



Full wwPDB EM Validation Report ⓘ

Apr 10, 2026 – 12:16 PM UTC

PDB ID : 9MNM / pdb_00009mmn
EMDB ID : EMD-48430
Title : SPA of purified HIV-1 CA protein in vitro assembled with IP6 (mature morphology). 500 uM LEN was added post assembly.
Authors : Ricana, C.L.; Dick, R.A.
Deposited on : 2024-12-22
Resolution : 3.50 Å(reported)
Based on initial model : 8G6M

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

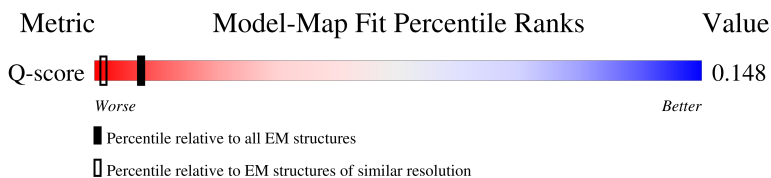
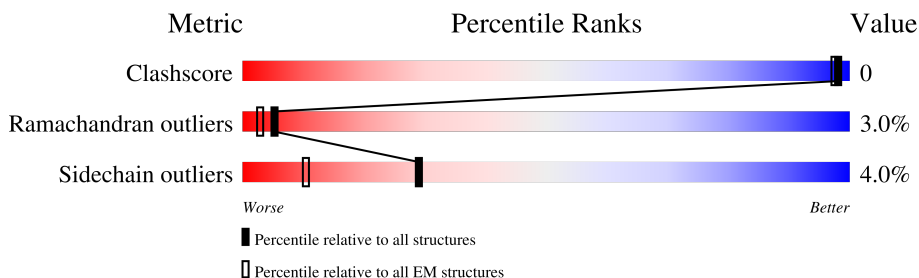
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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	13950 (3.00 - 4.00)

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	231	13% 72% 16% • 9%
1	B	231	31% 45% 10% 45%
1	C	231	38% 70% 14% • 14%
1	D	231	15% 25% 5% • 69%

2 Entry composition [i](#)

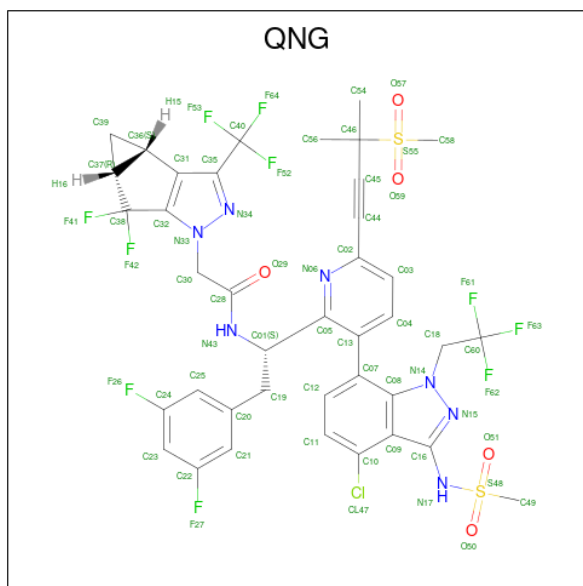
There are 3 unique types of molecules in this entry. The entry contains 9946 atoms, of which 4888 are hydrogens and 0 are deuteriums.

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 HIV-1 CA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	210	Total 3308	1041	1654	288	312	13	0	0
1	B	128	Total 2006	635	999	176	189	7	0	0
1	C	199	Total 3133	988	1563	273	297	12	0	0
1	D	71	Total 1127	353	564	97	108	5	0	0

- Molecule 2 is Lenacapavir (CCD ID: QNG) (formula: $C_{39}H_{32}ClF_{10}N_7O_5S_2$) (labeled as "Ligand of Interest" by depositor).



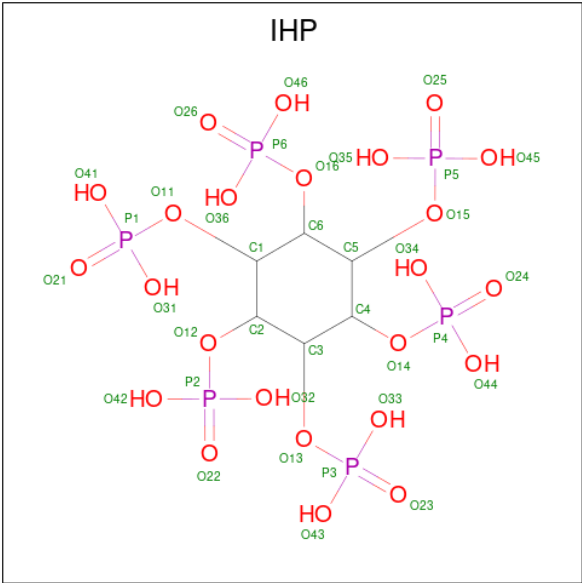
Mol	Chain	Residues	Atoms								AltConf
			Total	C	Cl	F	H	N	O	S	
2	A	1	Total 96	39	1	10	32	7	5	2	0
2	B	1	Total 96	39	1	10	32	7	5	2	0

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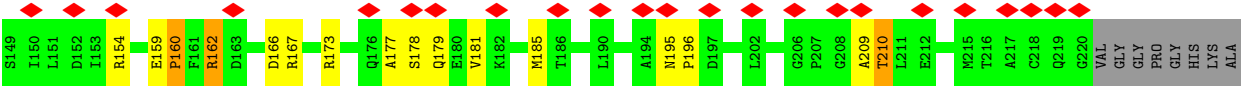
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Mol	Chain	Residues	Atoms								AltConf
			Total	C	Cl	F	H	N	O	S	
2	C	1	96	39	1	10	32	7	5	2	0

- Molecule 3 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	O	P	
3	A	1	42	6	6	24	6	0
3	A	1	42	6	6	24	6	0



ARG
VAL
LEU

● Molecule 1: HIV-1 CA



PRO ILE VAL GLN ASN LEU GLN GLY MET GLN THR HIS GLN ALA ILE SER PRO ARG THR LEU ASN TRP ALA TRP VAL LYS VAL VAL VAL GLU GLY LYS PHE ILE ALA

GLY HIS GLN ALA ALA MET GLN MET LEU LYS THR ILE ASN GLU GLU ALA ALA GLU THR ASP TRP ASP ARG LEU THR ILE ALA THR THR SER THR LEU GLN GLN ILE MET TRP MET THR HIS

ASN PRO PRO ILE PRO VAL GLY GLU TYR ARG TRP ILE ILE ILE LEU LEU GLY LEU ASN LYS ILE VAL ARG MET TYR SER PRO THR SER I150 I151 D152 I153 R154 E159 P160 F161 R162 D163 D166 R167 K170 T171 L172 R173 A174 E175 Q176 A177 S178 Q179 E180 V181 K182 N183 W184 M185

T186 L190 V191 Q192 N195 P196 D197 L202 K203 A204 L205 G206 A209 E212 M215 T216 A217 C218 Q219 G220 VAL GLY PRO GLY HIS LYS ARG VAL LEU

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	594567	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	0.009	Depositor
Minimum map value	-0.004	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.000	Depositor
Recommended contour level	0.0018	Depositor
Map size (Å)	295.92, 295.92, 295.92	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.822, 0.822, 0.822	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IHP, QNG

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	0.88	2/1688 (0.1%)	1.75	36/2289 (1.6%)
1	B	0.86	1/1030 (0.1%)	1.79	23/1399 (1.6%)
1	C	0.88	2/1603 (0.1%)	1.78	30/2174 (1.4%)
1	D	0.94	2/572 (0.3%)	1.80	10/772 (1.3%)
All	All	0.88	7/4893 (0.1%)	1.78	99/6634 (1.5%)

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	5
1	B	0	3
1	C	0	6
1	D	0	2
All	All	0	16

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	71	GLU	CD-OE2	6.44	1.37	1.25
1	B	71	GLU	CD-OE2	6.19	1.37	1.25
1	D	212	GLU	CD-OE2	6.11	1.36	1.25
1	A	166	ASP	CG-OD2	5.87	1.36	1.25
1	C	166	ASP	CG-OD2	5.87	1.36	1.25
1	C	71	GLU	CD-OE2	5.86	1.36	1.25
1	D	166	ASP	CG-OD2	5.80	1.36	1.25

