



wwPDB EM Validation Summary Report ⓘ

Nov 3, 2024 – 04:16 am GMT

PDB ID : 6G0L
EMDB ID : EMD-4336
Title : Structure of two molecules of the chromatin remodelling enzyme Chd1 bound to a nucleosome
Authors : Sundaramoorthy, R.; Owen-hughes, T.; Norman, D.G.; Hughes, A.
Deposited on : 2018-03-19
Resolution : 10.00 Å(reported)

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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
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

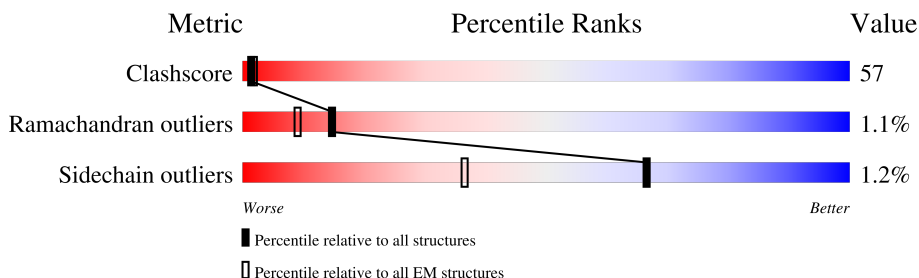
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 10.00 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.



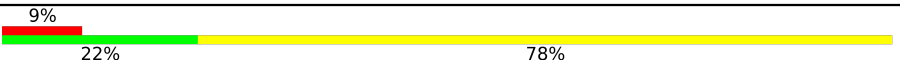

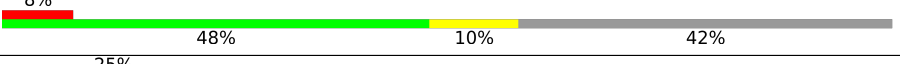
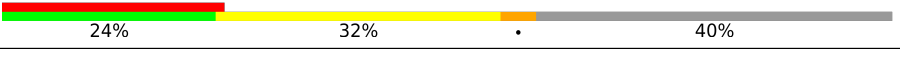
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	136	
1	E	136	
2	B	103	
2	F	103	
3	C	130	
4	D	126	
4	H	126	
5	G	130	

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Mol	Chain	Length	Quality of chain
6	I	176	
7	J	177	
8	M	1468	
8	W	1468	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	ADP	W	1502	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 27526 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 Histone H3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	97	Total	C	N	O	S	0	0
			800	504	155	138	3		
1	E	97	Total	C	N	O	S	0	0
			799	502	155	139	3		

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	83	Total	C	N	O	S	0	0
			662	418	129	114	1		
2	F	92	Total	C	N	O	S	0	0
			686	430	134	121	1		

- Molecule 3 is a protein called Histone H2A type 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	103	Total	C	N	O	0	0
			795	501	155	139		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	99	ARG	GLY	conflict	UNP P06897
C	106	ARG	GLY	conflict	UNP P06897

- Molecule 4 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	95	Total	C	N	O	S	0	0
			745	469	134	140	2		
4	H	93	Total	C	N	O	S	0	0
			726	457	130	137	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	29	THR	SER	conflict	UNP A0A1L8G0X3
H	29	THR	SER	conflict	UNP A0A1L8G0X3

- Molecule 5 is a protein called Histone H2A type 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	G	105	Total	C	N	O	0	0
			809	510	158	141		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	99	ARG	GLY	conflict	UNP P06897

- Molecule 6 is a DNA chain called DNA (176-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	176	Total	C	N	O	P	0	0
			3590	1704	657	1053	176		

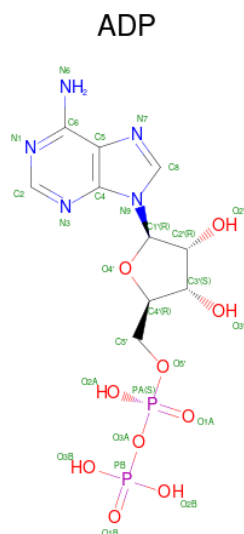
- Molecule 7 is a DNA chain called DNA (177-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	177	Total	C	N	O	P	0	0
			3646	1727	676	1066	177		

- Molecule 8 is a protein called Chromo domain-containing protein 1.

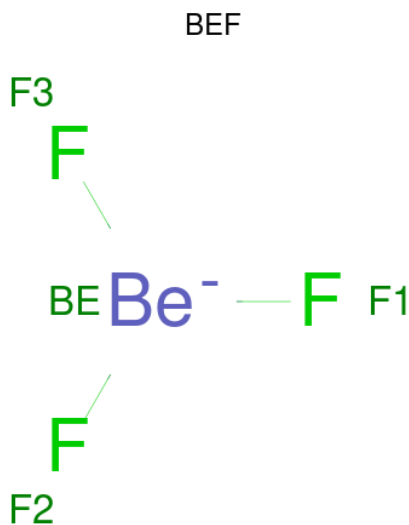
Mol	Chain	Residues	Atoms					AltConf	Trace
8	M	855	Total	C	N	O	S	0	0
			7017	4461	1221	1308	27		
8	W	878	Total	C	N	O	S	2	0
			7189	4568	1260	1334	27		

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					AltConf
9	M	1	Total 27	C 10	N 5	O 10	P 2	0
9	W	1	Total 27	C 10	N 5	O 10	P 2	0

- Molecule 10 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF_3).

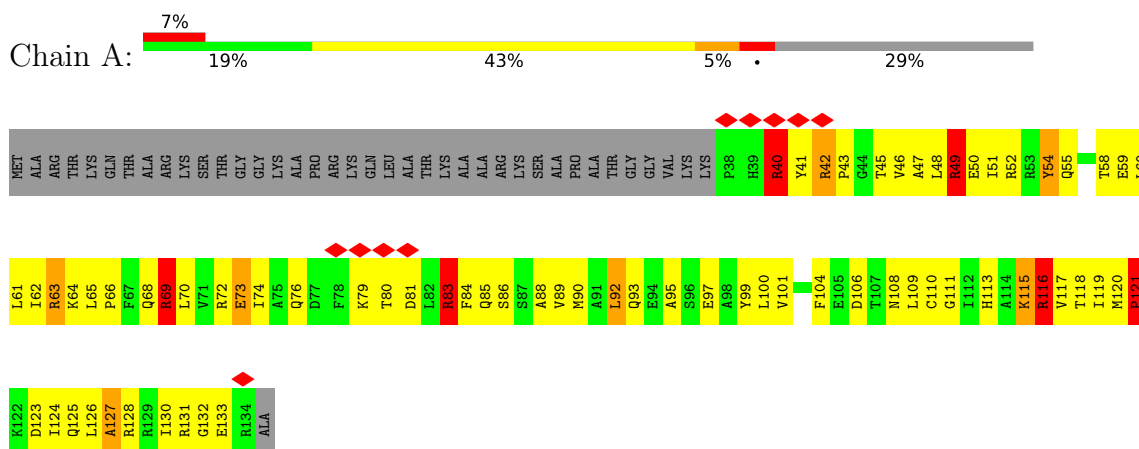


Mol	Chain	Residues	Atoms			AltConf
10	M	1	Total 4	Be 1	F 3	0
10	W	1	Total 4	Be 1	F 3	0

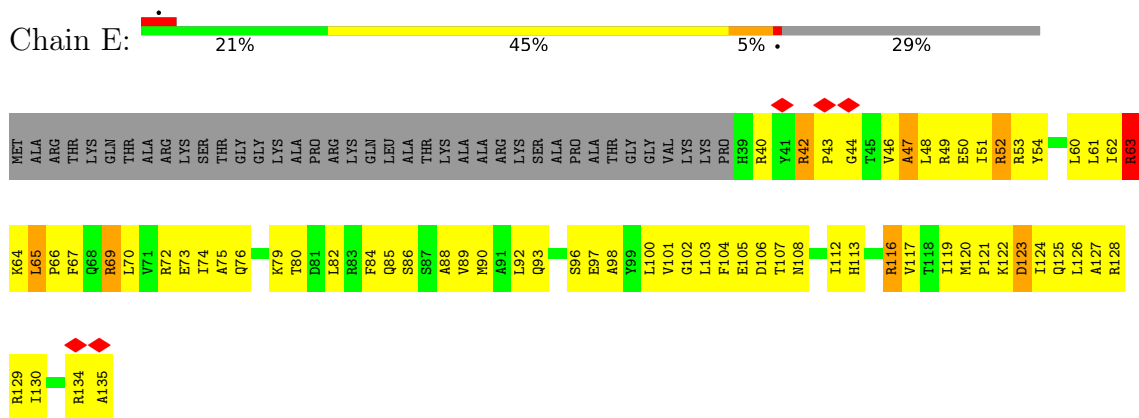
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

