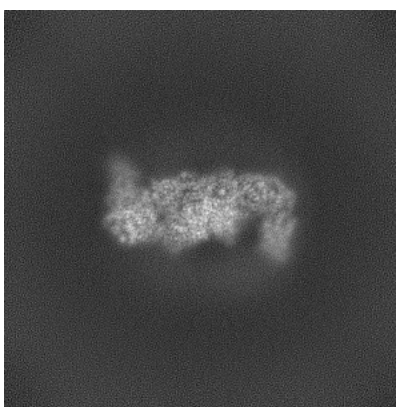


Z

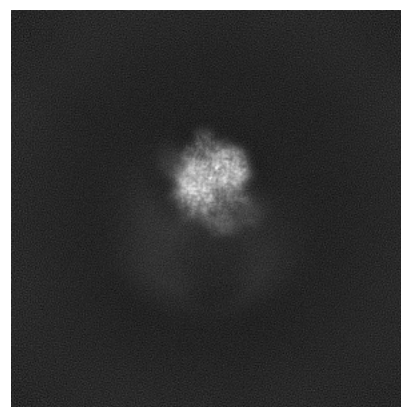
#### 6.1.2 Raw map



X



Y

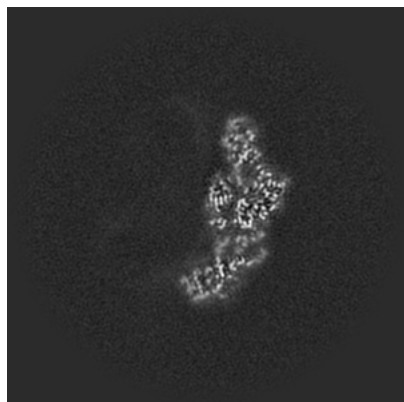


Z

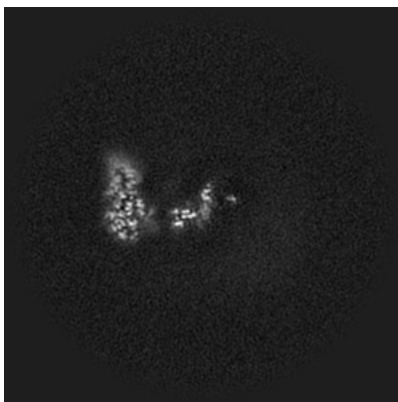
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

