



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 09:31 PM UTC

PDB ID : 9NVL / pdb_00009nvl
EMDB ID : EMD-49839
Title : ATPase Hybrid F1 with the ancestral core domains Binding Dwell
Authors : Stewart, A.G.; Noji, H.; Sobti, M.; Suzuki, A.K.
Deposited on : 2025-03-20
Resolution : 2.46 Å(reported)

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We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

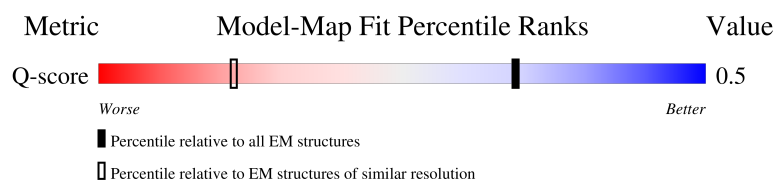
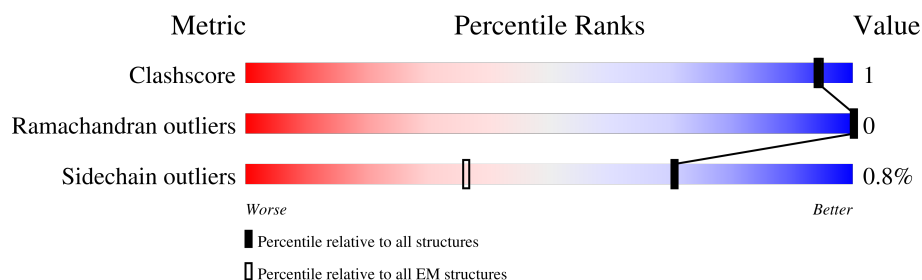
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMD 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) : 2.49

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 2.46 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	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6014 (1.96 - 2.96)

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	509	<div> <div>14%</div> <div>89%</div> <div>7%</div> </div>
1	B	509	<div> <div>11%</div> <div>90%</div> <div>7%</div> </div>
1	C	509	<div> <div>5%</div> <div>86%</div> <div>6%</div> <div>7%</div> </div>
2	D	482	<div> <div>7%</div> <div>90%</div> <div>7%</div> </div>

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Mol	Chain	Length	Quality of chain
2	E	482	
2	F	482	
3	G	285	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	PO4	C	603	-	X	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 24190 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 ATPase Hybrid F1 with the ancestral core domains Chain A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	474	Total	C	N	O	S	0	0
			3640	2299	630	699	12		
1	B	475	Total	C	N	O	S	0	0
			3651	2308	631	700	12		
1	C	473	Total	C	N	O	S	0	0
			3633	2295	629	697	12		

- Molecule 2 is a protein called ATPase Hybrid F1 with the ancestral core domains Chain D.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	469	Total	C	N	O	S	0	0
			3660	2319	632	695	14		
2	E	468	Total	C	N	O	S	0	0
			3651	2313	630	694	14		
2	F	468	Total	C	N	O	S	0	0
			3651	2313	630	694	14		

- Molecule 3 is a protein called ATP synthase gamma chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	282	Total	C	N	O	S	0	0
			2211	1393	388	420	10		

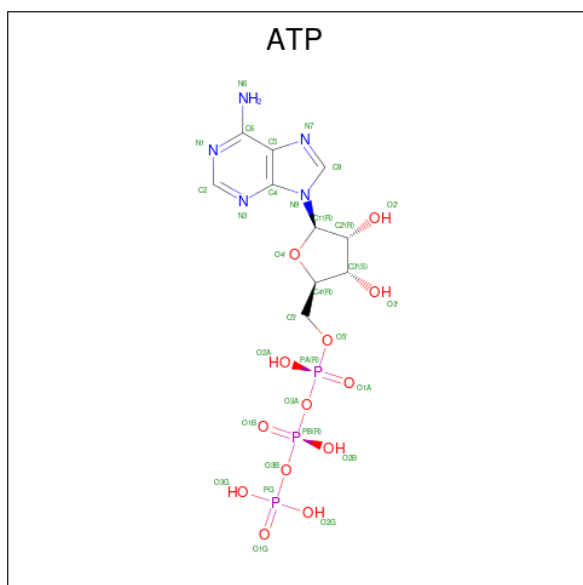
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	112	CYS	SER	conflict	UNP A0A0M4TPJ7
G	215	CYS	ILE	conflict	UNP A0A0M4TPJ7

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	C	2	Total	Mg	0
			2	2	
4	F	1	Total	Mg	0
			1	1	

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



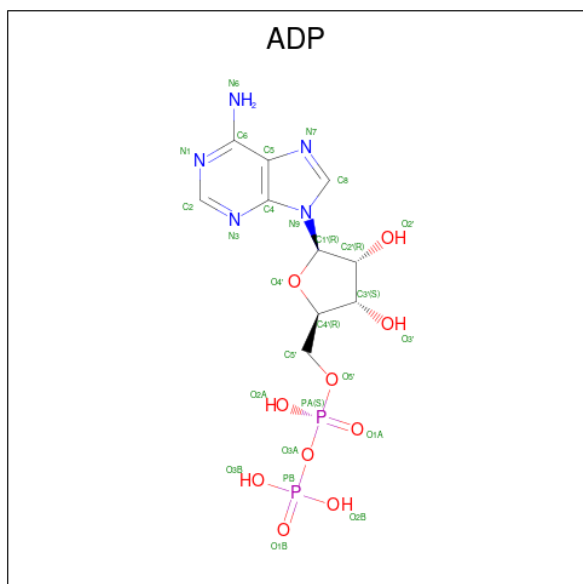
Mol	Chain	Residues	Atoms					AltConf
5	C	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P) (labeled as "Ligand of Interest" by depositor).

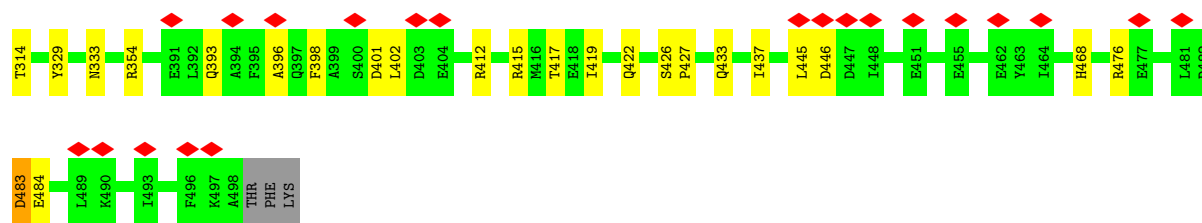


Mol	Chain	Residues	Atoms			AltConf
6	C	1	Total	O	P	0
			5	4	1	

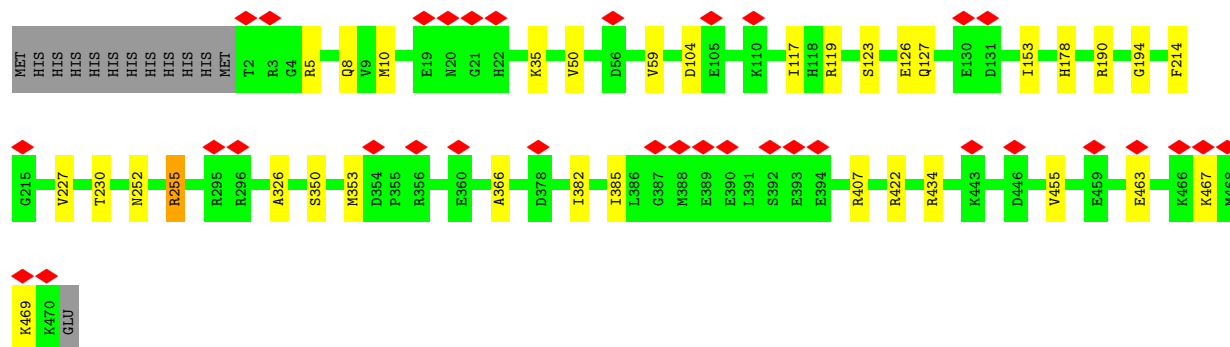
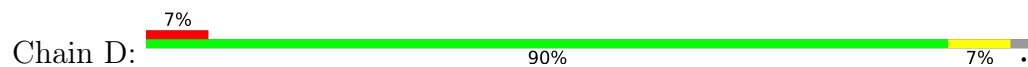
- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



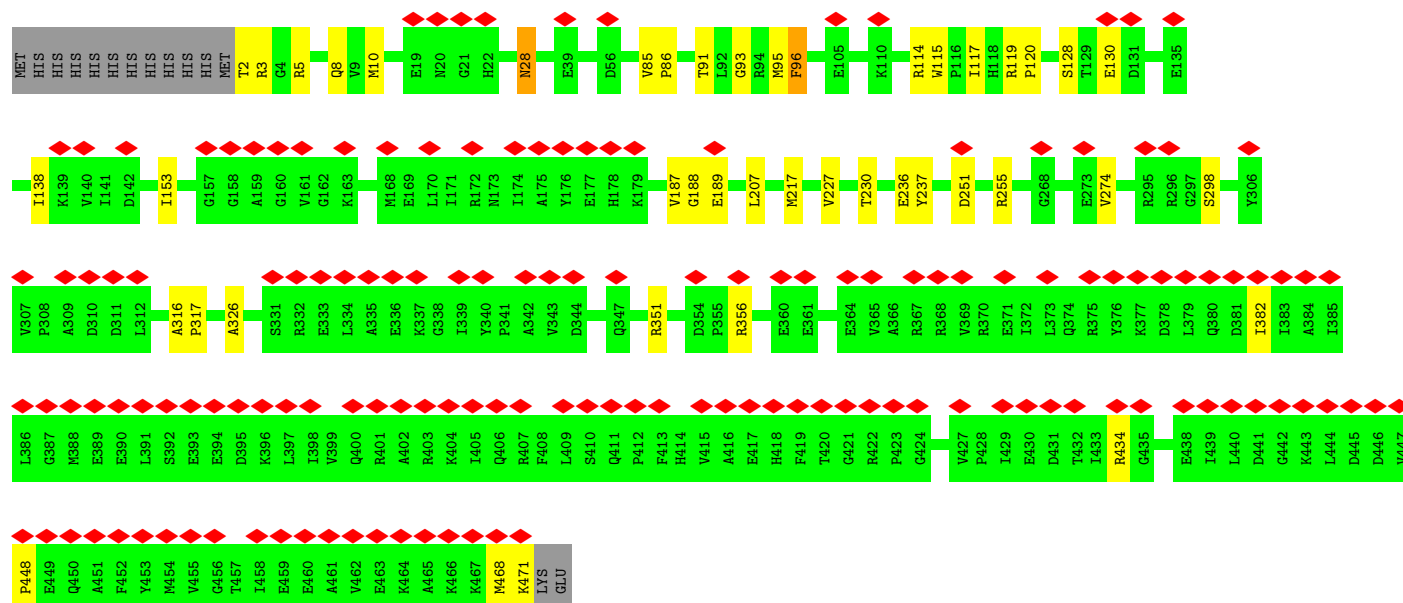
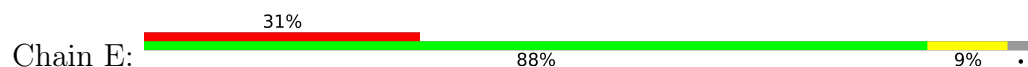
Mol	Chain	Residues	Atoms					AltConf
7	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
7	F	1	Total	C	N	O	P	0
			27	10	5	10	2	



