



Full wwPDB EM Validation Report ⓘ

Oct 20, 2025 – 04:09 PM EDT

PDB ID : 9DGQ / pdb_00009dgq
EMDB ID : EMD-46844
Title : Structure of dynein-1 on microtubules
Authors : Rao, Q.; Chai, P.; Zhang, K.
Deposited on : 2024-09-03
Resolution : 11.00 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:

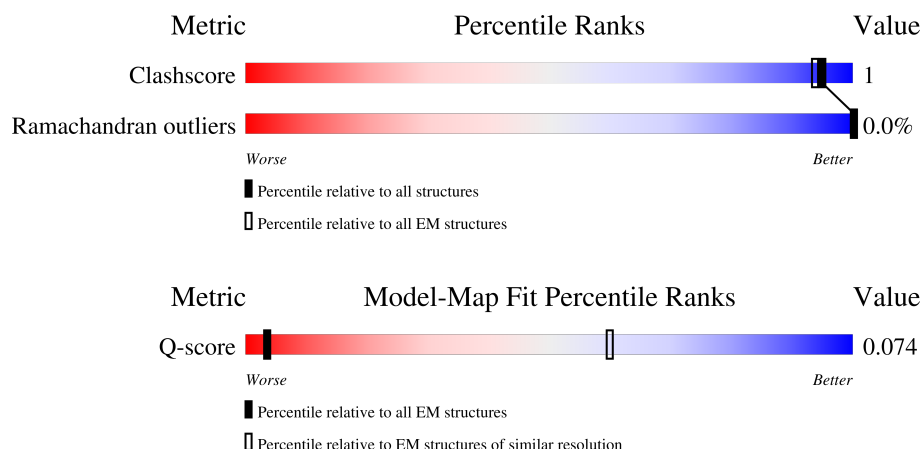
EMDB validation analysis : 0.0.1.dev129
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive 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) : 2.46

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 11.00 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Q-score	-	25397	97 (10.50 - 11.50)

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	m	4646	
1	n	4646	
2	q	492	
2	r	492	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 32970 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.

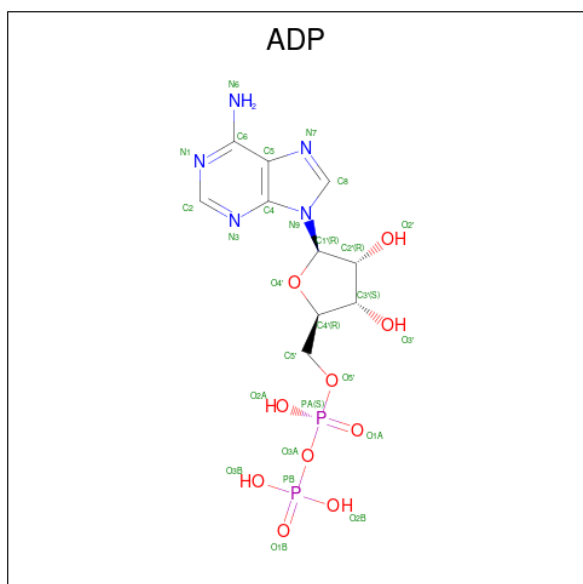
- Molecule 1 is a protein called Cytoplasmic dynein 1 heavy chain 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	m	3630	Total	C	N	O	0	0
			14572	7312	3630	3630		
1	n	3917	Total	C	N	O	0	0
			15722	7888	3917	3917		

- Molecule 2 is a protein called Dynein light intermediate chain.

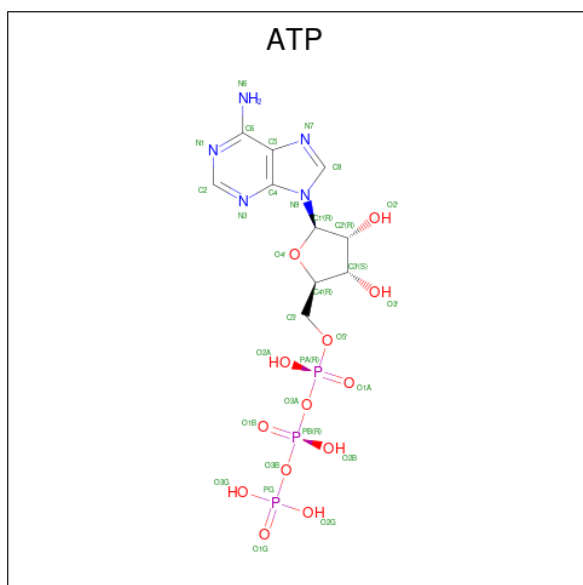
Mol	Chain	Residues	Atoms				AltConf	Trace
2	q	309	Total	C	N	O	0	0
			1241	623	309	309		
2	r	297	Total	C	N	O	0	0
			1193	599	297	297		

- Molecule 3 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
3	m	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	n	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
4	m	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	n	1	Total	C	N	O	P	0
			31	10	5	13	3	

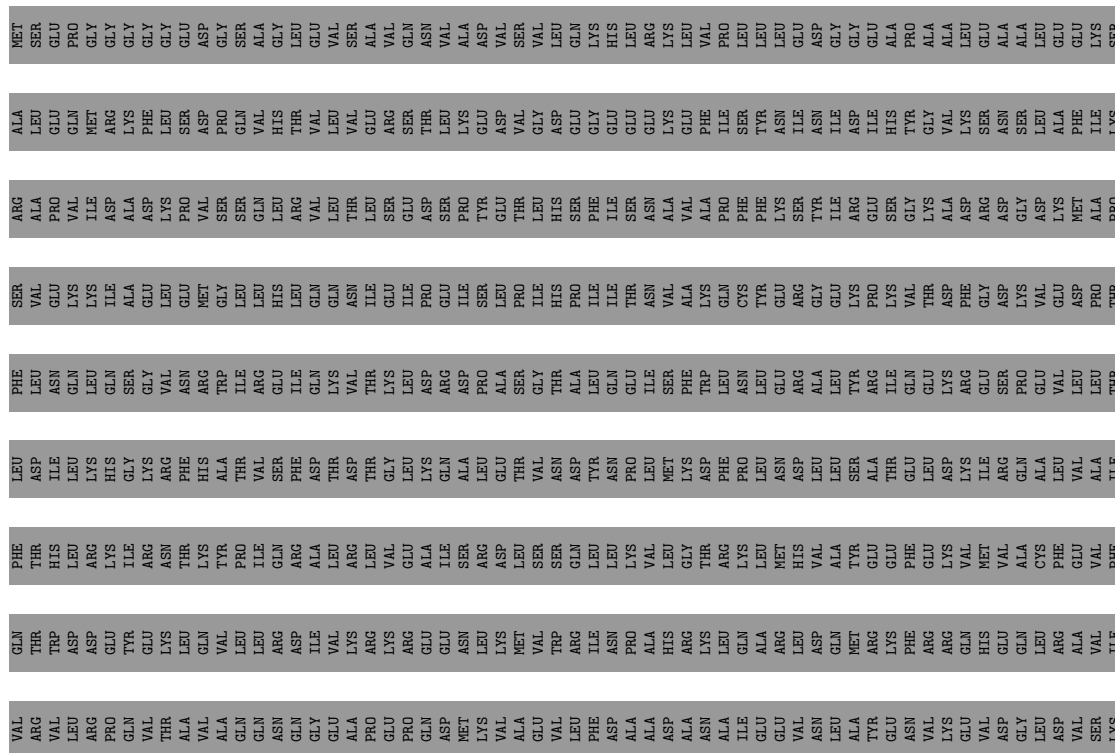
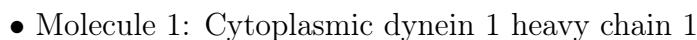
- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	m	1	Total	Mg	0
			1	1	
5	n	1	Total	Mg	0
			1	1	

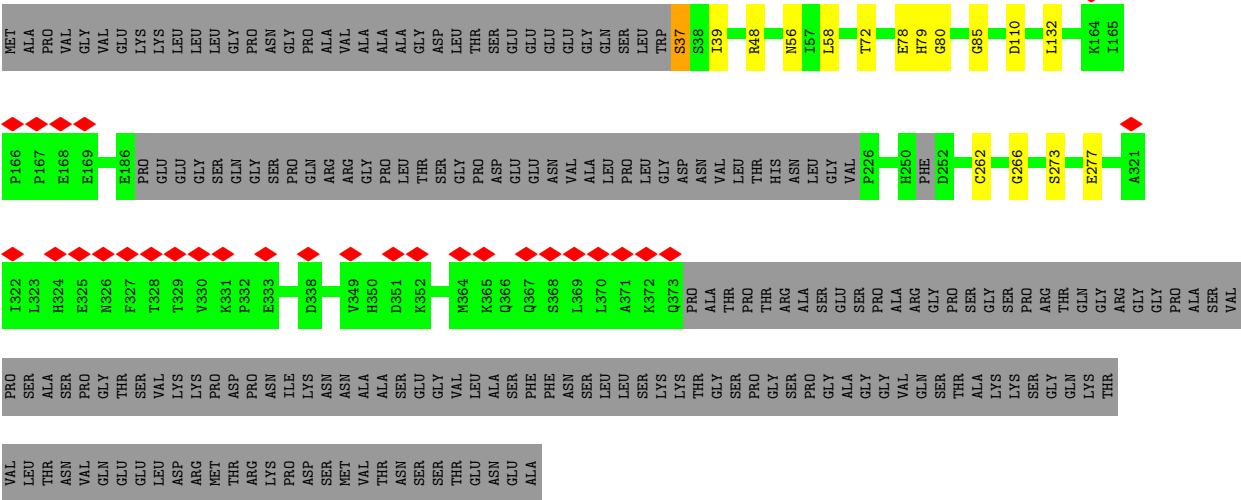
- Molecule 6 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
6	m	1	Total	C	N	O	P	0
			31	10	6	12	3	
6	m	1	Total	C	N	O	P	0
			31	10	6	12	3	
6	n	1	Total	C	N	O	P	0
			31	10	6	12	3	
6	n	1	Total	C	N	O	P	0
			31	10	6	12	3	



● Molecule 2: Dynein light intermediate chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	44792	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.661	Depositor
Minimum map value	-1.036	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.104	Depositor
Recommended contour level	0.2	Depositor
Map size (\AA)	666.624, 666.624, 666.624	wwPDB
Map dimensions	128, 128, 128	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	5.208, 5.208, 5.208	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: ATP, MG, ANP, 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	m	0.62	1/14569 (0.0%)	0.85	20/18245 (0.1%)
1	n	0.71	7/15718 (0.0%)	0.93	41/19681 (0.2%)
2	q	1.39	2/1237 (0.2%)	1.68	8/1543 (0.5%)
2	r	0.75	2/1190 (0.2%)	1.12	7/1486 (0.5%)
All	All	0.71	12/32714 (0.0%)	0.94	76/40955 (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
2	q	0	1
2	r	0	2
All	All	0	3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	n	1063	MET	C-O	8.25	1.33	1.24
1	n	1062	ASP	C-O	-8.16	1.14	1.24
2	r	79	HIS	C-N	7.91	1.38	1.33
1	n	1020	ARG	C-O	-7.26	1.14	1.24
1	n	1027	PRO	C-O	-6.35	1.16	1.24
1	n	3480	LYS	C-O	6.04	1.31	1.24
1	m	1273	PRO	C-O	5.90	1.31	1.24
2	q	353	GLU	C-O	5.59	1.30	1.24
2	q	43	VAL	C-O	-5.34	1.18	1.24
2	r	58	LEU	C-N	-5.34	1.26	1.33
1	n	3381	ILE	C-O	-5.17	1.18	1.24
1	n	1205	PRO	CA-C	5.01	1.54	1.51

