



wwPDB EM Validation Summary Report ⓘ

Mar 10, 2026 – 01:55 PM UTC

PDB ID : 6WG3 / pdb_00006wg3
EMDB ID : EMD-21658
Title : Cryo-EM structure of human Cohesin-NIPBL-DNA complex
Authors : Shi, Z.B.; Gao, H.; Bai, X.C.; Yu, H.
Deposited on : 2020-04-04
Resolution : 5.30 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

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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

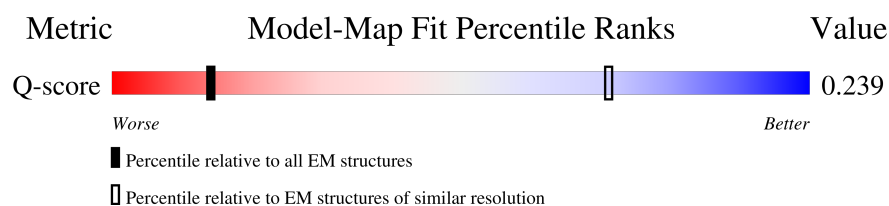
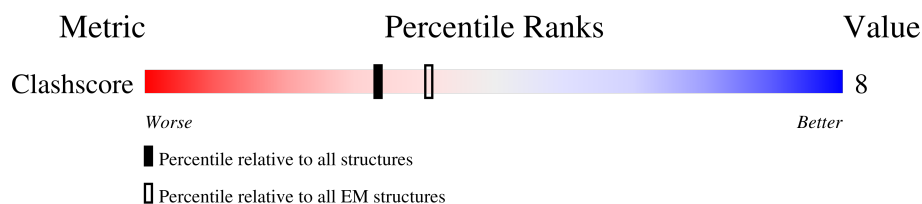
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

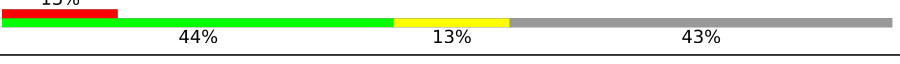
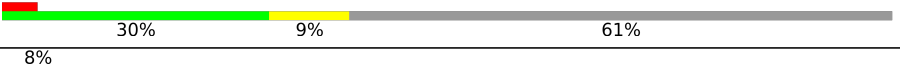
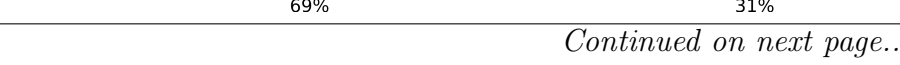
The reported resolution of this entry is 5.30 Å.

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	-
Q-score	-	25397	625 (4.80 - 5.80)

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	1233	 6% 36% 10% 55%
2	B	1217	 13% 44% 13% 43%
3	C	631	 30% 9% 61%
4	D	1272	 8% 56% 17% 27%
5	E	1652	 58% 16% 26%
6	F	51	 10% 69% 31%

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Mol	Chain	Length	Quality of chain
7	G	51	10% 92% 8%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 31683 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 Structural maintenance of chromosomes protein 1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	561	Total	C	N	O	S	0	0
			4458	2820	779	844	15		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1157	GLN	GLU	engineered mutation	UNP Q14683

- Molecule 2 is a protein called Structural maintenance of chromosomes protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	693	Total	C	N	O	S	0	0
			5636	3568	989	1050	29		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1144	GLN	GLU	engineered mutation	UNP Q9UQE7

- Molecule 3 is a protein called Double-strand-break repair protein rad21 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	248	Total	C	N	O	S	0	0
			1991	1278	352	350	11		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	172	ALA	ARG	engineered mutation	UNP O60216
C	279	ALA	ASP	engineered mutation	UNP O60216
C	450	ALA	ARG	engineered mutation	UNP O60216

- Molecule 4 is a protein called Cohesin subunit SA-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	932	Total	C	N	O	S	0	0
			7580	4817	1291	1425	47		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1259	GLY	-	expression tag	UNP Q8WVM7
D	1260	ALA	-	expression tag	UNP Q8WVM7
D	1261	PRO	-	expression tag	UNP Q8WVM7
D	1262	MET	-	expression tag	UNP Q8WVM7
D	1263	ARG	-	expression tag	UNP Q8WVM7
D	1264	SER	-	expression tag	UNP Q8WVM7
D	1265	GLY	-	expression tag	UNP Q8WVM7
D	1266	ALA	-	expression tag	UNP Q8WVM7
D	1267	LEU	-	expression tag	UNP Q8WVM7
D	1268	GLU	-	expression tag	UNP Q8WVM7
D	1269	VAL	-	expression tag	UNP Q8WVM7
D	1270	LEU	-	expression tag	UNP Q8WVM7
D	1271	PHE	-	expression tag	UNP Q8WVM7
D	1272	GLN	-	expression tag	UNP Q8WVM7

- Molecule 5 is a protein called Nipped-B-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	1226	Total	C	N	O	S	0	0
			9865	6290	1675	1829	71		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	1153	MET	-	expression tag	UNP Q6KC79
E	1154	SER	-	expression tag	UNP Q6KC79
E	1155	TYR	-	expression tag	UNP Q6KC79
E	1156	TYR	-	expression tag	UNP Q6KC79
E	1157	HIS	-	expression tag	UNP Q6KC79
E	1158	HIS	-	expression tag	UNP Q6KC79
E	1159	HIS	-	expression tag	UNP Q6KC79
E	1160	HIS	-	expression tag	UNP Q6KC79
E	1161	HIS	-	expression tag	UNP Q6KC79
E	1162	HIS	-	expression tag	UNP Q6KC79

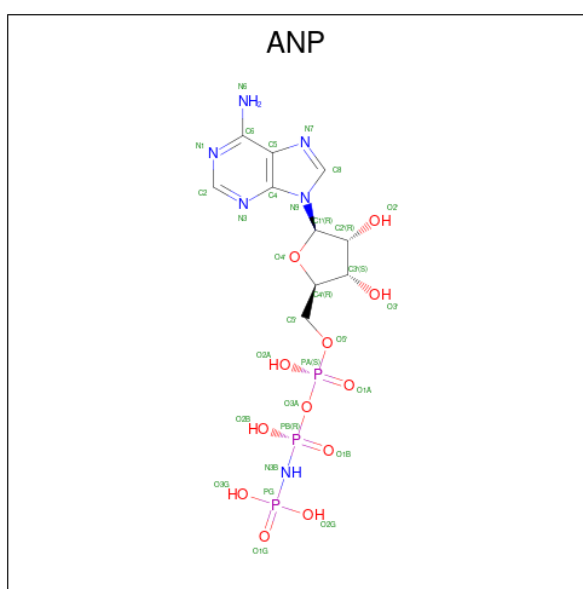
- Molecule 6 is a DNA chain called DNA (51-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	51	Total	C	N	O	P	0	0
			1071	510	255	255	51		

- Molecule 7 is a DNA chain called DNA (51-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	51	Total	C	N	O	P	0	0
			1020	510	102	357	51		

- Molecule 8 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).