- Molecule 2: ATPase Hybrid F1 with the ancestral core domains Chain D



- Molecule 2: ATPase Hybrid F1 with the ancestral core domains Chain D

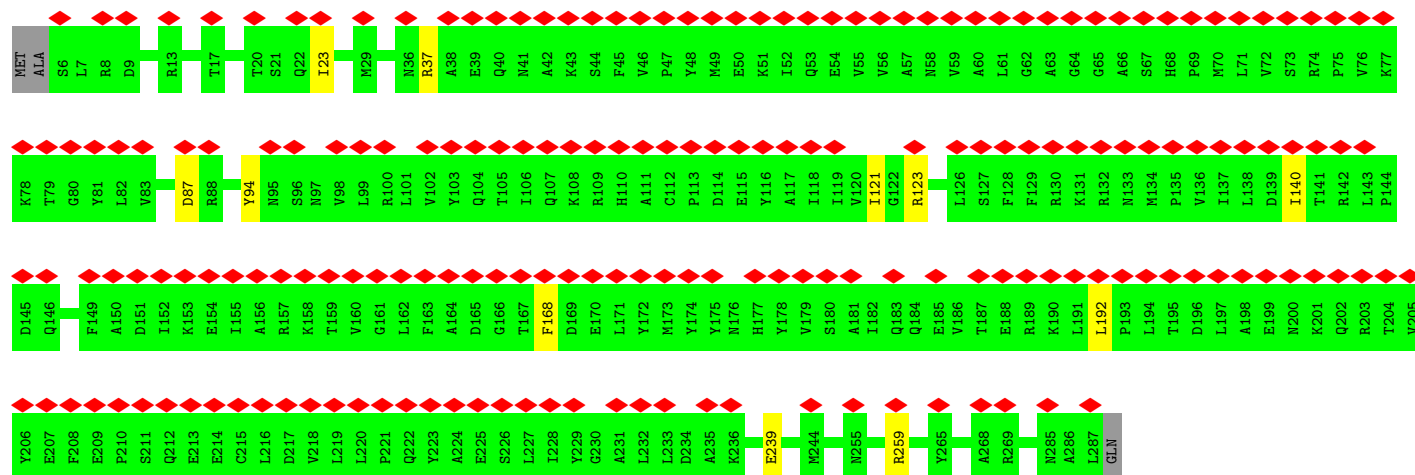


- Molecule 2: ATPase Hybrid F1 with the ancestral core domains Chain D





- Molecule 3: ATP synthase gamma chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	191889	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 ($e^-/\text{\AA}^2$)	62	Depositor
Minimum defocus (nm)	100	Depositor
Maximum defocus (nm)	1000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.206	Depositor
Minimum map value	-0.741	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.048	Depositor
Recommended contour level	0.16	Depositor
Map size (Å)	215.04, 215.04, 215.04	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84, 0.84, 0.84	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, PO4, ADP, 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	0.81	0/3695	1.42	12/4993 (0.2%)
1	B	0.79	0/3707	1.43	12/5009 (0.2%)
1	C	0.83	1/3688 (0.0%)	1.54	18/4983 (0.4%)
2	D	0.80	0/3726	1.44	14/5039 (0.3%)
2	E	0.83	0/3717	1.46	15/5028 (0.3%)
2	F	0.81	0/3717	1.48	16/5028 (0.3%)
3	G	0.79	0/2244	1.33	3/3036 (0.1%)
All	All	0.81	1/24494 (0.0%)	1.45	90/33116 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	2
2	D	0	2
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	484	GLU	N-CA	5.13	1.52	1.46