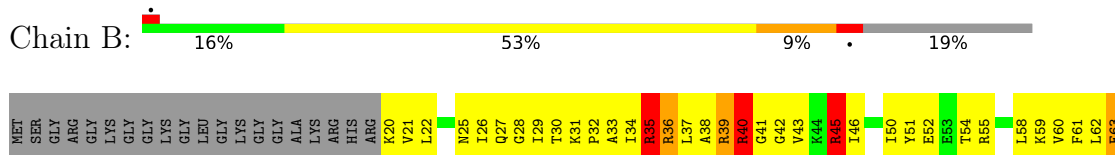
• Molecule 1: Histone H3



• Molecule 1: Histone H3

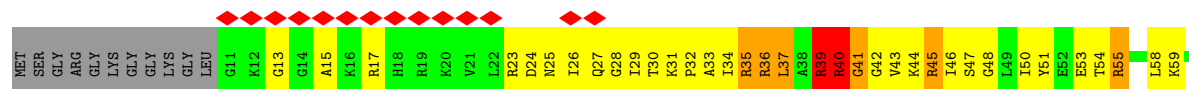


• Molecule 2: Histone H4

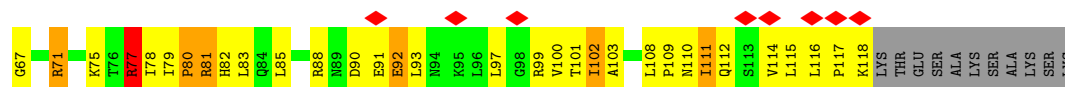




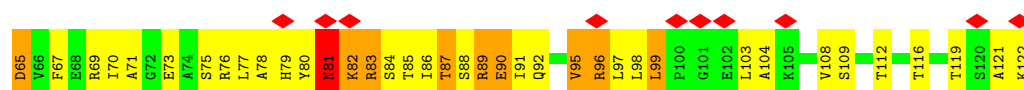
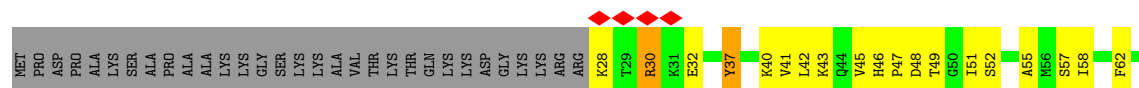
- Molecule 2: Histone H4



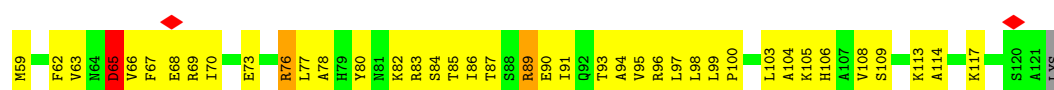
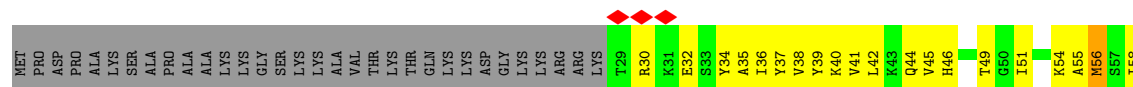
- Molecule 3: Histone H2A type 1



- Molecule 4: Histone H4



- Molecule 4: Histone H4



- Molecule 5: Histone H2A type 1

- Molecule 6: DNA (176-MER)

Chain I:

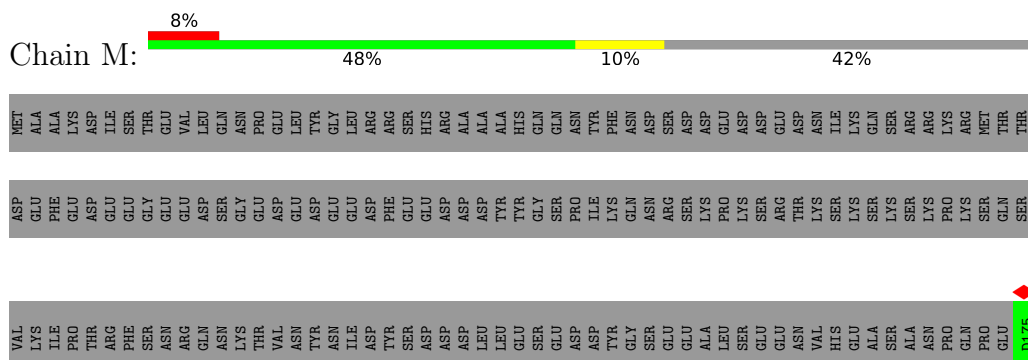
9% 22% 78%

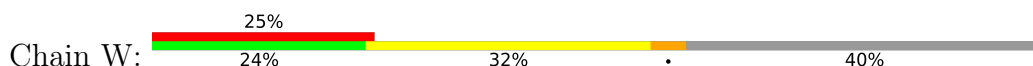
Items: T-26, A-25, G-24, C-37, T38, C-23, A-84, C-83, C-21, C-81, G-20, G-19, C-18, T-17, T-16, A-15, A-14, A-13, C-12, G-11, C-10, A-9, C-8, G-7, T-6, A-5, C-4, G-3, C-2, G-1, C0, T1, G2, T3, C4, C5, C6, C7, C8, G9, C10, T13, T14, T15, A16, A17, C18, C19, G20, C21, C22, A23, A24, G25, G26, C27, G28, A29, T30, T31, A32, C33, T34, A-86, T-85, A-84, C-83, C-82, G-81, G-80, G-79, C-78, C-77, G-76, C-75, C-74, C-73, C-72, T-71, C-70, G-69, A-68, A-67, A-66, T-65, C-64, C-63, C-62, G-61, G-60, T-59, G-58, C-57, C-56, G-55, A-54, G-53, G-52, C-51, C-50, G-49, C-48, T-47, C-46, A-45, A-44, T-43, T-42, G-41, G-40, T-39, C-38, G-37, T-36, A-35, G-34, A-33, C-32, A-31, G-30, C-29, T-28.

- Molecule 7: DNA (177-MER)

Chain J:

Category	Value
T-89	1
A-88	1
T-87	1
G-86	1
G-81	1
C-80	1
C-77	1
G-76	1
T-75	1
G-69	1
A-68	1
T-67	1
G-66	1
T-65	1
A-64	1
T-63	1
A-62	1
T-57	1
G-56	1
A-55	1
C-54	1
A-53	1
C-52	1
G-51	1
T-50	1
G-49	1
C-48	1
C-47	1
T-46	1
G-45	1
G-44	1
A-43	1
C-40	1
T-39	1
A-38	1
G-37	1
G-36	1
A-34	1
G-33	1
T-32	1
A-31	1
A-30	1
T-29	1
C-28	1
C-27	1
C-26	1
T-24	1
T-23	1
G-22	1
G-21	1
C-20	1
G-19	1
T-17	1
T-16	1
A-15	1
A-14	1
A-13	1
A-12	1
C-11	1
G-10	1
C-9	1
G-8	1
C-7	1
G-6	1
G-5	1
G-4	1
A-3	1
C-2	1
A-1	1
G0	1
C1	1
G2	1
C3	1
G4	1
T5	1
A6	1
C7	1
G8	1
C9	1
T9	1
C10	1
G11	1
T12	1
G13	1
T14	1
T15	1
A16	1
A17	1
G18	1
C19	1
G20	1
G21	1
T22	1
G23	1
C24	1
T25	1
A26	1
G27	1
A28	1
G29	1
C30	1
T31	1
G32	1
T33	1
C34	1
T35	1
A36	1
C37	1
G38	1
A39	1
C40	1
G41	1
T42	1
A43	1
T44	1
T45	1
G46	1
A47	1
G48	1
C49	1
G50	1
G51	1
C52	1
T53	1
G54	1
T55	1
C56	1
G57	1
C58	1
C59	1
A60	1
C61	1
C62	1
G63	1
G64	1
G65	1
A66	1
T67	1
T68	1
C69	1
T70	1
G71	1
A72	1
T73	1
G74	1
G75	1
G76	1
C77	1
G78	1
G79	1
C80	1
C81	1
C82	1
C83	1
G84	1
T85	1
A86	1
T87	1







