WORLDWIDE

wwPDB

PROTEIN DATA BANK

Full wwPDB EM Validation Report (i)

Nov 7, 2022 – 10:05 PM EST

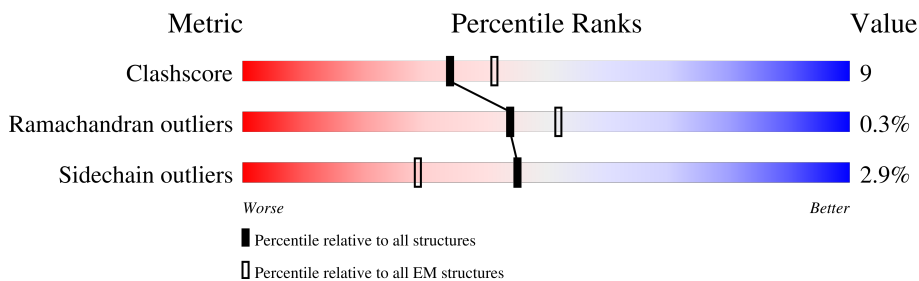|		
PDB ID	:	8DGI
EMDB ID	:	EMD-27423
Title	:	Structural Basis of MicroRNA Biogenesis by Dicer-1 and Its Partner Protein Loqs-PB - complex Ia
Authors	:	Jouravleva, K.; Golovenko, D.; Demo, G.; Dutcher, R.C.; Tanaka Hall, T.M.; Zamore, P.D.; Korostelev, A.A.
Deposited on	:	2022-06-23
Resolution	:	3.94 Å(reported)

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 3.94 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	Percentile Ranks	Value
Clashscore		9
Ramachandran outliers		0.3%
Sidechain outliers		2.9%

Worse   *Better*

■ Percentile relative to all structures
▯ Percentile relative to all EM structures

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	2249	6% / 52% / 18% · 30%
2	N	465	20% · 77%

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 13580 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.

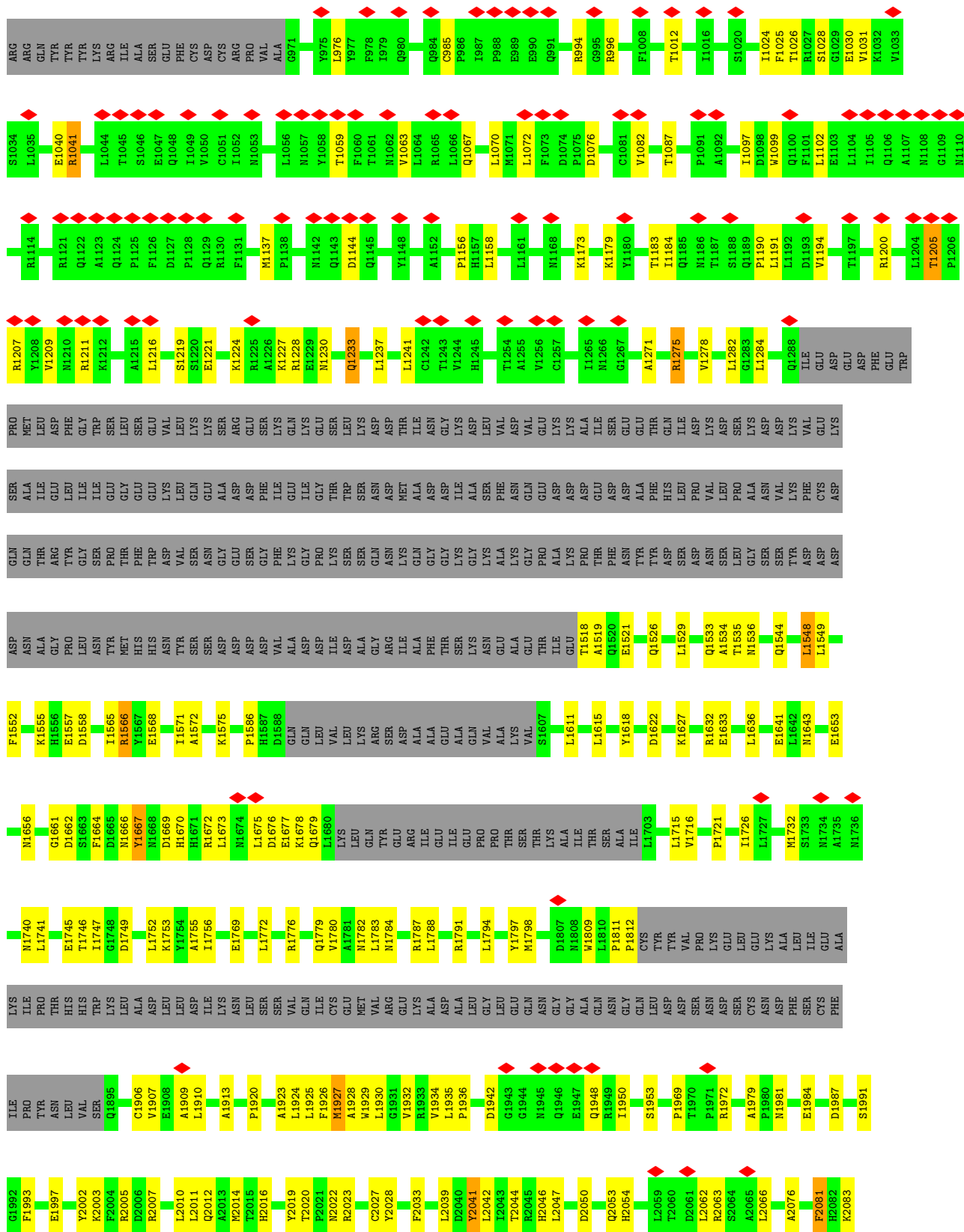- Molecule 1 is a protein called Endoribonuclease Dcr-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1582	Total 12733	C 8073	N 2236	O 2354	S 70	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	134	ARG	SER	conflict	UNP Q9VCU9
A	205	SER	THR	conflict	UNP Q9VCU9
A	416	LEU	MET	conflict	UNP Q9VCU9
A	702	SER	ALA	conflict	UNP Q9VCU9
A	796	CYS	SER	conflict	UNP Q9VCU9
A	1332	VAL	ALA	conflict	UNP Q9VCU9
A	1338	ALA	PRO	conflict	UNP Q9VCU9
A	1339	ILE	THR	conflict	UNP Q9VCU9
A	1345	ILE	LEU	conflict	UNP Q9VCU9

- Molecule 2 is a protein called Loquacious, isoform B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	N	108	Total 847	C 535	N 148	O 160	S 4	0	0

3   Residue-property plots (i)

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: Endoribonuclease Dcr-1

F2084 F2085 R2086 H2087 L2088 S2089 P2090 G2091 D2094 F2099 V2100 Q2103 N2106 G2107 H2108 C2109 I2110 S2111 Y2114 Y2115 L2116 L2117 S2118 E2121 C2122 ASP ASP ALA GLU ASP VAL E2129 A2133 L2134 G2135 D2136 E2139 S2140 I2141 A2142 G2143 F2146 L2147 D2148 S2149 N2150 W2157 H2158 V2159

Q2170 S2178 P2179 I2180 R2181 L2186 E2187 P2188 E2189 T2190 L2199 A2200 R2204 V2209 F2212 C2213 K2214 G2215 G2219 I2220 G2221 R2222 N2223 T2230 A2231 A2232 K2240 LYS GLN GLY LEU ILE ALA LYS LYS ASP

• Molecule 2: Loquacious, isoform B

Chain N: 20% • 77%

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

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

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

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

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

LYS LYS ILE ALA LYS ARG LEU ALA ALA HIS ARG MET TRP MET ARG LEU GLN GLU THR PRO ILE ASP SER GLY LYS ILE SER ASP SER ILE CYS GLY GLU LEU LEU GLU GLY LEU LEU PRO ARG SER SER GLU GLU ASN TYR TYR GLY GLU LEU LYS ASP ILE SER VAL PRO THR LEU THR T358 V364

H368 K372 N373 A374 D393 Y394 T410 L426 V427 S430 V434 H438 L456 M462 K465

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	112398	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose $(e^-/\text{Å}^2)$	48.06	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	57471	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.496	Depositor
Minimum map value	-0.340	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.0262	Depositor
Map size (Å)	360.18, 360.18, 360.18	wwPDB
Map dimensions	414, 414, 414	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.87, 0.87, 0.87	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.31	0/13020	0.68	21/17661 (0.1%)
2	N	0.31	0/859	0.65	1/1153 (0.1%)
All	All	0.31	0/13879	0.68	22/18814 (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	2