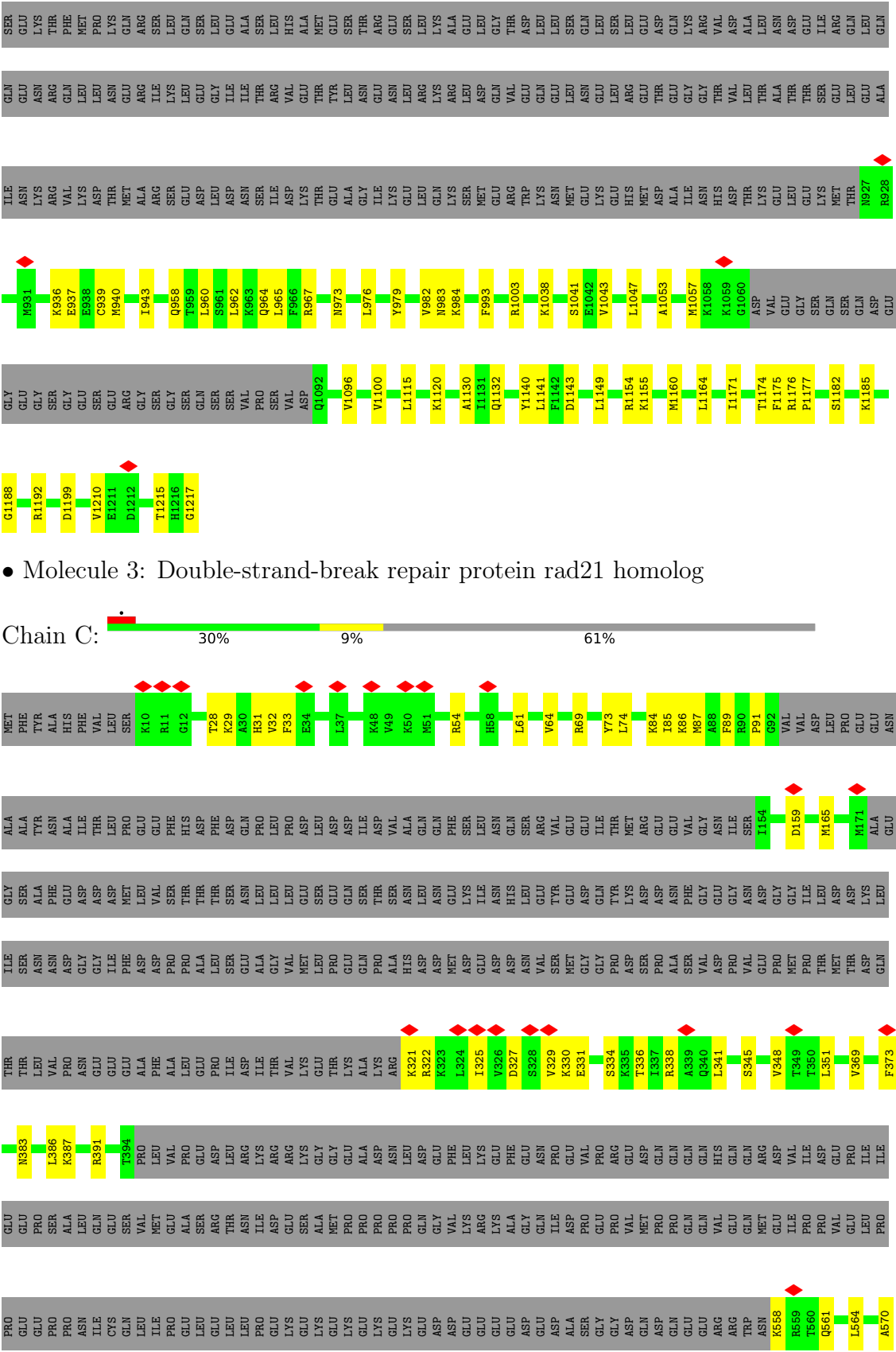


Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	N	O	P	0
			31	10	6	12	3	
8	B	1	Total	C	N	O	P	0
			31	10	6	12	3	

L1098
Y1107
I1111
R1121
F1122
R1123
P1124
N1127
G1130
K1133
F1152
L1155
D1163
N1164
T1167
A1171
Q1183
V1186
I1187
S1188
L1189
K1190
E1191
E1192
F1193
Y1194
T1195
K1196
L1200
C1210
V1211
T1217
Y1223
P1224
D1225
ALA
ASN
PRO
ASN
PRO
ASN
ASN
GLU
GLN

Chain B:





• Molecule 3: Double-strand-break repair protein rad21 homolog

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

● Molecule 5: Nipped-B-like protein



MET	GLY	D1298	L1406	ASP	LYS	MET	M1888	V2047	M2207	D2339
SER	ASP	L1299	L1406	SER	GLN	ASN	R1894	I2050	Q2210	L2342
THR	ASP	T1407	D1408	ALA	VAL	SER	D1746	L2053	L2210	L2342
HIS	GLU	R1303	I1411	GLU	GLY	GLY	A1753	L2054	N2214	E2343
HIS	PRO	D1309	I1411	ASP	GLU	GLU	I1756	V2055	L2215	E2344
HIS	GLN	D1313	V1414	SER	GLU	GLU	I1756	L2056	L2216	K2347
LYS	GLU	T1313	V1415	ASN	L1659	ASN	R1784	E1924	L2220	K2348
LYS	GLU	T1314	S1416	LYS	L1659	LYS	R1784	A1925	S2221	Y2349
ARG	L1232	I1315	T1420	ILE	T1663	ILE	T1768	M1926	D2222	M2363
THR	L1233	T1319	V1424	ASP	T1663	GLN	Q1768	V1937	K2230	L2371
LEU	S1245	M1323	V1427	GLN	D1524	GLN	F1770	C1940	K2230	T2372
SER	I1248	V1327	V1427	D1525	V1528	D1525	Q1776	R1941	L2234	THR
GLU	K1249	I1333	Q1431	T1528	G1580	G1580	I1777	K2075	L2234	CYS
VAL	G1252	F1342	R1449	G1580	Q1553	Q1553	I1778	L2076	L2241	LEU
ALA	M1254	H1343	E1454	E1556	E1556	E1556	R1779	I2077	K2257	LYS
VAL	K1256	T1347	T1458	E1556	L1570	L1570	R1779	Y1945	K2260	ASP
ARG	L1257	I1348	R1462	L1570	P1576	P1576	I1786	D1946	D2263	PRO
LYS	D1260	Y1349	L1463	L1570	E1577	E1577	T1790	W1947	L2264	VAL
GLN	K1261	P1350	S1469	E1582	E1577	E1577	K1791	F1948	ARG	ARG
LYS	K1264	Y1356	S1472	E1582	E1582	E1582	A1792	L1952	GLN	ARG
ARG	V1265	LEU	F1473	F1596	F1596	F1596	L1796	L1955	L2120	GLN
THR	L1266	ASP	R1474	F1596	F1596	F1596	P1804	L1955	L2120	ASP
GLY	M1267	PRO	S1597	N1598	N1598	N1598	S1805	C1971	D2127	GLU
ASP	L1268	GLY	L1475	N1598	N1598	N1598	I1806	L1974	R2142	SER
PHE	L1269	LYS	ASN	E1602	E1603	E1603	L1807	E1987	D2157	GLY
ALA	E1270	THR	GLY	E1602	M1603	M1603	R1819	LEU	D2160	THR
PRO	K1271	PRO	GLY	E1603	M1603	M1603	D1822	ALA	F2161	GLY
LEU	N1272	THR	GLY	M1603	M1603	M1603	N1823	ASP	K2162	ASP
THR	I1273	PRO	GLY	M1603	M1603	M1603	S1826	ASP	K2166	ASP
ILE	Q1274	PRO	GLY	M1603	M1603	M1603	V1827	ASN	K2170	ASP
PHE	D1275	GLU	SER	M1603	M1603	M1603	E1829	LYS	D2171	ASN
ASP	M1193	GLU	GLY	M1603	M1603	M1603	E1829	GLY	K2172	LYS
VAL	F1199	THR	ALA	M1603	M1603	M1603	E1833	VAL	N1998	VAL
MET	F1202	THR	ARG	M1603	M1603	M1603	V1839	M1998	L2006	M1998
MET	T1203	THR	ARG	M1603	M1603	M1603	R1842	L2006	L2015	L2015
SER	ALA	THR	ARG	M1603	M1603	M1603	A1846	L2015	K2022	K2022
ARG	A1204	THR	ARG	M1603	M1603	M1603	T1854	L2031	L2031	L2031
LEU	S1205	THR	ARG	M1603	M1603	M1603	I1862	N2039	N2039	N2039
GLN	I1206	THR	ARG	M1603	M1603	M1603	V1863	D2040	S1863	S1863
LEU	E1207	THR	ARG	M1603	M1603	M1603	R1865	F2041	P2041	P2041
VAL	N1208	THR	ARG	M1603	M1603	M1603	R1865	M2042	K2042	K2042
GLU	E1214	THR	ARG	M1603	M1603	M1603	R1867	V2043	V2043	V2043
ASP	D1215	THR	ARG	M1603	M1603	M1603	R1867	I2044	I2044	I2044
MET	M1216	THR	ARG	M1603	M1603	M1603	R1867	H2203	H2203	H2203
ASN	ASP	THR	ARG	M1603	M1603	M1603	R1867	H2203	H2203	H2203
GLU	P1294	THR	ARG	M1603	M1603	M1603	R1867	H2203	H2203	H2203
PHE	R1294	THR	ARG	M1603	M1603	M1603	R1867	H2203	H2203	H2203
GLU	E1293	THR	ARG	M1603	M1603	M1603	R1867	H2203	H2203	H2203
THR	W1296	THR	ARG	M1603	M1603	M1603	R1867	H2203	H2203	H2203
PHE	K1297	THR	ARG	M1603	M1603	M1603	R1867	H2203	H2203	H2203



