



Full wwPDB EM Validation Report ⓘ

Oct 21, 2024 – 12:36 PM JST

PDB ID : 7EJU
EMDB ID : EMD-31163
Title : Junin virus(JUNV) RNA polymerase L complexed with Z protein
Authors : Chen, Y.
Deposited on : 2021-04-02
Resolution : 3.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
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) : 2.39

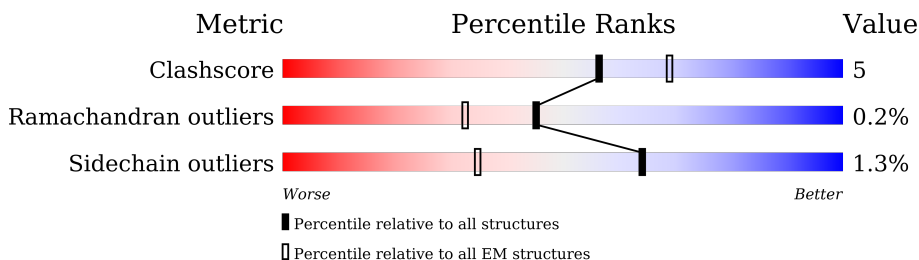
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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 ≥ 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	2210	
2	B	94	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 13713 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 RNA-directed RNA polymerase L.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1648	Total	C	N	O	S	0	0
			13287	8496	2247	2449	95		

- Molecule 2 is a protein called RING finger protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	52	Total	C	N	O	S	0	0
			423	265	75	74	9		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Zn	0
			1	1	
3	B	1	Total	Zn	0
			1	1	

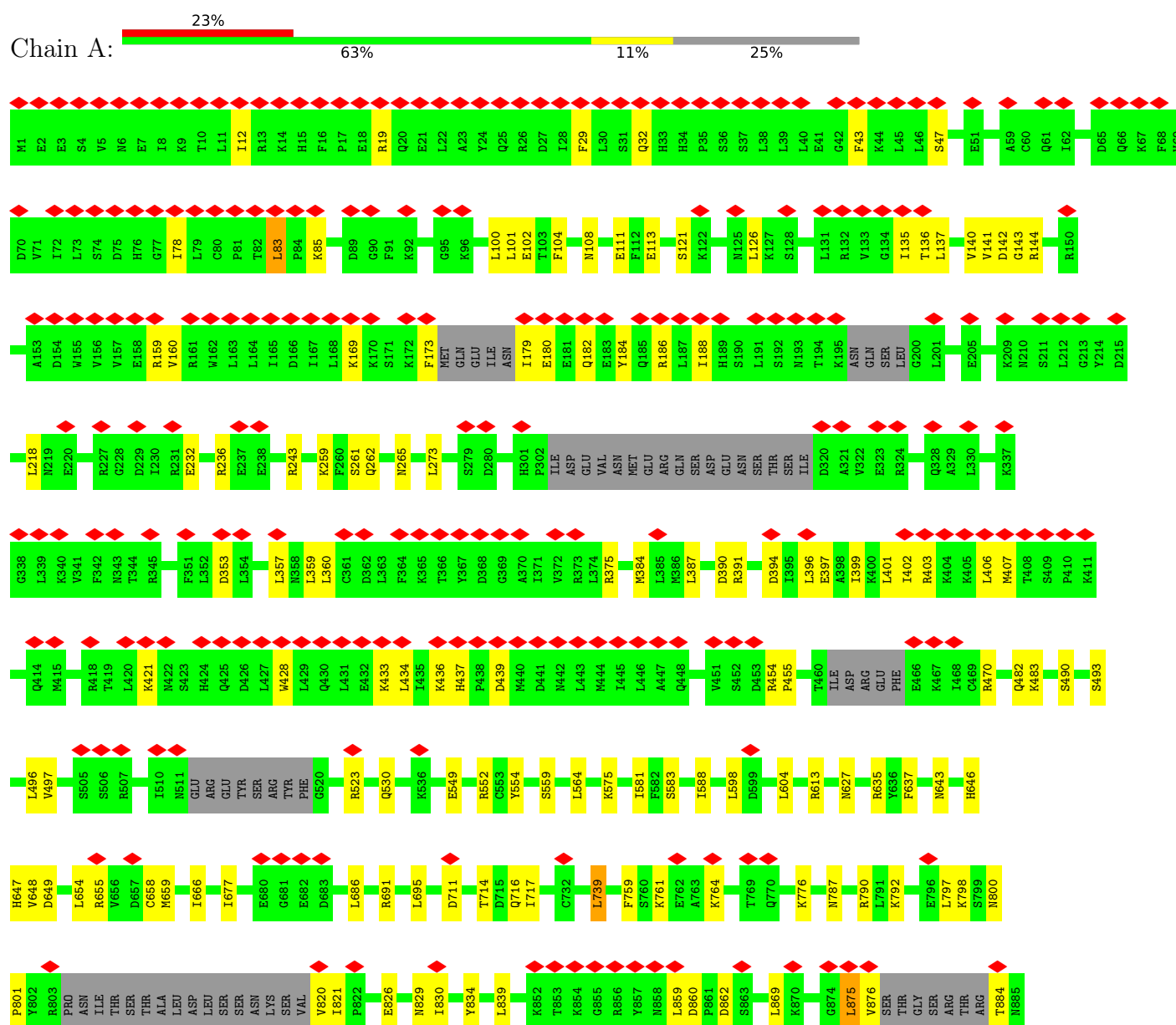
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Mg	0
			1	1	

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: RNA-directed RNA polymerase L

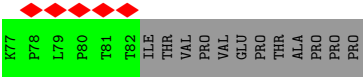
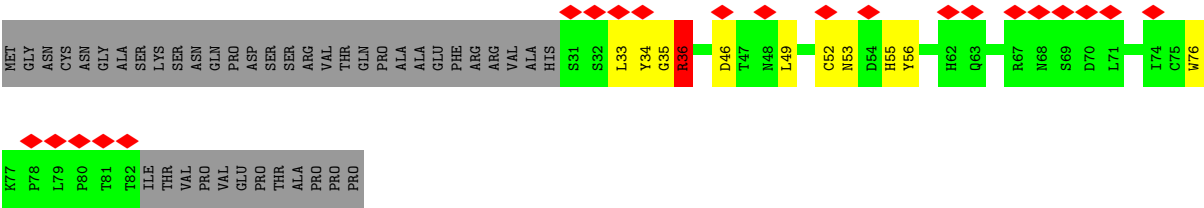