ASN	ALA	LYS	L1263	P1201	L1139	ARG	LYS
PHE	ILE	GLY	R1264	F1202	K1140	ALA	LEU
TRP	ARG	PRO	G1265	L1203		ASN	GLN
ALA	SER	ALA	G1266	G1204	K1143	D1005	GLU
ASP	LEU	LEU	I1205	I1205	L1077	D1007	GLN
VAL	ILE	ILE	T1206	T1206		S1008	LYS
ARG	ARG	ASN	D1207	D1207	T1082	I1009	ARG
THR	ARG	THR	K1208	K1208	Y1084	G1010	LYS
LYS	ARG	SER	I1209	I1209	R1085	E1011	ASP
LEU	GLY	ARG	F1210	F1210	A1086	S1012	GLU
LEU	GLY	SER	L1211	L1211	K1087	E1013	GLU
MET	GLY	SER	ALA	ASN	Y1150	V1014	TYR
ALA	LYS	PRO	ASP	GLU	R1151	E1015	VAL
MET	SER	ASN	ILE	VAL	D1152	K1089	LYS
TRP	LEU	PRO	GLY	HIS	D1153	S1090	LYS
ASP	SER	THR	SER	ASN	P1154	G1091	GLU
LYS	ARG	PRO	LYS	PRO	L1155	E1092	LEU
ILE	LYS	PRO	VAL	VAL	K1156	I1093	LEU
THR	GLU	PRO	ALA	ALA	F1157	K1094	GLU
GLU	TRP	LEU	LYS	LYS	S1158	A1020	LEU
GLU	TRP	LYS	PRO	THR	L1159	I1021	LEU
SER	LYS	LYS	ALA	ALA	G1160	L1022	ASN
GLN	LYS	SER	SER	SER	N1161	K1023	ARG
GLY	GLU	ARG	LYS	SER	N1162	F1024	ASP
LEU	ASP	ASP	LYS	SER	N1163	G1025	ALA
LEU	ASN	ASN	ARG	ASP	P1164	K1100	LEU
THR	THR	GLY	GLN	THR	T1165	D1101	LYS
THR	THR	ARG	ARG	THR	P1166	L1027	LYS
ILE	ILE	ARG	LYS	PRO	K1165	K1028	ILE
GLN	GLY	PRO	LYS	THR	P1166	E1029	LYS
ASN	SER	ASN	ALA	PRO	T1105	I1030	ASN
SER	HIS	SER	HIS	SER	R1166	L1031	SER
LYS	ILE	ASN	ASN	LYS	L1107	D1032	VAL
GLU	GLU	PRO	LYS	LYS	K1110	E1033	ASN
SER	SER	LYS	GLY	GLY	K1111	E1033	ASN
SER	SER	SER	LYS	LYS	R1112	L1034	GLY
GLN	GLN	MET	LYS	GLY	E1113	I1035	THR
LYS	GLY	THR	ILE	ILE	K1114	A1036	ALA
THR	GLY	PRO	ALA	THR	D1037	G1038	ALA
GLU	GLU	ILE	ILE	SER	A1116	T1039	ASN
LYS	LYS	THR	THR	SER	V1117	L1040	SER
GLU	GLU	SER	SER	K1244	L1118	P1041	ASP
TYR	TYR	GLU	GLU	K1245	F1119	V1042	ASP
ASP	PRO	ASP	GLU	V1246	N1120	S1044	ASP
GLU	GLU	MET	ALA	P1247	F1121	F1045	THR
GLN	LYS	ALA	ALA		K1122	E1046	SER
ASP	TYR	ASN	GLY	H1251	G1123	K1047	SER
GLU	GLY	GLY	GLY	L1252	V1124	S1044	ARG
PRO	PRO	PRO	PRO	G1253	K1125	F1045	SER
LEU	HIS	LEU	ASP	R1254	R1126	E1054	SER
LEU	CYS	SER	SER	R1255	S1126	K1047	ARG
TRP	TRP	ARG	ARG	V1256	L1127	Y1048	ARG
ARG	HIS	ARG	MET	D1257	N1128	G1049	ARG
SER	SER	LYS	LYS	F1187	E1050	T1051	ALA
THR	THR	ALA	ALA	K1188	L1132	Y1052	ARG
LEU	LEU	PRO	PRO	Y1189	L1133	D1053	ARG
PRO	PRO	LEU	LEU	G1190	S1134	E1054	ALA
				L1260	R1135	M1055	
				S1261	D1138	E1057	
				F1262		A1059	
						R1070	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	68000	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 ($e^-/\text{\AA}^2$)	1.56	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	98591	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.162	Depositor
Minimum map value	-0.047	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.044	Depositor
Map size (Å)	369.19998, 369.19998, 369.19998	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.42, 1.42, 1.42	Depositor

5 Model quality

5.1 Standard geometry

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

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	1.13	6/812 (0.7%)	1.47	10/1088 (0.9%)
1	E	1.03	4/810 (0.5%)	1.36	3/1084 (0.3%)
2	B	1.15	7/669 (1.0%)	1.69	10/894 (1.1%)
2	F	1.20	5/693 (0.7%)	1.57	12/929 (1.3%)
3	C	1.31	8/805 (1.0%)	1.54	5/1088 (0.5%)
4	D	1.20	6/756 (0.8%)	1.36	5/1015 (0.5%)
4	H	1.10	2/737 (0.3%)	1.40	5/993 (0.5%)
5	G	1.16	3/819 (0.4%)	1.37	5/1106 (0.5%)
6	I	0.32	0/4023	0.71	0/6199
7	J	0.33	0/4091	0.72	0/6315
8	M	0.23	0/7152	0.38	0/9632
8	W	1.03	22/7334 (0.3%)	1.14	20/9875 (0.2%)
All	All	0.77	63/28701 (0.2%)	0.97	75/40218 (0.2%)

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	7
1	E	0	6
2	B	0	5
2	F	0	7
3	C	0	7
4	D	0	3
4	H	0	4
5	G	0	4
8	W	0	19
All	All	0	62

The worst 5 of 63 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	W	669	GLU	CD-OE2	-10.85	1.13	1.25
4	D	73	GLU	CD-OE2	10.82	1.37	1.25
8	W	826	GLU	CD-OE2	-10.39	1.14	1.25
8	W	493	GLU	CD-OE2	9.68	1.36	1.25
4	D	90	GLU	CD-OE2	-9.00	1.15	1.25

The worst 5 of 75 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	40	ARG	NE-CZ-NH1	-15.85	112.38	120.30
3	C	50	TYR	CB-CG-CD1	-14.59	112.25	121.00
3	C	50	TYR	CB-CG-CD2	12.81	128.69	121.00
1	E	52	ARG	NE-CZ-NH1	-10.88	114.86	120.30
8	W	597	ARG	NE-CZ-NH2	-10.08	115.26	120.30

There are no chirality outliers.

5 of 62 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	40	ARG	Sidechain
1	A	42	ARG	Sidechain
1	A	49	ARG	Sidechain
1	A	63	ARG	Sidechain
1	A	69	ARG	Sidechain

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	800	0	837	194	0
1	E	799	0	834	154	0
2	B	662	0	709	172	0
2	F	686	0	693	186	0
3	C	795	0	844	177	0
4	D	745	0	773	133	0
4	H	726	0	746	112	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	G	809	0	864	174	0
6	I	3590	0	1969	643	0
7	J	3646	0	1989	703	0
8	M	7017	0	7011	171	0
8	W	7189	0	7206	938	0
9	M	27	0	12	1	0
9	W	27	0	12	13	0
10	M	4	0	0	1	0
10	W	4	0	0	0	0
All	All	27526	0	24499	2959	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 57.

The worst 5 of 2959 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)
7:J:26:DA:H2''	7:J:27:DG:C8	1.33	1.59
6:I:30:DT:C6	6:I:31:DT:H72	1.40	1.52
1:A:63:ARG:CZ	7:J:17:DA:H5'	1.40	1.50
6:I:22:DC:P	8:W:520:ASN:HB3	1.52	1.50
6:I:-84:DA:H2	7:J:86:DA:C2	1.30	1.48

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	95/136 (70%)	87 (92%)	7 (7%)	1 (1%)	12	47
1	E	95/136 (70%)	86 (90%)	5 (5%)	4 (4%)	2	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	81/103 (79%)	69 (85%)	10 (12%)	2 (2%)	4	26
2	F	90/103 (87%)	85 (94%)	5 (6%)	0	100	100
3	C	101/130 (78%)	83 (82%)	14 (14%)	4 (4%)	2	18
4	D	93/126 (74%)	85 (91%)	7 (8%)	1 (1%)	12	47
4	H	91/126 (72%)	81 (89%)	9 (10%)	1 (1%)	12	47
5	G	103/130 (79%)	93 (90%)	10 (10%)	0	100	100
8	M	839/1468 (57%)	749 (89%)	89 (11%)	1 (0%)	48	83
8	W	868/1468 (59%)	784 (90%)	70 (8%)	14 (2%)	8	38
All	All	2456/3926 (63%)	2202 (90%)	226 (9%)	28 (1%)	15	47

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	82	LYS
1	E	42	ARG
8	M	778	ILE
8	W	474	ASN
8	W	600	LYS

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	85/111 (77%)	85 (100%)	0	100	100
1	E	84/111 (76%)	83 (99%)	1 (1%)	67	78
2	B	68/79 (86%)	68 (100%)	0	100	100
2	F	63/79 (80%)	63 (100%)	0	100	100
3	C	82/102 (80%)	82 (100%)	0	100	100
4	D	81/105 (77%)	80 (99%)	1 (1%)	67	78
4	H	79/105 (75%)	78 (99%)	1 (1%)	65	77
5	G	83/101 (82%)	82 (99%)	1 (1%)	67	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	M	772/1313 (59%)	772 (100%)	0	100	100
8	W	787/1313 (60%)	764 (97%)	23 (3%)	37	56
All	All	2184/3419 (64%)	2157 (99%)	27 (1%)	66	78