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	r	79	HIS	CA-C-N	-14.02	108.88	122.20
2	r	79	HIS	C-N-CA	-14.02	108.88	122.20
1	m	1030	PRO	N-CA-C	-12.64	99.88	114.92
1	n	3407	LYS	N-CA-C	-10.61	99.72	111.07
1	m	3407	LYS	N-CA-C	-9.93	100.45	111.07
1	n	3470	ALA	N-CA-C	-9.14	100.14	111.11
1	n	1062	ASP	CA-C-N	8.97	136.56	122.74
1	n	1062	ASP	C-N-CA	8.97	136.56	122.74
1	m	3470	ALA	N-CA-C	-8.76	100.60	111.11
1	n	1027	PRO	CA-C-N	-8.14	109.39	122.66
1	n	1027	PRO	C-N-CA	-8.14	109.39	122.66
1	m	1313	SER	CA-C-O	-8.05	113.01	121.55
2	q	217	ASN	N-CA-C	-7.67	101.36	110.41
1	n	1313	SER	CA-C-O	-7.45	113.65	121.55
2	q	215	GLY	CA-C-O	-6.98	115.50	121.57
1	n	3405	MET	CA-C-O	-6.74	113.40	120.55
2	q	47	ALA	CA-C-N	6.57	130.48	120.82
2	q	47	ALA	C-N-CA	6.57	130.48	120.82
1	n	1058	GLN	N-CA-C	-6.54	105.41	113.19
1	n	3346	ASN	N-CA-C	-6.36	105.01	112.89
2	r	48	ARG	N-CA-C	-6.33	100.04	109.15
1	m	3405	MET	CA-C-O	-6.29	112.99	120.10
1	n	3313	PRO	N-CA-C	6.09	118.13	110.70
1	m	1058	GLN	N-CA-C	-6.08	104.98	113.37
1	m	1027	PRO	N-CA-C	6.02	121.90	113.53
1	n	3405	MET	O-C-N	5.98	128.46	122.12
1	n	1281	THR	N-CA-C	-5.97	104.16	112.45
1	n	3224	ILE	CA-C-O	-5.87	114.84	120.95
1	m	3313	PRO	N-CA-C	5.87	117.86	110.70
1	m	1069	TYR	CA-C-O	-5.86	114.86	120.90
1	m	3405	MET	N-CA-C	-5.86	104.97	111.71
1	n	3394	LYS	N-CA-C	-5.85	104.91	111.28
2	r	79	HIS	O-C-N	5.81	130.72	123.28
1	m	1275	GLU	CA-C-N	-5.79	111.00	121.14
1	m	1275	GLU	C-N-CA	-5.79	111.00	121.14
2	q	183	ASP	N-CA-C	-5.78	106.56	113.21
1	n	3402	TYR	CA-C-O	-5.71	114.50	120.55
1	m	1273	PRO	CA-C-O	5.65	130.88	120.60
1	n	3431	ASN	CA-C-O	-5.60	114.61	120.55
1	m	3401	ASN	N-CA-C	-5.49	105.29	111.28
1	n	1063	MET	N-CA-C	-5.49	99.48	108.76
1	n	3407	LYS	CA-C-N	-5.47	112.95	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	n	3407	LYS	C-N-CA	-5.47	112.95	120.28
1	n	970	TYR	CA-C-N	-5.43	115.44	123.05
1	n	970	TYR	C-N-CA	-5.43	115.44	123.05
1	n	3406	LEU	CA-C-N	-5.41	113.41	120.44
1	n	3406	LEU	C-N-CA	-5.41	113.41	120.44
1	n	3401	ASN	N-CA-C	-5.40	105.39	111.28
1	n	1272	ARG	CA-C-O	-5.38	113.92	120.54
1	n	3224	ILE	O-C-N	5.37	127.08	121.87
2	q	47	ALA	CA-C-O	-5.36	115.25	121.15
1	m	3405	MET	CA-C-N	5.35	127.88	120.29
1	m	3405	MET	C-N-CA	5.35	127.88	120.29
1	m	3406	LEU	CA-C-N	-5.34	113.49	120.44
1	m	3406	LEU	C-N-CA	-5.34	113.49	120.44
1	n	1064	GLN	CA-C-N	5.33	127.68	120.38
1	n	1064	GLN	C-N-CA	5.33	127.68	120.38
1	n	3401	ASN	O-C-N	5.33	127.77	122.12
2	r	72	THR	O-C-N	5.32	127.76	122.12
1	n	3461	ILE	CA-C-O	-5.31	115.43	120.95
2	q	50	LYS	CA-C-O	-5.27	115.50	121.72
1	n	1333	TRP	N-CA-C	-5.26	106.72	112.72
1	n	3230	GLU	CA-C-O	-5.26	115.30	120.82
1	n	1028	ASP	N-CA-C	-5.25	107.41	112.97
1	n	1027	PRO	N-CA-C	5.23	120.80	113.53
2	q	217	ASN	CA-C-O	-5.23	116.31	121.02
1	n	983	TYR	N-CA-C	-5.22	105.77	111.82
2	r	78	GLU	CA-C-N	-5.21	114.67	122.39
2	r	78	GLU	C-N-CA	-5.21	114.67	122.39
1	n	3444	ILE	CA-C-O	-5.19	115.56	120.95
1	n	1113	GLN	N-CA-C	-5.14	106.70	112.87
1	m	3402	TYR	CA-C-O	-5.13	115.11	120.55
1	n	3401	ASN	CA-C-O	-5.11	115.13	120.55
1	m	3387	LEU	N-CA-C	-5.09	106.84	113.16
1	n	3461	ILE	O-C-N	5.09	126.81	121.87
1	n	3405	MET	N-CA-C	-5.05	105.78	111.28

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	q	44	SER	Mainchain
2	r	37	SER	Mainchain
2	r	80	GLY	Mainchain

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	m	14572	0	3874	12	0
1	n	15722	0	4175	20	0
2	q	1241	0	329	2	0
2	r	1193	0	315	5	0
3	m	27	0	12	0	0
3	n	27	0	12	1	0
4	m	31	0	12	0	0
4	n	31	0	12	2	0
5	m	1	0	0	0	0
5	n	1	0	0	0	0
6	m	62	0	26	2	0
6	n	62	0	26	1	0
All	All	32970	0	8793	41	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 (41) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:n:918:GLY:HA2	1:n:950:GLY:HA2	1.48	0.93
1:n:918:GLY:HA2	1:n:950:GLY:CA	2.13	0.79
2:r:85:GLY:O	2:r:110:ASP:N	2.20	0.73
1:n:918:GLY:CA	1:n:950:GLY:HA2	2.20	0.72
1:m:1057:TYR:C	1:m:1059:CYS:H	1.97	0.71
1:n:4288:VAL:N	1:n:4292:LYS:O	2.26	0.68
1:m:4288:VAL:N	1:m:4292:LYS:O	2.26	0.68
2:r:262:CYS:O	2:r:266:GLY:N	2.26	0.68
1:m:3767:ILE:O	1:m:3771:GLU:N	2.29	0.66
1:n:3767:ILE:O	1:n:3771:GLU:N	2.29	0.66
6:n:4705:ANP:O1G	6:n:4705:ANP:O2B	2.18	0.62
1:n:1909:GLY:N	3:n:4701:ADP:O1B	2.27	0.62
2:r:37:SER:C	2:r:39:ILE:N	2.55	0.62
6:m:4705:ANP:O2B	6:m:4705:ANP:O1G	2.18	0.60
1:m:1057:TYR:C	1:m:1059:CYS:N	2.60	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:r:273:SER:O	2:r:277:GLU:N	2.36	0.59
2:r:56:ASN:O	2:r:132:LEU:N	2.27	0.53
1:m:3891:LYS:O	1:m:3895:THR:N	2.41	0.52
1:n:3891:LYS:O	1:n:3895:THR:N	2.42	0.52
1:n:2228:SER:N	4:n:4702:ATP:O2B	2.43	0.52
1:n:2373:MET:O	4:n:4702:ATP:H2	1.93	0.52
2:q:55:LYS:O	2:q:105:ASN:N	2.42	0.52
1:n:4087:ALA:O	1:n:4091:GLY:N	2.43	0.51
1:n:1054:TRP:C	1:n:1056:GLN:H	2.19	0.49
1:m:4087:ALA:O	1:m:4091:GLY:N	2.43	0.49
1:m:1029:GLY:C	1:m:1031:VAL:H	2.20	0.48
1:m:2694:ARG:O	1:m:2698:GLN:N	2.48	0.47
1:n:2694:ARG:O	1:n:2698:GLN:N	2.48	0.47
1:n:4549:GLN:O	1:n:4550:SER:CB	2.64	0.46
1:m:3407:LYS:O	1:m:3408:ARG:C	2.58	0.46
1:n:1057:TYR:C	1:n:1059:CYS:H	2.23	0.46
1:m:4549:GLN:O	1:m:4550:SER:CB	2.63	0.46
1:n:1054:TRP:C	1:n:1056:GLN:N	2.73	0.45
1:n:3407:LYS:O	1:n:3408:ARG:C	2.59	0.44
1:n:3378:ASN:C	1:n:3380:GLU:H	2.27	0.42
1:n:3410:GLU:O	1:n:3411:PRO:C	2.62	0.42
1:m:3410:GLU:O	1:m:3411:PRO:C	2.64	0.41
1:n:3469:GLU:O	1:n:3470:ALA:C	2.63	0.41
2:q:46:ARG:O	2:q:47:ALA:C	2.63	0.41
1:m:2943:LYS:O	6:m:4705:ANP:O2A	2.39	0.41
1:n:1057:TYR:C	1:n:1059:CYS:N	2.79	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	m	3624/4646 (78%)	3542 (98%)	81 (2%)	1 (0%)	100	100
1	n	3909/4646 (84%)	3823 (98%)	85 (2%)	1 (0%)	100	100
2	q	301/492 (61%)	292 (97%)	9 (3%)	0	100	100
2	r	291/492 (59%)	277 (95%)	14 (5%)	0	100	100
All	All	8125/10276 (79%)	7934 (98%)	189 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	m	1309	THR
1	n	1309	THR

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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](#)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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
4	ATP	n	4702	5	28,33,33	0.94	2 (7%)	34,52,52	0.96	1 (2%)
4	ATP	m	4702	5	28,33,33	0.92	2 (7%)	34,52,52	0.96	1 (2%)
6	ANP	m	4704	-	29,33,33	1.11	4 (13%)	31,52,52	0.92	1 (3%)
6	ANP	m	4705	-	29,33,33	1.12	4 (13%)	31,52,52	0.91	1 (3%)
3	ADP	n	4701	-	24,29,29	0.91	0	29,45,45	1.31	3 (10%)
6	ANP	n	4705	-	29,33,33	1.13	4 (13%)	31,52,52	0.91	1 (3%)
3	ADP	m	4701	-	24,29,29	0.91	0	29,45,45	1.32	3 (10%)
6	ANP	n	4704	-	29,33,33	1.11	4 (13%)	31,52,52	0.91	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
4	ATP	n	4702	5	-	2/18/38/38	0/3/3/3
4	ATP	m	4702	5	-	2/18/38/38	0/3/3/3
6	ANP	m	4704	-	-	7/14/38/38	0/3/3/3
6	ANP	m	4705	-	-	5/14/38/38	0/3/3/3
3	ADP	n	4701	-	-	5/12/32/32	0/3/3/3
6	ANP	n	4705	-	-	5/14/38/38	0/3/3/3
3	ADP	m	4701	-	-	5/12/32/32	0/3/3/3
6	ANP	n	4704	-	-	7/14/38/38	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	n	4704	ANP	PB-O3A	-2.70	1.55	1.59
4	n	4702	ATP	PB-O3B	-2.58	1.56	1.59
6	m	4704	ANP	PB-O3A	-2.57	1.55	1.59
6	m	4705	ANP	PB-O3A	-2.52	1.55	1.59
6	m	4704	ANP	PG-O1G	2.50	1.50	1.46
6	n	4705	ANP	PG-O1G	2.50	1.50	1.46
4	m	4702	ATP	PB-O3B	-2.49	1.56	1.59
6	m	4705	ANP	PG-O1G	2.48	1.49	1.46
6	n	4704	ANP	PG-O1G	2.42	1.49	1.46
6	n	4705	ANP	PB-O3A	-2.41	1.56	1.59
6	m	4704	ANP	PG-N3B	2.36	1.69	1.63
6	n	4704	ANP	PG-N3B	2.34	1.69	1.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	n	4705	ANP	PB-O1B	2.28	1.49	1.46
6	n	4705	ANP	PG-N3B	2.27	1.69	1.63
6	m	4705	ANP	PB-O1B	2.24	1.49	1.46
6	m	4705	ANP	PG-N3B	2.24	1.69	1.63
4	n	4702	ATP	PA-O3A	-2.13	1.57	1.59
6	m	4704	ANP	PB-O1B	2.09	1.49	1.46
6	n	4704	ANP	PB-O1B	2.09	1.49	1.46
4	m	4702	ATP	PA-O3A	-2.02	1.57	1.59