Q886	E887	E888	M892	T893	E894	T897	E898	D899	Q900	I907	R908	M913	T914	K917	N920	S921	GLY	SER	LYS	VAL	GLU	THR	SER	LYS	LEU	LEU	ASN	SER	VAL	ASP	GLU	ARG	E942	S943	L944	E945	L946	L947	W948	A949	P950	F951	G952	V953	M954	R955	E956	I957	K958																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
A959	E960	Y961	S962	M963	H964	E965	V966	K967	D968	F969	D970	P971	Y972	Y973	F974	R975	S976	D977	Y978	Y979	K980	E981	L982	C983	Y986	Y987	L988	S989	P990	Y991	K992	L993	L997	E998	A999	P1000	Q1001	D1002	I1003	C1004	P1005	L1006	G1007	L1008	L1009	L1010	K1011	N1012	L1013	I1016	A1017	Y1018	Q1019	E1020	E1021	E1022																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
F1023	F1024	E1025	C1026	F1027	K1028	L1031	I1032	Q1033	G1034	H1035	Y1036	D1037	Q1038	K1039	Y1040	G1041	S1042	TYR	GLY	HIS	SER	ARG	SER	ARG	LEU	GLY	SER	SER	VAL	LEU	LEU	ASP	GLY	VAL	ARG	LEU	SER	THR	THR	ARG	GLU	SER	ASN	SER	GLY	ALA	ILE	ALA	ASP	ASP	LYS	LEU	LEU	ASP	L1016	A1017	Y1018	Q1019	E1020	E1021	E1022																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
TYR	F1085	A1088	A1089	L1090	R1091	C1094	F1095	D1098	D1099	T1102	I1107	S1108	S1109	N1110	K1115	F1116	K1121	E1122	N1127	R1128	L1129	L1130	G1133	K1138	R1142	E1145	D1146	R1156	K1164	R1168	D1181	C1184	S1185	Y1186	S1189	P1193	P1197	F1200	L1207	E1208	L1209	P1212	R1213	D1214	K1217	E1221	N1225	W1229	H1232	V1235	N1240	V1241	A1242	E1243	C1246	V1247	K1249	L1250	K1251	ARG	SER	LEU	GLY	LEU	MET	GLY	CYS	ASP	CYS	THR	SER	VAL	G1265	E1266	F1269	H1270	Q1271	Y1272	L1273	R1276	D1277	Q1278	D1288	M1289																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
L1303	I1304	T1305	Q1307	D1314	L1315	D1318	T1325	Q1330	P1337	C1338	L1339	S1340	D1341	E1342	K1343	C1344	Q1345	D1346	R1347	V1354	F1359	S1362	K1363	L1364	S1369	V1373	I1374	F1377	F1385	I1426	V1435	R1441	V1442	N1443	G1450	T1454	P1455	F1456	G1457	A1458	E1461	Q1462	K1465	A1482	D1486	D1487	M1491	F1492	I1493	R1494	R1498	K1499	D1503	I1504	K1505	R1506	G1507	K1508	I1509	E1512	M1513	L1514	I1515	N1516	L1517	R1520	G1521	G1522	D1523	E1524	Q1531	Y1532	A1533	G1534	C1535	S1536	E1537	D1538	E1539	I1540	R1541	Q1542	T1543	L1544	V1548	V1549	M1550	L1551																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
G1555	K1564	L1565	M1566	T1567	SER	ARG	ARG	VAL	LEU	GLY	LYS	GLY	M1577	I1581	K1582	Q1585	S1586	L1587	L1588	S1589	R1590	ASN	PHE	THR	LYS	GLY	VAL	LYS	LEU	ALA	GLY	SER	ILE	ASN	SER	A1608	F1609	Q1610	S1611	R1630	D1631	K1633	G1634	G1635	F1636	L1637	D1641	I1642	C1651	G1652	T1653	M1566	T1567	SER	ARG	ARG	VAL	LEU	GLY	LYS	GLY	M1577	I1581	K1582	Q1585	S1586	L1587	L1588	S1589	R1590	ASN	PHE	THR	LYS	GLY	VAL	LYS	LEU	ALA	GLY	SER	ILE	ASN	SER	A1608	F1609	Q1610	S1611	R1630	D1631	K1633	G1634	G1635	F1636	L1637	D1641	I1642	C1651	G1652	T1653	M1566	T1567	SER	ARG	ARG	VAL	LEU	GLY	LYS	GLY	M1577	I1581	K1582	Q1585	S1586	L1587	L1588	S1589	R1590	ASN	PHE	THR	LYS	GLY	VAL	LYS	LEU	ALA	GLY	SER	ILE	ASN	SER	A1608	F1609	Q1610	S1611	R1630	D1631	K1633	G1634	G1635	F1636	L1637	D1641	I1642	C1651	G1652	T1653	M1566	T1567	SER	ARG	ARG	VAL	LEU	GLY	LYS	GLY	M1577	I1581	K1582	Q1585	S1586	L1587	L1588	S1589	R1590	ASN	PHE	THR	LYS	GLY	VAL	LYS	LEU	ALA	GLY	SER	ILE	ASN	SER	A1608	F1609	Q1610	S1611	R1630	D1631	K1633	G1634	G1635	F1636	L1637	D1641	I1642	C1651	G1652	T1653	M1566	T1567	SER	ARG	ARG	VAL	LEU	GLY	LYS	GLY	M1577	I1581	K1582	Q1585	S1586	L1587	L1588	S1589	R1590	ASN	PHE	THR	LYS	GLY	VAL	LYS	LEU	ALA	GLY	SER	ILE	ASN	SER	A1608	F1609	Q1610	S1611	R1630	D1631	K1633	G1634	G1635	F1636	L1637	D1641	I1642	C1651	G1652	T1653	M1566	T1567	SER	ARG	ARG	VAL	LEU	GLY	LYS	GLY	M1577	I1581	K1582	Q1585	S1586	L1587	L1588	S1589	R1590	ASN	PHE	THR	LYS	GLY	VAL	LYS	LEU	ALA	GLY	SER	ILE	ASN	SER	A1608	F1609	Q1610	S1611	R1630	D1631	K1633	G1634	G1635	F1636	L1637	D1641	I1642	C1651	G1652	T1653	M1566	T1567	SER	ARG	ARG	VAL	LEU	GLY	LYS	GLY	M1577	I1581	K1582	Q1585	S1586	L1587	L1588	S1589	R1590	ASN	PHE	THR	LYS	GLY	VAL	LYS	LEU	ALA	GLY	SER	ILE	ASN	SER	A1608	F1609	Q1610	S1611	R1630	D1631	K1633	G1634	G1635	F1636	L1637	D1641	I1642	C1651	G1652	T1653	M1566	T1567	SER	ARG	ARG	VAL	LEU	GLY	LYS	GLY	M1577	I1581	K1582	Q1585	S1586	L1587	L1588	S1589	R1590	ASN	PHE	THR	LYS	GLY	VAL	LYS	LEU	ALA	GLY	SER	ILE	ASN	SER	A1608	F1609	Q1610	S1611	R1630	D1631	K1633	G1634	G1635	F1636	L1637	D1641	I1642	C1651	G1652	T1653	M1566	T1567	SER	ARG	ARG	VAL	LEU	GLY	LYS	GLY	M1577	I1581	K1582	Q1585	S1586	L1587	L1588	S1589	R1590	ASN	PHE	THR	LYS	GLY	VAL	LYS	LEU	ALA	GLY	SER	ILE	ASN	SER	A1608	F1609	Q1610	S1611	R1630	D1631	K1633	G1634	G1635	F1636	L1637	D1641	I1642	C1651	G1652	T1653	M1566	T1567	SER	ARG	ARG	VAL	LEU	GLY	LYS	GLY	M1577	I1581	K1582	Q1585	S1586	L1587	L1588	S1589	R1590	ASN	PHE	THR	LYS	GLY	VAL	LYS	LEU	ALA	GLY	SER	ILE	ASN	SER	A1608	F1609	Q1610	S1611	R1630	D1631	K1633	G1634	G1635	F1636	L1637	D1641	I1642	C1651	G1652	T1653	M1566	T1567	SER	ARG	ARG	VAL	LEU	GLY	LYS	GLY	M1577	I1581	K1582	Q1585	S1586	L1587	L1588	S1589	R1590	ASN	PHE	THR	LYS	GLY	VAL	LYS	LEU	ALA	GLY	SER	ILE	ASN	SER	A1608	F1609	Q1610	S1611	R1630	D1631	K1633	G1634	G1635	F1636	L1637	D1641	I1642	C1651	G1652	T1653	M1566	T1567	SER	ARG	ARG	VAL	LEU	GLY	LYS	GLY	M1577	I1581	K1582	Q1585	S1586	L1587	L1588	S1589	R1590	ASN	PHE	THR	LYS	GLY	VAL	LYS	LEU	ALA	GLY	SER	ILE	ASN	SER	A1608	F1609	Q1610	S1611	R1630	D1631	K1633	G1634	G1635	F1636	L1637	D1641	I1642	C1651	G1652	T1653	M1566	T1567	SER	ARG	ARG	VAL	LEU	GLY	LYS	GLY	M1577	I1581	K1582	Q1585	S1586	L1587	L1588	S1589	R1590	ASN	PHE	THR	LYS	GLY	VAL	LYS	LEU	ALA	GLY	SER	ILE	ASN	SER	A1608	F1609	Q1610	S1611	R1630	D1631	K1633	G1634	G1635	F1636	L1637	D1641	I1642	C1651	G1652	T1653	M1566	T1567	SER	ARG	ARG	VAL	LEU	GLY	LYS	GLY	M1577	I1581	K1582	Q1585	S1586	L1587	L1588	S1589	R1590	ASN	PHE	THR	LYS	GLY	VAL	LYS	LEU	ALA	GLY	SER	ILE	ASN	SER	A1608	F1609	Q1610	S1611	R1630	D1631	K1633	G1634	G1635	F1636	L1637	D1641	I1642	C1651	G1652	T1653	M1566	T1567	SER	ARG	ARG	VAL	LEU	GLY	LYS	GLY	M1577	I1581	K1582	Q1585	S1586	L1587	L1588	S1589	R1590	ASN	PHE	THR	LYS	GLY	VAL	LYS	LEU	ALA	GLY	SER	ILE	ASN	SER	A1608	F1609	Q1610	S1611	R1630	D1631	K1633	G1634	G1635	F1636	L1637	D1641	I1642	C1651	G1652	T1653	M1566	T1567	SER	ARG	ARG	VAL	LEU	GLY	LYS	GLY	M1577	I1581	K1582	Q1585	S1586	L1587	L1588	S1589	R1590	ASN	PHE	THR	LYS	GLY	VAL	LYS	LEU	ALA	GLY	SER	ILE	ASN	SER	A1608	F1609	Q1610	S1611	R1630	D1631	K1633	G1634	G1635	F1636	L1637	D1641	I1642	C1651	G1652	T1653	M1566	T1567	SER	ARG	ARG	VAL	LEU	GLY	LYS	GLY	M1577	I1581	K1582	Q1585	S1586	L1587	L1588	S1589	R1590	ASN	PHE	THR	LYS	GLY	VAL	LYS	LEU	ALA	GLY	SER	ILE	ASN	SER	A1608	F1609	Q1610	S1611	R1630	D1631	K1633	G1634	G1635	F1636	L1637	D1641	I1642	C1651	G1652	T1653	M1566	T1567	SER	ARG	ARG	VAL	LEU	GLY	LYS	GLY	M1577	I1581	K1582	Q1585	S1586	L1587	L1588	S1589	R1590	ASN	PHE	THR	LYS	GLY	VAL	LYS	LEU	ALA	GLY	SER	ILE	ASN	SER	A1608	F1609	Q1610	S1611	R1630	D1631	K1633	G1634	G1635	F1636	L1637	D1641	I1642	C1651	G1652	T1653	M1566	T1567	SER	ARG	ARG	VAL	LEU	GLY	LYS	GLY	M1577	I1581	K1582	Q1585	S1586	L1587	L1588	S1589	R1590	ASN	PHE	THR	LYS	GLY	VAL	LYS	LEU	ALA	GLY	SER	ILE	ASN	SER	A1608	F1609	Q1610	S1611	R1630	D1631	K1633	G1634	G1635	F1636	L1637	D1641	I1642	C1651	G1652	T1653	M1566	T1567	SER	ARG	ARG	VAL	LEU	GLY	LYS	GLY	M1577	I1581	K1582	Q1585	S1586	L1587	L1588	S1589	R1590	ASN	PHE	THR	LYS	GLY	VAL	LYS	LEU	ALA	GLY	SER	ILE	ASN	SER	A1608	F1609	Q1610	S1611	R1630	D1631	K1633	G1634	G1635	F1636	L1637	D1641	I1642	C1651	G1652	T1653	M1566	T1567	SER	ARG	ARG	VAL	LEU	GLY	LYS	GLY	M1577	I1581	K1582	Q1585	S1586	L1587	L1588	S1589	R1590	ASN	PHE	THR	LYS	GLY	VAL	LYS	LEU	ALA	GLY	SER	ILE	ASN	SER	A1608	F1609	Q1610	S1611	R1630	D1631	K1633	G1634	G1635	F1636	L1637	D1641	I1642	C1651	G1652	T1653	M1566	T1567	SER	ARG	ARG	VAL	LEU	GLY	LYS	GLY	M1577	I1581	K1582	Q1585	S1586	L1587	L1588	S1589	R1590	ASN	PHE	THR	LYS	GLY	VAL	LYS	LEU	ALA	GLY	SER	ILE	ASN	SER	A1608	F1609	Q1610	S1611	R1630	D1631	K1633	G1634	G1635	F1636	L1637	D1641	I1642	C1651	G1652	T1653	M1566	T1567	SER	ARG	ARG	VAL	LEU	GLY	LYS	GLY	M1577	I1581	K1582	Q1585	S1586	L1587	L1588	S1589	R1590	ASN	PHE	THR	LYS	GLY	VAL	LYS	LEU	ALA	GLY	SER	ILE	ASN	SER	A1608	F1609	Q1610	S1611	R1630	D1631	K1633	G1634	G1635	F1636	L1637	D1641	I1642	C1651	G1652	T1653	M1566	T1567	SER	ARG	ARG	VAL	LEU	GLY	LYS	GLY	M1577	I1581	K1582	Q1585	S1586	L1587	L1588	S1589	R1590	ASN	PHE	THR	LYS	GLY	VAL	LYS	LEU	ALA	GLY	SER	ILE	ASN	SER	A1608	F1609	Q1610	S1611	R1630	D1631	K1633	G1634	G1635	F1636	L1637	D1641	I1642	C1651	G1652	T1653	M1566	T1567	SER	ARG	ARG	VAL	LEU</

