



## Full wwPDB EM Validation Report ⓘ

Dec 8, 2025 – 12:22 PM JST

PDB ID : 9KJY / pdb\_00009kjy  
EMDB ID : EMD-62379  
Title : Cryo-EM structure of the Retron-Eco7 complex (state 2)  
Authors : Ishikawa, J.; Yoneyama, K.; Yamashita, K.; Nishimasu, H.  
Deposited on : 2024-11-12  
Resolution : 2.61 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](mailto: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>.

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

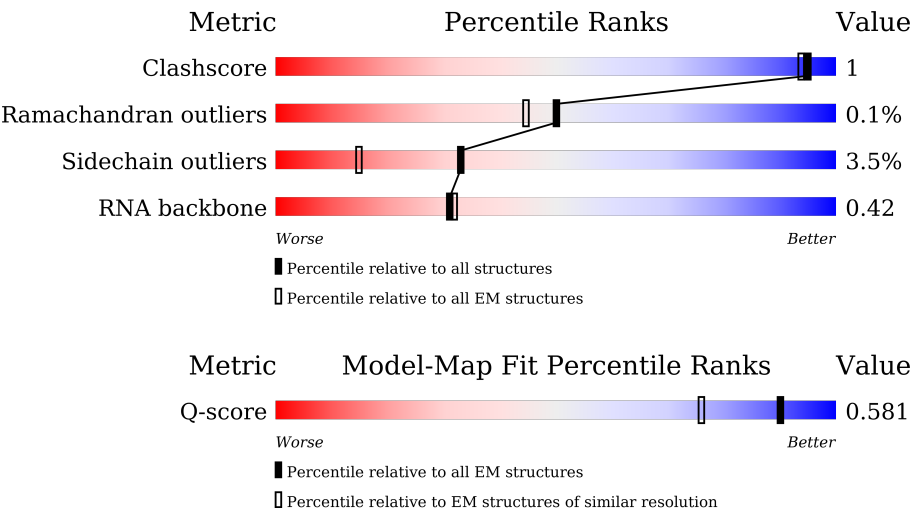
EMDB validation analysis : 0.0.1.dev129  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.47

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.61 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
RNA backbone	6643	2191	-
Q-score	-	25397	8735 ( 2.11 - 3.11 )

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  $\geq 3$ , 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	322	<div><div></div><div>91%</div><div>9%</div><div>0%</div><div>0%</div><div>0%</div></div>
2	B	550	<div><div></div><div>88%</div><div>7%</div><div>0%</div><div>0%</div><div>5%</div></div>
2	C	550	<div><div></div><div>89%</div><div>8%</div><div>0%</div><div>0%</div><div>5%</div></div>

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Mol	Chain	Length	Quality of chain
2	D	550	<div><div><div></div><div></div><div></div></div><div>9%89%8%</div><div></div></div>
2	E	550	<div><div><div></div><div></div><div></div></div><div>9%85%7%8%</div><div></div></div>
3	F	266	<div><div><div></div><div></div><div></div></div><div>5%75%••21%</div><div></div></div>
3	G	266	<div><div><div></div><div></div><div></div></div><div>11%75%•21%</div><div></div></div>
4	H	146	<div><div><div></div><div></div><div></div></div><div>•19%5%•72%</div><div></div></div>
5	I	77	<div><div><div></div><div></div><div></div></div><div>•84%10%5%</div><div></div></div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 25275 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called RNA-directed DNA polymerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	308	Total	C	N	O	S	0	0
			2473	1588	434	442	9		

- Molecule 2 is a protein called AAA family ATPase.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	528	Total	C	N	O	S	1	0
			4245	2672	746	814	13		
2	C	535	Total	C	N	O	S	1	0
			4290	2699	754	824	13		
2	D	535	Total	C	N	O	S	3	0
			4309	2713	760	823	13		
2	E	508	Total	C	N	O	S	3	0
			4102	2590	717	783	12		

- Molecule 3 is a protein called TIGR02646 family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	210	Total	C	N	O	S	0	0
			1701	1074	292	324	11		
3	G	210	Total	C	N	O	S	0	0
			1701	1074	292	324	11		

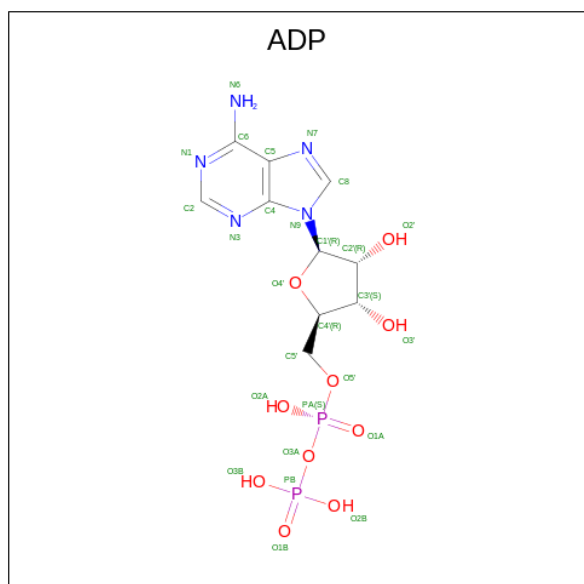
- Molecule 4 is a RNA chain called msrRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	41	Total	C	N	O	P	0	0
			869	389	149	290	41		

- Molecule 5 is a DNA chain called msdDNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	73	Total	C	N	O	P	0	0
			1501	711	285	432	73		

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
6	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
6	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
6	E	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
7	F	1	Total	Zn	0
			1	1	
7	G	1	Total	Zn	0
			1	1	


- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

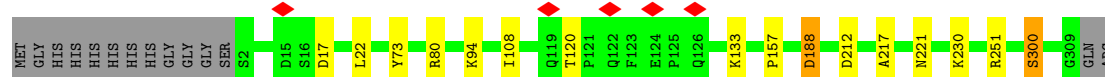
Mol	Chain	Residues	Atoms		AltConf
8	H	1	Total	Mg	0
			1	1	

### 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.

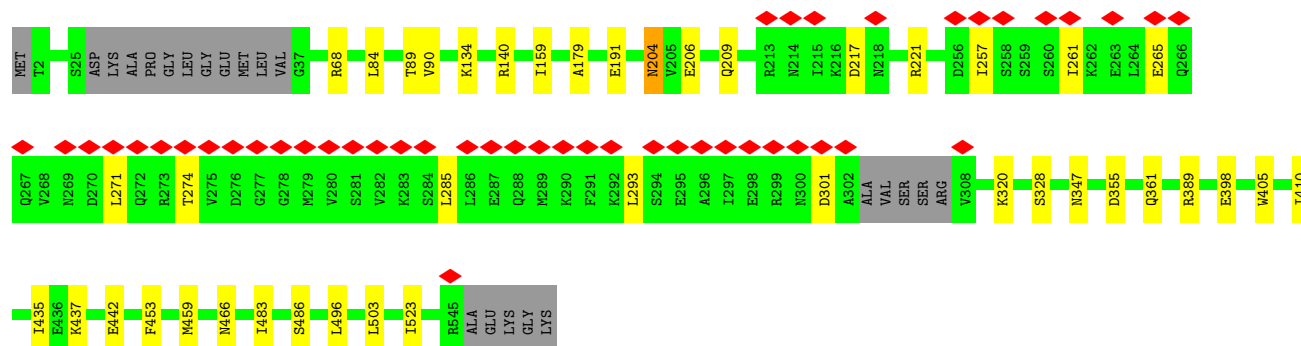
- Molecule 1: RNA-directed DNA polymerase

Chain A:  91%




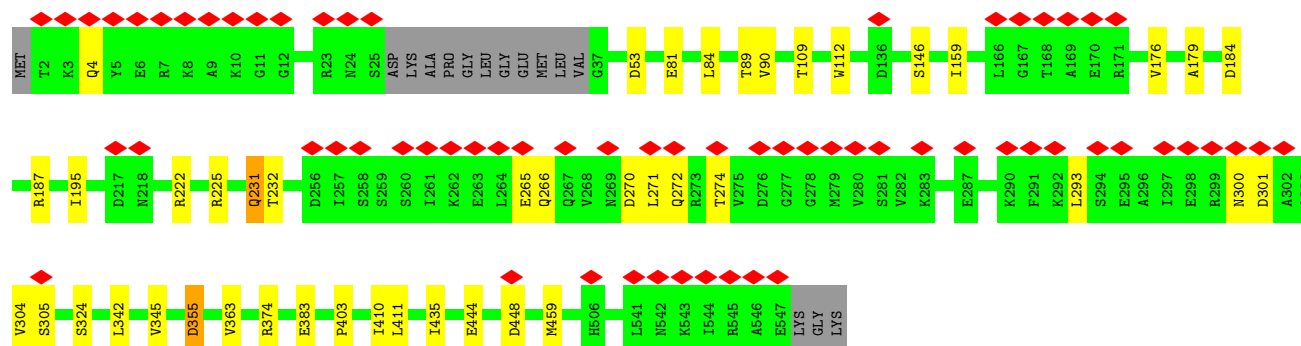
- Molecule 2: AAA family ATPase

Chain B:  9% 88% 7%



- Molecule 2: AAA family ATPase

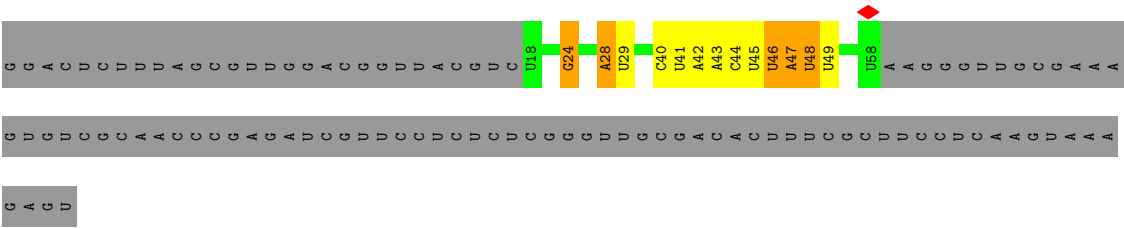
Chain C:  12% 89% 8%



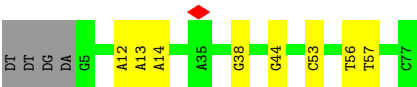
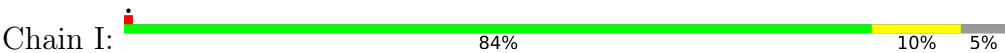