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	483	ASP	O-C-N	-20.41	95.45	122.59
2	E	227	VAL	N-CA-C	7.15	117.91	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	354	ARG	N-CA-C	7.13	121.90	112.35
1	A	483	ASP	CA-C-O	6.70	127.47	120.30
1	A	399	ALA	N-CA-C	6.68	118.25	110.97
1	C	333	ASN	CA-CB-CG	6.67	119.27	112.60
2	E	298	SER	N-CA-C	6.67	119.56	109.23
1	C	468	HIS	CB-CA-C	6.63	116.77	111.00
1	A	483	ASP	N-CA-CB	6.53	120.84	110.65
2	D	214	PHE	CA-CB-CG	6.50	120.30	113.80
1	C	483	ASP	CA-CB-CG	6.23	118.83	112.60
1	B	144	GLU	CA-C-N	6.21	126.42	119.90
1	B	144	GLU	C-N-CA	6.21	126.42	119.90
1	A	163	GLN	OE1-CD-NE2	-6.16	116.44	122.60
2	F	119	ARG	NE-CZ-NH2	6.08	124.67	119.20
1	B	283	ARG	NE-CZ-NH1	-6.07	115.43	121.50
2	E	351	ARG	NE-CZ-NH2	6.02	124.62	119.20
2	F	186	GLY	CA-C-N	6.01	129.00	120.53
2	F	186	GLY	C-N-CA	6.01	129.00	120.53
1	C	57	ASN	CA-CB-CG	6.00	118.61	112.60
1	C	161	ARG	NE-CZ-NH2	6.00	124.60	119.20
2	D	119	ARG	NE-CZ-NH2	5.98	124.58	119.20
1	A	406	THR	CB-CA-C	5.96	118.68	109.03
3	G	168	PHE	CA-CB-CG	5.95	119.75	113.80
2	E	120	PRO	CB-CA-C	-5.87	103.76	110.92
1	C	163	GLN	OE1-CD-NE2	-5.84	116.76	122.60
2	F	434	ARG	NE-CZ-NH2	5.70	124.33	119.20
2	E	8	GLN	OE1-CD-NE2	-5.67	116.92	122.60
2	F	225	PHE	CA-CB-CG	5.62	119.42	113.80
2	D	8	GLN	OE1-CD-NE2	-5.62	116.98	122.60
1	B	57	ASN	CA-CB-CG	5.58	118.18	112.60
2	E	138	ILE	CA-C-N	5.58	128.52	120.38
2	E	138	ILE	C-N-CA	5.58	128.52	120.38
2	E	434	ARG	NE-CZ-NH2	5.57	124.22	119.20
1	B	127	ARG	NE-CZ-NH2	5.47	124.13	119.20
2	E	120	PRO	N-CA-C	5.47	117.38	110.70
2	E	28	ASN	CA-CB-CG	5.46	118.06	112.60
2	F	175	ALA	CA-C-N	5.45	127.86	120.44
2	F	175	ALA	C-N-CA	5.45	127.86	120.44
3	G	259	ARG	NE-CZ-NH2	5.45	124.11	119.20
2	F	362	HIS	CA-CB-CG	5.44	119.24	113.80
1	C	417	THR	CA-C-N	5.43	127.56	120.28
1	C	417	THR	C-N-CA	5.43	127.56	120.28
1	A	271	ARG	NE-CZ-NH2	5.41	124.07	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	422	ARG	CA-C-N	5.37	126.56	119.84
2	D	422	ARG	C-N-CA	5.37	126.56	119.84
2	F	252	ASN	N-CA-C	5.37	116.83	107.49
2	E	448	PRO	CA-C-N	5.36	127.78	120.54
2	E	448	PRO	C-N-CA	5.36	127.78	120.54
1	B	371	GLN	N-CA-CB	-5.36	102.45	110.17
2	D	227	VAL	N-CA-C	5.34	116.07	110.62
1	A	470	ASP	CA-CB-CG	5.33	117.93	112.60
1	C	354	ARG	NE-CZ-NH2	5.29	123.96	119.20
1	C	65	ASN	CA-CB-CG	5.28	117.88	112.60
1	B	250	ARG	CD-NE-CZ	5.28	131.79	124.40
1	C	225	ALA	N-CA-C	5.25	116.98	108.26
1	A	277	LEU	CA-C-N	5.24	130.00	122.40
1	A	277	LEU	C-N-CA	5.24	130.00	122.40
1	B	164	ARG	NE-CZ-NH2	5.24	123.92	119.20
2	F	264	SER	N-CA-C	5.24	116.99	111.28
2	D	455	VAL	N-CA-C	5.22	120.20	109.34
2	D	190	ARG	NE-CZ-NH2	5.21	123.89	119.20
2	D	5	ARG	NE-CZ-NH2	5.20	123.88	119.20
2	F	374	GLN	OE1-CD-NE2	-5.20	117.41	122.60
2	E	96	PHE	N-CA-C	5.18	117.55	109.52
2	E	356	ARG	NE-CZ-NH2	5.18	123.86	119.20
2	E	5	ARG	NE-CZ-NH2	5.17	123.86	119.20
1	C	412	ARG	NE-CZ-NH2	5.17	123.85	119.20
1	B	68	GLU	CB-CA-C	-5.16	102.22	110.79
1	B	261	ASP	N-CA-C	5.16	118.35	111.75
1	B	296	ARG	NE-CZ-NH2	5.15	123.84	119.20
2	D	194	GLY	CA-C-N	5.14	127.44	120.44
2	D	194	GLY	C-N-CA	5.14	127.44	120.44
1	C	329	TYR	N-CA-C	5.13	116.56	110.97
2	F	216	GLN	N-CA-C	5.10	117.11	110.43
1	C	422	GLN	OE1-CD-NE2	-5.08	117.52	122.60
3	G	37	ARG	NE-CZ-NH2	5.07	123.76	119.20
2	D	178	HIS	CB-CG-CD2	-5.05	124.63	131.20
1	C	294	HIS	CB-CG-CD2	-5.04	124.64	131.20
2	F	368	ARG	NE-CZ-NH2	5.04	123.74	119.20
1	C	476	ARG	NE-CZ-NH2	5.04	123.74	119.20
2	F	28	ASN	CA-CB-CG	5.04	117.64	112.60
1	A	294	HIS	CB-CG-CD2	-5.03	124.66	131.20
2	D	434	ARG	NE-CZ-NH2	5.03	123.73	119.20
2	F	138	ILE	CA-C-N	5.02	127.71	120.38
2	F	138	ILE	C-N-CA	5.02	127.71	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	403	ASP	CA-C-N	5.02	127.25	120.38
1	A	403	ASP	C-N-CA	5.02	127.25	120.38
1	B	90	ARG	NE-CZ-NH2	5.01	123.71	119.20
2	D	104	ASP	CA-CB-CG	5.00	117.60	112.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	405	ALA	Mainchain
1	C	161	ARG	Sidechain
1	C	483	ASP	Mainchain
2	D	255	ARG	Sidechain
2	D	407	ARG	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3640	0	3706	6	0
1	B	3651	0	3715	3	0
1	C	3633	0	3699	9	0
2	D	3660	0	3711	12	0
2	E	3651	0	3698	20	0
2	F	3651	0	3697	6	0
3	G	2211	0	2257	4	0
4	C	2	0	0	0	0
4	F	1	0	0	0	0
5	C	31	0	12	0	0
6	C	5	0	0	0	0
7	D	27	0	12	0	0
7	F	27	0	12	0	0
All	All	24190	0	24519	57	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 (57) 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:E:91:THR:HG23	2:E:96:PHE:CE2	2.25	0.72
2:E:2:THR:HG23	2:E:3:ARG:H	1.55	0.71
2:E:117:ILE:HD12	2:E:230:THR:HA	1.76	0.66
2:E:189:GLU:HB2	2:E:251:ASP:OD2	2.01	0.60
2:E:86:PRO:HD3	2:E:114:ARG:NH1	2.22	0.54
1:A:295:SER:HB2	2:E:217:MET:HG2	1.90	0.53
2:F:254:PHE:CZ	2:F:308:PRO:HG3	2.44	0.53
2:E:119:ARG:NH2	2:E:236:GLU:OE1	2.42	0.52
2:E:128:SER:OG	2:E:130:GLU:HG2	2.10	0.52
1:A:133:ALA:HB1	1:A:134:PRO:HD2	1.92	0.51
2:E:85:VAL:CG2	2:E:117:ILE:HD11	2.41	0.51
2:F:463:GLU:O	2:F:467:LYS:HG3	2.11	0.51
3:G:87:ASP:OD1	3:G:123:ARG:HG3	2.12	0.50
3:G:94:TYR:CZ	3:G:239:GLU:HG3	2.48	0.48
1:C:149:GLY:HA3	1:C:427:PRO:HB3	1.95	0.48
2:E:2:THR:HG23	2:E:3:ARG:N	2.26	0.48
2:D:353:MET:HE1	2:D:366:ALA:HB3	1.95	0.48
2:E:115:TRP:CH2	2:E:237:TYR:HA	2.49	0.48
2:D:463:GLU:HG3	2:D:467:LYS:HE3	1.96	0.48
2:D:326:ALA:HA	2:D:350:SER:HA	1.96	0.47
1:A:137:VAL:CG1	2:E:95:MET:HE1	2.45	0.47
1:C:415:ARG:HD3	1:C:446:ASP:HA	1.97	0.47
2:D:123:SER:HG	2:D:126:GLU:HG2	1.79	0.47
1:B:183:ILE:HG22	1:B:183:ILE:O	2.15	0.47
1:A:175:LYS:HE3	1:A:320:GLU:HG2	1.97	0.47
2:D:469:LYS:N	2:D:469:LYS:HD2	2.30	0.46
1:C:419:ILE:HD11	1:C:445:LEU:HD13	1.96	0.46
1:A:250:ARG:HG2	1:A:250:ARG:HH21	1.81	0.46
2:D:50:VAL:HG13	2:D:59:VAL:CG1	2.46	0.46
1:B:250:ARG:HG2	1:B:250:ARG:HH21	1.81	0.46
2:E:382:ILE:HD12	2:E:382:ILE:H	1.81	0.46
1:C:393:GLN:HA	1:C:396:ALA:HB2	1.97	0.45
2:D:123:SER:OG	2:D:126:GLU:HG2	2.16	0.45
2:D:382:ILE:HD12	2:D:382:ILE:H	1.83	0.44
2:E:93:GLY:HA2	2:E:207:LEU:O	2.17	0.44
3:G:121:ILE:HG23	3:G:140:ILE:HG23	1.99	0.44
2:E:316:ALA:HB3	2:E:317:PRO:HD3	1.99	0.44
2:F:50:VAL:HG13	2:F:59:VAL:CG1	2.48	0.44
1:C:250:ARG:HH21	1:C:250:ARG:HG2	1.83	0.43
1:C:426:SER:N	1:C:427:PRO:HD3	2.32	0.43
2:F:438:GLU:HG2	2:F:444:LEU:HD13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:251:ASP:O	2:F:304:ALA:HB3	2.18	0.43
2:E:188:GLY:HA3	2:E:255:ARG:HG2	2.01	0.43
1:C:398:PHE:O	1:C:402:LEU:HG	2.19	0.42
1:C:398:PHE:HB2	1:C:401:ASP:OD1	2.19	0.42
1:B:175:LYS:HE3	1:B:320:GLU:HG2	2.00	0.42
2:D:252:ASN:HB3	2:D:255:ARG:HD3	2.02	0.42
2:E:91:THR:HG23	2:E:96:PHE:HE2	1.80	0.42
1:A:389:TYR:CG	1:A:413:GLY:HA3	2.54	0.42
2:E:117:ILE:CD1	2:E:230:THR:HA	2.48	0.42
2:D:123:SER:O	2:D:127:GLN:HG2	2.19	0.41
2:E:153:ILE:HD12	2:E:326:ALA:HB3	2.02	0.41
1:C:433:GLN:O	1:C:437:ILE:HG13	2.21	0.41
2:F:382:ILE:H	2:F:382:ILE:HD12	1.87	0.40
2:E:468:MET:O	2:E:471:LYS:HB2	2.21	0.40
2:D:385:ILE:HD11	3:G:23:ILE:HD12	2.03	0.40
2:D:117:ILE:HD12	2:D:230:THR:HA	2.03	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	472/509 (93%)	460 (98%)	12 (2%)	0	100	100
1	B	473/509 (93%)	455 (96%)	18 (4%)	0	100	100
1	C	471/509 (92%)	455 (97%)	16 (3%)	0	100	100
2	D	467/482 (97%)	455 (97%)	12 (3%)	0	100	100
2	E	466/482 (97%)	451 (97%)	15 (3%)	0	100	100
2	F	466/482 (97%)	450 (97%)	16 (3%)	0	100	100
3	G	280/285 (98%)	273 (98%)	7 (2%)	0	100	100
All	All	3095/3258 (95%)	2999 (97%)	96 (3%)	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	383/415 (92%)	380 (99%)	3 (1%)	73	83
1	B	384/415 (92%)	381 (99%)	3 (1%)	73	83
1	C	382/415 (92%)	379 (99%)	3 (1%)	73	83
2	D	395/408 (97%)	392 (99%)	3 (1%)	73	83
2	E	394/408 (97%)	390 (99%)	4 (1%)	68	77
2	F	394/408 (97%)	390 (99%)	4 (1%)	68	77
3	G	238/240 (99%)	237 (100%)	1 (0%)	84	89
All	All	2570/2709 (95%)	2549 (99%)	21 (1%)	70	83

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	142	VAL
1	A	264	SER
1	A	313	LEU
1	B	53	VAL
1	B	326	VAL
1	B	327	SER
1	C	53	VAL
1	C	142	VAL
1	C	314	THR
2	D	10	MET
2	D	35	LYS
2	D	153	ILE
2	E	10	MET
2	E	28	ASN
2	E	187	VAL
2	E	274	VAL
2	F	28	ASN
2	F	153	ILE

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Mol	Chain	Res	Type
2	F	167	ILE
2	F	274	VAL
3	G	192	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	ASN
1	A	69	ASN
1	A	70	ASN
1	A	186	GLN
1	A	294	HIS
1	B	69	ASN
1	B	235	GLN
1	B	294	HIS
1	C	42	HIS
1	C	69	ASN
1	C	70	ASN
1	C	186	GLN
1	C	189	GLN
1	C	202	GLN
1	C	235	GLN
1	C	409	GLN
2	D	216	GLN
2	D	218	ASN
2	D	288	GLN
2	D	303	GLN
2	D	347	GLN
2	D	362	HIS
2	D	380	GLN
2	D	418	HIS
2	E	374	GLN
2	E	380	GLN
2	F	34	HIS
2	F	127	GLN
2	F	258	GLN
2	F	362	HIS
2	F	374	GLN
2	F	380	GLN
3	G	104	GLN
3	G	240	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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$
5	ATP	C	602	4	32,33,33	1.10	2 (6%)	48,52,52	1.25	6 (12%)
6	PO4	C	603	4	4,4,4	2.63	4 (100%)	6,6,6	2.90	3 (50%)
7	ADP	F	500	4	28,29,29	1.20	3 (10%)	43,45,45	1.30	7 (16%)
7	ADP	D	500	4	28,29,29	1.14	2 (7%)	43,45,45	1.38	7 (16%)

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
5	ATP	C	602	4	-	0/22/38/38	0/3/3/3
7	ADP	D	500	4	-	4/16/32/32	0/3/3/3
7	ADP	F	500	4	-	2/16/32/32	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	F	500	ADP	PA-O3A	-3.32	1.55	1.59
6	C	603	PO4	P-O3	-2.83	1.46	1.54
6	C	603	PO4	P-O2	-2.82	1.46	1.54
6	C	603	PO4	P-O4	-2.53	1.47	1.54
7	D	500	ADP	PA-O3A	-2.45	1.56	1.59
6	C	603	PO4	P-O1	-2.32	1.45	1.50
7	F	500	ADP	C5-C4	-2.23	1.35	1.39
7	F	500	ADP	PB-O3B	-2.12	1.46	1.54
5	C	602	ATP	PB-O3A	-2.07	1.57	1.59
7	D	500	ADP	C5-C4	-2.04	1.35	1.39
5	C	602	ATP	C5-C4	-2.02	1.35	1.39