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	m	4701	ADP	N3-C2-N1	-4.24	122.92	128.67
3	n	4701	ADP	N3-C2-N1	-4.21	122.96	128.67
3	m	4701	ADP	C4-C5-N7	-2.40	106.80	109.34
3	n	4701	ADP	C4-C5-N7	-2.34	106.87	109.34
6	m	4704	ANP	C5-C6-N6	2.33	123.86	120.31
6	n	4704	ANP	C5-C6-N6	2.30	123.81	120.31
4	m	4702	ATP	C5-C6-N6	2.29	123.80	120.31
4	n	4702	ATP	C5-C6-N6	2.26	123.76	120.31
6	n	4705	ANP	C5-C6-N6	2.23	123.70	120.31
6	m	4705	ANP	C5-C6-N6	2.18	123.63	120.31
3	m	4701	ADP	C2'-C3'-C4'	2.04	106.55	102.61
3	n	4701	ADP	C2'-C3'-C4'	2.03	106.52	102.61

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	m	4701	ADP	PA-O3A-PB-O2B
3	m	4701	ADP	C5'-O5'-PA-O2A
3	m	4701	ADP	C5'-O5'-PA-O3A
3	n	4701	ADP	PA-O3A-PB-O2B
3	n	4701	ADP	C5'-O5'-PA-O2A
3	n	4701	ADP	C5'-O5'-PA-O3A
4	m	4702	ATP	PB-O3B-PG-O2G
4	n	4702	ATP	PB-O3B-PG-O2G
6	m	4704	ANP	PG-N3B-PB-O1B
6	m	4704	ANP	PG-N3B-PB-O3A
6	m	4705	ANP	PB-N3B-PG-O1G
6	m	4705	ANP	PG-N3B-PB-O1B
6	m	4705	ANP	C5'-O5'-PA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	m	4705	ANP	C5'-O5'-PA-O3A
6	n	4704	ANP	PG-N3B-PB-O1B
6	n	4704	ANP	PG-N3B-PB-O3A
6	n	4705	ANP	PB-N3B-PG-O1G
6	n	4705	ANP	PG-N3B-PB-O1B
6	n	4705	ANP	C5'-O5'-PA-O1A
6	n	4705	ANP	C5'-O5'-PA-O3A
6	m	4704	ANP	O4'-C4'-C5'-O5'
6	n	4704	ANP	O4'-C4'-C5'-O5'
4	m	4702	ATP	PB-O3B-PG-O3G
4	n	4702	ATP	PB-O3B-PG-O3G
6	m	4704	ANP	C3'-C4'-C5'-O5'
6	n	4704	ANP	C3'-C4'-C5'-O5'
3	m	4701	ADP	C5'-O5'-PA-O1A
3	n	4701	ADP	C5'-O5'-PA-O1A
6	m	4704	ANP	C5'-O5'-PA-O1A
6	m	4704	ANP	C5'-O5'-PA-O2A
6	m	4704	ANP	C5'-O5'-PA-O3A
6	m	4705	ANP	C5'-O5'-PA-O2A
6	n	4704	ANP	C5'-O5'-PA-O1A
6	n	4704	ANP	C5'-O5'-PA-O2A
6	n	4704	ANP	C5'-O5'-PA-O3A
6	n	4705	ANP	C5'-O5'-PA-O2A
3	m	4701	ADP	PA-O3A-PB-O1B
3	n	4701	ADP	PA-O3A-PB-O1B

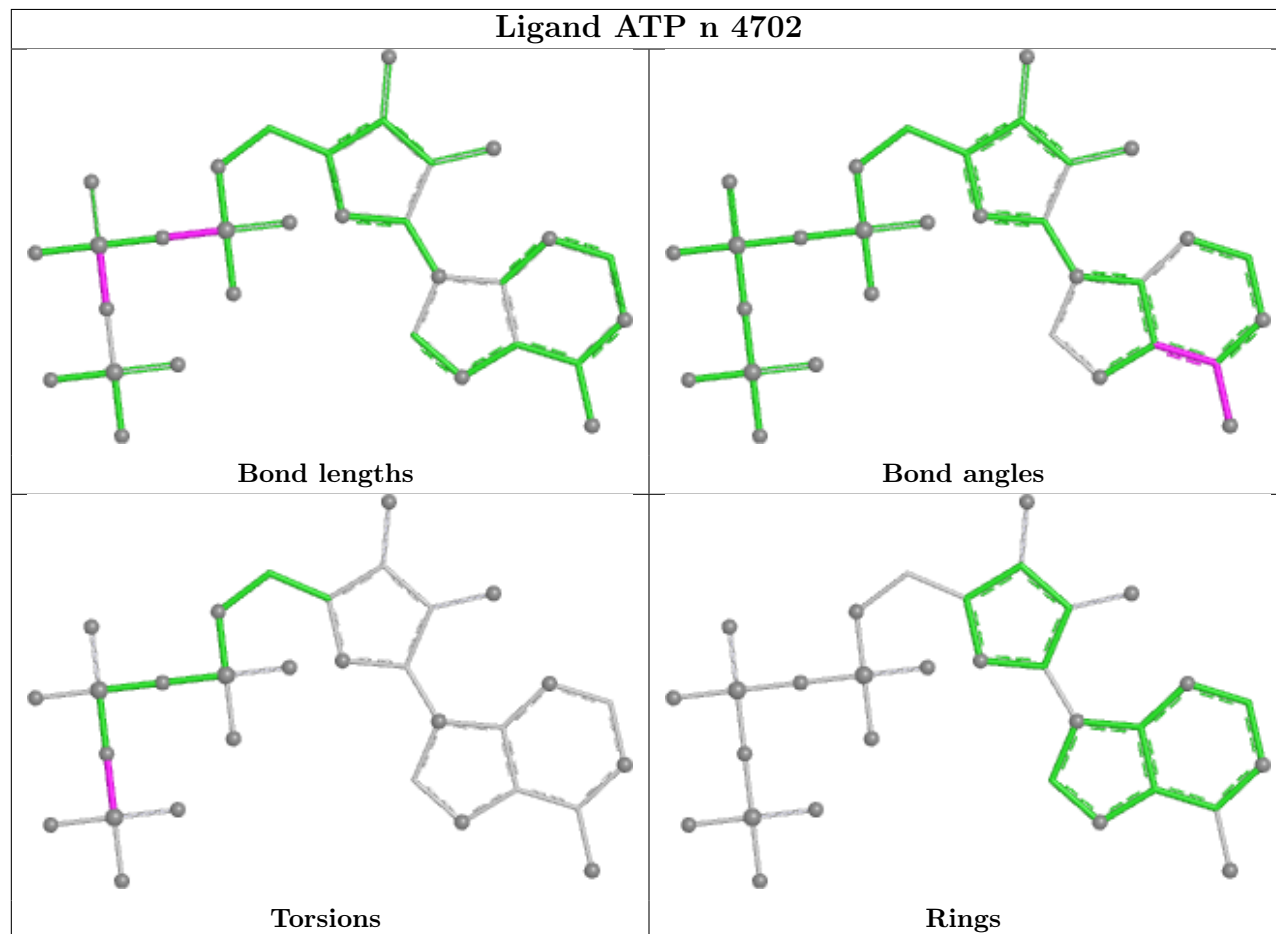
There are no ring outliers.

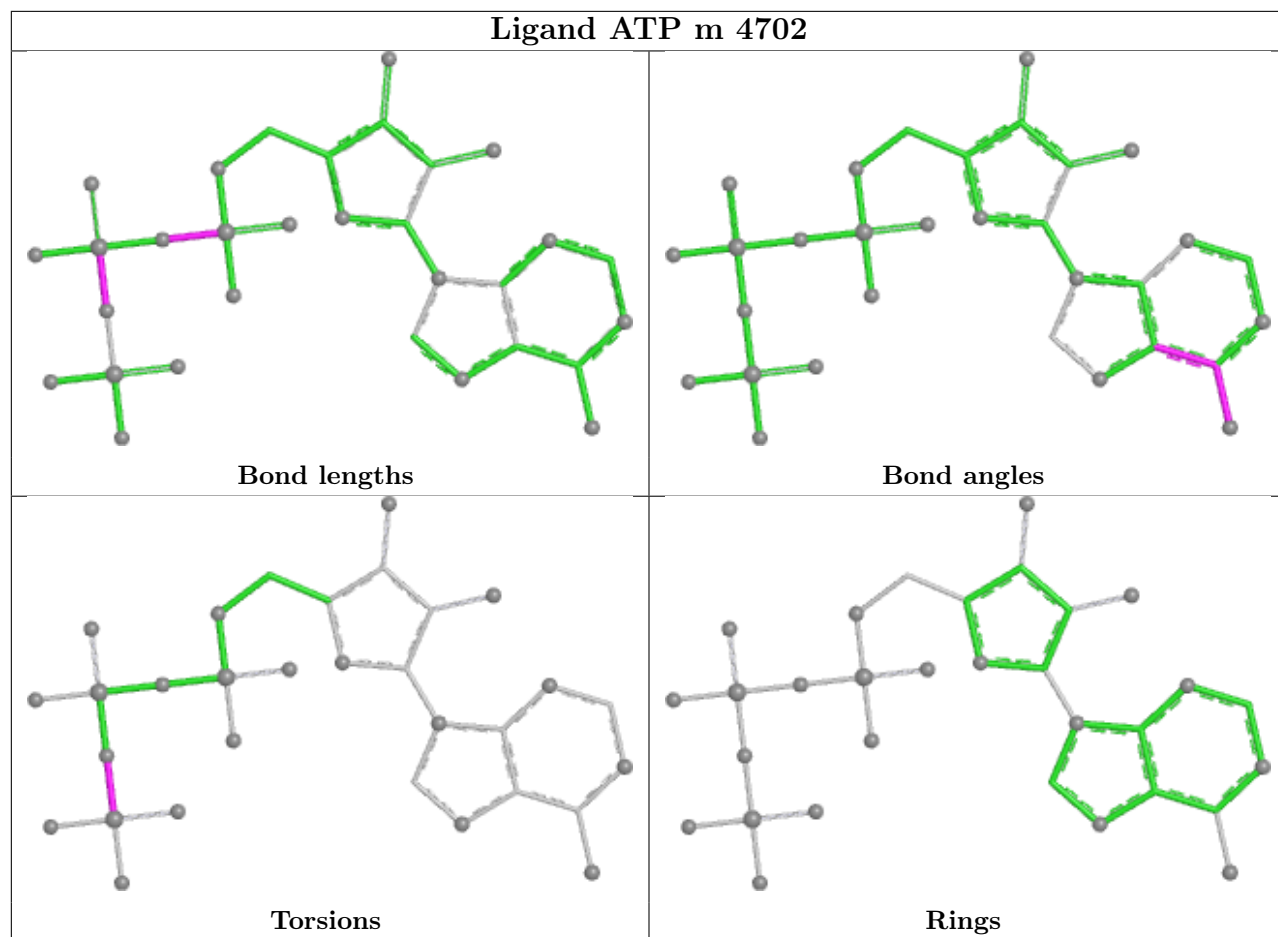
4 monomers are involved in 6 short contacts:

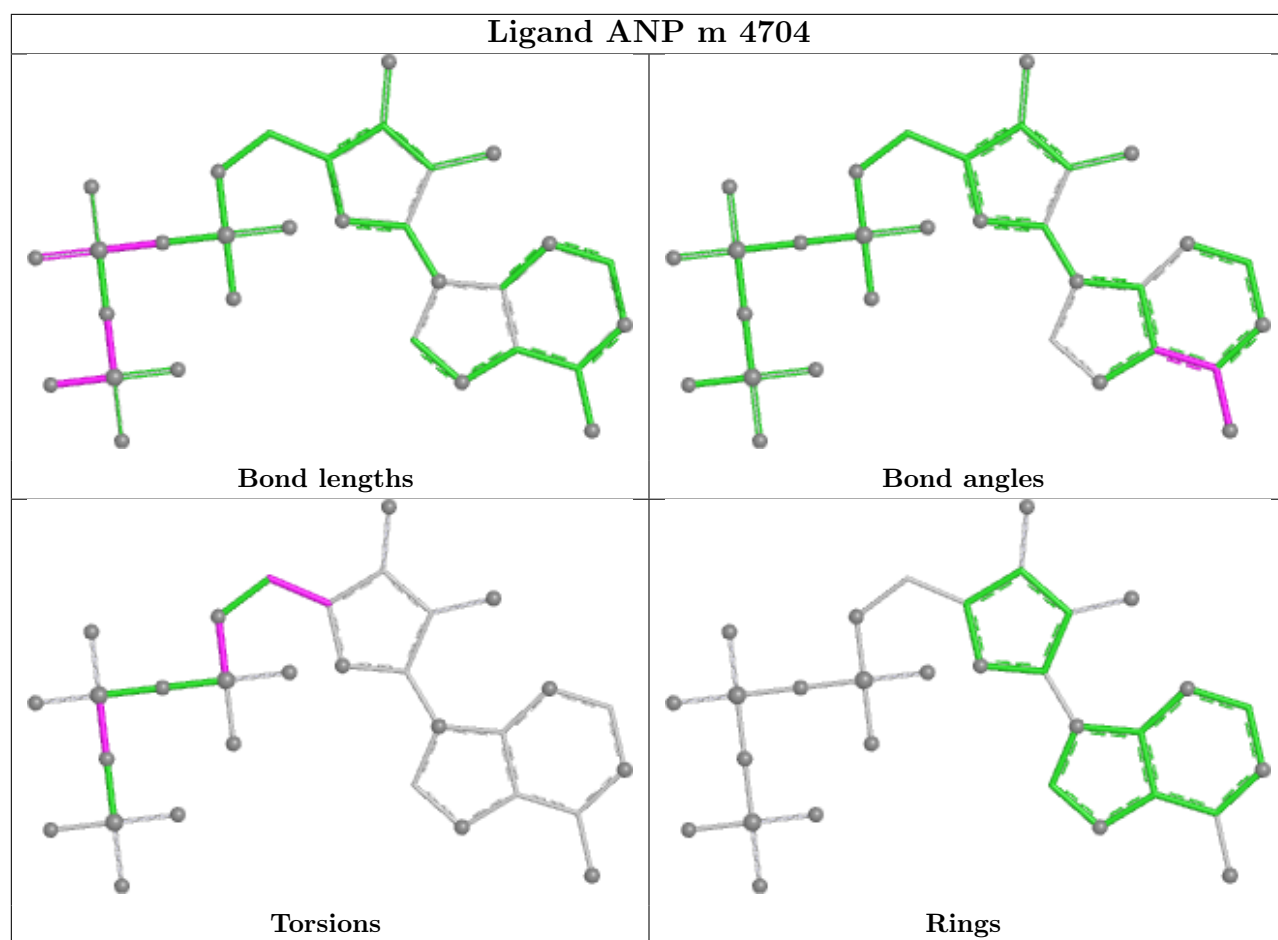
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	n	4702	ATP	2	0
6	m	4705	ANP	2	0
3	n	4701	ADP	1	0
6	n	4705	ANP	1	0

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

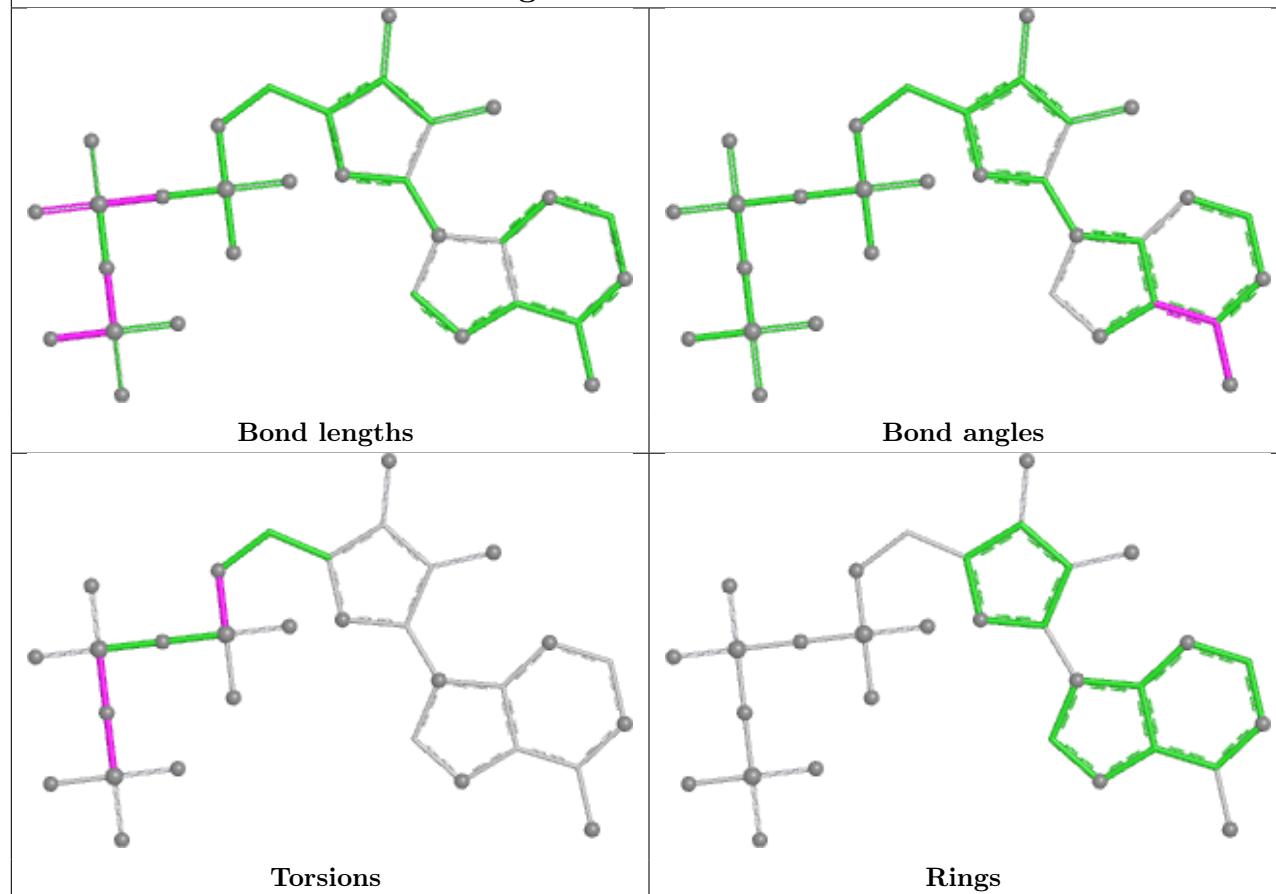
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