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	6857	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.073	Depositor
Minimum map value	-0.022	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	321.6, 321.6, 321.6	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	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: ANP

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	0.28	0/4532	0.68	0/6086
2	B	0.26	0/5727	0.67	2/7675 (0.0%)
3	C	0.25	0/2026	0.69	0/2721
4	D	0.28	0/7715	0.69	0/10403
5	E	0.29	0/10021	0.70	3/13509 (0.0%)
6	F	0.32	0/1223	0.61	0/1883
7	G	0.38	0/1121	0.66	1/1730 (0.1%)
All	All	0.28	0/32365	0.69	6/44007 (0.0%)

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
5	E	1974	LEU	CA-CB-CG	6.42	138.78	116.30
2	B	74	ILE	N-CA-C	-6.34	107.69	113.71
5	E	2606	ILE	CA-C-N	5.50	132.05	121.54
5	E	2606	ILE	C-N-CA	5.50	132.05	121.54
7	G	27	DT	P-O3'-C3'	5.04	127.75	120.20

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	4458	0	4500	83	0
2	B	5636	0	5709	101	0
3	C	1991	0	2083	47	0
4	D	7580	0	7582	139	0
5	E	9865	0	10101	179	0
6	F	1071	0	562	11	0
7	G	1020	0	613	2	0
8	A	31	0	13	2	0
8	B	31	0	13	2	0
All	All	31683	0	31176	523	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 523 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)
4:D:187:ARG:HE	4:D:235:ASN:HD22	1.30	0.80
5:E:1303:ARG:HG2	5:E:1343:HIS:HE1	1.52	0.73
2:B:962:LEU:H	2:B:965:LEU:HD23	1.53	0.73
1:A:1091:ASN:ND2	5:E:2269:ASP:OD2	2.23	0.71
5:E:2392:CYS:SG	5:E:2434:ASN:ND2	2.63	0.71

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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](#)

2 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	$\# Z > 2$
8	ANP	B	2000	-	33,33,33	1.07	5 (15%)	45,52,52	0.88	1 (2%)
8	ANP	A	2000	-	33,33,33	1.06	5 (15%)	45,52,52	0.92	2 (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
8	ANP	B	2000	-	-	3/18/38/38	0/3/3/3
8	ANP	A	2000	-	-	6/18/38/38	0/3/3/3

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	2000	ANP	PG-O1G	3.29	1.51	1.46
8	B	2000	ANP	PG-O1G	2.95	1.50	1.46
8	B	2000	ANP	PB-O1B	2.86	1.50	1.46
8	A	2000	ANP	PB-O1B	2.65	1.50	1.46
8	A	2000	ANP	PB-O2B	-2.34	1.50	1.56

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2000	ANP	O2B-PB-O1B	4.02	118.48	109.87
8	B	2000	ANP	O2B-PB-O1B	3.82	118.06	109.87
8	A	2000	ANP	O2G-PG-O1G	-2.41	107.42	113.45