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	603	PO4	O4-P-O2	4.73	122.63	107.91
6	C	603	PO4	O3-P-O1	-4.33	95.65	110.95
7	D	500	ADP	O2B-PB-O3A	3.72	117.11	104.64
5	C	602	ATP	C5-C4-N3	-2.98	122.62	126.72
7	F	500	ADP	C5-C4-N3	-2.93	122.68	126.72
5	C	602	ATP	C4-C5-N7	2.89	113.89	110.58
7	D	500	ADP	O2A-PA-O3A	2.85	114.98	107.27
7	D	500	ADP	C5-C4-N3	-2.85	122.80	126.72
7	D	500	ADP	C4-C5-N7	2.83	113.82	110.58
7	F	500	ADP	O2B-PB-O3A	2.76	113.90	104.64
5	C	602	ATP	O2B-PB-O3B	2.72	114.62	107.27
7	F	500	ADP	C4-C5-N7	2.70	113.67	110.58
7	F	500	ADP	C3'-C2'-C1'	2.69	106.55	101.46
6	C	603	PO4	O2-P-O1	-2.40	102.45	110.95
5	C	602	ATP	N3-C4-N9	2.31	131.09	127.17
7	F	500	ADP	C2-N1-C6	-2.27	115.00	118.73
7	D	500	ADP	O3B-PB-O3A	2.17	111.93	104.64
5	C	602	ATP	O2B-PB-O3A	2.15	113.09	107.27
7	F	500	ADP	N3-C4-N9	2.08	130.71	127.17
5	C	602	ATP	O2A-PA-O3A	2.07	112.86	107.27
7	D	500	ADP	O3B-PB-O2B	-2.06	100.09	107.80
7	D	500	ADP	C2-N1-C6	-2.04	115.38	118.73
7	F	500	ADP	C5-C6-N1	2.01	122.62	117.51

There are no chirality outliers.

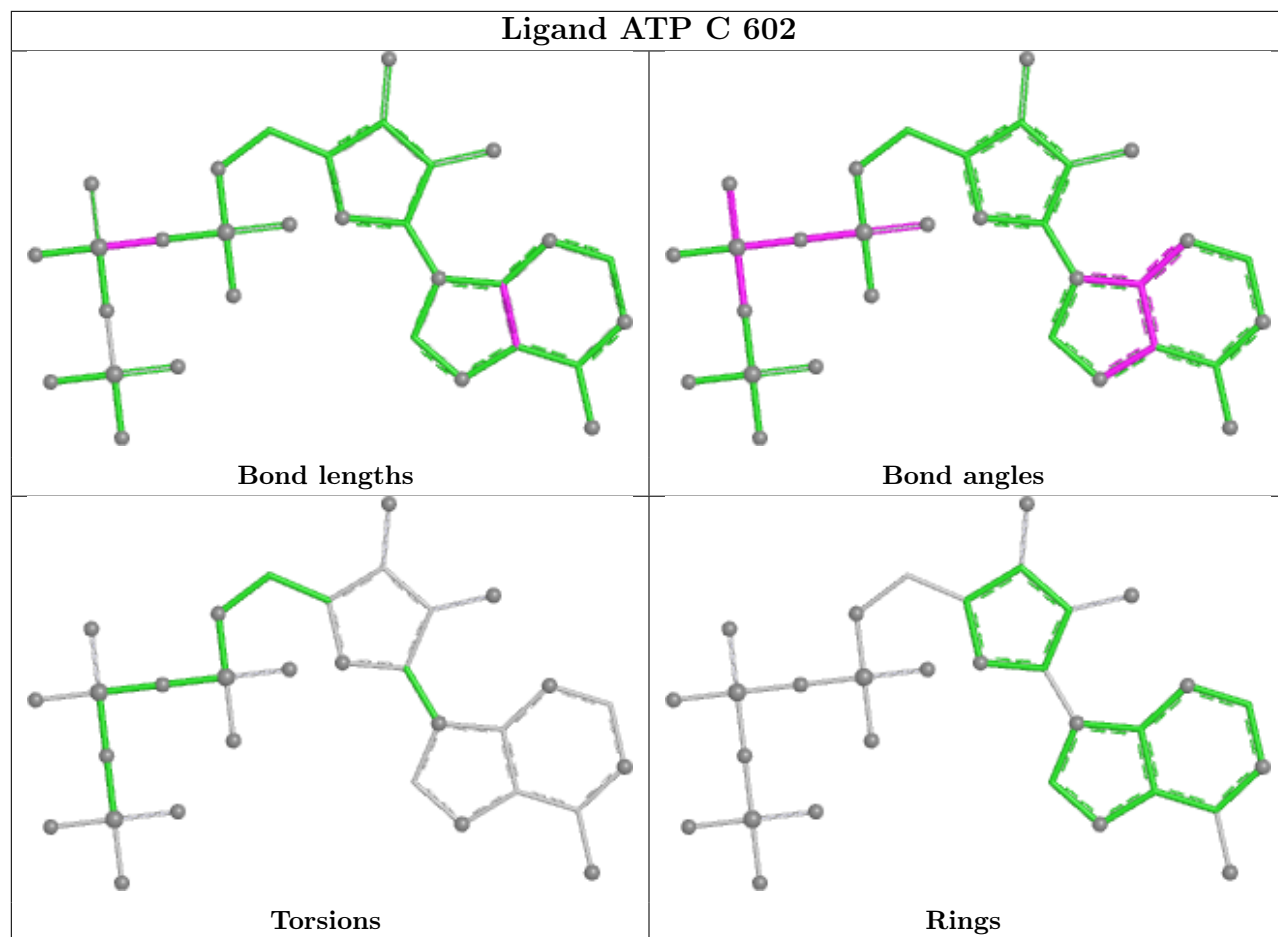
All (6) torsion outliers are listed below:

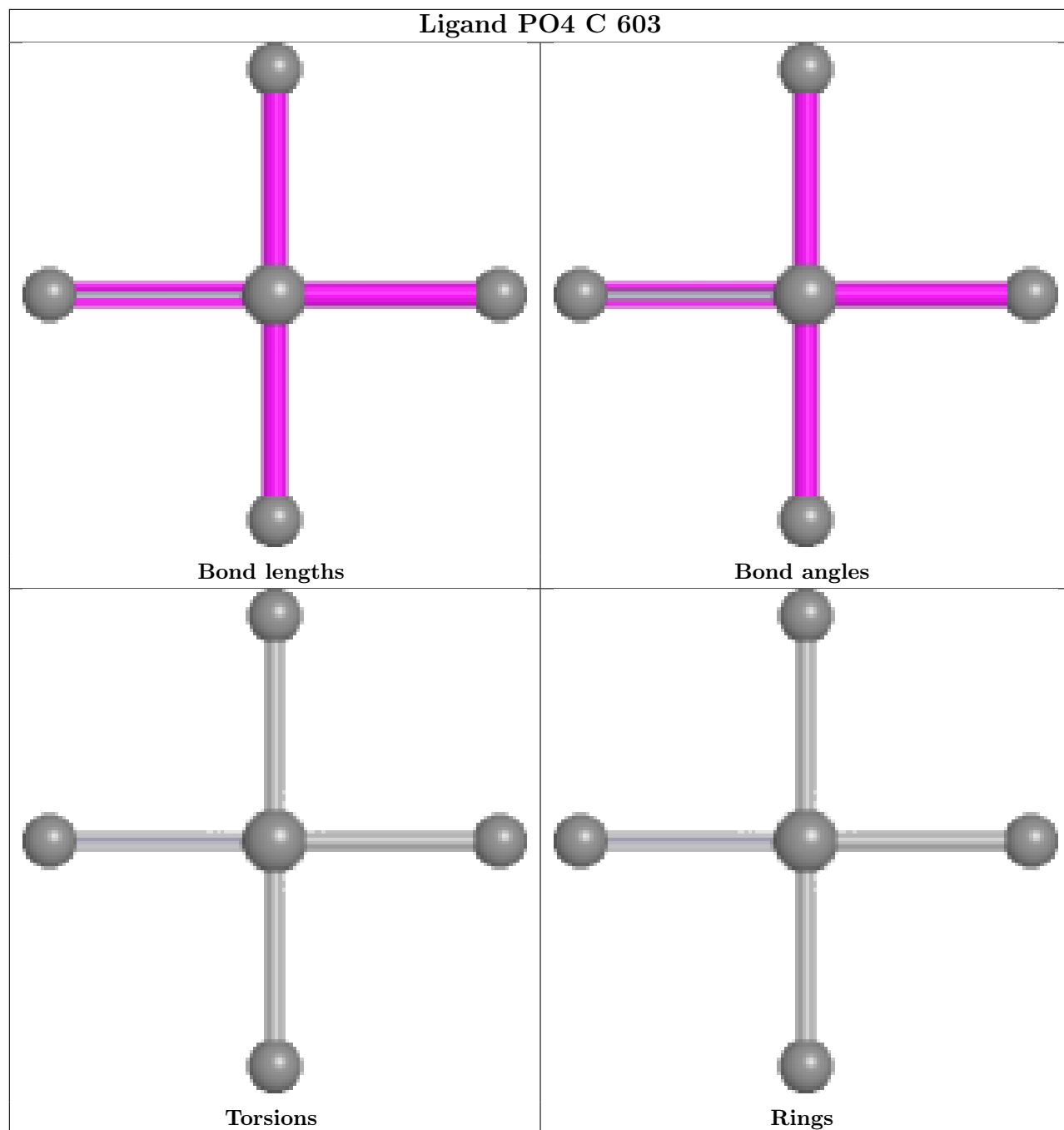
Mol	Chain	Res	Type	Atoms
7	D	500	ADP	PA-O3A-PB-O2B
7	F	500	ADP	PA-O3A-PB-O2B
7	D	500	ADP	PA-O3A-PB-O1B
7	D	500	ADP	C3'-C4'-C5'-O5'
7	D	500	ADP	O4'-C4'-C5'-O5'
7	F	500	ADP	PA-O3A-PB-O3B