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	18	ARG	NE-CZ-NH2	8.31	126.68	119.20
1	C	59	VAL	N-CA-C	7.86	119.58	110.62
1	D	209	ALA	CA-C-N	7.71	132.03	120.31
1	D	209	ALA	C-N-CA	7.71	132.03	120.31
1	B	100	ARG	NE-CZ-NH2	7.56	126.01	119.20
1	B	132	ARG	NE-CZ-NH2	7.56	126.01	119.20
1	D	178	SER	N-CA-C	7.43	119.28	111.03
1	B	124	ILE	CA-C-N	7.30	126.97	119.82
1	B	124	ILE	C-N-CA	7.30	126.97	119.82
1	B	143	ARG	NE-CZ-NH2	7.18	125.67	119.20
1	A	100	ARG	NE-CZ-NH2	6.97	125.48	119.20
1	B	31	ALA	N-CA-C	6.93	119.72	111.33
1	C	173	ARG	NE-CZ-NH2	6.83	125.34	119.20
1	C	126	VAL	N-CA-C	6.69	118.24	110.62
1	B	34	PRO	CA-C-N	6.56	129.72	120.28
1	B	34	PRO	C-N-CA	6.56	129.72	120.28
1	A	115	ILE	CA-C-N	6.53	128.30	120.14
1	A	115	ILE	C-N-CA	6.53	128.30	120.14
1	C	178	SER	N-CA-C	6.52	118.27	111.03
1	A	31	ALA	N-CA-C	6.50	119.19	111.33
1	A	63	GLN	N-CA-C	6.48	120.05	111.75
1	C	82	ARG	NE-CZ-NH2	6.35	124.91	119.20
1	A	209	ALA	CA-C-N	6.32	129.92	120.31
1	A	209	ALA	C-N-CA	6.32	129.92	120.31
1	C	162	ARG	NE-CZ-NH2	6.28	124.85	119.20
1	C	147	PRO	CA-N-CD	-6.21	103.31	112.00
1	C	63	GLN	N-CA-C	6.19	119.68	111.75
1	C	31	ALA	N-CA-C	6.17	118.80	111.33
1	A	124	ILE	CA-C-N	6.13	125.83	119.82
1	A	124	ILE	C-N-CA	6.13	125.83	119.82
1	C	143	ARG	NE-CZ-NH2	6.13	124.72	119.20
1	D	159	GLU	CA-C-N	6.13	127.50	119.84
1	D	159	GLU	C-N-CA	6.13	127.50	119.84
1	C	36	VAL	CA-C-N	6.08	125.19	120.33
1	C	36	VAL	C-N-CA	6.08	125.19	120.33
1	A	147	PRO	CA-N-CD	-6.07	103.50	112.00
1	B	147	PRO	CA-N-CD	-6.06	103.51	112.00
1	B	148	THR	N-CA-C	6.03	118.79	110.35
1	D	160	PRO	CA-C-N	5.99	129.80	120.82
1	D	160	PRO	C-N-CA	5.99	129.80	120.82
1	C	124	ILE	N-CA-C	5.97	115.53	108.96
1	A	36	VAL	CA-C-N	5.95	125.09	120.33
1	A	36	VAL	C-N-CA	5.95	125.09	120.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	159	GLU	CA-C-N	5.89	127.20	119.84
1	A	159	GLU	C-N-CA	5.89	127.20	119.84
1	C	132	ARG	NE-CZ-NH2	5.85	124.46	119.20
1	C	154	ARG	NE-CZ-NH2	5.79	124.41	119.20
1	A	84	HIS	CA-C-O	-5.77	110.98	120.80
1	A	96	MET	N-CA-C	5.75	117.55	111.28
1	A	154	ARG	NE-CZ-NH2	5.74	124.37	119.20
1	A	16	SER	N-CA-C	5.73	119.97	112.17
1	B	143	ARG	NE-CZ-NH1	-5.73	115.77	121.50
1	B	18	ARG	NE-CZ-NH2	5.72	124.35	119.20
1	C	159	GLU	CA-C-N	5.70	126.97	119.84
1	C	159	GLU	C-N-CA	5.70	126.97	119.84
1	B	47	ALA	N-CA-C	5.70	118.27	110.24
1	A	176	GLN	N-CA-C	5.69	122.92	110.80
1	A	95	GLN	CA-C-N	5.66	127.87	120.28
1	A	95	GLN	C-N-CA	5.66	127.87	120.28
1	A	100	ARG	NE-CZ-NH1	-5.65	115.85	121.50
1	C	19	THR	N-CA-C	5.64	117.51	111.36
1	A	97	ARG	NE-CZ-NH2	5.64	124.27	119.20
1	B	63	GLN	N-CA-C	5.61	118.92	111.75
1	C	209	ALA	CA-C-N	5.56	128.76	120.31
1	C	209	ALA	C-N-CA	5.56	128.76	120.31
1	A	143	ARG	NE-CZ-NH2	5.51	124.16	119.20
1	C	115	ILE	CA-C-N	5.51	127.03	120.14
1	C	115	ILE	C-N-CA	5.51	127.03	120.14
1	B	45	GLU	N-CA-C	5.48	118.42	110.42
1	A	82	ARG	NE-CZ-NH2	5.46	124.12	119.20
1	A	167	ARG	NE-CZ-NH2	5.45	124.10	119.20
1	B	101	GLY	CA-C-N	5.45	128.12	120.28
1	B	101	GLY	C-N-CA	5.45	128.12	120.28
1	A	132	ARG	NE-CZ-NH2	5.37	124.03	119.20
1	A	160	PRO	CA-C-N	5.37	131.79	121.54
1	A	160	PRO	C-N-CA	5.37	131.79	121.54
1	A	125	PRO	N-CA-C	5.37	120.90	113.98
1	B	132	ARG	NE-CZ-NH1	-5.37	116.13	121.50
1	B	29	GLU	N-CA-C	5.36	116.98	111.03
1	C	18	ARG	NE-CZ-NH2	5.35	124.02	119.20
1	C	124	ILE	CA-C-N	5.34	125.05	119.82
1	C	124	ILE	C-N-CA	5.34	125.05	119.82
1	C	179	GLN	N-CA-C	5.32	116.89	111.14
1	B	84	HIS	CA-C-O	-5.27	111.84	120.80
1	A	178	SER	N-CA-C	5.16	117.89	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	147	PRO	CA-C-N	5.12	131.33	121.54
1	C	147	PRO	C-N-CA	5.12	131.33	121.54
1	D	174	ALA	N-CA-C	5.12	116.86	111.28
1	A	18	ARG	N-CA-C	5.11	116.66	111.14
1	C	210	THR	CA-C-N	5.11	127.38	120.38
1	C	210	THR	C-N-CA	5.11	127.38	120.38
1	D	209	ALA	CA-C-O	5.08	125.84	119.59
1	D	153	ILE	N-CA-C	5.05	111.61	106.21
1	B	147	PRO	CA-C-N	5.04	128.83	121.31
1	B	147	PRO	C-N-CA	5.04	128.83	121.31
1	A	210	THR	CA-C-N	5.04	127.35	120.54
1	A	210	THR	C-N-CA	5.04	127.35	120.54
1	A	162	ARG	NE-CZ-NH2	5.03	123.73	119.20
1	B	125	PRO	N-CA-C	5.01	120.45	113.98

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	ARG	Sidechain
1	A	132	ARG	Sidechain
1	A	146	SER	Peptide
1	A	15	ILE	Peptide
1	A	169	TYR	Sidechain
1	B	100	ARG	Sidechain
1	B	146	SER	Peptide
1	B	16	SER	Peptide
1	C	100	ARG	Sidechain
1	C	146	SER	Peptide
1	C	16	SER	Peptide
1	C	160	PRO	Peptide
1	C	162	ARG	Sidechain
1	C	177	ALA	Peptide
1	D	173	ARG	Sidechain
1	D	178	SER	Peptide

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	1654	1654	1653	1	0
1	B	1007	999	997	0	0
1	C	1570	1563	1561	2	0
1	D	563	564	563	1	0
2	A	64	32	0	0	0
2	B	64	32	0	0	0
2	C	64	32	0	0	0
3	A	72	12	12	0	0
All	All	5058	4888	4786	4	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 0.

All (4) 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:181:VAL:HG12	1:C:185:MET:HE2	1.81	0.61
1:A:120:HIS:CG	1:A:121:ASN:N	2.88	0.41
1:C:27:VAL:HG11	1:C:59:VAL:HG13	2.01	0.41
1:D:162:ARG:HA	1:D:215:MET:HE3	2.02	0.41

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	206/231 (89%)	186 (90%)	13 (6%)	7 (3%)	3	23
1	B	124/231 (54%)	116 (94%)	6 (5%)	2 (2%)	7	36
1	C	195/231 (84%)	180 (92%)	9 (5%)	6 (3%)	3	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	69/231 (30%)	62 (90%)	4 (6%)	3 (4%)	2	18
All	All	594/924 (64%)	544 (92%)	32 (5%)	18 (3%)	5	25

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	147	PRO
1	A	176	GLN
1	A	195	ASN
1	B	147	PRO
1	C	147	PRO
1	C	195	ASN
1	D	195	ASN
1	A	160	PRO
1	C	160	PRO
1	D	160	PRO
1	A	177	ALA
1	A	196	PRO
1	B	17	PRO
1	C	17	PRO
1	C	196	PRO
1	D	196	PRO
1	C	110	THR
1	A	17	PRO

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	181/194 (93%)	173 (96%)	8 (4%)	25	51
1	B	110/194 (57%)	105 (96%)	5 (4%)	24	50
1	C	171/194 (88%)	165 (96%)	6 (4%)	32	57
1	D	61/194 (31%)	59 (97%)	2 (3%)	33	58
All	All	523/776 (67%)	502 (96%)	21 (4%)	29	54

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

Mol	Chain	Res	Type
1	A	1	PRO
1	A	9	GLN
1	A	15	ILE
1	A	20	LEU
1	A	25	LYS
1	A	147	PRO
1	A	148	THR
1	A	200	THR
1	B	39	MET
1	B	50	GLN
1	B	74	ASN
1	B	112	GLN
1	B	147	PRO
1	C	107	THR
1	C	124	ILE
1	C	147	PRO
1	C	148	THR
1	C	167	ARG
1	C	210	THR
1	D	162	ARG
1	D	205	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	HIS
1	B	74	ASN
1	C	74	ASN
1	C	95	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 ligands are modelled in this entry.

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
3	IHP	A	303	-	36,36,36	0.82	0	60,60,60	1.13	3 (5%)
3	IHP	A	302	-	36,36,36	0.95	1 (2%)	60,60,60	1.17	5 (8%)
2	QNG	B	301	-	64,70,70	1.66	9 (14%)	82,114,114	3.79	22 (26%)
2	QNG	A	301	-	64,70,70	1.70	11 (17%)	82,114,114	3.66	20 (24%)
2	QNG	C	301	-	64,70,70	1.73	11 (17%)	82,114,114	3.61	21 (25%)

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
3	IHP	A	303	-	-	3/30/54/54	0/1/1/1
3	IHP	A	302	-	-	4/30/54/54	0/1/1/1
2	QNG	B	301	-	-	11/45/72/72	0/7/7/7
2	QNG	A	301	-	-	4/45/72/72	0/7/7/7
2	QNG	C	301	-	-	7/45/72/72	0/7/7/7

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	QNG	C32-C31	-7.32	1.28	1.37
2	B	301	QNG	C32-C31	-7.26	1.28	1.37
2	A	301	QNG	C32-C31	-7.22	1.28	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	QNG	C07-C08	5.29	1.47	1.41
2	C	301	QNG	C36-C31	-5.26	1.45	1.51
2	A	301	QNG	C36-C31	-4.87	1.46	1.51
2	B	301	QNG	C07-C08	4.74	1.46	1.41
2	A	301	QNG	C07-C08	4.72	1.46	1.41
2	B	301	QNG	C36-C31	-4.67	1.46	1.51
2	A	301	QNG	C35-N34	3.70	1.38	1.32
2	B	301	QNG	C35-N34	3.68	1.38	1.32
2	C	301	QNG	C35-N34	3.64	1.38	1.32
2	A	301	QNG	C16-N15	2.70	1.36	1.31
2	B	301	QNG	C09-C08	-2.69	1.37	1.41
3	A	302	IHP	P2-O12	-2.60	1.55	1.59
2	A	301	QNG	C39-C37	2.56	1.54	1.50
2	C	301	QNG	C39-C37	2.54	1.54	1.50
2	B	301	QNG	C16-N15	2.52	1.35	1.31
2	A	301	QNG	C09-C08	-2.51	1.37	1.41
2	A	301	QNG	C58-S55	2.37	1.79	1.76
2	B	301	QNG	C39-C37	2.36	1.54	1.50
2	A	301	QNG	C44-C45	2.32	1.22	1.19
2	C	301	QNG	C18-N14	2.29	1.48	1.45
2	A	301	QNG	N33-N34	2.19	1.40	1.36
2	C	301	QNG	C58-S55	2.15	1.79	1.76
2	C	301	QNG	N33-N34	2.15	1.40	1.36
2	C	301	QNG	C09-C08	-2.09	1.38	1.41
2	B	301	QNG	C44-C45	2.07	1.22	1.19
2	B	301	QNG	N33-N34	2.07	1.40	1.36
2	A	301	QNG	C18-N14	2.05	1.48	1.45
2	C	301	QNG	C44-C45	2.04	1.22	1.19
2	C	301	QNG	C08-N14	2.02	1.38	1.37