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	W	635	SER
8	W	660	ASN
8	W	1132	LEU
8	W	652	MET
8	W	720	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
5	G	84	GLN
5	G	112	GLN
8	W	667	ASN
8	M	653	ASN
1	E	108	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
10	BEF	W	1501	9	0,3,3	-	-	-		
9	ADP	M	1501	10	24,29,29	0.97	1 (4%)	29,45,45	1.49	4 (13%)
9	ADP	W	1502	10	24,29,29	1.46	4 (16%)	29,45,45	1.89	7 (24%)
10	BEF	M	1502	9	0,3,3	-	-	-		

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
9	ADP	M	1501	10	-	5/12/32/32	0/3/3/3
9	ADP	W	1502	10	-	3/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	W	1502	ADP	C5-C4	3.08	1.49	1.40
9	M	1501	ADP	C5-C4	2.50	1.47	1.40
9	W	1502	ADP	PB-O1B	2.35	1.58	1.50
9	W	1502	ADP	PB-O2B	-2.23	1.46	1.54
9	W	1502	ADP	C2-N3	2.23	1.35	1.32

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	W	1502	ADP	C3'-C2'-C1'	4.96	108.45	100.98
9	M	1501	ADP	PA-O3A-PB	-3.63	120.37	132.83
9	W	1502	ADP	N3-C2-N1	-3.49	123.23	128.68
9	M	1501	ADP	C3'-C2'-C1'	3.45	106.17	100.98
9	W	1502	ADP	PA-O3A-PB	-3.39	121.21	132.83

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

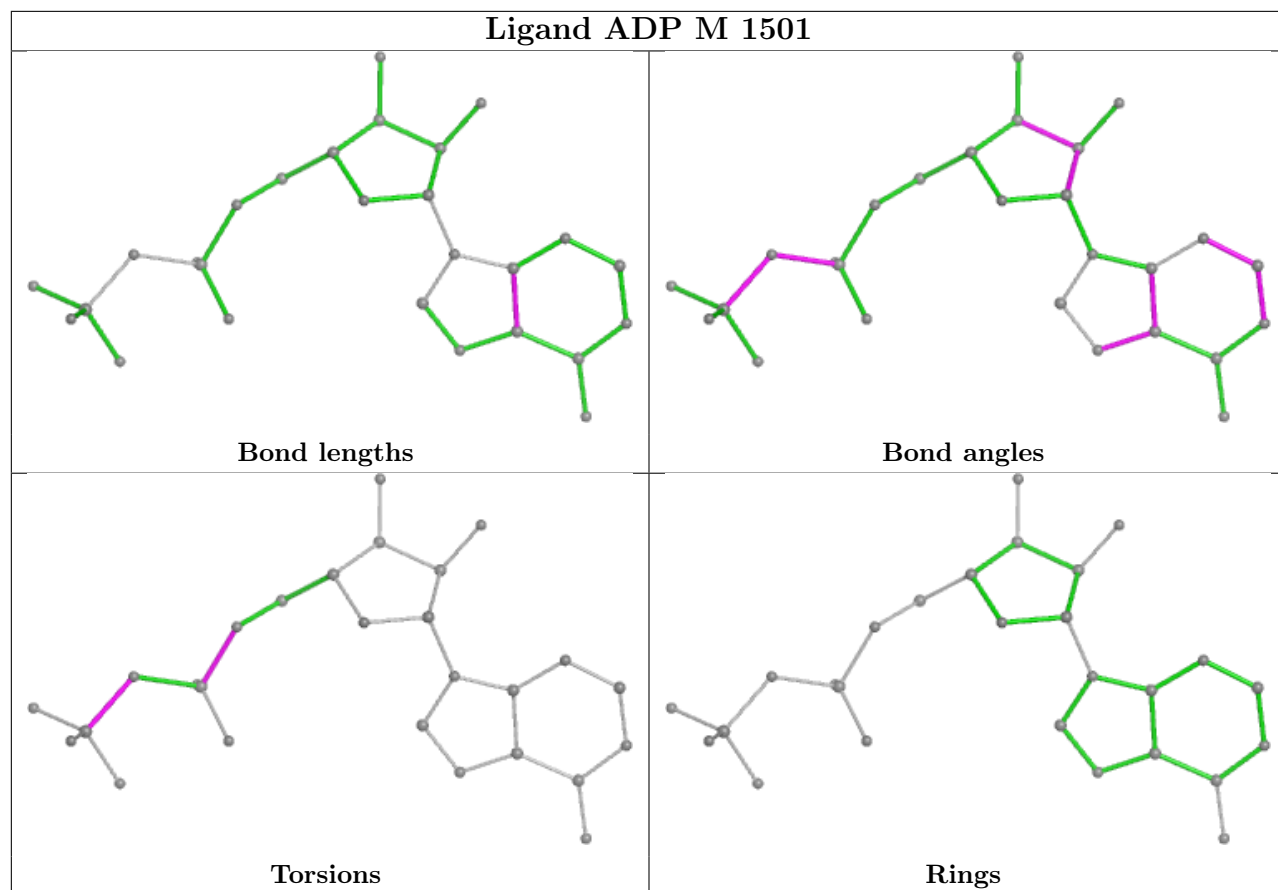
Mol	Chain	Res	Type	Atoms
9	M	1501	ADP	C5'-O5'-PA-O2A
9	M	1501	ADP	C5'-O5'-PA-O3A
9	W	1502	ADP	PA-O3A-PB-O2B
9	M	1501	ADP	PA-O3A-PB-O1B
9	W	1502	ADP	O4'-C4'-C5'-O5'

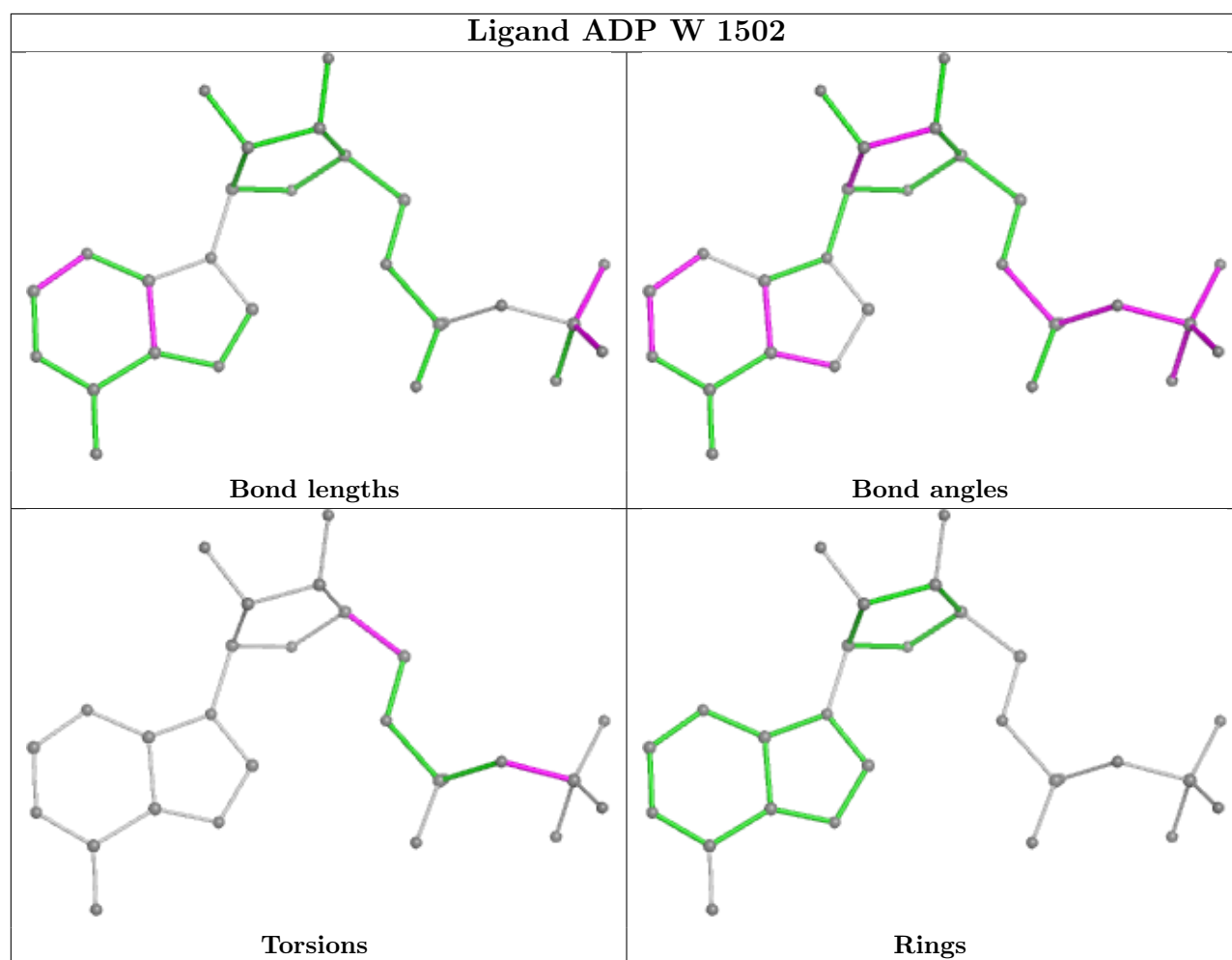
There are no ring outliers.

