



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 07:40 AM UTC

PDB ID : 9NVM / pdb_00009nvm
EMDB ID : EMD-49840
Title : ATPase Hybrid F1 with the ancestral core domains Catalytic Dwell
Authors : Stewart, A.G.; Noji, H.; Sobti, M.; Suzuki, A.K.
Deposited on : 2025-03-20
Resolution : 2.58 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.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 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) : 2.49

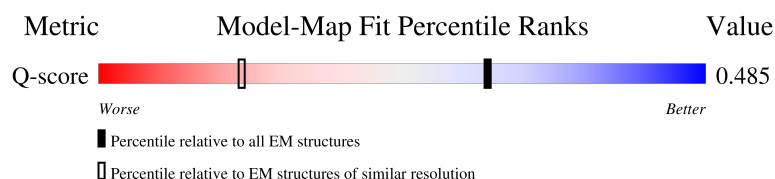
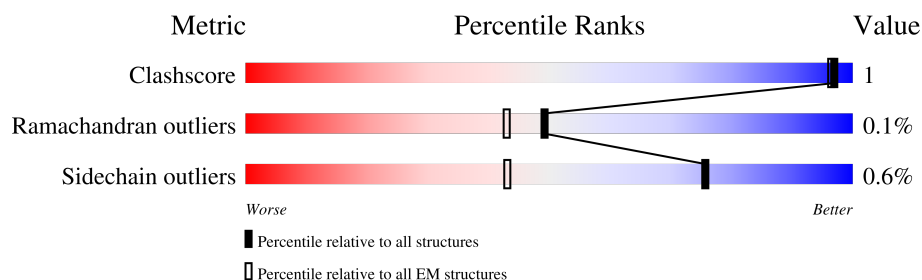
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.58 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	7675 (2.08 - 3.08)

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	14% 89% 6%
1	B	509	17% 90% 7%
1	C	509	13% 90% 7%
2	D	482	15% 94% 7%

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Mol	Chain	Length	Quality of chain
2	E	482	21% 94% ..
2	F	482	8% 93% ..
3	G	285	75% 97% ..

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 24284 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 alpha chains.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	476	Total	C	N	O	S	0	0
			3661	2314	633	702	12		
1	B	475	Total	C	N	O	S	0	0
			3655	2311	632	700	12		
1	C	475	Total	C	N	O	S	0	0
			3655	2311	632	700	12		

- Molecule 2 is a protein called ATPase hybrid F1 with the ancestral core domains beta chains.

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
			3650	2312	629	694	15		
2	F	470	Total	C	N	O	S	0	0
			3668	2324	633	696	15		

- 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 Q5KUJ2
G	215	CYS	ILE	conflict	UNP Q5KUJ2

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



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

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

Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total Mg 1 1	0
5	C	1	Total Mg 1 1	0
5	D	1	Total Mg 1 1	0
5	F	1	Total Mg 1 1	0

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).

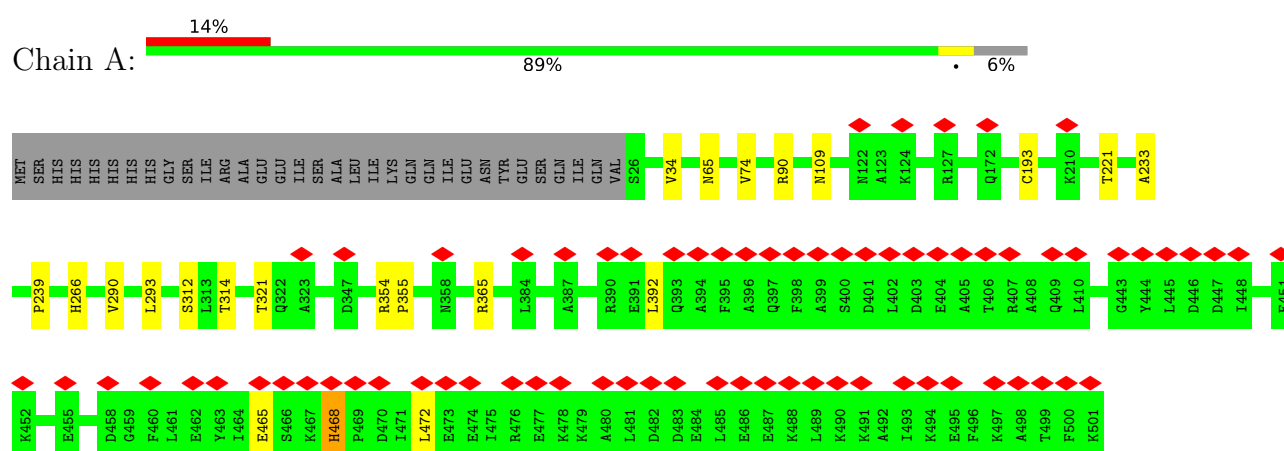


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
6	F	1	27	10	5	10	2	0

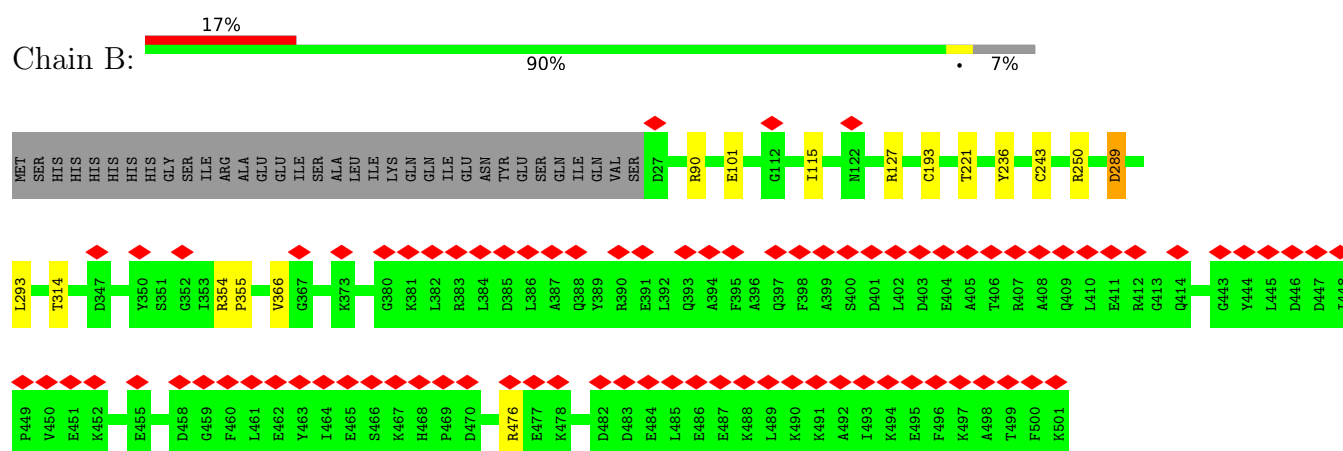
3 Residue-property plots

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

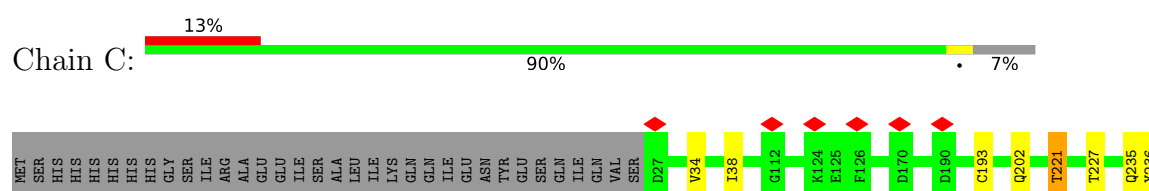
- Molecule 1: ATPase hybrid F1 with the ancestral core domains alpha chains