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

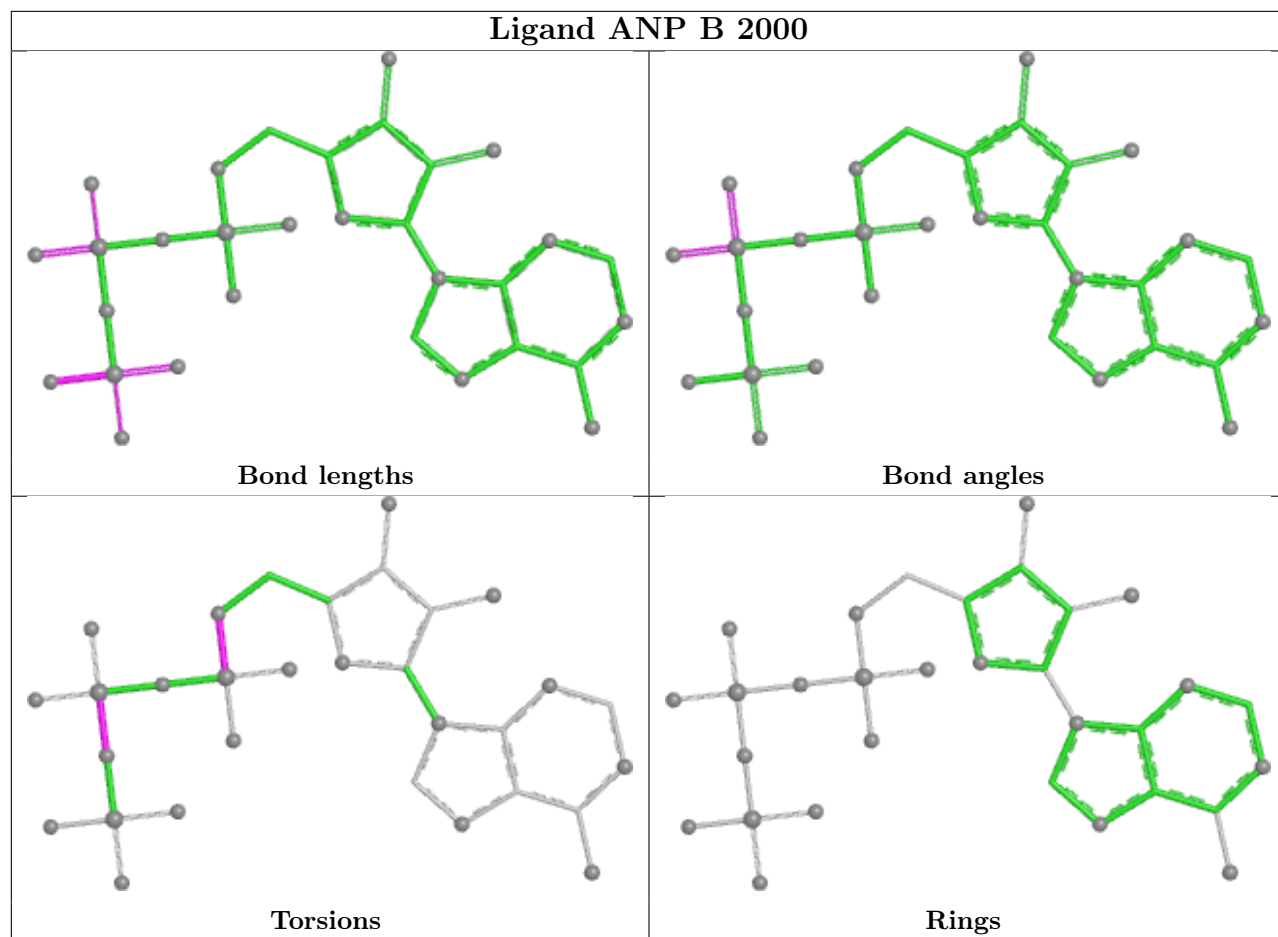
Mol	Chain	Res	Type	Atoms
8	A	2000	ANP	PG-N3B-PB-O1B
8	A	2000	ANP	PG-N3B-PB-O3A
8	B	2000	ANP	PG-N3B-PB-O1B
8	B	2000	ANP	PG-N3B-PB-O3A
8	A	2000	ANP	O4'-C4'-C5'-O5'

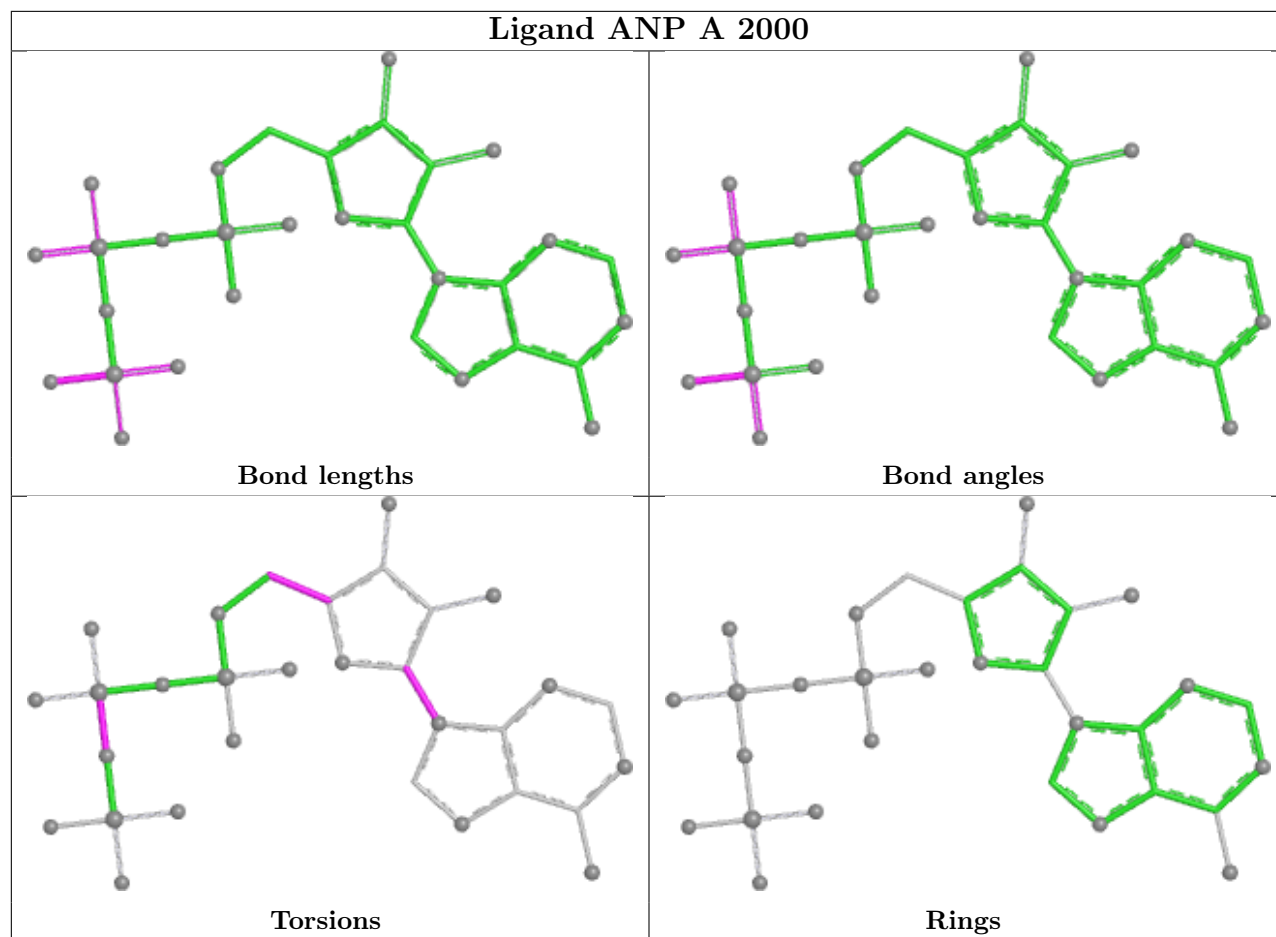
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	2000	ANP	2	0
8	A	2000	ANP	2	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.

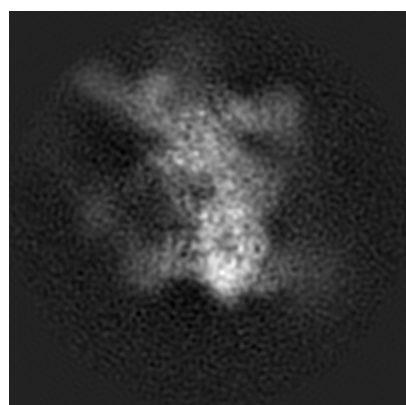
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21658. These allow visual inspection of the internal detail of the map and identification of artifacts.