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	QNG	C40-C35-C31	26.20	145.18	128.38
2	A	301	QNG	C40-C35-C31	24.90	144.34	128.38
2	C	301	QNG	C40-C35-C31	23.26	143.29	128.38
2	C	301	QNG	C38-C37-C36	8.56	114.87	108.40
2	A	301	QNG	C38-C37-C36	8.29	114.67	108.40
2	B	301	QNG	C38-C37-C36	8.18	114.58	108.40
2	A	301	QNG	F42-C38-C32	-8.06	91.10	111.26
2	B	301	QNG	F42-C38-C32	-7.96	91.36	111.26
2	C	301	QNG	F42-C38-C32	-7.84	91.65	111.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	QNG	C40-C35-N34	-7.75	109.33	118.50
2	C	301	QNG	C31-C35-N34	-7.64	104.31	113.09
2	B	301	QNG	C31-C35-N34	-7.36	104.64	113.09
2	A	301	QNG	C31-C35-N34	-7.35	104.65	113.09
2	A	301	QNG	C02-N06-C05	6.82	122.72	117.29
2	C	301	QNG	F42-C38-F41	6.47	135.99	105.19
2	A	301	QNG	F42-C38-F41	6.43	135.83	105.19
2	B	301	QNG	F42-C38-F41	6.38	135.56	105.19
2	A	301	QNG	C40-C35-N34	-6.34	111.00	118.50
2	C	301	QNG	C02-N06-C05	6.29	122.30	117.29
2	C	301	QNG	C40-C35-N34	-5.54	111.95	118.50
2	B	301	QNG	C37-C36-C31	-5.38	97.85	104.31
2	A	301	QNG	C37-C36-C31	-5.14	98.13	104.31
2	C	301	QNG	C37-C36-C31	-5.03	98.27	104.31
2	C	301	QNG	C60-C18-N14	4.88	117.21	112.09
2	B	301	QNG	C36-C31-C35	-4.64	132.32	145.10
2	C	301	QNG	C36-C31-C35	-4.58	132.50	145.10
2	A	301	QNG	C36-C31-C35	-4.52	132.66	145.10
2	C	301	QNG	N17-C16-N15	-4.52	109.89	119.03
2	B	301	QNG	C02-N06-C05	4.36	120.76	117.29
3	A	302	IHP	P2-O12-C2	3.82	133.62	123.43
2	C	301	QNG	F53-C40-C35	3.73	117.71	112.39
2	B	301	QNG	C03-C02-C44	-3.50	113.85	120.35
2	B	301	QNG	C44-C02-N06	3.40	123.37	116.62
2	C	301	QNG	C37-C38-C32	-3.34	92.00	100.73
2	B	301	QNG	C37-C38-C32	-3.29	92.14	100.73
2	A	301	QNG	C37-C38-C32	-3.28	92.15	100.73
3	A	303	IHP	C6-C5-C4	-3.26	103.27	110.43
2	B	301	QNG	C32-N33-N34	-3.20	108.26	111.67
2	A	301	QNG	C32-N33-N34	-3.15	108.30	111.67
2	B	301	QNG	C60-C18-N14	3.06	115.29	112.09
2	C	301	QNG	C32-N33-N34	-3.04	108.42	111.67
2	A	301	QNG	F41-C38-C32	2.96	118.65	111.26
2	B	301	QNG	F41-C38-C32	2.89	118.48	111.26
2	C	301	QNG	C09-C10-CL47	2.81	123.24	119.62
2	C	301	QNG	F41-C38-C32	2.80	118.25	111.26
3	A	302	IHP	C3-C2-C1	-2.76	104.37	110.43
2	C	301	QNG	C09-C16-N17	2.73	137.11	125.87
2	C	301	QNG	C39-C36-C37	2.71	60.94	59.26
2	B	301	QNG	C13-C07-C08	-2.64	120.75	124.44
2	A	301	QNG	C39-C36-C37	2.55	60.85	59.26
3	A	303	IHP	C3-C2-C1	-2.52	104.89	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	QNG	C13-C07-C08	-2.50	120.94	124.44
2	A	301	QNG	F52-C40-C35	2.37	115.76	112.39
2	B	301	QNG	C04-C13-C07	-2.32	114.05	118.74
2	B	301	QNG	C36-C31-C32	2.30	114.87	110.21
2	C	301	QNG	C54-C46-C45	2.27	112.16	109.99
2	A	301	QNG	C36-C31-C32	2.26	114.79	110.21
2	B	301	QNG	C39-C36-C37	2.25	60.66	59.26
3	A	302	IHP	C6-C5-C4	-2.24	105.50	110.43
2	C	301	QNG	C36-C31-C32	2.19	114.66	110.21
2	B	301	QNG	C02-C44-C45	-2.16	171.79	176.12
2	A	301	QNG	C60-C18-N14	2.16	114.35	112.09
3	A	303	IHP	P5-O15-C5	2.16	129.19	123.43
2	C	301	QNG	O50-S48-N17	2.10	111.07	106.83
3	A	302	IHP	O16-C6-C1	2.08	113.19	108.76
2	A	301	QNG	C08-N14-N15	-2.07	110.76	111.71
2	B	301	QNG	C08-N14-N15	-2.03	110.78	111.71
2	A	301	QNG	C56-C46-C45	2.03	111.93	109.99
3	A	302	IHP	C5-C6-C1	-2.01	106.01	110.43
2	A	301	QNG	C03-C02-C44	2.01	124.08	120.35
2	B	301	QNG	O57-S55-C58	-2.00	105.89	108.42

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	QNG	C28-C30-N33-C32
2	B	301	QNG	C28-C30-N33-C32
2	C	301	QNG	C60-C18-N14-C08
2	C	301	QNG	C16-N17-S48-C49
2	C	301	QNG	C16-N17-S48-O51
2	B	301	QNG	C31-C35-C40-F52
2	B	301	QNG	C31-C35-C40-F64
2	B	301	QNG	C31-C35-C40-F53
2	C	301	QNG	C28-C30-N33-C32
2	B	301	QNG	C60-C18-N14-C08
2	B	301	QNG	N34-C35-C40-F64
2	A	301	QNG	N06-C02-C44-C45
3	A	302	IHP	C3-O13-P3-O43
3	A	302	IHP	C6-O16-P6-O36
3	A	303	IHP	C4-O14-P4-O34
2	B	301	QNG	N34-C35-C40-F53
2	B	301	QNG	N34-C35-C40-F52

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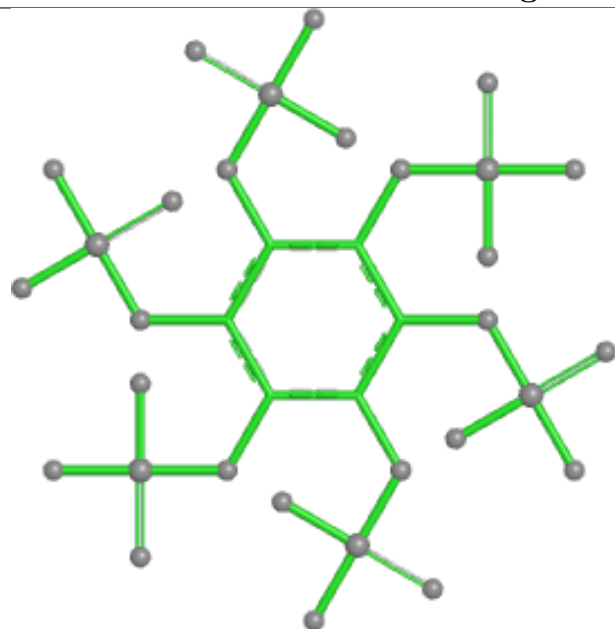
Mol	Chain	Res	Type	Atoms
3	A	302	IHP	C6-O16-P6-O26
3	A	303	IHP	C1-O11-P1-O21
2	C	301	QNG	C09-C16-N17-S48
2	C	301	QNG	N43-C28-C30-N33
2	B	301	QNG	C02-C44-C45-C46
3	A	302	IHP	C4-O14-P4-O44
3	A	303	IHP	C1-O11-P1-O31
2	A	301	QNG	C28-C30-N33-N34
2	B	301	QNG	C28-C30-N33-N34
2	C	301	QNG	C28-C30-N33-N34
2	B	301	QNG	C54-C46-S55-O57
2	A	301	QNG	N34-C35-C40-F52

There are no ring outliers.

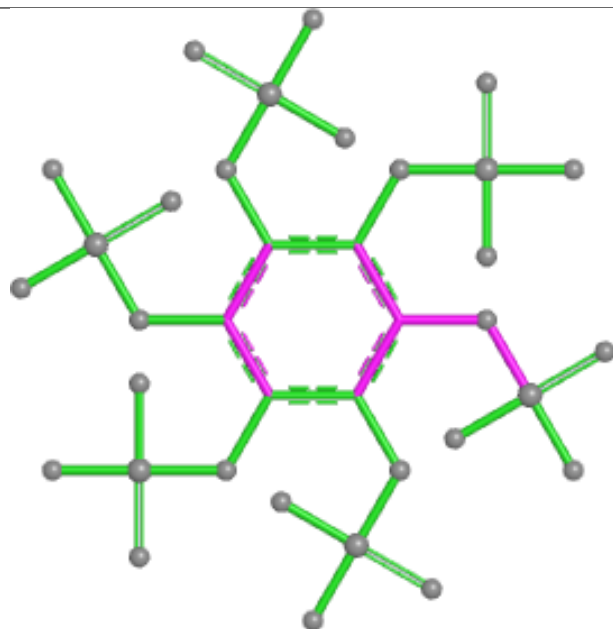
No monomer is involved in short contacts.

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.