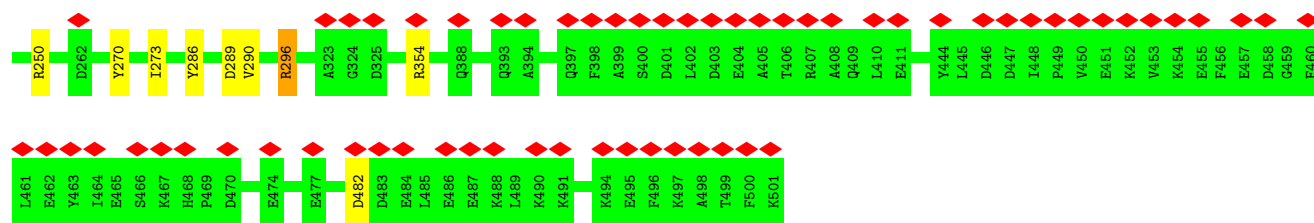


- Molecule 1: ATPase hybrid F1 with the ancestral core domains alpha chains

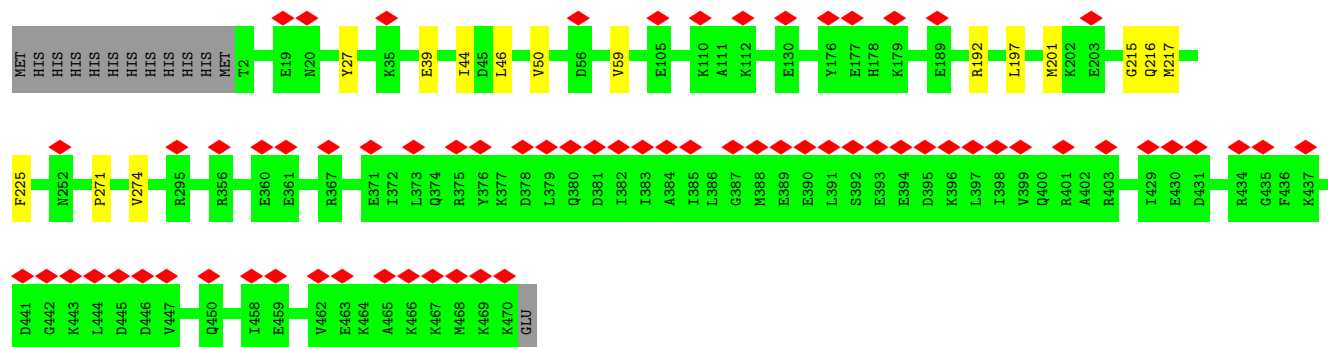


- Molecule 1: ATPase hybrid F1 with the ancestral core domains alpha chains

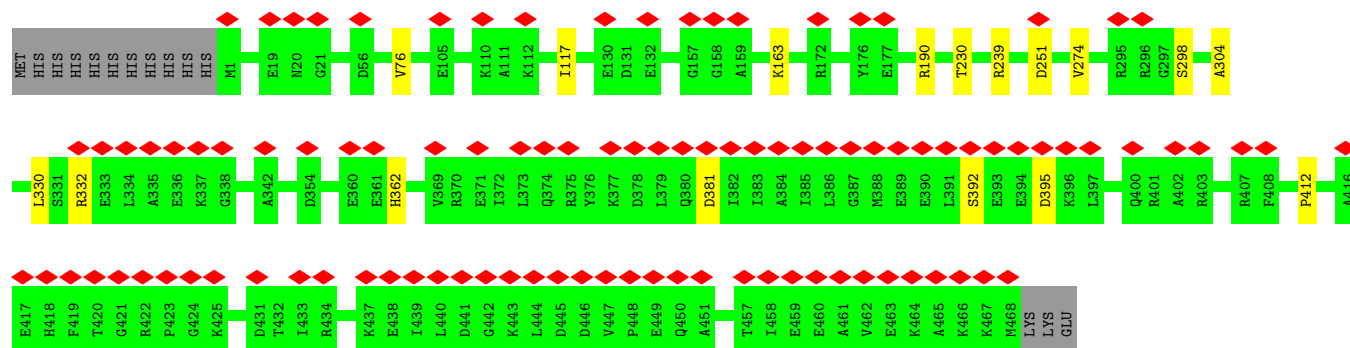




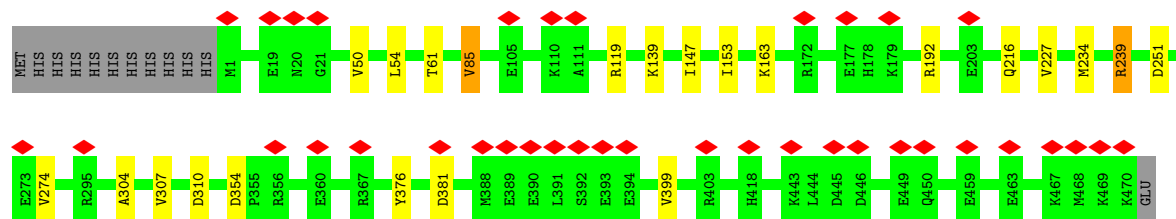
- Molecule 2: ATPase hybrid F1 with the ancestral core domains beta chains



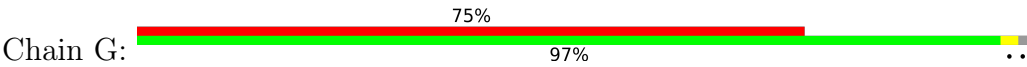
- Molecule 2: ATPase hybrid F1 with the ancestral core domains beta chains



- Molecule 2: ATPase hybrid F1 with the ancestral core domains beta chains



- Molecule 3: ATP synthase gamma chain



A198	E199	N200	K201	Q202	R203	T204	V205	Y206	E207	F208	E209	P210	S211	Q212	E213	E214	C215	L216	D217	V218	L219	L220	P221	Q222	Y223	A224	E225	S226	L227	I228	Y229	G230	A231	L232	L233	D234	A235	K236	A237	S238			A241	A242			K248			D252	E256			R259			N285	A286	L287	GLN	
L138	D139	I140	T141	R142	L143	F144	D145	Q146	P147	S148	F149	A150	D151	I152	K153	E154	I155	A156	R157	K158	T159	V160	G161	L162	F163	A164	D165	G166	T167	F168	D169	E170	L171	Y172	M173	Y174	Y175	N176	H177	Y178	V179	S180	A181	I182	Q183	Q184	E185	V186	T187	E188	R189	K190	L191	L192	P193	L194	T195	D196	L197		
V76	K77	K78	T79	G80	Y81	L82	V83	I84	D87	R88	G89	L90	A91	G92					N95	S96	N97	V98	L99	R100	L101	V102	Y103	Q104	T105	I106	Q107	K108	R109	H110	A111	C112	P113	D114	E115	Y116	A117	I118	I119	V120	I121	G122	R123	V124	G125	L126	S127	F128	F129	R130	K131	R132	N133	M134	P135	V136	I137
MET	ALA	S6	L7	R8	D9	I10	K19	Q22			E28	M29	V30	S31	T32	S33	K34	L35	N36	R37	A38	E39	Q40	N41	A42	K43	S44	F45	V46	P47	Y48	M49	E50	K51	I52	Q53	E54	V55	V56	A57	N58	V59	A60	L61	G62	A63	G64	G65	A66	S67	H68	P69	M70	L71	V72	S73	R74	P75			

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	206455	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)	200	Depositor
Maximum defocus (nm)	1000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.326	Depositor
Minimum map value	-0.834	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.047	Depositor
Recommended contour level	0.15	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: MG, ATP, 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	0.81	0/3717	1.44	7/5020 (0.1%)
1	B	0.82	1/3711 (0.0%)	1.43	8/5012 (0.2%)
1	C	0.81	0/3711	1.43	6/5012 (0.1%)
2	D	0.82	0/3726	1.41	7/5039 (0.1%)
2	E	0.82	0/3716	1.41	8/5027 (0.2%)
2	F	0.81	0/3734	1.44	16/5049 (0.3%)
3	G	0.82	0/2244	1.41	4/3036 (0.1%)
All	All	0.82	1/24559 (0.0%)	1.43	56/33195 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	2
2	D	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	90	ARG	CZ-NH2	-8.81	1.22	1.33

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	216	GLN	N-CA-C	6.86	118.70	110.19
2	E	239	ARG	NE-CZ-NH2	6.64	125.17	119.20
1	C	289	ASP	CA-CB-CG	6.59	119.19	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	ASN	CA-CB-CG	6.56	119.16	112.60
1	B	366	VAL	CA-C-N	6.53	126.31	120.10
1	B	366	VAL	C-N-CA	6.53	126.31	120.10
2	E	412	PRO	N-CA-CB	6.51	106.57	102.92
2	E	190	ARG	NE-CZ-NH2	6.35	124.92	119.20
2	F	54	LEU	N-CA-CB	-6.26	101.21	110.53
1	B	289	ASP	CA-CB-CG	6.25	118.85	112.60
2	D	192	ARG	NE-CZ-NH2	6.13	124.72	119.20
3	G	146	GLN	CB-CA-C	6.04	116.50	110.33
2	F	239	ARG	NE-CZ-NH2	6.00	124.60	119.20
1	C	250	ARG	NE-CZ-NH2	5.76	124.38	119.20
1	A	365	ARG	NE-CZ-NH2	5.71	124.34	119.20
1	C	482	ASP	CA-CB-CG	5.67	118.27	112.60
2	E	381	ASP	CA-CB-CG	5.65	118.25	112.60
1	A	392	LEU	N-CA-C	5.65	117.24	111.14
2	E	395	ASP	CA-CB-CG	5.62	118.22	112.60
1	B	250	ARG	NE-CZ-NH2	5.59	124.23	119.20
2	F	119	ARG	NE-CZ-NH2	5.58	124.22	119.20
2	F	119	ARG	CA-C-N	5.57	123.67	119.66
2	F	119	ARG	C-N-CA	5.57	123.67	119.66
2	F	381	ASP	CA-CB-CG	5.53	118.13	112.60
3	G	259	ARG	NE-CZ-NH2	5.53	124.17	119.20
2	D	217	MET	N-CA-C	5.52	118.01	111.33
1	B	127	ARG	NE-CZ-NH2	5.51	124.16	119.20
1	B	101	GLU	CA-C-N	5.47	128.16	120.28
1	B	101	GLU	C-N-CA	5.47	128.16	120.28
1	A	312	SER	N-CA-C	5.47	117.53	108.13
2	D	215	GLY	CA-C-N	5.46	130.78	121.29
2	D	215	GLY	C-N-CA	5.46	130.78	121.29
2	F	227	VAL	N-CA-C	5.45	116.18	110.62
2	E	332	ARG	NE-CZ-NH2	5.40	124.06	119.20
3	G	109	ARG	NE-CZ-NH2	5.34	124.00	119.20
1	C	296	ARG	NE-CZ-NH2	5.33	123.99	119.20
1	B	476	ARG	NE-CZ-NH2	5.32	123.99	119.20
1	C	235	GLN	OE1-CD-NE2	-5.28	117.32	122.60
2	F	216	GLN	OE1-CD-NE2	-5.24	117.36	122.60
2	D	216	GLN	OE1-CD-NE2	-5.23	117.37	122.60
2	F	85	VAL	N-CA-C	5.23	113.59	107.89
2	F	307	VAL	CA-C-N	5.22	125.52	119.47
2	F	307	VAL	C-N-CA	5.22	125.52	119.47
2	D	225	PHE	CA-CB-CG	5.21	119.01	113.80
2	F	354	ASP	CA-CB-CG	5.18	117.78	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	468	HIS	CB-CG-CD2	-5.15	124.51	131.20
1	A	90	ARG	NE-CZ-NH2	5.13	123.82	119.20
2	E	362	HIS	CB-CG-CD2	-5.12	124.54	131.20
2	F	139	LYS	N-CA-C	5.10	117.23	111.11
1	A	109	ASN	CA-CB-CG	5.09	117.69	112.60
2	F	192	ARG	NE-CZ-NH2	5.07	123.76	119.20
1	C	221	THR	CA-CB-CG2	5.05	119.08	110.50
2	F	310	ASP	CA-C-N	5.03	130.20	122.95
2	F	310	ASP	C-N-CA	5.03	130.20	122.95
3	G	157	ARG	NE-CZ-NH2	5.02	123.72	119.20
2	E	298	SER	N-CA-C	5.01	117.42	109.50