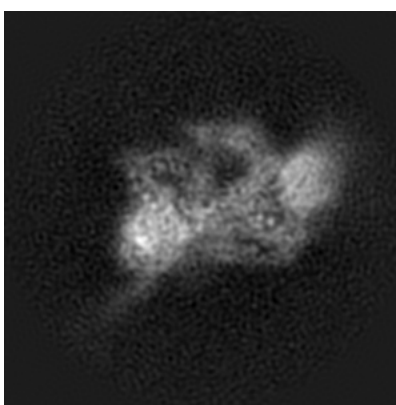
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

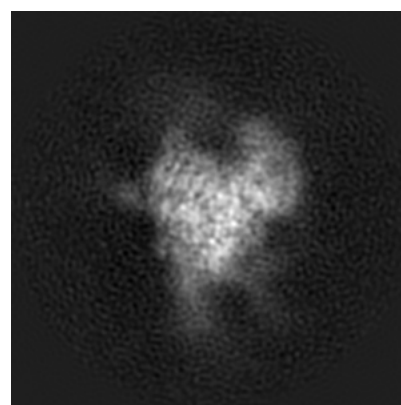
6.1.1 Primary map



X



Y

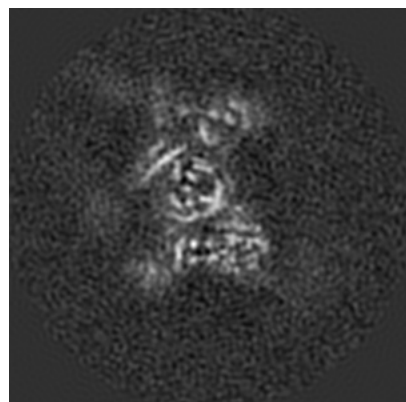


Z

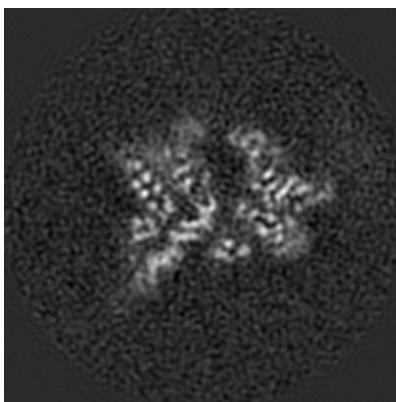
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

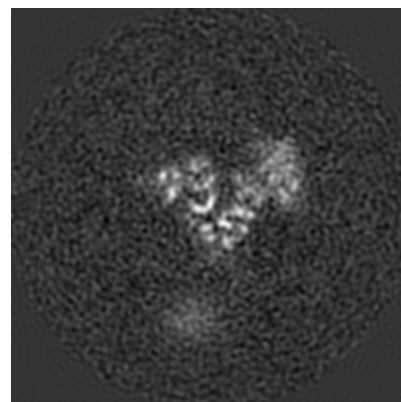
6.2.1 Primary map



X Index: 120



Y Index: 120

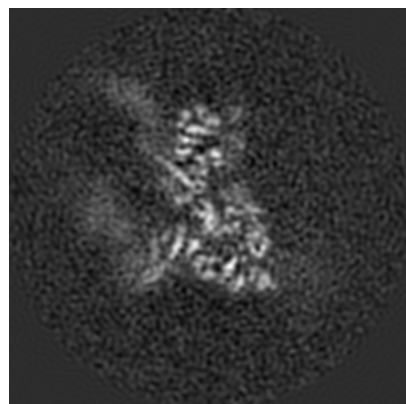


Z Index: 120

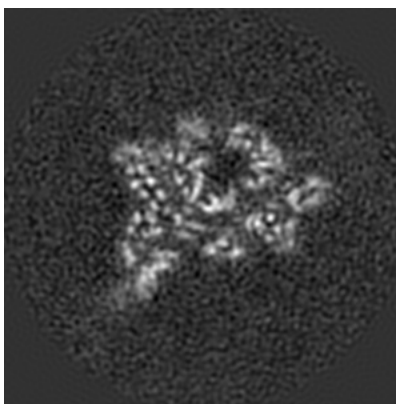
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

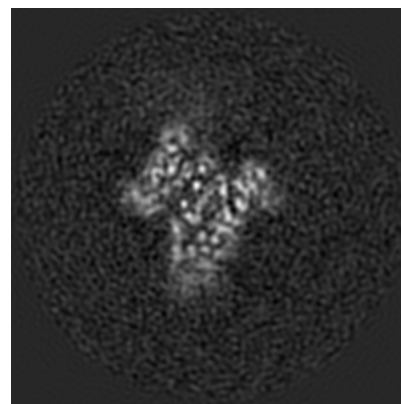
6.3.1 Primary map



X Index: 110



Y Index: 124

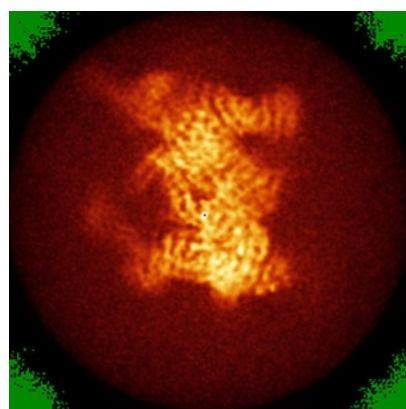


Z Index: 86

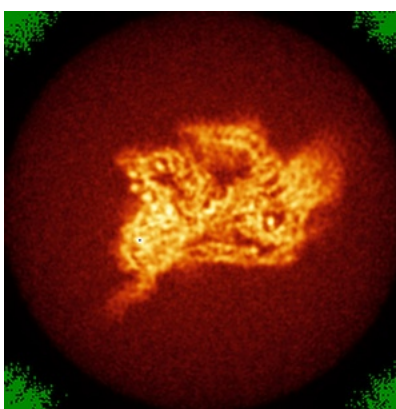
The images above show the largest variance slices of the map in three orthogonal directions.

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

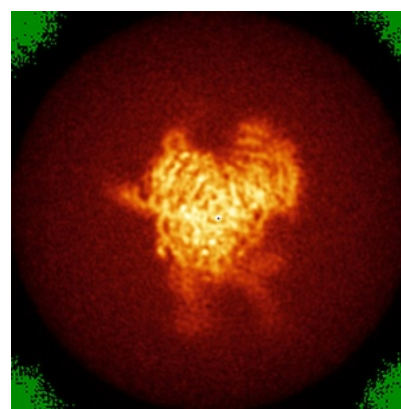
6.4.1 Primary map



X



Y



Z

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 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