● Molecule 4: msrRNA



● Molecule 5: msdDNA



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	125298	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	49.7	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.275	Depositor
Minimum map value	-0.746	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	398.4, 398.4, 398.4	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.996, 0.996, 0.996	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, 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	0.61	0/2526	1.14	3/3408 (0.1%)
2	B	0.64	0/4316	1.14	6/5820 (0.1%)
2	C	0.62	0/4366	1.13	6/5891 (0.1%)
2	D	0.63	0/4389	1.16	10/5922 (0.2%)
2	E	0.62	0/4175	1.12	5/5635 (0.1%)
3	F	0.69	0/1740	1.36	7/2352 (0.3%)
3	G	0.71	0/1740	1.33	5/2352 (0.2%)
4	H	0.57	0/970	1.11	6/1508 (0.4%)
5	I	0.41	0/1686	1.12	8/2600 (0.3%)
All	All	0.62	0/25908	1.17	56/35488 (0.2%)

There are no bond length outliers.

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	42	A	O3'-P-O5'	-12.21	85.68	104.00
2	B	453	PHE	CA-CB-CG	9.62	123.42	113.80
1	A	17	ASP	CA-CB-CG	8.69	121.29	112.60
4	H	47	A	O3'-P-O5'	-8.58	91.14	104.00
2	E	301	ASP	CA-CB-CG	8.06	120.66	112.60
2	C	53	ASP	CA-CB-CG	8.03	120.63	112.60
5	I	14	DA	O3'-P-O5'	-7.15	93.27	104.00
1	A	188	ASP	CA-CB-CG	7.09	119.69	112.60
5	I	44	DG	O3'-P-O5'	-7.07	93.39	104.00
2	D	444	GLU	CB-CA-C	7.00	117.93	110.65
2	E	409	VAL	N-CA-CB	6.75	119.71	110.54
2	D	268	VAL	N-CA-CB	6.62	120.51	110.58
2	E	348	ASP	CA-CB-CG	6.47	119.07	112.60
3	G	48	CYS	CB-CA-C	-6.36	98.38	109.64
2	C	355	ASP	CA-CB-CG	6.25	118.85	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	13	DA	O3'-P-O5'	-6.10	94.85	104.00
3	F	180	PHE	CA-CB-CG	6.01	119.81	113.80
2	D	414	ARG	CA-CB-CG	6.01	126.12	114.10
1	A	212	ASP	CA-CB-CG	5.90	118.50	112.60
2	E	389	ARG	CB-CA-C	-5.79	99.70	109.83
4	H	48	U	O3'-P-O5'	-5.75	95.38	104.00
2	B	68	ARG	CD-NE-CZ	5.73	132.42	124.40
2	D	185	ILE	N-CA-CB	5.71	116.85	110.51
3	G	9	ARG	CB-CA-C	5.69	116.19	109.47
3	F	9	ARG	CB-CA-C	5.64	116.25	109.31
2	B	209	GLN	CB-CA-C	-5.57	102.34	109.92
3	F	1	MET	CG-SD-CE	5.51	113.01	100.90
3	G	110	ASP	CA-CB-CG	5.49	118.09	112.60
2	B	389	ARG	CB-CA-C	-5.46	100.27	109.83
5	I	38	DG	O3'-P-O5'	-5.44	95.84	104.00
5	I	53	DC	O3'-P-O5'	-5.44	95.84	104.00
2	D	193	ASN	CA-CB-CG	5.44	118.04	112.60
5	I	12	DA	O3'-P-O5'	-5.41	95.89	104.00
2	C	374	ARG	CD-NE-CZ	5.38	131.93	124.40
2	D	217	ASP	CA-CB-CG	5.37	117.97	112.60
2	D	225	ARG	CD-NE-CZ	5.32	131.84	124.40
2	E	139	ASP	CA-CB-CG	5.31	117.91	112.60
2	D	238	ARG	NE-CZ-NH2	5.31	123.97	119.20
3	F	116	ASP	CA-CB-CG	5.30	117.90	112.60
4	H	46	U	C1'-C2'-O2'	-5.28	103.87	111.80
2	D	455	ASP	CA-CB-CG	5.27	117.87	112.60
4	H	45	U	O3'-P-O5'	-5.23	96.15	104.00
2	C	383	GLU	N-CA-CB	5.22	117.58	110.01
2	C	448	ASP	CA-CB-CG	5.20	117.80	112.60
5	I	56	DT	O3'-P-O5'	-5.18	96.23	104.00
3	G	105	ASP	CA-CB-CG	5.17	117.77	112.60
2	D	275	VAL	N-CA-CB	5.16	118.31	110.58
5	I	57	DT	O3'-P-O5'	-5.14	96.30	104.00
3	F	105	ASP	CA-CB-CG	5.13	117.73	112.60
3	G	180	PHE	CA-CB-CG	5.13	118.93	113.80
2	B	217	ASP	CA-CB-CG	5.12	117.72	112.60
3	F	191	ASP	CA-CB-CG	5.11	117.71	112.60
4	H	28	A	O3'-P-O5'	-5.05	96.42	104.00
2	C	222	ARG	CD-NE-CZ	5.05	131.47	124.40
2	B	301	ASP	CA-CB-CG	5.02	117.62	112.60
3	F	9	ARG	NE-CZ-NH2	5.01	123.71	119.20

There are no chirality outliers.

There are no planarity outliers.

## 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	2473	0	2532	4	0
2	B	4245	0	4238	12	0
2	C	4290	0	4282	12	0
2	D	4309	0	4310	10	0
2	E	4102	0	4092	11	0
3	F	1701	0	1631	0	0
3	G	1701	0	1631	0	0
4	H	869	0	438	1	0
5	I	1501	0	818	0	0
6	B	27	0	12	0	0
6	C	27	0	12	0	0
6	E	27	0	12	0	0
7	F	1	0	0	0	0
7	G	1	0	0	0	0
8	H	1	0	0	0	0
All	All	25275	0	24008	48	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 1.

All (48) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:184:ASP:OD1	2:C:187:ARG:NH1	2.24	0.68
2:E:184:ASP:OD1	2:E:187:ARG:NH1	2.22	0.65
2:E:194:THR:OG1	2:E:304:VAL:O	2.14	0.65
2:C:301:ASP:O	2:C:305:SER:N	2.32	0.61
2:D:184:ASP:OD1	2:D:187:ARG:NH1	2.30	0.61
2:E:90:VAL:HG21	2:E:435:ILE:HD13	1.82	0.60
2:C:265:GLU:HG3	2:C:293:LEU:HD11	1.85	0.58
2:B:90:VAL:HG21	2:B:435:ILE:HD13	1.84	0.58
2:C:90:VAL:HG21	2:C:435:ILE:HD13	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:265:GLU:HG3	2:B:293:LEU:HD11	1.86	0.56
2:E:200:PHE:O	2:E:232:THR:OG1	2.16	0.53
2:D:160:ARG:CZ	2:D:175:GLU:OE1	2.56	0.53
2:B:204:ASN:ND2	2:B:206:GLU:HB2	2.25	0.52
2:E:410:ILE:HD13	2:E:435:ILE:HD11	1.92	0.51
2:B:134:LYS:O	2:B:140:ARG:NH2	2.45	0.50
2:C:112:TRP:CZ3	2:C:176:VAL:HG21	2.47	0.49
2:C:195:ILE:O	2:C:225:ARG:NH2	2.34	0.49
2:C:159:ILE:CD1	2:C:179:ALA:HB2	2.43	0.49
2:D:248:TYR:OH	2:D:252:ARG:NH1	2.43	0.49
2:B:84:LEU:HD23	2:B:89:THR:HG21	1.95	0.48
2:D:402[B]:HIS:CE1	2:D:405:TRP:CD1	3.01	0.48
1:A:73:TYR:CG	1:A:157:PRO:HB3	2.49	0.47
2:B:483:ILE:O	2:B:486:SER:OG	2.30	0.47
1:A:251:ARG:NH2	4:H:24:G:O6	2.48	0.47
2:D:300:ASN:O	2:D:304:VAL:HG23	2.15	0.47
2:D:321:ALA:HB2	2:D:386:LEU:HD11	1.96	0.47
1:A:22:LEU:O	1:A:133:LYS:HD3	2.15	0.47
2:E:410:ILE:HD12	2:E:431:VAL:HG13	1.97	0.47
2:D:301:ASP:O	2:D:305:SER:N	2.40	0.46
2:E:232:THR:HG23	2:E:233:LEU:HG	1.97	0.46
2:B:257:ILE:O	2:B:261:ILE:N	2.46	0.46
2:C:300:ASN:O	2:C:304:VAL:HG23	2.15	0.45
2:B:361:GLN:HG2	2:B:405:TRP:HH2	1.82	0.45
2:D:84:LEU:HD23	2:D:89:THR:HG21	1.99	0.45
2:B:410:ILE:HG13	2:B:435:ILE:HD11	2.00	0.43
2:C:109:THR:HG21	2:C:146:SER:OG	2.19	0.43
2:C:84:LEU:HD23	2:C:89:THR:HG21	1.99	0.43
2:C:270:ASP:OD2	2:D:281:SER:OG	2.32	0.43
2:B:204:ASN:HD21	2:B:206:GLU:HB2	1.83	0.43
2:B:159:ILE:CD1	2:B:179:ALA:HB2	2.50	0.42
1:A:108:ILE:HD11	1:A:217:ALA:HB1	2.00	0.42
2:B:328:SER:HB2	2:B:347:ASN:OD1	2.20	0.41
2:D:401:LEU:HD22	2:D:405:TRP:HE3	1.85	0.41
2:E:246:TYR:OH	2:E:319:GLU:OE2	2.37	0.41
2:E:141:TYR:CD1	2:E:172:ARG:HD2	2.56	0.41
2:E:410:ILE:CD1	2:E:435:ILE:HD11	2.50	0.40
2:E:195:ILE:O	2:E:225:ARG:NH2	2.38	0.40
2:C:410:ILE:HG12	2:C:435:ILE:HD11	2.02	0.40