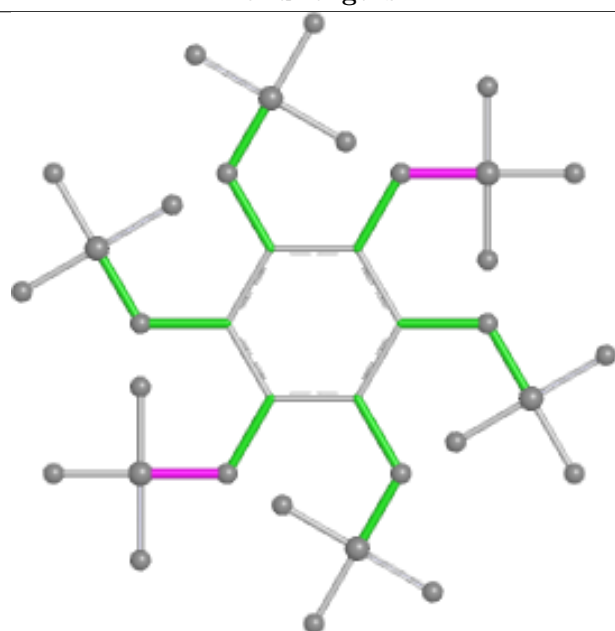
Ligand IHP A 303



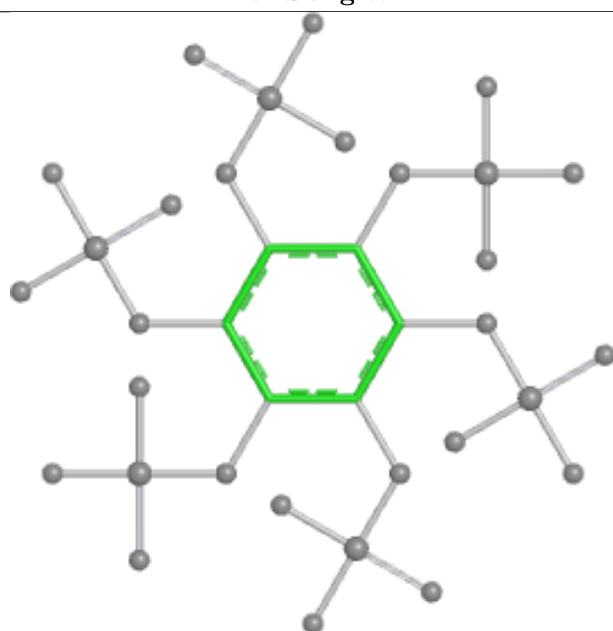
Bond lengths



Bond angles

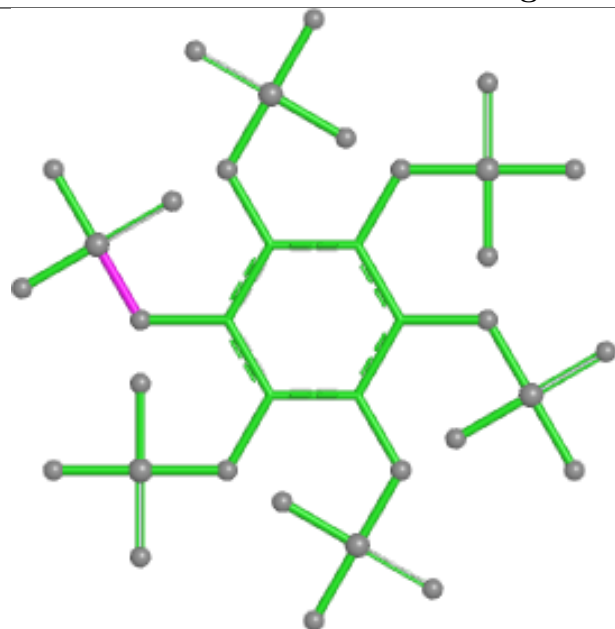


Torsions

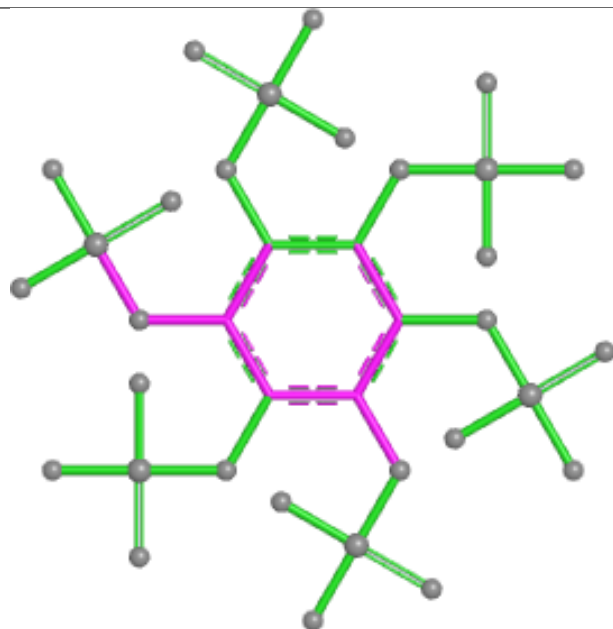


Rings

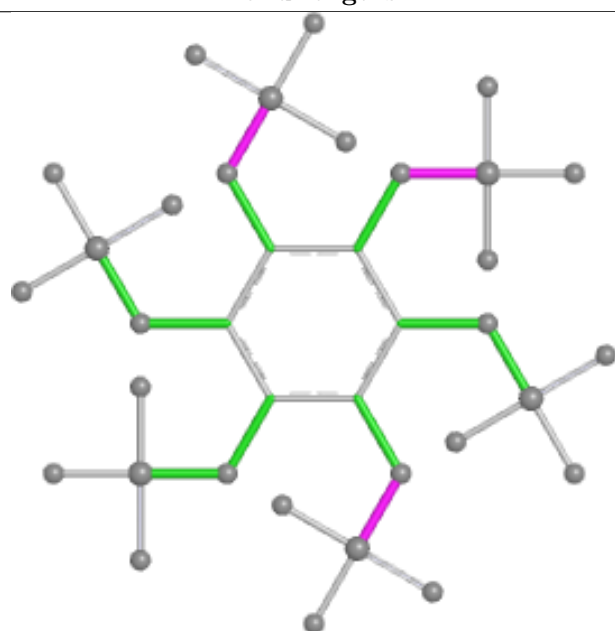
Ligand IHP A 302



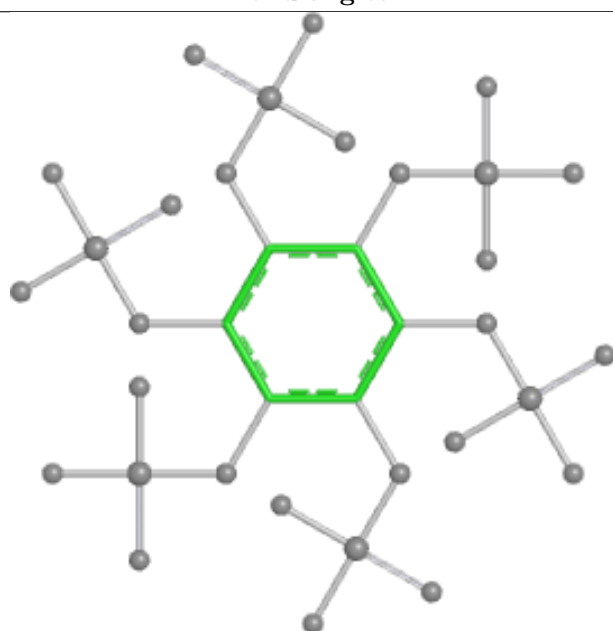
Bond lengths



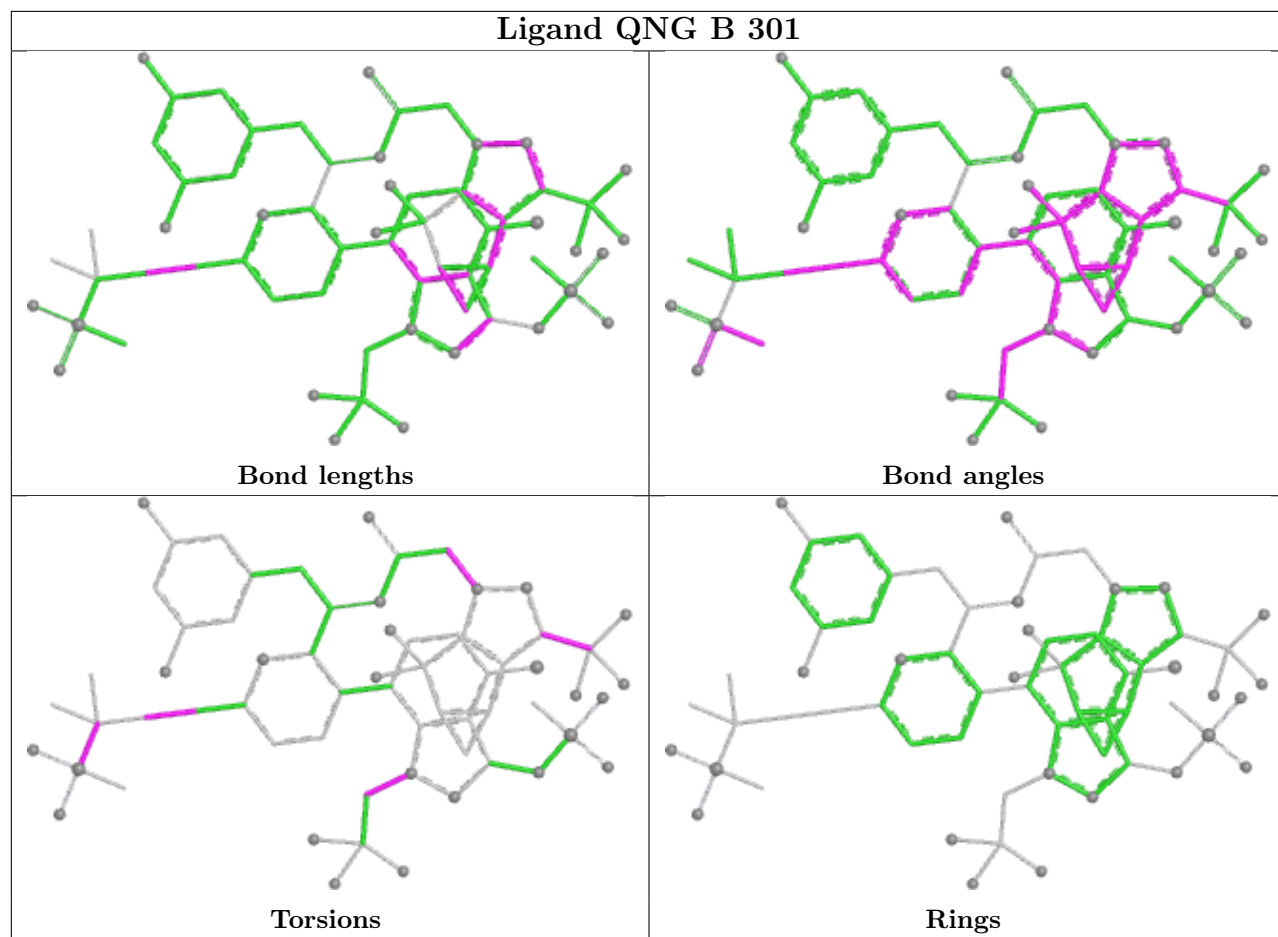
Bond angles

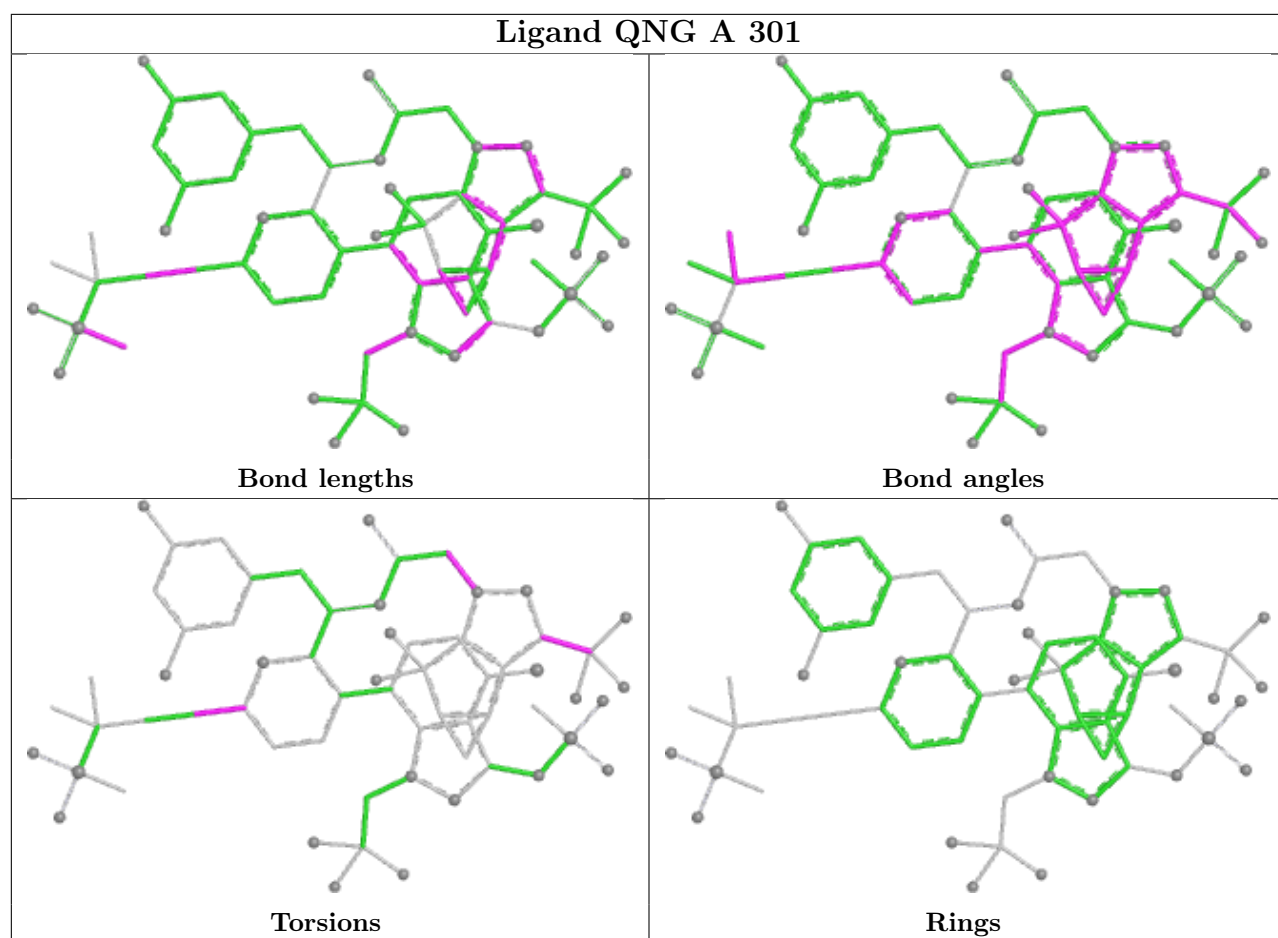


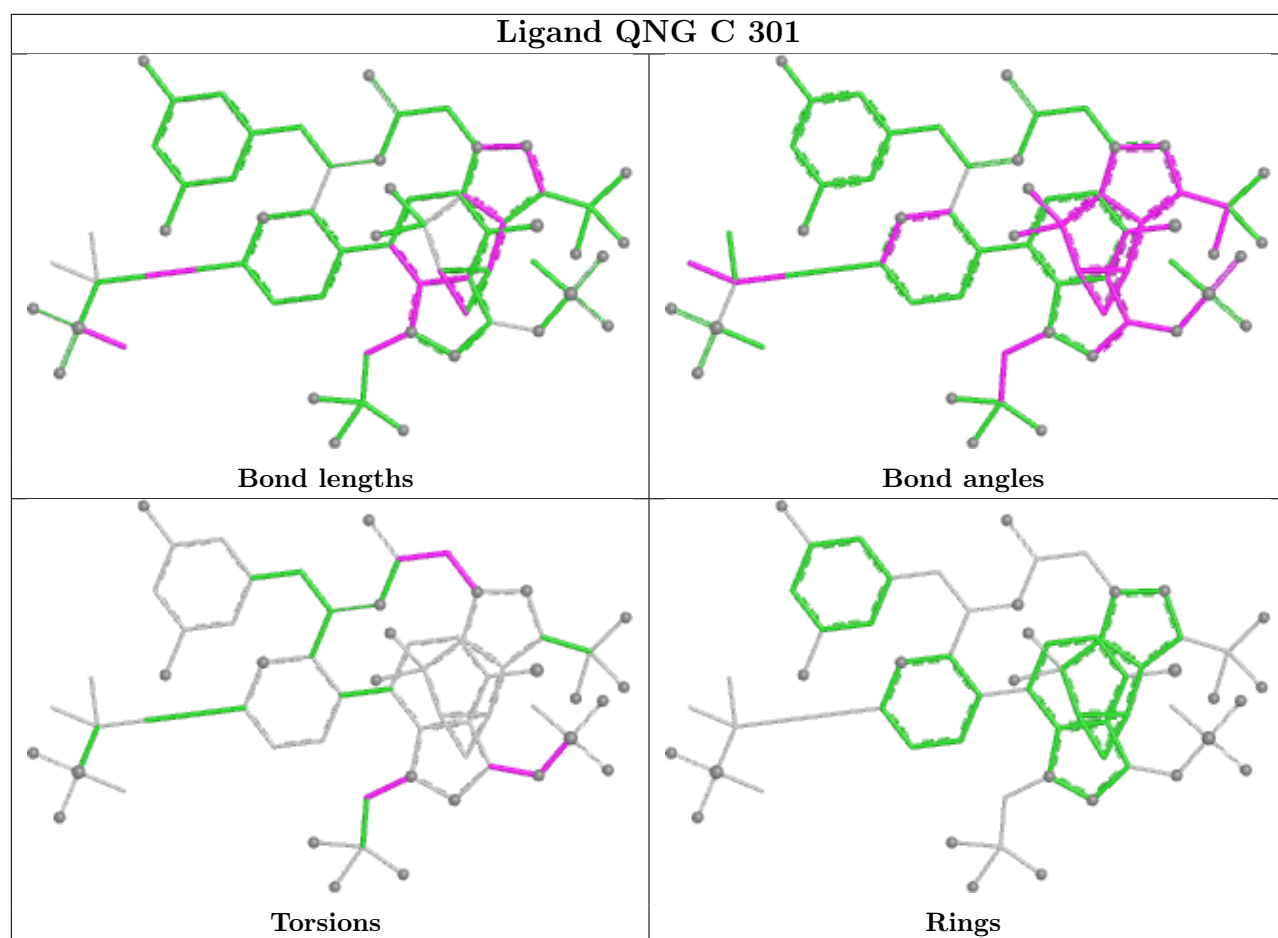
Torsions



Rings







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.

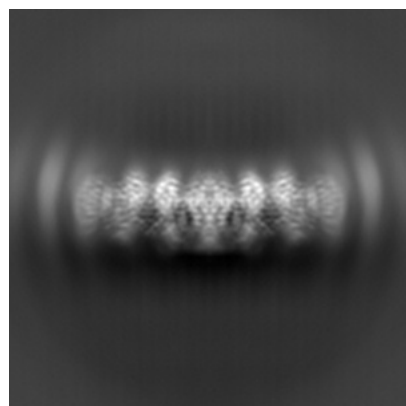
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48430. These allow visual inspection of the internal detail of the map and identification of artifacts.

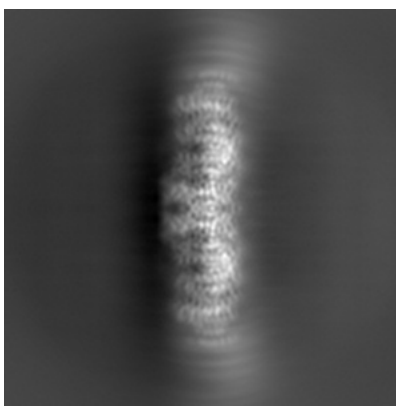
