



Full wwPDB EM Validation Report ⓘ

Apr 15, 2025 – 05:50 PM EDT

PDB ID : 9CQ3 / pdb_00009cq3
EMDB ID : EMD-45807
Title : The gap-filling complex with Pol mu engaged in the NHEJ pathway
Authors : Li, J.; Liu, L.; Gellert, M.; Yang, W.
Deposited on : 2024-07-19
Resolution : 2.80 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:

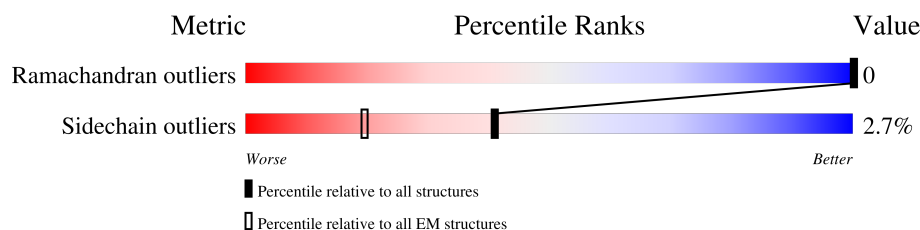
EMDB validation analysis : 0.0.1.dev117
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

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 2.80 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.



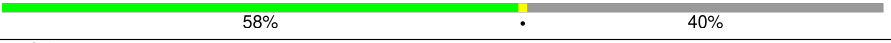









Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	612	
1	a	612	
2	B	732	
2	b	732	
3	C	302	
3	c	302	
4	D	336	
4	E	336	
4	d	336	

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Mol	Chain	Length	Quality of chain
4	e	336	
5	F	914	
5	f	914	
6	G	218	
6	H	218	
7	I	68	
8	J	68	
9	K	51	
10	L	50	
11	M	512	
11	m	512	

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 43972 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 X-ray repair cross-complementing protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	516	Total	C	N	O	S	1	0
			4188	2678	708	783	19		
1	a	505	Total	C	N	O	S	0	0
			4081	2610	691	762	18		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P12956
A	-1	PRO	-	expression tag	UNP P12956
A	0	VAL	-	expression tag	UNP P12956
a	-2	GLY	-	expression tag	UNP P12956
a	-1	PRO	-	expression tag	UNP P12956
a	0	VAL	-	expression tag	UNP P12956

- Molecule 2 is a protein called X-ray repair cross-complementing protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	526	Total	C	N	O	S	0	0
			4211	2697	707	784	23		
2	b	525	Total	C	N	O	S	0	0
			4204	2692	706	783	23		

- Molecule 3 is a protein called Non-homologous end-joining factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	231	Total	C	N	O	S	0	0
			1831	1170	306	340	15		
3	c	228	Total	C	N	O	S	0	0
			1813	1158	303	337	15		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP Q9H9Q4
C	-1	PRO	-	expression tag	UNP Q9H9Q4
C	0	VAL	-	expression tag	UNP Q9H9Q4
c	-2	GLY	-	expression tag	UNP Q9H9Q4
c	-1	PRO	-	expression tag	UNP Q9H9Q4
c	0	VAL	-	expression tag	UNP Q9H9Q4

- Molecule 4 is a protein called DNA repair protein XRCC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	202	Total	C	N	O	S	0	0
			1633	1034	279	313	7		
4	E	201	Total	C	N	O	S	0	0
			1628	1031	278	312	7		
4	d	200	Total	C	N	O	S	0	0
			1623	1028	277	311	7		
4	e	200	Total	C	N	O	S	0	0
			1623	1028	277	311	7		

- Molecule 5 is a protein called DNA ligase 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	679	Total	C	N	O	S	0	0
			5503	3504	945	1021	33		
5	f	255	Total	C	N	O	S	0	0
			2069	1315	349	392	13		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-2	GLY	-	expression tag	UNP P49917
F	-1	PRO	-	expression tag	UNP P49917
F	0	VAL	-	expression tag	UNP P49917
f	-2	GLY	-	expression tag	UNP P49917
f	-1	PRO	-	expression tag	UNP P49917
f	0	VAL	-	expression tag	UNP P49917

- Molecule 6 is a protein called Protein PAXX.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	164	Total	C	N	O	S	0	0
			1219	767	210	236	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	149	Total	C	N	O	S	0	0
			1114	710	192	206	6		

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-13	MET	-	expression tag	UNP Q9BUH6
G	-12	GLY	-	expression tag	UNP Q9BUH6
G	-11	SER	-	expression tag	UNP Q9BUH6
G	-10	SER	-	expression tag	UNP Q9BUH6
G	-9	HIS	-	expression tag	UNP Q9BUH6
G	-8	HIS	-	expression tag	UNP Q9BUH6
G	-7	HIS	-	expression tag	UNP Q9BUH6
G	-6	HIS	-	expression tag	UNP Q9BUH6
G	-5	HIS	-	expression tag	UNP Q9BUH6
G	-4	HIS	-	expression tag	UNP Q9BUH6
G	-3	SER	-	expression tag	UNP Q9BUH6
G	-2	GLN	-	expression tag	UNP Q9BUH6
G	-1	ASP	-	expression tag	UNP Q9BUH6
G	0	PRO	-	expression tag	UNP Q9BUH6
H	-13	MET	-	expression tag	UNP Q9BUH6
H	-12	GLY	-	expression tag	UNP Q9BUH6
H	-11	SER	-	expression tag	UNP Q9BUH6
H	-10	SER	-	expression tag	UNP Q9BUH6
H	-9	HIS	-	expression tag	UNP Q9BUH6
H	-8	HIS	-	expression tag	UNP Q9BUH6
H	-7	HIS	-	expression tag	UNP Q9BUH6
H	-6	HIS	-	expression tag	UNP Q9BUH6
H	-5	HIS	-	expression tag	UNP Q9BUH6
H	-4	HIS	-	expression tag	UNP Q9BUH6
H	-3	SER	-	expression tag	UNP Q9BUH6
H	-2	GLN	-	expression tag	UNP Q9BUH6
H	-1	ASP	-	expression tag	UNP Q9BUH6
H	0	PRO	-	expression tag	UNP Q9BUH6

- Molecule 7 is a DNA chain called DNA (38-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	38	Total	C	N	O	P	0	0
			771	370	131	232	38		

- Molecule 8 is a DNA chain called DNA (42-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	42	Total	C	N	O	P	0	0
			857	410	154	251	42		

- Molecule 9 is a DNA chain called DNA (34-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	34	Total	C	N	O	P	0	0
			702	335	136	198	33		

- Molecule 10 is a DNA chain called DNA (37-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	37	Total	C	N	O	P	0	0
			763	364	137	225	37		

- Molecule 11 is a protein called DNA-directed DNA/RNA polymerase mu.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	426	Total	C	N	O	S	0	0
			3375	2129	620	612	14		
11	m	96	Total	C	N	O	S	0	0
			732	457	135	134	6		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-17	HIS	-	expression tag	UNP Q9NP87
M	-16	HIS	-	expression tag	UNP Q9NP87
M	-15	HIS	-	expression tag	UNP Q9NP87
M	-14	HIS	-	expression tag	UNP Q9NP87
M	-13	HIS	-	expression tag	UNP Q9NP87
M	-12	HIS	-	expression tag	UNP Q9NP87
M	-11	SER	-	expression tag	UNP Q9NP87
M	-10	SER	-	expression tag	UNP Q9NP87
M	-9	GLY	-	expression tag	UNP Q9NP87
M	-8	LEU	-	expression tag	UNP Q9NP87
M	-7	GLU	-	expression tag	UNP Q9NP87
M	-6	VAL	-	expression tag	UNP Q9NP87
M	-5	LEU	-	expression tag	UNP Q9NP87
M	-4	PHE	-	expression tag	UNP Q9NP87
M	-3	GLN	-	expression tag	UNP Q9NP87
M	-2	GLY	-	expression tag	UNP Q9NP87
M	-1	PRO	-	expression tag	UNP Q9NP87

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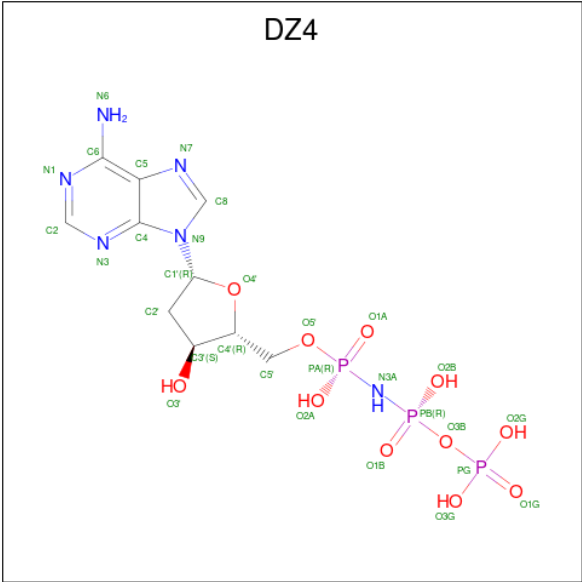
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Chain	Residue	Modelled	Actual	Comment	Reference
M	0	HIS	-	expression tag	UNP Q9NP87
m	-17	HIS	-	expression tag	UNP Q9NP87
m	-16	HIS	-	expression tag	UNP Q9NP87
m	-15	HIS	-	expression tag	UNP Q9NP87
m	-14	HIS	-	expression tag	UNP Q9NP87
m	-13	HIS	-	expression tag	UNP Q9NP87
m	-12	HIS	-	expression tag	UNP Q9NP87
m	-11	SER	-	expression tag	UNP Q9NP87
m	-10	SER	-	expression tag	UNP Q9NP87
m	-9	GLY	-	expression tag	UNP Q9NP87
m	-8	LEU	-	expression tag	UNP Q9NP87
m	-7	GLU	-	expression tag	UNP Q9NP87
m	-6	VAL	-	expression tag	UNP Q9NP87
m	-5	LEU	-	expression tag	UNP Q9NP87
m	-4	PHE	-	expression tag	UNP Q9NP87
m	-3	GLN	-	expression tag	UNP Q9NP87
m	-2	GLY	-	expression tag	UNP Q9NP87
m	-1	PRO	-	expression tag	UNP Q9NP87
m	0	HIS	-	expression tag	UNP Q9NP87