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

SER
ASP
PRO
GLN
GLY
GLN
PHE
ARG
LEU
LYS
GLY
VAL
THR
CYS
ARG
PRO
GLN
LEU
LYS
HIS
PHE
LYS
VAL
VAL
ILE
ILE
LYS
ASP
ASP
ILE
ASP

● Molecule 2: RING finger protein Z



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	362657	Depositor
Resolution determination method	Not provided	
CTF correction method	PHASE FLIPPING ONLY	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 K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.067	Depositor
Minimum map value	-0.048	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0123	Depositor
Map size (\AA)	166.4, 166.4, 166.4	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.65, 0.65, 0.65	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.44	0/13530	0.71	10/18230 (0.1%)
2	B	0.45	0/434	0.71	0/590
All	All	0.44	0/13964	0.71	10/18820 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
2	B	0	3
All	All	0	7

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	396	LEU	CA-CB-CG	7.07	131.56	115.30
1	A	434	LEU	CA-CB-CG	6.95	131.27	115.30
1	A	1544	LEU	CA-CB-CG	6.25	129.66	115.30
1	A	353	ASP	CB-CG-OD1	6.03	123.73	118.30
1	A	1692	LEU	CA-CB-CG	5.95	128.98	115.30
1	A	1637	LEU	CA-CB-CG	5.21	127.27	115.30
1	A	83	LEU	CA-CB-CG	5.16	127.17	115.30
1	A	1650	LEU	CA-CB-CG	5.09	127.00	115.30
1	A	739	LEU	CA-CB-CG	5.08	126.98	115.30
1	A	218	LEU	CA-CB-CG	5.06	126.94	115.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1364	LEU	Peptide
1	A	1506	ARG	Peptide
1	A	19	ARG	Peptide
1	A	949	ALA	Peptide
2	B	35	GLY	Peptide
2	B	36	ARG	Peptide
2	B	76	TRP	Peptide

5.2 Too-close contacts

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	13287	0	13459	124	0
2	B	423	0	403	6	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
All	All	13713	0	13862	129	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 5.