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	306/322 (95%)	301 (98%)	4 (1%)	1 (0%)	37	57
2	B	523/550 (95%)	511 (98%)	12 (2%)	0	100	100
2	C	532/550 (97%)	518 (97%)	13 (2%)	1 (0%)	44	65
2	D	534/550 (97%)	523 (98%)	11 (2%)	0	100	100
2	E	501/550 (91%)	493 (98%)	8 (2%)	0	100	100
3	F	208/266 (78%)	196 (94%)	12 (6%)	0	100	100
3	G	208/266 (78%)	194 (93%)	14 (7%)	0	100	100
All	All	2812/3054 (92%)	2736 (97%)	74 (3%)	2 (0%)	50	70

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	231	GLN
1	A	300	SER

### 5.3.2 Protein sidechains [i](#)

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	269/279 (96%)	262 (97%)	7 (3%)	41	66
2	B	474/489 (97%)	457 (96%)	17 (4%)	30	54
2	C	479/489 (98%)	462 (96%)	17 (4%)	31	55
2	D	482/489 (99%)	463 (96%)	19 (4%)	27	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	459/489 (94%)	442 (96%)	17 (4%)	29	53
3	F	179/216 (83%)	172 (96%)	7 (4%)	27	51
3	G	179/216 (83%)	173 (97%)	6 (3%)	32	56
All	All	2521/2667 (94%)	2431 (96%)	90 (4%)	33	54

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	ARG
1	A	94	LYS
1	A	120	THR
1	A	188	ASP
1	A	221	ASN
1	A	230	LYS
1	A	300	SER
2	B	191	GLU
2	B	204	ASN
2	B	221[A]	ARG
2	B	221[B]	ARG
2	B	271	LEU
2	B	274	THR
2	B	285	LEU
2	B	320	LYS
2	B	355	ASP
2	B	398	GLU
2	B	437	LYS
2	B	442	GLU
2	B	459	MET
2	B	466	ASN
2	B	496	LEU
2	B	503	LEU
2	B	523	ILE
2	C	4	GLN
2	C	81	GLU
2	C	231	GLN
2	C	232	THR
2	C	266	GLN
2	C	271	LEU
2	C	272	GLN
2	C	274	THR
2	C	324	SER

*Continued on next page...*



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Mol	Chain	Res	Type
2	C	342	LEU
2	C	345	VAL
2	C	355	ASP
2	C	363	VAL
2	C	403	PRO
2	C	411	LEU
2	C	444	GLU
2	C	459	MET
2	D	4	GLN
2	D	35	LEU
2	D	41	GLU
2	D	72	LYS
2	D	119	LYS
2	D	172	ARG
2	D	219	THR
2	D	225	ARG
2	D	271	LEU
2	D	274	THR
2	D	282	VAL
2	D	286	LEU
2	D	293	LEU
2	D	337	ILE
2	D	403	PRO
2	D	479	THR
2	D	496	LEU
2	D	503	LEU
2	D	540	LYS
2	E	97	LYS
2	E	159	ILE
2	E	170	GLU
2	E	204	ASN
2	E	249	LEU
2	E	263	GLU
2	E	266	GLN
2	E	271	LEU
2	E	273	ARG
2	E	275	VAL
2	E	298	GLU
2	E	320	LYS
2	E	353	THR
2	E	365	LEU
2	E	373	ARG

*Continued on next page...*

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Mol	Chain	Res	Type
2	E	444	GLU
2	E	459	MET
3	F	9	ARG
3	F	11	GLU
3	F	28	GLN
3	F	80	ASP
3	F	161	THR
3	F	169	ASN
3	F	180	PHE
3	G	11	GLU
3	G	17	ILE
3	G	63	LYS
3	G	80	ASP
3	G	161	THR
3	G	179	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	263	GLN
2	B	204	ASN
2	B	267	GLN
2	B	466	ASN
2	B	499	ASN
2	B	535	ASN
2	B	542	ASN
2	C	116	ASN
2	C	241	HIS
2	C	267	GLN
2	C	466	ASN
2	C	468	GLN
2	C	472	GLN
2	C	499	ASN
2	C	505	ASN
2	D	125	GLN
2	D	499	ASN
2	D	542	ASN
2	E	116	ASN
2	E	272	GLN
2	E	350	HIS
2	E	499	ASN
2	E	505	ASN

*Continued on next page...*

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Mol	Chain	Res	Type
3	F	54	HIS

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	H	40/146 (27%)	9 (22%)	3 (7%)

All (9) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	H	24	G
4	H	28	A
4	H	29	U
4	H	40	C
4	H	43	A
4	H	44	C
4	H	46	U
4	H	47	A
4	H	49	U

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	H	41	U
4	H	46	U
4	H	48	U

## 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 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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	$\# Z  > 2$
6	ADP	E	601	-	24,29,29	0.71	0	29,45,45	0.73	0
6	ADP	B	601	-	24,29,29	0.75	0	29,45,45	0.86	1 (3%)
6	ADP	C	601	-	24,29,29	0.63	0	29,45,45	0.86	1 (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
6	ADP	E	601	-	-	1/12/32/32	0/3/3/3
6	ADP	B	601	-	-	4/12/32/32	0/3/3/3
6	ADP	C	601	-	-	4/12/32/32	0/3/3/3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	601	ADP	C5-C6-N6	2.67	124.40	120.35
6	C	601	ADP	C5-C6-N6	2.18	123.66	120.35

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	601	ADP	O4'-C4'-C5'-O5'
6	B	601	ADP	C3'-C4'-C5'-O5'
6	C	601	ADP	PA-O3A-PB-O2B
6	E	601	ADP	PA-O3A-PB-O2B
6	B	601	ADP	PB-O3A-PA-O1A
6	B	601	ADP	PB-O3A-PA-O2A
6	C	601	ADP	C3'-C4'-C5'-O5'

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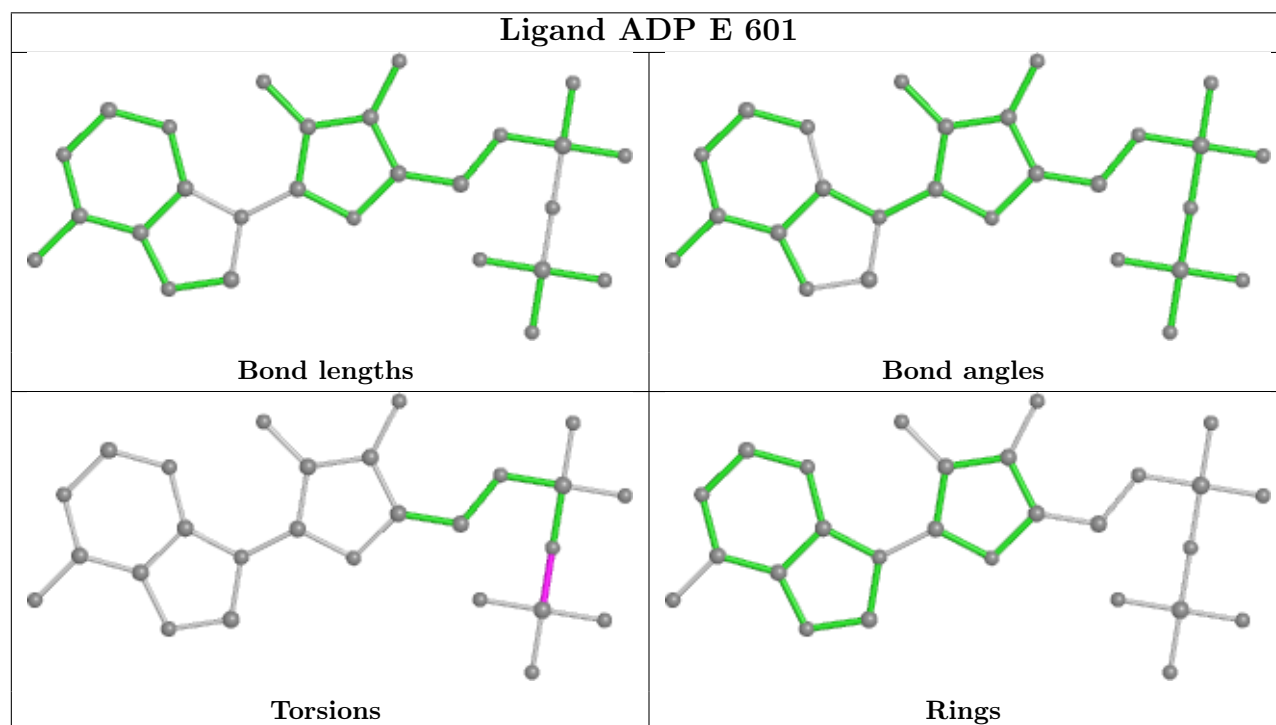
*Continued from previous page...*