3 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	M	1501	ADP	1	0
9	W	1502	ADP	13	0
10	M	1502	BEF	1	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
7	J	1
6	I	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	J	-46:DT	O3'	-45:DG	P	3.92
1	I	45:DC	O3'	46:DA	P	3.25

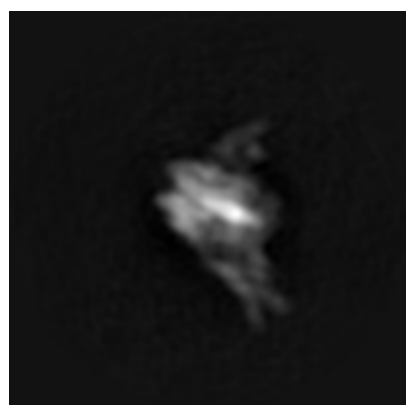
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4336. These allow visual inspection of the internal detail of the map and identification of artifacts.

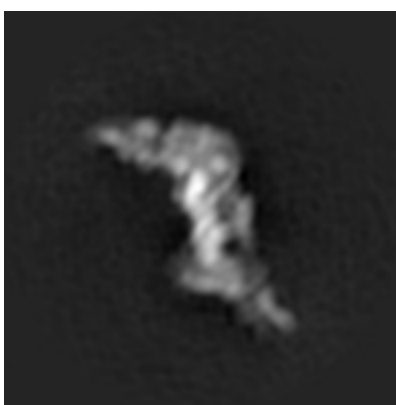
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

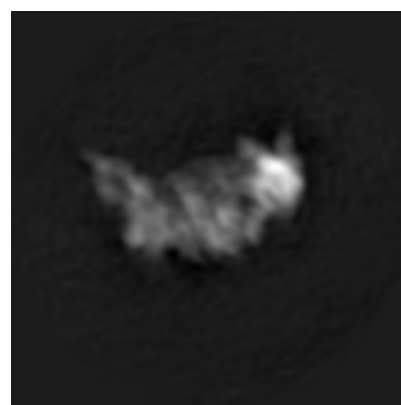
6.1.1 Primary map



X



Y

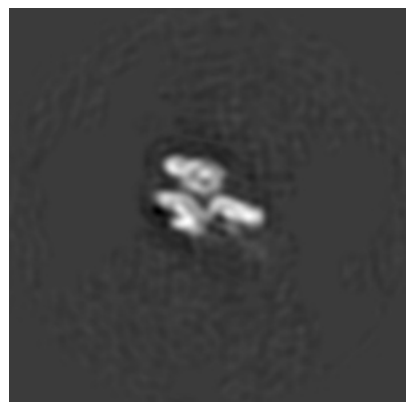


Z

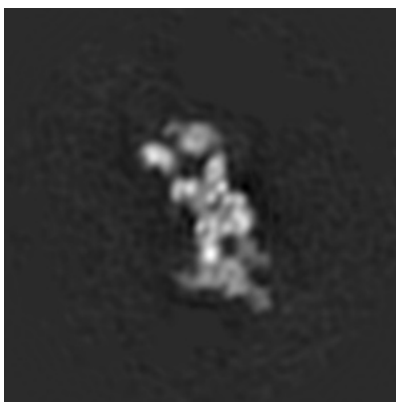
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

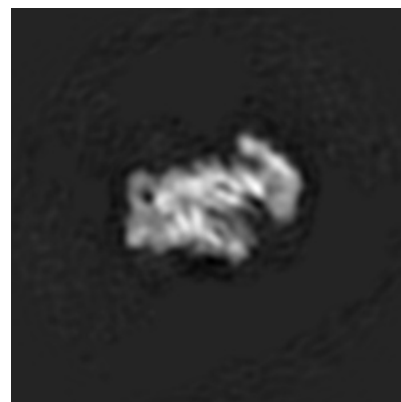
6.2.1 Primary map



X Index: 130



Y Index: 130

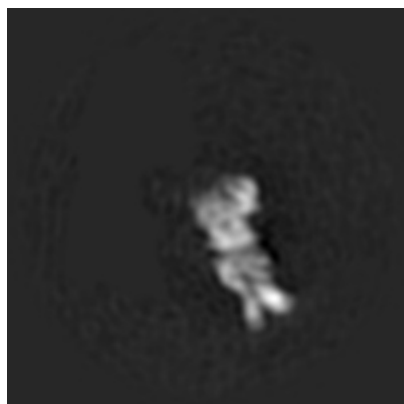


Z Index: 130

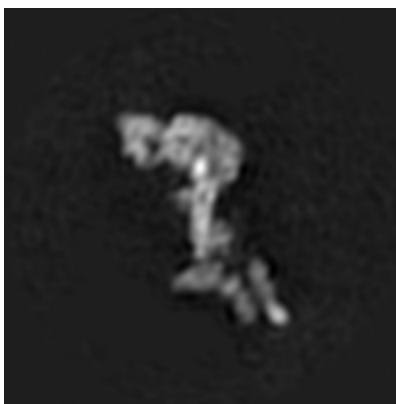
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

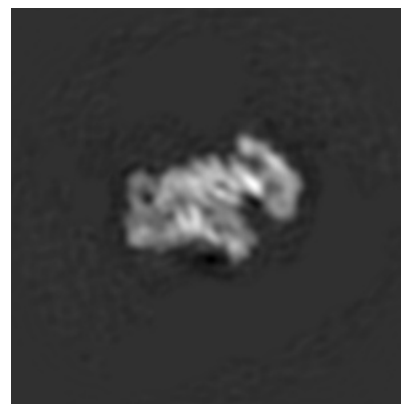
6.3.1 Primary map



X Index: 177



Y Index: 146

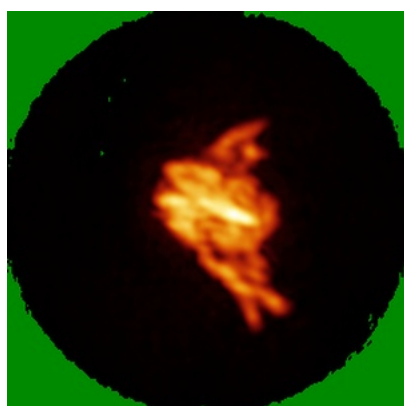


Z Index: 128

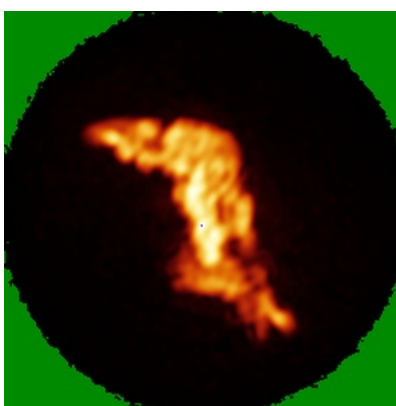
The images above show the largest variance slices of the map in three orthogonal directions.