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	88	LEU	CB-CG-CD2	-8.55	96.46	111.00
1	A	323	LEU	CA-CB-CG	7.86	133.38	115.30
1	A	511	LEU	CA-CB-CG	7.74	133.11	115.30
1	A	577	ASP	CB-CG-OD2	7.72	125.25	118.30
1	A	1749	ASP	CB-CG-OD1	7.50	125.05	118.30
2	N	393	ASP	CB-CG-OD1	6.99	124.59	118.30
1	A	236	LEU	CA-CB-CG	6.86	131.07	115.30
1	A	532	ASP	CB-CG-OD1	6.74	124.37	118.30
1	A	88	LEU	CA-CB-CG	6.70	130.70	115.30
1	A	161	MET	CA-CB-CG	6.24	123.90	113.30
1	A	1070	LEU	CA-CB-CG	6.21	129.59	115.30
1	A	1783	LEU	CA-CB-CG	6.20	129.56	115.30
1	A	1241	LEU	CA-CB-CG	6.08	129.28	115.30
1	A	2186	LEU	CA-CB-CG	6.00	129.10	115.30
1	A	2041	TYR	CB-CG-CD2	-5.89	117.47	121.00
1	A	1548	LEU	CA-CB-CG	5.70	128.40	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	195	LEU	CA-CB-CG	5.67	128.35	115.30
1	A	1924	LEU	CA-CB-CG	5.42	127.76	115.30
1	A	1566	ARG	CA-CB-CG	5.41	125.30	113.40
1	A	256	PRO	N-CD-CG	-5.31	95.23	103.20
1	A	274	ASP	CB-CG-OD1	5.31	123.08	118.30
1	A	312	LEU	CA-CB-CG	5.00	126.80	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1205	THR	Peptide
1	A	2116	LEU	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	12733	0	12650	234	0
2	N	847	0	873	8	0
All	All	13580	0	13523	242	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (242) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1278:VAL:O	1:A:1282:LEU:HB3	1.79	0.81
1:A:1920:PRO:O	1:A:1923:ALA:HB3	1.83	0.78
1:A:1529:LEU:O	1:A:1533:GLN:HB2	1.84	0.78
1:A:2117:LEU:O	1:A:2121:GLU:HB3	1.92	0.70
1:A:59:ARG:HB3	1:A:1991:SER:HB3	1.77	0.67
1:A:95:GLN:HB2	1:A:115:ILE:HD12	1.77	0.67
1:A:1907:VAL:O	1:A:1910:LEU:HB2	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:ARG:HB2	1:A:111:TYR:HA	1.80	0.63
1:A:1794:LEU:O	1:A:1797:TYR:HB2	1.98	0.63
1:A:2062:LEU:O	1:A:2066:LEU:HB2	1.98	0.63
1:A:528:GLN:NE2	1:A:529:TYR:O	2.32	0.62
1:A:67:TYR:HB3	1:A:115:ILE:HG23	1.81	0.62
1:A:88:LEU:O	1:A:2087:HIS:NE2	2.33	0.62
1:A:985:CYS:HB3	1:A:1030:GLU:HB3	1.80	0.62
1:A:79:CYS:SG	1:A:80:SER:N	2.73	0.61
1:A:976:LEU:H	1:A:1041:ARG:HH21	1.48	0.61
1:A:153:ARG:O	1:A:157:GLU:HB2	2.01	0.60
1:A:878:VAL:O	1:A:895:GLN:NE2	2.35	0.60
1:A:2042:LEU:HD22	1:A:2157:TRP:HB2	1.84	0.59
1:A:2106:ASN:ND2	1:A:2108:HIS:O	2.35	0.59
1:A:204:GLU:HG3	1:A:206:ALA:HB2	1.84	0.59
1:A:48:LEU:HG	1:A:89:THR:HG23	1.84	0.59
1:A:43:LYS:HD2	1:A:174:LEU:HB3	1.85	0.59
1:A:1627:LYS:NZ	1:A:1641:GLU:OE2	2.35	0.59
1:A:1779:GLN:O	1:A:1784:ASN:ND2	2.36	0.58
1:A:1221:GLU:HB3	1:A:1224:LYS:HB3	1.86	0.58
1:A:329:SER:HA	1:A:332:LEU:HD12	1.87	0.57
1:A:1746:THR:O	1:A:2063:ARG:NH2	2.37	0.57
1:A:1927:MET:HA	1:A:1930:LEU:HB2	1.87	0.57
1:A:1662:ASP:HB2	1:A:1664:PHE:H	1.70	0.57
1:A:832:TYR:HD1	1:A:912:PRO:HB3	1.70	0.56
1:A:573:GLU:O	1:A:598:GLN:NE2	2.38	0.56
1:A:2016:HIS:HB2	1:A:2087:HIS:HA	1.87	0.56
1:A:214:ARG:NH2	1:A:785:CYS:SG	2.75	0.56
1:A:1776:ARG:NH2	1:A:2033:PHE:O	2.38	0.56
1:A:2076:ALA:HA	1:A:2081:PHE:HD2	1.70	0.56
1:A:52:GLN:NE2	1:A:2085:PHE:O	2.38	0.56
1:A:1275:ARG:HG2	1:A:1721:PRO:HG2	1.86	0.56
1:A:578:VAL:O	1:A:604:ARG:NH1	2.40	0.55
2:N:430:SER:HA	2:N:434:VAL:HG23	1.88	0.55
1:A:375:PHE:HB3	1:A:493:LEU:HD11	1.89	0.55
1:A:495:ALA:HB3	1:A:565:VAL:HG22	1.89	0.55
1:A:1565:ILE:HA	1:A:1568:GLU:HG2	1.88	0.55
1:A:586:ARG:NH1	1:A:595:SER:OG	2.40	0.55
1:A:1278:VAL:O	1:A:1282:LEU:CB	2.55	0.55
1:A:1173:LYS:HE2	1:A:1184:ILE:H	1.72	0.54
1:A:89:THR:HB	1:A:91:LEU:HD12	1.90	0.54
1:A:1997:GLU:OE1	1:A:2003:LYS:NZ	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:880:LEU:H	1:A:891:LEU:HD23	1.73	0.54
1:A:1927:MET:HB3	1:A:1932:VAL:HB	1.89	0.54
1:A:1158:LEU:HB3	1:A:1191:LEU:HD12	1.89	0.53
1:A:87:HIS:CG	1:A:2100:VAL:HB	2.43	0.53
1:A:247:SER:O	1:A:251:ASP:HB2	2.09	0.53
1:A:1910:LEU:O	1:A:1913:ALA:HB3	2.09	0.53
1:A:930:LEU:HA	1:A:1787:ARG:HD3	1.90	0.53
1:A:205:SER:HB2	1:A:210:VAL:HG11	1.91	0.53
1:A:895:GLN:HG2	1:A:1636:LEU:HD21	1.90	0.53
1:A:1059:THR:HA	1:A:1063:VAL:HB	1.91	0.53
1:A:877:ILE:HD13	1:A:896:ALA:HA	1.91	0.53
1:A:909:GLN:O	1:A:911:GLN:NE2	2.42	0.53
1:A:1935:LEU:HD12	1:A:1936:PRO:HD2	1.90	0.53
1:A:1076:ASP:OD1	1:A:1076:ASP:N	2.42	0.53
1:A:1284:LEU:HD12	1:A:1715:LEU:HA	1.91	0.53
1:A:2005:ARG:HH12	1:A:2150:ASN:HB2	1.72	0.53
1:A:1667:TYR:O	1:A:1672:ARG:NH1	2.42	0.52
1:A:1548:LEU:HG	1:A:1549:LEU:HG	1.91	0.52
1:A:848:TRP:HB3	1:A:865:LEU:HD13	1.90	0.52
1:A:1678:LYS:HG3	1:A:1679:GLN:HB3	1.90	0.52
1:A:2143:GLY:O	1:A:2146:PHE:HB3	2.09	0.52
1:A:559:ARG:NH2	1:A:577:ASP:OD2	2.43	0.52
1:A:802:SER:OG	1:A:890:ARG:NH1	2.37	0.52
1:A:141:GLU:HA	1:A:174:LEU:HB2	1.90	0.52
1:A:492:THR:O	1:A:582:ASN:ND2	2.42	0.52
1:A:1622:ASP:OD1	1:A:1622:ASP:N	2.41	0.52
1:A:1752:LEU:HD23	1:A:1780:VAL:HA	1.92	0.52
1:A:81:ILE:HG13	1:A:115:ILE:HD13	1.92	0.52
1:A:931:GLU:HG2	1:A:1787:ARG:HG2	1.92	0.52
1:A:117:ARG:HB2	1:A:120:GLY:H	1.76	0.51
1:A:221:GLU:OE1	1:A:596:TYR:OH	2.27	0.51
1:A:586:ARG:NH1	1:A:599:CYS:SG	2.84	0.51
1:A:52:GLN:HE21	1:A:2086:ARG:HA	1.76	0.51
1:A:64:VAL:HB	1:A:135:VAL:HG12	1.92	0.51
1:A:223:ILE:HG23	1:A:767:LEU:HD23	1.92	0.51
1:A:1179:LYS:NZ	1:A:1230:ASN:O	2.42	0.51
1:A:1228:ARG:HB2	1:A:1233:GLN:HA	1.92	0.51
1:A:1662:ASP:OD1	1:A:1662:ASP:N	2.36	0.51
1:A:242:LEU:HD21	1:A:335:LEU:HD11	1.93	0.51
1:A:2103:GLN:O	1:A:2107:GLY:N	2.44	0.51
1:A:219:PRO:HD2	1:A:600:LYS:HE3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1282:LEU:HG	1:A:1284:LEU:H	1.75	0.50
1:A:822:LEU:HB3	1:A:890:ARG:HB3	1.92	0.50
1:A:221:GLU:OE2	1:A:600:LYS:NZ	2.44	0.50
1:A:1572:ALA:HA	1:A:1575:LYS:HD2	1.93	0.50
1:A:614:VAL:HB	1:A:767:LEU:HD22	1.93	0.50
1:A:31:ARG:O	1:A:170:ARG:NH2	2.41	0.49
1:A:256:PRO:HB2	1:A:269:LEU:HD13	1.95	0.49
1:A:1653:GLU:H	1:A:1675:LEU:HD11	1.77	0.49
1:A:2178:SER:HB3	1:A:2181:ARG:HB2	1.94	0.49
1:A:520:PRO:HA	1:A:523:LYS:HB2	1.94	0.49
1:A:1676:ASP:OD1	1:A:1676:ASP:N	2.43	0.49
1:A:508:LEU:HA	1:A:511:LEU:HG	1.95	0.49
1:A:1788:LEU:HD13	1:A:1791:ARG:HD3	1.94	0.49
1:A:1571:ILE:O	1:A:1575:LYS:N	2.43	0.49
1:A:18:ARG:O	1:A:843:LYS:NZ	2.42	0.49
1:A:1670:HIS:HA	1:A:1673:LEU:HG	1.95	0.48
1:A:1566:ARG:O	1:A:1566:ARG:NH1	2.32	0.48
1:A:1643:ASN:HB3	1:A:1678:LYS:HZ1	1.78	0.48
1:A:2047:LEU:HD11	1:A:2066:LEU:HD12	1.94	0.48