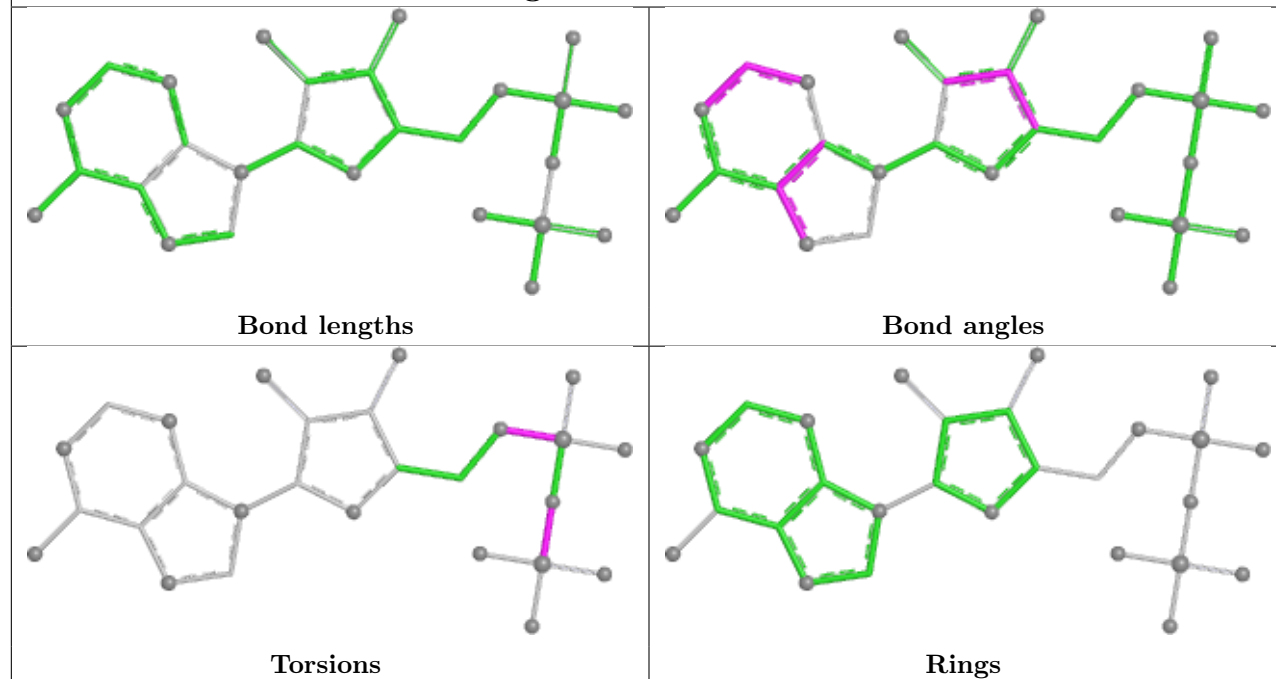


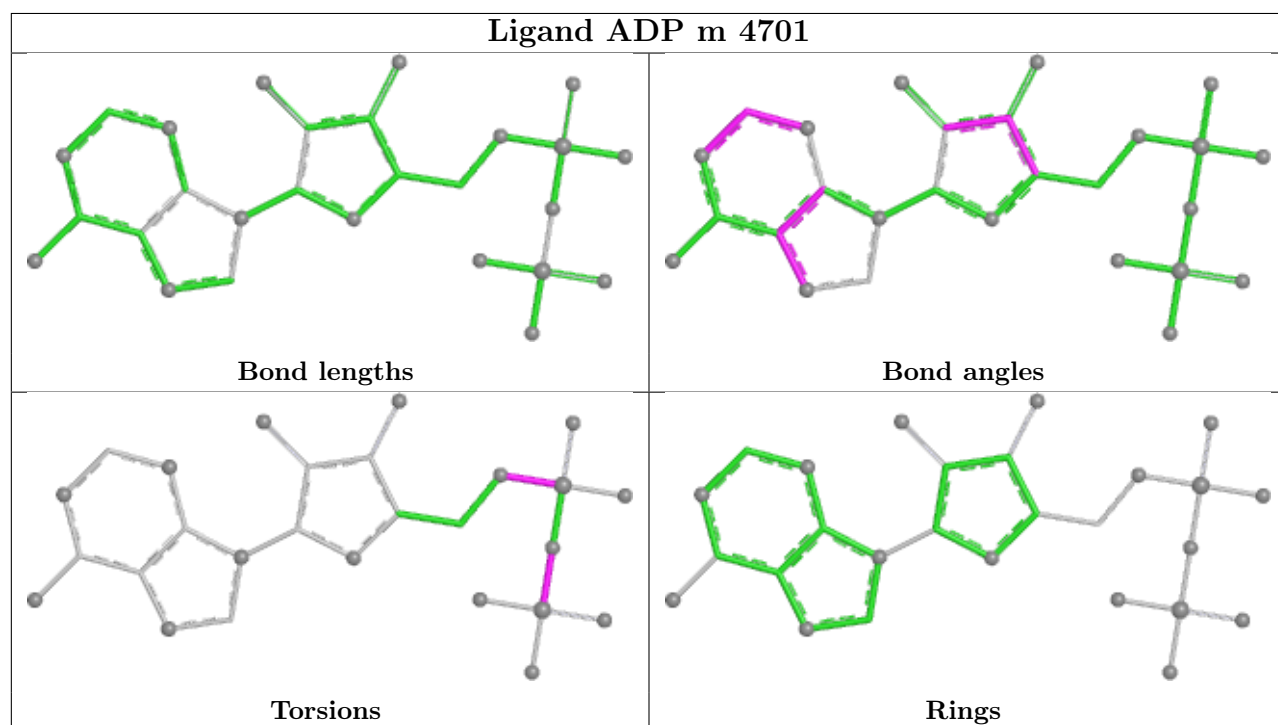
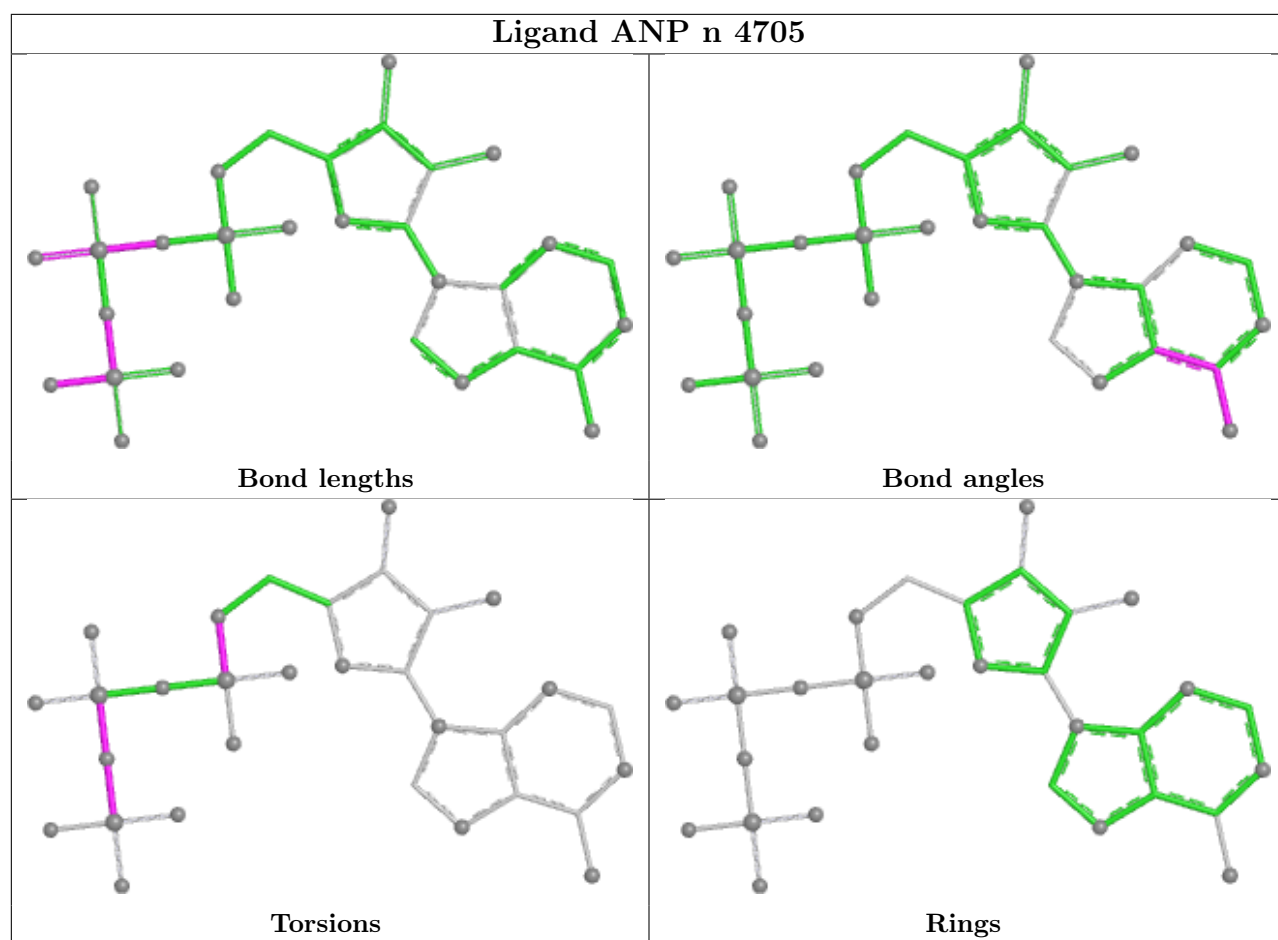


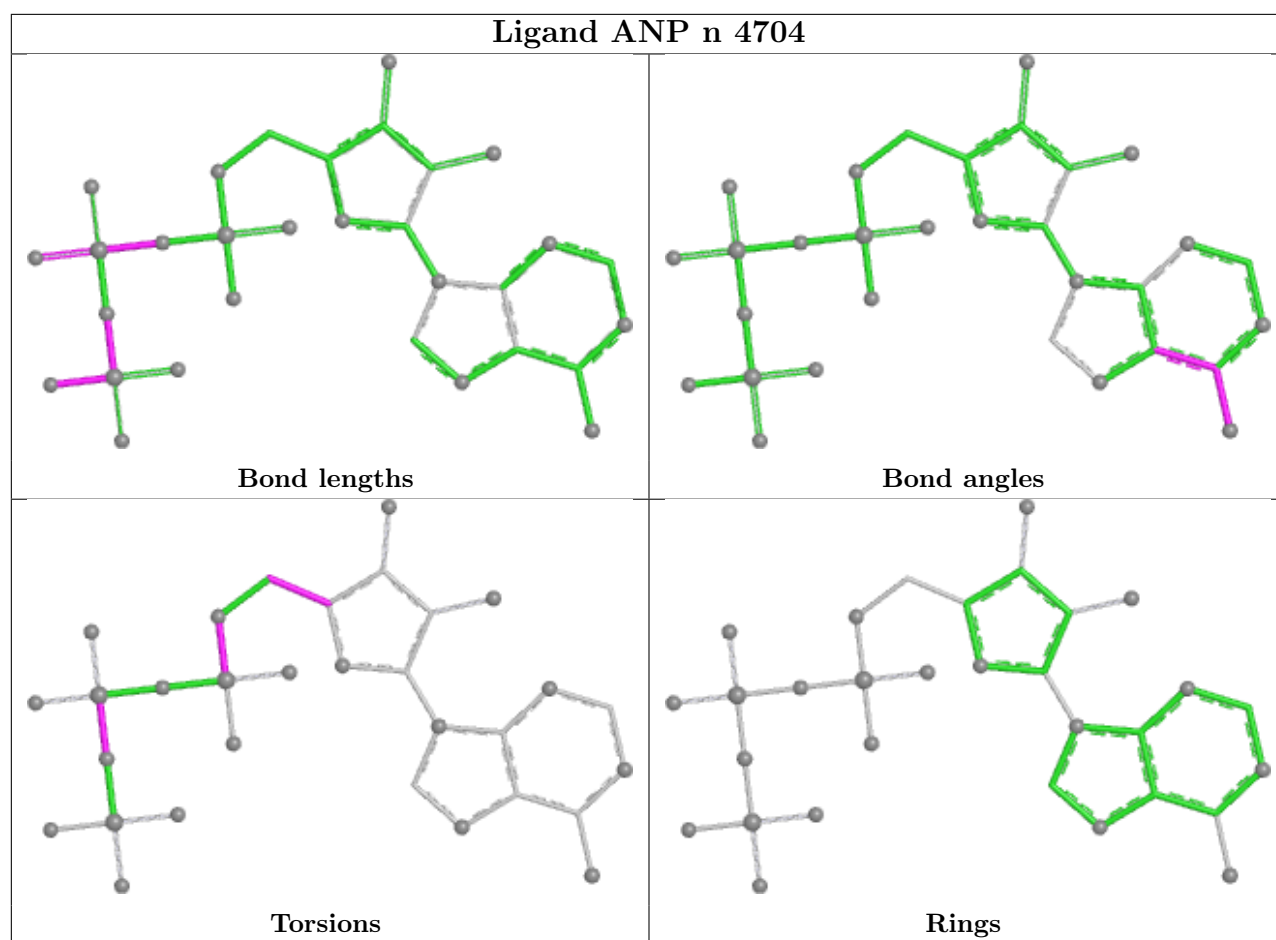
Ligand ANP m 4705



Ligand ADP n 4701







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.

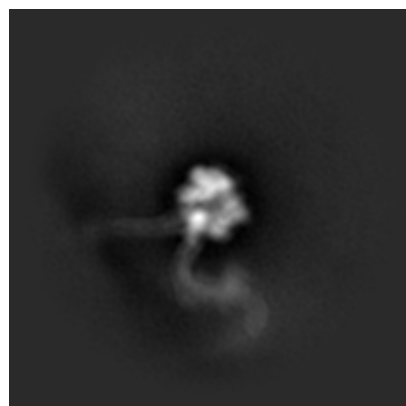
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46844. These allow visual inspection of the internal detail of the map and identification of artifacts.

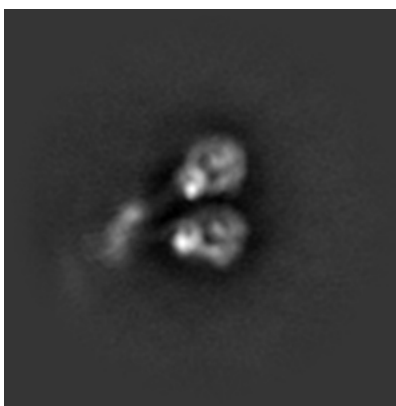
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

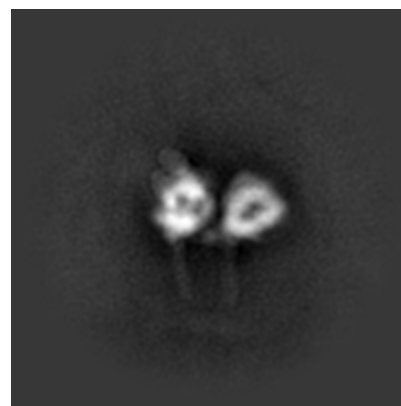
6.1.1 Primary map



X

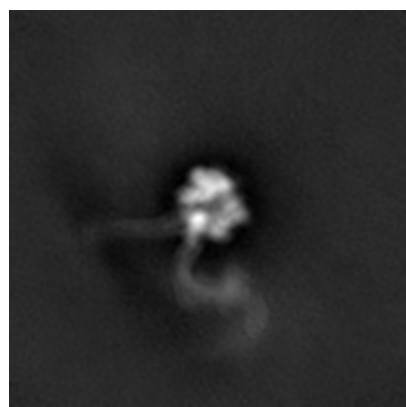


Y

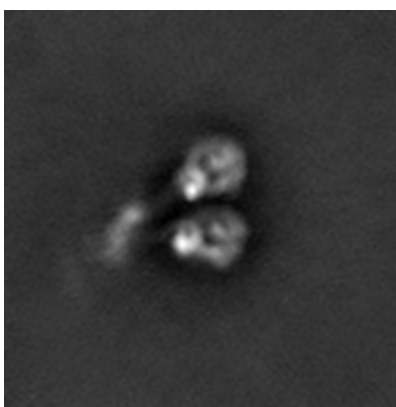


Z

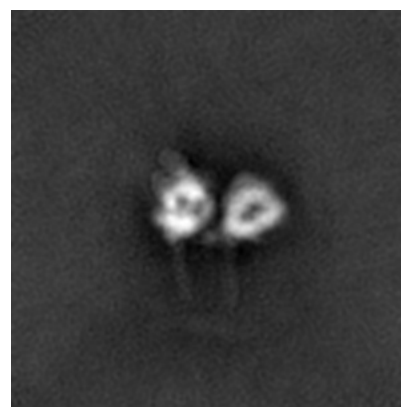
6.1.2 Raw map



X



Y

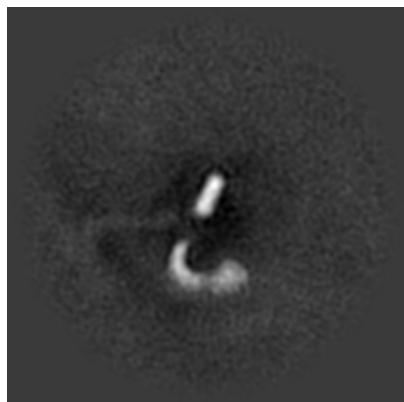


Z

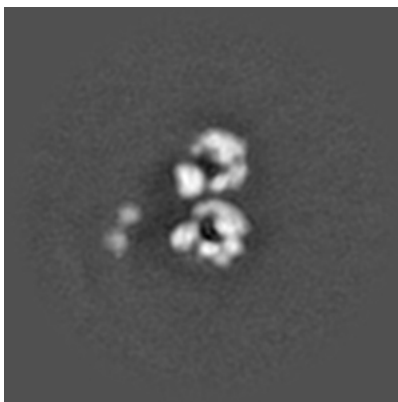
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