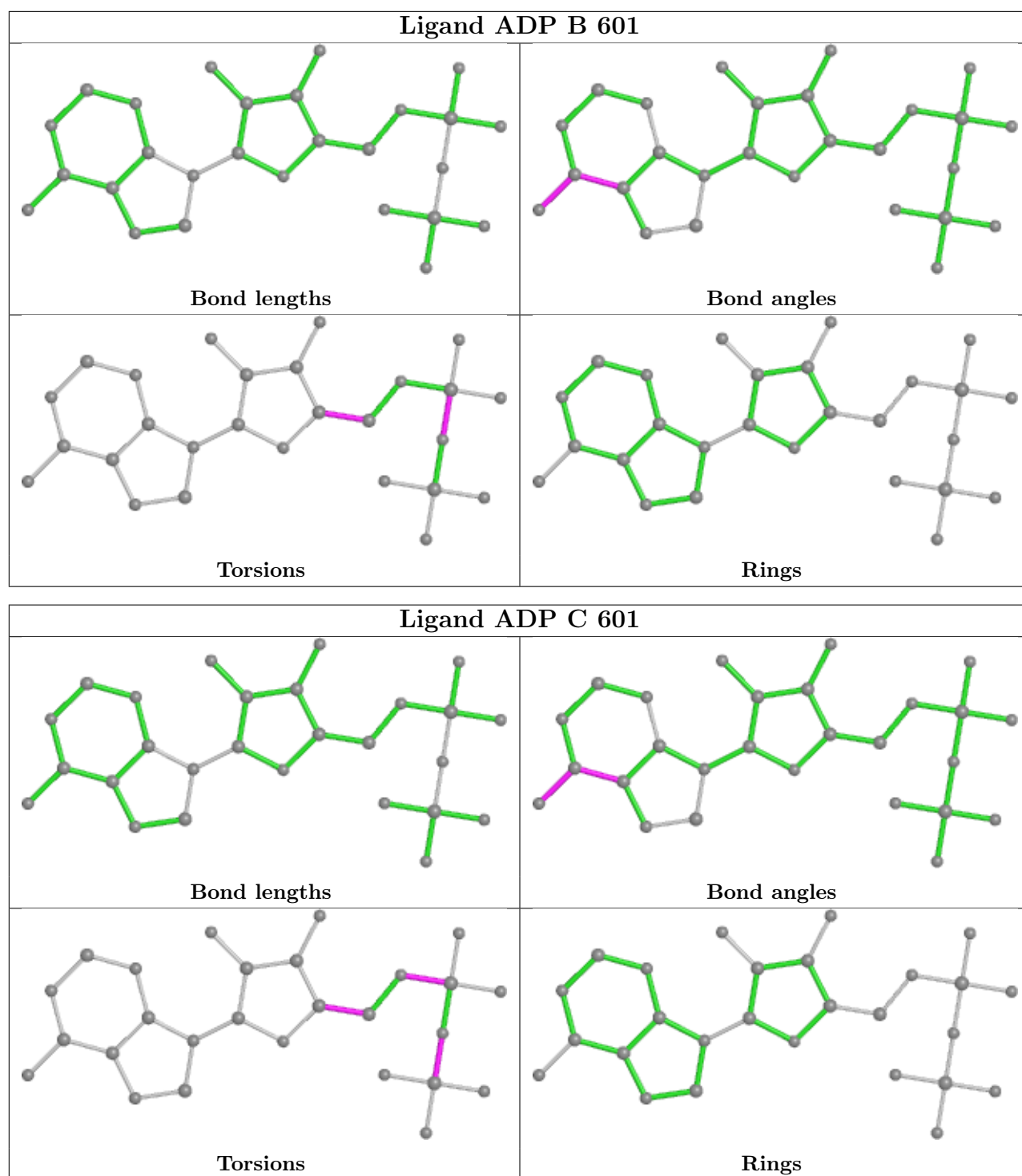
Mol	Chain	Res	Type	Atoms
6	C	601	ADP	C5'-O5'-PA-O3A
6	C	601	ADP	C5'-O5'-PA-O1A

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 ⓘ

There are no chain breaks in this entry.

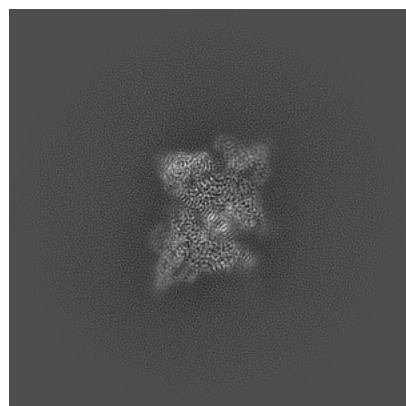
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62379. These allow visual inspection of the internal detail of the map and identification of artifacts.

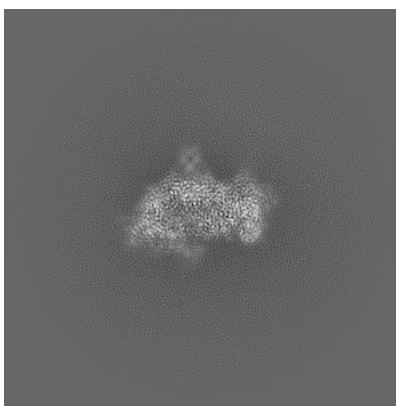
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