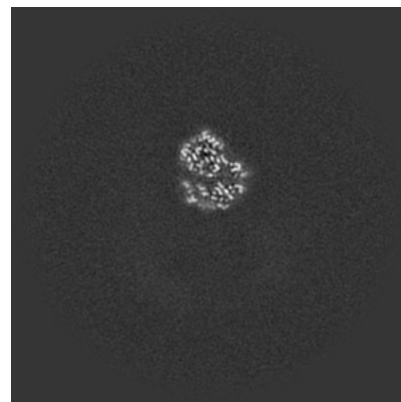
### 6.2.1 Primary map



X Index: 180

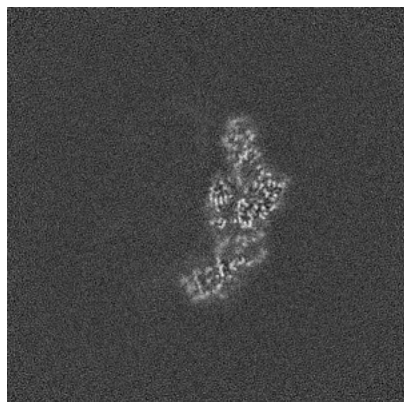


Y Index: 180



Z Index: 180

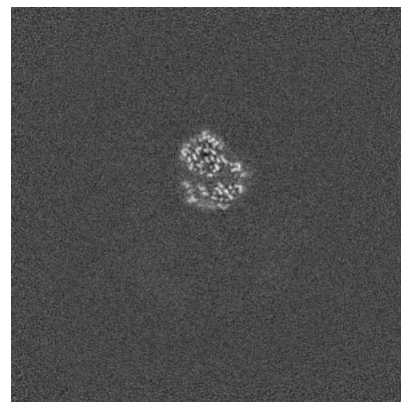
### 6.2.2 Raw map



X Index: 180



Y Index: 180



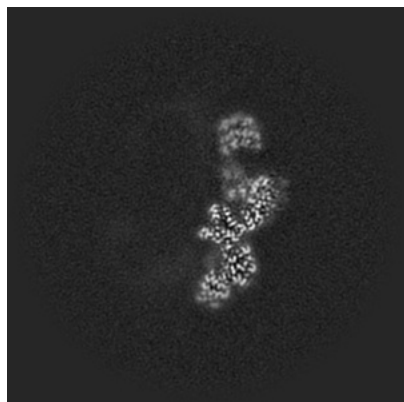
Z Index: 180

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

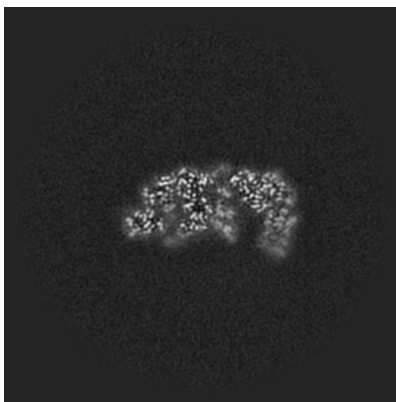


## 6.3 Largest variance slices [i](#)

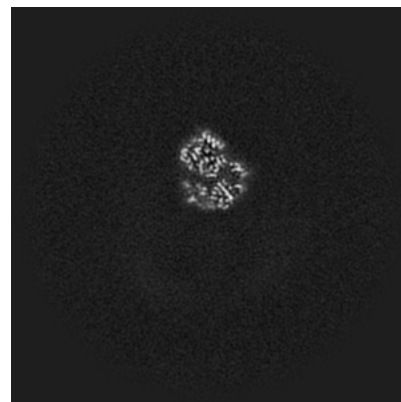
### 6.3.1 Primary map



X Index: 164

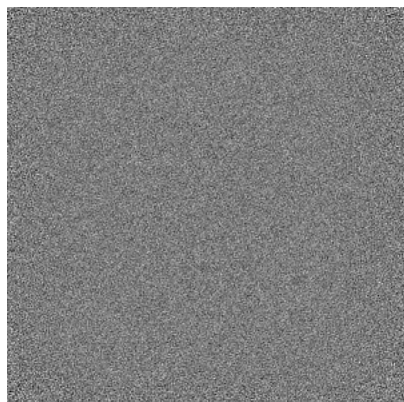


Y Index: 214

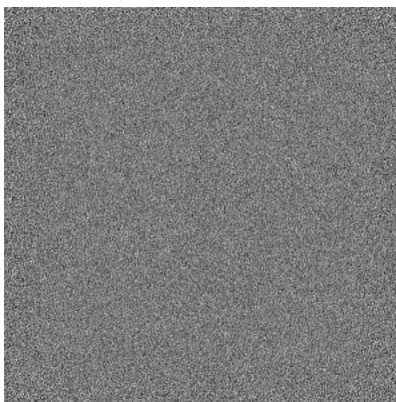


Z Index: 181

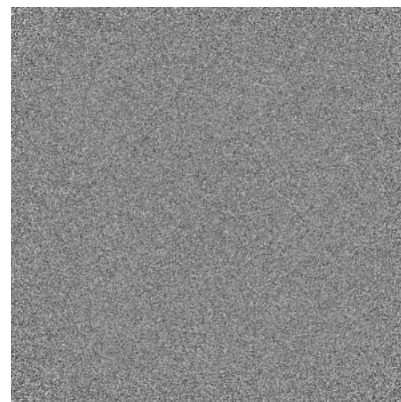
### 6.3.2 Raw map



X Index: 0



Y Index: 0



Z Index: 359

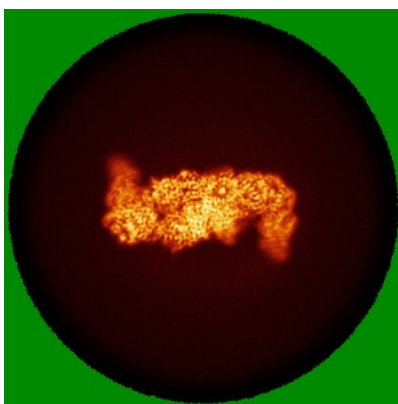
The images above show the largest variance slices of the map in three orthogonal directions.