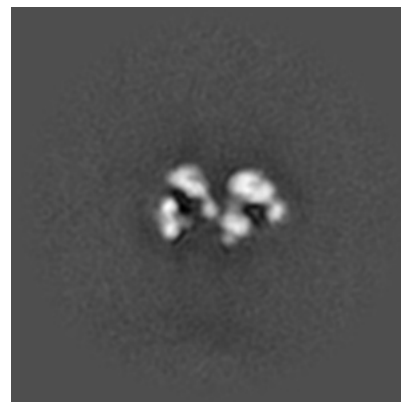
6.2.1 Primary map



X Index: 64

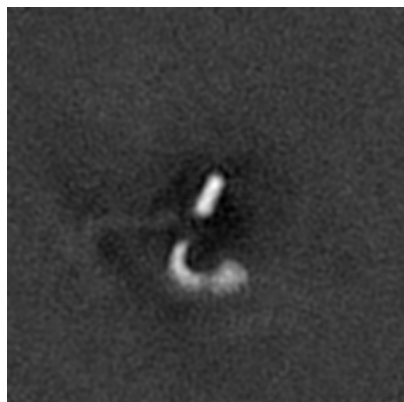


Y Index: 64

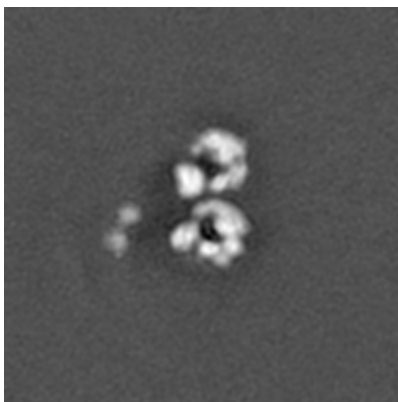


Z Index: 64

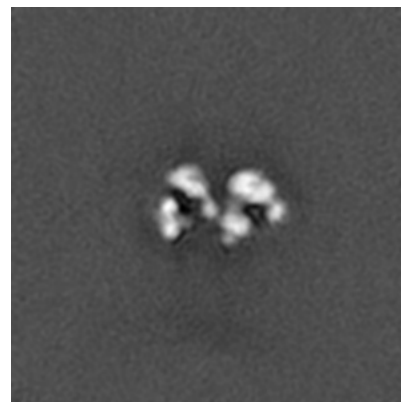
6.2.2 Raw map



X Index: 64



Y Index: 64

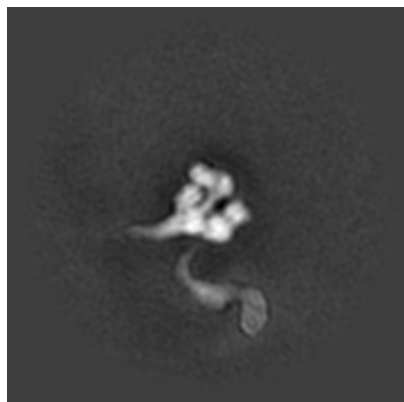


Z Index: 64

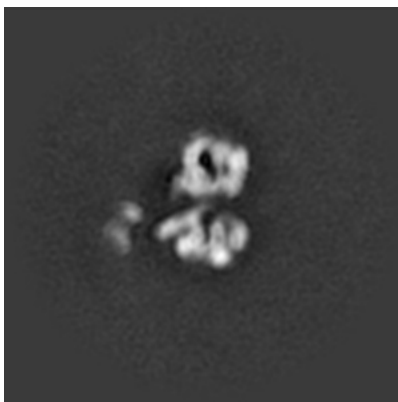
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

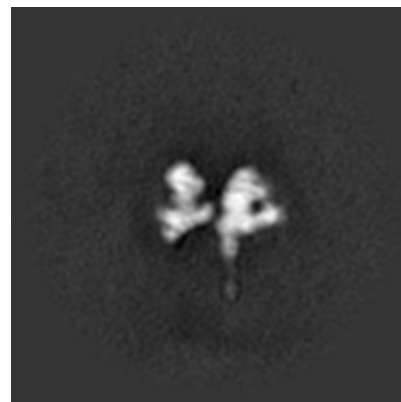
6.3.1 Primary map



X Index: 52

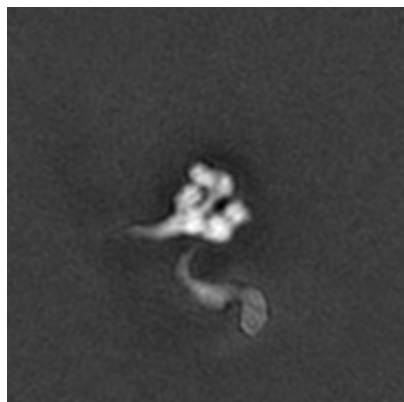


Y Index: 60

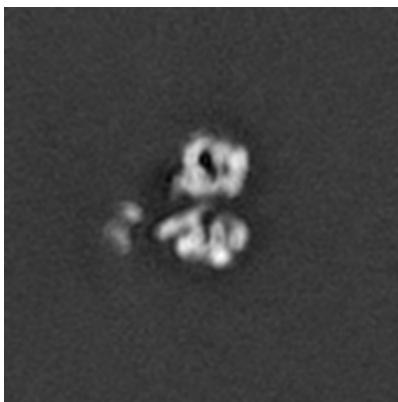


Z Index: 61

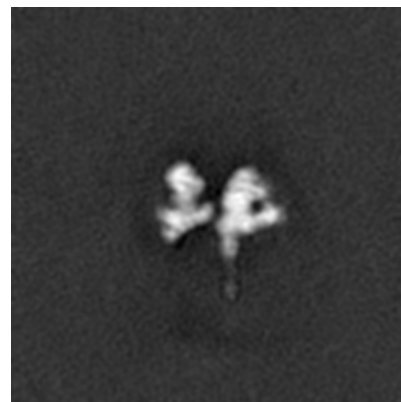
6.3.2 Raw map



X Index: 52



Y Index: 60



Z Index: 61

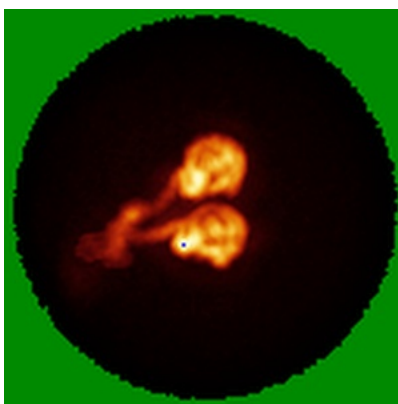
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X



Y

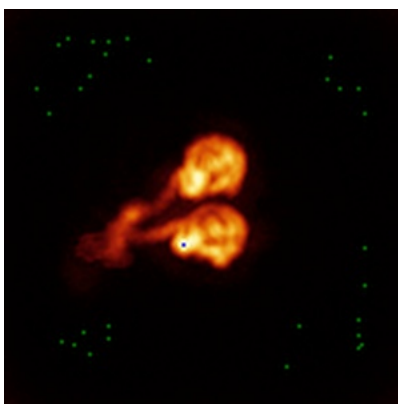


Z

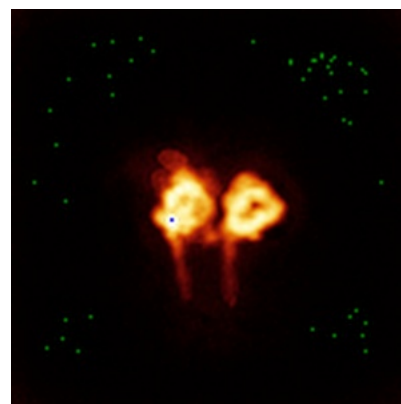
6.4.2 Raw map



X



Y

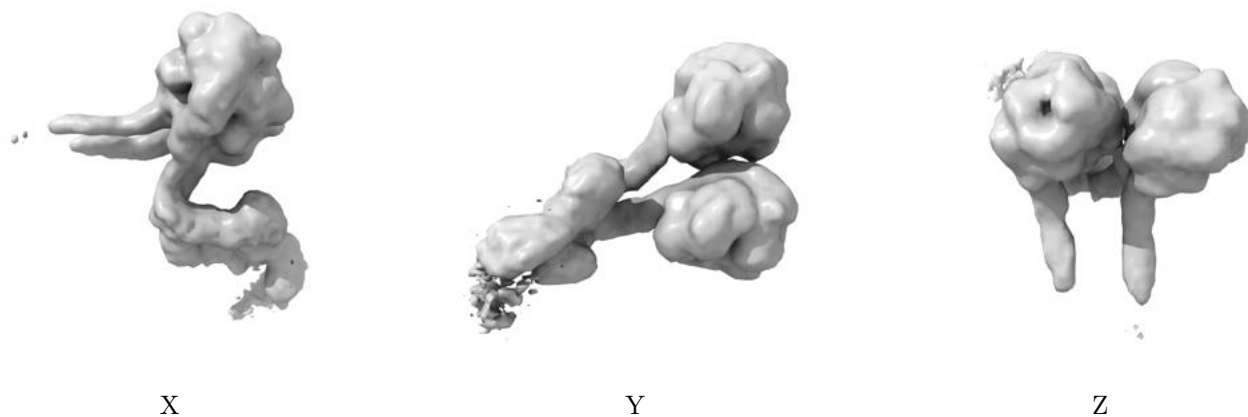


Z

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.

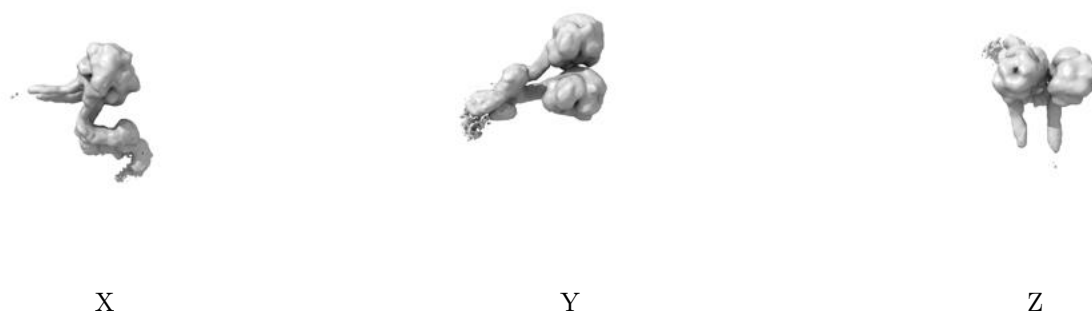
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. 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.