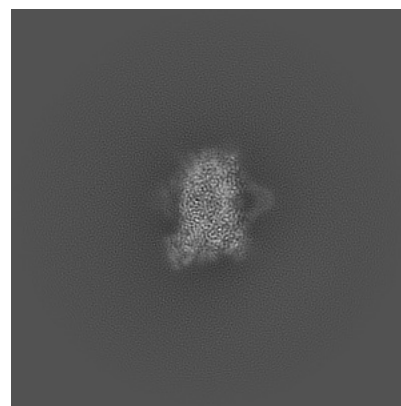
#### 6.1.1 Primary map



X

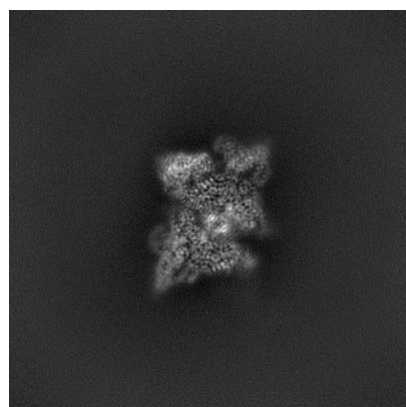


Y

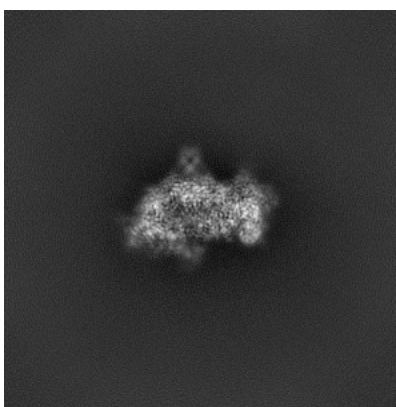


Z

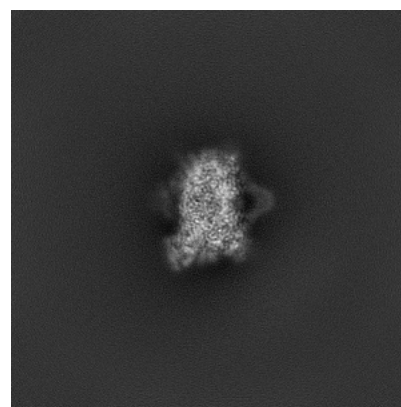
#### 6.1.2 Raw map



X



Y



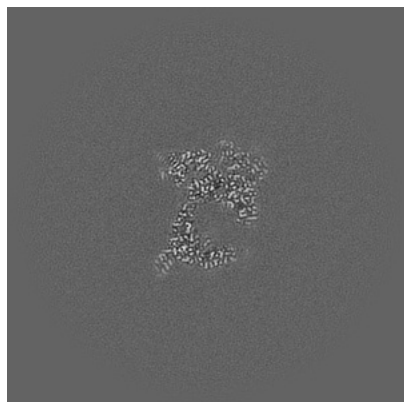
Z

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

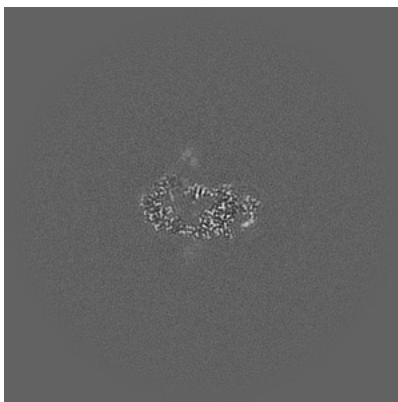


## 6.2 Central slices [i](#)

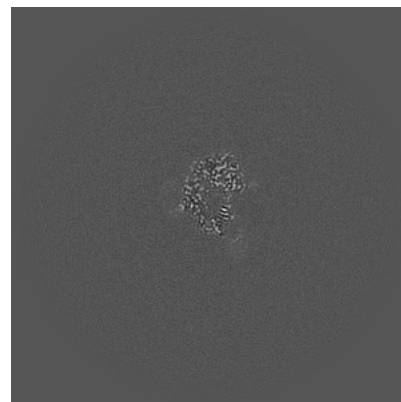
### 6.2.1 Primary map



X Index: 200

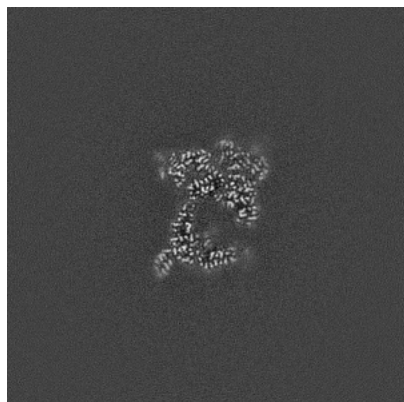


Y Index: 200

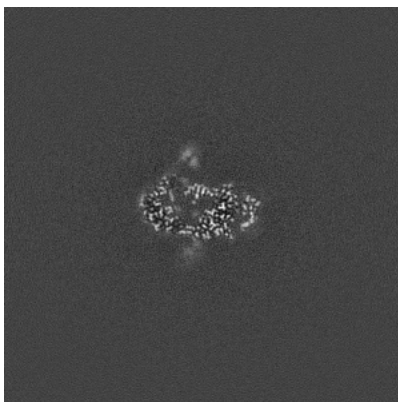


Z Index: 200

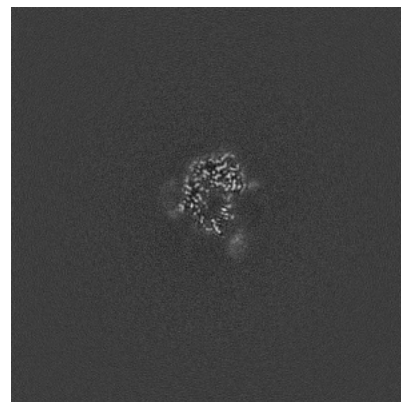
### 6.2.2 Raw map



X Index: 200



Y Index: 200

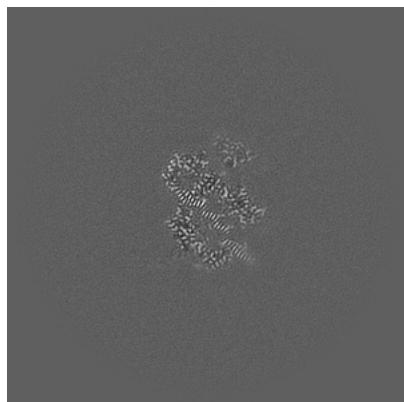


Z Index: 200

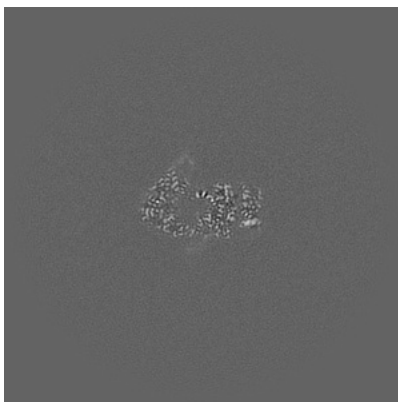
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

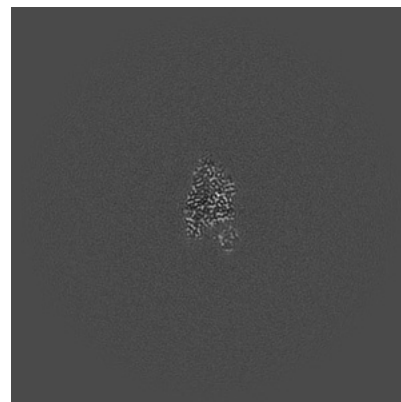
### 6.3.1 Primary map



X Index: 210

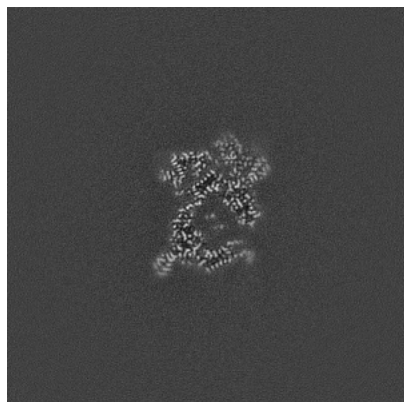


Y Index: 196

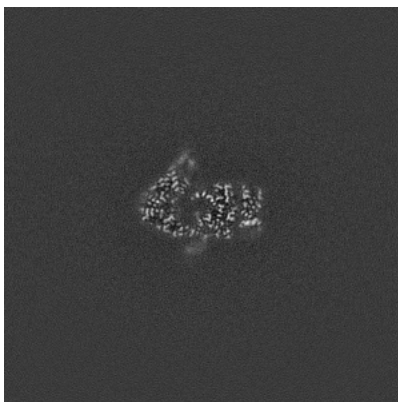


Z Index: 219

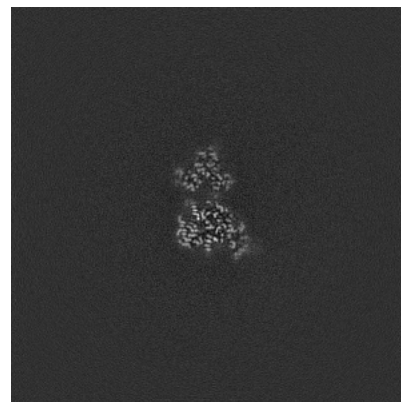
### 6.3.2 Raw map



X Index: 203



Y Index: 196

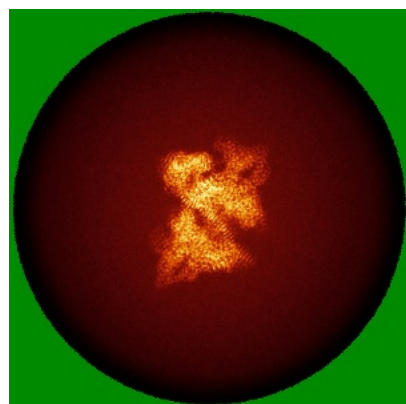


Z Index: 243

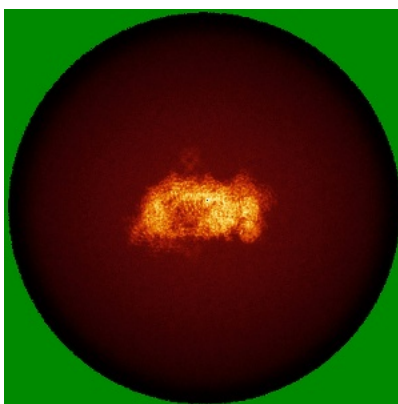
The images above show the largest variance slices of the map in three orthogonal directions.

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

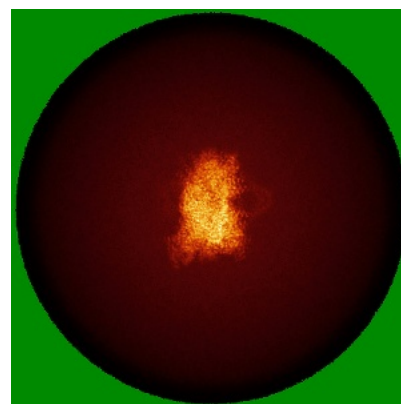
### 6.4.1 Primary map



X

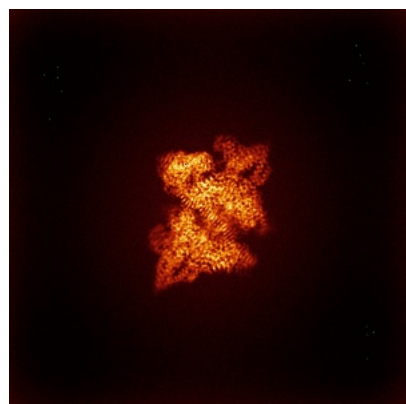


Y

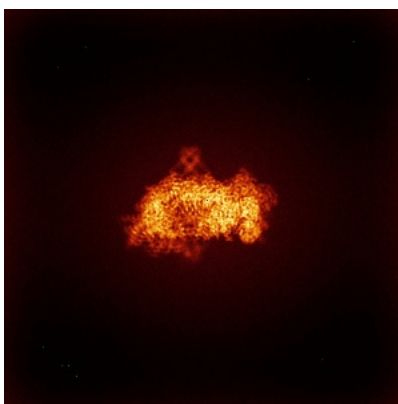


Z

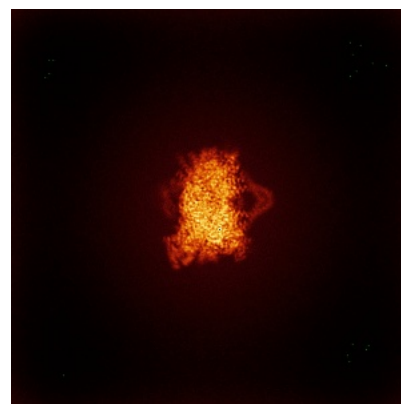
### 6.4.2 Raw map



X



Y

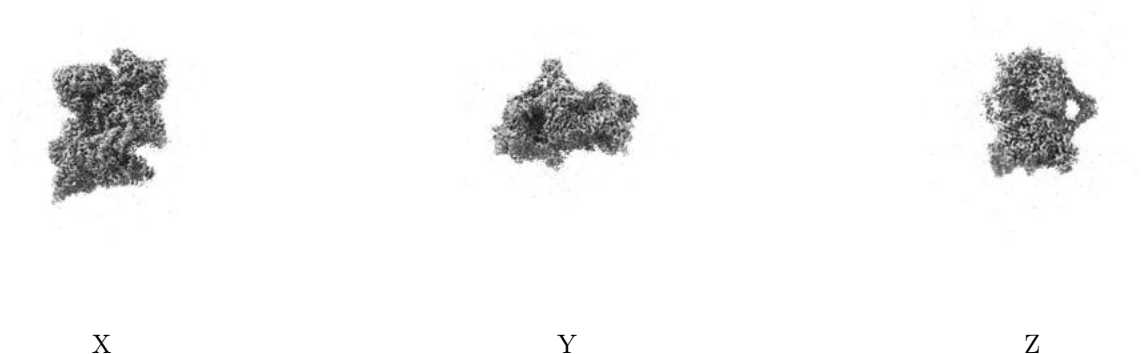


Z

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 0.1. 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.