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	296	ARG	Sidechain
1	C	354	ARG	Sidechain
2	D	27	TYR	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	3661	0	3727	6	0
1	B	3655	0	3723	4	0
1	C	3655	0	3722	8	0
2	D	3660	0	3710	4	0
2	E	3650	0	3697	4	0
2	F	3668	0	3722	6	0
3	G	2211	0	2257	1	0
4	A	31	0	12	0	0
4	C	31	0	12	0	0
4	D	31	0	12	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	1	0	0	0	0
6	F	27	0	12	0	0
All	All	24284	0	24606	32	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 (32) 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:C:193:CYS:HB2	1:C:221:THR:HG22	1.65	0.77
1:A:193:CYS:HB2	1:A:221:THR:HG22	1.74	0.69
1:C:236:TYR:CZ	1:C:273:ILE:HD12	2.33	0.63
1:C:202:GLN:HG2	1:C:227:THR:HG21	1.80	0.62
2:D:197:LEU:HD11	2:D:201:MET:HE2	1.81	0.61
2:E:251:ASP:O	2:E:304:ALA:HB3	2.01	0.61
1:A:239:PRO:HD3	1:A:266:HIS:CE1	2.38	0.59
1:B:193:CYS:HB2	1:B:221:THR:HG22	1.84	0.57
1:C:236:TYR:CE2	1:C:273:ILE:HD12	2.41	0.56
1:C:236:TYR:CZ	1:C:270:TYR:HA	2.43	0.53
1:C:286:TYR:HB3	1:C:290:VAL:HG21	1.91	0.53
1:B:236:TYR:CE1	1:B:293:LEU:HD11	2.45	0.52
2:D:50:VAL:HG13	2:D:59:VAL:CG1	2.41	0.51
1:C:38:ILE:HD11	1:C:273:ILE:HG23	1.93	0.50
2:F:147:ILE:HG23	2:F:153:ILE:HD11	1.93	0.49
2:E:163:LYS:HG2	2:E:330:LEU:HD12	1.95	0.48
1:B:236:TYR:HE1	1:B:293:LEU:HD11	1.78	0.48
2:F:376:TYR:CE1	2:F:399:VAL:HG23	2.50	0.47
2:F:251:ASP:O	2:F:304:ALA:HB3	2.16	0.46
2:E:117:ILE:HD12	2:E:230:THR:HA	1.98	0.46
2:F:85:VAL:CG1	2:F:234:MET:HE3	2.46	0.45
2:F:50:VAL:HA	2:F:61:THR:HG22	1.97	0.45
2:D:271:PRO:HD3	3:G:287:LEU:HD12	1.98	0.45
1:A:74:VAL:HG12	1:A:233:ALA:HB2	1.98	0.44
1:C:202:GLN:CG	1:C:227:THR:HG21	2.45	0.44
2:E:163:LYS:HG2	2:E:330:LEU:CD1	2.48	0.44
1:B:354:ARG:HA	1:B:355:PRO:C	2.45	0.42
1:A:465:GLU:HA	1:A:468:HIS:CD2	2.56	0.41
1:A:354:ARG:HA	1:A:355:PRO:C	2.45	0.41
2:F:163:LYS:HB2	2:F:163:LYS:HE3	1.87	0.40
1:A:472:LEU:HD13	1:A:472:LEU:C	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:39:GLU:CD	2:D:39:GLU:H	2.30	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	474/509 (93%)	465 (98%)	9 (2%)	0	100	100
1	B	473/509 (93%)	461 (98%)	12 (2%)	0	100	100
1	C	473/509 (93%)	462 (98%)	11 (2%)	0	100	100
2	D	467/482 (97%)	451 (97%)	15 (3%)	1 (0%)	43	63
2	E	466/482 (97%)	452 (97%)	13 (3%)	1 (0%)	43	63
2	F	468/482 (97%)	453 (97%)	14 (3%)	1 (0%)	43	63
3	G	280/285 (98%)	275 (98%)	5 (2%)	0	100	100
All	All	3101/3258 (95%)	3019 (97%)	79 (2%)	3 (0%)	49	69

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	274	VAL
2	E	274	VAL
2	D	274	VAL

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	385/415 (93%)	380 (99%)	5 (1%)	61	81
1	B	384/415 (92%)	380 (99%)	4 (1%)	68	84
1	C	384/415 (92%)	383 (100%)	1 (0%)	86	94
2	D	395/408 (97%)	393 (100%)	2 (0%)	81	91
2	E	394/408 (97%)	392 (100%)	2 (0%)	81	91
2	F	396/408 (97%)	395 (100%)	1 (0%)	86	94
3	G	238/240 (99%)	237 (100%)	1 (0%)	84	92
All	All	2576/2709 (95%)	2560 (99%)	16 (1%)	76	89

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	VAL
1	A	290	VAL
1	A	293	LEU
1	A	314	THR
1	A	321	THR
1	B	115	ILE
1	B	243	CYS
1	B	289	ASP
1	B	314	THR
1	C	34	VAL
2	D	44	ILE
2	D	46	LEU
2	E	76	VAL
2	E	392	SER
2	F	239	ARG
3	G	90	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	GLN
1	A	442	ASN
1	B	140	GLN
1	B	172	GLN
1	B	186	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	202	GLN
1	B	272	GLN
1	B	397	GLN
1	C	202	GLN
1	C	235	GLN
1	C	272	GLN
1	C	409	GLN
2	D	118	HIS
2	D	195	ASN
2	D	288	GLN
2	D	303	GLN
2	D	347	GLN
2	D	380	GLN
2	D	414	HIS
2	E	33	GLN
2	E	195	ASN
2	E	288	GLN
2	E	303	GLN
2	E	362	HIS
2	E	414	HIS
2	F	178	HIS
2	F	374	GLN
2	F	380	GLN

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 8 ligands modelled in this entry, 4 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	$\# Z > 2$
6	ADP	F	500	-	28,29,29	1.09	2 (7%)	43,45,45	1.23	6 (13%)
4	ATP	C	601	5	32,33,33	1.11	0	48,52,52	1.24	4 (8%)
4	ATP	A	601	5	32,33,33	1.20	3 (9%)	48,52,52	1.25	6 (12%)
4	ATP	D	501	5	32,33,33	1.32	4 (12%)	48,52,52	1.22	6 (12%)

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	F	500	-	-	3/16/32/32	0/3/3/3
4	ATP	C	601	5	-	0/22/38/38	0/3/3/3
4	ATP	A	601	5	-	1/22/38/38	0/3/3/3
4	ATP	D	501	5	-	3/22/38/38	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	501	ATP	PB-O3A	-2.94	1.56	1.59
4	D	501	ATP	PB-O3B	-2.88	1.56	1.59
4	D	501	ATP	PA-O3A	-2.77	1.56	1.59
6	F	500	ADP	PA-O3A	-2.60	1.56	1.59
4	A	601	ATP	PB-O3A	-2.52	1.56	1.59
4	A	601	ATP	PA-O3A	-2.48	1.56	1.59
4	D	501	ATP	C5-C4	-2.18	1.35	1.39
6	F	500	ADP	C5-C4	-2.07	1.35	1.39
4	A	601	ATP	PG-O3G	-2.05	1.47	1.54

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	601	ATP	C5-C4-N3	-3.19	122.32	126.72

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	ATP	C5-C4-N3	-3.08	122.47	126.72
4	D	501	ATP	C4-C5-N7	3.07	114.10	110.58
4	D	501	ATP	O2A-PA-O3A	2.98	115.31	107.27
6	F	500	ADP	C4-C5-N7	2.89	113.88	110.58
4	A	601	ATP	C4-C5-N7	2.86	113.85	110.58
4	C	601	ATP	C4-C5-N7	2.69	113.66	110.58
4	D	501	ATP	O3G-PG-O3B	2.65	113.52	104.64
6	F	500	ADP	C5-C4-N3	-2.58	123.17	126.72
6	F	500	ADP	O2B-PB-O3A	2.56	113.23	104.64
4	D	501	ATP	C5-C4-N3	-2.30	123.54	126.72
4	A	601	ATP	N3-C4-N9	2.29	131.05	127.17
4	A	601	ATP	O2A-PA-O3A	2.27	113.41	107.27
4	C	601	ATP	N3-C4-N9	2.25	130.99	127.17
4	D	501	ATP	O3G-PG-O1G	-2.24	102.09	110.83
4	C	601	ATP	C2-N1-C6	-2.11	115.27	118.73
6	F	500	ADP	C5-C6-N1	2.08	122.78	117.51
6	F	500	ADP	C2-N1-C6	-2.05	115.36	118.73
4	A	601	ATP	C2-N1-C6	-2.04	115.37	118.73
4	D	501	ATP	O2B-PB-O3A	2.04	112.78	107.27
4	A	601	ATP	O3G-PG-O3B	2.03	111.43	104.64
6	F	500	ADP	O2A-PA-O3A	2.01	112.70	107.27

There are no chirality outliers.

All (7) torsion outliers are listed below:

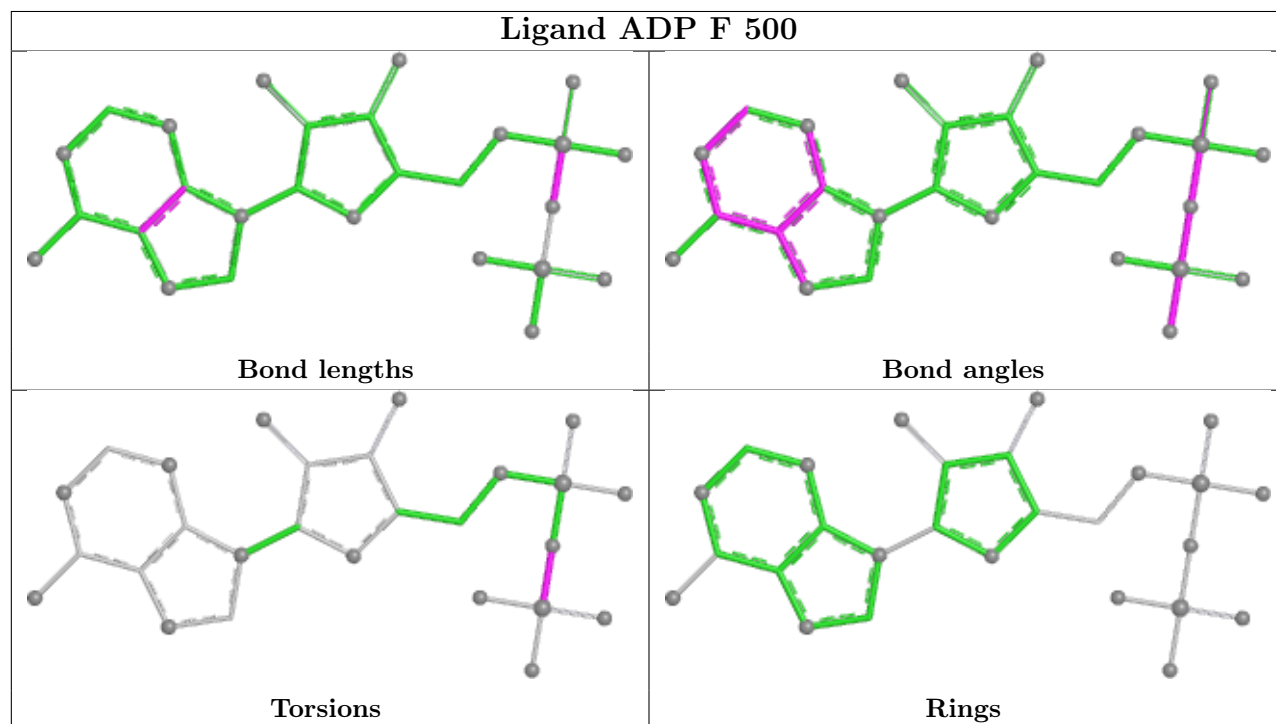
Mol	Chain	Res	Type	Atoms
6	F	500	ADP	PA-O3A-PB-O2B
6	F	500	ADP	PA-O3A-PB-O3B
4	D	501	ATP	O4'-C4'-C5'-O5'
4	D	501	ATP	PG-O3B-PB-O2B
4	A	601	ATP	O4'-C4'-C5'-O5'
6	F	500	ADP	PA-O3A-PB-O1B
4	D	501	ATP	PG-O3B-PB-O1B

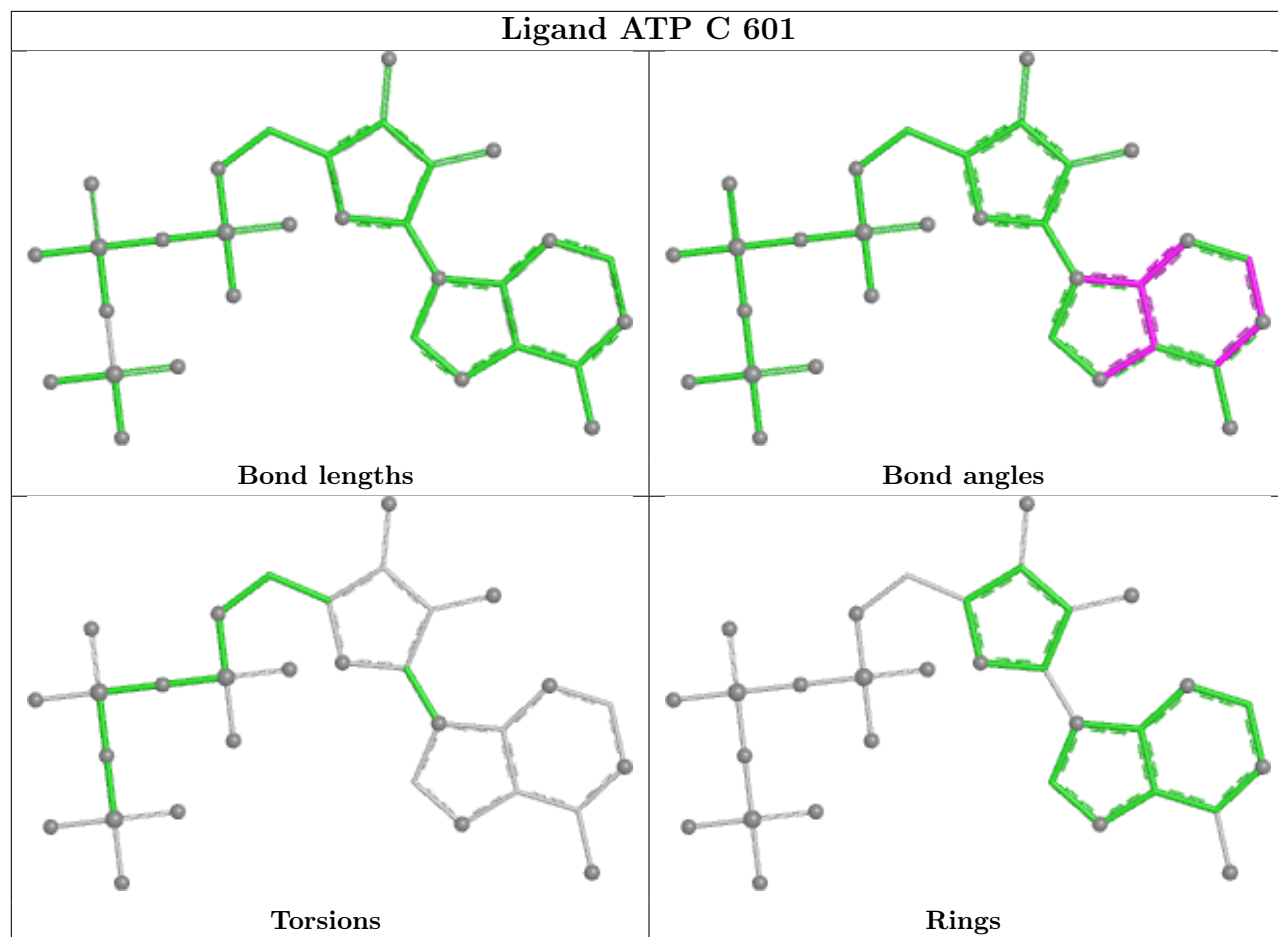
There are no ring outliers.

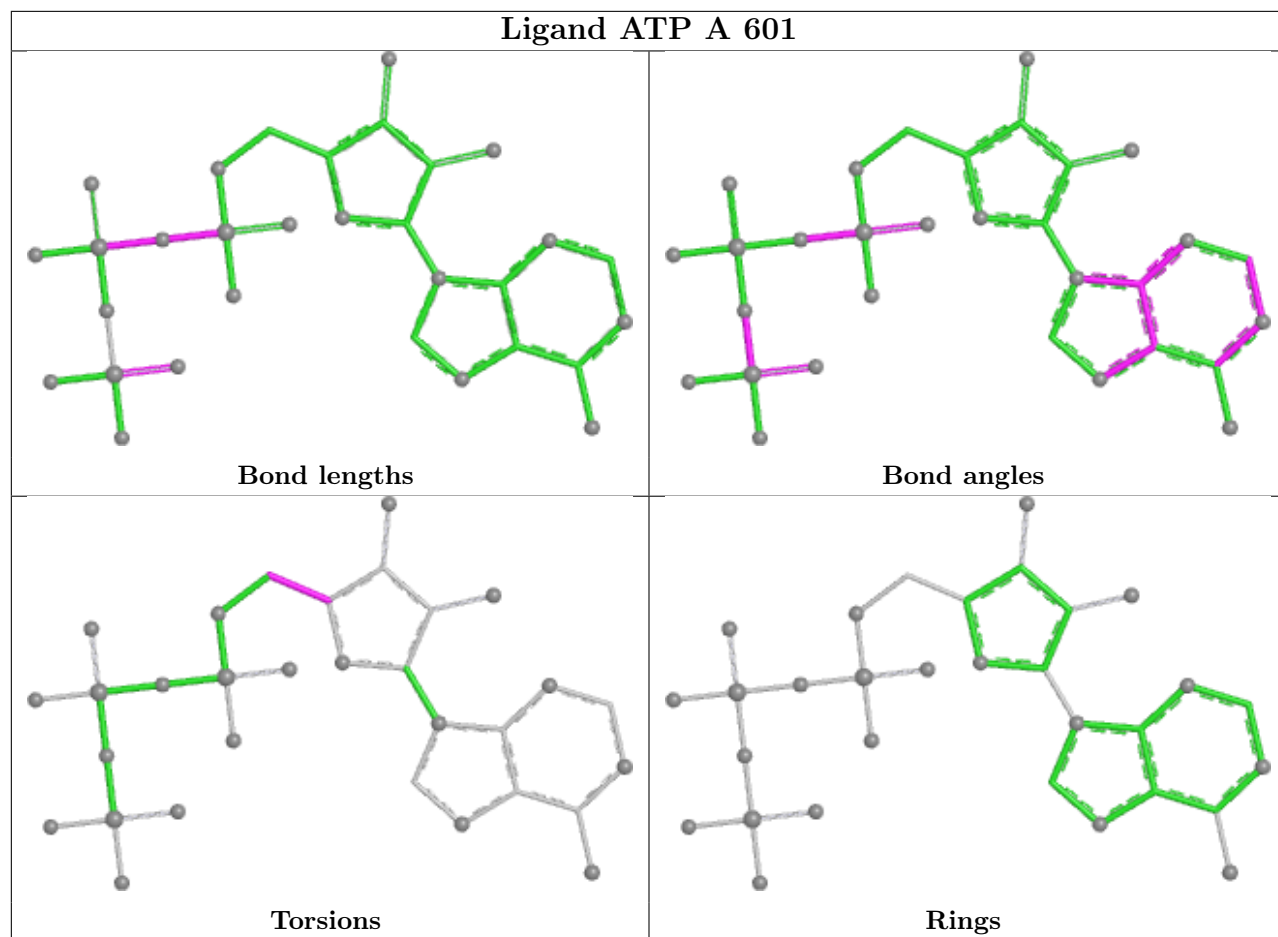
No monomer is involved in short contacts.