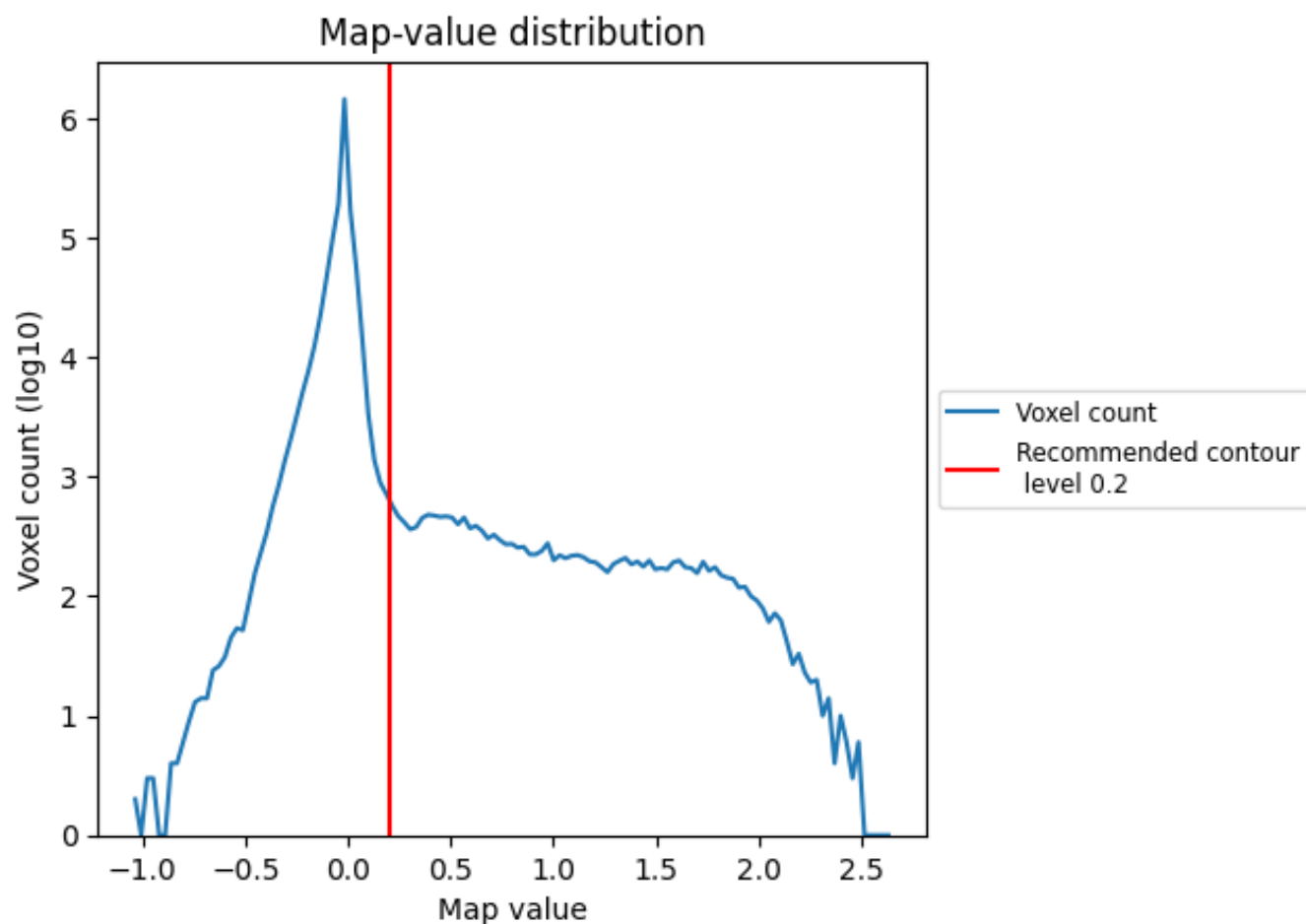
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

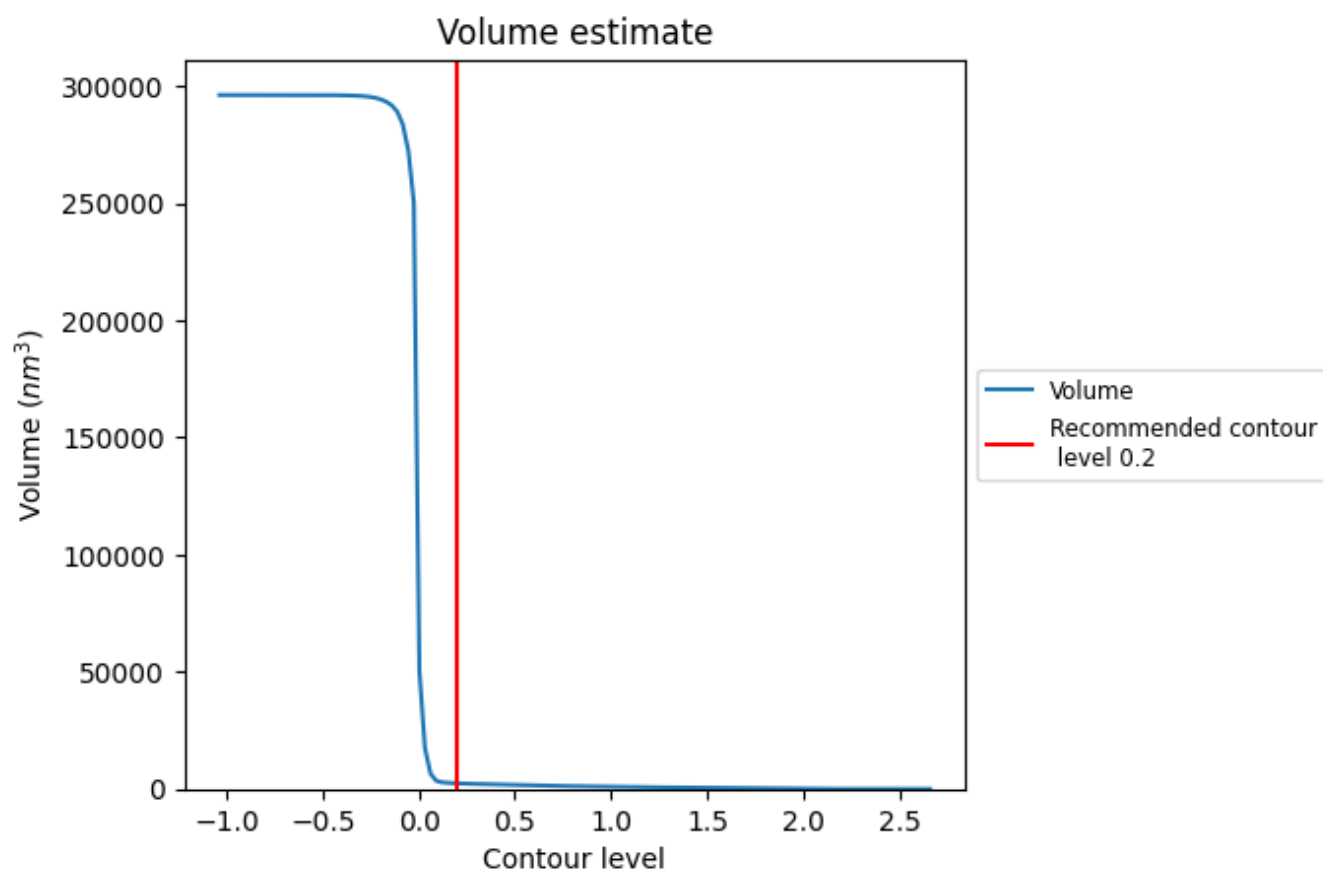
This section contains the results of statistical analysis of the map.

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.

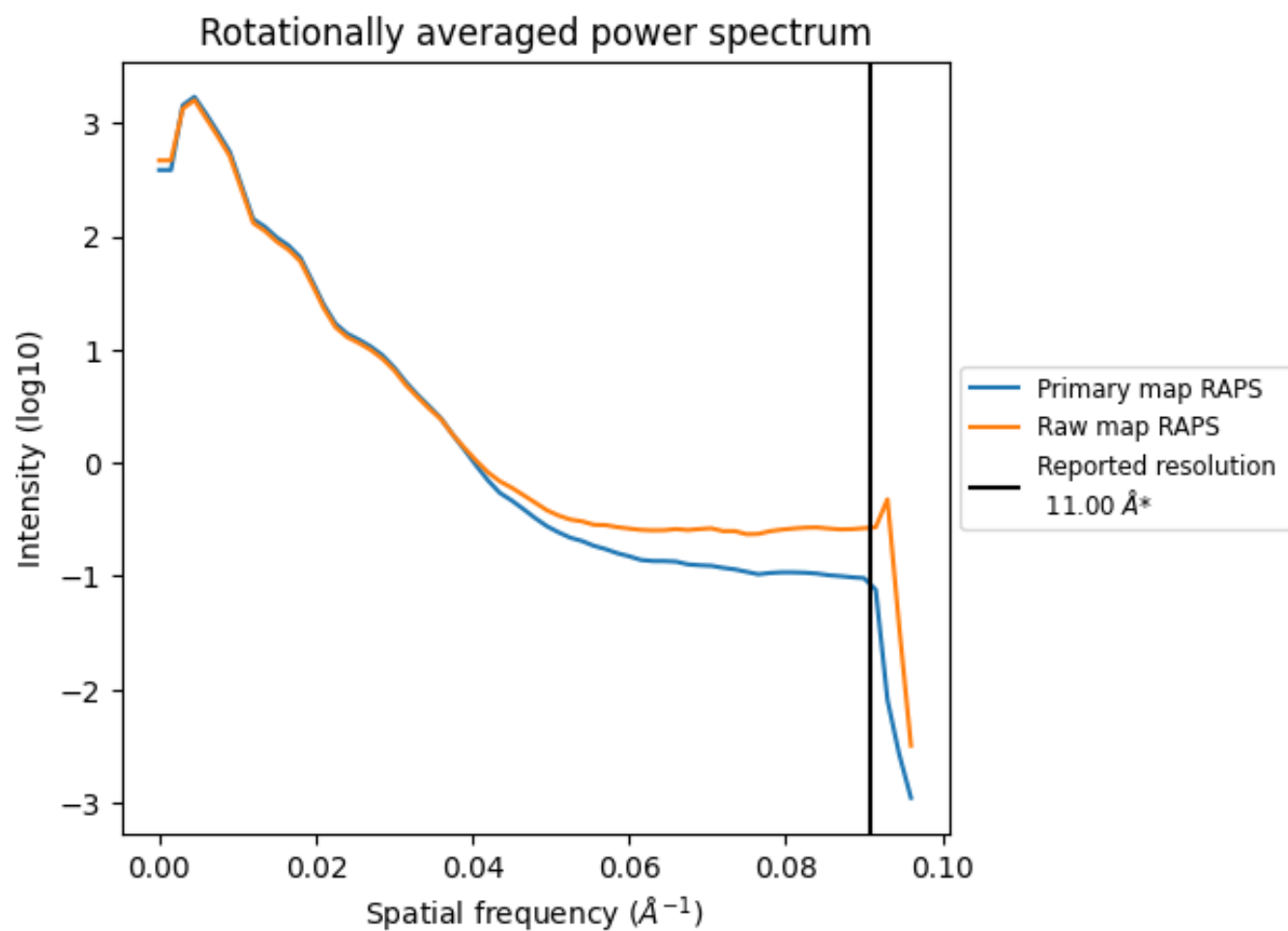
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2391 nm^3 ; this corresponds to an approximate mass of 2160 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 ⓘ