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

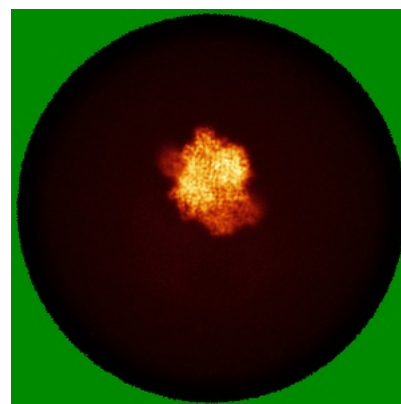
### 6.4.1 Primary map



X

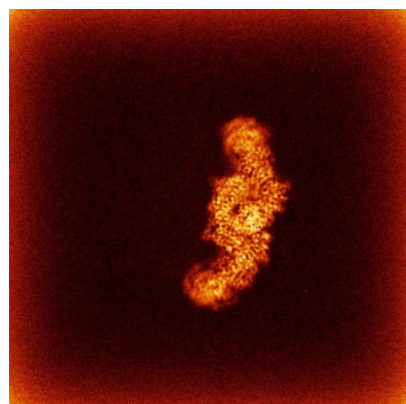


Y

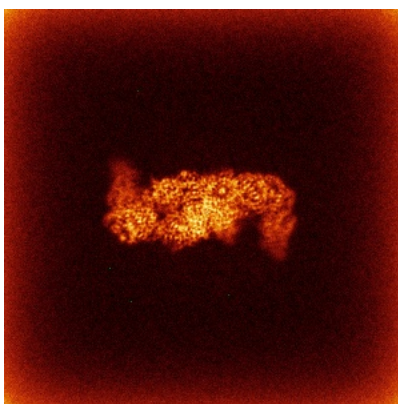


Z

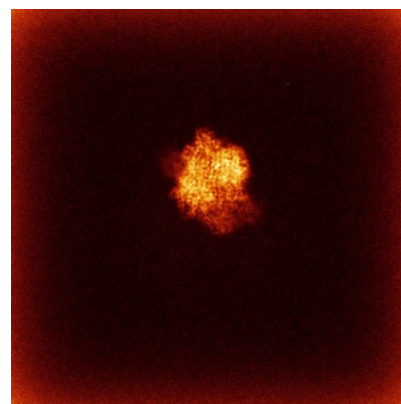
### 6.4.2 Raw map



X



Y



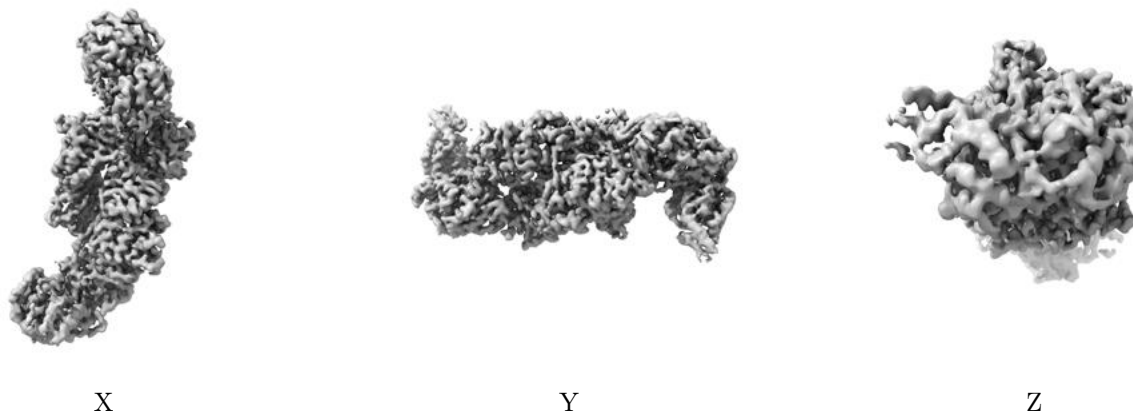
Z

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 0.221. 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.

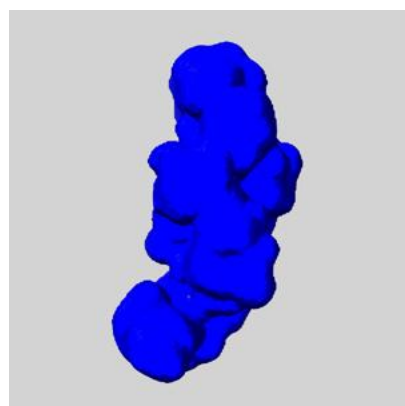
## 6.6 Mask visualisation [i](#)

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

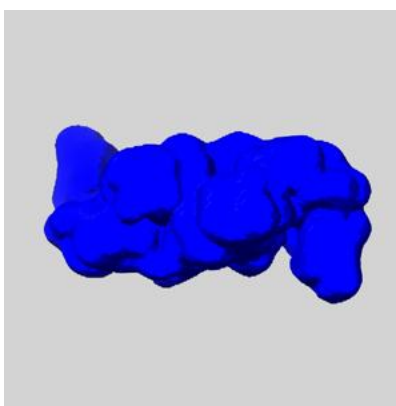
A mask typically either:

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

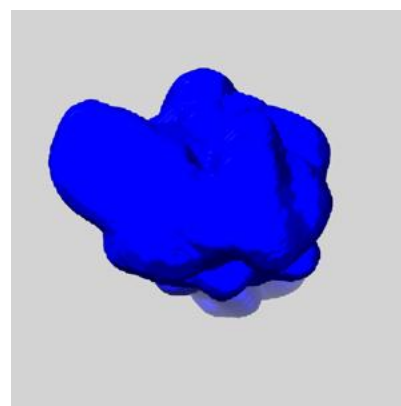
### 6.6.1 emd\_43187\_msk\_1.map [i](#)