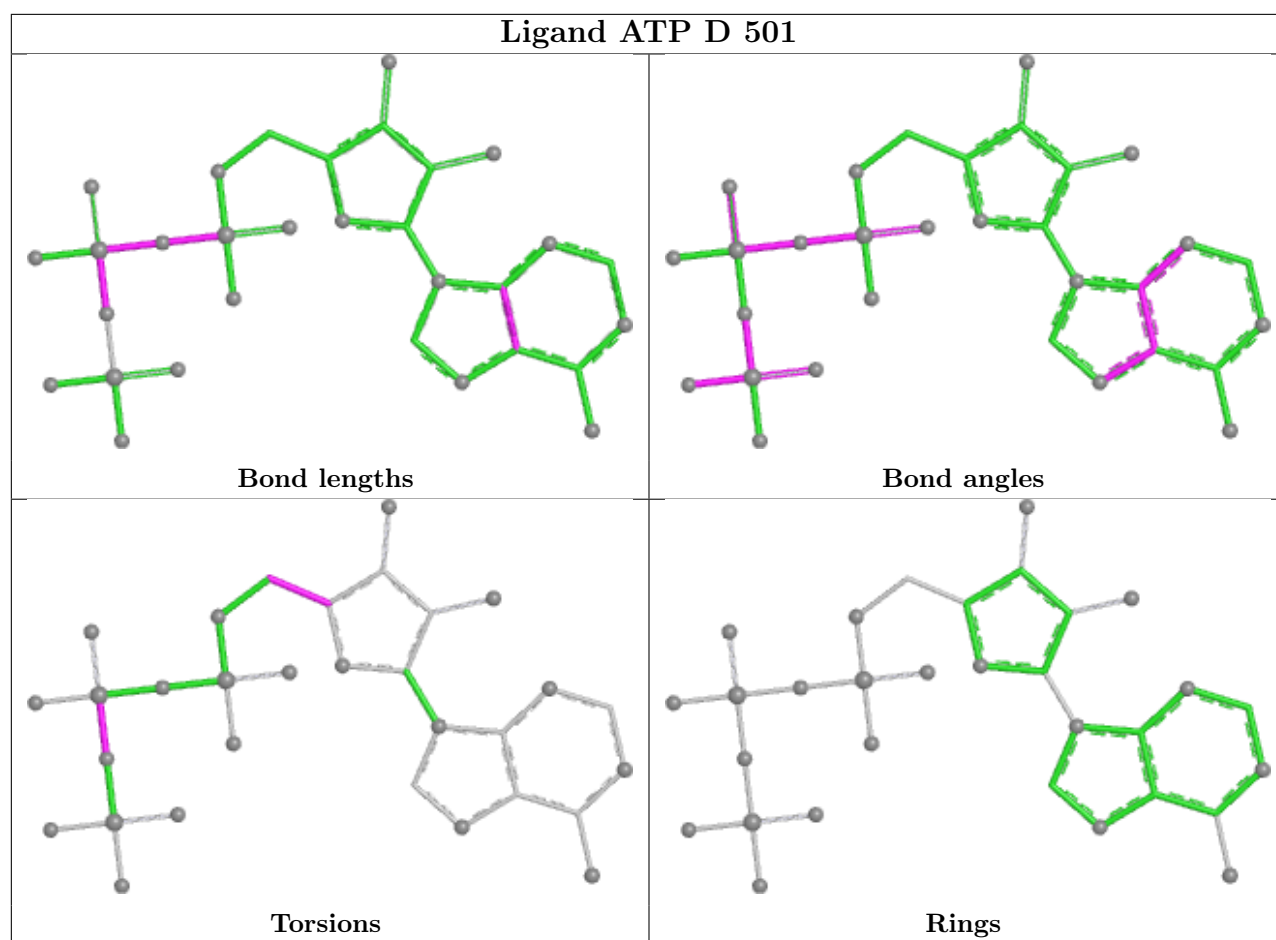
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

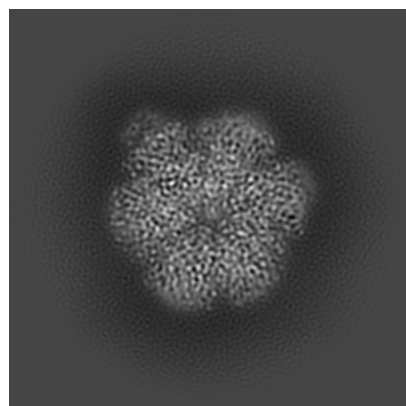
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49840. These allow visual inspection of the internal detail of the map and identification of artifacts.

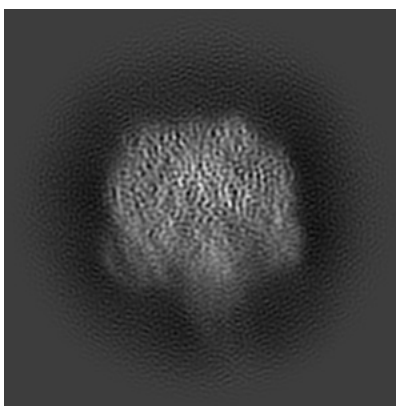
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

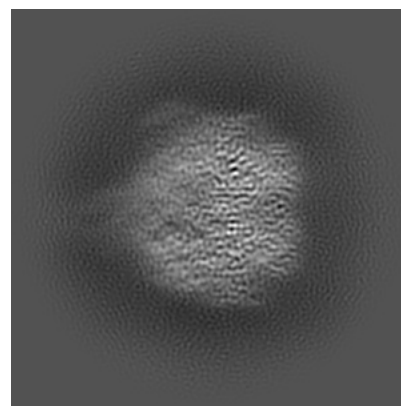
6.1.1 Primary map



X

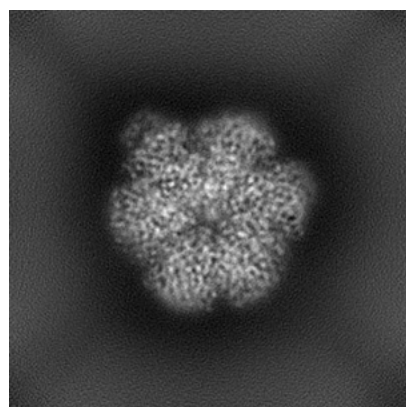


Y

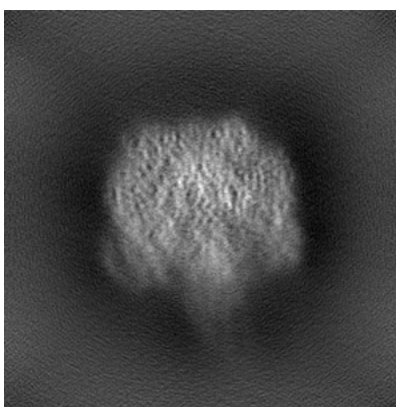


Z

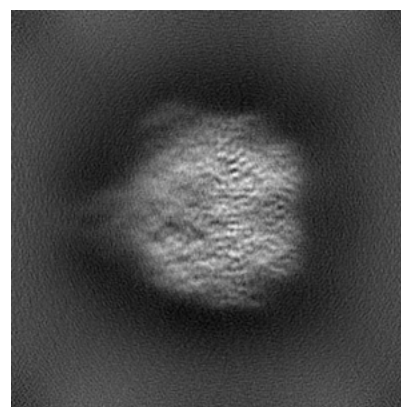
6.1.2 Raw map



X



Y

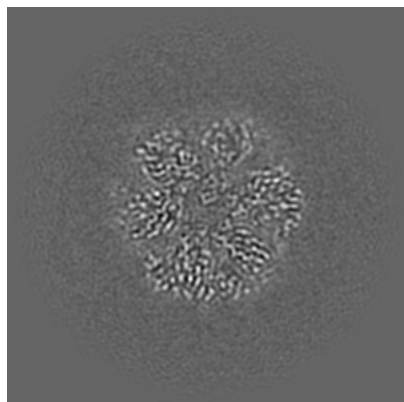


Z

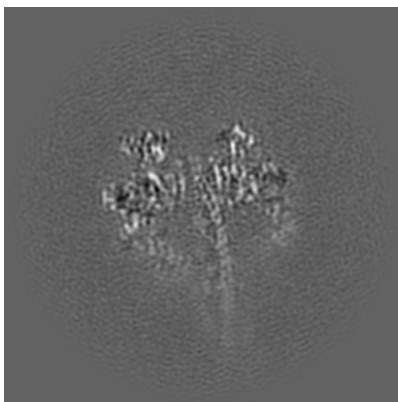
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

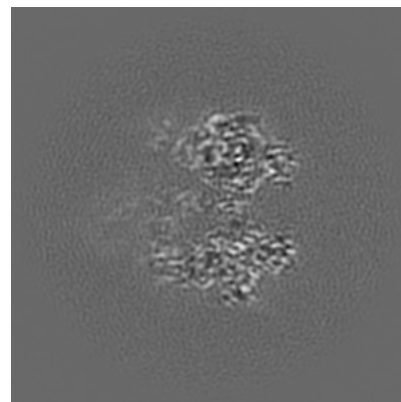
6.2.1 Primary map



X Index: 128

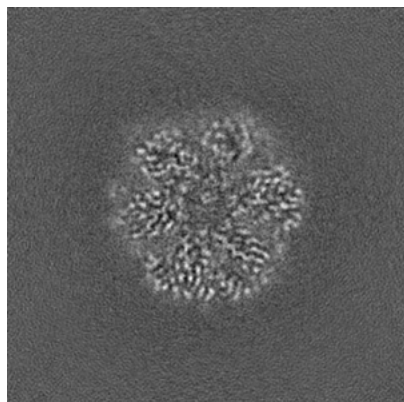


Y Index: 128

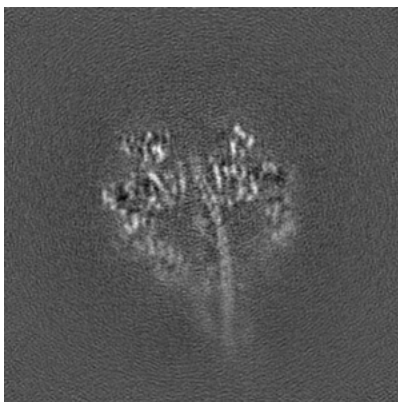


Z Index: 128

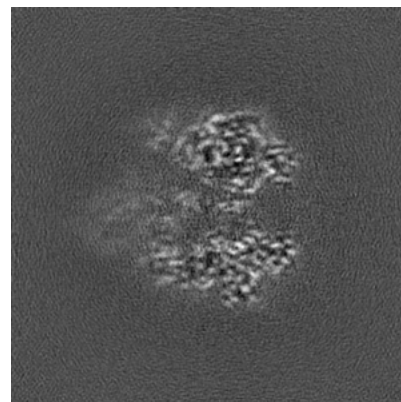
6.2.2 Raw map



X Index: 128



Y Index: 128

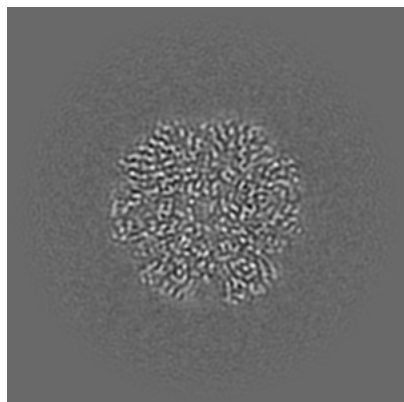


Z Index: 128

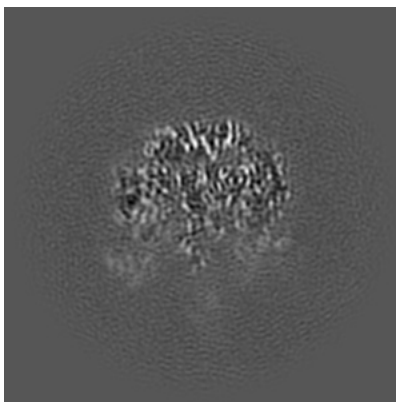
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