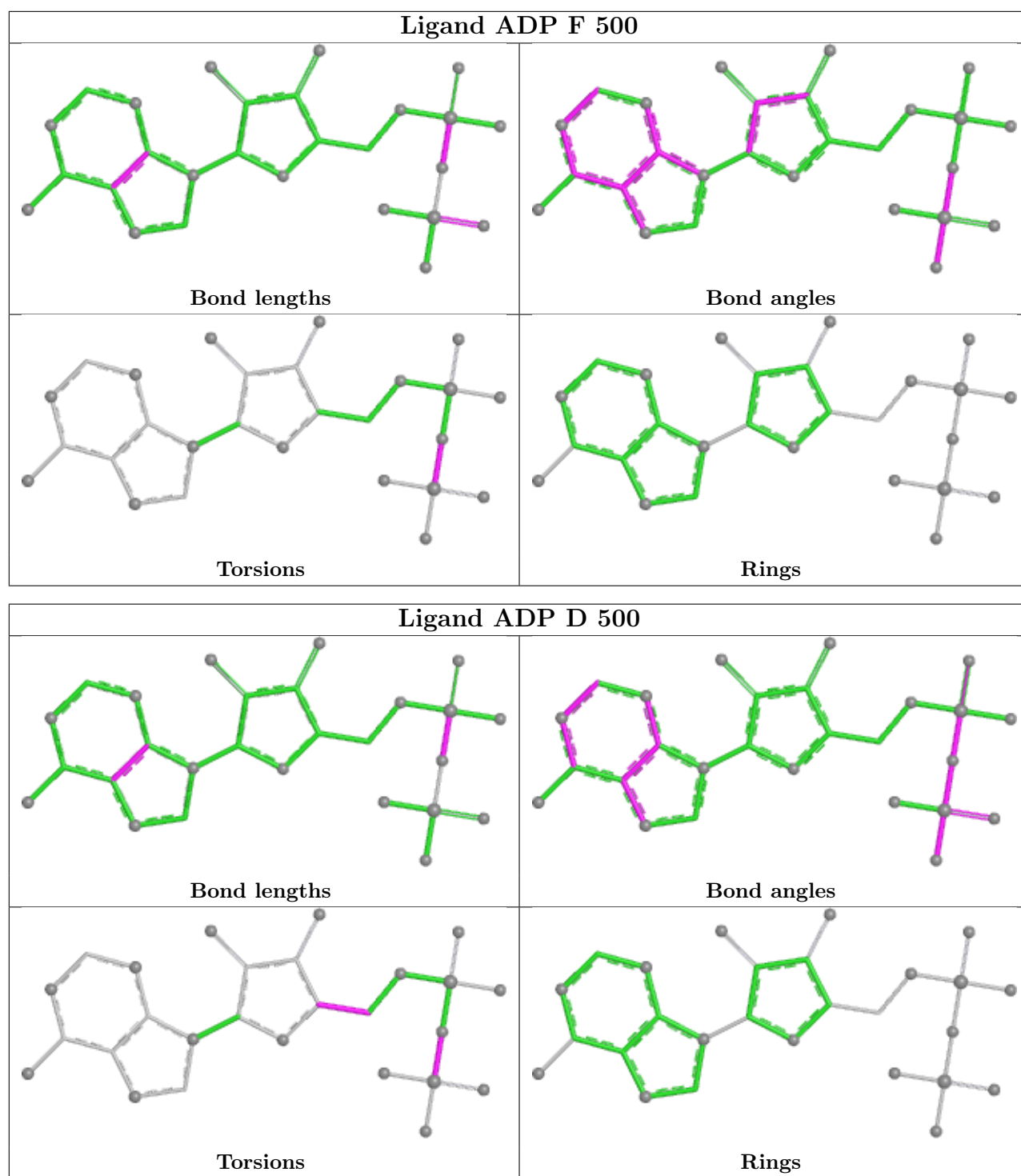
There are no ring outliers.

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

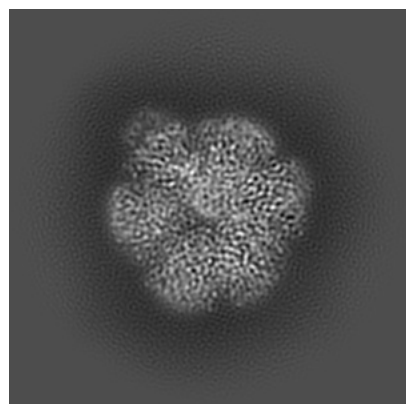
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49839. These allow visual inspection of the internal detail of the map and identification of artifacts.

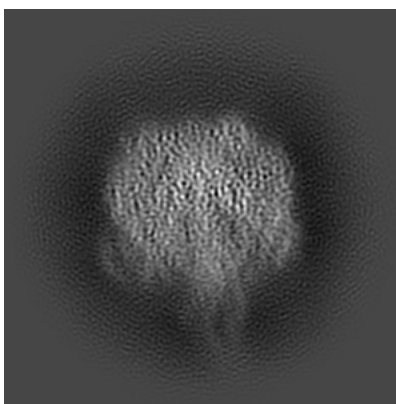
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

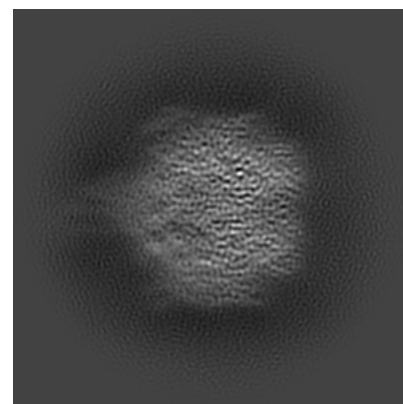
6.1.1 Primary map



X

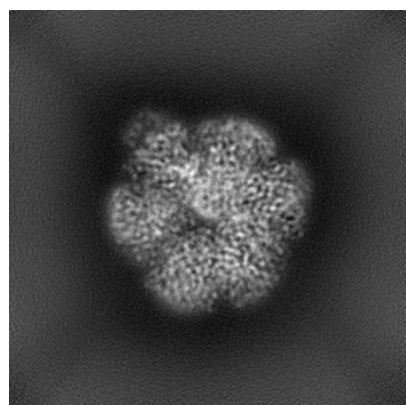


Y

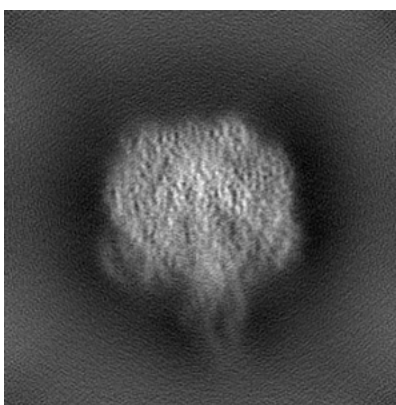


Z

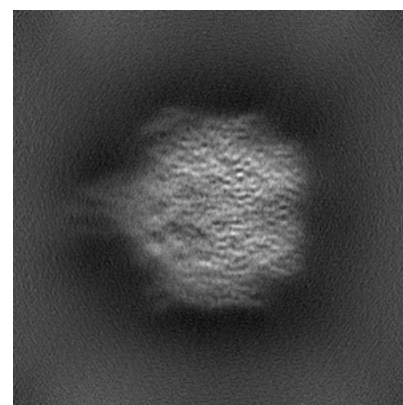
6.1.2 Raw map



X



Y

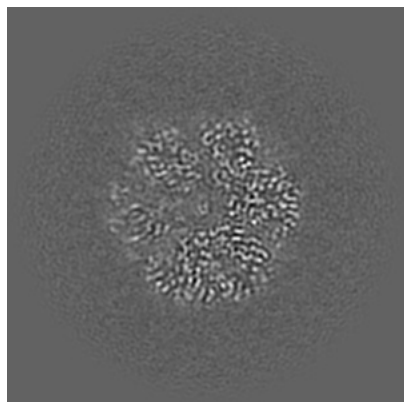


Z

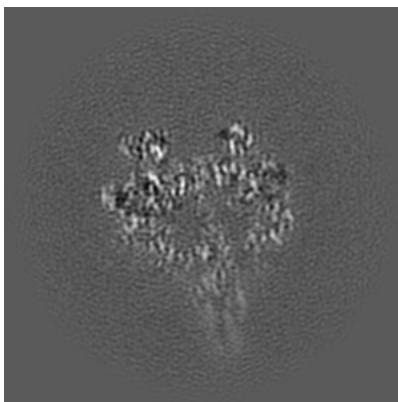
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