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

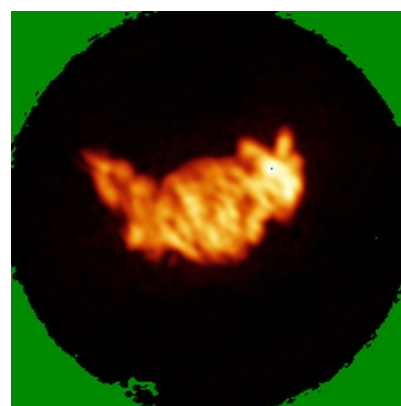
6.4.1 Primary map



X



Y

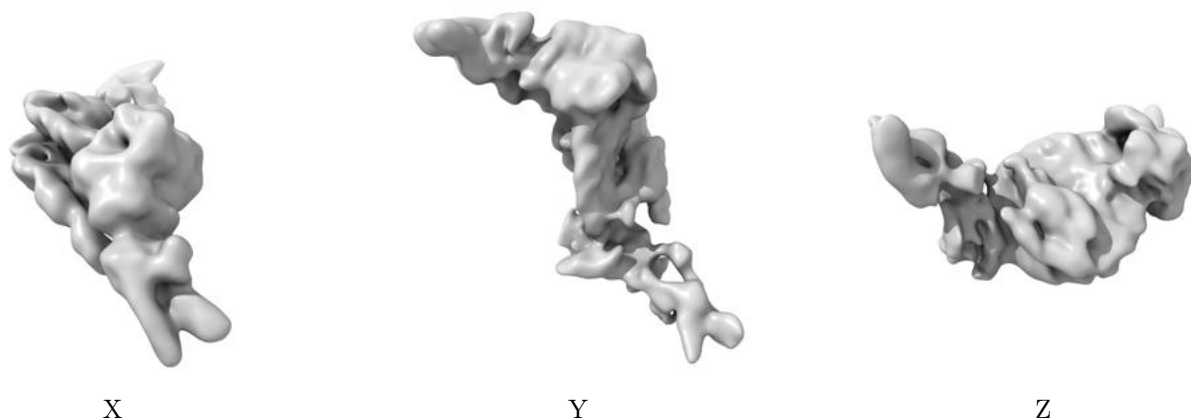


Z

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

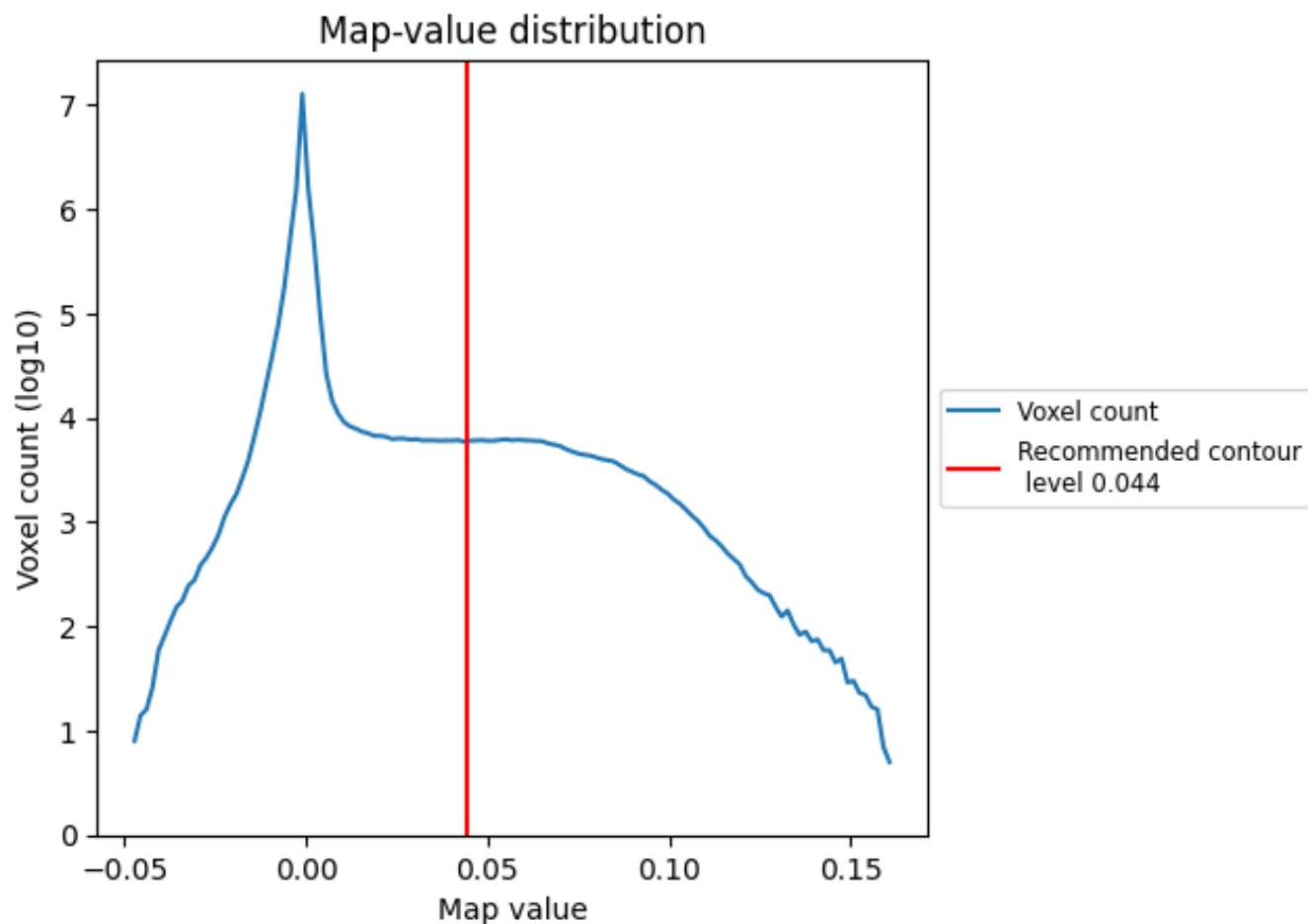
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

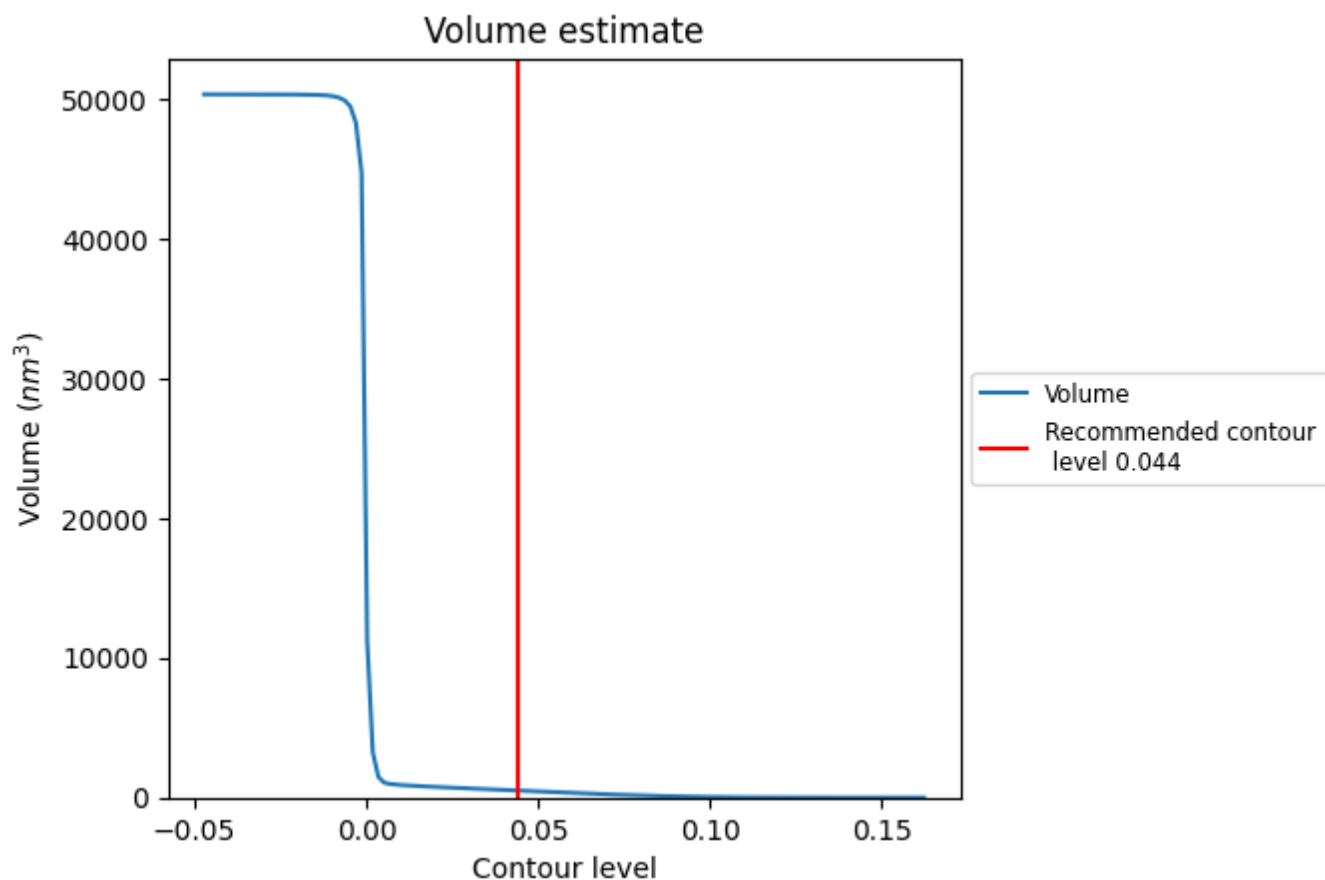
This section contains the results of statistical analysis of the map.

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.