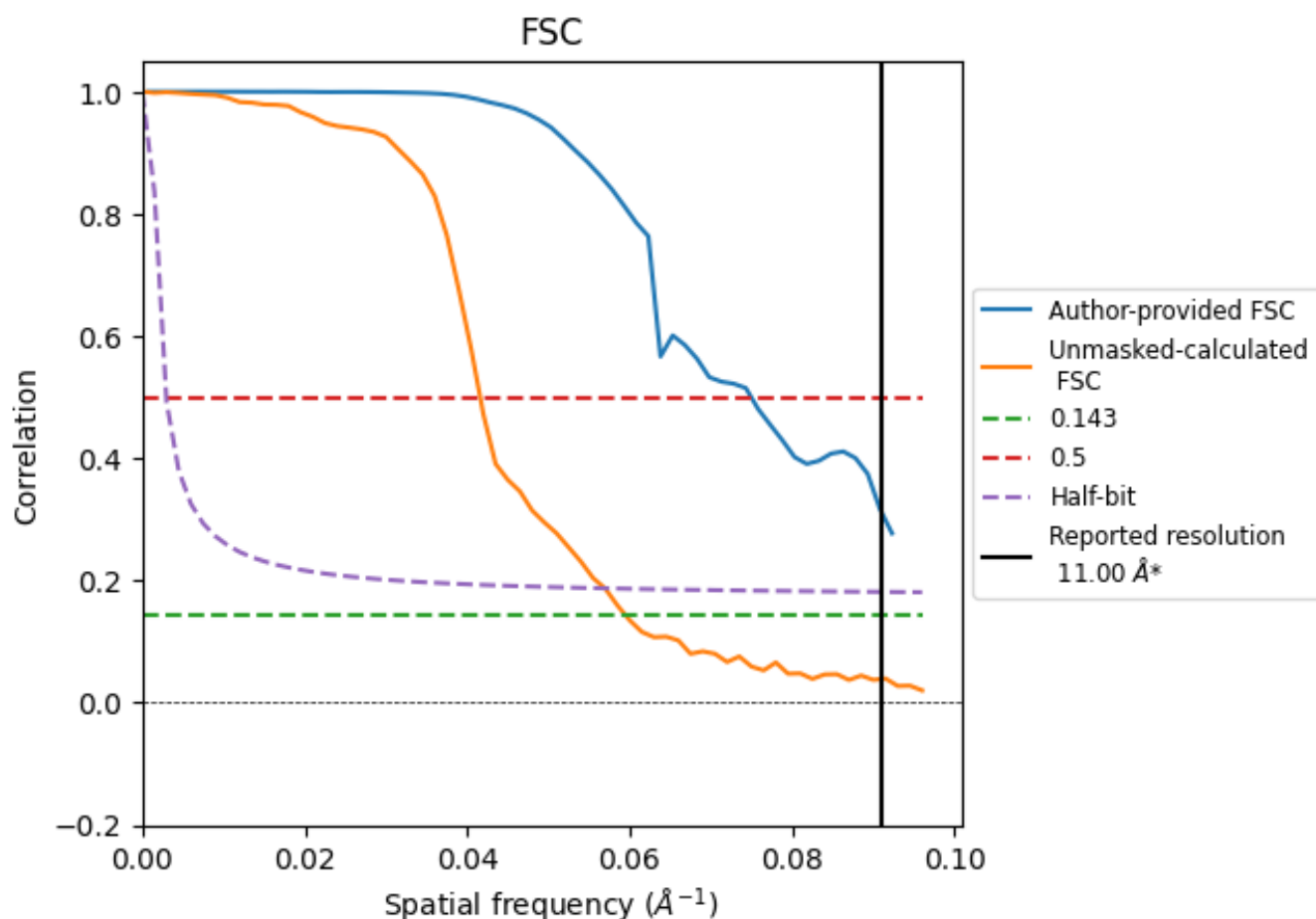


*Reported resolution corresponds to spatial frequency of 0.091 Å⁻¹

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 0.091 \AA^{-1}

8.2 Resolution estimates [i](#)

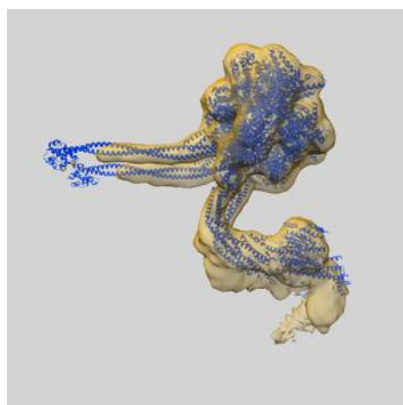
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	11.00	-	-
Author-provided FSC curve	-	13.35	-
Unmasked-calculated*	16.81	24.04	17.54

*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 16.81 differs from the reported value 11.0 by more than 10 %

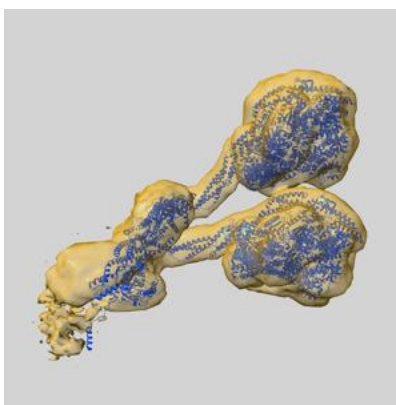
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-46844 and PDB model 9DGQ. Per-residue inclusion information can be found in section [3](#) on page [6](#).

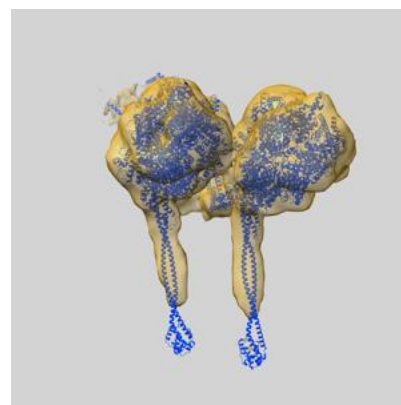
9.1 Map-model overlay [i](#)



X



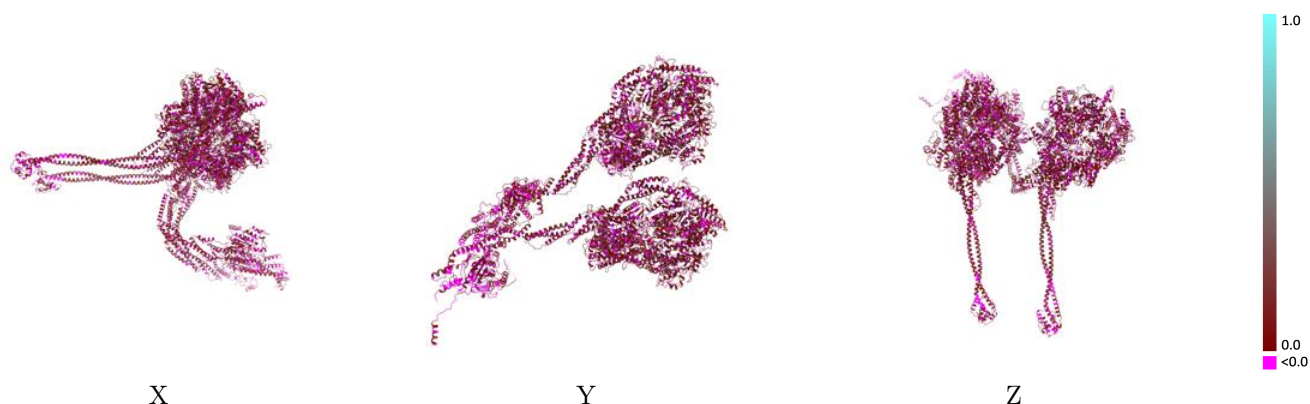
Y



Z

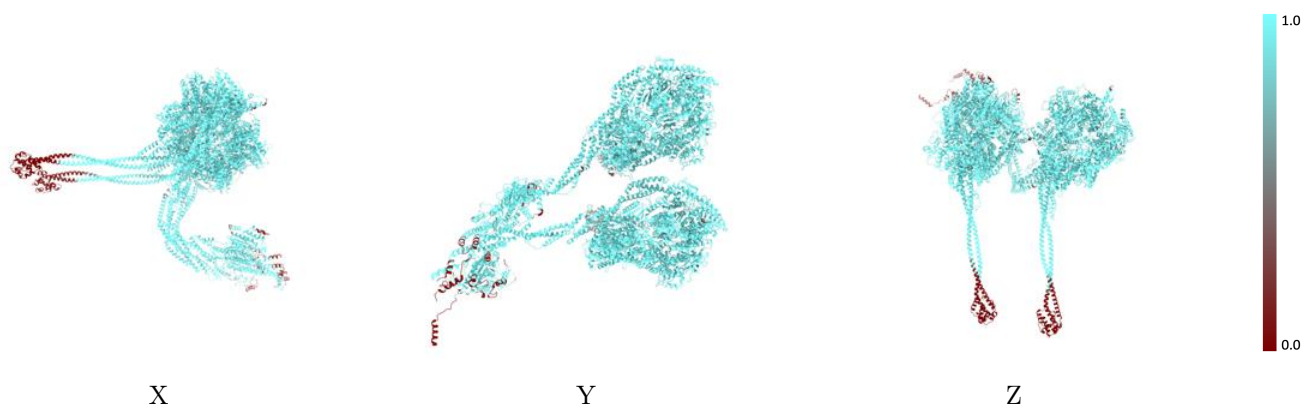
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



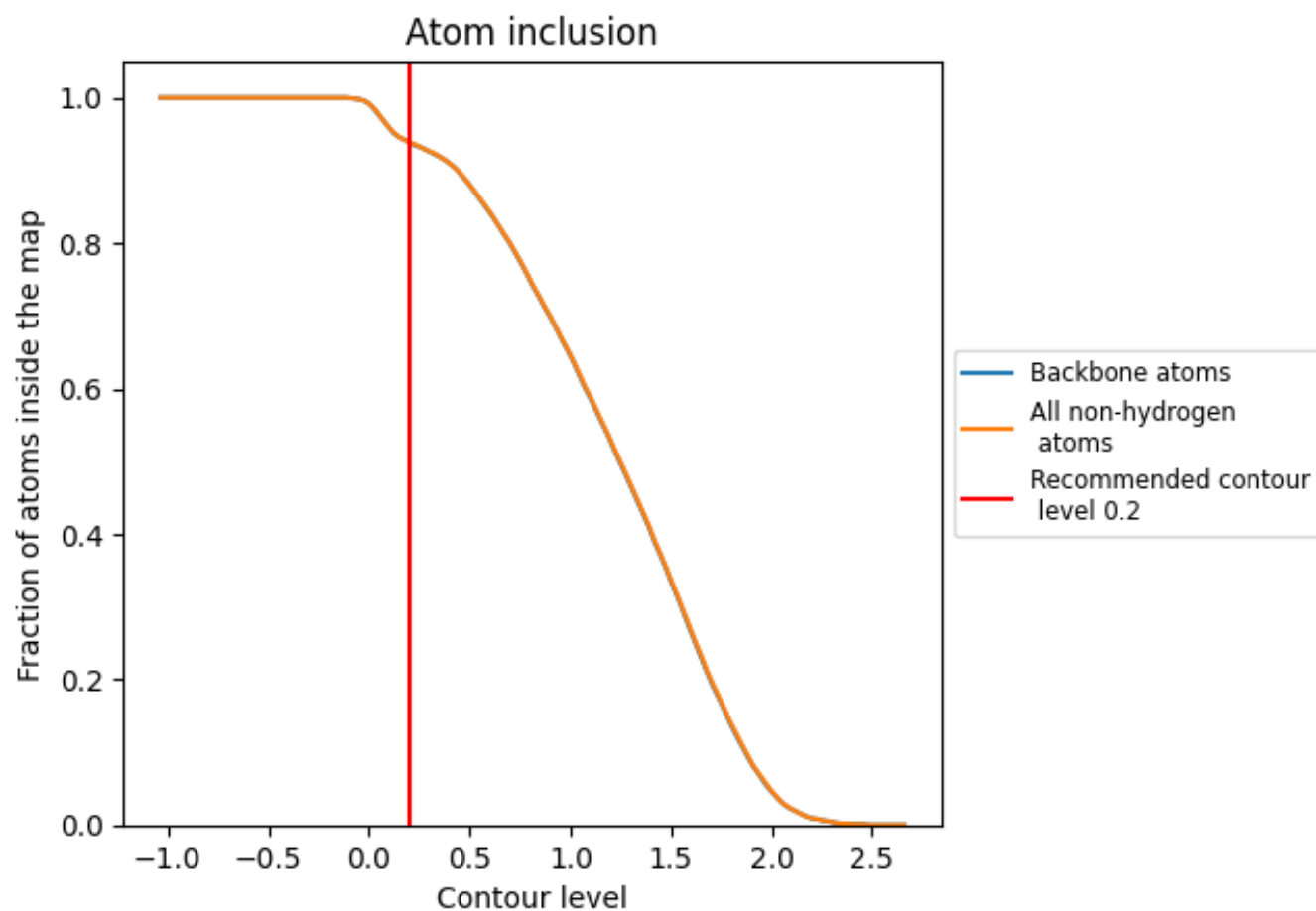
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

9.4 Atom inclusion ⓘ



At the recommended contour level, 94% of all backbone atoms, 94% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9390	<div></div> 0.0740
m	<div></div> 0.9520	<div></div> 0.0770
n	<div></div> 0.9430	<div></div> 0.0770
q	<div></div> 0.7730	<div></div> 0.0300
r	<div></div> 0.8980	<div></div> 0.0400