1:A:2136:ASP:O	1:A:2140:SER:N	2.47	0.48
1:A:210:VAL:HA	1:A:213:LEU:HB2	1.95	0.48
1:A:2050:ASP:OD2	1:A:2050:ASP:N	2.44	0.48
2:N:410:THR:O	2:N:427:VAL:HA	2.14	0.48
1:A:573:GLU:O	1:A:602:ARG:NH2	2.46	0.48
1:A:363:PRO:O	1:A:367:ARG:HB2	2.14	0.48
1:A:578:VAL:HG22	1:A:602:ARG:HH11	1.78	0.48
1:A:2117:LEU:O	1:A:2121:GLU:CB	2.61	0.48
1:A:574:GLU:OE1	1:A:598:GLN:NE2	2.47	0.47
1:A:181:ALA:HA	1:A:1552:PHE:HB2	1.96	0.47
1:A:502:ASN:OD1	1:A:502:ASN:N	2.47	0.47
1:A:509:PHE:HB2	1:A:529:TYR:HB3	1.95	0.47
1:A:1271:ALA:HB1	1:A:1726:ILE:HB	1.96	0.47
1:A:1611:LEU:O	1:A:1615:LEU:HB2	2.14	0.47
1:A:849:ARG:HA	1:A:1661:GLY:HA3	1.97	0.47
1:A:802:SER:HG	1:A:890:ARG:HH11	1.60	0.47
1:A:928:PHE:O	1:A:1787:ARG:NH1	2.47	0.47
1:A:853:ASN:ND2	1:A:1653:GLU:OE1	2.47	0.47
1:A:1776:ARG:O	1:A:1780:VAL:HB	2.13	0.47
1:A:1156:PRO:HA	1:A:1190:PRO:HB3	1.96	0.47
1:A:40:ARG:NH1	1:A:71:GLU:OE2	2.48	0.47
1:A:1026:THR:HG23	1:A:1028:SER:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2209:VAL:HG12	1:A:2231:ALA:HB1	1.98	0.46
1:A:19:ASP:HA	1:A:845:THR:HG21	1.97	0.46
1:A:900:LEU:HD22	1:A:905:GLU:HB2	1.97	0.46
1:A:139:VAL:HG22	1:A:172:LEU:HB3	1.97	0.46
1:A:852:ARG:HG2	1:A:1656:ASN:HB2	1.97	0.46
1:A:1099:TRP:HA	1:A:1102:LEU:HD12	1.97	0.46
1:A:2187:GLU:HB3	1:A:2190:THR:HB	1.96	0.46
2:N:465:LYS:H	2:N:465:LYS:HG3	1.62	0.46
1:A:180:SER:HA	1:A:593:TYR:HB3	1.97	0.46
1:A:218:ARG:NH1	1:A:778:GLU:OE2	2.49	0.46
1:A:320:ARG:HH11	1:A:323:LEU:HD13	1.80	0.46
1:A:1950:ILE:HB	1:A:1953:SER:HB3	1.98	0.46
2:N:394:TYR:HD1	2:N:456:LEU:HD12	1.81	0.45
1:A:1205:THR:O	1:A:1205:THR:OG1	2.31	0.45
1:A:87:HIS:ND1	1:A:2100:VAL:HB	2.32	0.45
1:A:869:ILE:HD12	1:A:2020:THR:HA	1.98	0.45
1:A:1173:LYS:HE2	1:A:1183:THR:HA	1.98	0.45
1:A:1926:PHE:O	1:A:1929:TRP:HB3	2.17	0.45
1:A:2007:ARG:HD2	1:A:2010:LEU:HD23	1.98	0.45
1:A:23:GLU:OE2	1:A:214:ARG:NH1	2.50	0.45
1:A:33:THR:O	1:A:172:LEU:HA	2.15	0.45
1:A:866:ARG:NH1	1:A:1664:PHE:O	2.49	0.45
1:A:1518:THR:OG1	1:A:1519:ALA:N	2.49	0.45
1:A:49:LYS:HD2	1:A:2088:LEU:HA	1.98	0.45
1:A:862:GLN:NE2	1:A:879:GLY:O	2.46	0.45
1:A:236:LEU:O	1:A:240:ASP:HB2	2.16	0.45
1:A:1798:MET:H	1:A:1798:MET:HE2	1.82	0.45
1:A:280:LEU:O	1:A:284:ASN:HB2	2.18	0.44
1:A:586:ARG:HH12	1:A:595:SER:HG	1.65	0.44
1:A:597:VAL:HA	1:A:600:LYS:HB3	2.00	0.44
1:A:224:VAL:HB	1:A:613:LEU:HD23	2.00	0.44
1:A:1667:TYR:HB3	1:A:1979:ALA:HB2	1.99	0.44
1:A:39:HIS:HA	1:A:1544:GLN:HG3	1.99	0.44
1:A:1732:MET:HA	1:A:1741:LEU:HG	1.99	0.44
1:A:1756:ILE:HD13	1:A:1779:GLN:HB3	2.00	0.44
1:A:275:PRO:HB2	1:A:324:LEU:HD12	1.99	0.44
1:A:560:MET:SD	1:A:560:MET:N	2.91	0.44
1:A:83:THR:HA	1:A:86:THR:HG22	2.00	0.44
1:A:947:GLY:O	1:A:1782:ASN:ND2	2.51	0.44
1:A:1981:ASN:HB2	1:A:1984:GLU:HB2	1.99	0.44
1:A:1811:PRO:HA	1:A:1812:PRO:HD3	1.89	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1906:CYS:O	1:A:1909:ALA:HB3	2.18	0.43
1:A:1936:PRO:HG3	1:A:1969:PRO:HD3	1.99	0.43
1:A:847:LEU:HD13	1:A:866:ARG:HH21	1.83	0.43
1:A:333:ILE:O	1:A:337:SER:OG	2.34	0.43
1:A:2109:CYS:HB3	1:A:2110:ILE:H	1.66	0.43
1:A:17:PRO:HG3	1:A:834:ALA:HB2	2.00	0.43
1:A:367:ARG:NH2	1:A:1586:PRO:O	2.52	0.43
1:A:1278:VAL:HG22	1:A:1282:LEU:HD22	2.00	0.43
1:A:1534:ALA:O	1:A:1536:ASN:N	2.52	0.43
1:A:1769:GLU:HA	1:A:1772:LEU:HD12	1.99	0.43
1:A:60:ARG:NH1	1:A:1987:ASP:O	2.52	0.43
1:A:90:ASP:OD1	1:A:2083:LYS:N	2.52	0.43
1:A:494:CYS:HB3	1:A:581:CYS:HA	1.99	0.43
1:A:915:LYS:H	1:A:915:LYS:HG2	1.64	0.43
2:N:462:MET:HB2	2:N:462:MET:HE2	1.77	0.43
1:A:1745:GLU:HB2	1:A:1909:ALA:HB2	2.01	0.43
1:A:569:THR:HG22	1:A:570:SER:H	1.83	0.43
1:A:996:ARG:NH2	1:A:1194:VAL:O	2.52	0.43
1:A:2223:ASN:OD1	1:A:2223:ASN:N	2.52	0.43
1:A:855:ARG:NH1	1:A:1618:TYR:OH	2.52	0.43
1:A:862:GLN:HE22	1:A:1677:GLU:HB3	1.84	0.43
1:A:48:LEU:HD12	1:A:85:LEU:HD23	2.01	0.42
1:A:1755:ALA:HB1	1:A:1934:VAL:HG21	2.01	0.42
1:A:348:GLY:N	1:A:351:SER:OG	2.53	0.42
1:A:1925:LEU:O	1:A:1928:ALA:HB3	2.19	0.42
1:A:2002:TYR:HB2	1:A:2159:VAL:HG21	2.01	0.42
1:A:2011:LEU:HG	1:A:2022:ASN:HD21	1.84	0.42
1:A:2012:GLN:NE2	1:A:2027:CYS:O	2.52	0.42
1:A:51:LEU:O	1:A:55:SER:OG	2.31	0.42
1:A:2039:LEU:HD23	1:A:2039:LEU:HA	1.83	0.42
1:A:90:ASP:OD1	1:A:2084:PHE:N	2.39	0.42
1:A:2002:TYR:OH	1:A:2148:ASP:OD1	2.31	0.42
1:A:88:LEU:O	1:A:90:ASP:N	2.53	0.42
1:A:1024:ILE:HG13	1:A:1031:VAL:HB	2.01	0.42
1:A:1087:THR:HG22	1:A:1097:ILE:HA	2.02	0.42
1:A:1643:ASN:HB3	1:A:1678:LYS:NZ	2.34	0.42
1:A:49:LYS:NZ	1:A:2089:SER:H	2.18	0.42
1:A:841:PHE:CZ	1:A:2091:GLY:HA3	2.55	0.42
1:A:2134:LEU:HD23	1:A:2134:LEU:HA	1.92	0.42
1:A:255:ASP:HB3	1:A:258:GLU:HB2	2.02	0.41
1:A:92:ARG:O	1:A:112:HIS:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1200:ARG:HB3	1:A:1219:SER:HB2	2.01	0.41
1:A:1518:THR:HG23	1:A:1521:GLU:H	1.85	0.41
1:A:866:ARG:HD3	1:A:2023:ARG:HH12	1.85	0.41
2:N:456:LEU:HD23	2:N:456:LEU:HA	1.91	0.41
1:A:319:GLU:O	1:A:323:LEU:HD12	2.20	0.41
1:A:873:LEU:HD11	1:A:899:GLU:HG3	2.02	0.41
1:A:588:ASP:N	1:A:588:ASP:OD1	2.53	0.41
1:A:944:PRO:HB3	1:A:950:LYS:HG3	2.03	0.41
1:A:1716:VAL:HG22	1:A:1948:GLN:HG2	2.01	0.41
1:A:194:THR:OG1	1:A:1557:GLU:OE2	2.37	0.41
2:N:426:LEU:HA	2:N:438:HIS:HA	2.03	0.41
1:A:45:PHE:CE1	1:A:49:LYS:HG3	2.56	0.41
1:A:868:PRO:O	1:A:871:SER:OG	2.29	0.41
1:A:1666:ASN:HA	1:A:1670:HIS:HB2	2.03	0.41
1:A:1012:THR:HG22	1:A:1082:VAL:HG22	2.02	0.41
1:A:1747:ILE:HG13	1:A:2044:THR:HG22	2.03	0.41
1:A:1993:PHE:CE2	1:A:2014:MET:HG3	2.56	0.41
1:A:1194:VAL:HG11	1:A:1237:LEU:HD12	2.03	0.41
1:A:2199:LEU:HD12	1:A:2204:ARG:HB2	2.03	0.41
1:A:1025:PHE:HB2	1:A:1209:VAL:HB	2.03	0.40
1:A:2139:GLU:O	1:A:2142:ALA:HB3	2.21	0.40
1:A:1753:LYS:HB2	1:A:1753:LYS:HE3	1.94	0.40
1:A:87:HIS:CE1	1:A:2099:PHE:HB3	2.56	0.40
1:A:1224:LYS:HA	1:A:1227:LYS:HE2	2.03	0.40
1:A:1740:ASN:OD1	1:A:1740:ASN:N	2.54	0.40
1:A:2019:TYR:HA	1:A:2088:LEU:HD12	2.04	0.40
1:A:2066:LEU:HD23	1:A:2066:LEU:HA	1.93	0.40
1:A:226:CYS:HB2	1:A:615:ALA:HB2	2.03	0.40
1:A:1067:GLN:HA	1:A:1809:TRP:HZ3	1.87	0.40
2:N:364:VAL:O	2:N:368:HIS:ND1	2.55	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	1562/2249 (70%)	1460 (94%)	97 (6%)	5 (0%)	41	74
2	N	106/465 (23%)	105 (99%)	1 (1%)	0	100	100
All	All	1668/2714 (62%)	1565 (94%)	98 (6%)	5 (0%)	44	74