- Molecule 12 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

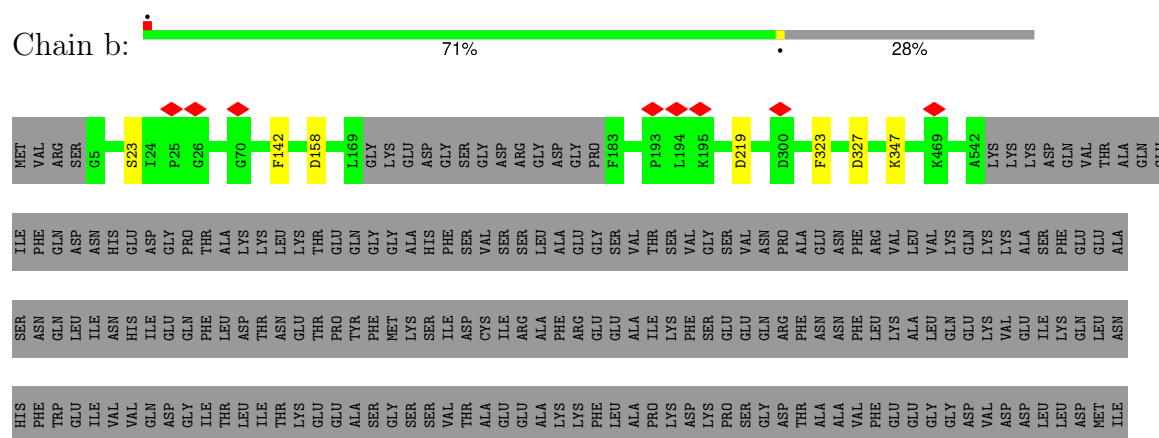
Mol	Chain	Residues	Atoms	AltConf
12	M	2	Total Mg 2 2	0

- Molecule 13 is 2'-deoxy-5'-O-[(R)-hydroxy{[(R)-hydroxy(phosphonooxy)phosphoryl]amino}phosphoryl]adenosine (CCD ID: DZ4) (formula: C₁₀H₁₇N₆O₁₁P₃) (labeled as "Ligand of Interest" by depositor).

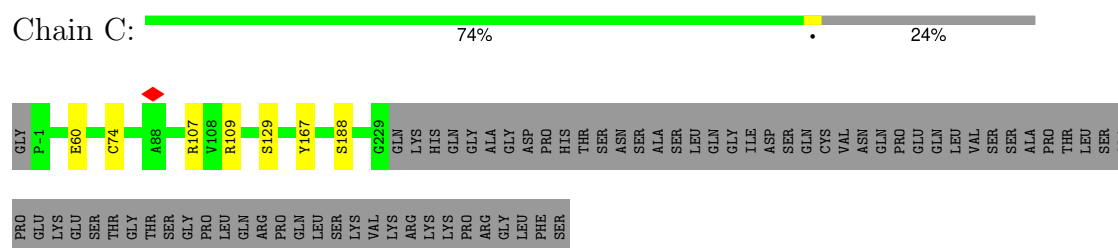


Mol	Chain	Residues	Atoms					AltConf
13	M	1	Total	C	N	O	P	0
			30	10	6	11	3	

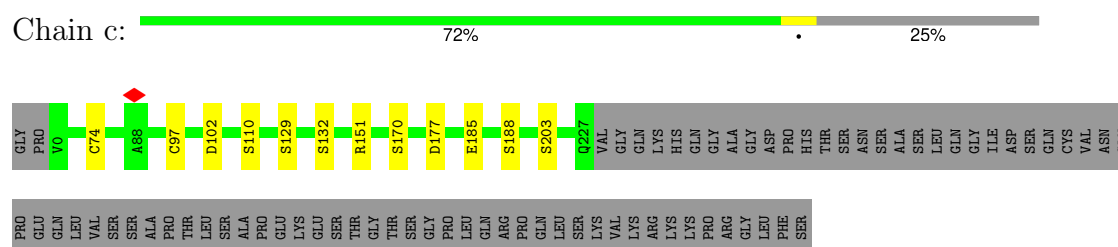
- Molecule 2: X-ray repair cross-complementing protein 5



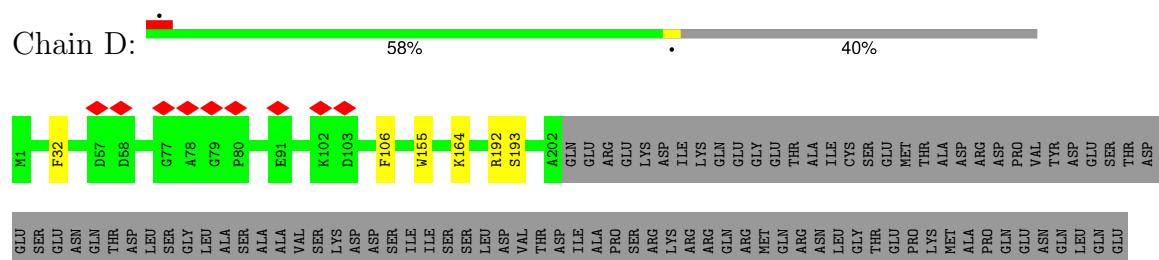
- Molecule 3: Non-homologous end-joining factor 1