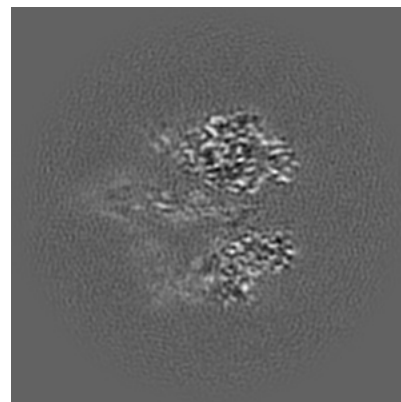
6.2.1 Primary map



X Index: 128

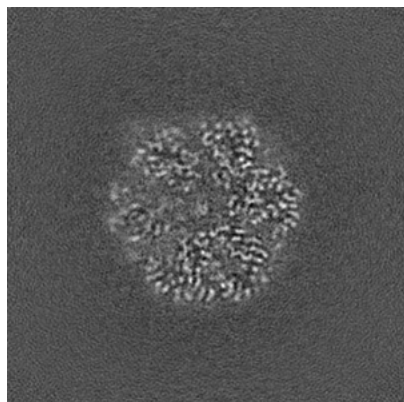


Y Index: 128

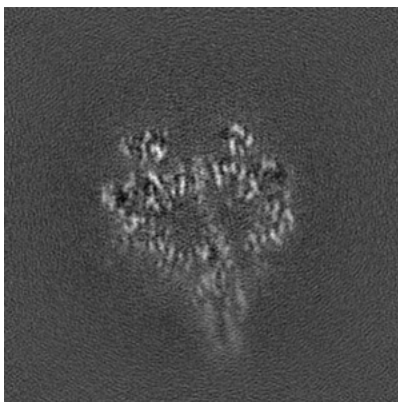


Z Index: 128

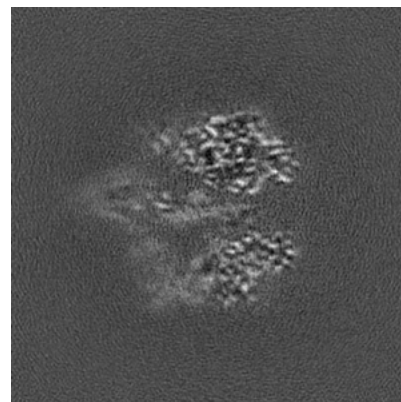
6.2.2 Raw map



X Index: 128



Y Index: 128

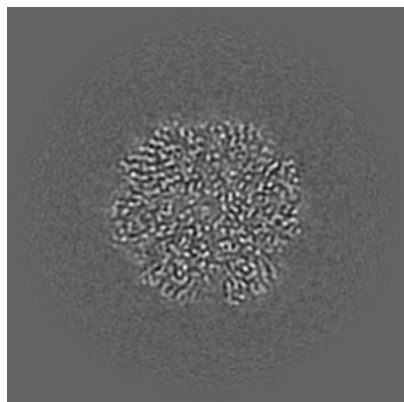


Z Index: 128

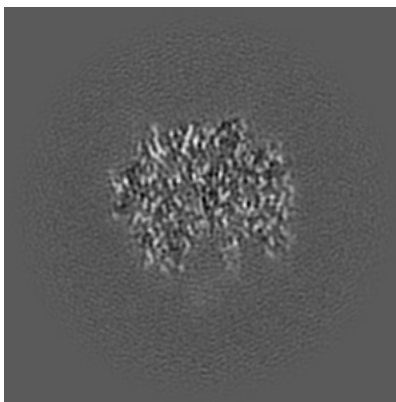
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

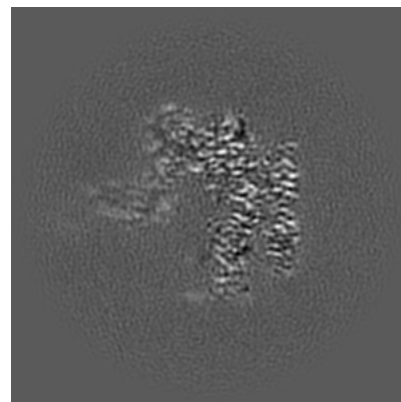
6.3.1 Primary map



X Index: 143

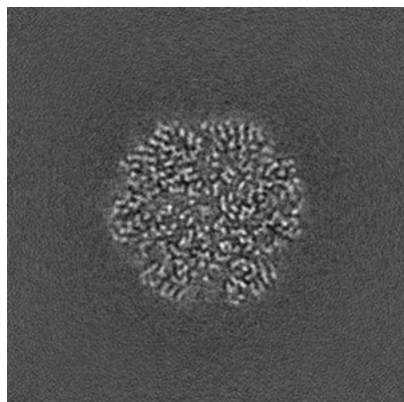


Y Index: 151

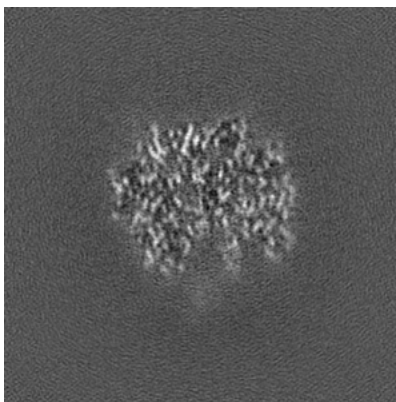


Z Index: 141

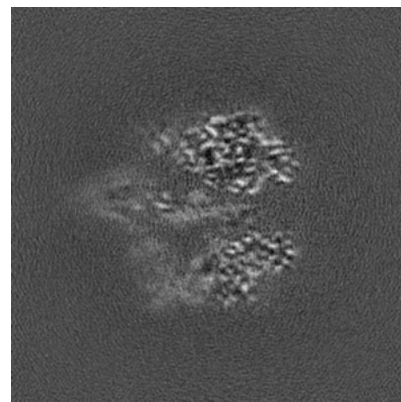
6.3.2 Raw map



X Index: 144



Y Index: 151

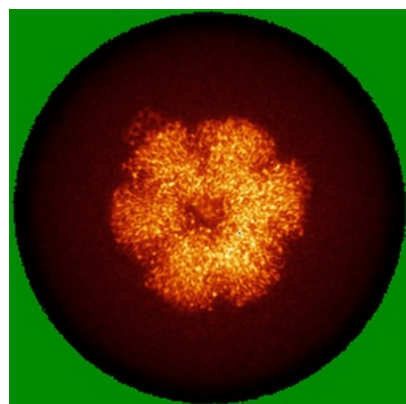


Z Index: 128

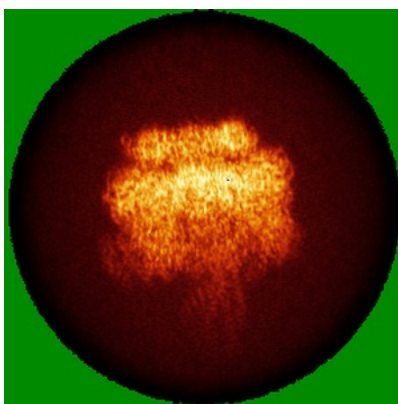
The images above show the largest variance slices of the map in three orthogonal directions.

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

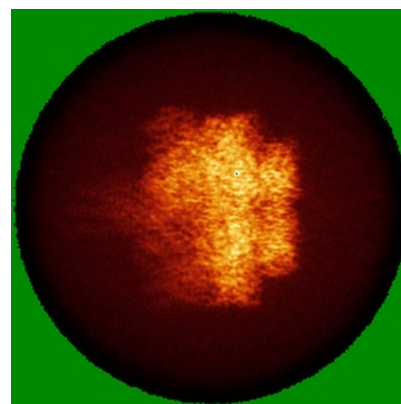
6.4.1 Primary map



X

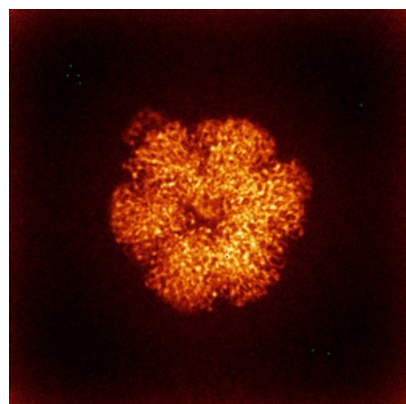


Y

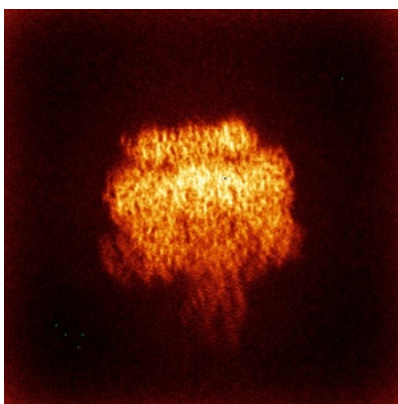


Z

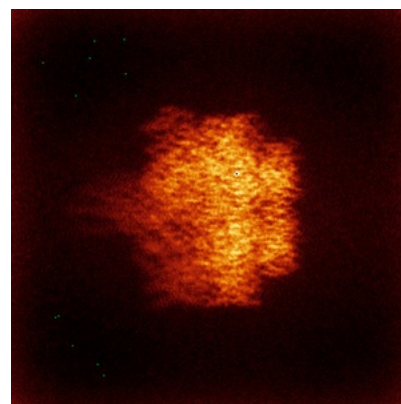
6.4.2 Raw map



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

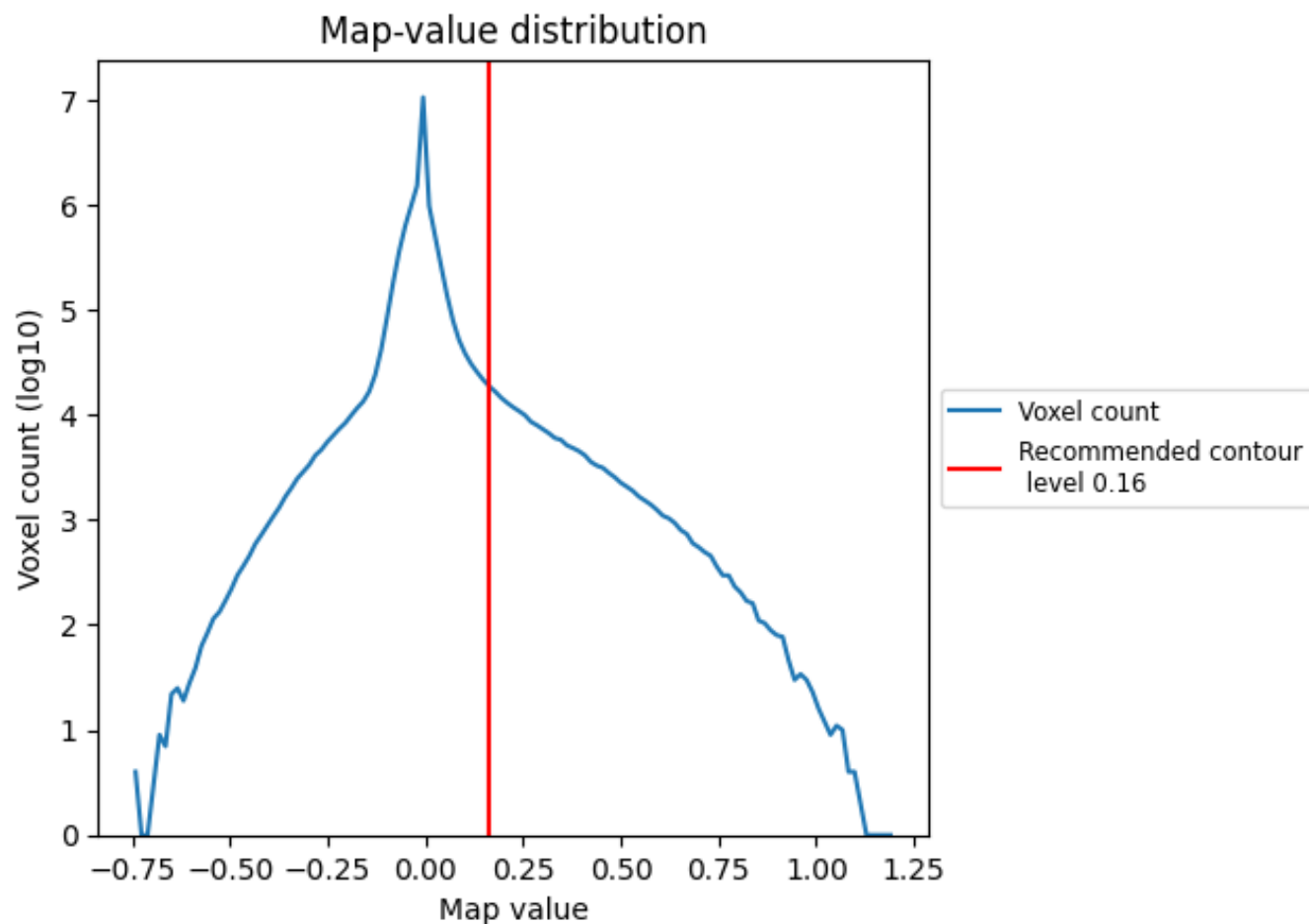
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