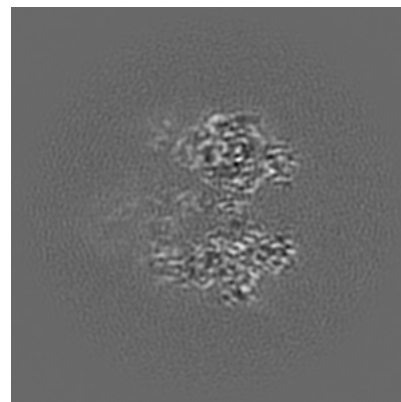
6.3.1 Primary map



X Index: 143

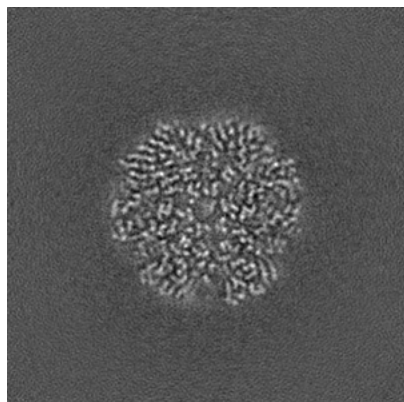


Y Index: 103

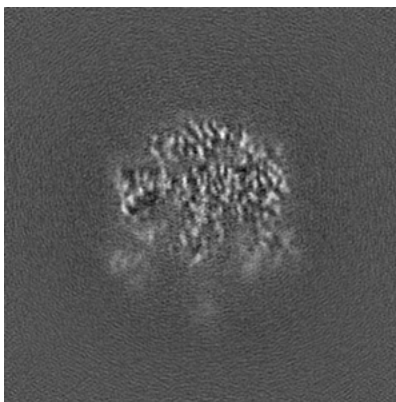


Z Index: 128

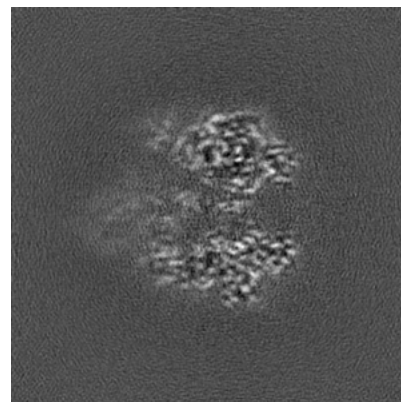
6.3.2 Raw map



X Index: 143



Y Index: 100

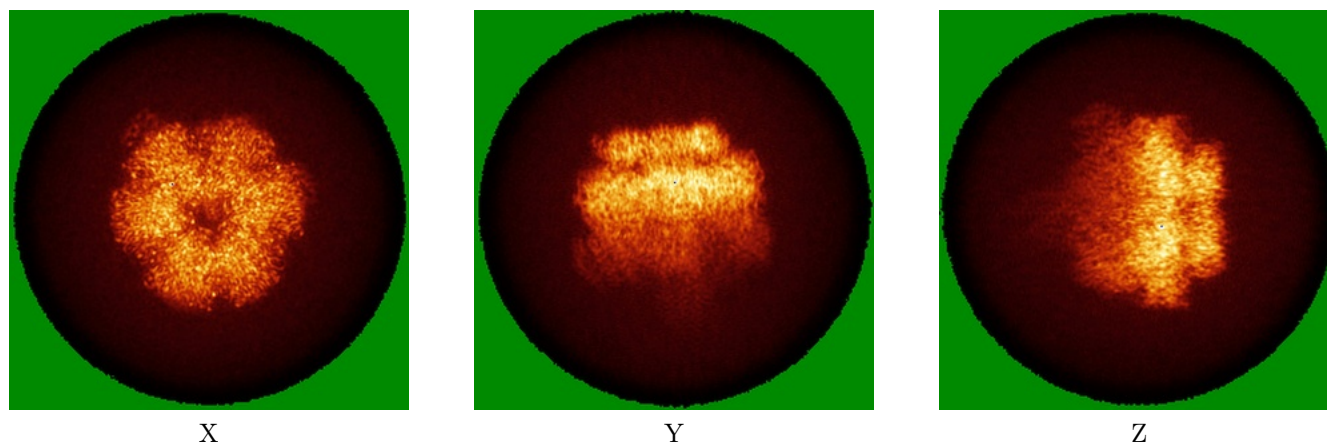


Z Index: 128

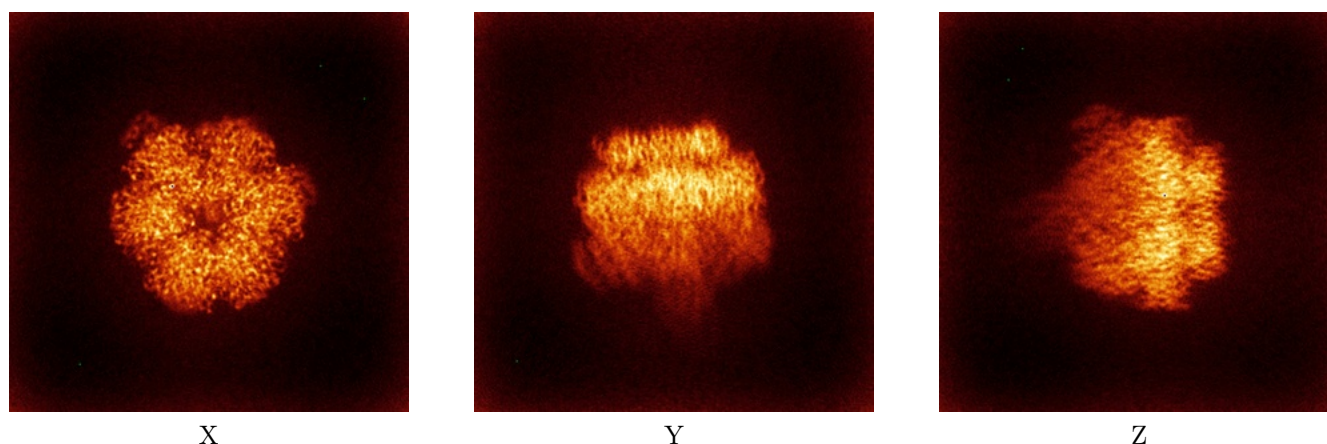
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

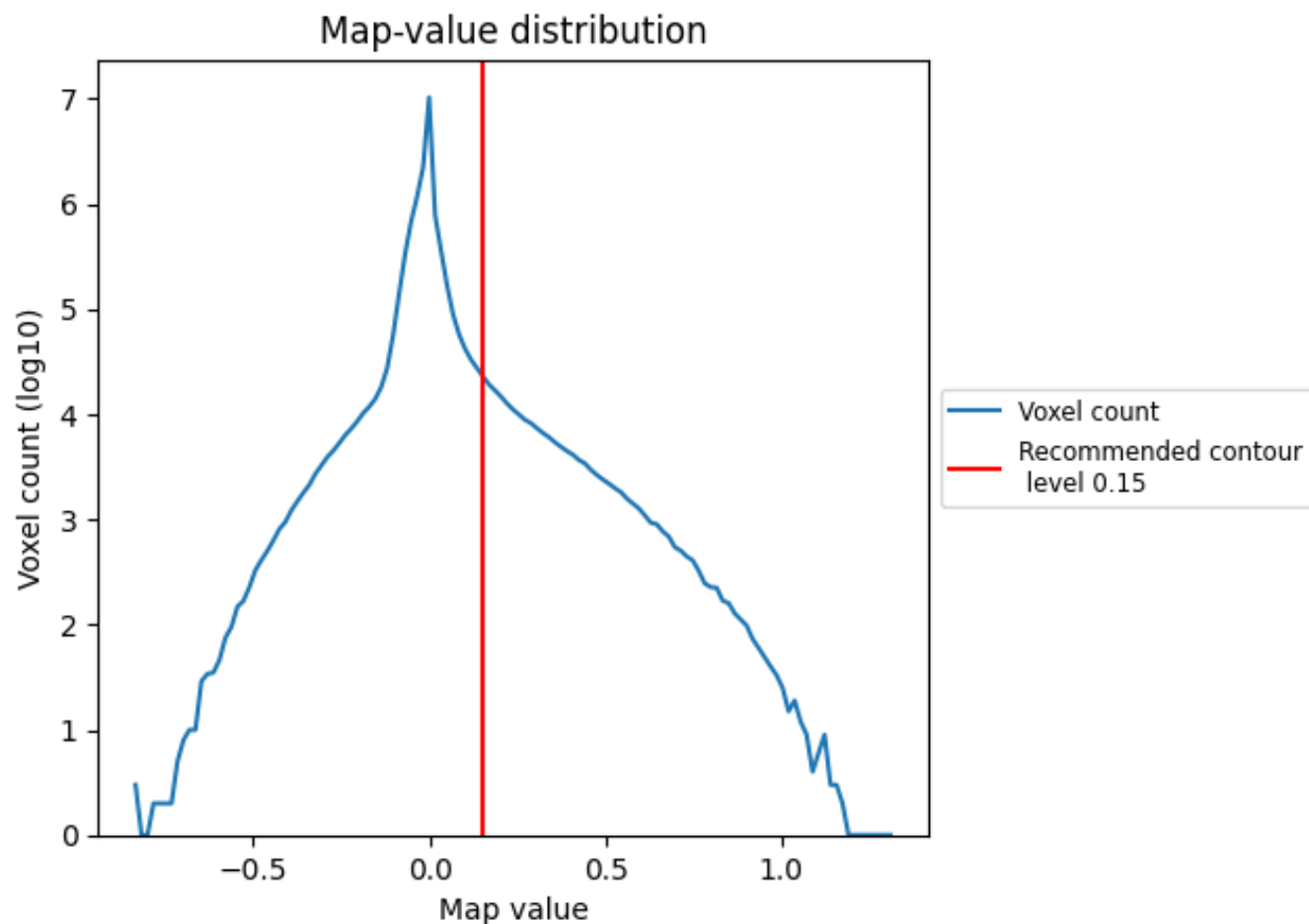
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