X



Y

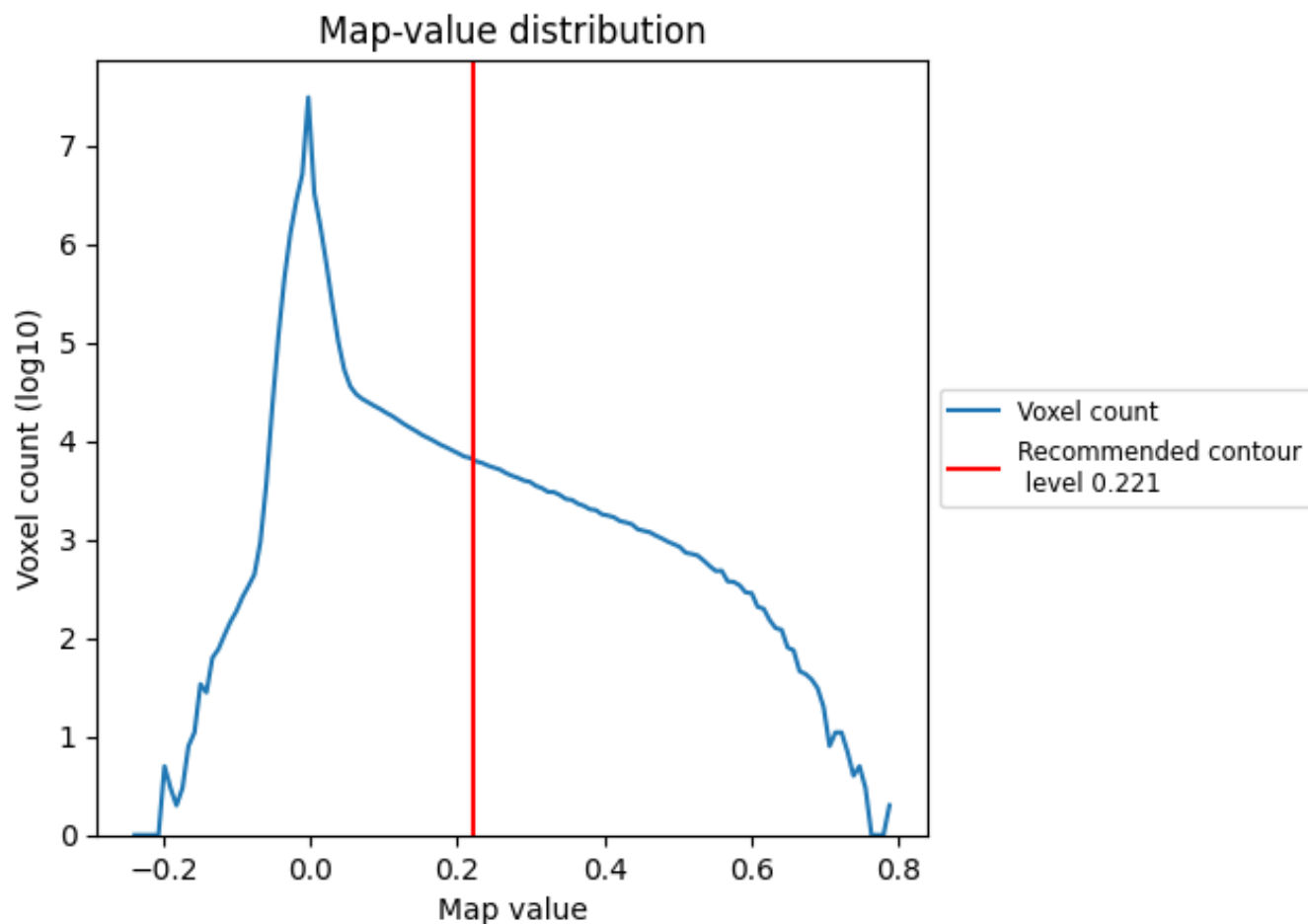


Z

## 7 Map analysis [i](#)

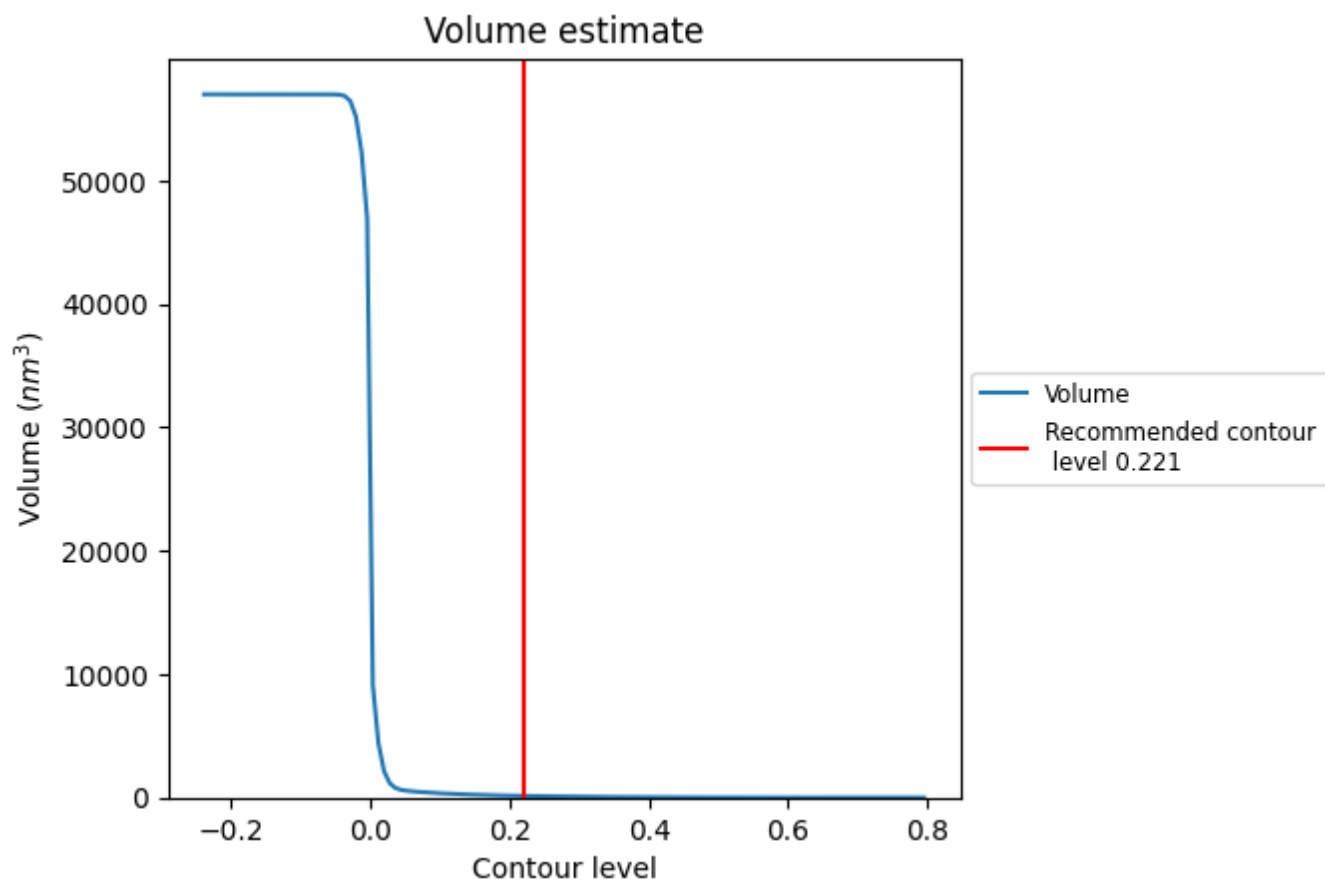
This section contains the results of statistical analysis of the map.

### 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.