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

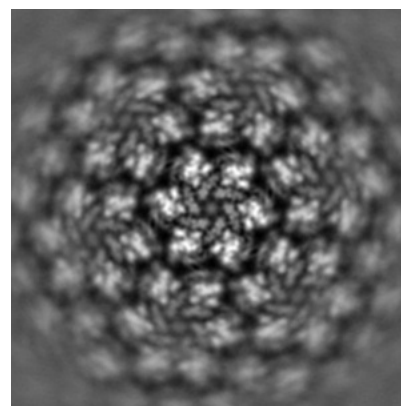
6.1.1 Primary map



X

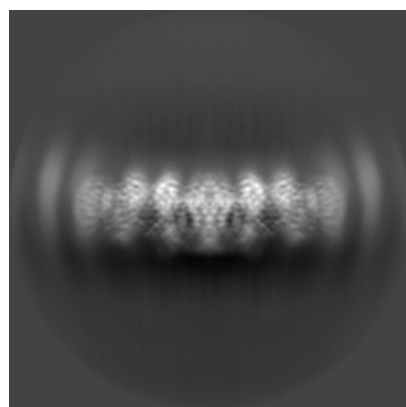


Y

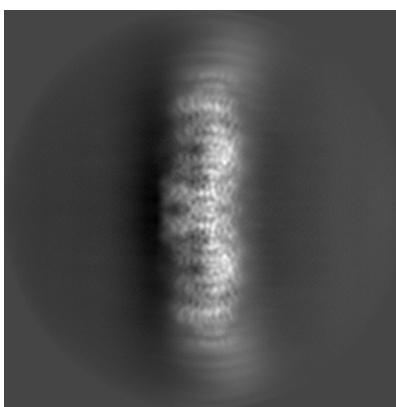


Z

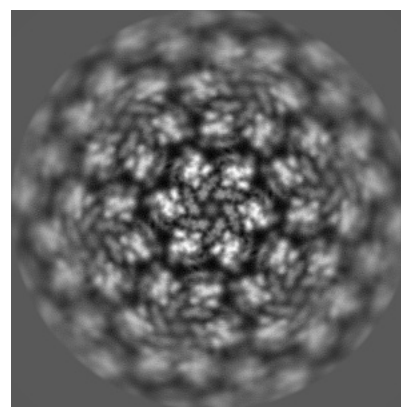
6.1.2 Raw map



X



Y

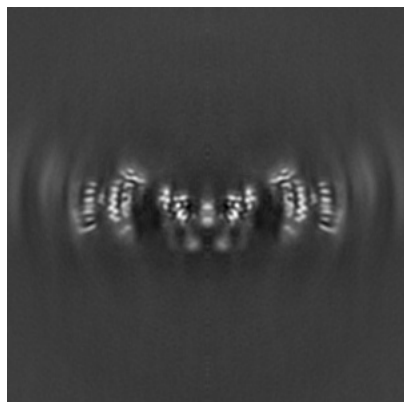


Z

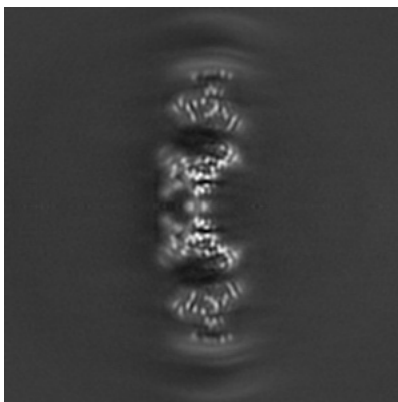
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

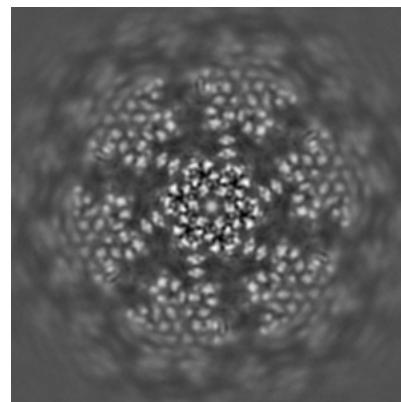
6.2.1 Primary map



X Index: 180

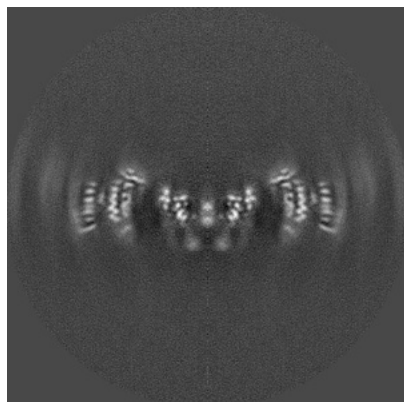


Y Index: 180

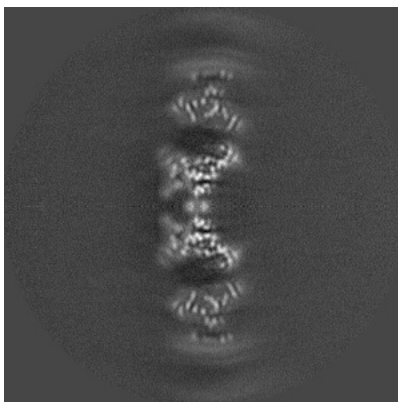


Z Index: 180

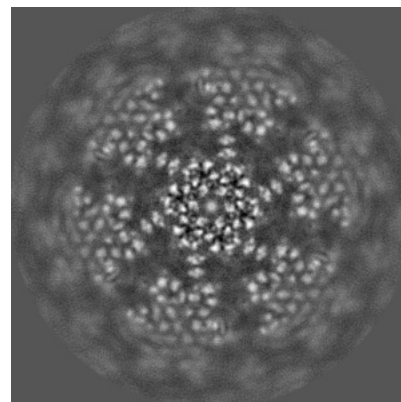
6.2.2 Raw map



X Index: 180



Y Index: 180

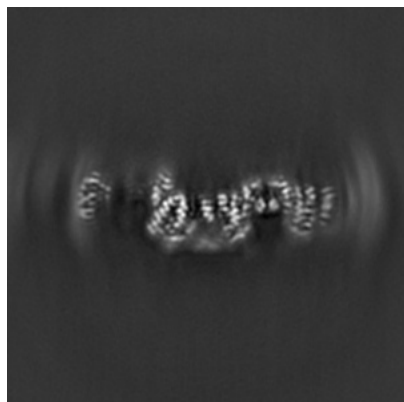


Z Index: 180

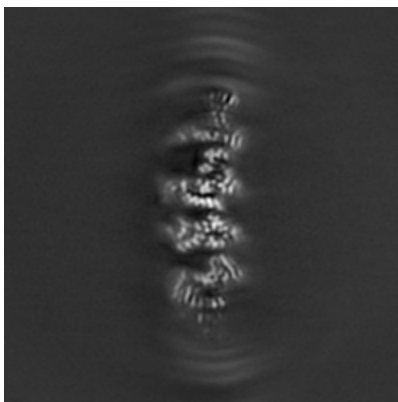
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