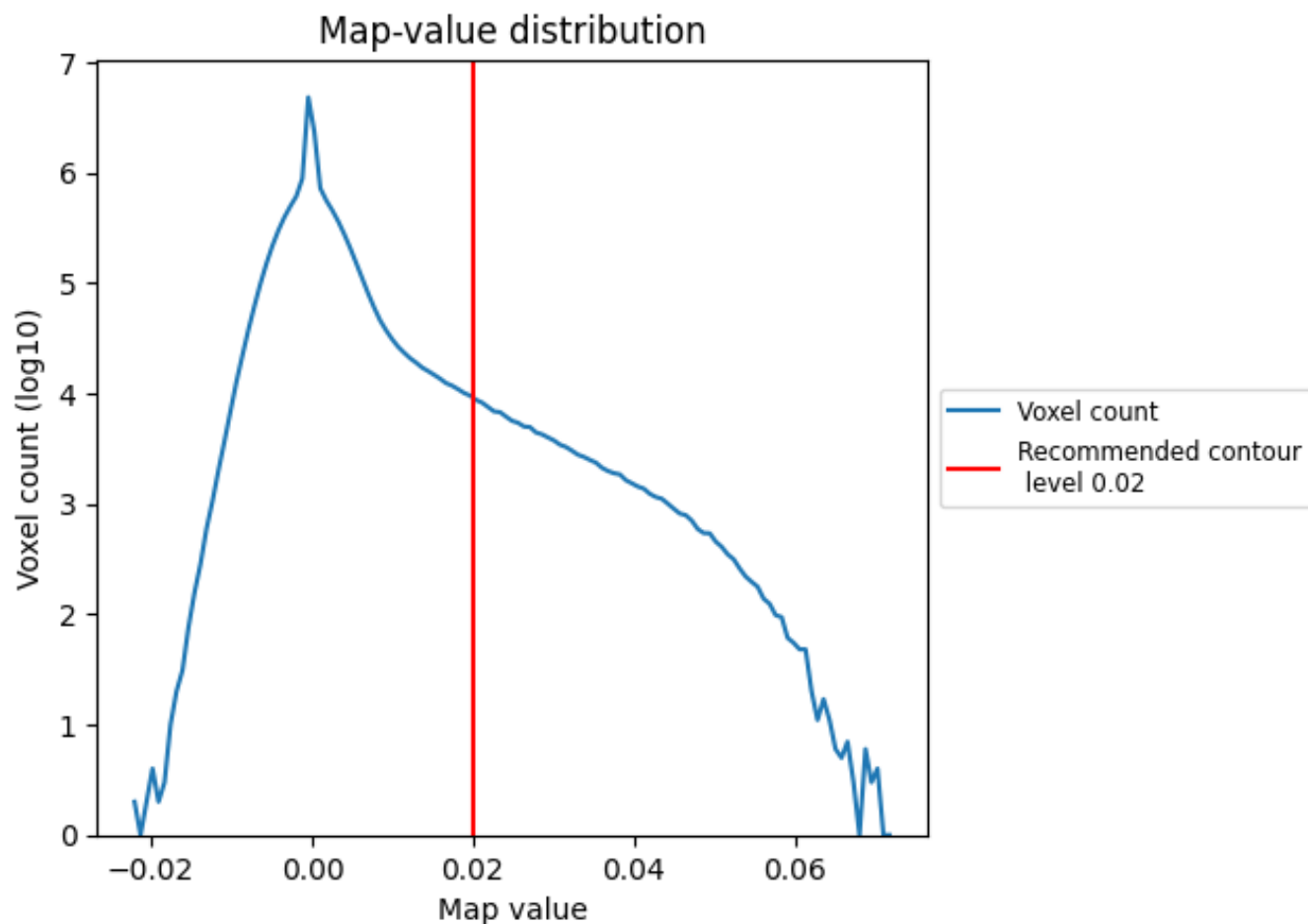
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

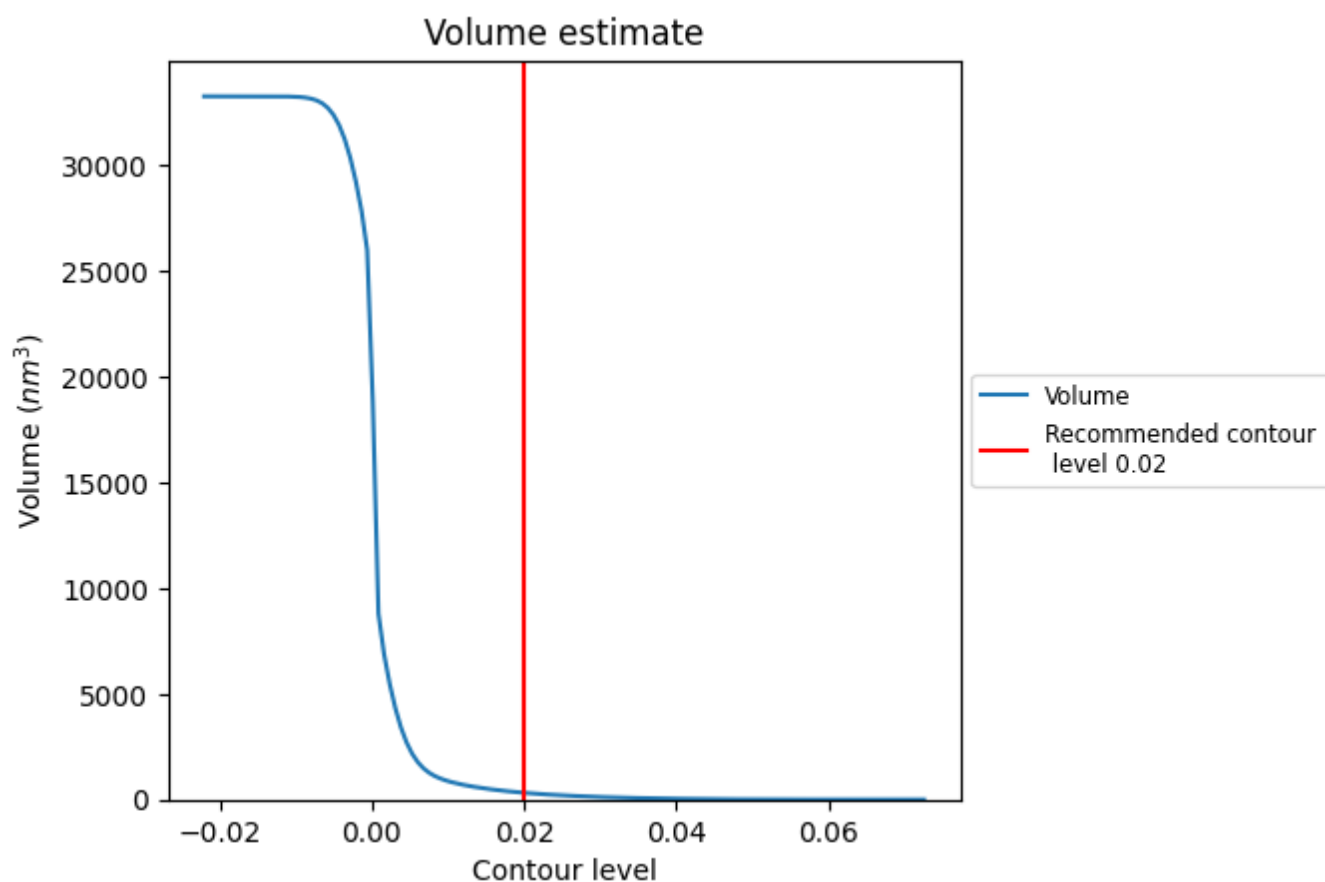
This section contains the results of statistical analysis of the map.

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.