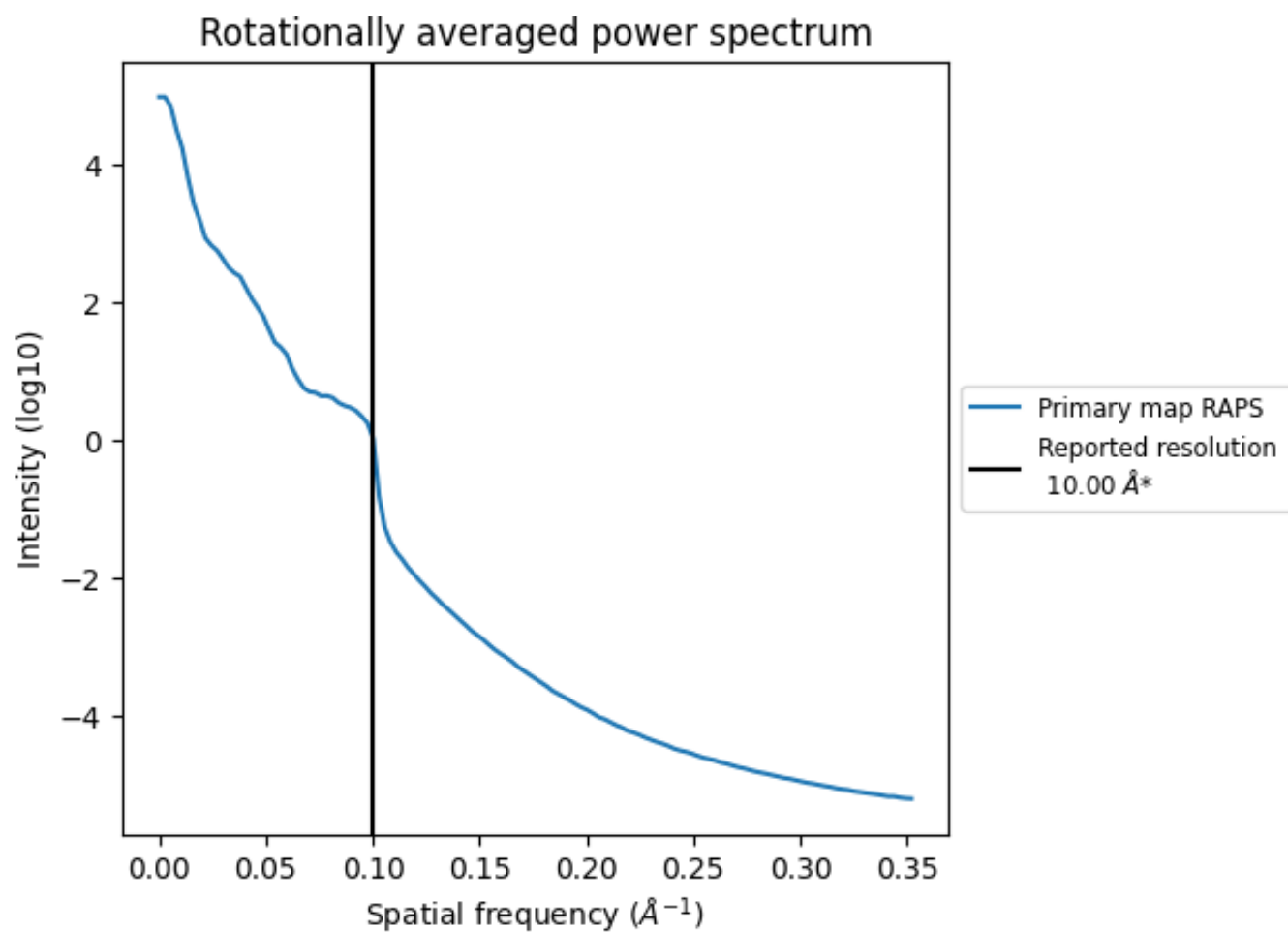
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 503 nm³; this corresponds to an approximate mass of 454 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 ⓘ

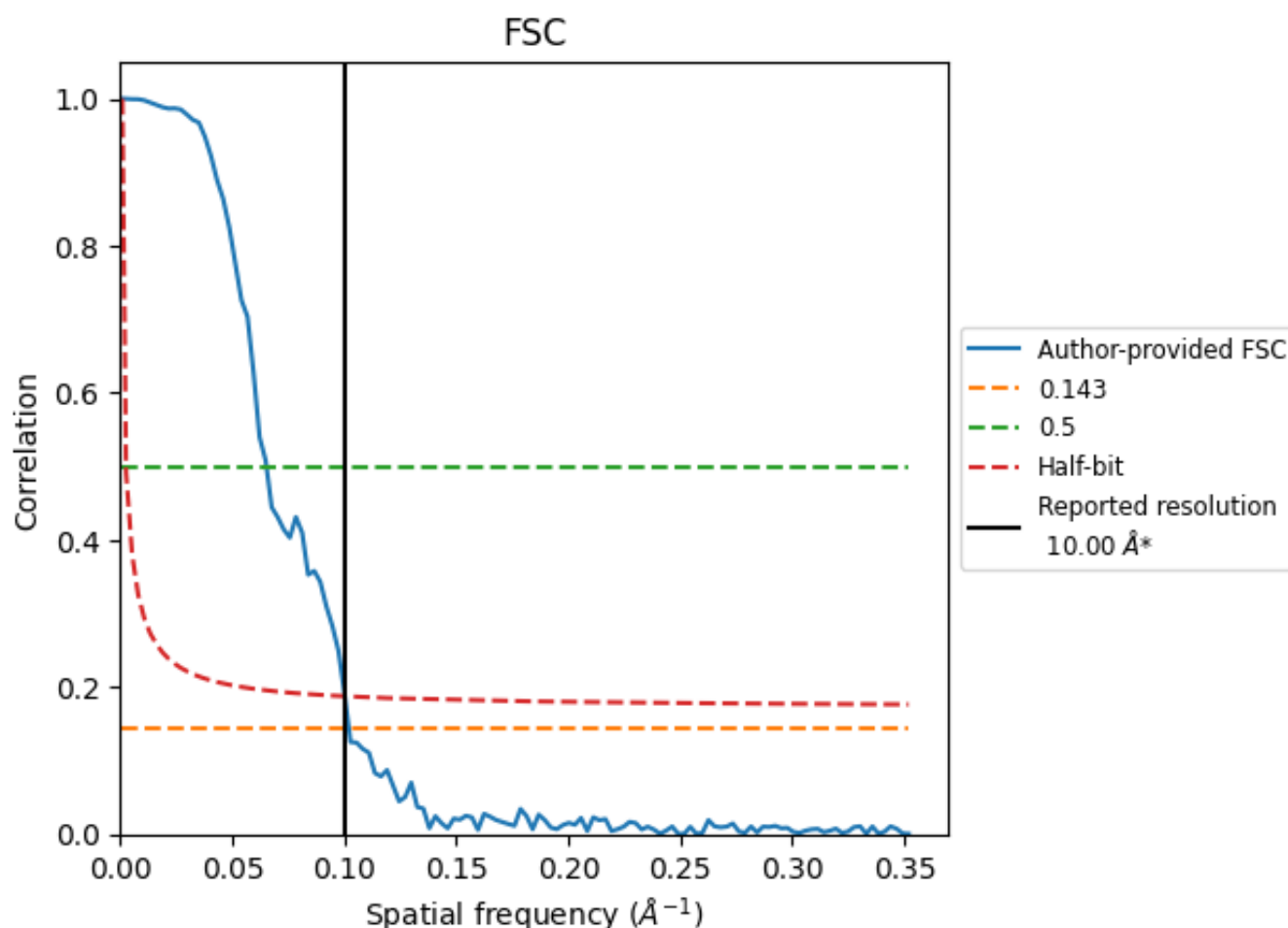


*Reported resolution corresponds to spatial frequency of 0.100 Å⁻¹

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 0.100 Å⁻¹

8.2 Resolution estimates [i](#)

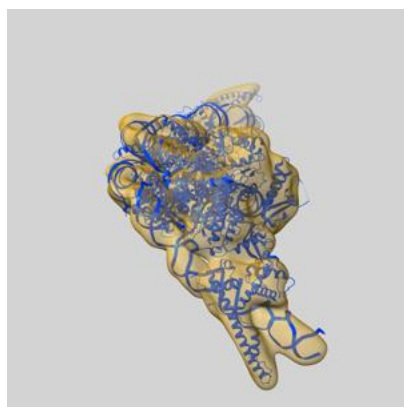
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	10.00	-	-
Author-provided FSC curve	9.78	15.31	9.96
Unmasked-calculated*	-	-	-

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

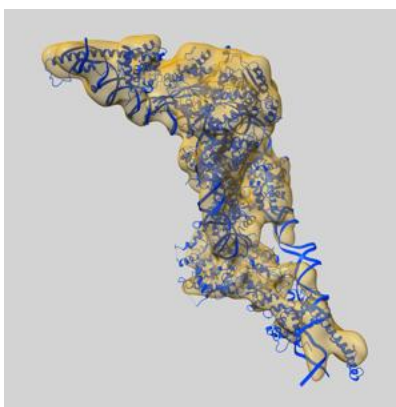
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4336 and PDB model 6G0L. Per-residue inclusion information can be found in section [3](#) on page [7](#).