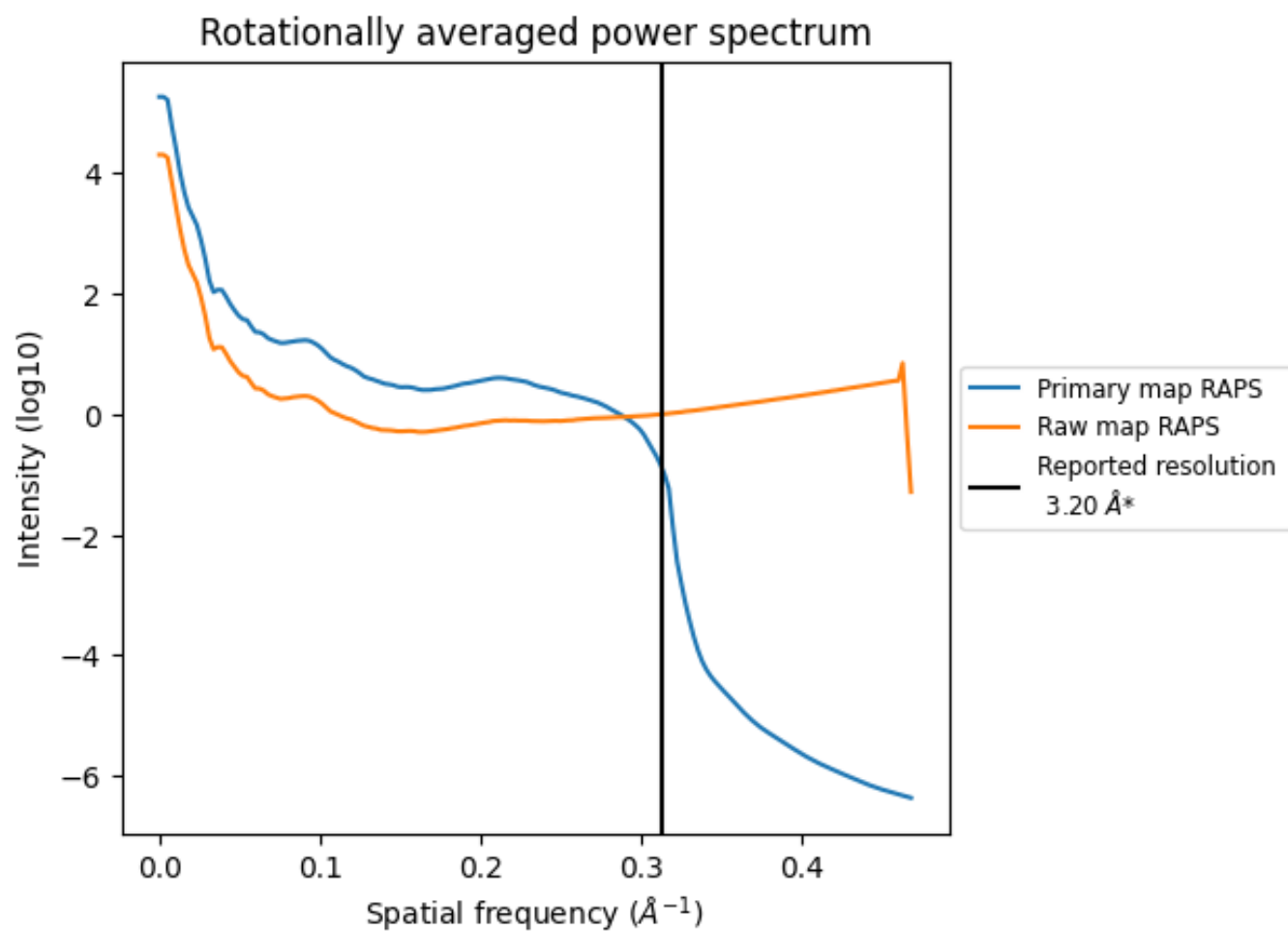
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 131 nm<sup>3</sup>; this corresponds to an approximate mass of 119 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 ⓘ