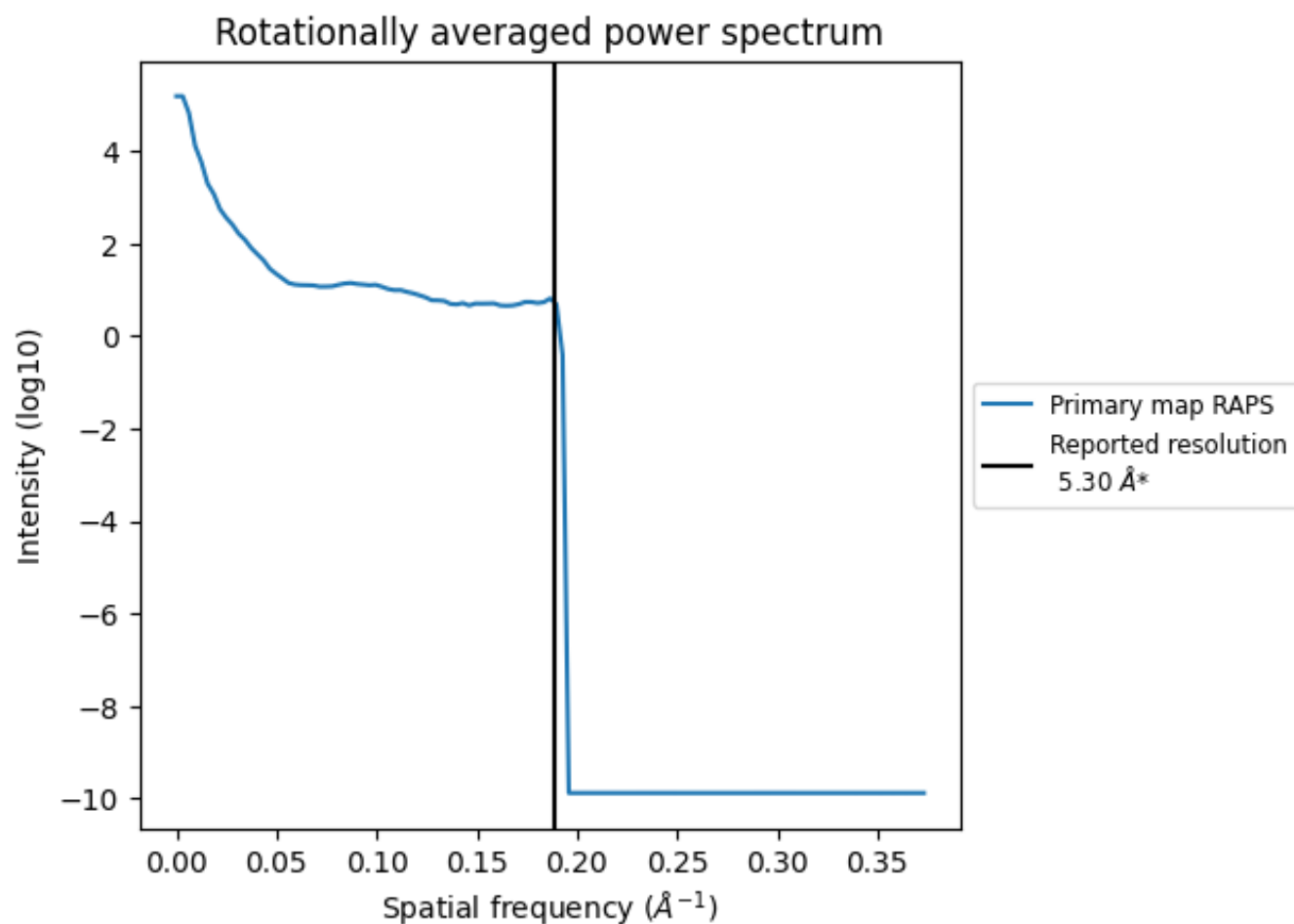
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 320 nm³; this corresponds to an approximate mass of 289 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 ⓘ

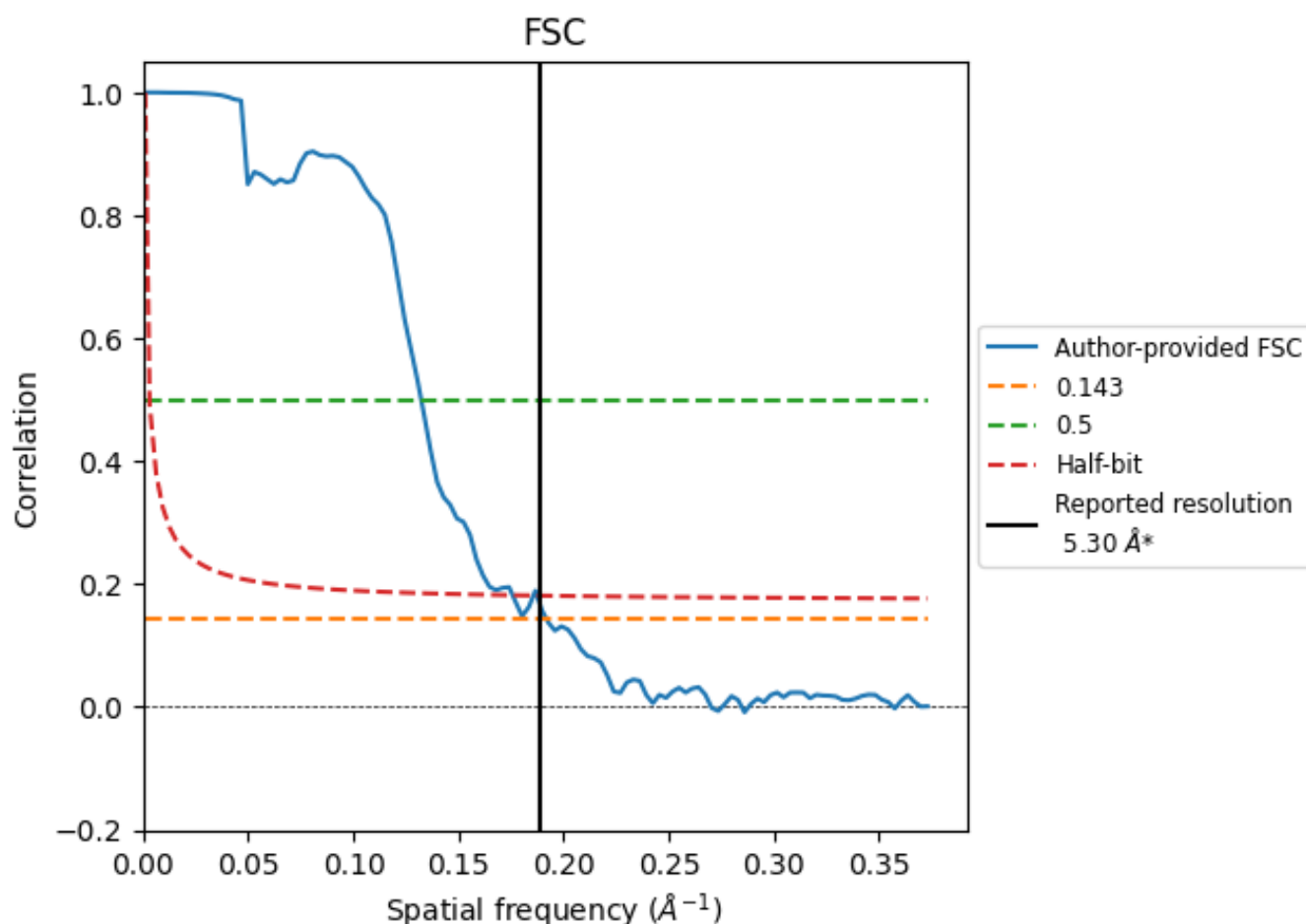


*Reported resolution corresponds to spatial frequency of 0.189 Å⁻¹

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 0.189 Å⁻¹

8.2 Resolution estimates [i](#)

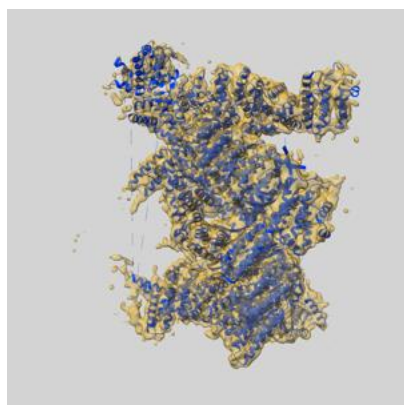
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.30	-	-
Author-provided FSC curve	5.21	7.56	5.69
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