- Molecule 3: Non-homologous end-joining factor 1

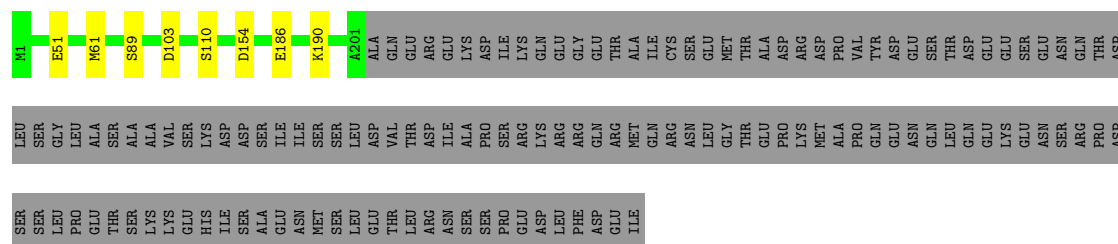


- Molecule 4: DNA repair protein XRCC4



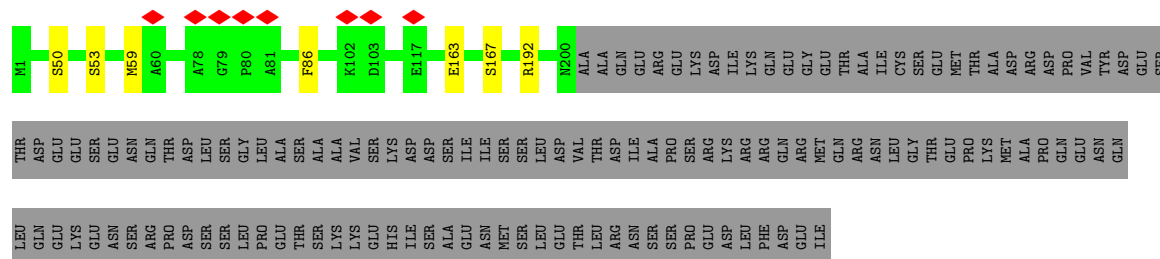
- Molecule 4: DNA repair protein XRCC4

Chain E:  57% . 40%



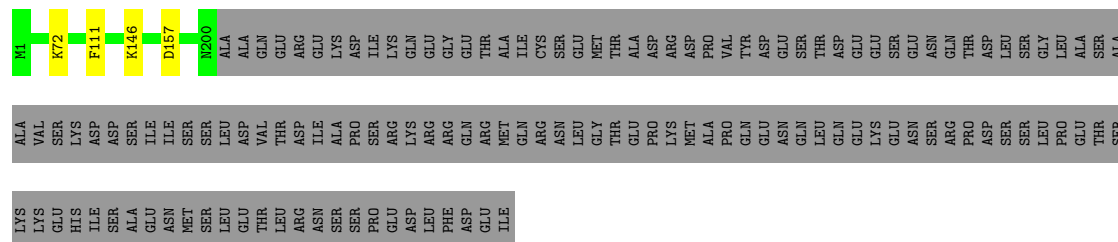
- Molecule 4: DNA repair protein XRCC4

Chain d:  57% 40%



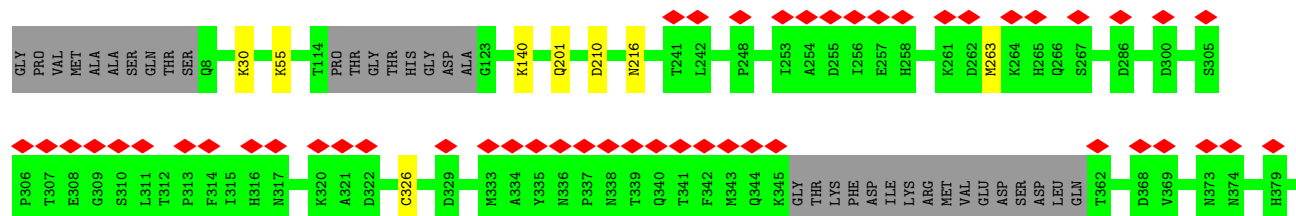
- Molecule 4: DNA repair protein XRCC4

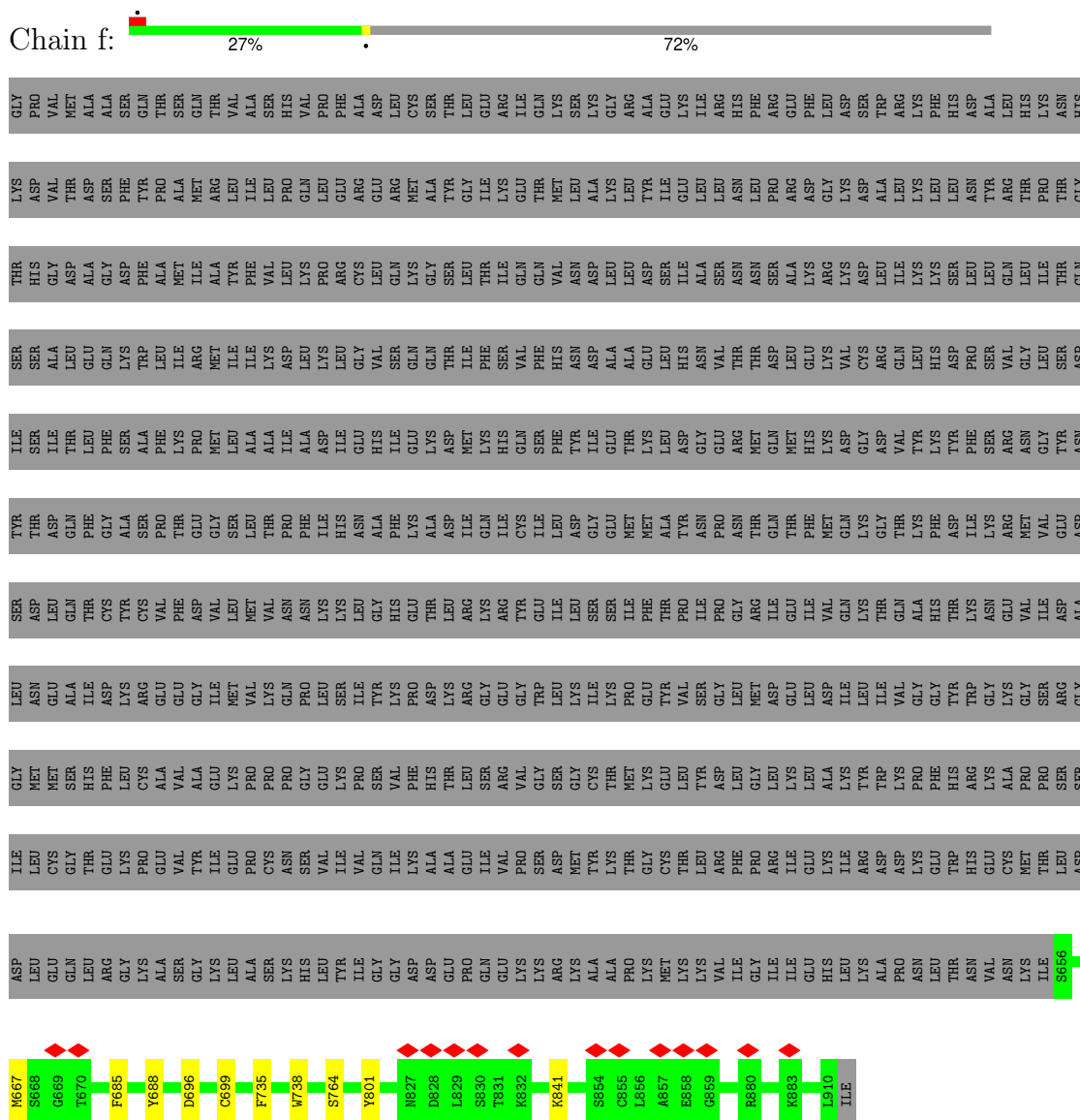
Chain e:  58% . 40%



- Molecule 5: DNA ligase 4

Chain F:  9% 73% 26%





LEU
GLU
TYR
LEU
PRO
PRO
GLU
GLN
ARG
ASN
ALA

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	891208	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 ($e^-/\text{\AA}^2$)	54.4	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	83.840	Depositor
Minimum map value	-45.605	Depositor
Average map value	0.010	Depositor
Map value standard deviation	1.448	Depositor
Recommended contour level	8	Depositor
Map size (Å)	426.496, 426.496, 426.496	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.833, 0.833, 0.833	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DZ4, 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	0.25	0/4272	0.48	0/5755
1	a	0.25	0/4162	0.48	0/5609
2	B	0.25	0/4298	0.45	0/5800
2	b	0.24	0/4290	0.45	0/5788
3	C	0.24	0/1869	0.46	0/2536
3	c	0.24	0/1850	0.46	0/2510
4	D	0.25	0/1662	0.46	0/2235
4	E	0.26	0/1657	0.46	0/2228
4	d	0.25	0/1652	0.47	0/2221
4	e	0.25	0/1652	0.45	0/2221
5	F	0.25	0/5617	0.46	0/7568
5	f	0.24	0/2118	0.46	0/2862
6	G	0.25	0/1247	0.48	0/1695
6	H	0.25	0/1140	0.49	0/1549
7	I	0.55	0/861	0.98	0/1325
8	J	0.51	0/960	0.94	0/1478
9	K	0.54	0/790	0.92	0/1219
10	L	0.63	1/855 (0.1%)	0.94	0/1317
11	M	0.25	0/3452	0.52	0/4671
11	m	0.25	0/749	0.54	0/1017
All	All	0.28	1/45153 (0.0%)	0.53	0/61604

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	L	1	DG	OP3-P	-10.63	1.48	1.61

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	513/612 (84%)	506 (99%)	7 (1%)	0	100	100
1	a	503/612 (82%)	490 (97%)	13 (3%)	0	100	100
2	B	522/732 (71%)	509 (98%)	13 (2%)	0	100	100
2	b	521/732 (71%)	510 (98%)	11 (2%)	0	100	100
3	C	229/302 (76%)	223 (97%)	6 (3%)	0	100	100
3	c	226/302 (75%)	221 (98%)	5 (2%)	0	100	100
4	D	200/336 (60%)	194 (97%)	6 (3%)	0	100	100
4	E	199/336 (59%)	196 (98%)	3 (2%)	0	100	100
4	d	198/336 (59%)	197 (100%)	1 (0%)	0	100	100
4	e	198/336 (59%)	196 (99%)	2 (1%)	0	100	100
5	F	671/914 (73%)	656 (98%)	15 (2%)	0	100	100
5	f	253/914 (28%)	244 (96%)	9 (4%)	0	100	100
6	G	160/218 (73%)	159 (99%)	1 (1%)	0	100	100
6	H	141/218 (65%)	139 (99%)	2 (1%)	0	100	100
11	M	418/512 (82%)	409 (98%)	9 (2%)	0	100	100
11	m	94/512 (18%)	93 (99%)	1 (1%)	0	100	100
All	All	5046/7924 (64%)	4942 (98%)	104 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	470/550 (86%)	463 (98%)	7 (2%)	60	86
1	a	459/550 (84%)	447 (97%)	12 (3%)	41	75
2	B	474/649 (73%)	462 (98%)	12 (2%)	42	75
2	b	473/649 (73%)	466 (98%)	7 (2%)	60	86
3	C	204/264 (77%)	197 (97%)	7 (3%)	32	66
3	c	202/264 (76%)	190 (94%)	12 (6%)	16	44
4	D	180/303 (59%)	174 (97%)	6 (3%)	33	67
4	E	180/303 (59%)	172 (96%)	8 (4%)	24	56
4	d	180/303 (59%)	173 (96%)	7 (4%)	27	61
4	e	180/303 (59%)	176 (98%)	4 (2%)	47	79
5	F	611/810 (75%)	598 (98%)	13 (2%)	48	80
5	f	231/810 (28%)	221 (96%)	10 (4%)	25	57
6	G	127/173 (73%)	123 (97%)	4 (3%)	35	69
6	H	117/173 (68%)	113 (97%)	4 (3%)	32	66
11	M	358/428 (84%)	351 (98%)	7 (2%)	50	81
11	m	77/428 (18%)	77 (100%)	0	100	100
All	All	4523/6960 (65%)	4403 (97%)	120 (3%)	41	74

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	SER
1	A	133	ASP
1	A	162	SER
1	A	184	SER
1	A	201	ASP
1	A	409	TYR
1	A	500	PRO
2	B	13	CYS

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Mol	Chain	Res	Type
2	B	52	ASP
2	B	104	GLN
2	B	142	PHE
2	B	183	PHE
2	B	209	LYS
2	B	228	SER
2	B	233	LYS
2	B	241	GLU
2	B	246	HIS
2	B	309	ASP
2	B	329	GLU
3	C	60	GLU
3	C	74	CYS
3	C	107	ARG
3	C	109	ARG
3	C	129	SER
3	C	167	TYR
3	C	188	SER
4	D	32	PHE
4	D	106	PHE
4	D	155	TRP
4	D	164	LYS
4	D	192	ARG
4	D	193	SER
4	E	51	GLU
4	E	61	MET
4	E	89	SER
4	E	103	ASP
4	E	110	SER
4	E	154	ASP
4	E	186	GLU
4	E	190	LYS
5	F	30	LYS
5	F	55	LYS
5	F	140	LYS
5	F	201	GLN
5	F	210	ASP
5	F	216	ASN
5	F	263	MET
5	F	326	CYS
5	F	418	LEU
5	F	680	ASN

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Mol	Chain	Res	Type
5	F	699	CYS
5	F	754	PHE
5	F	769	THR
6	G	20	PHE
6	G	24	CYS
6	G	409	LYS
6	G	418	ASP
6	H	24	CYS
6	H	37	PHE
6	H	80	CYS
6	H	120	ARG
11	M	38	ARG
11	M	156	LEU
11	M	205	PHE
11	M	255	TYR
11	M	285	ASP
11	M	448	SER
11	M	470	PHE
1	a	57	LEU
1	a	62	MET
1	a	142	SER
1	a	162	SER
1	a	192	ASP
1	a	206	LYS
1	a	299	LYS
1	a	342	ASP
1	a	373	SER
1	a	409	TYR
1	a	441	ASP
1	a	471	PHE
2	b	23	SER
2	b	142	PHE
2	b	158	ASP
2	b	219	ASP
2	b	323	PHE
2	b	327	ASP
2	b	347	LYS
3	c	74	CYS
3	c	97	CYS
3	c	102	ASP
3	c	110	SER
3	c	129	SER