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1667	TYR
1	A	2117	LEU
1	A	1535	THR
1	A	1233	GLN
1	A	1216	LEU

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	1407/1994 (71%)	1365 (97%)	42 (3%)	41	64
2	N	94/380 (25%)	93 (99%)	1 (1%)	73	84
All	All	1501/2374 (63%)	1458 (97%)	43 (3%)	45	64

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	PHE
1	A	60	ARG
1	A	100	MET
1	A	128	ARG
1	A	142	ASP
1	A	178	LEU
1	A	252	HIS
1	A	323	LEU

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Mol	Chain	Res	Type
1	A	354	ARG
1	A	521	ASP
1	A	588	ASP
1	A	841	PHE
1	A	852	ARG
1	A	863	TYR
1	A	994	ARG
1	A	1040	GLU
1	A	1041	ARG
1	A	1072	LEU
1	A	1137	MET
1	A	1144	ASP
1	A	1207	ARG
1	A	1211	ARG
1	A	1275	ARG
1	A	1526	GLN
1	A	1555	LYS
1	A	1558	ASP
1	A	1632	ARG
1	A	1633	GLU
1	A	1669	ASP
1	A	1927	MET
1	A	1942	ASP
1	A	1972	ARG
1	A	2028	TYR
1	A	2041	TYR
1	A	2046	HIS
1	A	2053	GLN
1	A	2054	HIS
1	A	2081	PHE
1	A	2089	SER
1	A	2099	PHE
1	A	2158	HIS
1	A	2170	GLN
2	N	465	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	598	GLN
1	A	895	GLN
1	A	2106	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-27423. 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
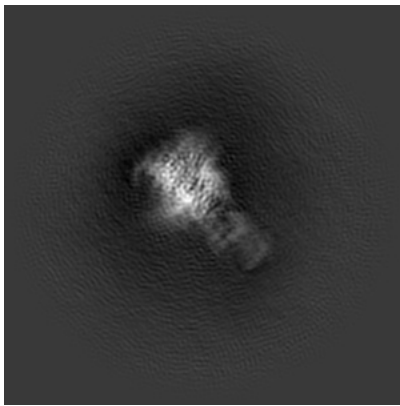
X
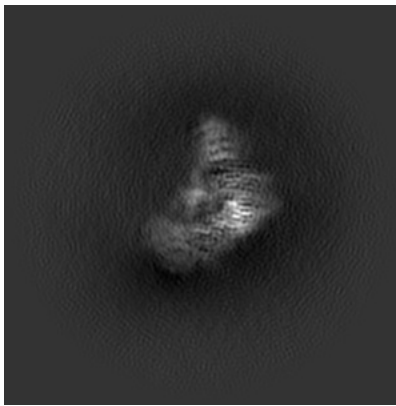
Y
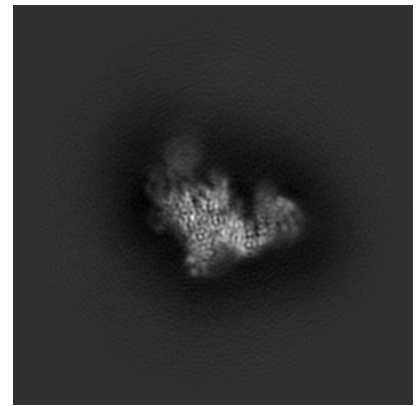
Z

6.1.2 Raw map

X

Y

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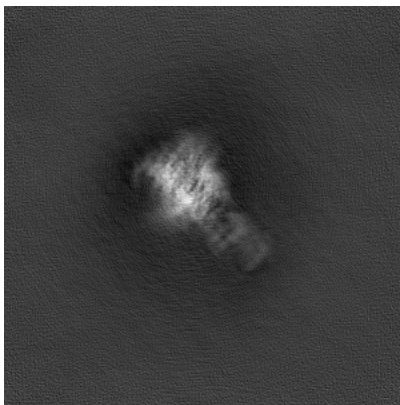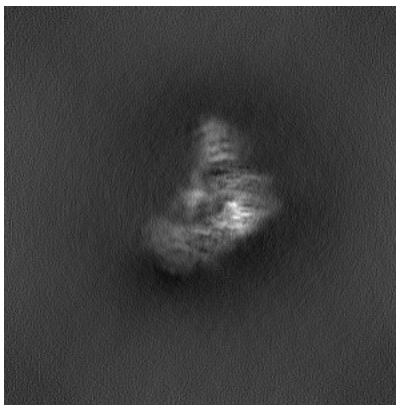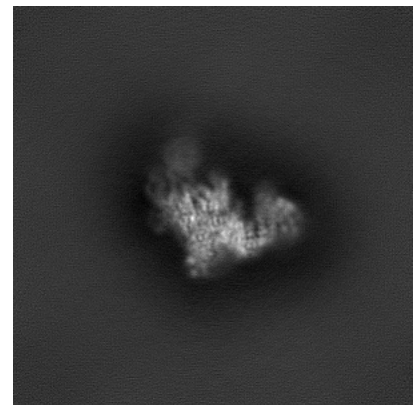
The images above show the map projected in three orthogonal directions.