All (129) 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:52:CYS:HB3	2:B:55:HIS:O	1.92	0.69
1:A:716:GLN:HE22	1:A:1240:ASN:HD22	1.42	0.67
1:A:101:LEU:HA	1:A:140:VAL:O	1.94	0.67
1:A:169:LYS:HD3	1:A:188:ILE:HD11	1.76	0.67
1:A:677:ILE:O	1:A:691:ARG:NH1	2.28	0.66
1:A:1377:PHE:H	2:B:36:ARG:HH22	1.46	0.62
1:A:1122:GLU:HA	1:A:1127:ASN:HD22	1.64	0.62
2:B:52:CYS:SG	2:B:53:ASN:N	2.74	0.61
1:A:1305:THR:HB	1:A:1364:LEU:HD13	1.82	0.61
1:A:390:ASP:OD2	1:A:530:GLN:NE2	2.34	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:ILE:HG21	1:A:135:ILE:HD11	1.83	0.59
1:A:1221:GLU:OE2	1:A:1225:ASN:ND2	2.36	0.59
1:A:1189:SER:HB3	1:A:1369:SER:HB3	1.85	0.58
1:A:1443:ASN:ND2	1:A:1461:GLU:OE2	2.36	0.58
1:A:454:ARG:HG3	1:A:523:ARG:HD2	1.86	0.58
1:A:1108:SER:O	1:A:1229:TRP:NE1	2.37	0.57
1:A:1133:GLY:O	1:A:1138:LYS:NZ	2.37	0.57
1:A:83:LEU:HD23	1:A:85:LYS:H	1.70	0.57
1:A:262:GLN:OE1	1:A:265:ASN:ND2	2.38	0.57
1:A:897:THR:H	1:A:900:GLN:HE21	1.53	0.57
1:A:759:PHE:HB3	1:A:776:LYS:HE3	1.87	0.56
1:A:113:GLU:HB3	1:A:821:ILE:HG22	1.88	0.56
1:A:1747:PHE:HA	1:A:1750:HIS:HB2	1.88	0.56
1:A:717:ILE:HG12	1:A:1241:VAL:HG23	1.88	0.56
1:A:236:ARG:HG3	1:A:1315:LEU:HD21	1.89	0.55
1:A:997:LEU:HB2	1:A:1011:LYS:HB3	1.88	0.55
1:A:384:MET:HA	1:A:394:ASP:HA	1.89	0.55
1:A:136:THR:HG21	1:A:914:THR:HG22	1.88	0.55
1:A:635:ARG:HE	1:A:1385:PHE:HZ	1.56	0.54
1:A:1548:TRP:CD1	1:A:1677:ILE:HG23	2.43	0.54
1:A:1493:ILE:HG13	1:A:1678:LEU:HD12	1.89	0.54
1:A:261:SER:OG	1:A:646:HIS:ND1	2.40	0.54
1:A:559:SER:HB3	1:A:564:LEU:HD23	1.90	0.54
1:A:273:LEU:HD11	1:A:655:ARG:HB2	1.90	0.53
1:A:1354:VAL:HG11	1:A:1374:ILE:HD13	1.89	0.53
1:A:43:PHE:HB2	1:A:1095:PHE:HZ	1.73	0.53
1:A:1338:CYS:SG	1:A:1339:LEU:N	2.81	0.53
1:A:1184:CYS:HB3	1:A:1374:ILE:HG23	1.91	0.53
1:A:869:LEU:HD12	1:A:892:MET:HB3	1.90	0.52
1:A:1494:ARG:NH1	1:A:1698:SER:O	2.42	0.52
1:A:875:LEU:HD23	1:A:876:VAL:H	1.73	0.52
1:A:637:PHE:HB2	1:A:654:LEU:HD21	1.91	0.51
2:B:49:LEU:HD13	2:B:56:TYR:HB3	1.92	0.51
1:A:677:ILE:HG13	1:A:695:LEU:HD21	1.93	0.51
1:A:1754:PHE:HA	1:A:1758:LEU:HB2	1.93	0.51
1:A:359:LEU:HD12	1:A:433:LYS:HG2	1.93	0.51
1:A:820:VAL:HG12	1:A:821:ILE:HG12	1.93	0.51
1:A:761:LYS:NZ	1:A:1362:SER:O	2.43	0.50
1:A:399:ILE:HA	1:A:402:ILE:HG22	1.92	0.50
1:A:397:GLU:O	1:A:401:LEU:HB2	2.11	0.50
1:A:102:GLU:HB2	1:A:141:VAL:HG12	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:LYS:HG3	1:A:428:TRP:HZ2	1.77	0.49
1:A:1498:ARG:NH2	1:A:1697:PHE:O	2.45	0.49
1:A:1677:ILE:HD12	1:A:1678:LEU:HD22	1.94	0.49
1:A:797:LEU:HD22	1:A:1209:LEU:HB3	1.94	0.49
1:A:552:ARG:NH2	1:A:554:TYR:OH	2.45	0.49
1:A:1121:LYS:HD2	1:A:1130:LEU:HD13	1.95	0.49
1:A:108:ASN:HB2	1:A:111:GLU:HG2	1.94	0.48
1:A:121:SER:OG	1:A:834:TYR:OH	2.30	0.48
1:A:826:GLU:HB3	1:A:829:ASN:HD22	1.77	0.48
1:A:1186:TYR:HD2	1:A:1330:GLN:HE21	1.59	0.48
1:A:1585:GLN:HE22	1:A:1749:GLU:HB2	1.77	0.48
1:A:184:TYR:HB3	1:A:186:ARG:H	1.78	0.48
1:A:711:ASP:HB3	1:A:714:THR:HG22	1.95	0.48
1:A:159:ARG:HG3	1:A:160:VAL:H	1.79	0.48
1:A:1487:ASP:OD1	1:A:1494:ARG:NH2	2.46	0.48
1:A:1537:GLU:HA	1:A:1540:ILE:HG22	1.96	0.48
1:A:1426:ILE:HD12	1:A:1435:VAL:HG21	1.96	0.48
1:A:839:LEU:HD23	1:A:907:ILE:HD13	1.95	0.48
1:A:104:PHE:O	1:A:143:GLY:HA2	2.13	0.48
1:A:173:PHE:O	1:A:179:ILE:N	2.47	0.48
1:A:439:ASP:OD1	1:A:439:ASP:N	2.47	0.48
1:A:1642:ILE:HG23	1:A:1670:VAL:HG11	1.96	0.48
1:A:1465:LYS:HB2	1:A:1810:ALA:HB1	1.95	0.47
1:A:739:LEU:HD21	1:A:1115:LYS:HE3	1.95	0.47
1:A:1108:SER:OG	1:A:1109:SER:N	2.47	0.47
1:A:259:LYS:HD3	1:A:648:VAL:HG12	1.95	0.47
1:A:357:LEU:HD21	1:A:399:ILE:HG22	1.96	0.47
1:A:860:ASP:N	1:A:860:ASP:OD1	2.45	0.47
1:A:1193:PRO:HA	1:A:1288:ASP:HA	1.96	0.47
1:A:1454:THR:HG22	1:A:1456:PHE:H	1.80	0.47
1:A:180:GLU:OE1	1:A:1085:PHE:N	2.48	0.47
2:B:46:ASP:N	2:B:46:ASP:OD1	2.48	0.47
1:A:482:GLN:OE1	1:A:613:ARG:NH1	2.47	0.46
1:A:12:ILE:HG13	1:A:159:ARG:HH22	1.80	0.46
1:A:830:ILE:HD13	1:A:900:GLN:HB3	1.97	0.45
1:A:1121:LYS:HD3	1:A:1128:ARG:HD3	1.98	0.45
1:A:1517:LEU:HA	1:A:1520:ARG:HE	1.81	0.45
1:A:1339:LEU:O	1:A:1347:ARG:NH1	2.49	0.45
1:A:47:SER:HG	1:A:1094:CYS:HG	1.65	0.45
1:A:967:LYS:HD3	1:A:968:ASP:HB2	1.98	0.45
1:A:1303:LEU:HA	1:A:1325:THR:HG21	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:ARG:HH11	1:A:406:LEU:HD23	1.82	0.44
1:A:436:LYS:HG3	1:A:437:HIS:H	1.82	0.44
1:A:232:GLU:OE1	1:A:790:ARG:NH1	2.50	0.44
1:A:798:LYS:HA	1:A:1212:PRO:HB3	2.00	0.44
1:A:792:LYS:HB2	1:A:1307:GLN:HE21	1.83	0.44
1:A:859:LEU:HD12	1:A:1003:ILE:HG21	2.00	0.43
1:A:647:HIS:HD2	1:A:649:ASP:H	1.66	0.43
1:A:800:ASN:HA	1:A:801:PRO:HD3	1.87	0.43
1:A:598:LEU:HD23	1:A:604:LEU:HG	2.01	0.43
1:A:787:ASN:HD21	1:A:1207:LEU:HA	1.83	0.43
1:A:1359:PHE:O	1:A:1362:SER:OG	2.26	0.43
1:A:490:SER:OG	1:A:581:ILE:O	2.32	0.43
1:A:583:SER:HB3	1:A:1441:ARG:HD2	2.01	0.42
1:A:1116:PHE:HB2	1:A:1235:VAL:HG12	2.01	0.42
1:A:1197:PRO:HA	1:A:1200:PHE:HD2	1.84	0.42
1:A:483:LYS:HG2	1:A:588:ILE:HD13	2.02	0.42
1:A:830:ILE:HA	1:A:1564:LYS:HZ1	1.85	0.42
1:A:549:GLU:O	1:A:575:LYS:NZ	2.47	0.42
1:A:142:ASP:OD1	1:A:142:ASP:N	2.52	0.42
1:A:1107:ILE:HG22	1:A:1232:HIS:CG	2.55	0.42
1:A:29:PHE:HA	1:A:32:GLN:HE22	1.84	0.42
1:A:100:LEU:HD12	1:A:137:LEU:HD11	2.02	0.41
1:A:643:ASN:HD22	1:A:1373:VAL:HG12	1.85	0.41
1:A:1734:HIS:HA	1:A:1737:HIS:HB3	2.02	0.41
1:A:387:LEU:HD23	1:A:391:ARG:HH11	1.85	0.41
1:A:884:THR:HA	1:A:888:GLU:HG2	2.03	0.41
1:A:958:LYS:O	1:A:962:SER:OG	2.26	0.41
1:A:658:CYS:SG	1:A:659:MET:N	2.93	0.41
1:A:360:LEU:HA	1:A:375:ARG:HH12	1.85	0.41
1:A:1550:ASN:OD1	1:A:1551:LEU:N	2.54	0.41
1:A:454:ARG:HA	1:A:455:PRO:HD3	1.80	0.41
2:B:33:LEU:HA	2:B:34:TYR:HA	1.81	0.41
1:A:1514:LEU:HD21	1:A:1532:TYR:HE2	1.86	0.41
1:A:1555:GLY:HA3	1:A:1630:ARG:HD2	2.02	0.40
1:A:493:SER:HA	1:A:496:LEU:HD12	2.04	0.40
1:A:497:VAL:HG21	1:A:581:ILE:HD11	2.03	0.40
1:A:627:ASN:ND2	1:A:666:ILE:HG21	2.37	0.40