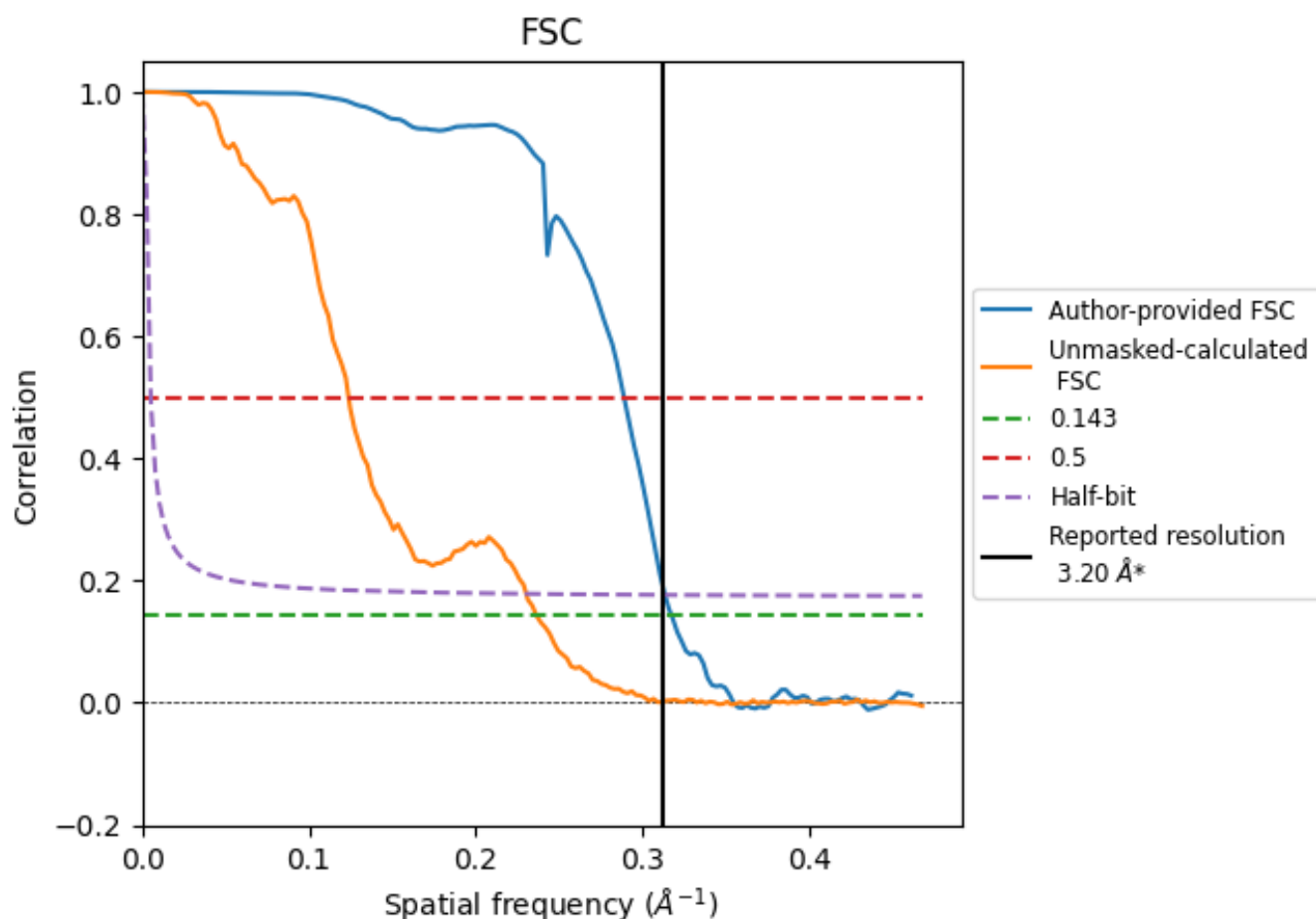


\*Reported resolution corresponds to spatial frequency of 0.312  $\text{\AA}^{-1}$