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Mol	Chain	Res	Type
3	c	132	SER
3	c	151	ARG
3	c	170	SER
3	c	177	ASP
3	c	185	GLU
3	c	188	SER
3	c	203	SER
4	d	50	SER
4	d	53	SER
4	d	59	MET
4	d	86	PHE
4	d	163	GLU
4	d	167	SER
4	d	192	ARG
4	e	72	LYS
4	e	111	PHE
4	e	146	LYS
4	e	157	ASP
5	f	667	MET
5	f	685	PHE
5	f	688	TYR
5	f	696	ASP
5	f	699	CYS
5	f	735	PHE
5	f	738	TRP
5	f	764	SER
5	f	801	TYR
5	f	841	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	132	GLN
3	C	149	GLN
4	D	21	GLN
5	F	27	GLN
3	c	6	GLN

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, 2 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z > 2$
13	DZ4	M	503	12	28,32,32	3.38	14 (50%)	33,50,50	1.73	5 (15%)

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
13	DZ4	M	503	12	-	5/15/34/34	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	503	DZ4	C2'-C3'	-8.42	1.31	1.52
13	M	503	DZ4	O4'-C4'	-6.88	1.29	1.45
13	M	503	DZ4	O4'-C1'	6.60	1.57	1.42
13	M	503	DZ4	PB-O3B	5.77	1.66	1.59
13	M	503	DZ4	C1'-N9	-5.25	1.34	1.49
13	M	503	DZ4	C3'-C4'	3.69	1.62	1.53
13	M	503	DZ4	C6-N6	3.50	1.46	1.34
13	M	503	DZ4	PB-N3A	3.43	1.72	1.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	503	DZ4	PA-N3A	3.20	1.71	1.63
13	M	503	DZ4	PA-O1A	3.10	1.50	1.46
13	M	503	DZ4	C2-N3	2.83	1.36	1.32
13	M	503	DZ4	PB-O1B	2.83	1.50	1.46
13	M	503	DZ4	PB-O2B	-2.13	1.51	1.56
13	M	503	DZ4	PA-O2A	-2.09	1.51	1.56

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	503	DZ4	N3-C2-N1	-6.30	120.12	128.67
13	M	503	DZ4	C5-C6-N6	4.23	126.75	120.31
13	M	503	DZ4	O1A-PA-N3A	-3.24	107.00	111.77
13	M	503	DZ4	N6-C6-N1	-2.39	113.23	118.33
13	M	503	DZ4	O5'-PA-O1A	-2.02	108.28	114.27

There are no chirality outliers.

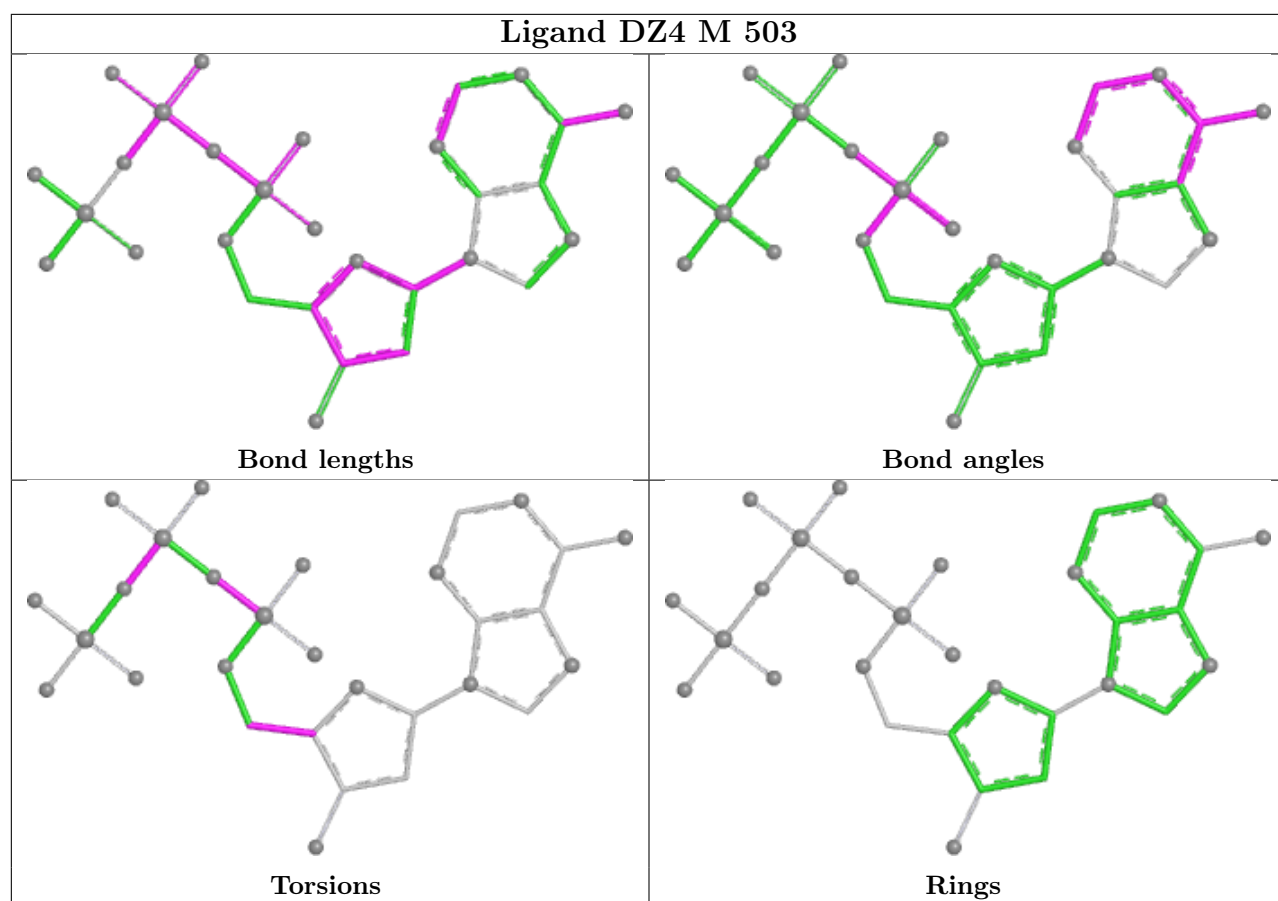
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	M	503	DZ4	PB-N3A-PA-O5'
13	M	503	DZ4	PG-O3B-PB-O1B
13	M	503	DZ4	PG-O3B-PB-O2B
13	M	503	DZ4	O4'-C4'-C5'-O5'
13	M	503	DZ4	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

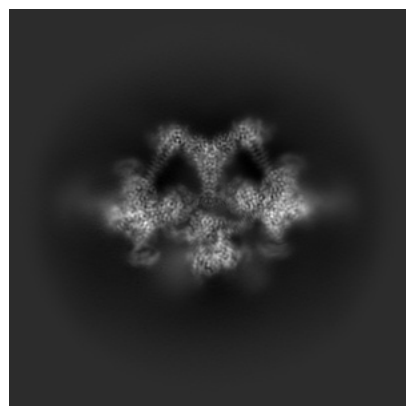
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45807. These allow visual inspection of the internal detail of the map and identification of artifacts.

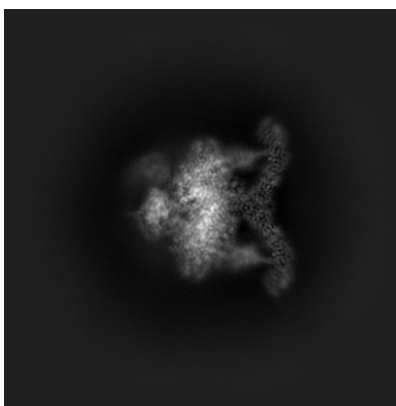
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

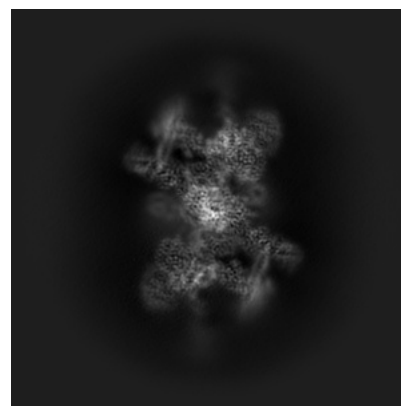
6.1.1 Primary map



X

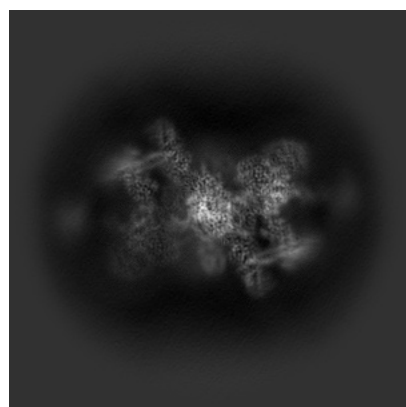


Y

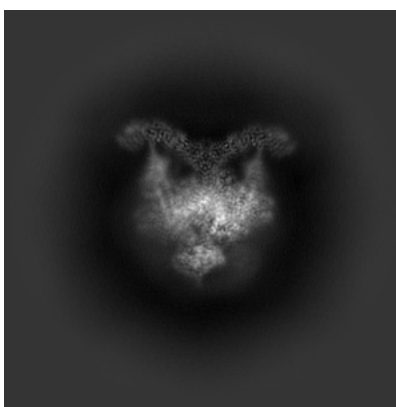


Z

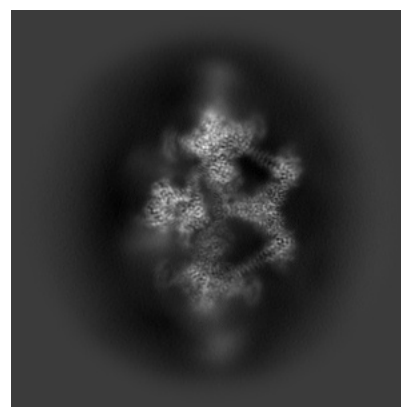
6.1.2 Raw map



X



Y

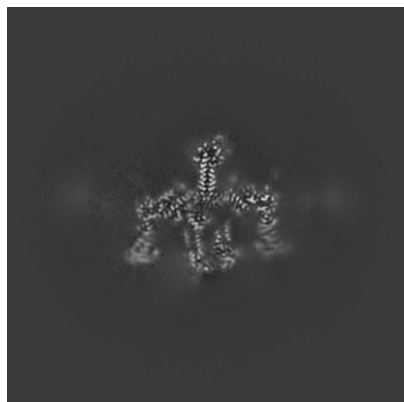


Z

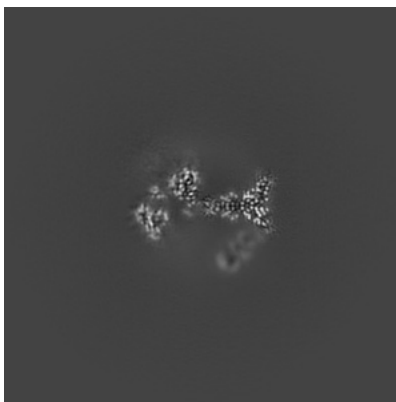
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