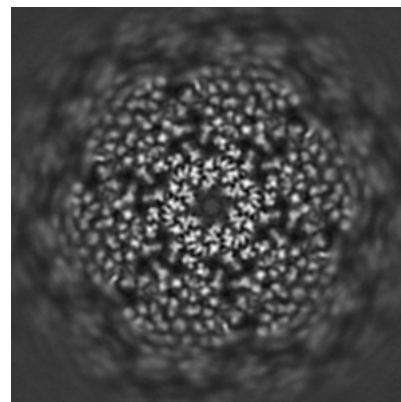
6.3.1 Primary map



X Index: 194

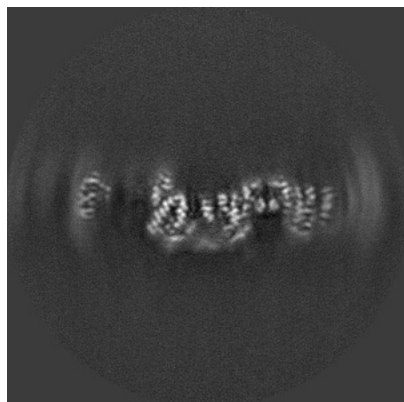


Y Index: 144

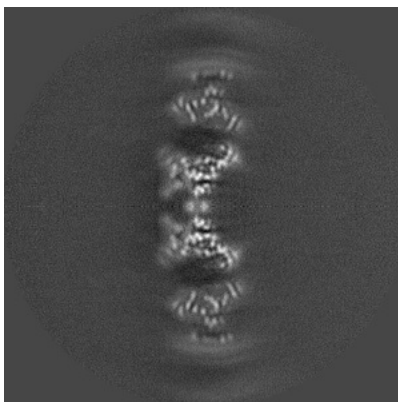


Z Index: 187

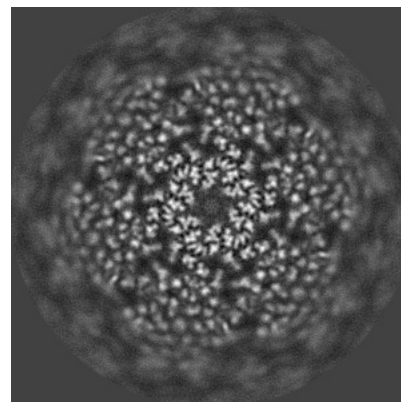
6.3.2 Raw map



X Index: 194



Y Index: 180

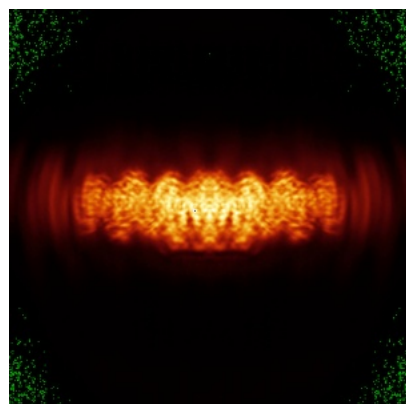


Z Index: 187

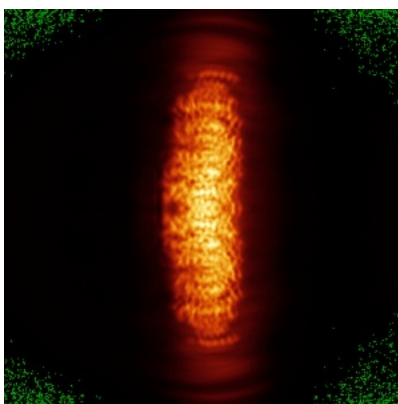
The images above show the largest variance slices of the map in three orthogonal directions.

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

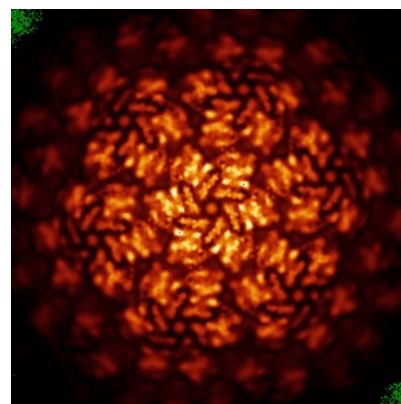
6.4.1 Primary map



X

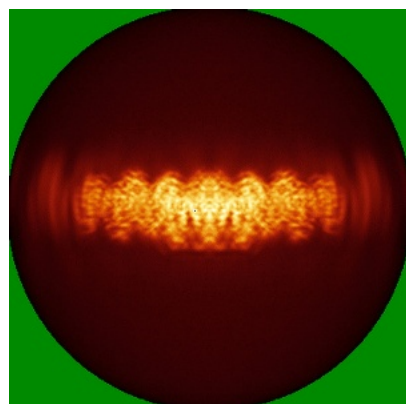


Y

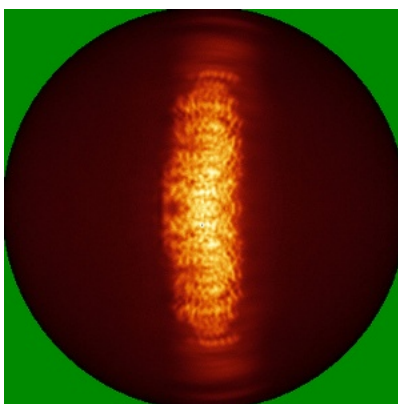


Z

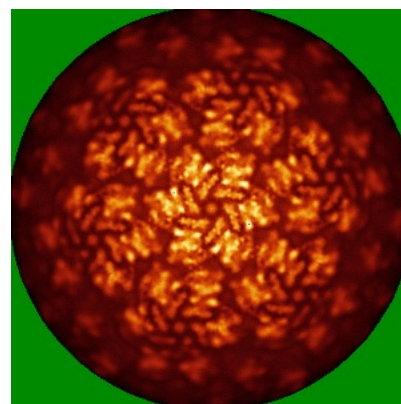
6.4.2 Raw map



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.

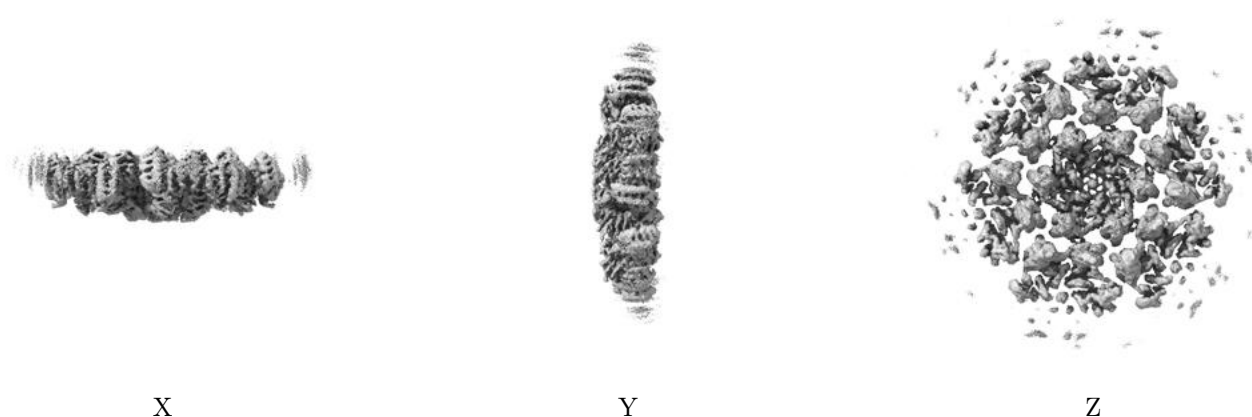
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0018. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

6.6 Mask visualisation [i](#)

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

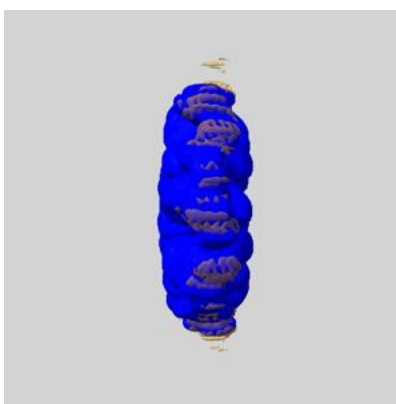
A mask typically either:

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

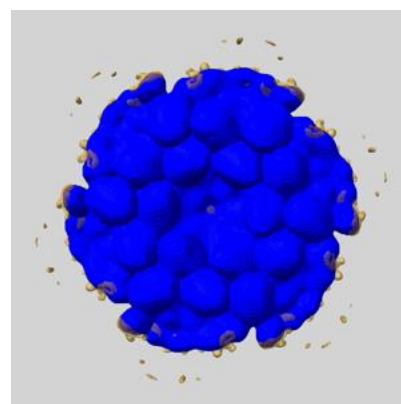
6.6.1 emd_48430_msk_1.map [i](#)