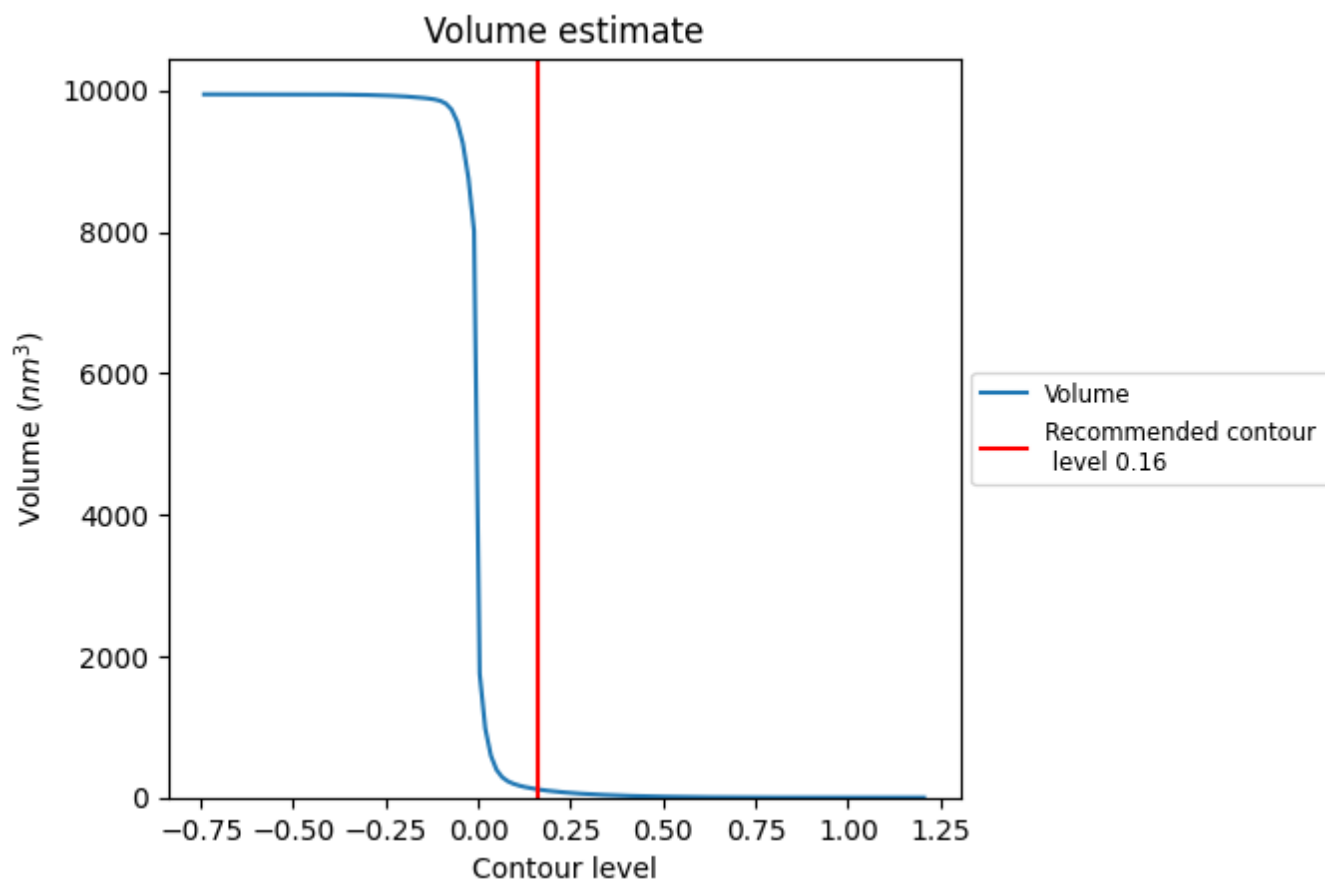
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

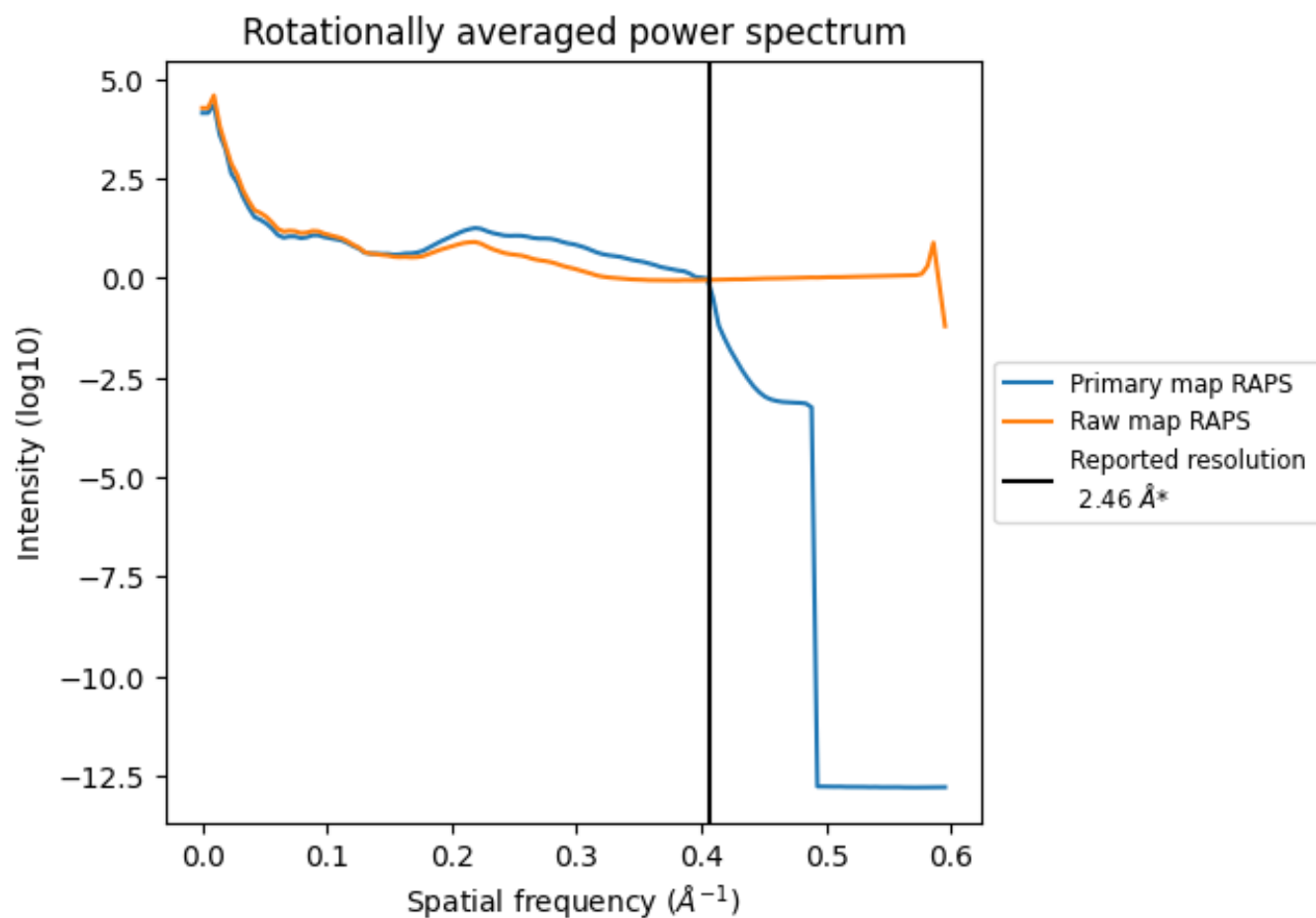
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 117 nm³; this corresponds to an approximate mass of 106 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 ⓘ

