WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB EM Validation Summary Report (i)

May 4, 2025 – 11:36 PM EDT

PDB ID	:	8SNH / pdb_00008snh
EMDB ID	:	EMD-40625
Title	:	cytochrome bc1-cbb3 supercomplex from Pseudomonas aeruginosa
Authors	:	Di Trani, J.M.; Rubinstein, J.L.
Deposited on	:	2023-04-27
Resolution	:	2.70 Å(reported)

This is a wwPDB EM Validation Summary 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 (i) 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 (i)) were used in the production of this report:

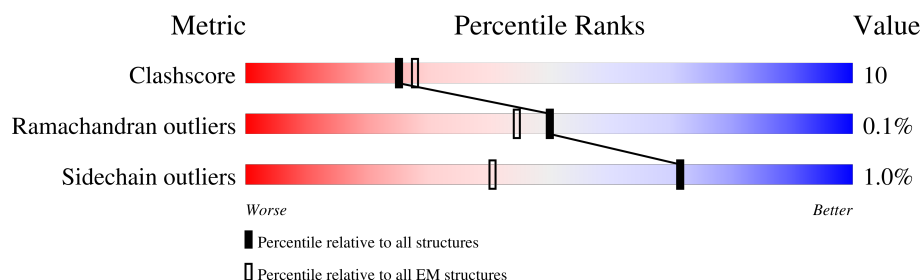|		
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 2.70 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	Percentile Ranks	Value
Clashscore		10
Ramachandran outliers		0.1%
Sidechain outliers		1.0%

Worse   *Better*

∎ Percentile relative to all structures

▯ Percentile relative to all EM structures

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 <=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	E	468	7% / 71% 28% •
2	C	194	11% / 80% 18% •
2	Z	194	16% / 87% 13% •
3	D	403	83% 17%
3	I	403	83% 16%
4	J	233	79% 21%
4	M	233	81% 6% 12%
5	K	181	88% 12%

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Mol	Chain	Length	Quality of chain
5	N	181	91% 9%
6	L	136	9% 88%
6	O	136	11% 88%
7	F	200	18% 80% 19%
8	G	304	38% 65% 35%

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
12	FES	Z	201	-	-	X	-

2   Entry composition ⓘ

There are 15 unique types of molecules in this entry. The entry contains 44205 atoms, of which 20040 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 cytochrome-c oxidase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	468	Total 3719	C 2478	N 607	O 609	S 25	0	0

- Molecule 2 is a protein called Ubiquinol-cytochrome c reductase iron-sulfur subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	C	190	Total 2827	C 910	H 1407	N 245	O 260	S 5	0	0
2	Z	194	Total 2883	C 926	H 1434	N 251	O 267	S 5	0	0

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	I	403	Total 6556	C 2207	H 3289	N 508	O 533	S 19	0	0
3	D	403	Total 6556	C 2207	H 3289	N 508	O 533	S 19	0	0

- Molecule 4 is a protein called Cytochrome c1.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	J	232	Total 3663	C 1188	H 1821	N 309	O 334	S 11	0	0
4	M	204	Total 3250	C 1059	H 1619	N 273	O 290	S 9	0	0

- Molecule 5 is a protein called Cytochrome c4.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	K	181	Total 2585	C 805	H 1279	N 235	O 256	S 10	0	0

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Mol	Chain	Residues	Atoms						AltConf	Trace
5	N	181	Total 2585	C 805	H 1279	N 235	O 256	S 10	0	0

- Molecule 6 is a protein called Cytochrome C5.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	L	16	Total 244	C 73	H 129	N 22	O 19	S 1	0	0
6	O	16	Total 244	C 73	H 129	N 22	O 19	S 1	0	0

- Molecule 7 is a protein called Cbb3-type Cytochrome C oxidase subunit II.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	F	200	Total 2917	C 944	H 1418	N 268	O 280	S 7	0	0

- Molecule 8 is a protein called Cbb3-type cytochrome c oxidase subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	G	304	Total 4655	C 1516	H 2299	N 394	O 432	S 14	0	0

- Molecule 9 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
9	E	1	Total 1	Cu 1	0

- Molecule 10 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
10	E	2	Total 2	Ca 2	0