6.2　Central slices (i)

6.2.1　Primary map
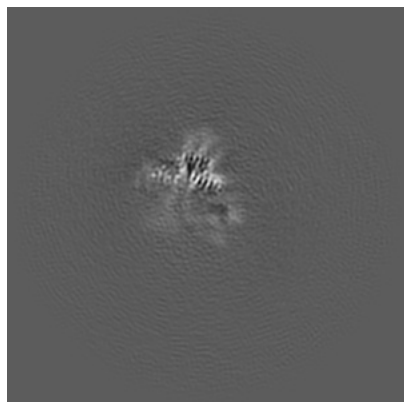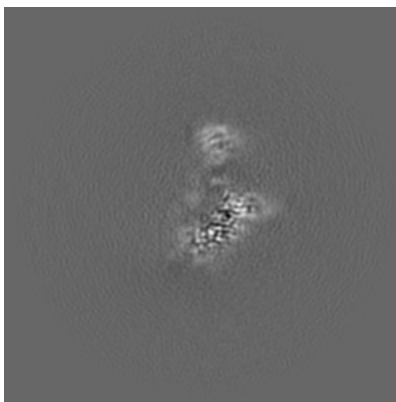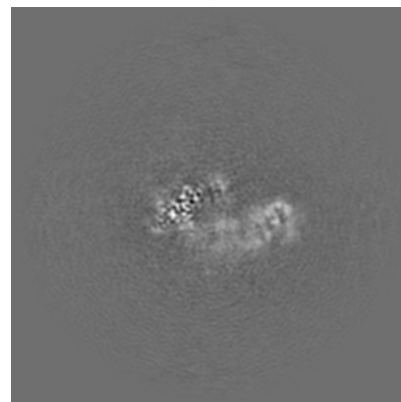
| X Index: 207 | Y Index: 207 | Z Index: 207 |

6.2.2　Raw map
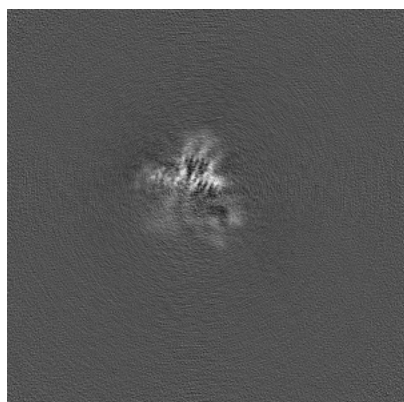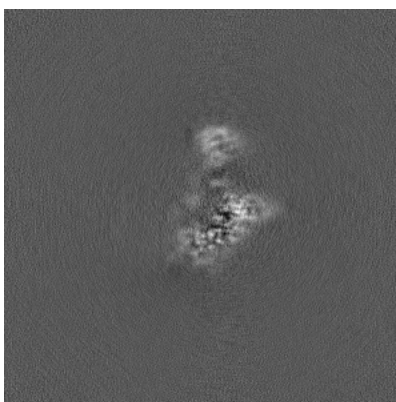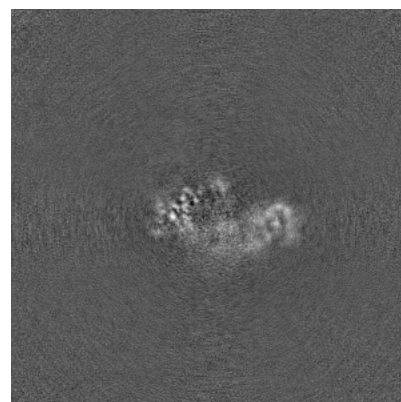
| X Index: 207 | Y Index: 207 | Z Index: 207 |

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

6.3 Largest variance slices (i)

6.3.1 Primary map
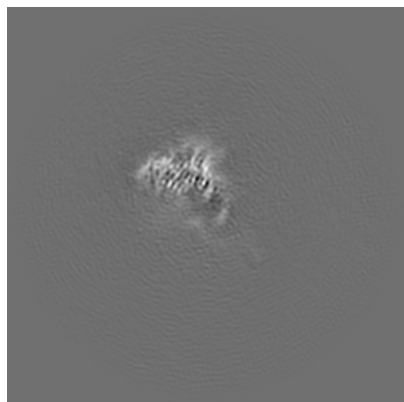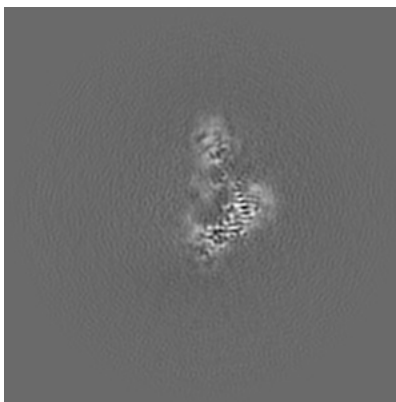
| X Index: 198 | Y Index: 193 | Z Index: 238 |
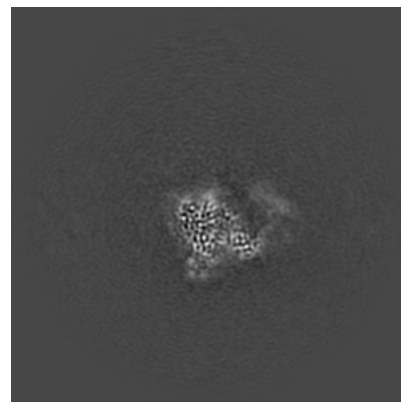
6.3.2 Raw map
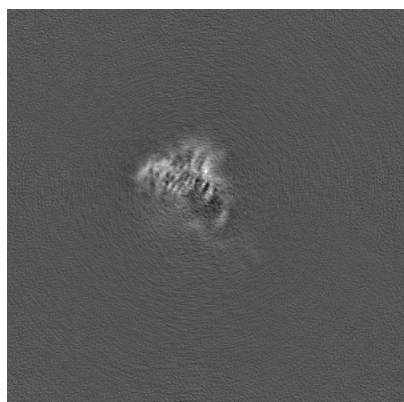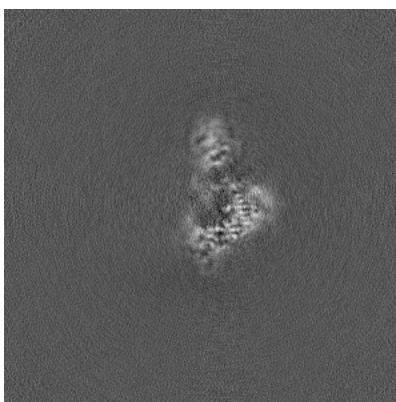
| X Index: 198 | Y Index: 194 | Z Index: 238 |
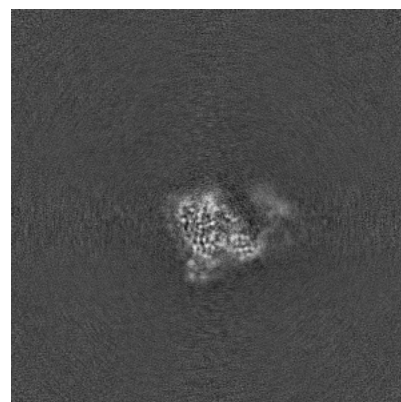
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views ⓘ

6.4.1 Primary map

| X | Y | Z |
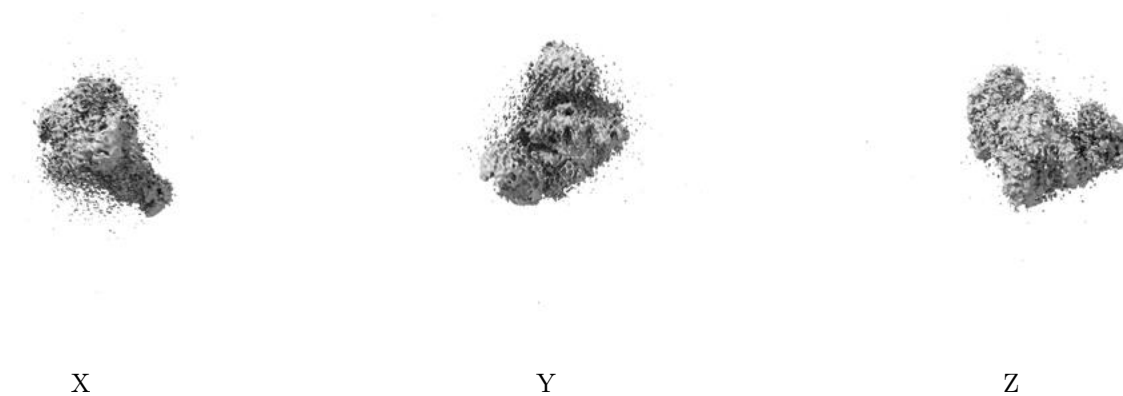
The images above show the 3D surface view of the map at the recommended contour level 0.0262. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