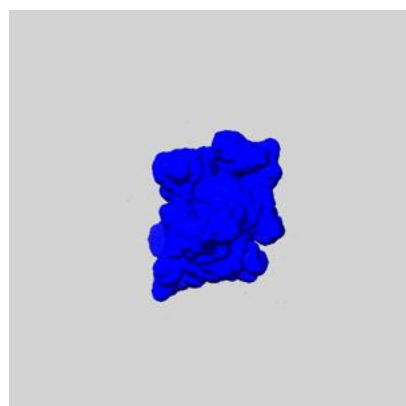
## 6.6 Mask visualisation [i](#)

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

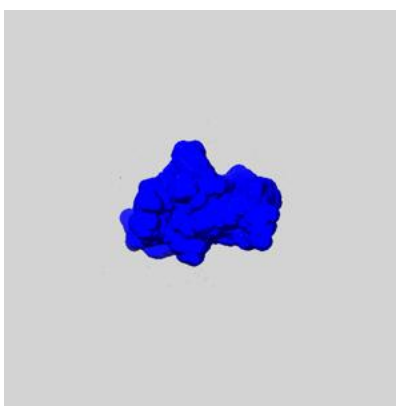
A mask typically either:

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

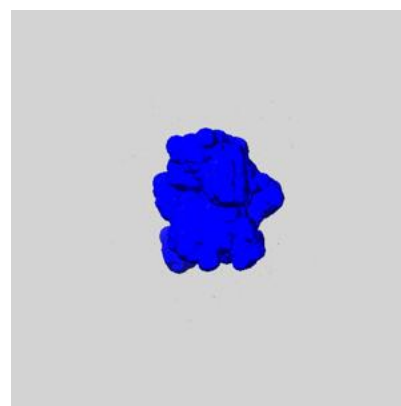
### 6.6.1 emd\_62379\_msk\_1.map [i](#)



X



Y

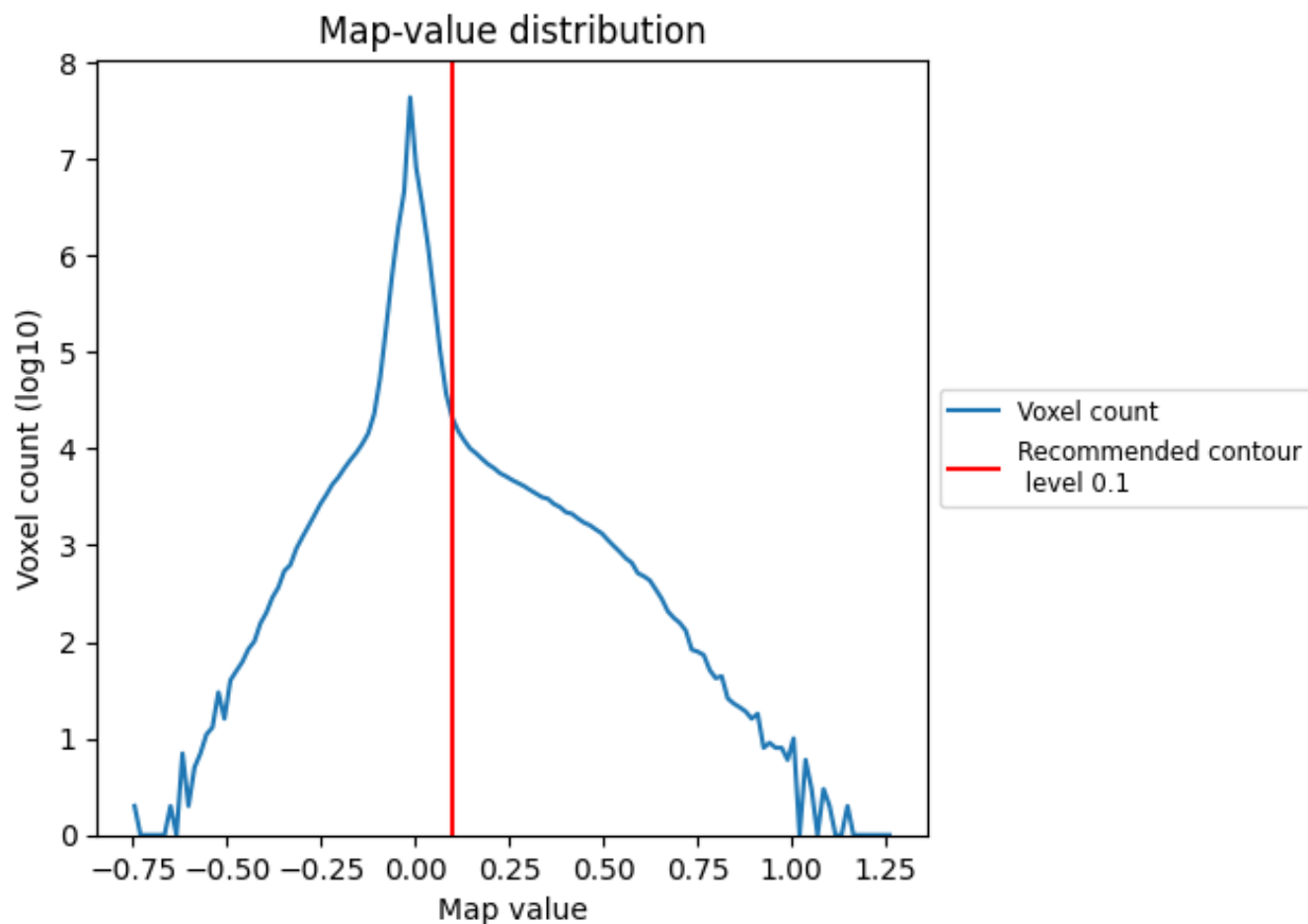


Z

## 7 Map analysis [i](#)

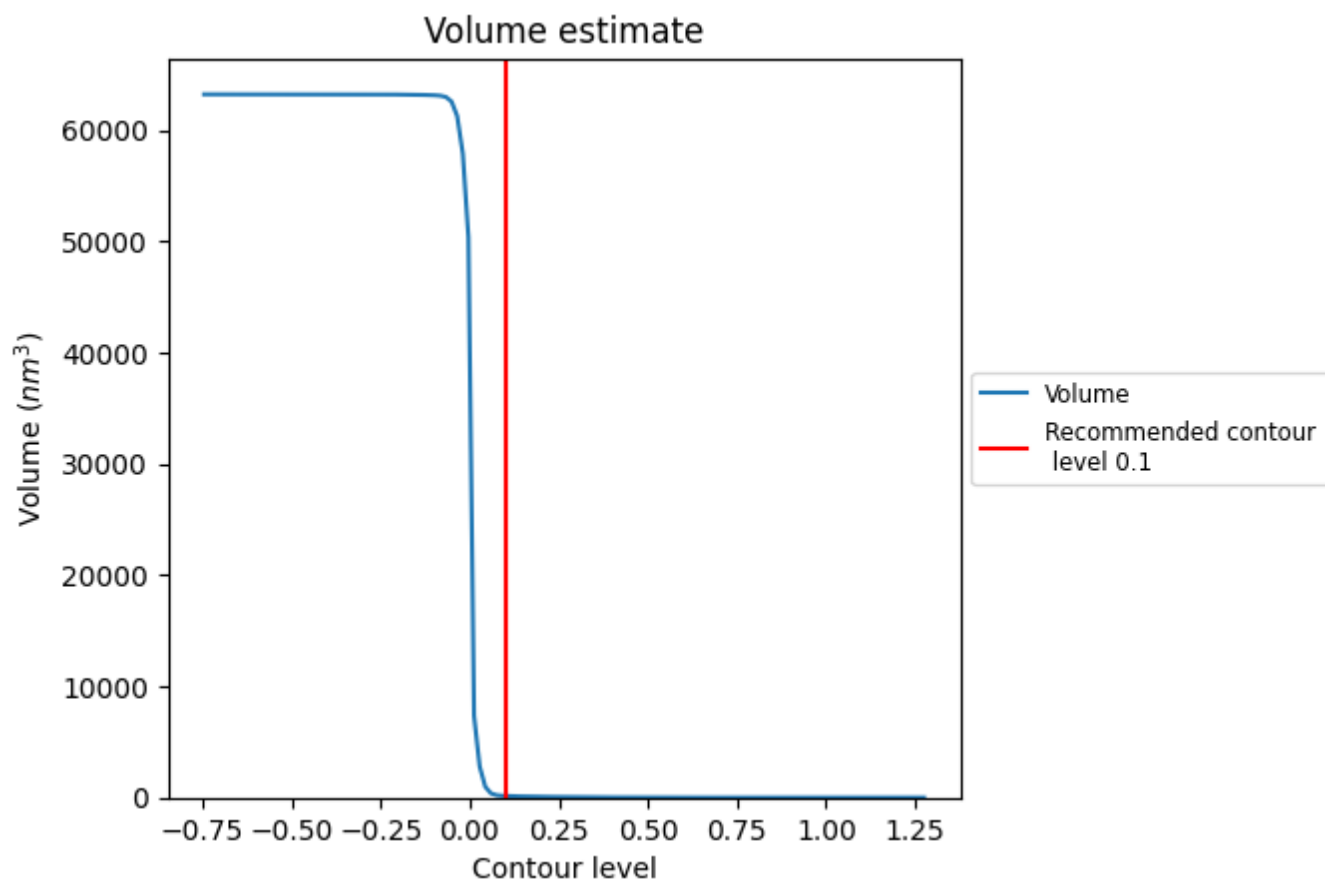
This section contains the results of statistical analysis of the map.