## 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 0.312 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

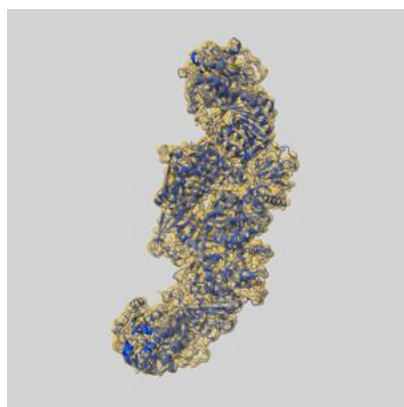
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.15	3.46	3.19
Unmasked-calculated*	4.23	8.08	4.34

\*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 4.23 differs from the reported value 3.2 by more than 10 %

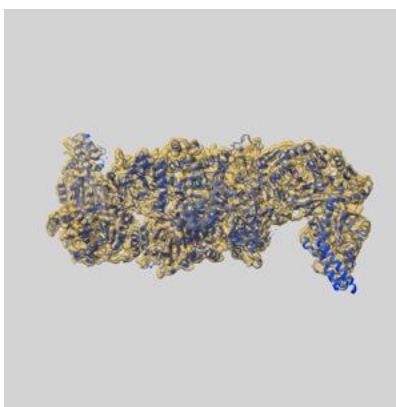
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-43187 and PDB model 8VF7. Per-residue inclusion information can be found in section [3](#) on page [7](#).

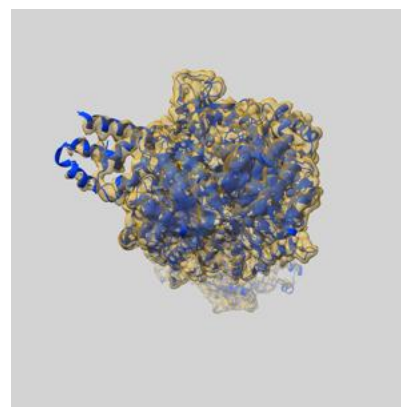
### 9.1 Map-model overlay [i](#)



X



Y

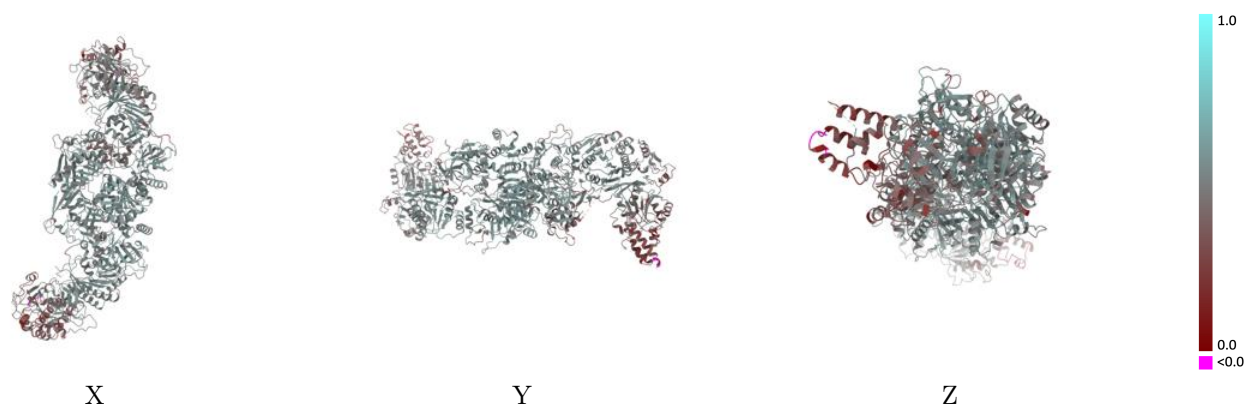


Z

The images above show the 3D surface view of the map at the recommended contour level 0.221 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.