| X | Y | Z |
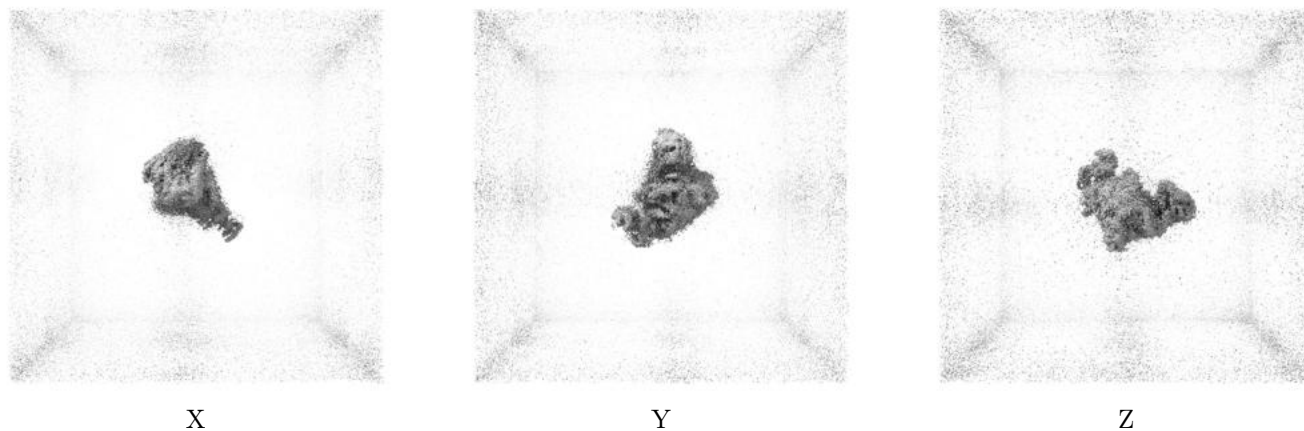
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.5 Mask visualisation ⓘ

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

7   Map analysis ⓘ

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

7.1   Map-value distribution ⓘ
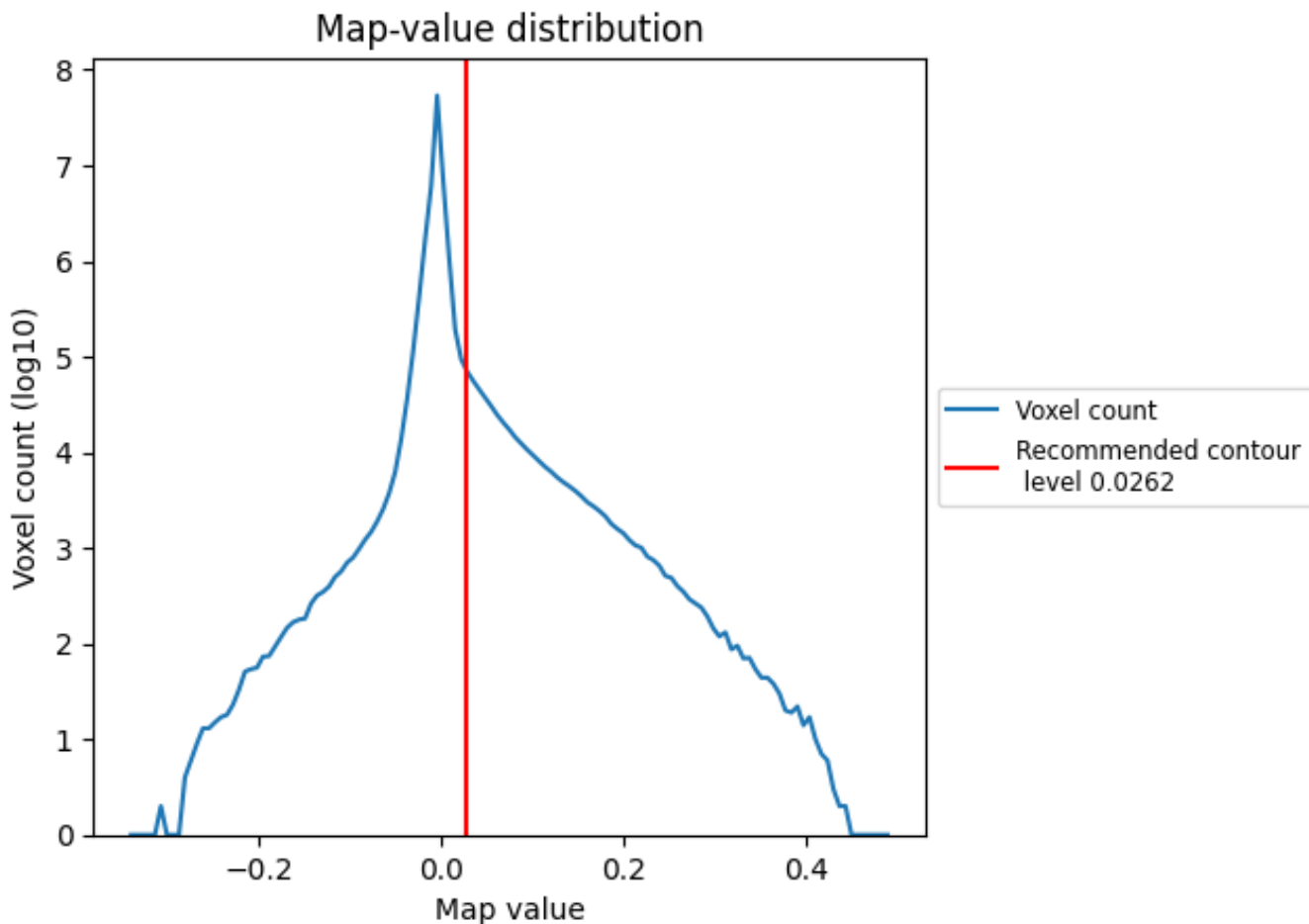
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate (i)
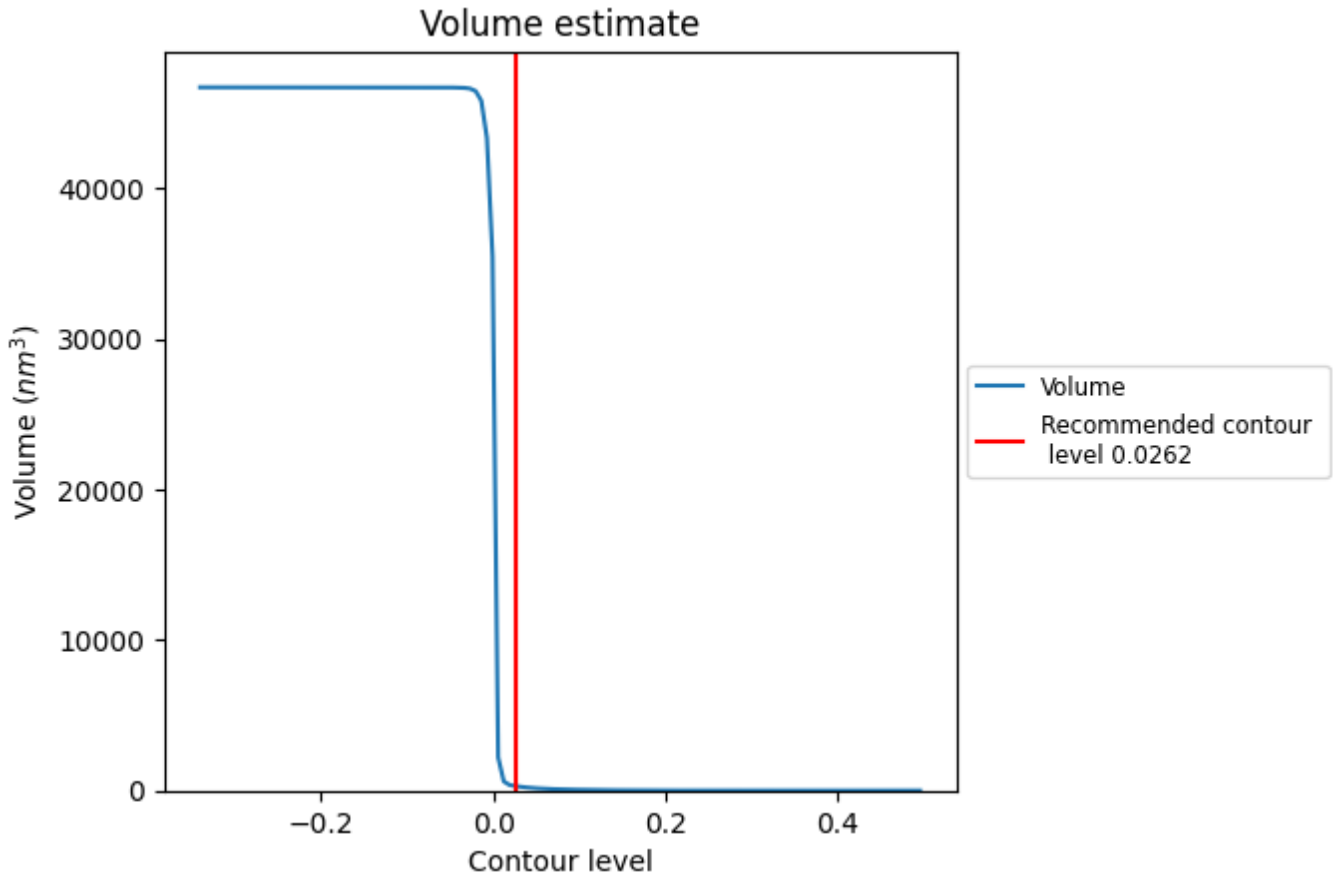
The volume at the recommended contour level is 291 nm^3; this corresponds to an approximate mass of 263 kDa.