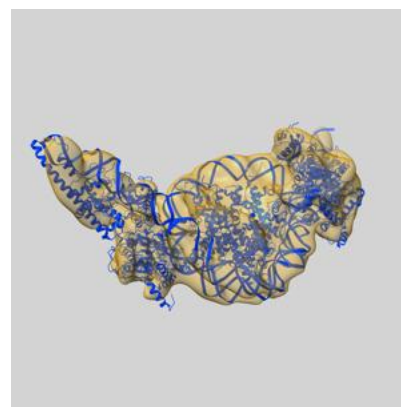
9.1 Map-model overlay [i](#)



X



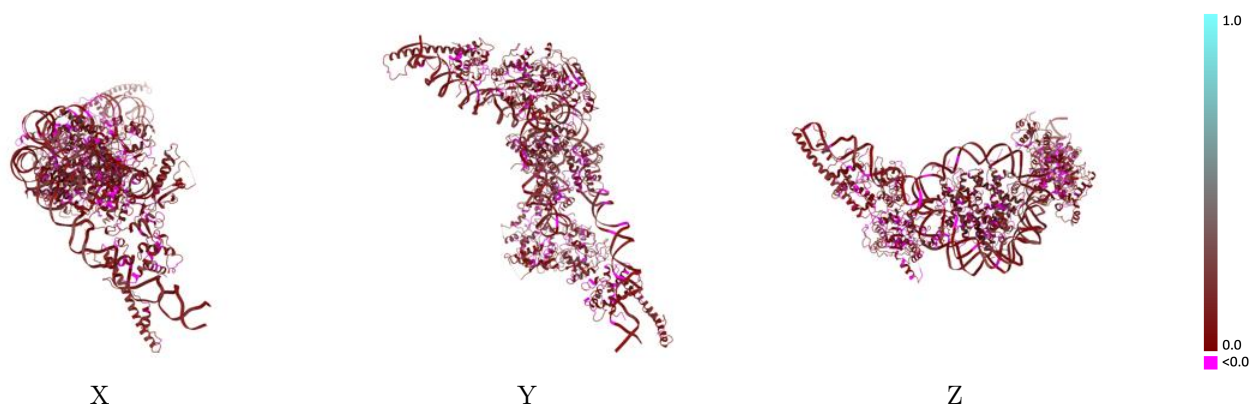
Y



Z

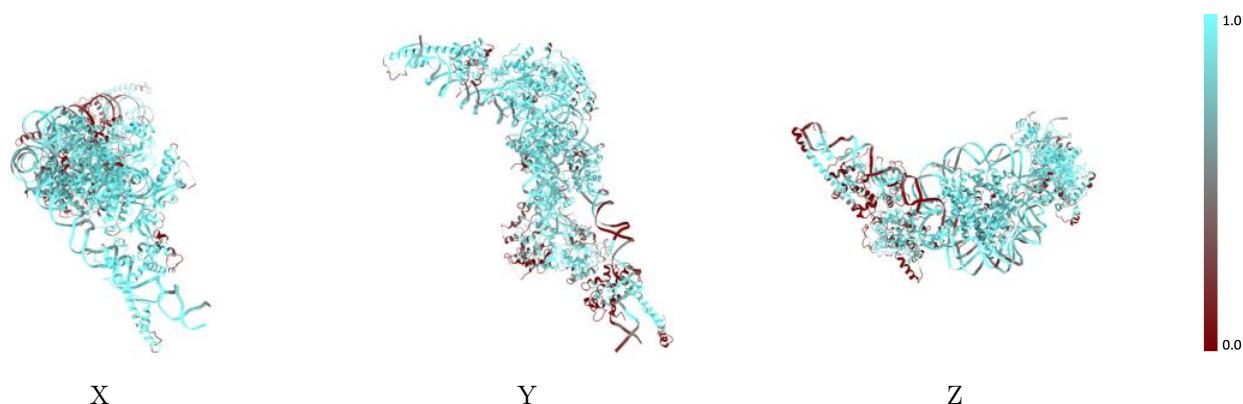
The images above show the 3D surface view of the map at the recommended contour level 0.044 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



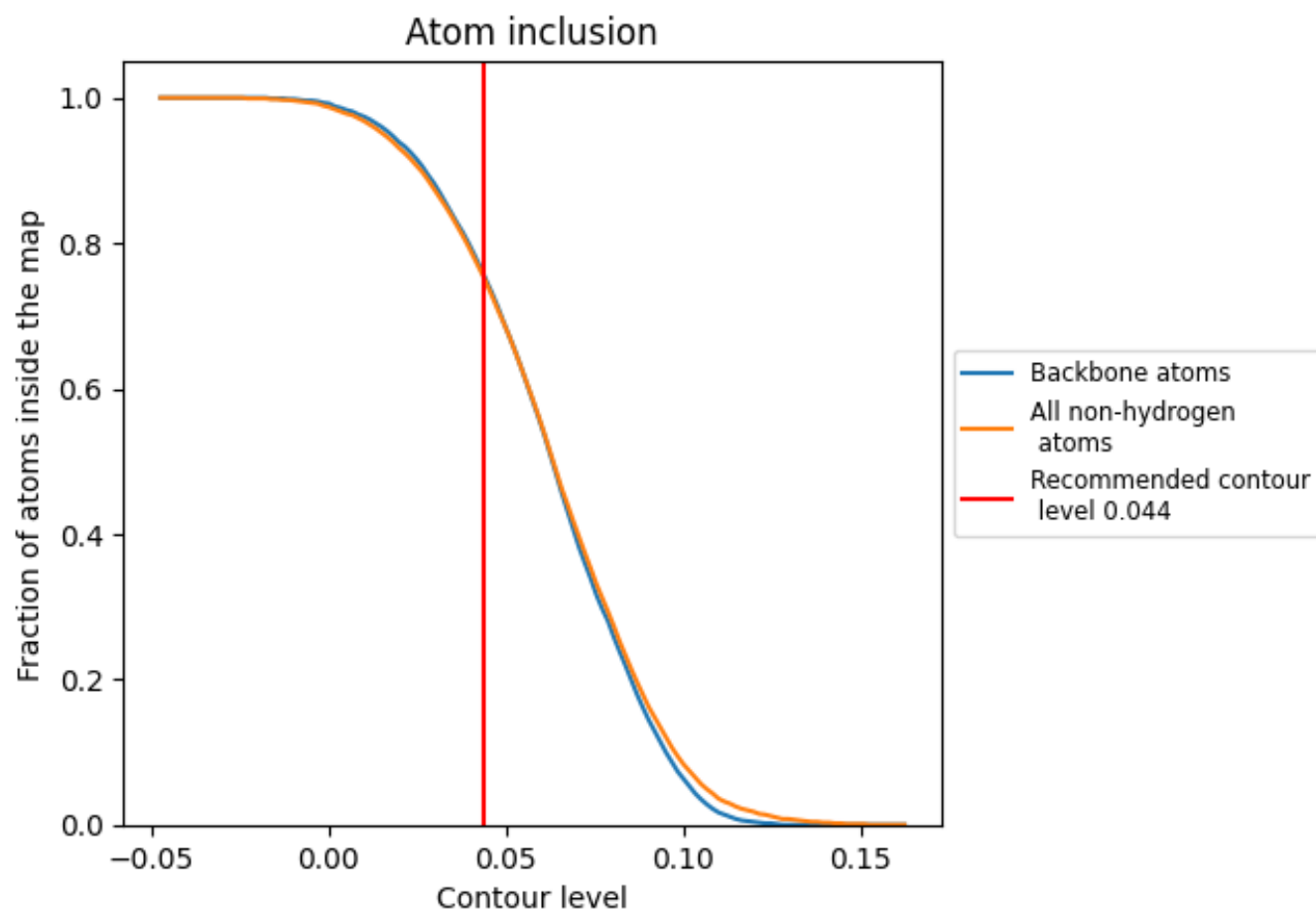
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.044).

9.4 Atom inclusion ⓘ



At the recommended contour level, 75% of all backbone atoms, 75% 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 (0.044) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.7510</div>	<div><div></div>0.0950</div>
A	<div><div></div>0.8440</div>	<div><div></div>0.1140</div>
B	<div><div></div>0.9500</div>	<div><div></div>0.1000</div>
C	<div><div></div>0.8830</div>	<div><div></div>0.0650</div>
D	<div><div></div>0.8120</div>	<div><div></div>0.1020</div>
E	<div><div></div>0.9270</div>	<div><div></div>0.1220</div>
F	<div><div></div>0.8510</div>	<div><div></div>0.0640</div>
G	<div><div></div>0.7410</div>	<div><div></div>0.0690</div>
H	<div><div></div>0.8980</div>	<div><div></div>0.1310</div>
I	<div><div></div>0.7910</div>	<div><div></div>0.1190</div>
J	<div><div></div>0.7580</div>	<div><div></div>0.1190</div>
M	<div><div></div>0.8330</div>	<div><div></div>0.0930</div>
W	<div><div></div>0.5540</div>	<div><div></div>0.0730</div>

1.0

0.0

<0.0