- Molecule 11 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

HEM
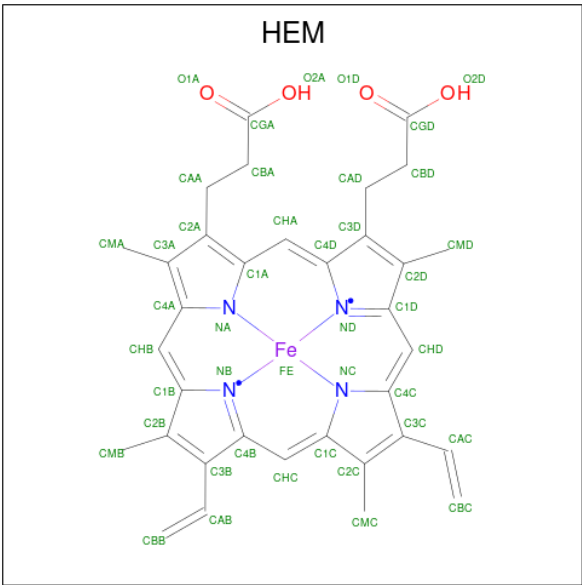
Mol	Chain	Residues	Atoms						AltConf
11	E	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
11	E	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
11	I	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
11	I	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
11	D	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
11	D	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	

- Molecule 12 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).
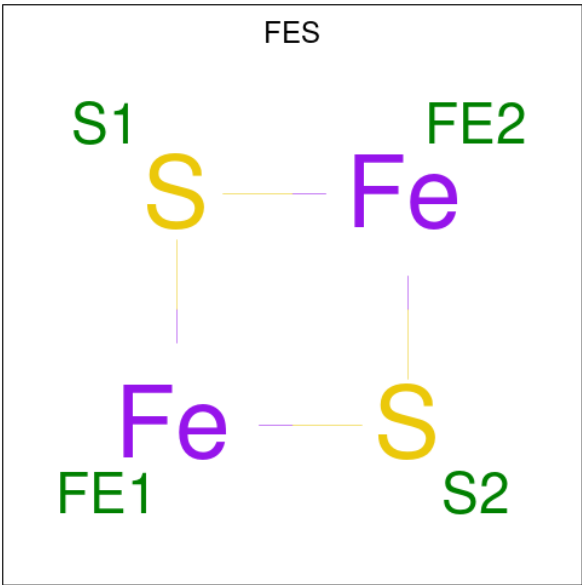
Mol	Chain	Residues	Atoms			AltConf
12	C	1	Total	Fe	S	0
			4	2	2	
12	Z	1	Total	Fe	S	0
			4	2	2	

- Molecule 13 is (2R)-2-(methoxymethyl)-4-{[(25R)-spirost-5-en-3beta-yl]oxy}butyl 4-O-alpha-D-glucopyranosyl-beta-D-glucopyranoside (CCD ID: I7Y) (formula: $C_{45}H_{74}O_{15}$).
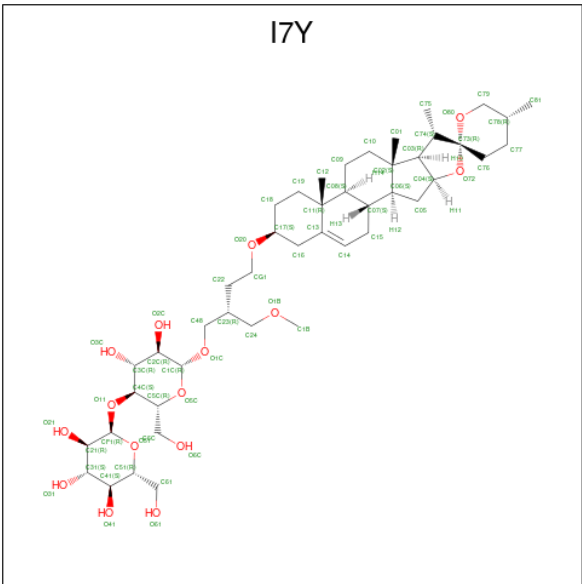
Mol	Chain	Residues	Atoms			AltConf
13	I	1	Total	C	O	0
			31	28	3	

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Mol	Chain	Residues	Atoms			AltConf
13	Z	1	Total 60	C 45	O 15	0

- Molecule 14 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$).