X



Y

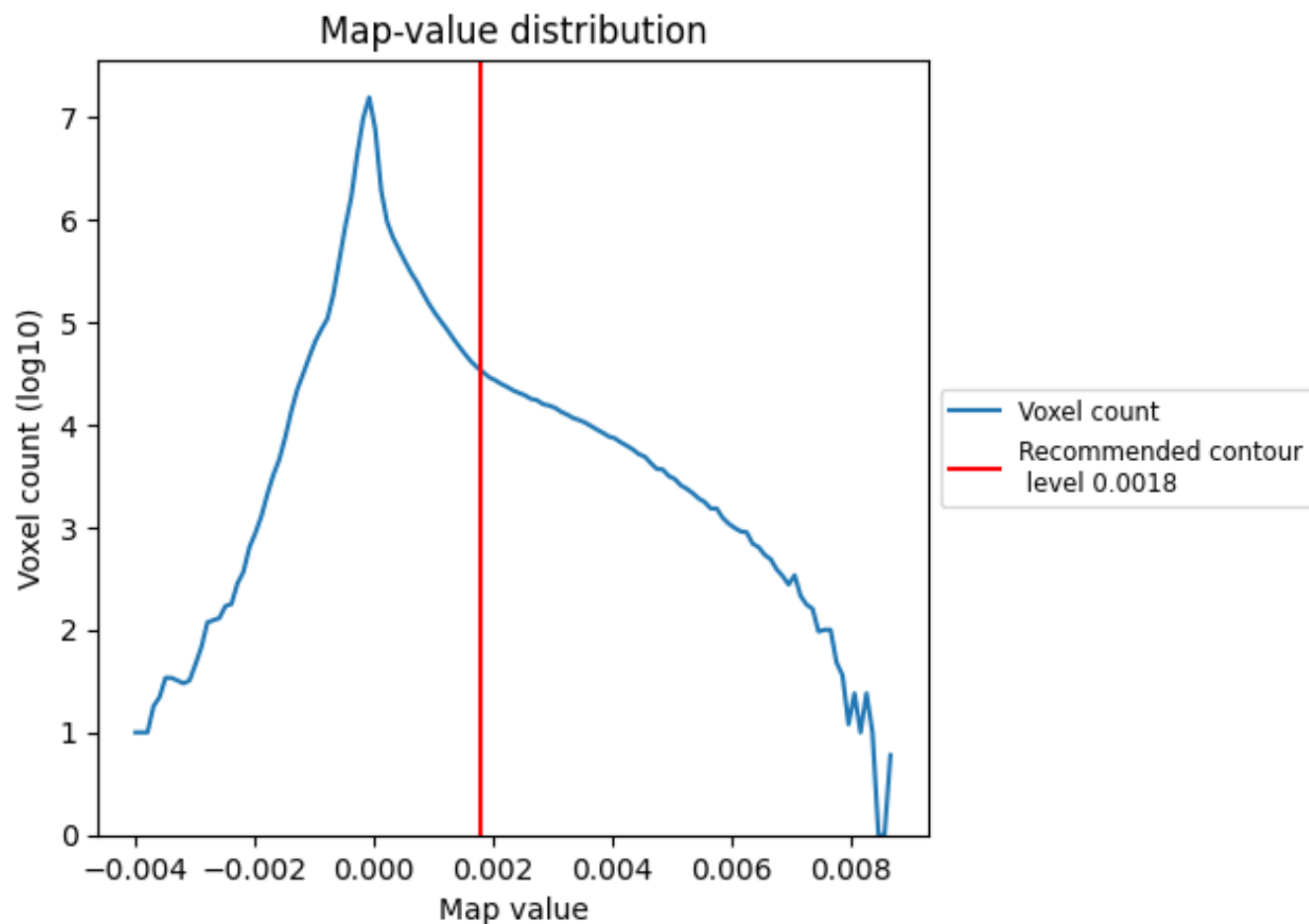


Z

7 Map analysis [i](#)

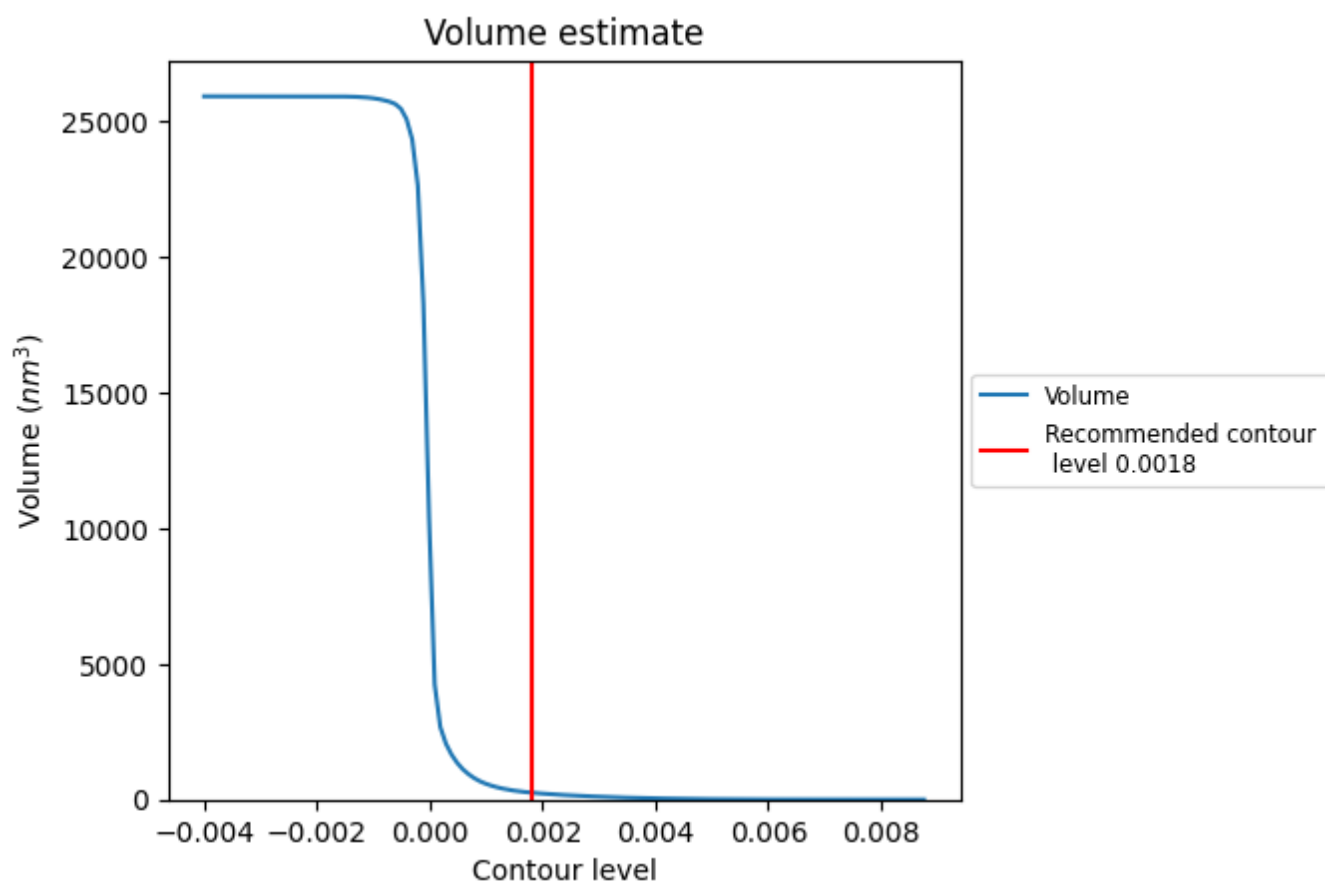
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

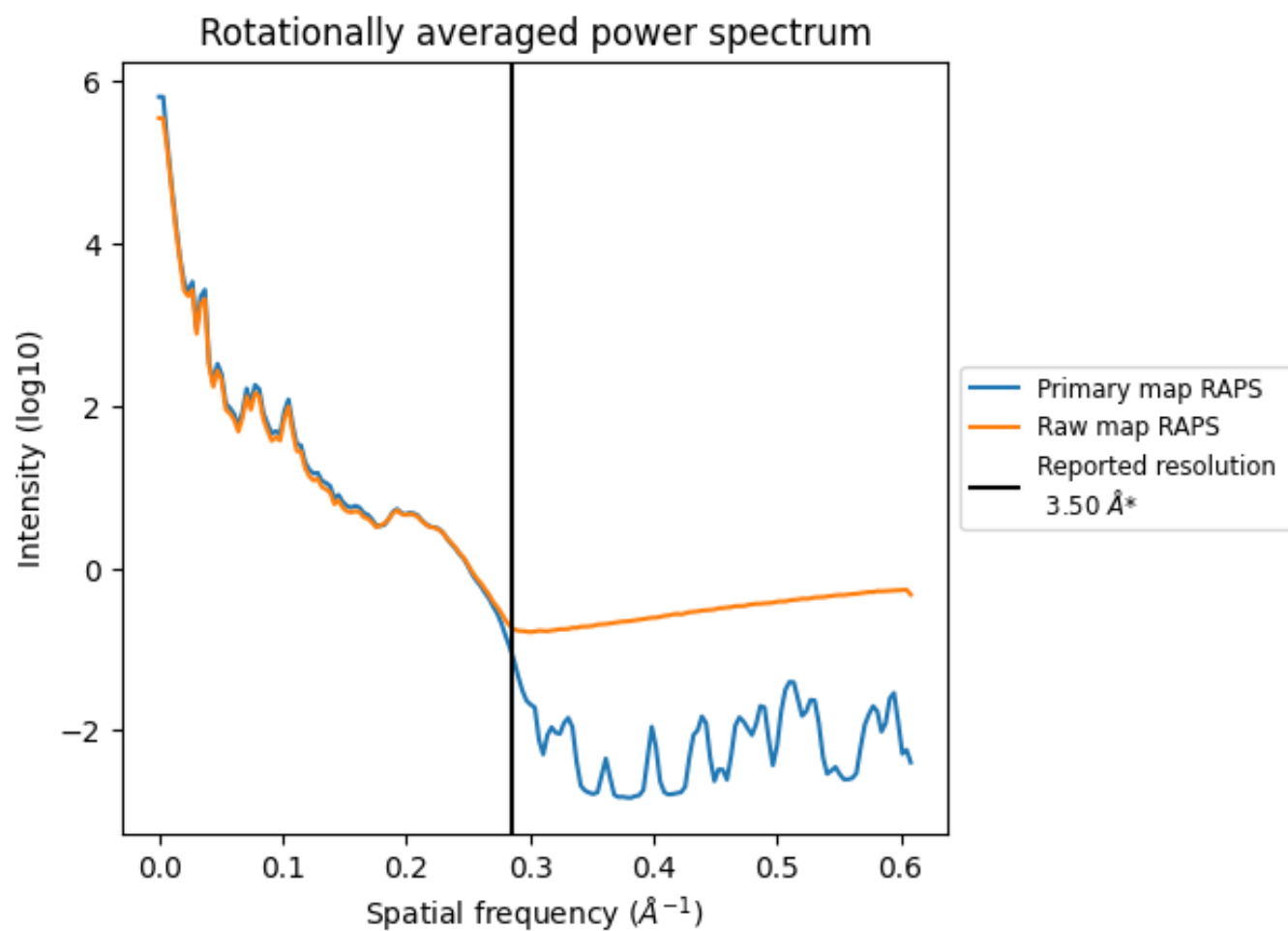
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 255 nm³; this corresponds to an approximate mass of 230 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 ⓘ

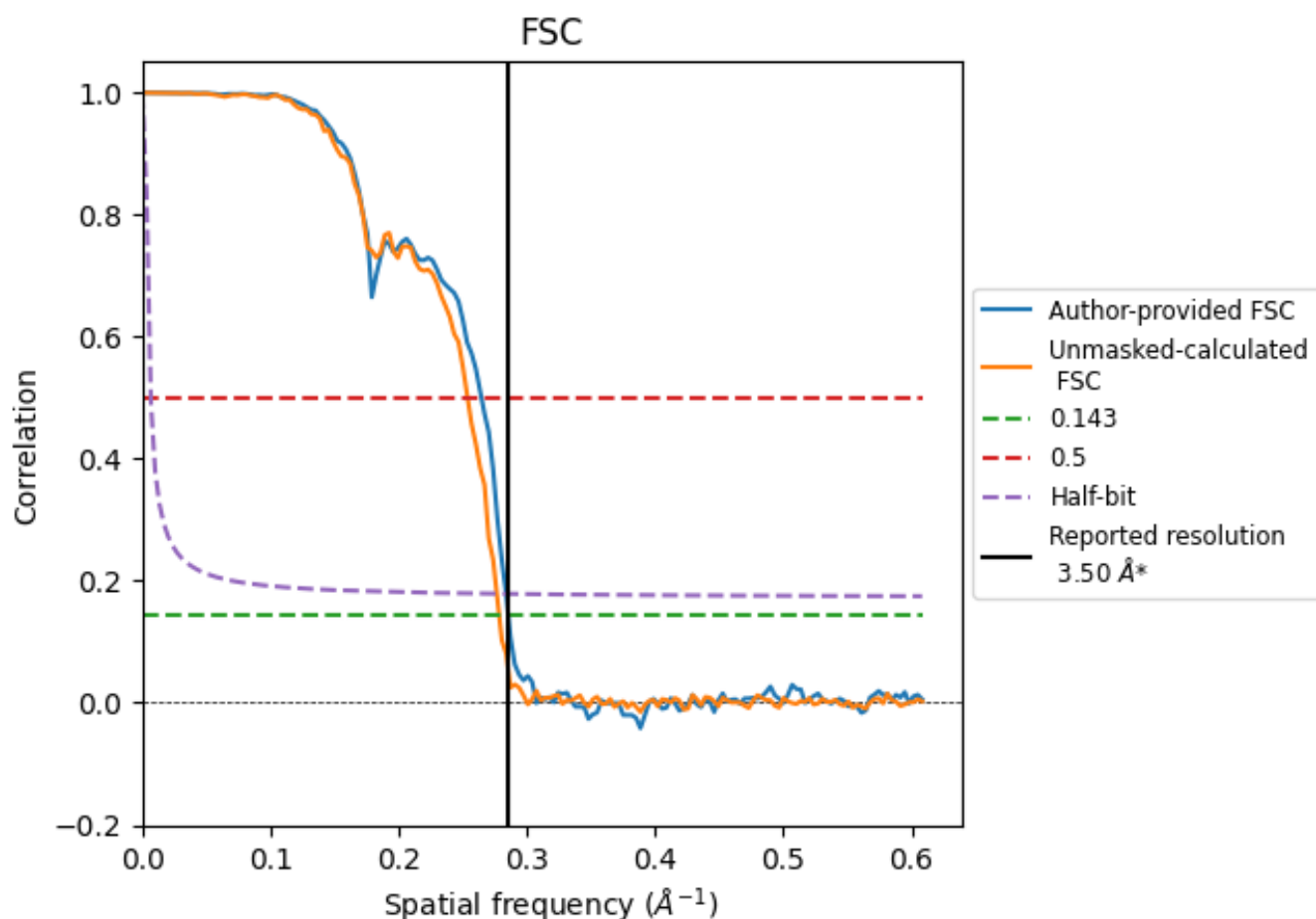


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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 0.286 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.50	3.78	3.52
Unmasked-calculated*	3.59	3.94	3.62