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	1620/2210 (73%)	1353 (84%)	265 (16%)	2 (0%)	48	79
2	B	50/94 (53%)	30 (60%)	19 (38%)	1 (2%)	6	33
All	All	1670/2304 (72%)	1383 (83%)	284 (17%)	3 (0%)	45	75

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	36	ARG
1	A	862	ASP
1	A	1798	ASN

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	1514/2034 (74%)	1494 (99%)	20 (1%)	65	81
2	B	50/85 (59%)	50 (100%)	0	100	100
All	All	1564/2119 (74%)	1544 (99%)	20 (1%)	64	81

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	126	LEU
1	A	144	ARG
1	A	182	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	243	ARG
1	A	407	MET
1	A	470	ARG
1	A	686	LEU
1	A	764	LYS
1	A	875	LEU
1	A	908	ARG
1	A	975	ARG
1	A	1091	ARG
1	A	1110	ASN
1	A	1156	ARG
1	A	1271	GLN
1	A	1289	MET
1	A	1339	LEU
1	A	1633	LYS
1	A	1686	LEU
1	A	1724	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	HIS
1	A	265	ASN
1	A	347	ASN
1	A	471	HIS
1	A	787	ASN
1	A	900	GLN
1	A	1110	ASN
1	A	1127	ASN
1	A	1232	HIS
1	A	1240	ASN
1	A	1307	GLN
1	A	1585	GLN
1	A	1734	HIS
1	A	1790	HIS

5.3.3 RNA ⓘ

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](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

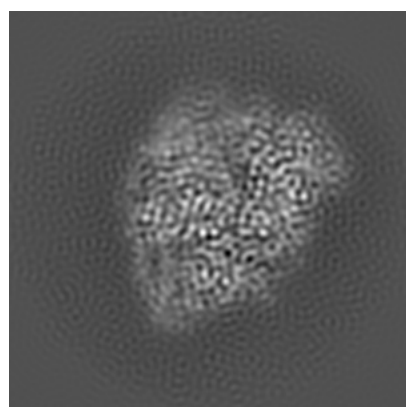
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31163. These allow visual inspection of the internal detail of the map and identification of artifacts.

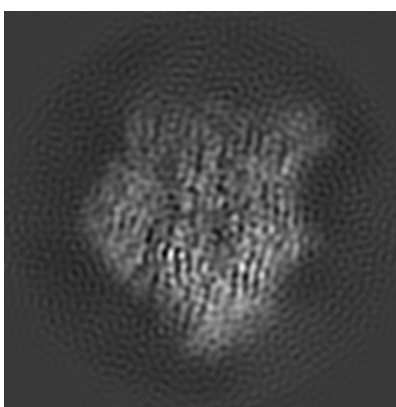
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

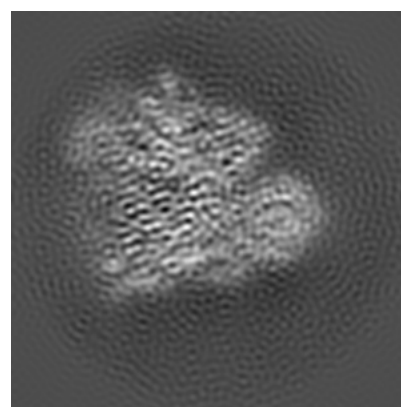
6.1.1 Primary map



X



Y

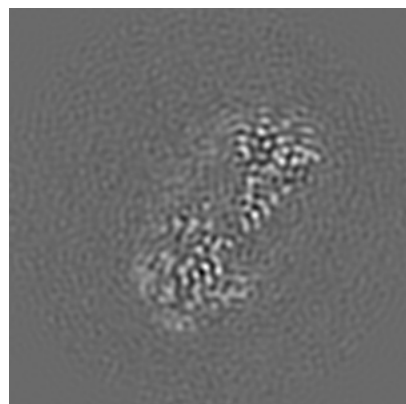


Z

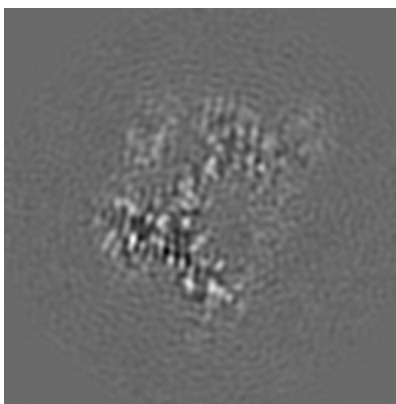
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

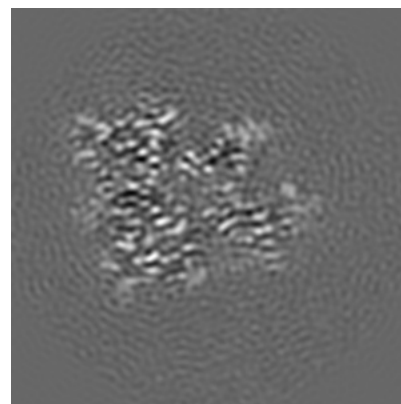
6.2.1 Primary map



X Index: 128



Y Index: 128

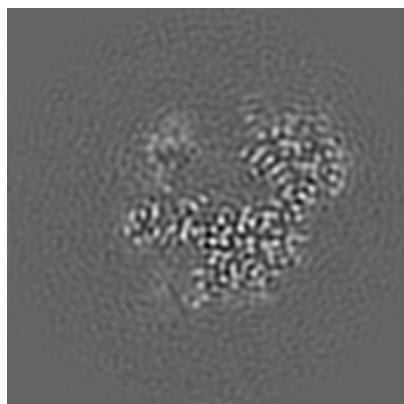


Z Index: 128

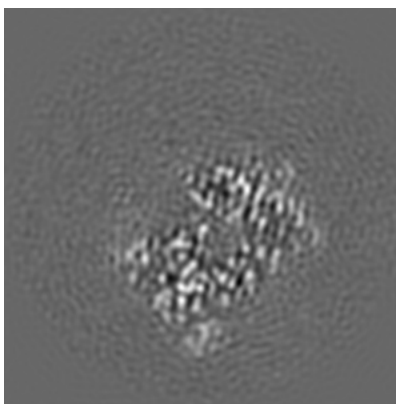
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