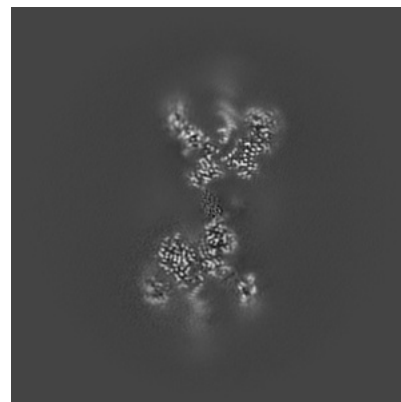
6.2.1 Primary map



X Index: 256

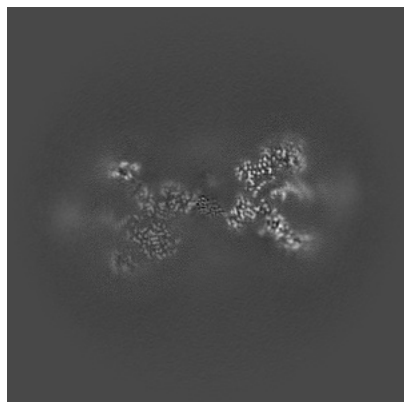


Y Index: 256

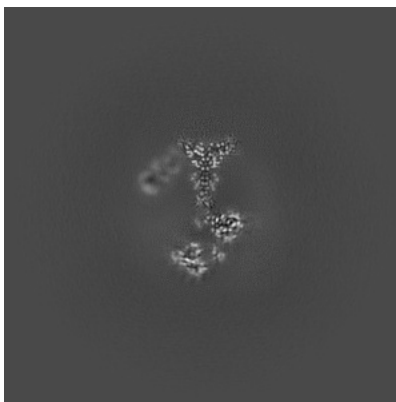


Z Index: 256

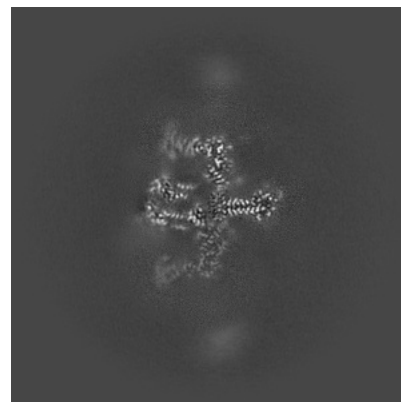
6.2.2 Raw map



X Index: 256



Y Index: 256

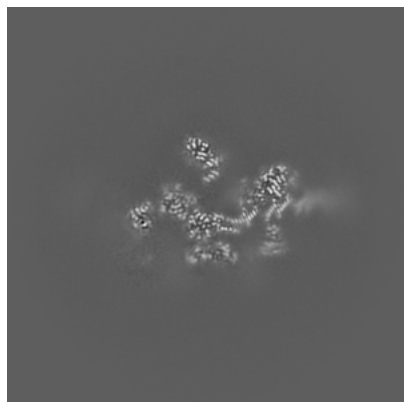


Z Index: 256

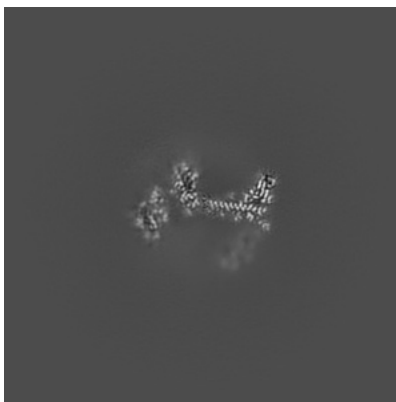
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

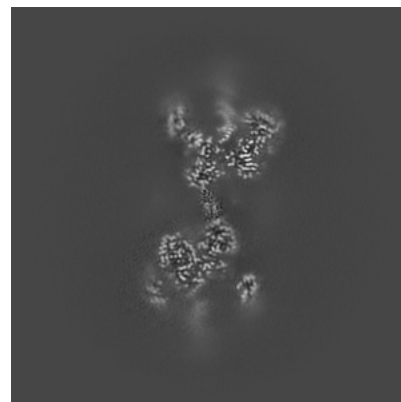
6.3.1 Primary map



X Index: 273

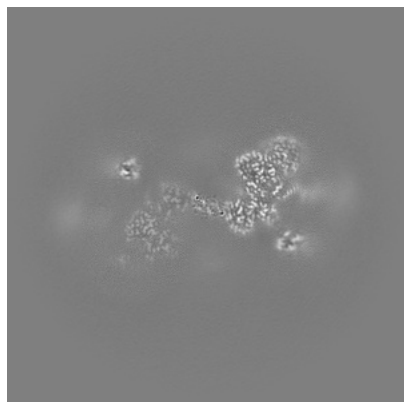


Y Index: 251

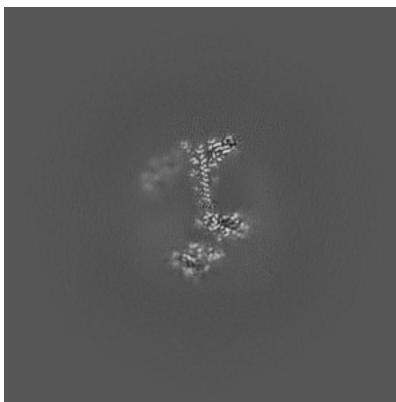


Z Index: 259

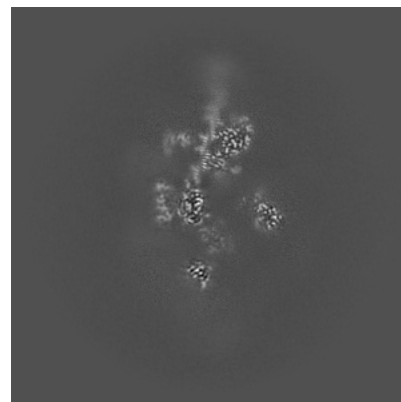
6.3.2 Raw map



X Index: 264



Y Index: 251

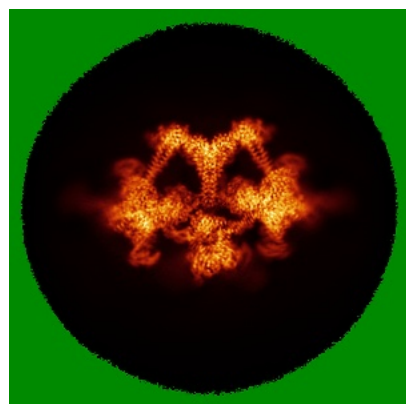


Z Index: 277

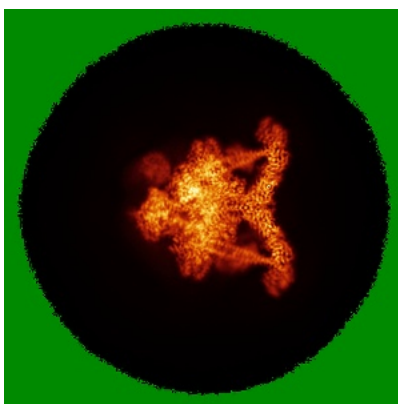
The images above show the largest variance slices of the map in three orthogonal directions.