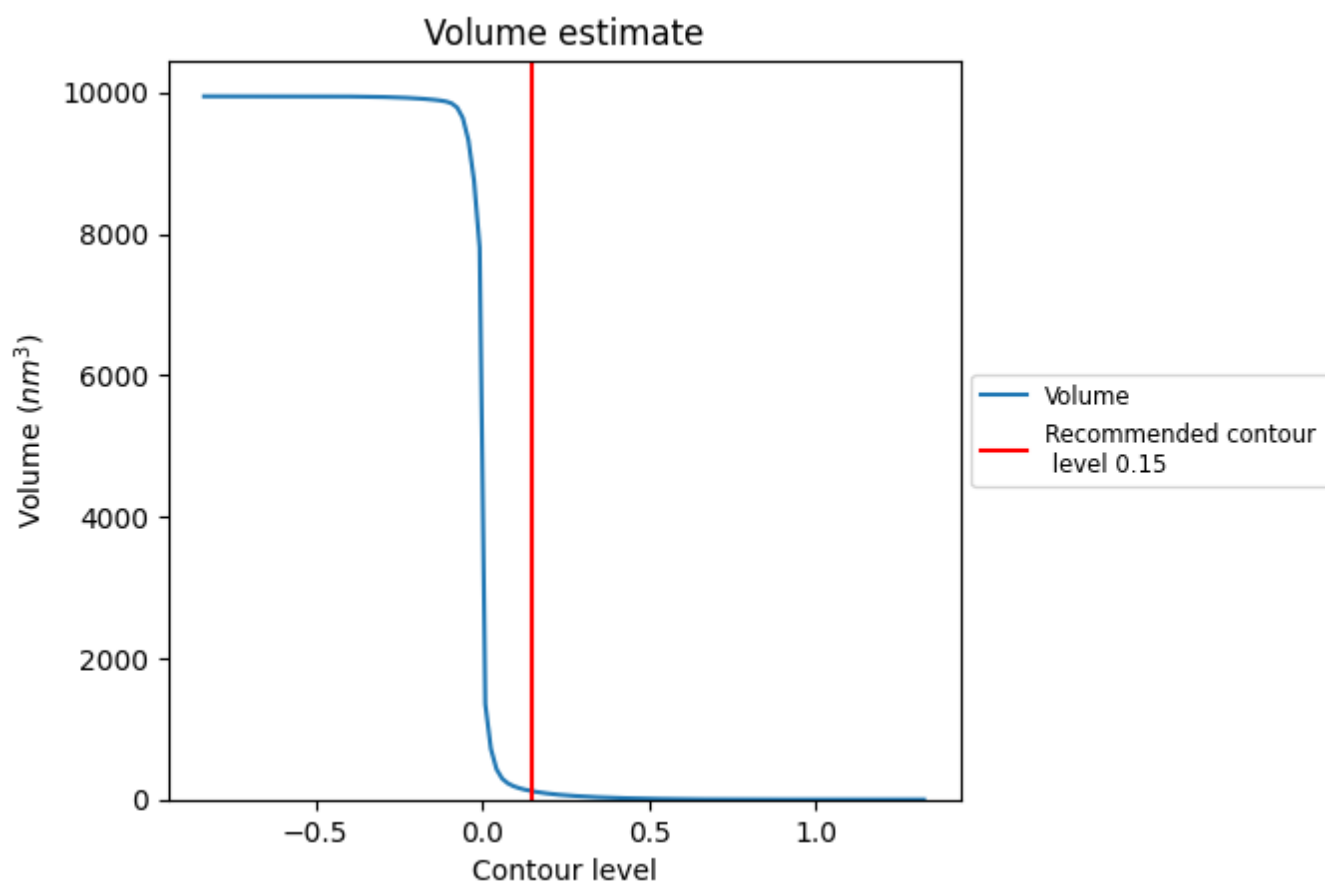
This section contains the results of statistical analysis of the map.

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.

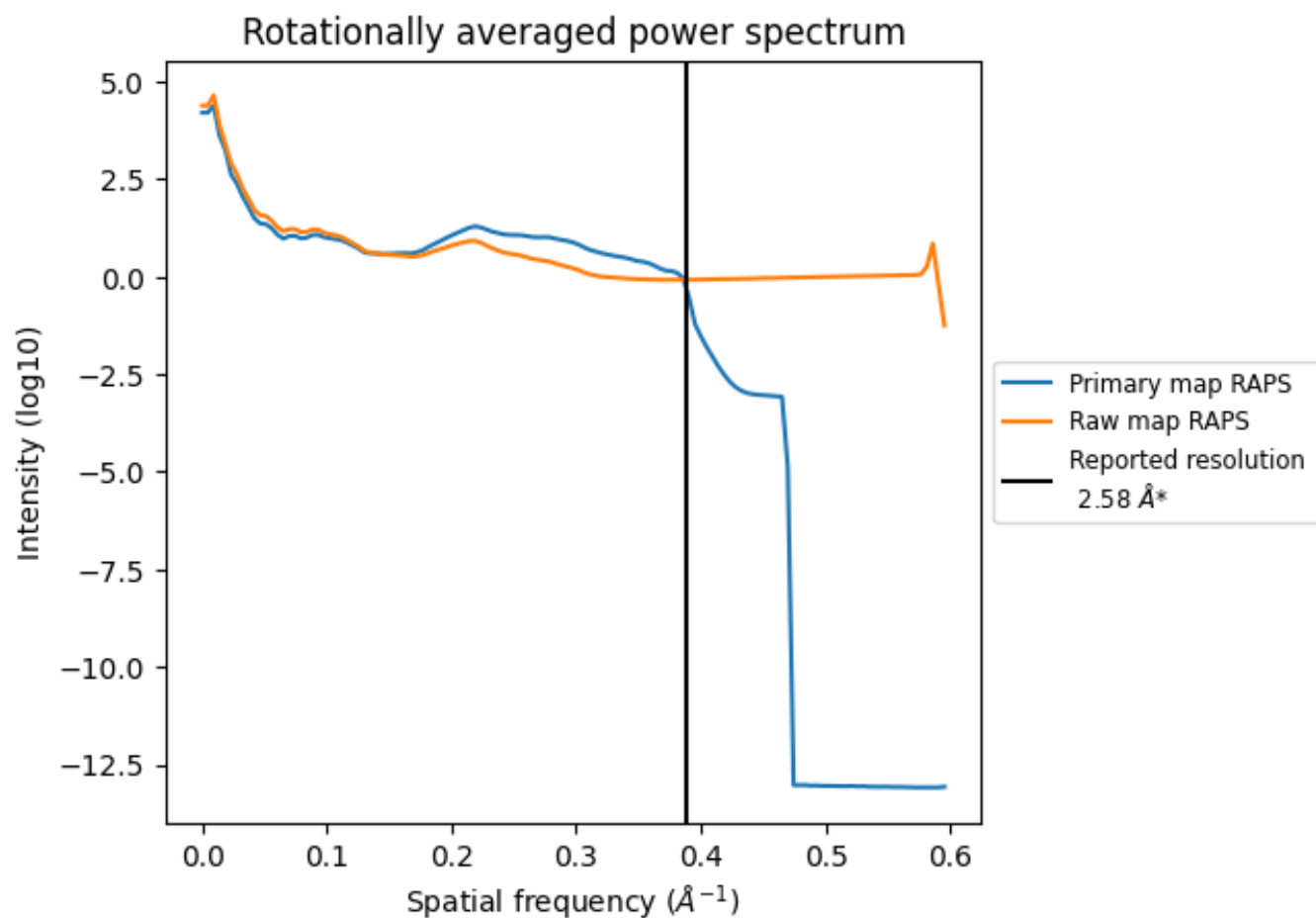
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 119 nm³; this corresponds to an approximate mass of 107 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 ⓘ