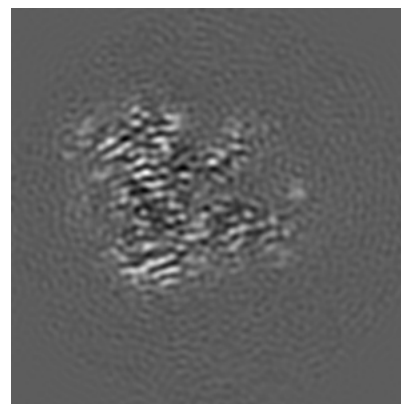
6.3.1 Primary map



X Index: 98



Y Index: 162

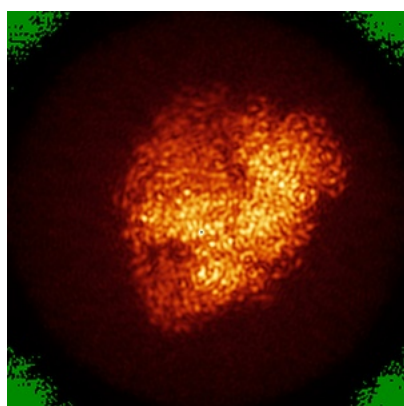


Z Index: 123

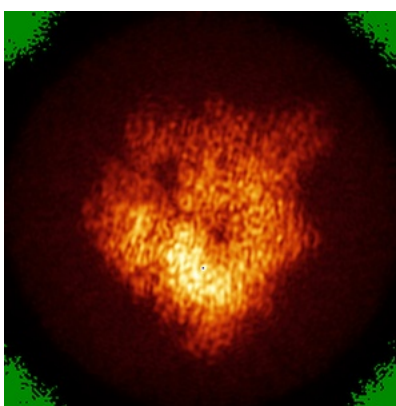
The images above show the largest variance slices of the map in three orthogonal directions.

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

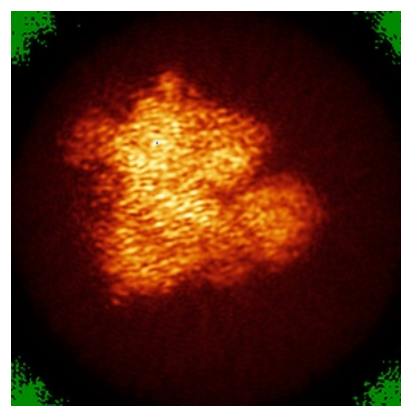
6.4.1 Primary map



X



Y

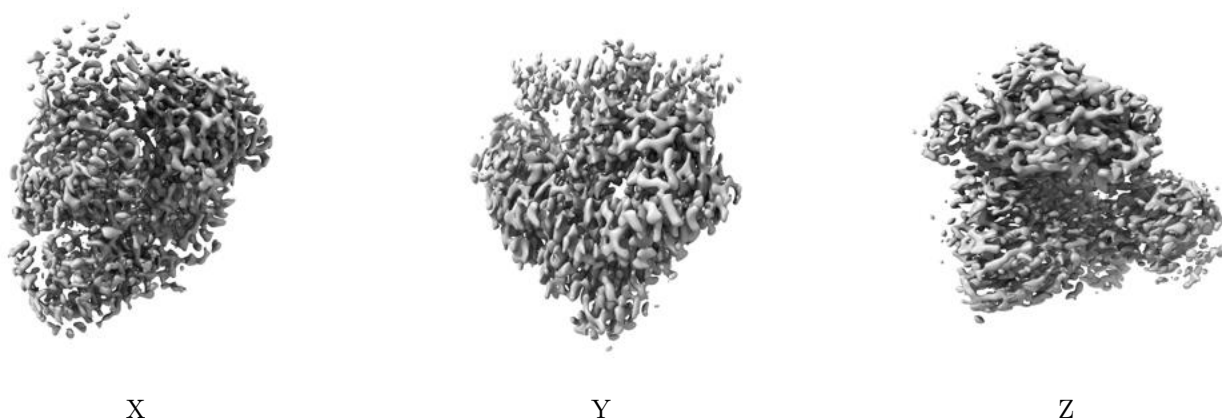


Z

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 0.0123. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

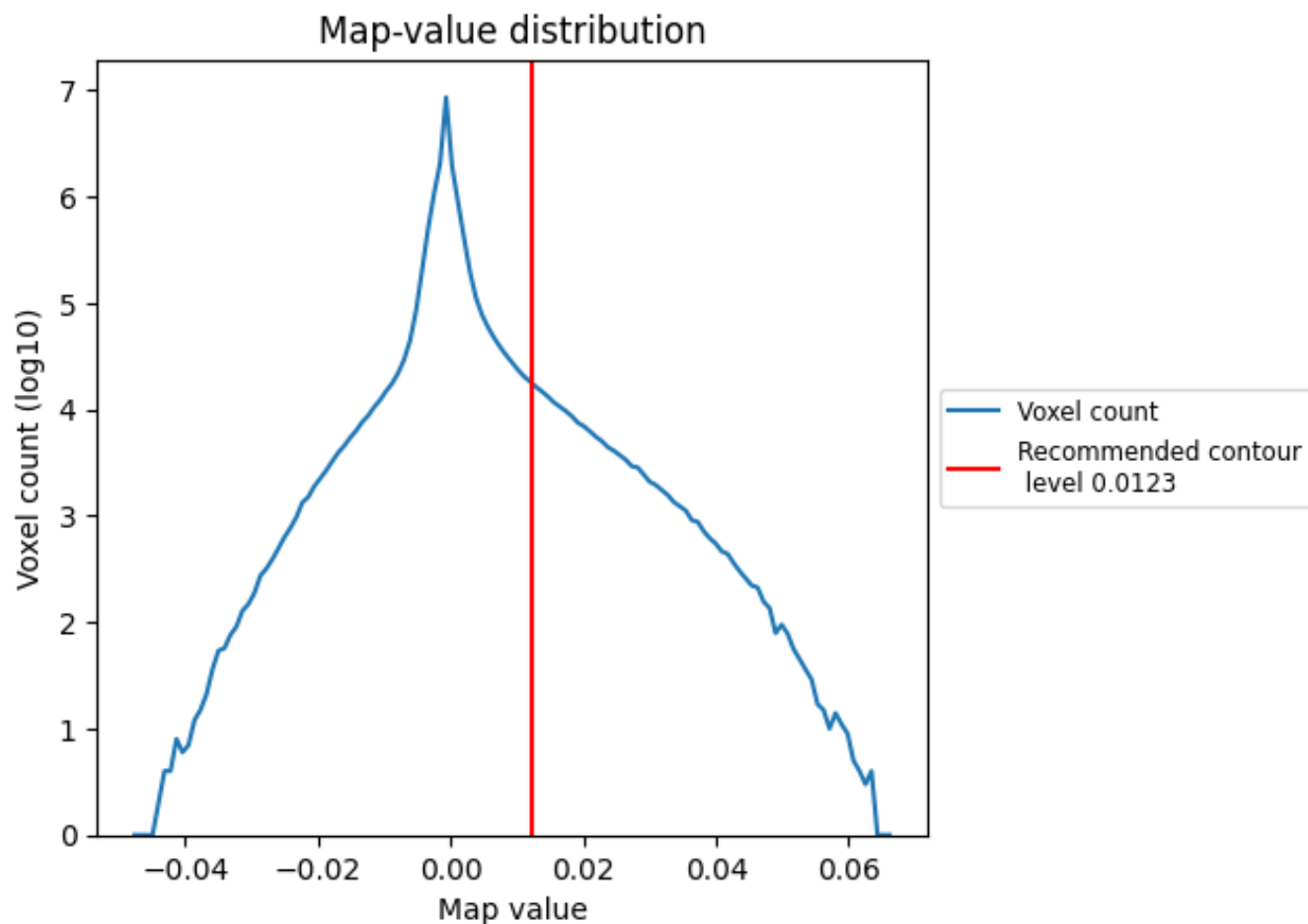
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