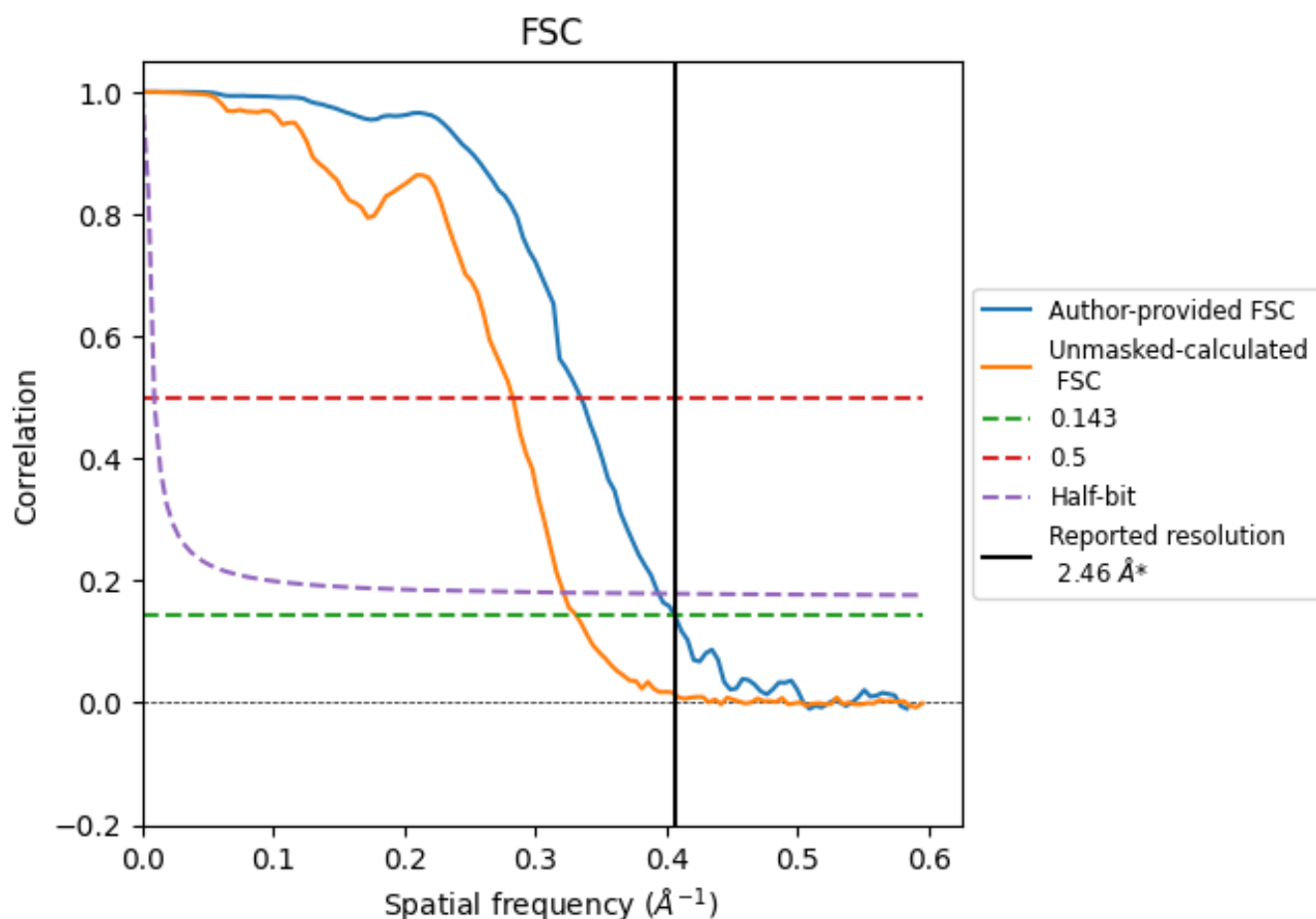


*Reported resolution corresponds to spatial frequency of 0.407 \AA^{-1}

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 0.407 \AA^{-1}

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.46	-	-
Author-provided FSC curve	2.46	2.99	2.54
Unmasked-calculated*	3.02	3.54	3.11

*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 3.02 differs from the reported value 2.46 by more than 10 %

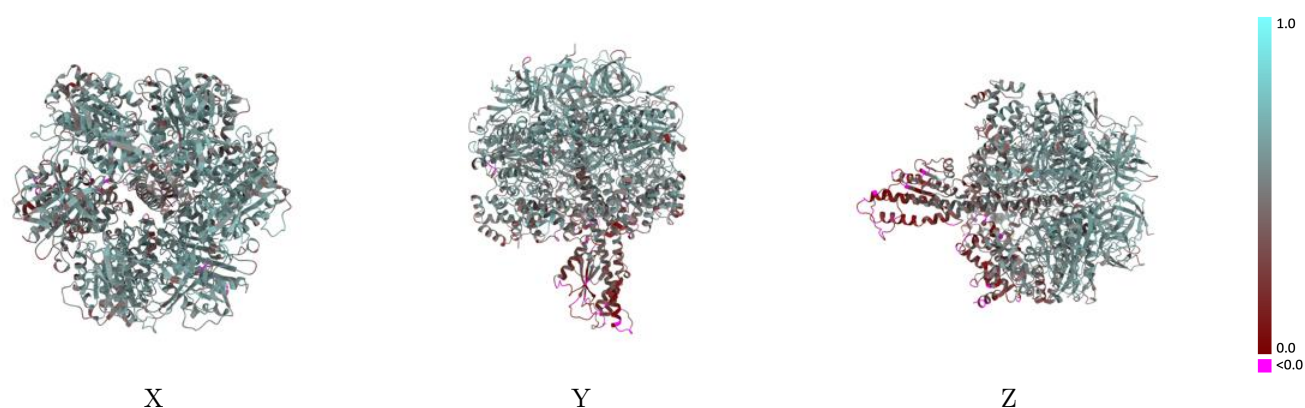
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-49839 and PDB model 9NVL. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)

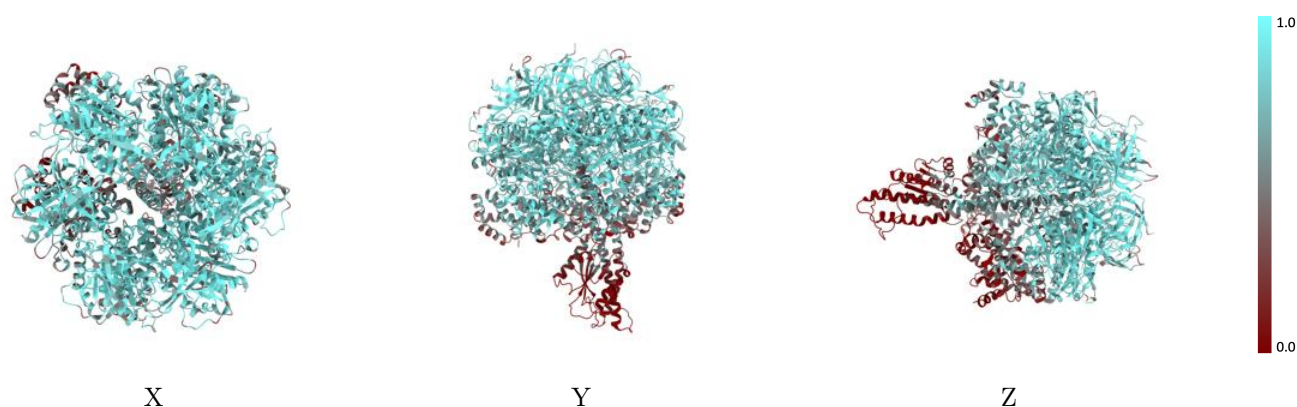
This section was not generated.

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



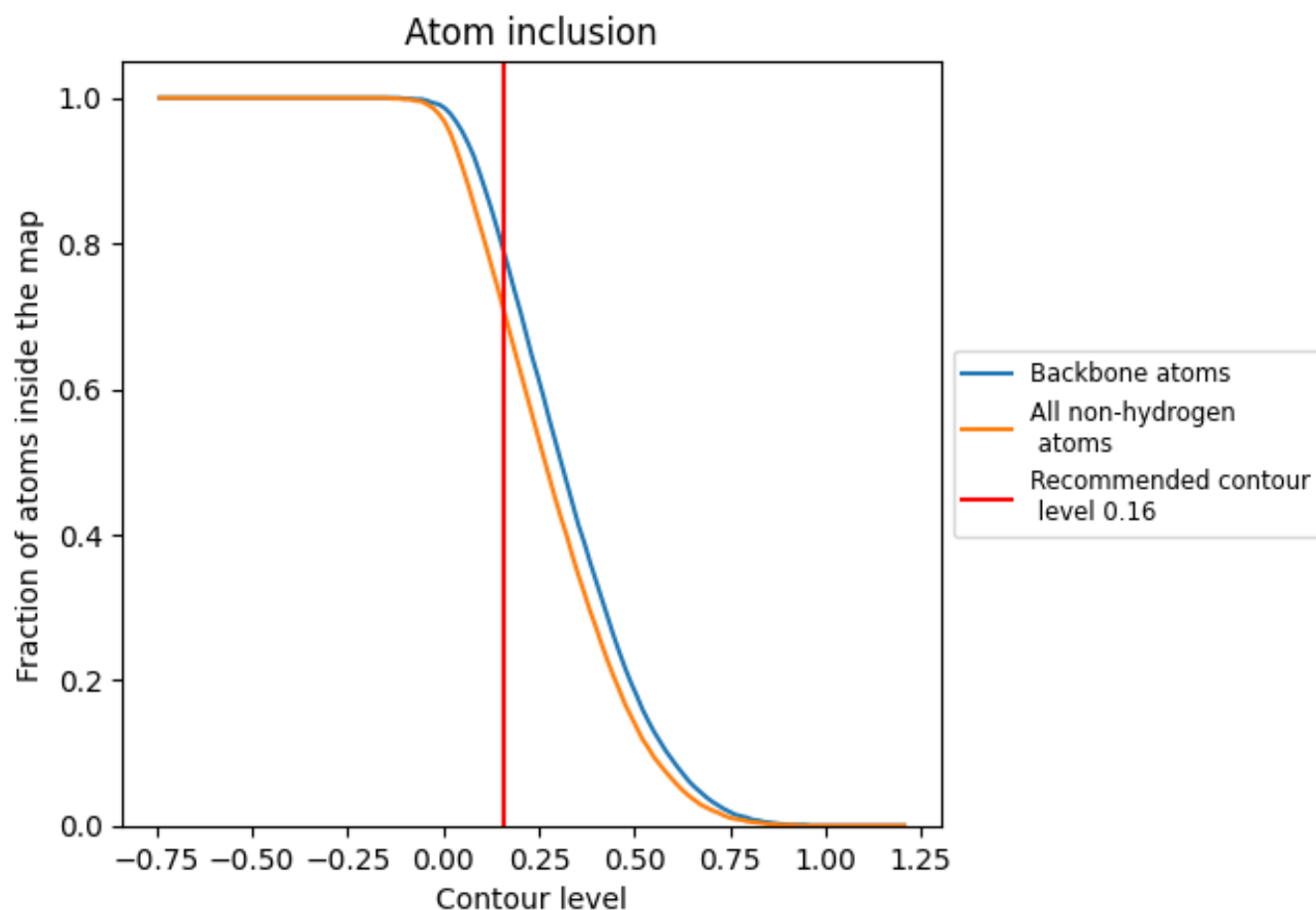
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [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 (0.16).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 70% 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 (0.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7050	<div></div> 0.5000
A	<div></div> 0.7310	<div></div> 0.5320
B	<div></div> 0.7360	<div></div> 0.5200
C	<div></div> 0.8150	<div></div> 0.5510
D	<div></div> 0.8100	<div></div> 0.5570
E	<div></div> 0.5800	<div></div> 0.4230
F	<div></div> 0.8230	<div></div> 0.5480
G	<div></div> 0.2650	<div></div> 0.2780

1.0

0.0

<0.0