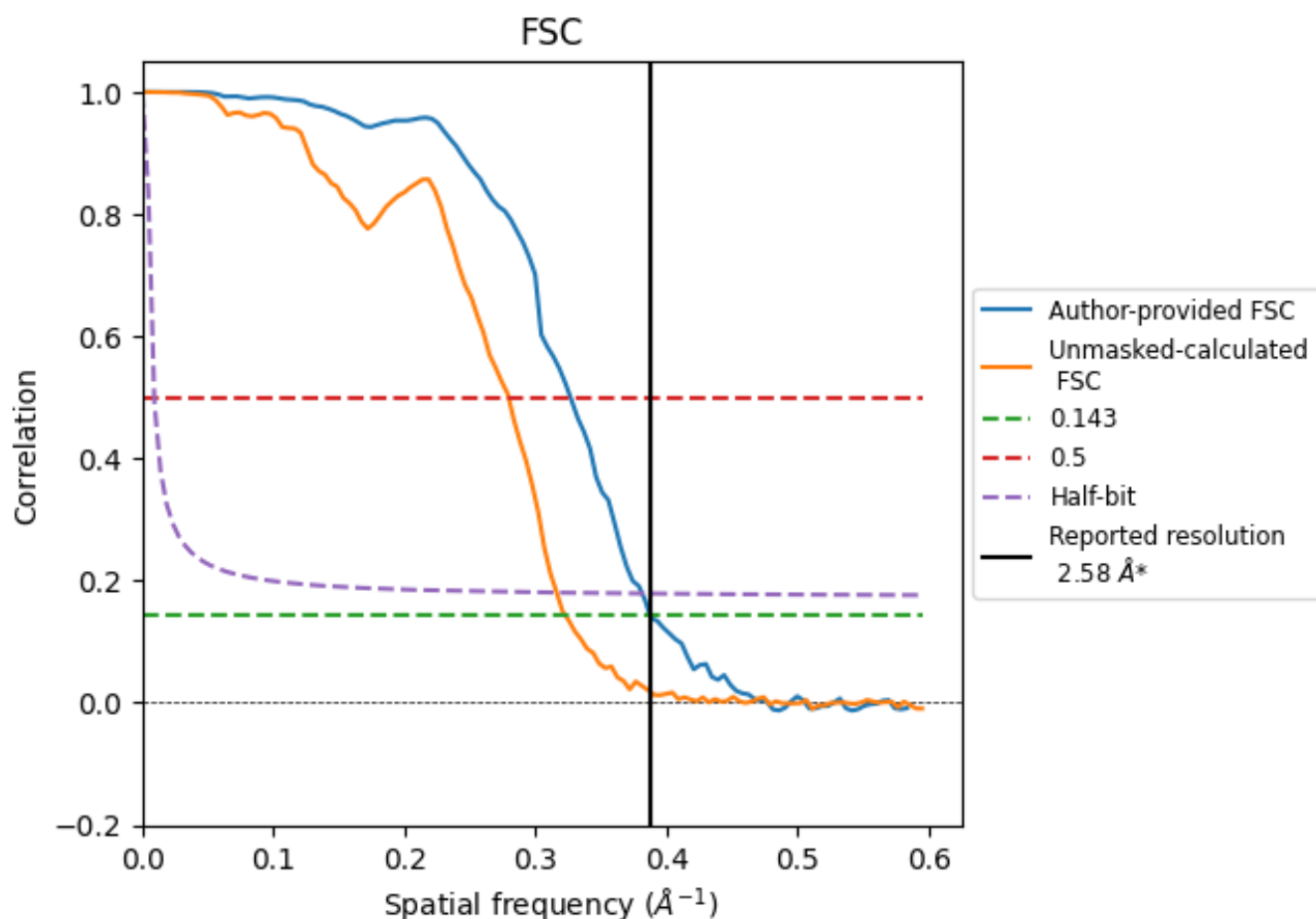


*Reported resolution corresponds to spatial frequency of 0.388 $\text{\AA}^{-1}$

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 0.388 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.58	-	-
Author-provided FSC curve	2.58	3.06	2.62
Unmasked-calculated*	3.10	3.58	3.16

*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 3.10 differs from the reported value 2.58 by more than 10 %

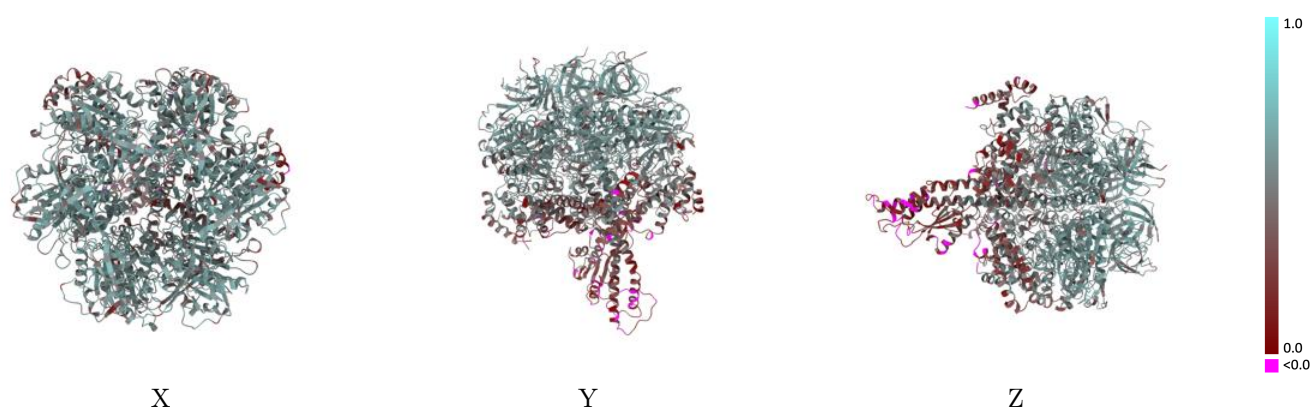
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-49840 and PDB model 9NVM. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)

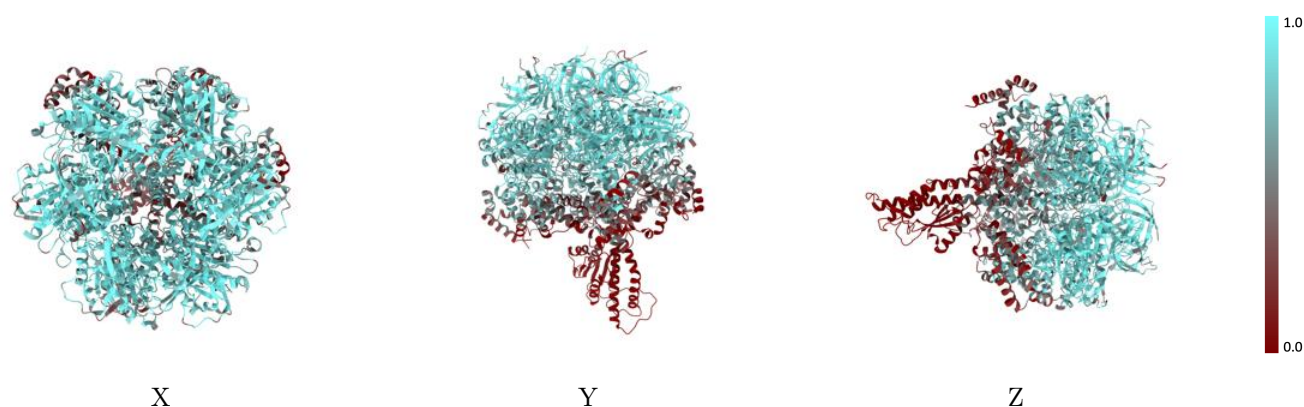
This section was not generated.

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



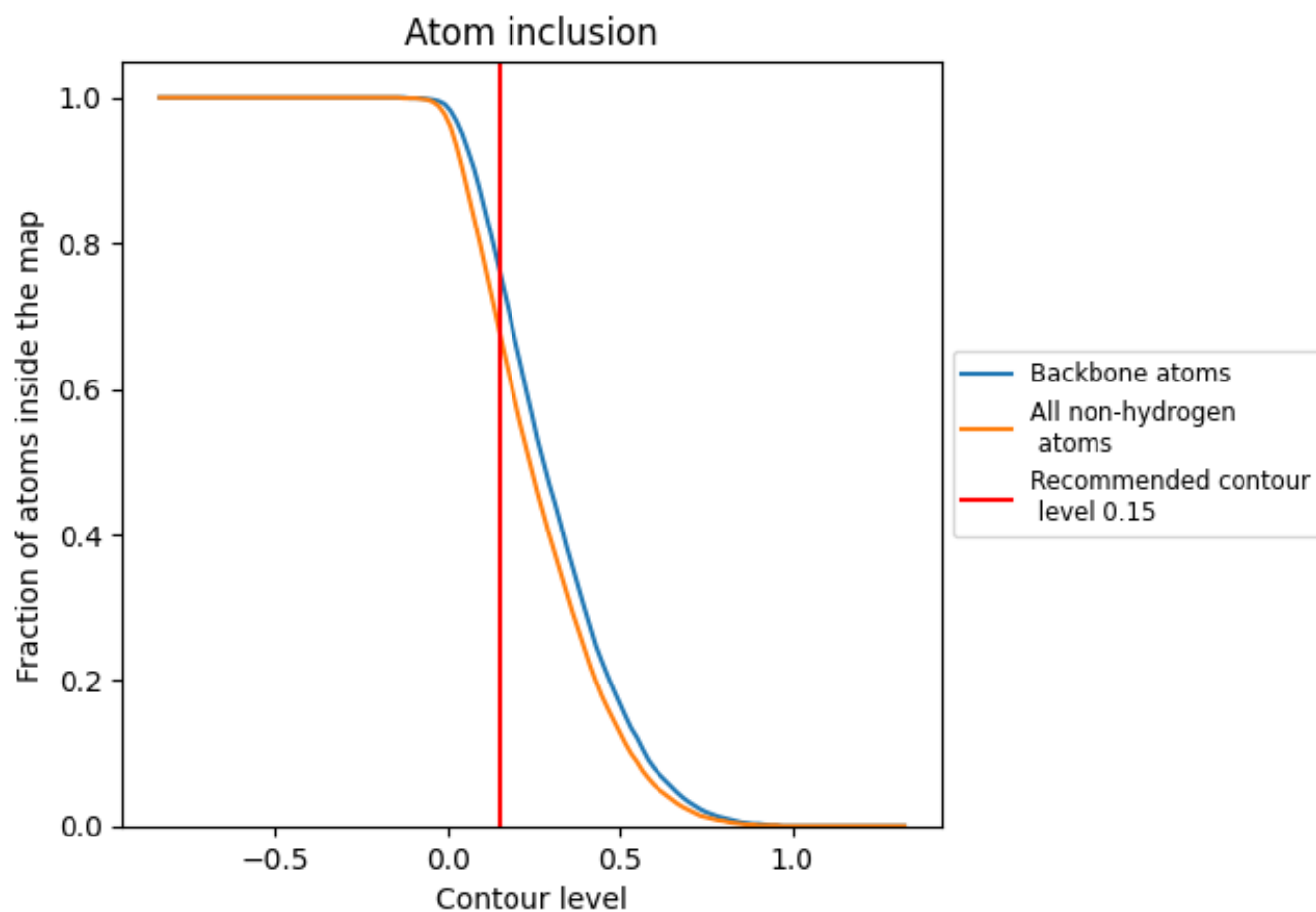
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 68% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6800	0.4850
A	0.7230	0.5030
B	0.7140	0.5020
C	0.7320	0.5110
D	0.7280	0.4920
E	0.6820	0.4940
F	0.7910	0.5330
G	0.1940	0.2730

1.0

0.0

<0.0