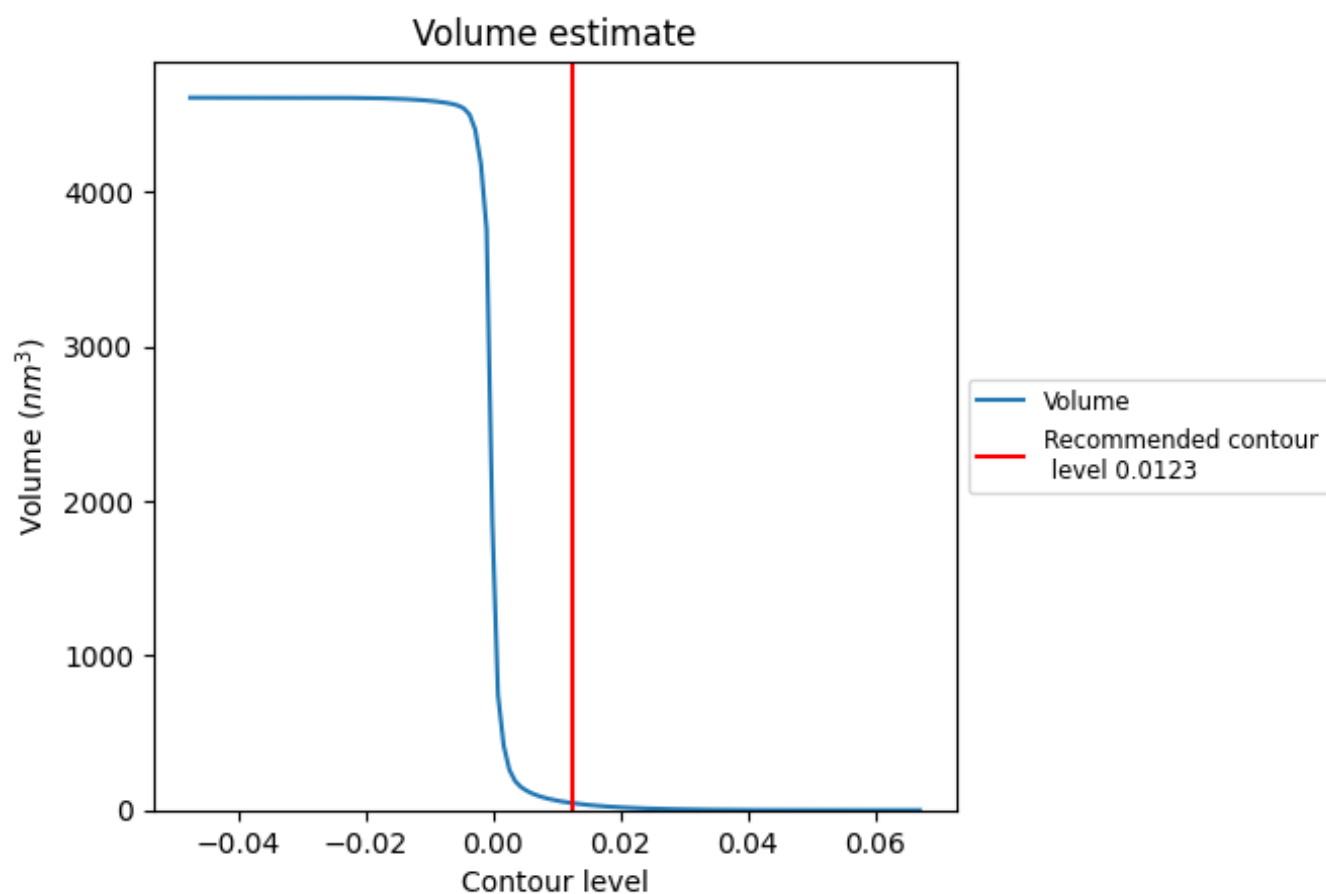
This section contains the results of statistical analysis of the map.

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.

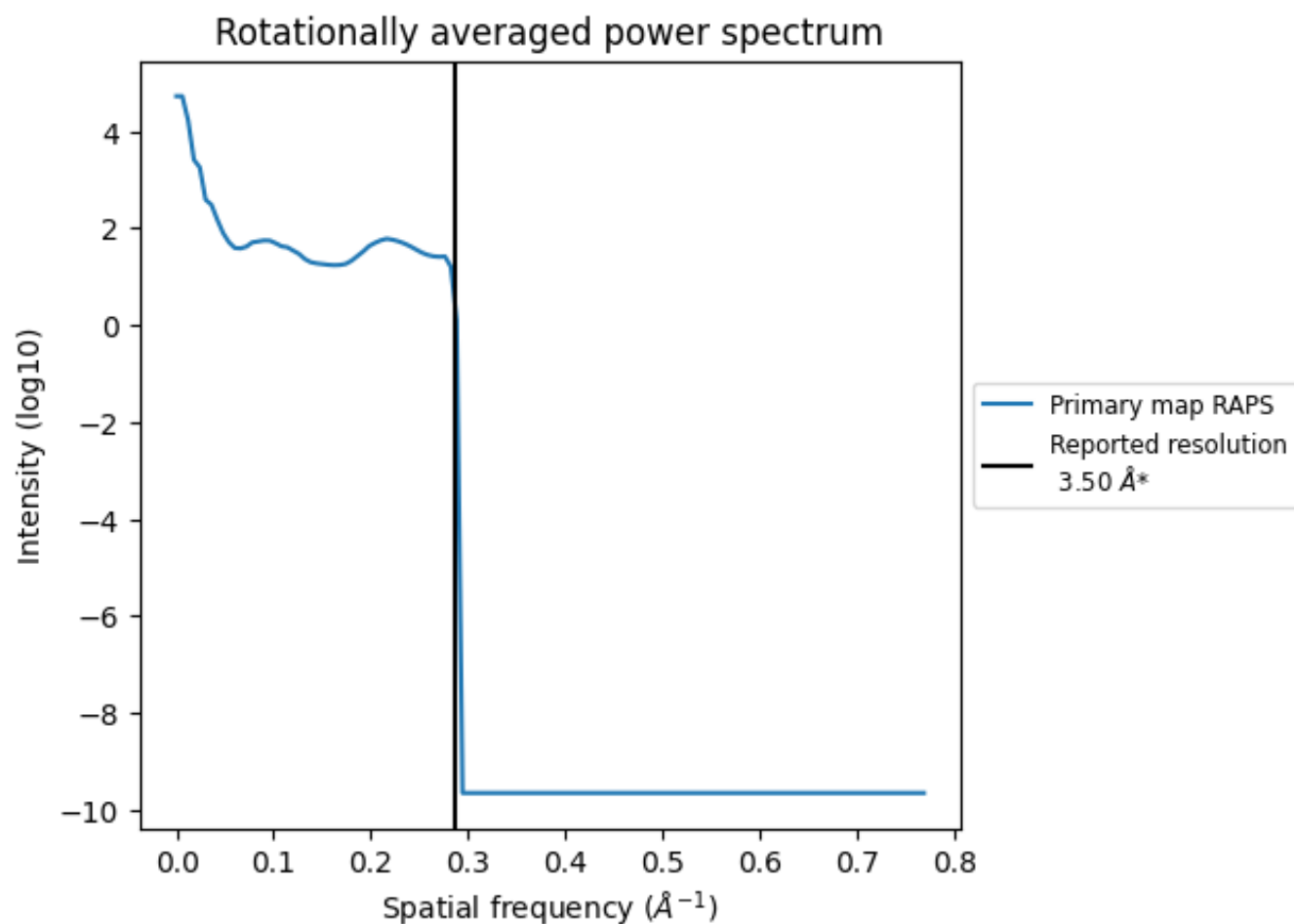
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 46 nm³; this corresponds to an approximate mass of 42 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 0.286 Å⁻¹

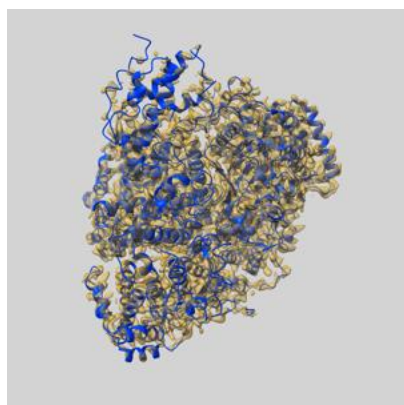
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

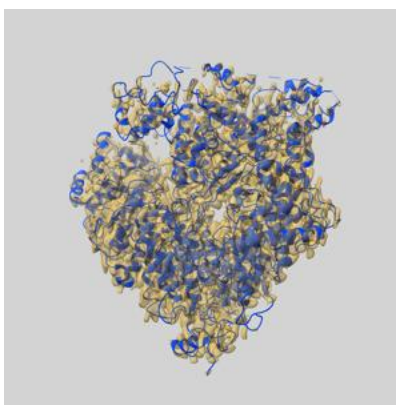
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-31163 and PDB model 7EJU. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