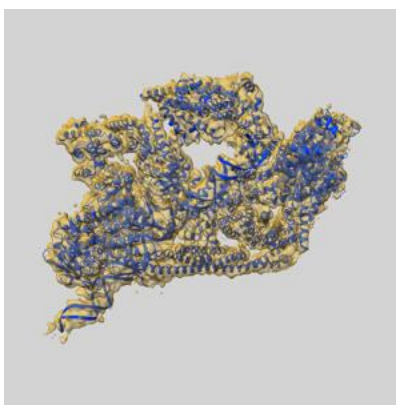
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21658 and PDB model 6WG3. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

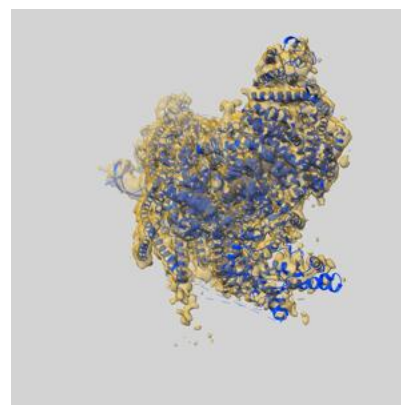
9.1 Map-model overlay [i](#)



X



Y



Z

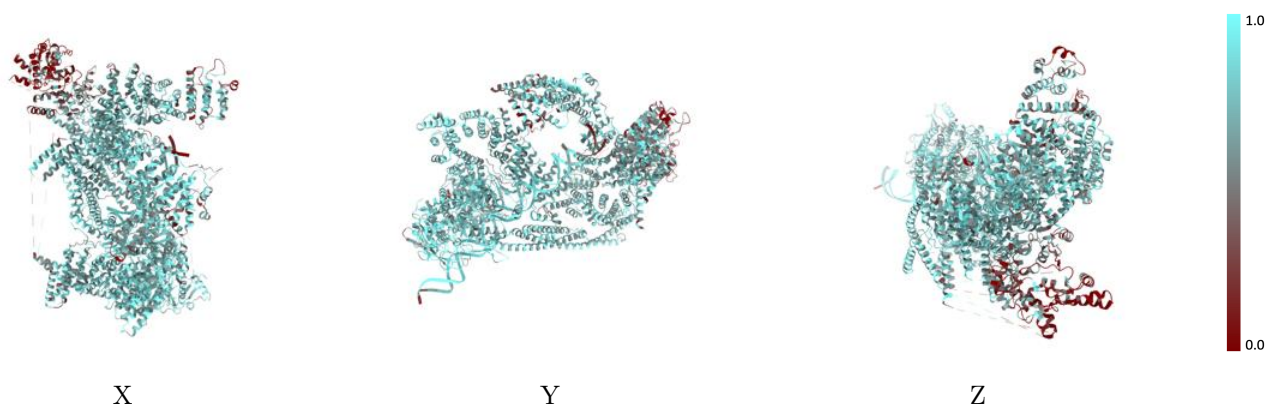
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



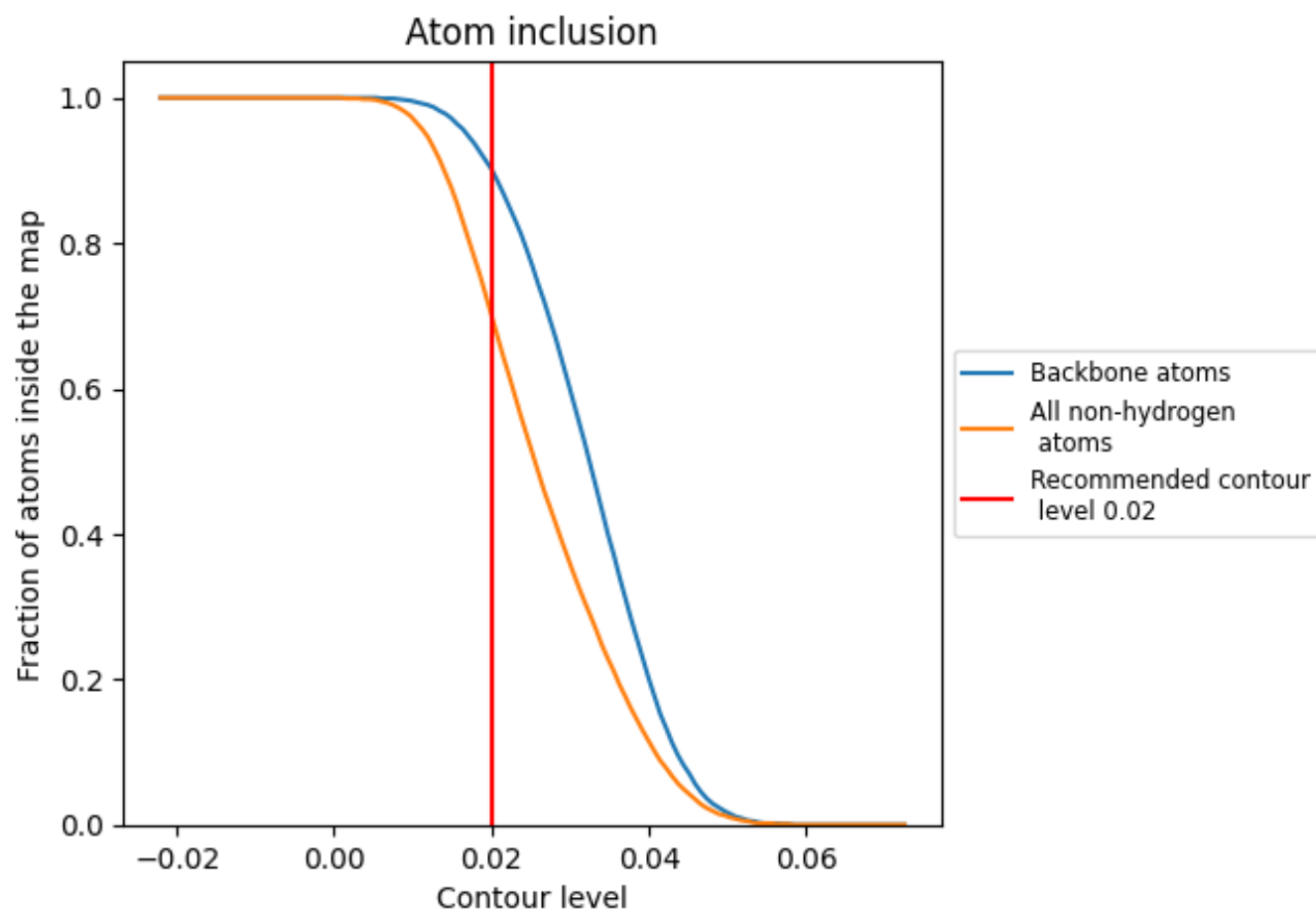
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 70% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7010	0.2390
A	0.6670	0.2470
B	0.6110	0.2320
C	0.7190	0.2550
D	0.6860	0.2150
E	0.7480	0.2510
F	0.8340	0.2520
G	0.8220	0.2520

1.0

0.0

<0.0