### 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.

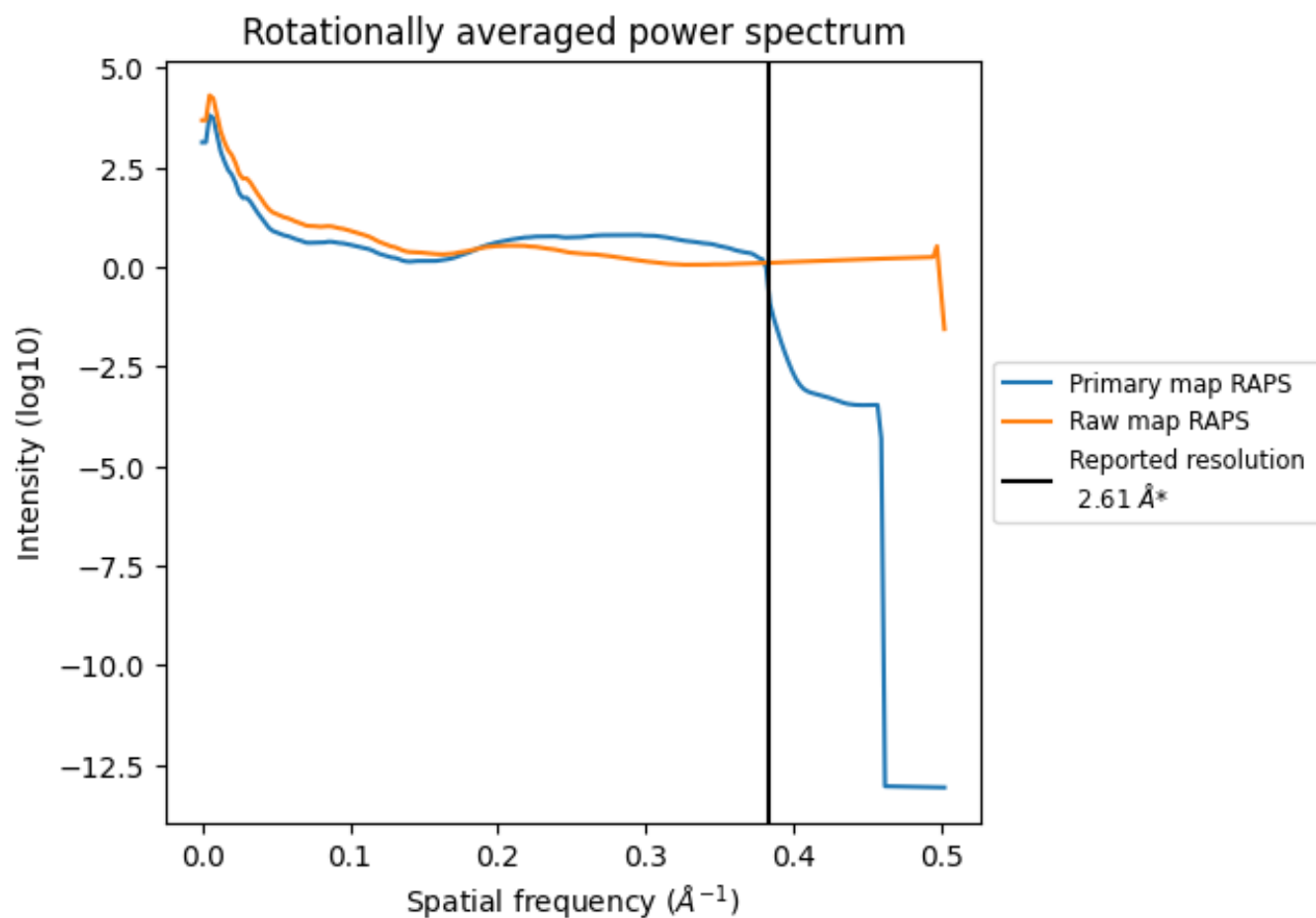
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 147 nm<sup>3</sup>; this corresponds to an approximate mass of 133 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 ⓘ



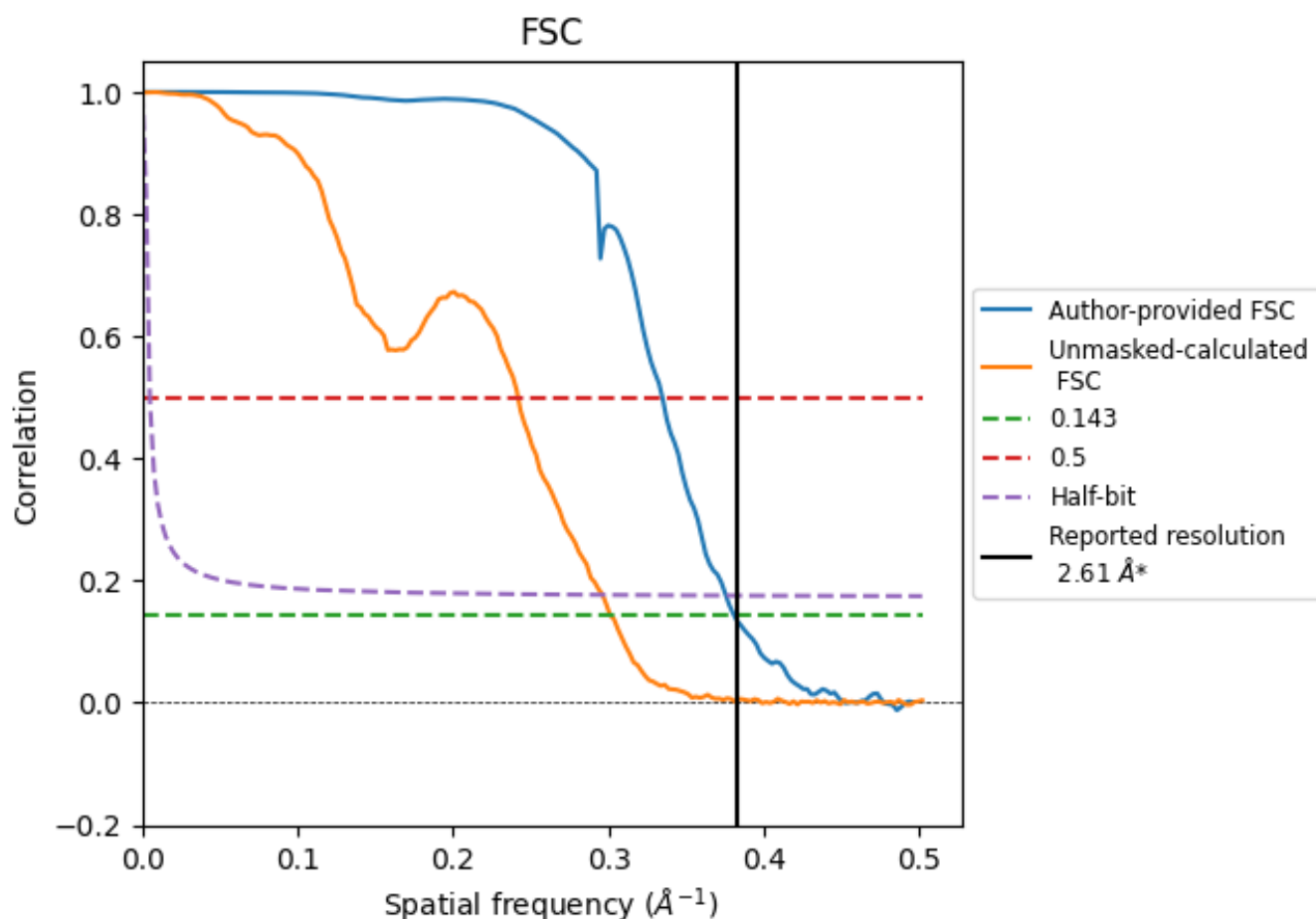
\*Reported resolution corresponds to spatial frequency of 0.383  $\text{\AA}^{-1}$