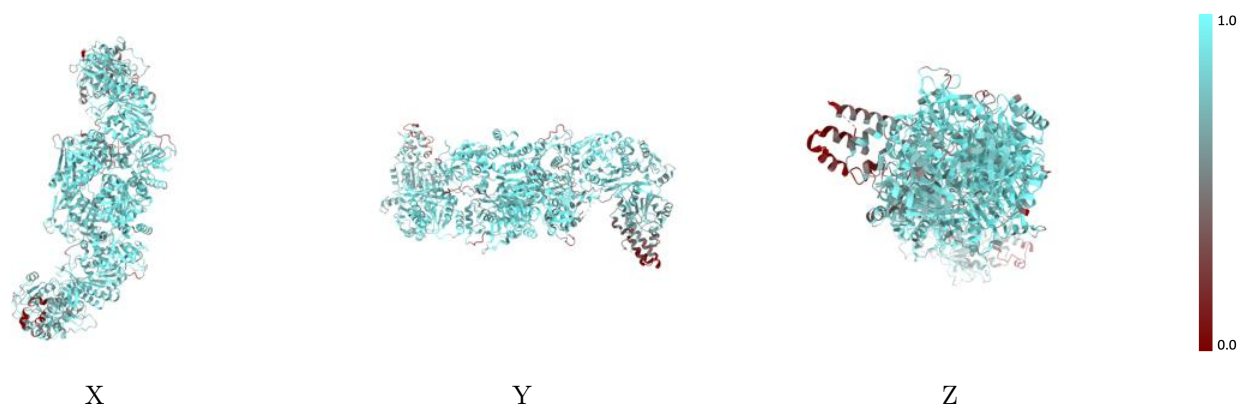


## 9.2 Q-score mapped to coordinate model [i](#)



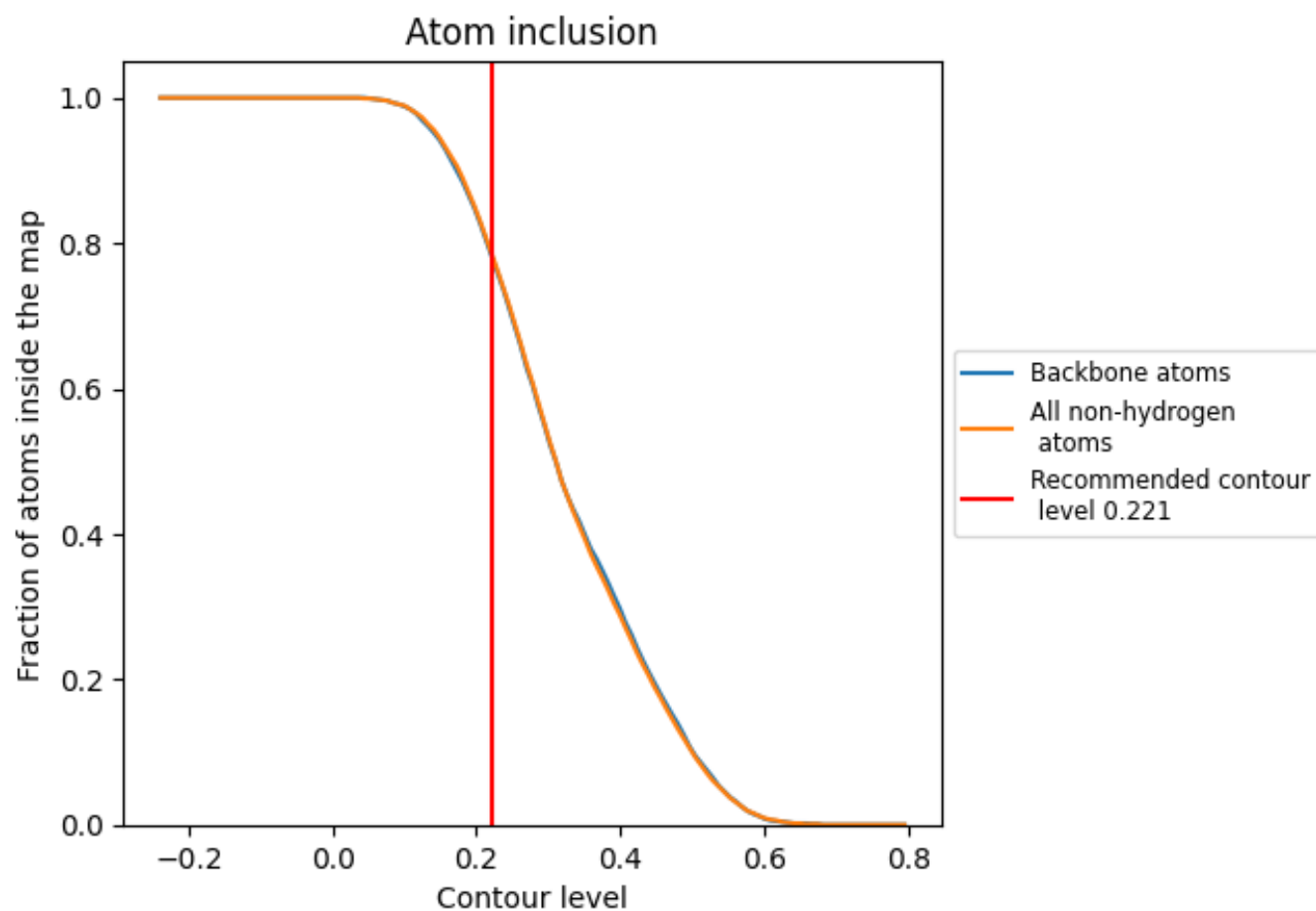
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.221).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 79% 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 (0.221) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7870	<div></div> 0.4870
A	<div></div> 0.8130	<div></div> 0.4970
B	<div></div> 0.7850	<div></div> 0.4770