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   ⓘ
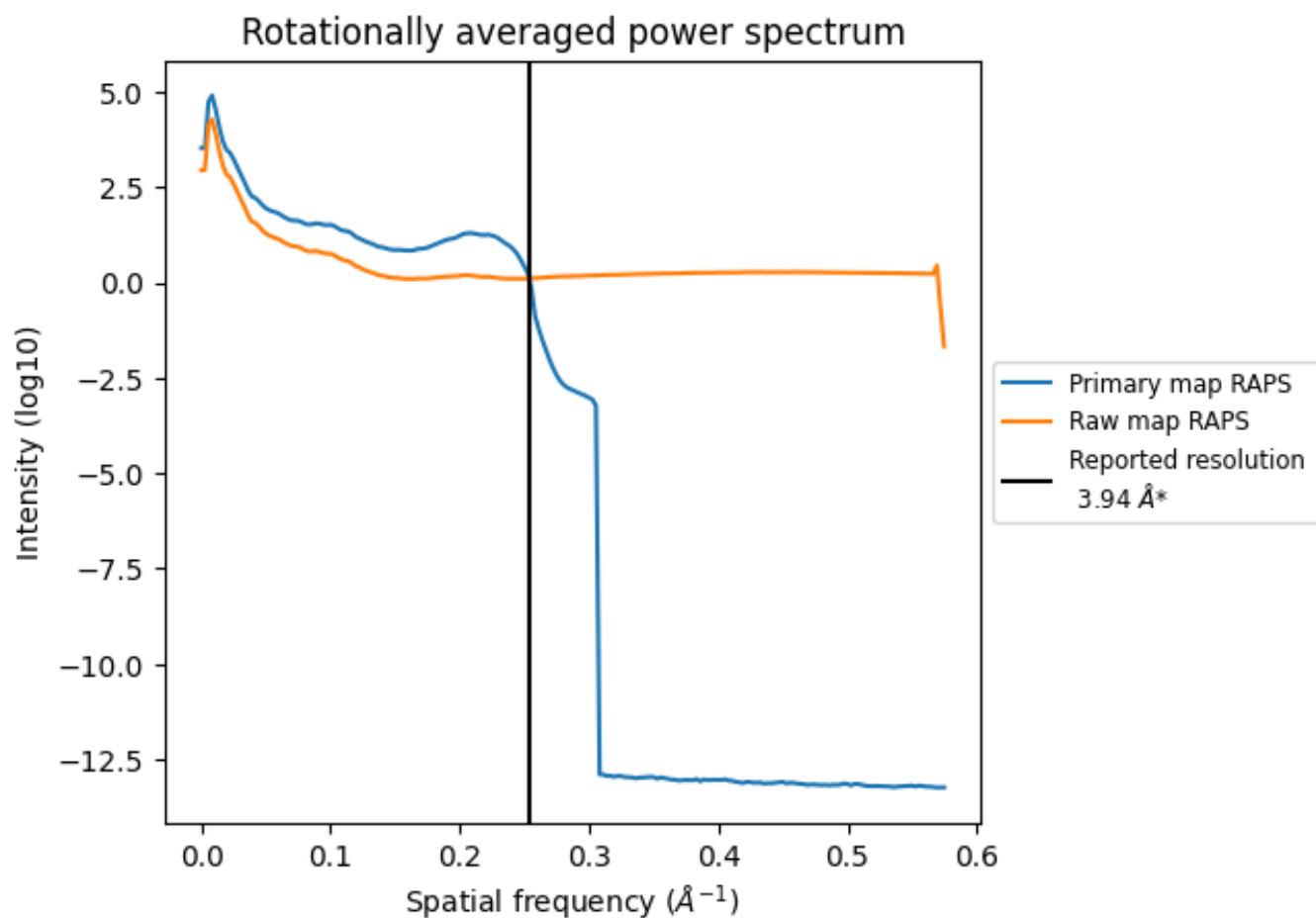
*Reported resolution corresponds to spatial frequency of 0.254 Å^{-1}

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)
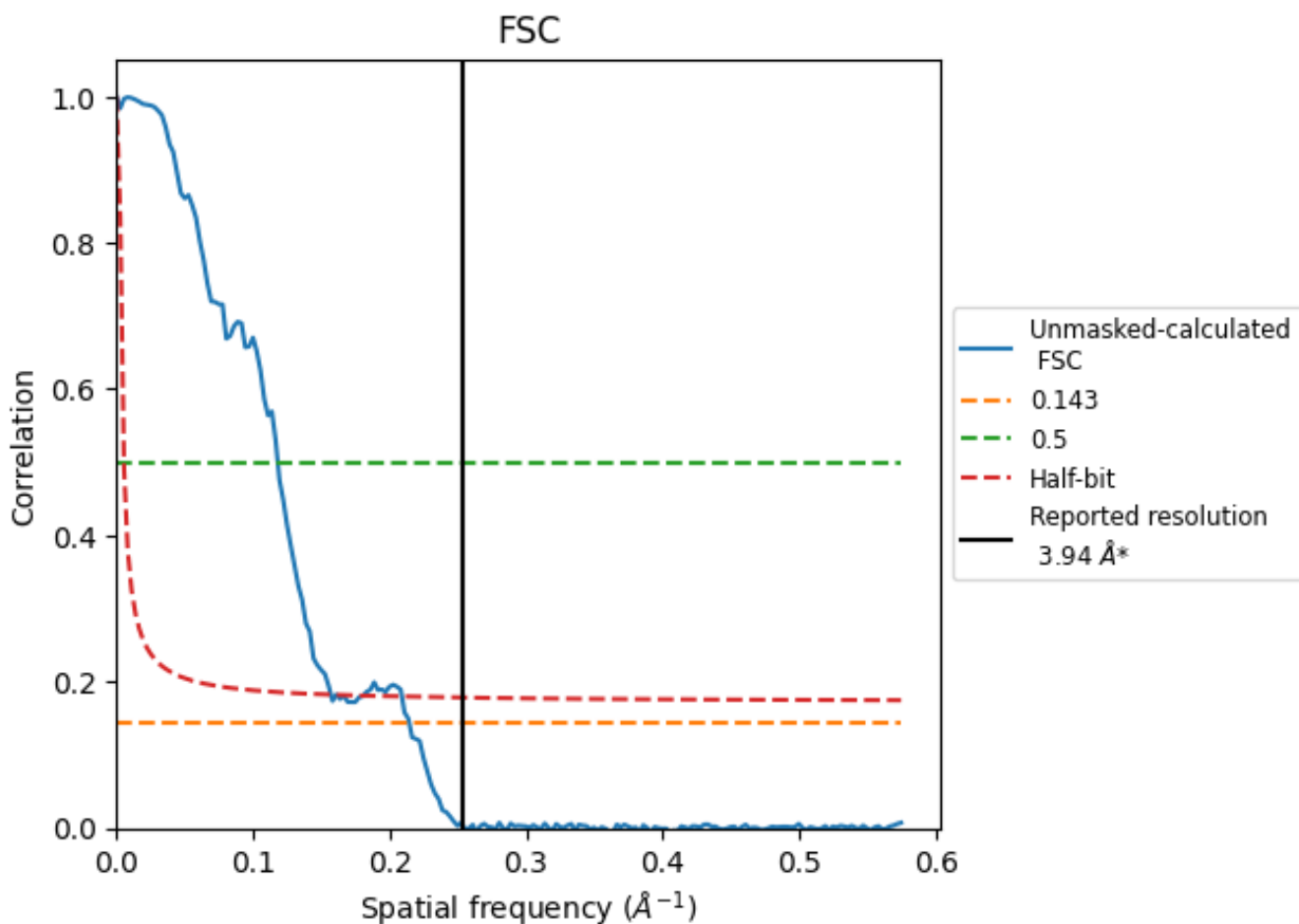
*Reported resolution corresponds to spatial frequency of 0.254 Å^{-1}

8.2   Resolution estimates ⓘ

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.94	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.66	8.46	6.37

*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 4.66 differs from the reported value 3.94 by more than 10 %