## 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 0.383  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

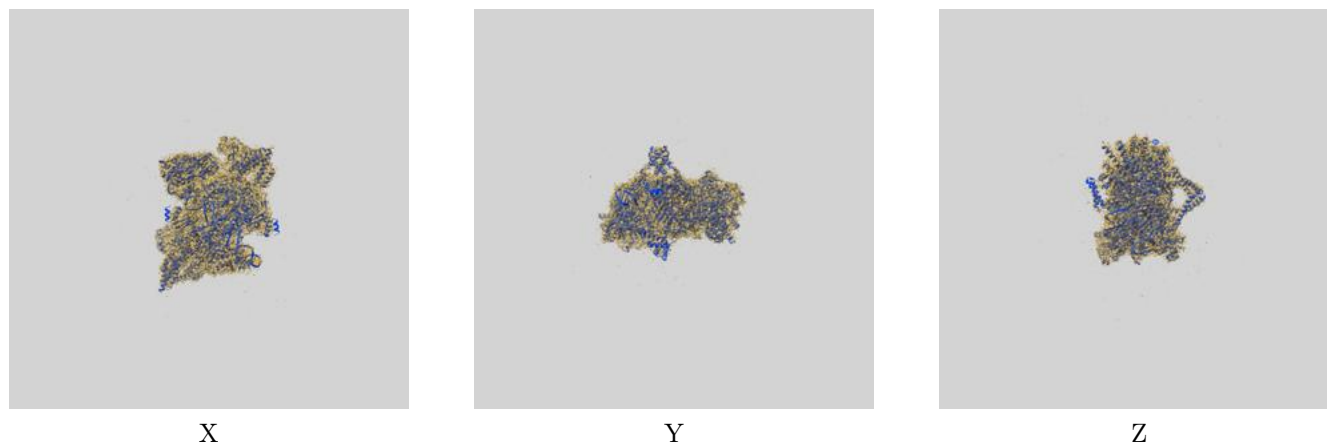
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.61	-	-
Author-provided FSC curve	2.62	2.99	2.66
Unmasked-calculated*	3.32	4.13	3.37

\*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 3.32 differs from the reported value 2.61 by more than 10 %

## 9 Map-model fit [i](#)

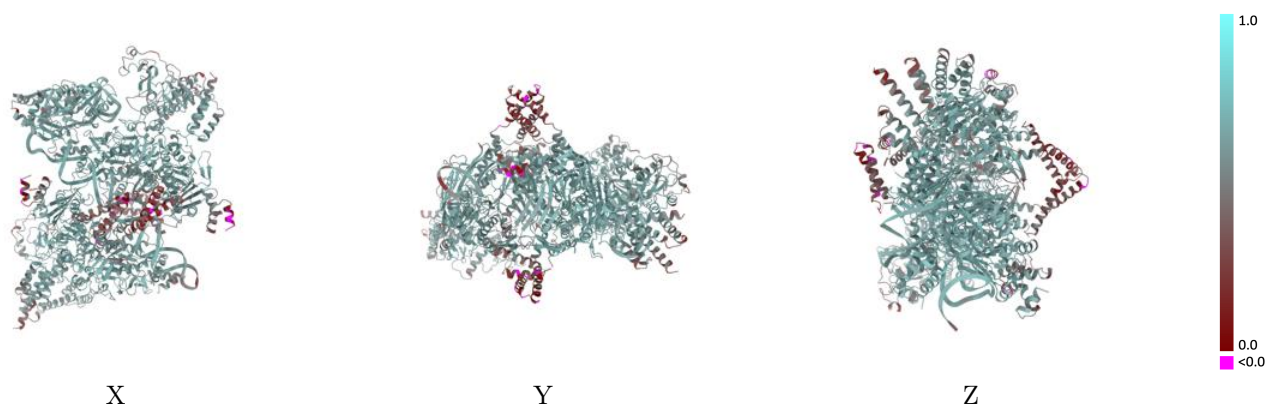
This section contains information regarding the fit between EMDB map EMD-62379 and PDB model 9KJY. Per-residue inclusion information can be found in section 3 on page 7.

### 9.1 Map-model overlay [i](#)



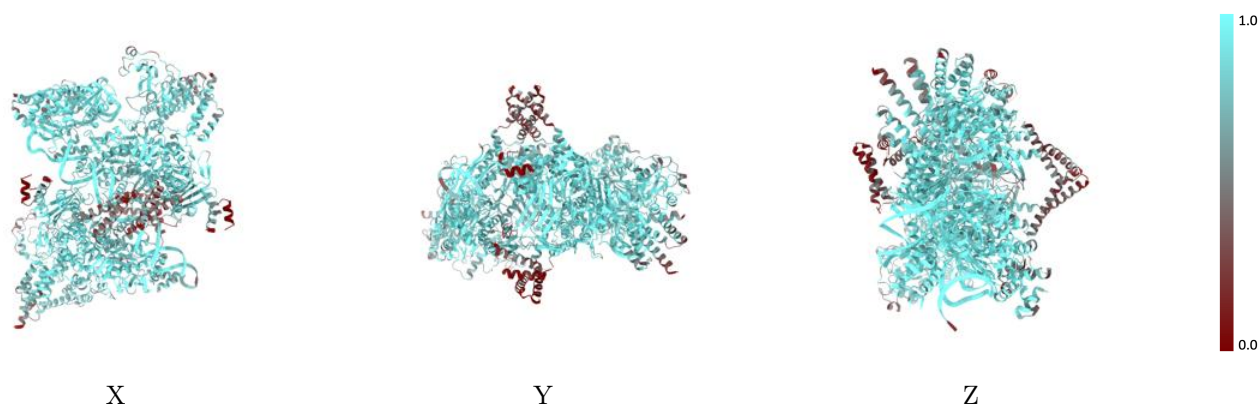
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



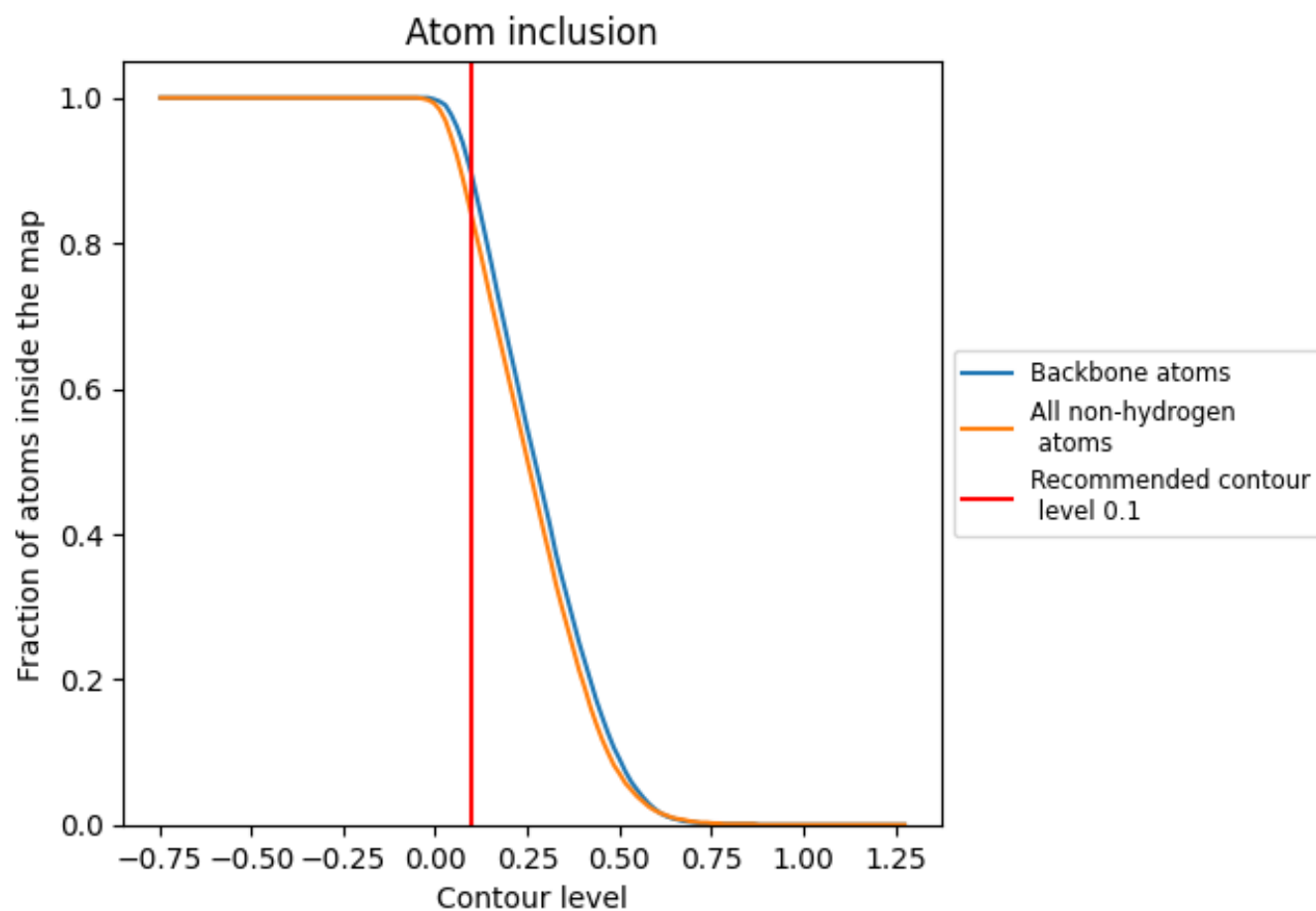
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 89% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.8360</div>	<div><div></div>0.5810</div>
A	<div><div></div>0.9090</div>	<div><div></div>0.6210</div>
B	<div><div></div>0.8550</div>	<div><div></div>0.6030</div>
C	<div><div></div>0.7860</div>	<div><div></div>0.5480</div>
D	<div><div></div>0.8220</div>	<div><div></div>0.5770</div>
E	<div><div></div>0.8270</div>	<div><div></div>0.5830</div>
F	<div><div></div>0.7920</div>	<div><div></div>0.5550</div>
G	<div><div></div>0.7430</div>	<div><div></div>0.5180</div>
H	<div><div></div>0.9620</div>	<div><div></div>0.6310</div>
I	<div><div></div>0.9520</div>	<div><div></div>0.6270</div>

1.0

0.0

<0.0