U10
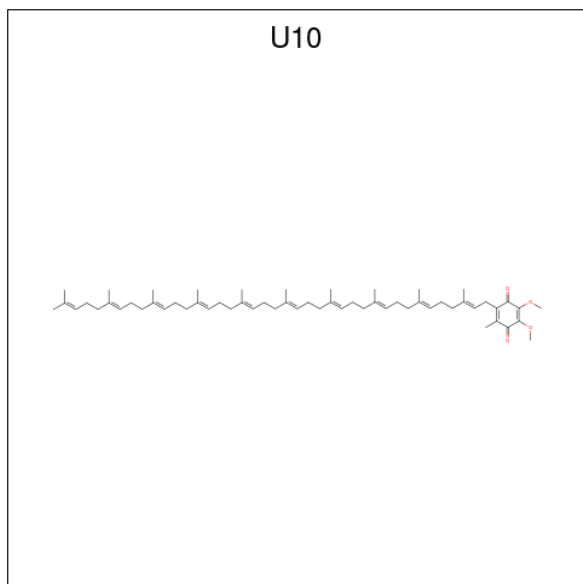
Mol	Chain	Residues	Atoms				AltConf
14	I	1	Total 153	C 59	H 90	O 4	0
14	D	1	Total 153	C 59	H 90	O 4	0

- Molecule 15 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).

HEC
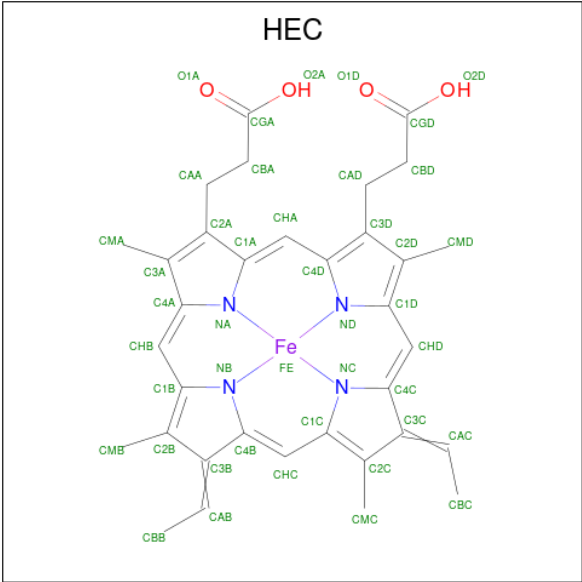
Mol	Chain	Residues	Atoms						AltConf
15	J	1	Total	C	Fe	H	N	O	0
			75	34	1	32	4	4	
15	K	1	Total	C	Fe	H	N	O	0
			75	34	1	32	4	4	
15	K	1	Total	C	Fe	H	N	O	0
			75	34	1	32	4	4	
15	M	1	Total	C	Fe	H	N	O	0
			75	34	1	32	4	4	
15	N	1	Total	C	Fe	H	N	O	0
			75	34	1	32	4	4	
15	N	1	Total	C	Fe	H	N	O	0
			75	34	1	32	4	4	
15	F	1	Total	C	Fe	H	N	O	0
			75	34	1	32	4	4	
15	G	1	Total	C	Fe	H	N	O	0
			75	34	1	32	4	4	
15	G	1	Total	C	Fe	H	N	O	0
			75	34	1	32	4	4	

3   Residue-property plots (i)

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

- Molecule 1: cytochrome-c oxidase

Chain E:

- Molecule 2: Ubiquinol-cytochrome c reductase iron-sulfur subunit

Chain C:

- Molecule 2: Ubiquinol-cytochrome c reductase iron-sulfur subunit
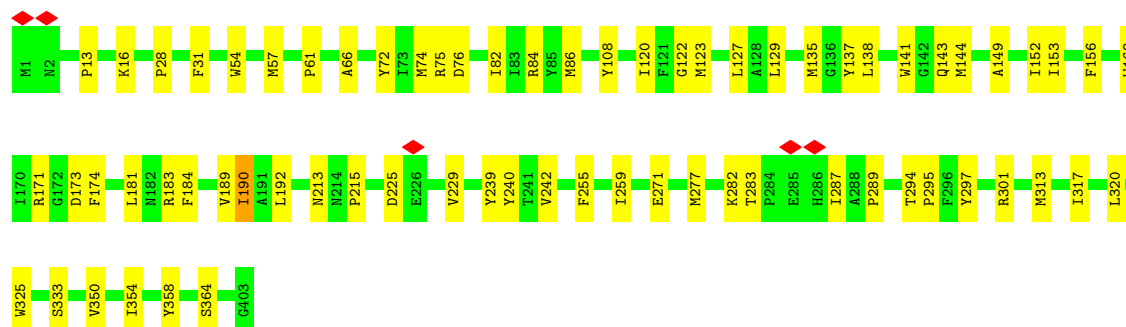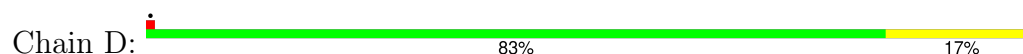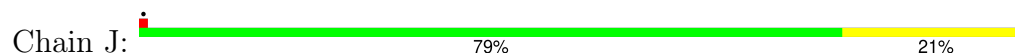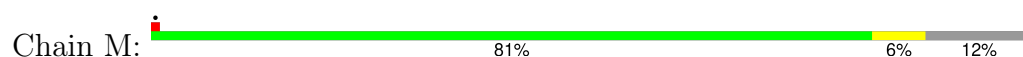
Chain Z:

N3 D4 G5 V21 A46 G47 N53 V54 G55 K56 I57 D58 I64 A65 E66 K79 E80 M81 L82 D83 E89 D96 S97 K98 P103 E104 Y105 V106 K109 K114 P115 E116 V121 C124 T125 H126 L127 G128 C129 S130 A140 D141 L142 D145 W146

C154 H155 G156 S157 Q169 P170 A171 P178 D183 A184 D185 D186 V192 D193 Q194 E195 K196

- Molecule 3: Cytochrome b

Chain I:

83%   16%

M1 V8 F12 F31 I53 M57 P61 A66 Y72 D76 Y85 Y108 G109 S110 Y111 Q112 R115 I120 F121 G122 M123 L129 E132 A133 F134 M135 G136 Y137 L138 S145 A149 Q150 V151 I152 I153 S154 L155 W169 I170 R171 G172 D173

F174 L181 F185 H188 V189 I190 A191 L192 H203 L207 G211 S212 N213 N214 P215 V218 E226 Y239 Y240 T241 V242 F253 I254 F255 I259 E285 H286 I287 A288 P289 V290 W291 T294 Y297 R301 M308 M313 L320 W325 L326 D327

S333 V350 I354 Y358 G403

- Molecule 3: Cytochrome b

Chain D:

83%   17%

M1 N2 P13 K16 P28 F31 W54 M57 P61 A66 Y72 I73 M74 R75 D76 I82 I83 R84 Y85 M86 Y108 I120 F121 G122 M123 L127 A128 L129 M135 G136 Y137 L138 W141 G142 Q143 M144 A149 I152 I153 F156 W169

I170 R171 G172 D173 F174 L181 N182 R183 F184 V189 I190 A191 L192 N213 N214 P215 D225 E226 V229 Y239 Y240 T241 V242 F255 I259 E271 M277 K282 T283 P284 E285 H286 I287 A288 P289 T294 Y295 F296 Y297 R301 M313 I317 L320
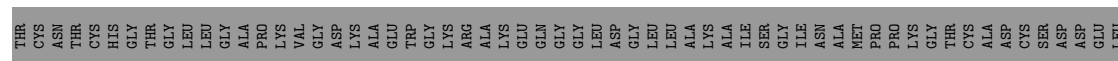
W325 S333 V350 I354 Y358 S364 G403

- Molecule 4: Cytochrome c1

Chain J:

79%   21%

PRO Q26 I32 D33 L34 Y50 C51 M52 H55 S56 Y62 E63 L75 M76 M77 L80 V81 F82 T83 G84 A85 K86 I87 P108 P109 D110 R116 T120 L127 R128 E132 R160 I163 G164 C165 V170 V171 E172 D173 G174 K175 K176 D179 P180

L186 E189 A190 C191 V197 P198 K199 T200 D209 E210 K211 V212 L215 V216 Y240 L241 R253 E254 K257

- Molecule 4: Cytochrome c1

Chain M:

81%   6%   12%

P25 Q26 L27 D28 Y50 R64 M76 L80 A100 P108 L127 R128 V153 L157 I163 GLY CYS LYS GLN VAL GLN VAL VAL GLU ASP GLY LYS LYS GLN PHE ASP PRO LEU THR GLY THR PRO LEU THR HIS GLU ALA CYS ASP Q193 V197 P198 K199 T200

L215 Y240 K257

• Molecule 5: Cytochrome c4

Chain K:

88%   12%

A21 A26 K30 F49 Q55 K62 I67 E76 M77 L81 T82 N83 M105 I123 T131 G132 C133 H134 S135 V139 H148 T162 E166 N171 D174 I193 H201

• Molecule 5: Cytochrome c4

Chain N:

91%   9%

A21 K30 Q55 K62 L75 E76 M77 T78 L81 T82 N83 L84 S85 D88 D91 S135 V139 F146 P147 H148 N171 K188 H201

• Molecule 6: Cytochrome C5

Chain L: 9% • 88%

MET LEU ALA ALA GLN ALA ALA VAL LEU ALA LEU TRP ALA VAL SER ALA GLN ALA THR THR ASP ASP A24 I25 A26 E30 P31 V32 Q38 G39 LYS GLU CYS GLU GLY VAL ALA VAL ALA ALA ALA GLY GLY GLY GLY ALA ARG SER GLY GLU ASP ILE VAL GLY LYS

THR CYS ASN THR CYS HIS GLY THR GLY LEU GLY LEU GLY ALA PRO LYS VAL GLY ASP LYS ALA GLU TRP GLY LYS ALA GLU LYS GLU GLN GLY GLY LEU ASP GLY LEU LEU ALA LYS ALA ILE SER GLY ILE ASN ALA MET PRO PRO LYS GLY THR CYS ALA ASP CYS SER ASP ASP GLU LEU

LYS ALA ALA ILE LYS HIS MET SER GLY LEU

• Molecule 6: Cytochrome C5

Chain O: 11% • 88%

MET LEU ALA ALA GLN ALA ALA VAL LEU ALA LEU TRP ALA VAL SER ALA GLN ALA THR THR ASP ASP A24 V32 Q38 G39 LYS GLU CYS GLU GLY VAL GLY VAL ALA ALA ALA GLY GLY GLY ALA ARG SER GLY GLU ASP ILE VAL GLY LYS THR CYS ASN THR

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

LYS HIS MET SER GLY LEU

• Molecule 7: Cbb3-type Cytochrome C oxidase subunit II

18%

Chain F:

80%   19%

• Molecule 8: Cbb3-type cytochrome c oxidase subunit

Chain G:

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	48594	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	51	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	15.242	Depositor
Minimum map value	-7.411	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.182	Depositor
Recommended contour level	1.24	Depositor
Map size (Å)	341.96, 341.96, 341.96	wwPDB
Map dimensions	332, 332, 332	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: HEC, CU, CA, U10, I7Y, FES, HEM

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	E	0.22	0/3847	0.45	2/5252 (0.0%)
2	C	0.13	0/1461	0.32	0/1997
2	Z	0.12	0/1490	0.31	0/2035
3	D	0.15	0/3381	0.31	0/4606
3	I	0.14	0/3381	0.32	0/4606
4	J	0.14	0/1889	0.29	0/2564
4	M	0.11	0/1674	0.26	0/2271
5	K	0.10	0/1327	0.24	0/1788
5	N	0.10	0/1327	0.23	0/1788
6	L	0.11	0/115	0.30	0/153
6	O	0.07	0/115	0.21	0/153
7	F	0.10	0/1533	0.29	0/2083
8	G	0.20	0/2422	0.54	1/3288 (0.0%)
All	All	0.15	0/23962	0.35	3/32584 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	G	70	VAL	N-CA-C	-6.51	106.12	111.91
1	E	464	ARG	CA-C-N	6.06	127.42	119.84
1	E	464	ARG	C-N-CA	6.06	127.42	119.84