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

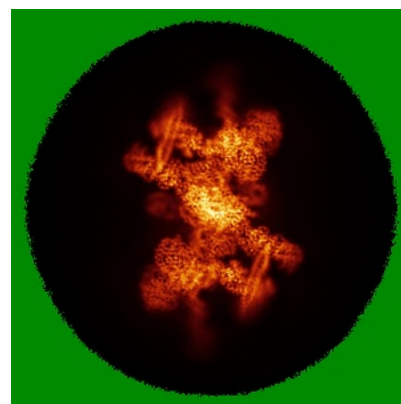
6.4.1 Primary map



X

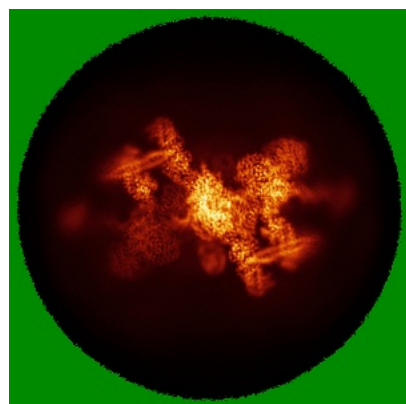


Y



Z

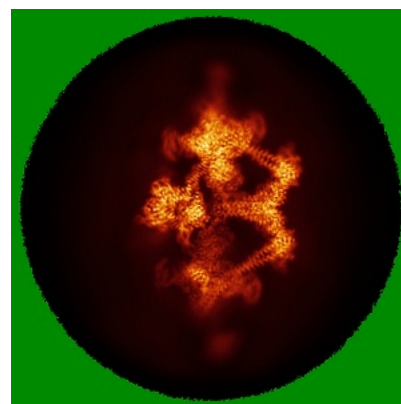
6.4.2 Raw map



X



Y

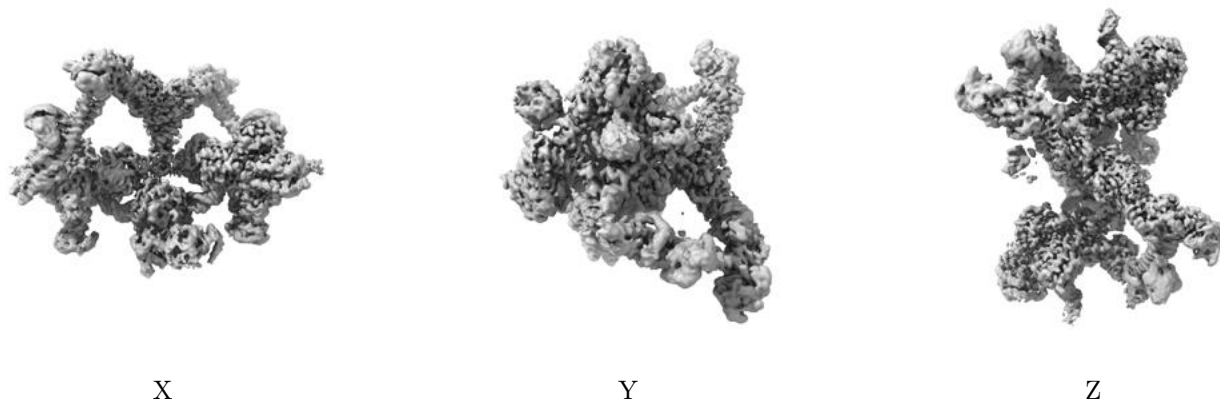


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

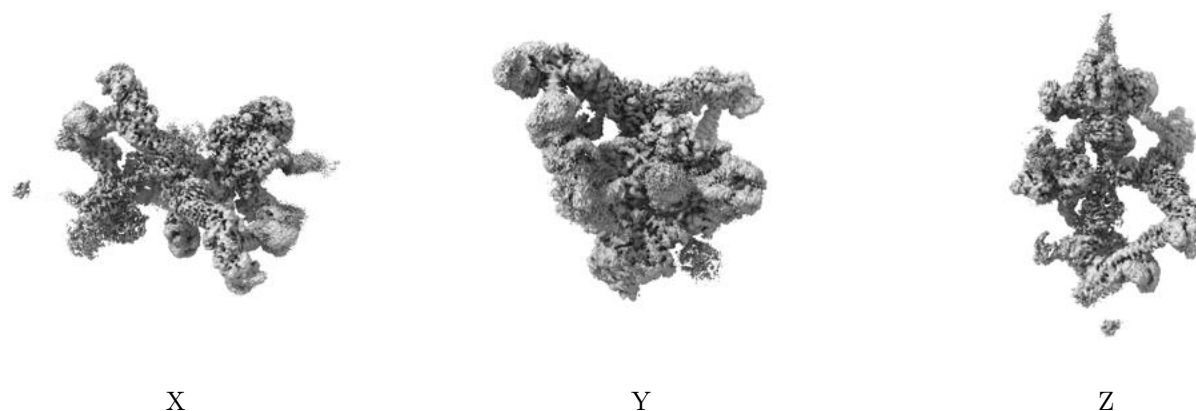
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 8.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

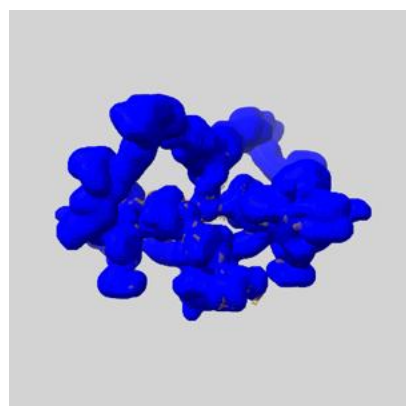
6.6 Mask visualisation [i](#)

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

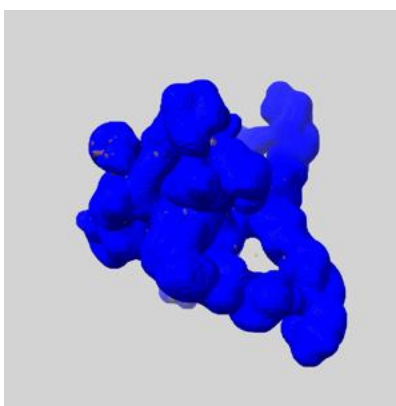
A mask typically either:

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

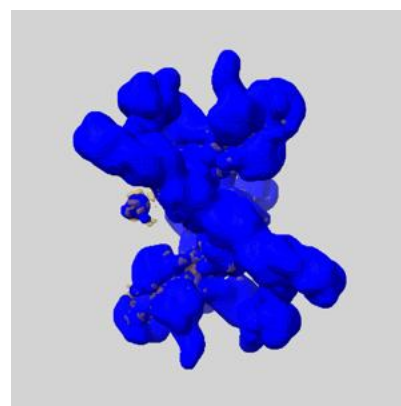
6.6.1 emd_45807_msk_1.map [i](#)