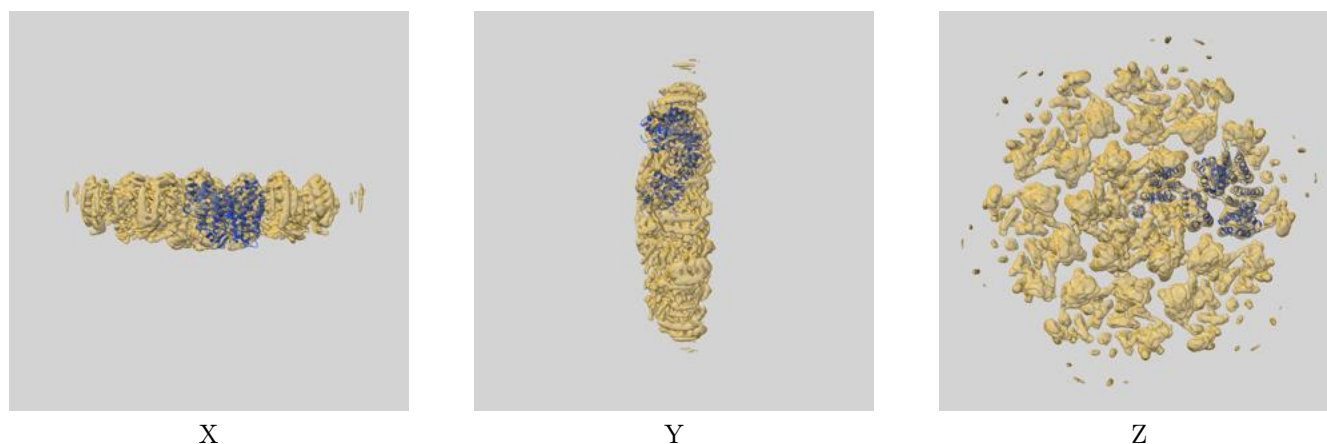
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

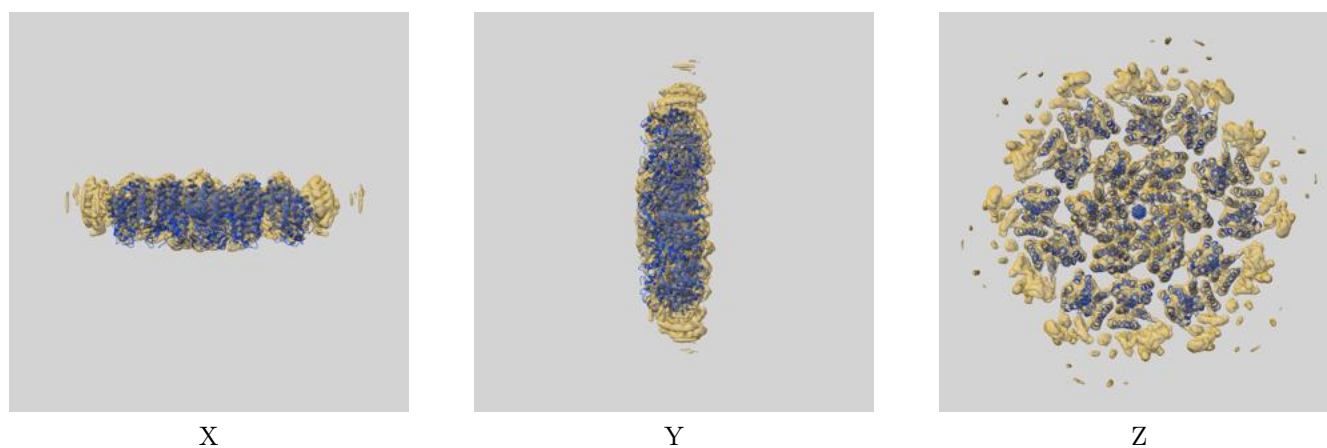
This section contains information regarding the fit between EMDB map EMD-48430 and PDB model 9MNM. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

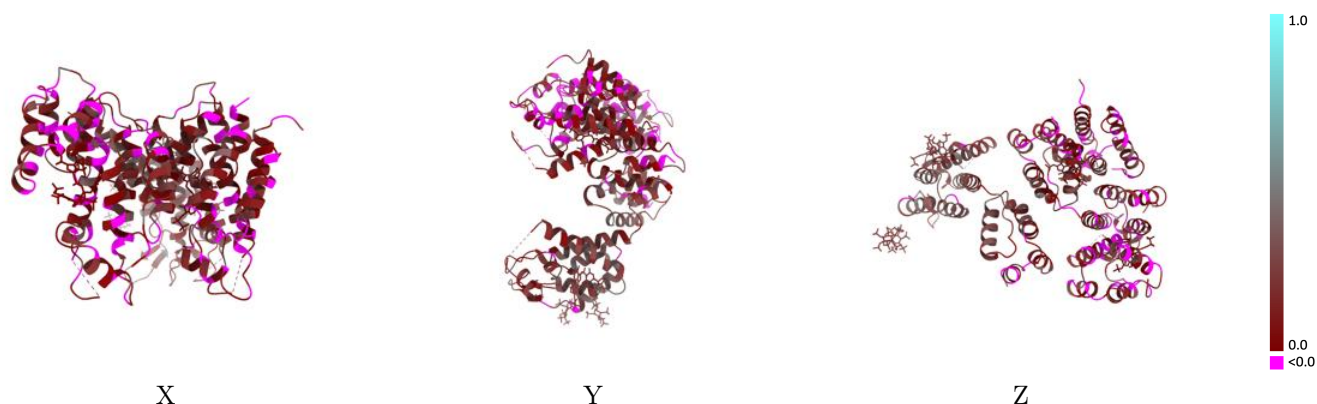


9.1.2 Map-model assembly overlay [i](#)



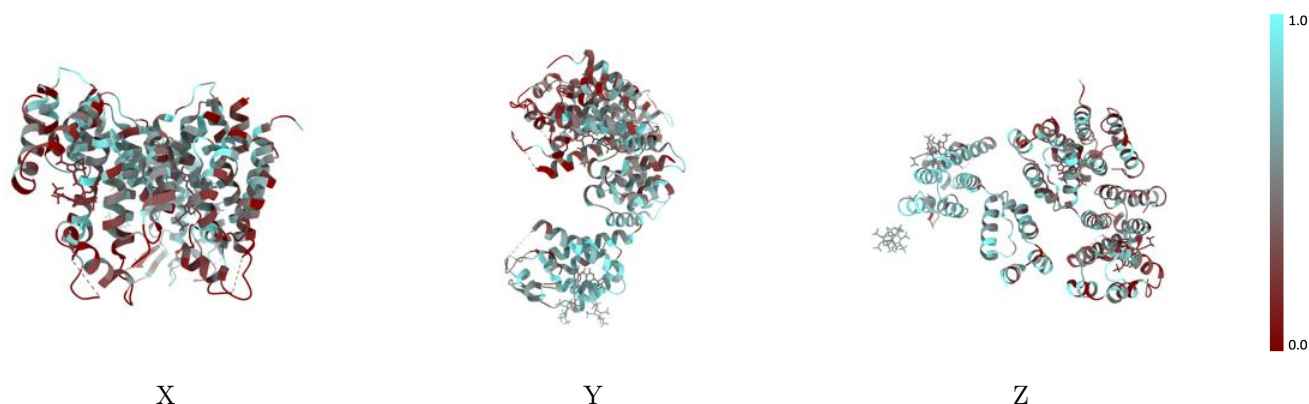
The images above show the 3D surface view of the map at the recommended contour level 0.0018 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



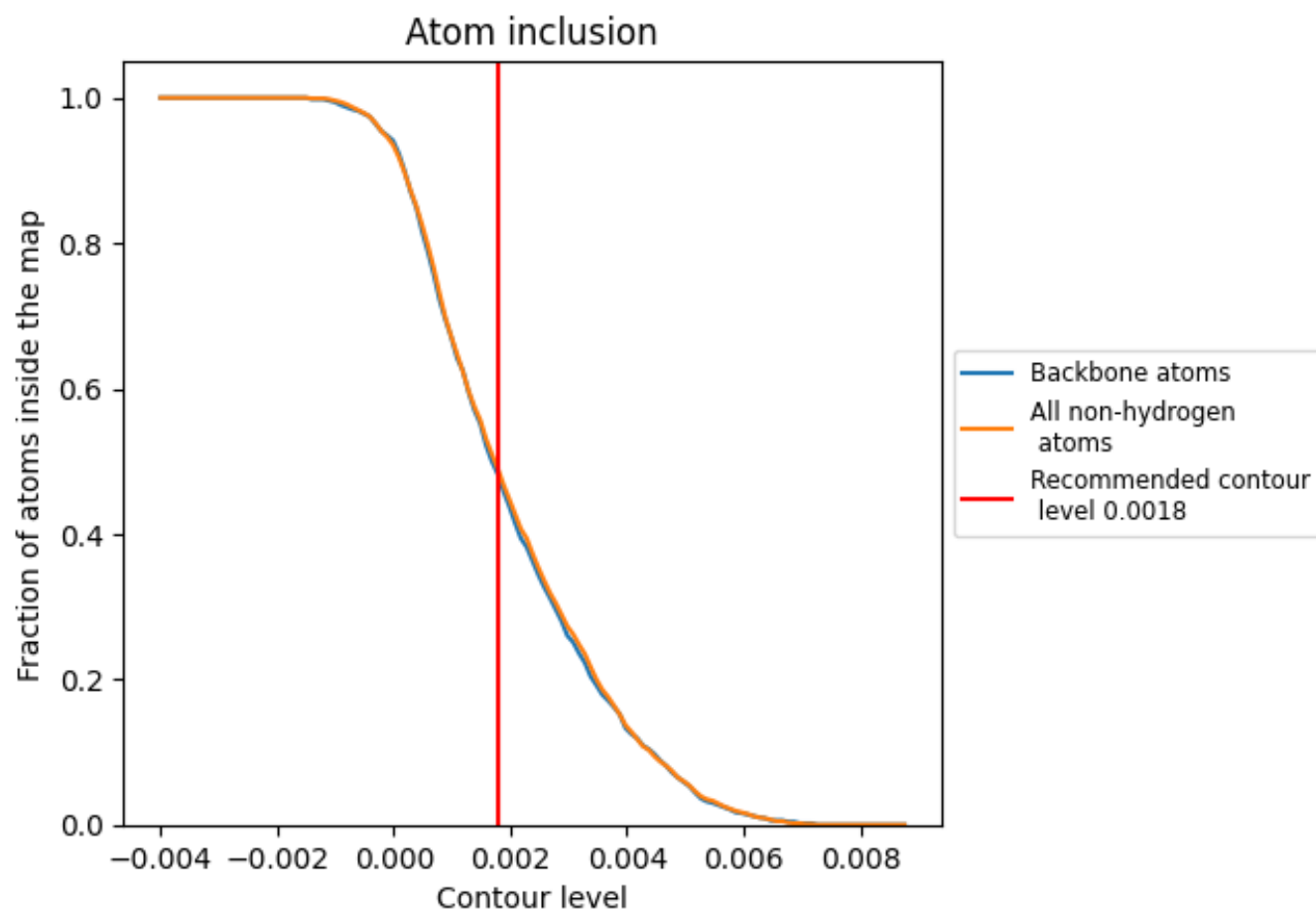
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0018).

9.4 Atom inclusion [i](#)



At the recommended contour level, 48% of all backbone atoms, 49% 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 (0.0018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4870	0.1480
A	0.6270	0.2330
B	0.3950	0.0930
C	0.4390	0.1150
D	0.4420	0.0820