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3719	0	3712	128	0
2	C	1420	1407	1407	29	0
2	Z	1449	1434	1434	23	0
3	D	3267	3289	3289	60	0
3	I	3267	3289	3289	49	0
4	J	1842	1821	1821	37	0
4	M	1631	1619	1619	12	0
5	K	1306	1279	1279	18	0
5	N	1306	1279	1279	9	0
6	L	115	129	129	4	0
6	O	115	129	129	1	0
7	F	1499	1418	1418	31	0
8	G	2356	2299	2296	102	0
9	E	1	0	0	0	0
10	E	2	0	0	0	0
11	D	86	60	60	9	0
11	E	86	60	60	12	0
11	I	86	60	60	11	0
12	C	4	0	0	1	0
12	Z	4	0	0	2	0
13	I	31	0	0	3	0
13	Z	60	0	0	6	0
14	D	63	90	90	10	0
14	I	63	90	90	13	0
15	F	43	32	30	7	0
15	G	86	64	60	12	0
15	J	43	32	30	5	0
15	K	86	64	60	5	0
15	M	43	32	30	5	0
15	N	86	64	60	2	0
All	All	24165	20040	23731	487	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 10.

The worst 5 of 487 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)
13:I:501:I7Y:C15	13:I:501:I7Y:C07	1.78	1.59
13:Z:202:I7Y:C15	13:Z:202:I7Y:C07	1.77	1.58
1:E:417:ASP:OD1	8:G:137:ARG:NH2	1.91	1.03
2:Z:169:GLN:HE22	13:Z:202:I7Y:C61	1.74	1.01
2:Z:3:ASN:HD22	2:Z:3:ASN:N	1.54	1.00

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	E	466/468 (100%)	446 (96%)	19 (4%)	1 (0%)	44	68
2	C	188/194 (97%)	185 (98%)	3 (2%)	0	100	100
2	Z	192/194 (99%)	185 (96%)	7 (4%)	0	100	100
3	D	401/403 (100%)	394 (98%)	7 (2%)	0	100	100
3	I	401/403 (100%)	394 (98%)	7 (2%)	0	100	100
4	J	230/233 (99%)	224 (97%)	6 (3%)	0	100	100
4	M	200/233 (86%)	197 (98%)	3 (2%)	0	100	100
5	K	179/181 (99%)	176 (98%)	3 (2%)	0	100	100
5	N	179/181 (99%)	174 (97%)	5 (3%)	0	100	100
6	L	14/136 (10%)	14 (100%)	0	0	100	100
6	O	14/136 (10%)	14 (100%)	0	0	100	100
7	F	198/200 (99%)	192 (97%)	6 (3%)	0	100	100
8	G	302/304 (99%)	280 (93%)	20 (7%)	2 (1%)	19	42
All	All	2964/3266 (91%)	2875 (97%)	86 (3%)	3 (0%)	50	73

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	G	33	LYS
8	G	208	GLU
1	E	473	ARG

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	E	383/383 (100%)	375 (98%)	8 (2%)	48	76
2	C	148/151 (98%)	147 (99%)	1 (1%)	81	93
2	Z	151/151 (100%)	149 (99%)	2 (1%)	65	85
3	D	342/342 (100%)	340 (99%)	2 (1%)	84	94
3	I	342/342 (100%)	340 (99%)	2 (1%)	84	94
4	J	195/196 (100%)	194 (100%)	1 (0%)	86	95
4	M	171/196 (87%)	171 (100%)	0	100	100
5	K	130/130 (100%)	130 (100%)	0	100	100
5	N	130/130 (100%)	130 (100%)	0	100	100
6	L	12/90 (13%)	12 (100%)	0	100	100
6	O	12/90 (13%)	12 (100%)	0	100	100
7	F	147/167 (88%)	144 (98%)	3 (2%)	50	78
8	G	237/237 (100%)	231 (98%)	6 (2%)	42	72
All	All	2400/2605 (92%)	2375 (99%)	25 (1%)	71	89

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	190	ILE
7	F	50	THR
8	G	301	LEU
7	F	43	VAL
7	F	81	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11

such sidechains are listed below:

Mol	Chain	Res	Type
4	M	90	HIS
4	M	161	GLN
8	G	95	GLN
5	N	83	ASN
5	K	179	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 24 ligands modelled in this entry, 3 are monoatomic - leaving 21 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	#$|Z| > 2$
14	U10	I	504	-	63,63,63	2.80	17 (26%)	78,79,79	1.69	22 (28%)
12	FES	C	201	2	0,4,4	-	-	-		
11	HEM	E	505	1,10	42,50,50	1.51	5 (11%)	46,82,82	1.22	4 (8%)
14	U10	D	503	-	63,63,63	2.81	17 (26%)	78,79,79	1.64	22 (28%)
11	HEM	D	502	3	42,50,50	1.49	6 (14%)	46,82,82	1.37	6 (13%)
15	HEC	G	401	8	32,50,50	2.20	3 (9%)	30,82,82	2.07	6 (20%)
15	HEC	G	402	8	32,50,50	2.13	3 (9%)	30,82,82	2.17	7 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
15	HEC	N	502	5	32,50,50	2.11	3 (9%)	30,82,82	2.30	6 (20%)
15	HEC	K	502	5	32,50,50	2.12	3 (9%)	30,82,82	2.32	4 (13%)
15	HEC	M	500	4	32,50,50	2.11	3 (9%)	30,82,82	2.27	7 (23%)
12	FES	Z	201	2	0,4,4	-	-	-		
15	HEC	J	500	4	32,50,50	2.15	3 (9%)	30,82,82	2.25	6 (20%)
11	HEM	D	501	3	42,50,50	1.44	5 (11%)	46,82,82	1.56	10 (21%)
11	HEM	E	504	1,10	42,50,50	1.48	4 (9%)	46,82,82	1.36	6 (13%)
15	HEC	N	501	5	32,50,50	2.17	3 (9%)	30,82,82	2.23	4 (13%)
15	HEC	K	501	5	32,50,50	2.09	3 (9%)	30,82,82	2.12	6 (20%)
13	I7Y	I	501	-	36,36,67	6.20	22 (61%)	59,59,103	3.45	18 (30%)
11	HEM	I	502	3	42,50,50	1.45	5 (11%)	46,82,82	1.54	8 (17%)
15	HEC	F	301	7	32,50,50	2.11	3 (9%)	30,82,82	2.14	3 (10%)
13	I7Y	Z	202	-	67,67,67	4.67	29 (43%)	99,103,103	2.81	24 (24%)
11	HEM	I	503	3	42,50,50	1.50	5 (11%)	46,82,82	1.41	6 (13%)

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
14	U10	I	504	-	-	20/63/87/87	0/1/1/1
12	FES	C	201	2	-	-	0/1/1/1
11	HEM	E	505	1,10	-	4/12/54/54	-
14	U10	D	503	-	-	25/63/87/87	0/1/1/1
15	HEC	G	402	8	-	1/10/54/54	-
11	HEM	D	502	3	-	2/12/54/54	-
15	HEC	G	401	8	-	8/10/54/54	-
15	HEC	N	502	5	-	1/10/54/54	-
15	HEC	K	502	5	-	2/10/54/54	-
15	HEC	M	500	4	-	2/10/54/54	-
12	FES	Z	201	2	-	-	0/1/1/1
15	HEC	J	500	4	-	0/10/54/54	-
11	HEM	D	501	3	-	2/12/54/54	-
11	HEM	E	504	1,10	-	2/12/54/54	-
15	HEC	N	501	5	-	1/10/54/54	-
15	HEC	K	501	5	-	2/10/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	I7Y	I	501	-	-	1/2/90/150	0/6/6/8
11	HEM	I	502	3	-	7/12/54/54	-
15	HEC	F	301	7	-	2/10/54/54	-
13	I7Y	Z	202	-	-	10/22/150/150	0/8/8/8
11	HEM	I	503	3	-	4/12/54/54	-

The worst 5 of 142 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	I	501	I7Y	C15-C07	15.39	1.78	1.53
13	Z	202	I7Y	C15-C07	15.36	1.77	1.53
13	Z	202	I7Y	C07-C08	-14.85	1.25	1.53
13	I	501	I7Y	C07-C08	-14.84	1.25	1.53
13	I	501	I7Y	C10-C02	-13.87	1.30	1.54

The worst 5 of 175 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	I	501	I7Y	C76-C73-C74	17.95	148.17	115.66
13	Z	202	I7Y	C76-C73-C74	17.94	148.16	115.66
13	I	501	I7Y	O80-C73-C74	-9.18	79.89	107.26
13	Z	202	I7Y	O80-C73-C74	-9.18	79.90	107.26
15	F	301	HEC	CBB-CAB-C3B	-7.52	109.90	127.49

There are no chirality outliers.