X



Y

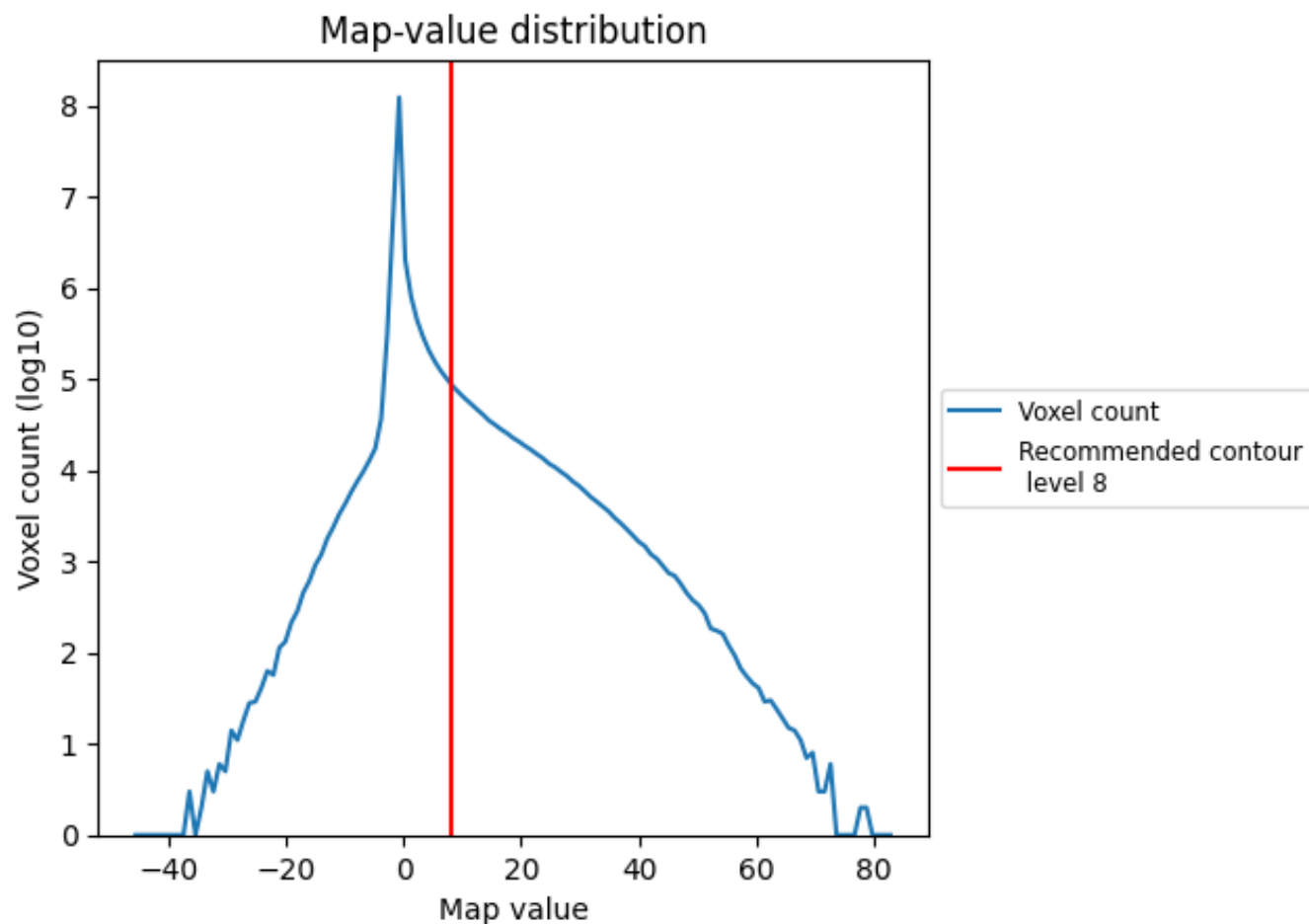


Z

7 Map analysis [i](#)

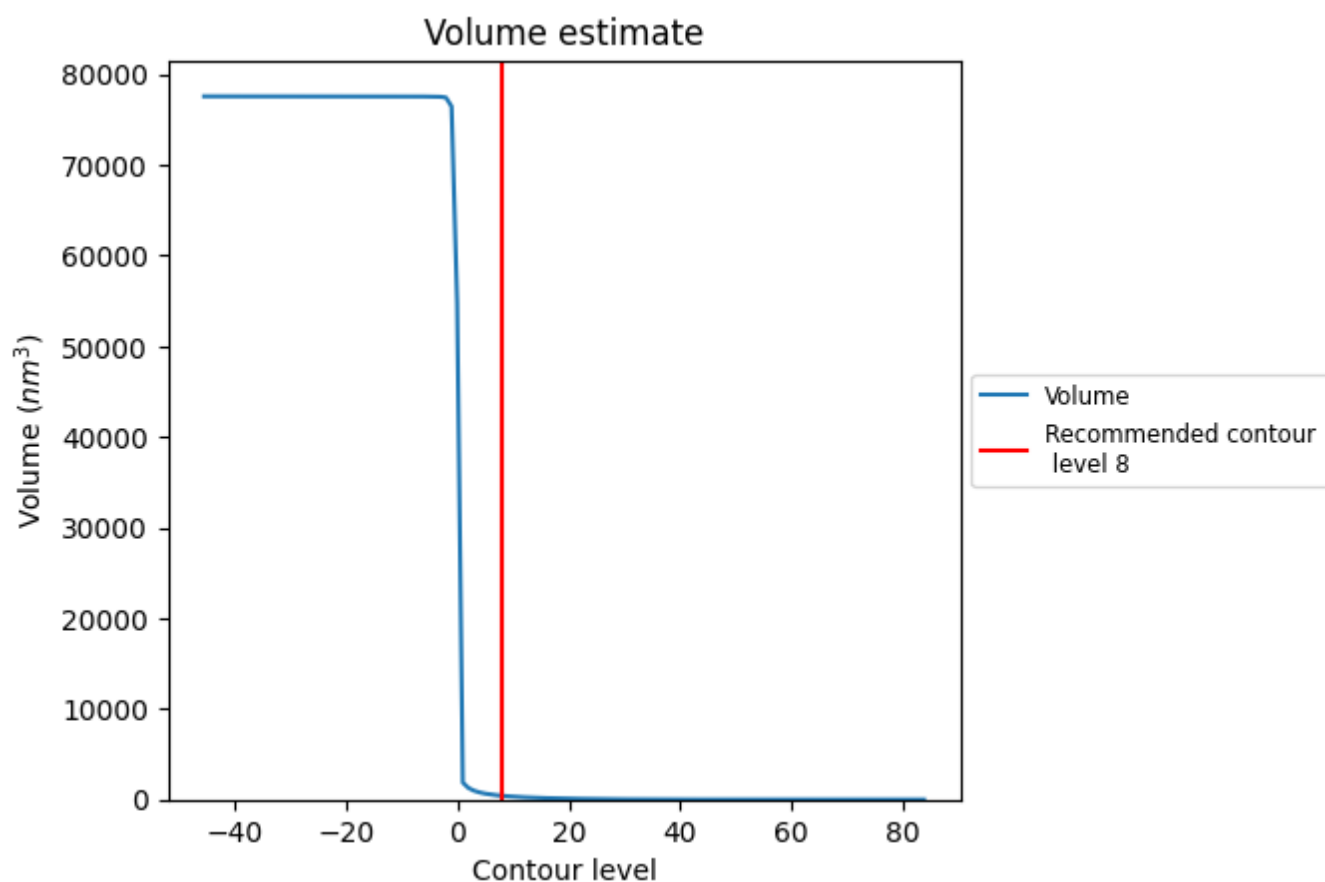
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

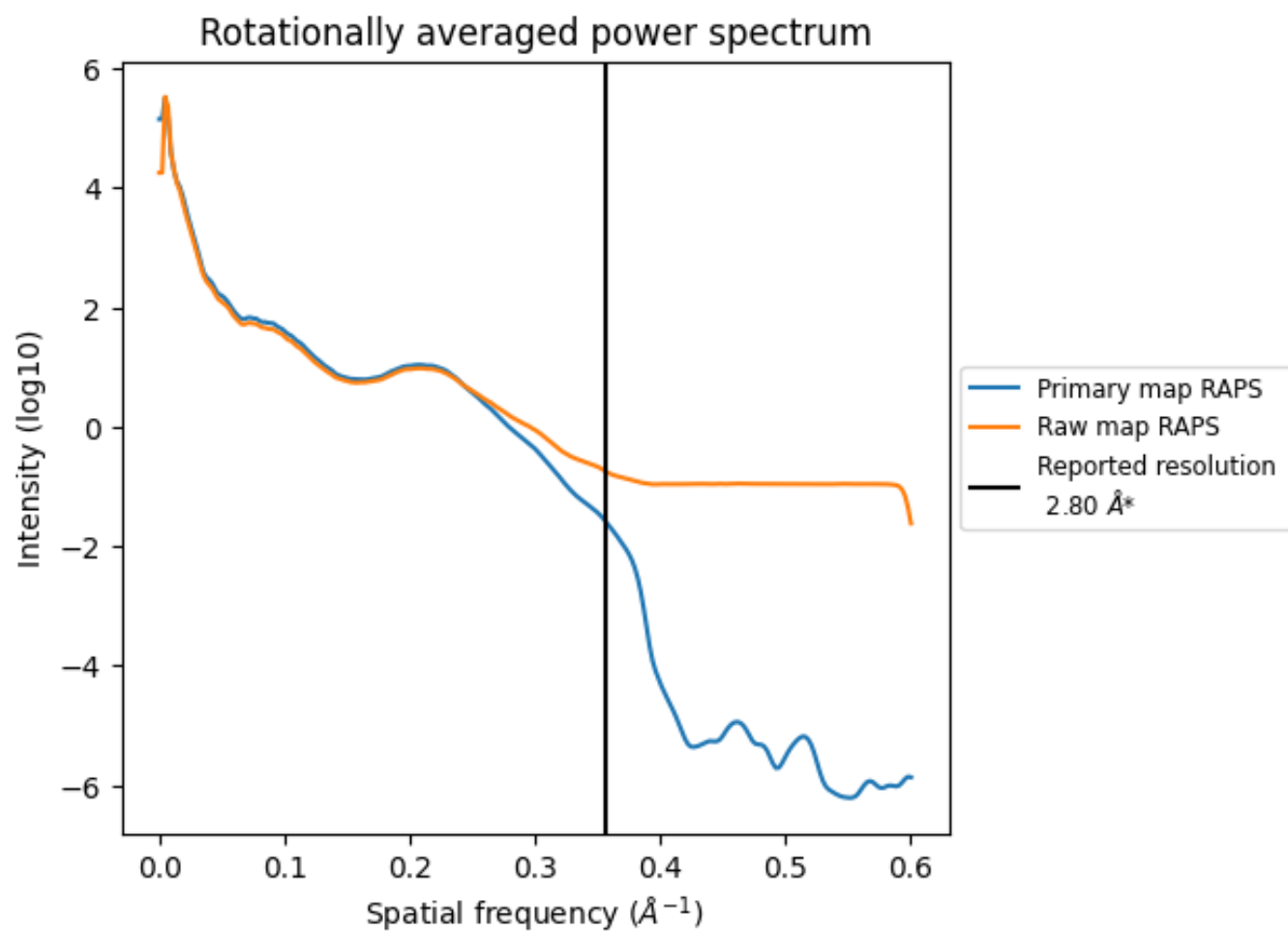
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 416 nm³; this corresponds to an approximate mass of 375 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 ⓘ

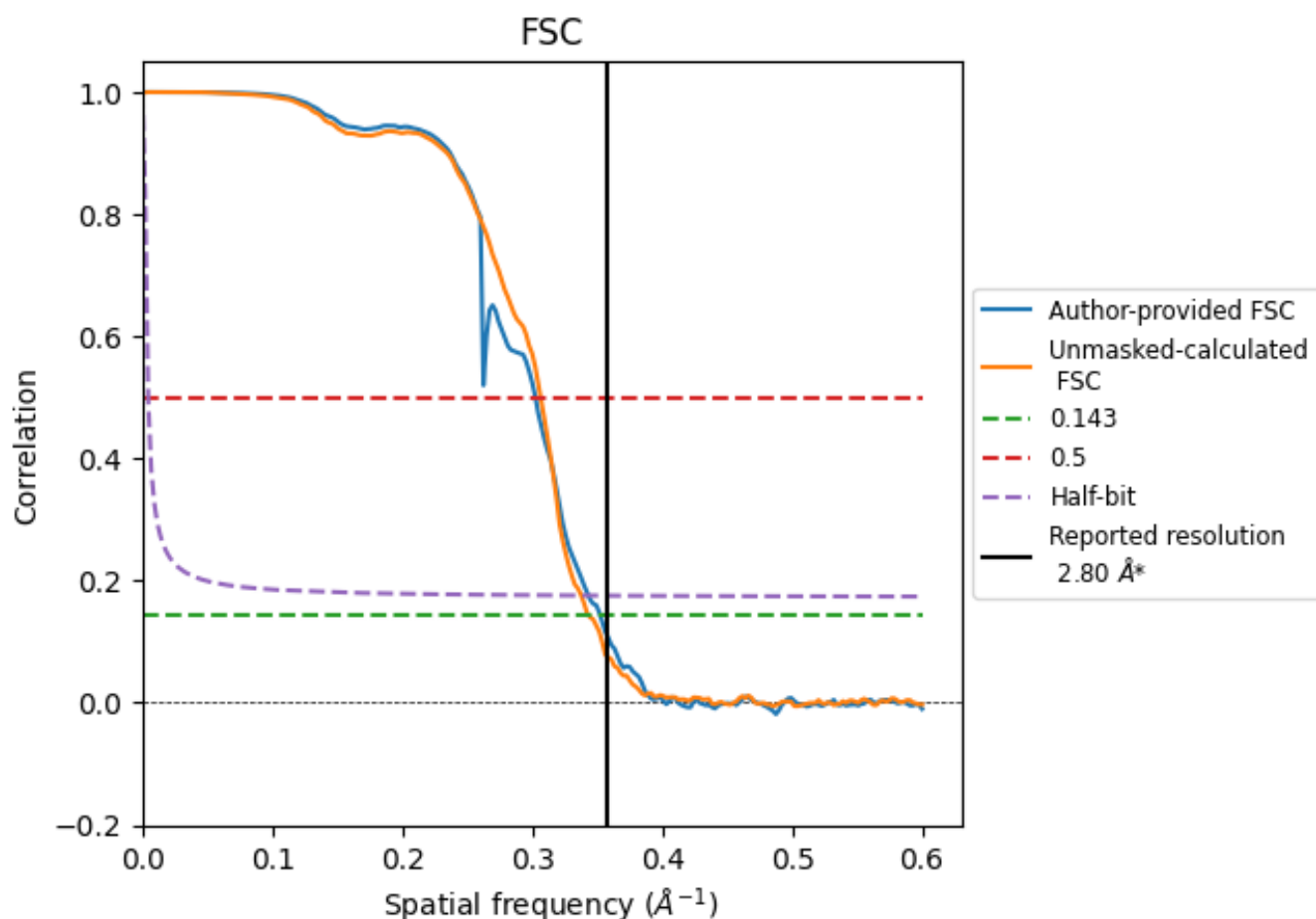


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

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 0.357 \AA^{-1}

8.2 Resolution estimates [i](#)

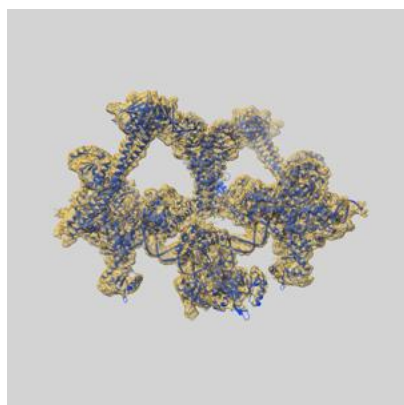
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.84	3.30	2.91
Unmasked-calculated*	2.91	3.26	2.96