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-27423 and PDB model 8DGI. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay ⓘ
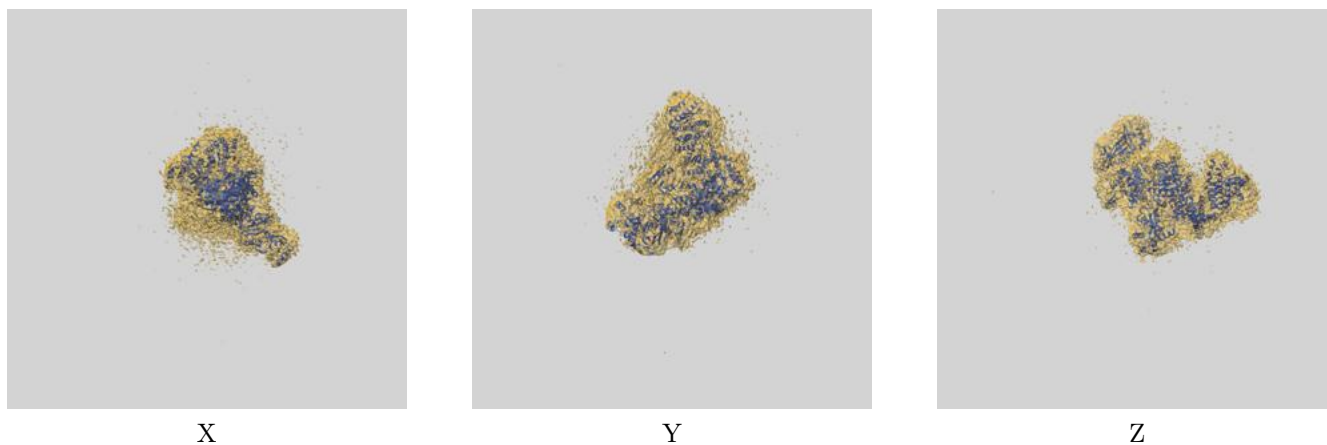
| X | Y | Z |

The images above show the 3D surface view of the map at the recommended contour level 0.0262 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 ⓘ

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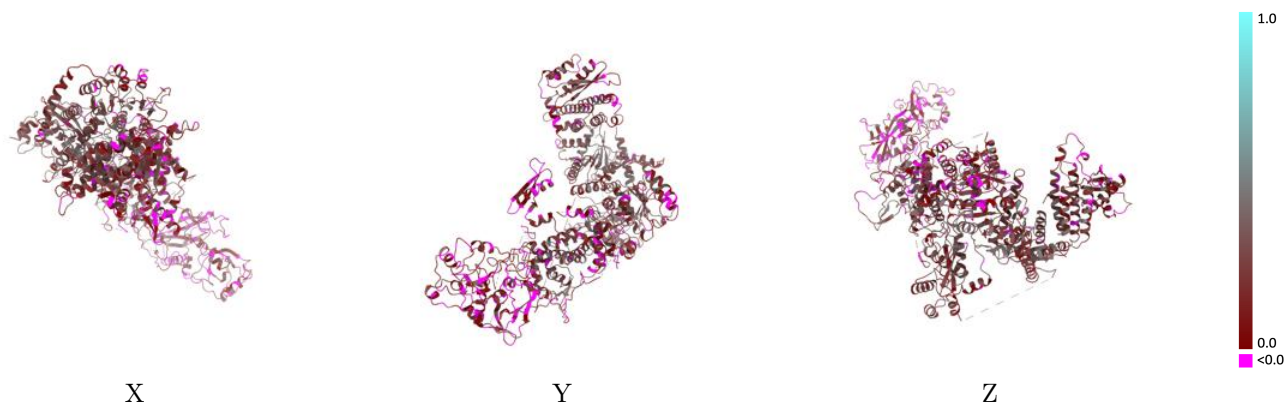
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

X　　　　　　　　　Y　　　　　　　　　Z
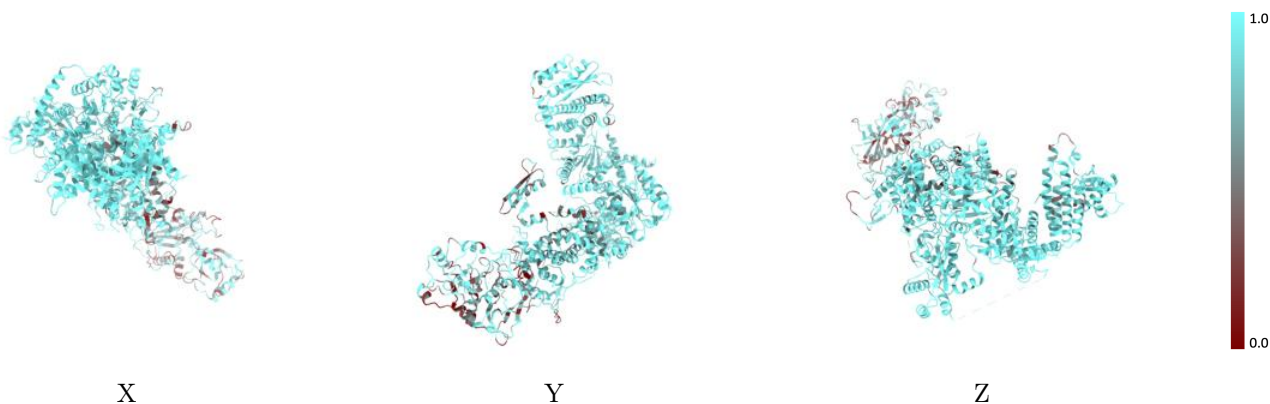
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0262).

9.4 Atom inclusion ⓘ
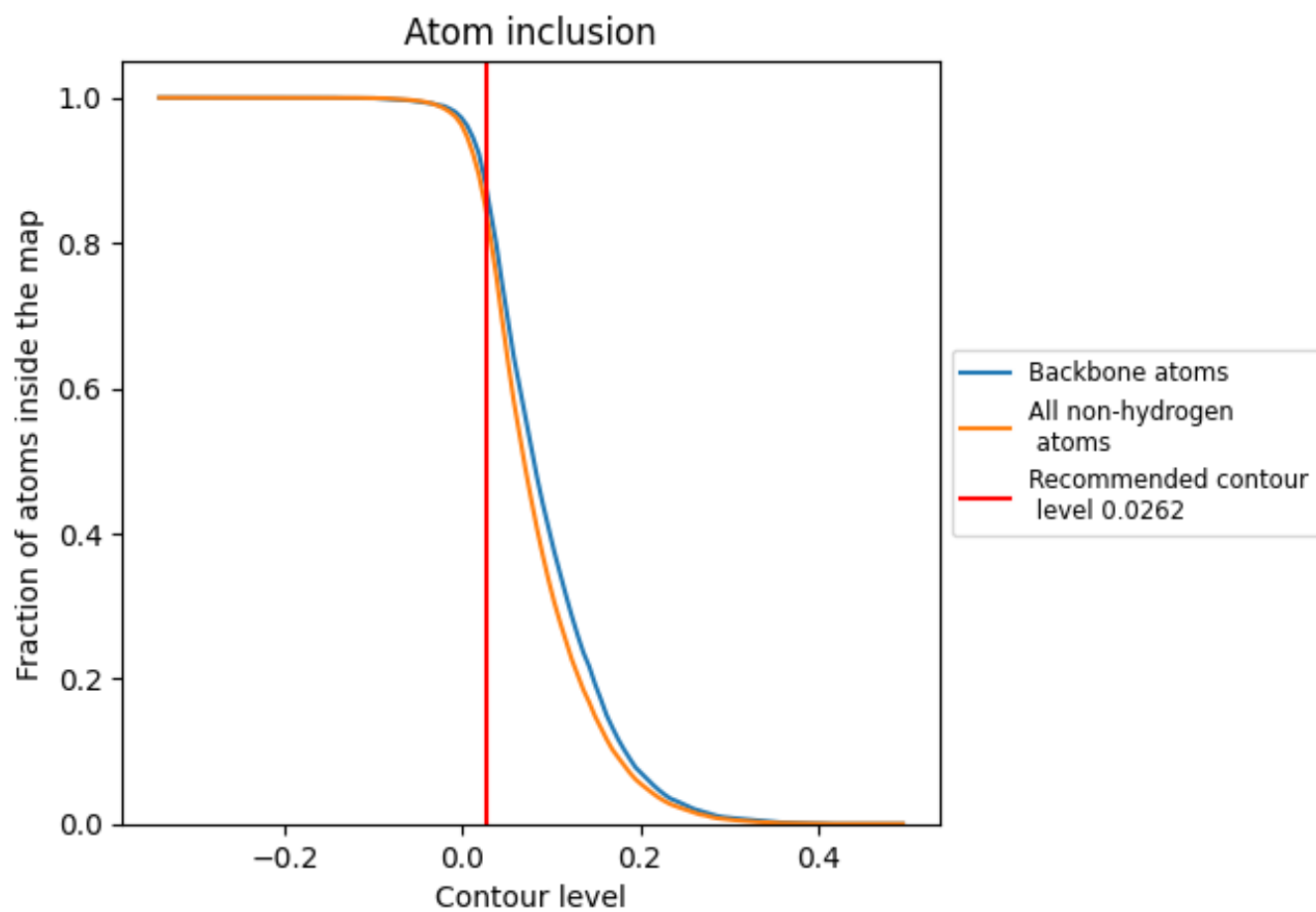
At the recommended contour level, 88% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5　Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0262) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8493	0.2060
A	0.8430	0.2090
N	0.9418	0.1610

1.0

0.0
<0.0