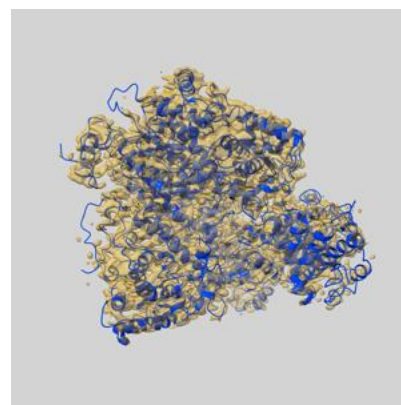
9.1 Map-model overlay [i](#)



X



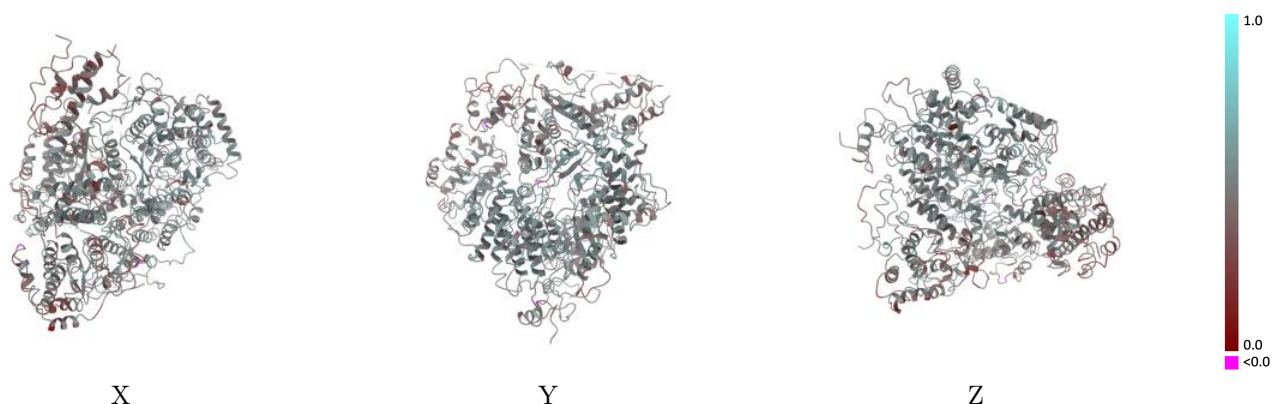
Y



Z

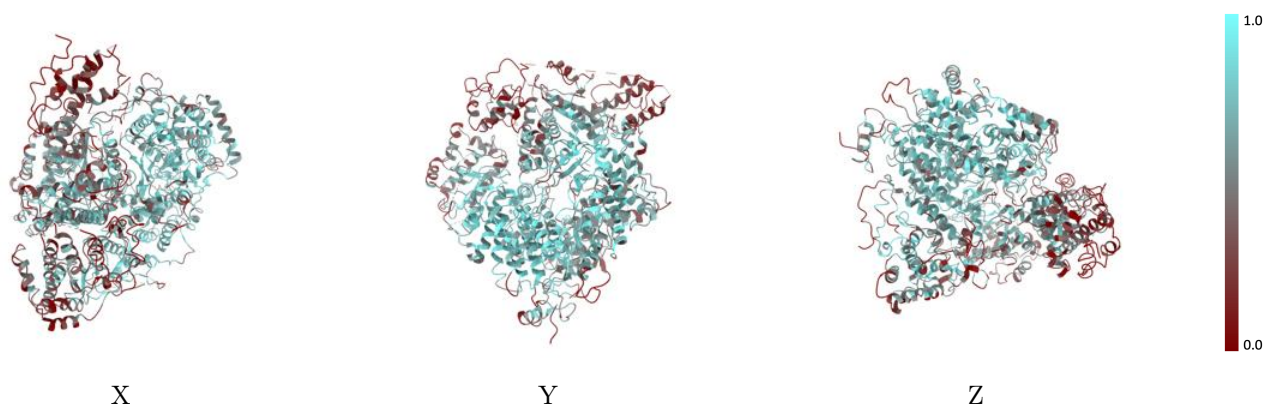
The images above show the 3D surface view of the map at the recommended contour level 0.0123 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



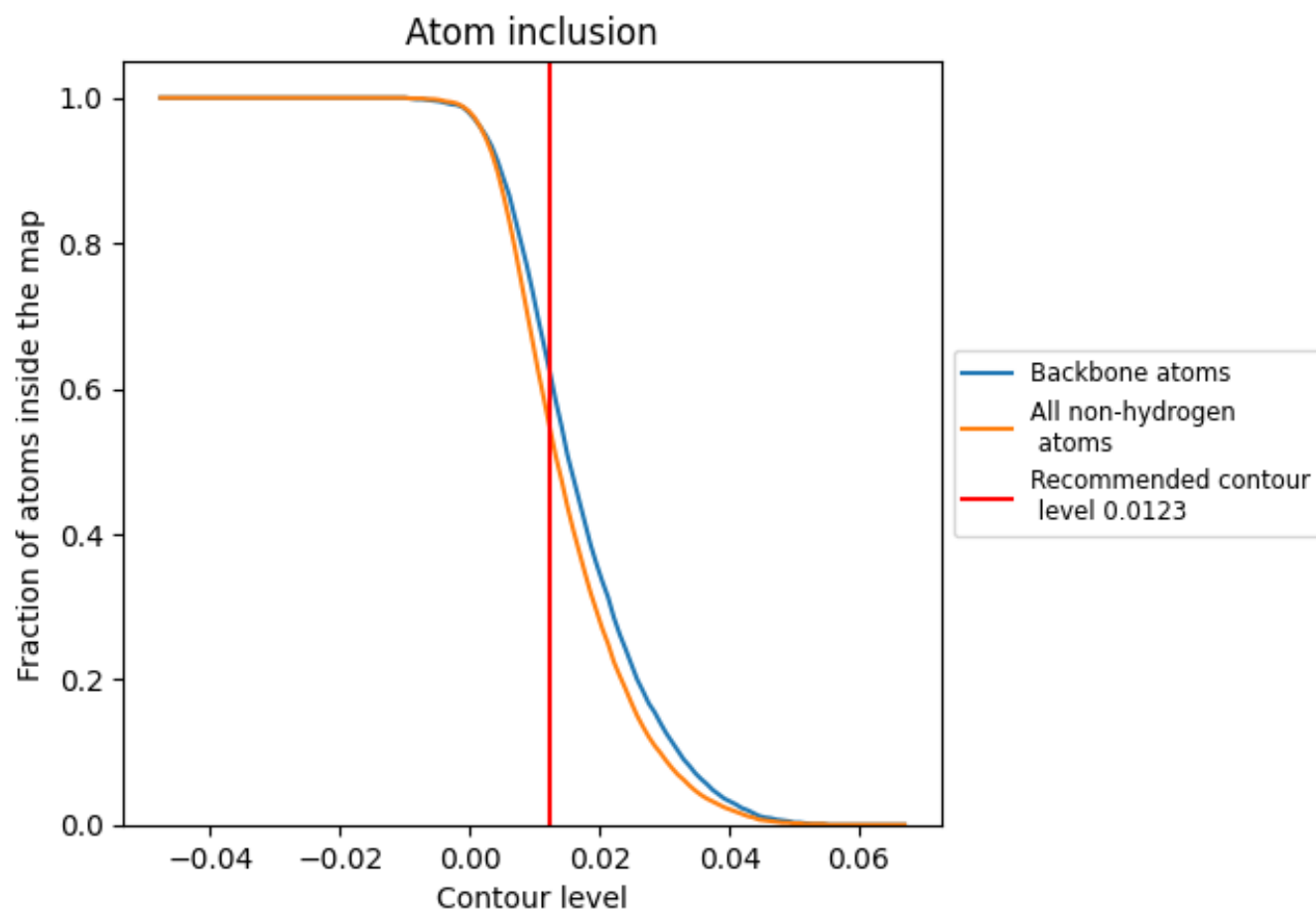
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0123).

9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 55% 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 (0.0123) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5490	<div></div> 0.4730
A	<div></div> 0.5510	<div></div> 0.4740
B	<div></div> 0.4870	<div></div> 0.4520