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

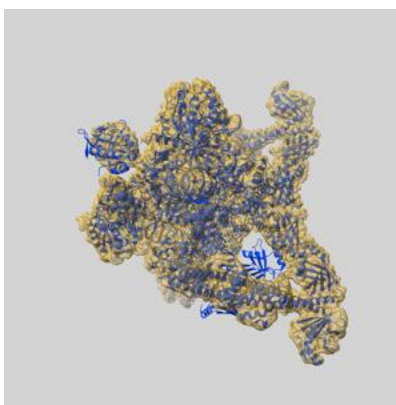
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-45807 and PDB model 9CQ3. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

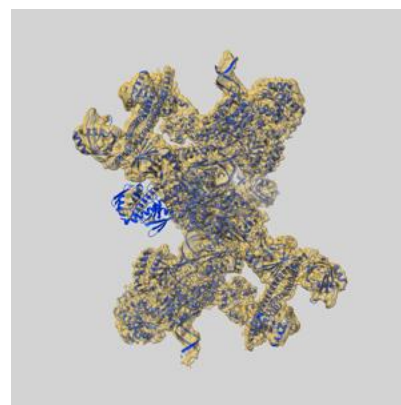
9.1 Map-model overlay [i](#)



X



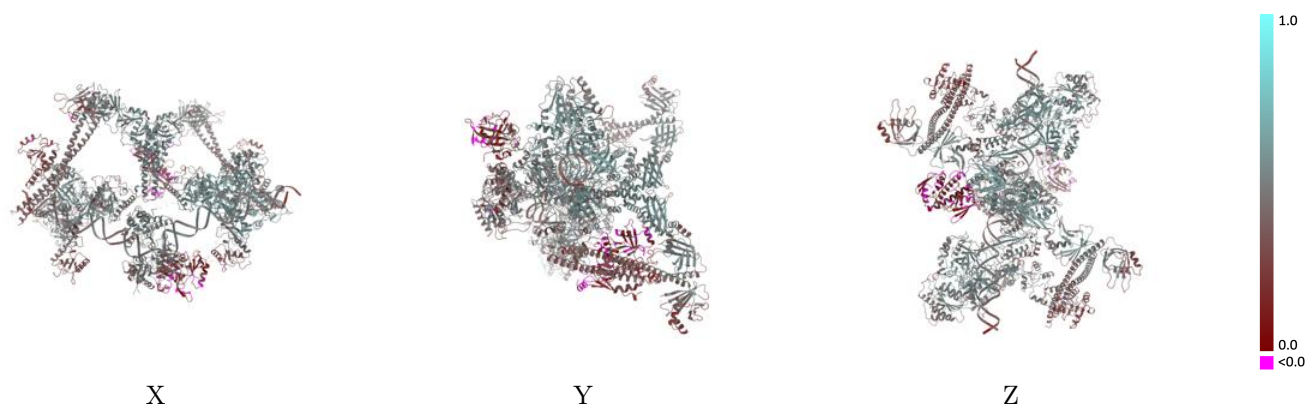
Y



Z

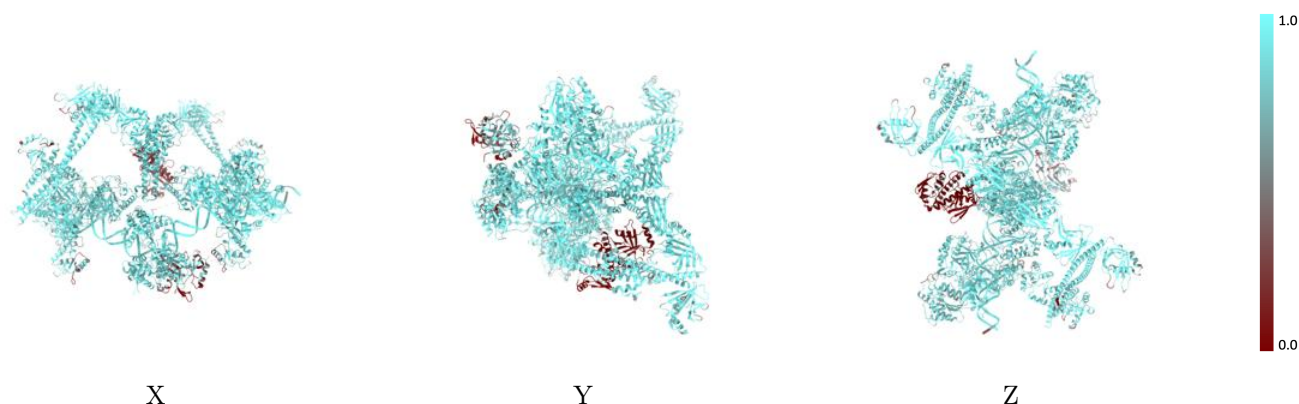
The images above show the 3D surface view of the map at the recommended contour level 8.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



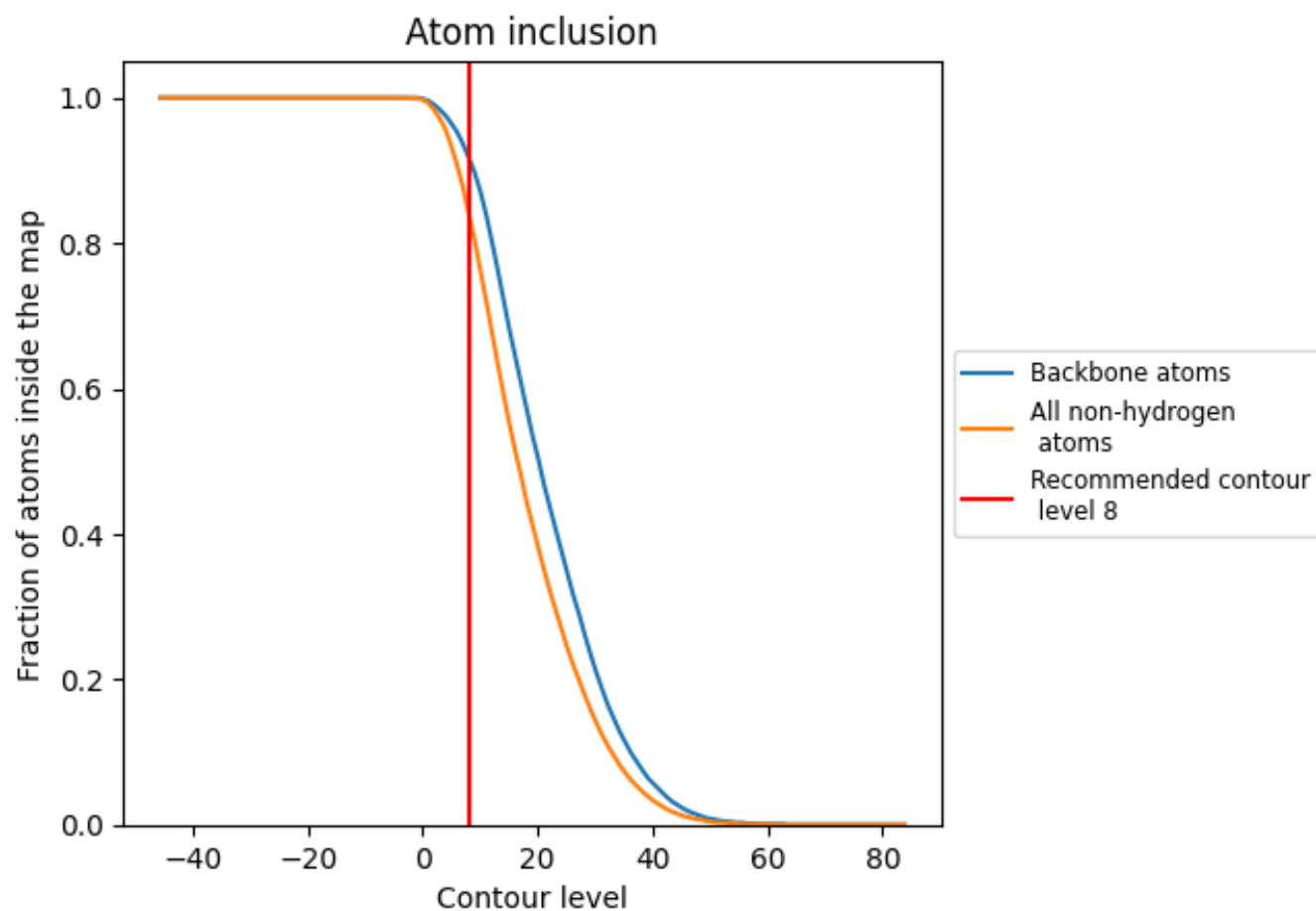
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (8).











































9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 84% 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 (8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8420	 0.4430
A	 0.9170	 0.5270
B	 0.9110	 0.5300
C	 0.9270	 0.5360
D	 0.8710	 0.3780
E	 0.9270	 0.4370
F	 0.7650	 0.3540
G	 0.1550	 0.1860
H	 0.2380	 0.1630
I	 0.9490	 0.4200
J	 0.9630	 0.4860
K	 0.9700	 0.4230
L	 0.9500	 0.4840
M	 0.8760	 0.4300
a	 0.8780	 0.5000
b	 0.8570	 0.4960
c	 0.9330	 0.5270
d	 0.8750	 0.4070
e	 0.9250	 0.4690
f	 0.8520	 0.3730
m	 0.7520	 0.3110