5 of 96 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	E	505	HEM	C1A-C2A-CAA-CBA
11	E	505	HEM	C3A-C2A-CAA-CBA
13	Z	202	I7Y	C16-C17-O20-CG1
13	Z	202	I7Y	C2C-C1C-O1C-C48
13	Z	202	I7Y	O5C-C1C-O1C-C48

There are no ring outliers.

21 monomers are involved in 103 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	I	504	U10	13	0
12	C	201	FES	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	E	505	HEM	5	0
14	D	503	U10	10	0
11	D	502	HEM	5	0
15	G	401	HEC	4	0
15	G	402	HEC	8	0
15	N	502	HEC	1	0
15	K	502	HEC	1	0
15	M	500	HEC	5	0
12	Z	201	FES	2	0
15	J	500	HEC	5	0
11	D	501	HEM	4	0
11	E	504	HEM	7	0
15	N	501	HEC	1	0
15	K	501	HEC	4	0
13	I	501	I7Y	3	0
11	I	502	HEM	5	0
15	F	301	HEC	7	0
13	Z	202	I7Y	6	0
11	I	503	HEM	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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 U10 I 504

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM E 505

Bond lengths

Bond angles

Torsions

Rings

Ligand U10 D 503

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM D 502

Bond lengths

Bond angles

Torsions

Rings

Ligand HEC G 401

Bond lengths

Bond angles

Torsions

Rings

Ligand HEC G 402

Bond lengths

Bond angles

Torsions

Rings

Ligand HEC N 502

Bond lengths

Bond angles

Torsions

Rings

Ligand HEC K 502

Bond lengths

Bond angles

Torsions

Rings

Ligand HEC M 500

Bond lengths

Bond angles

Torsions

Rings

Ligand HEC J 500

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM D 501

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM E 504

Bond lengths

Bond angles

Torsions

Rings

Ligand HEC N 501

Bond lengths

Bond angles

Torsions

Rings

Ligand HEC K 501

Bond lengths

Bond angles

Torsions

Rings

Ligand I7Y I 501

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM I 502
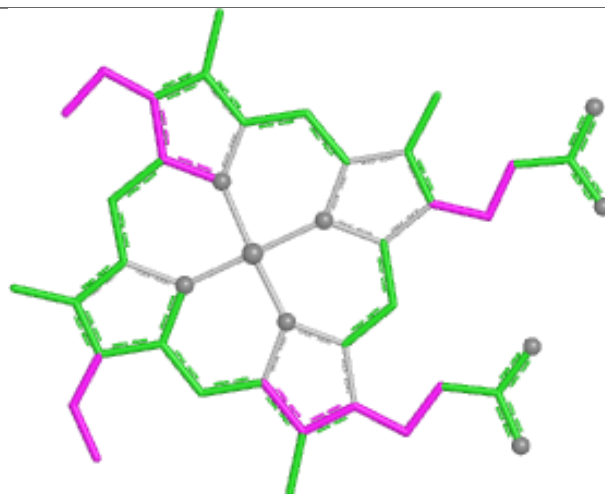
Bond lengths
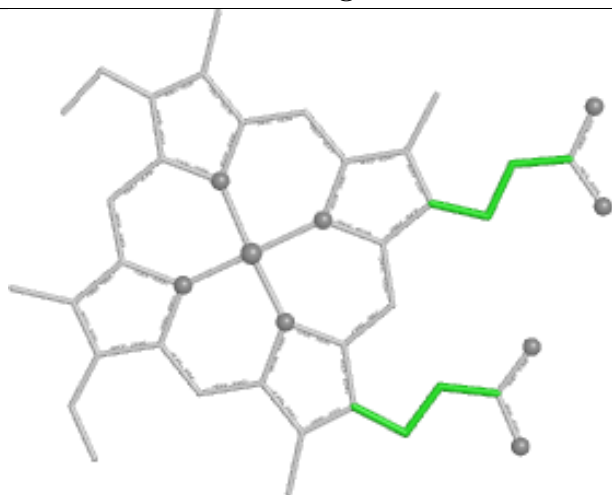
Bond angles
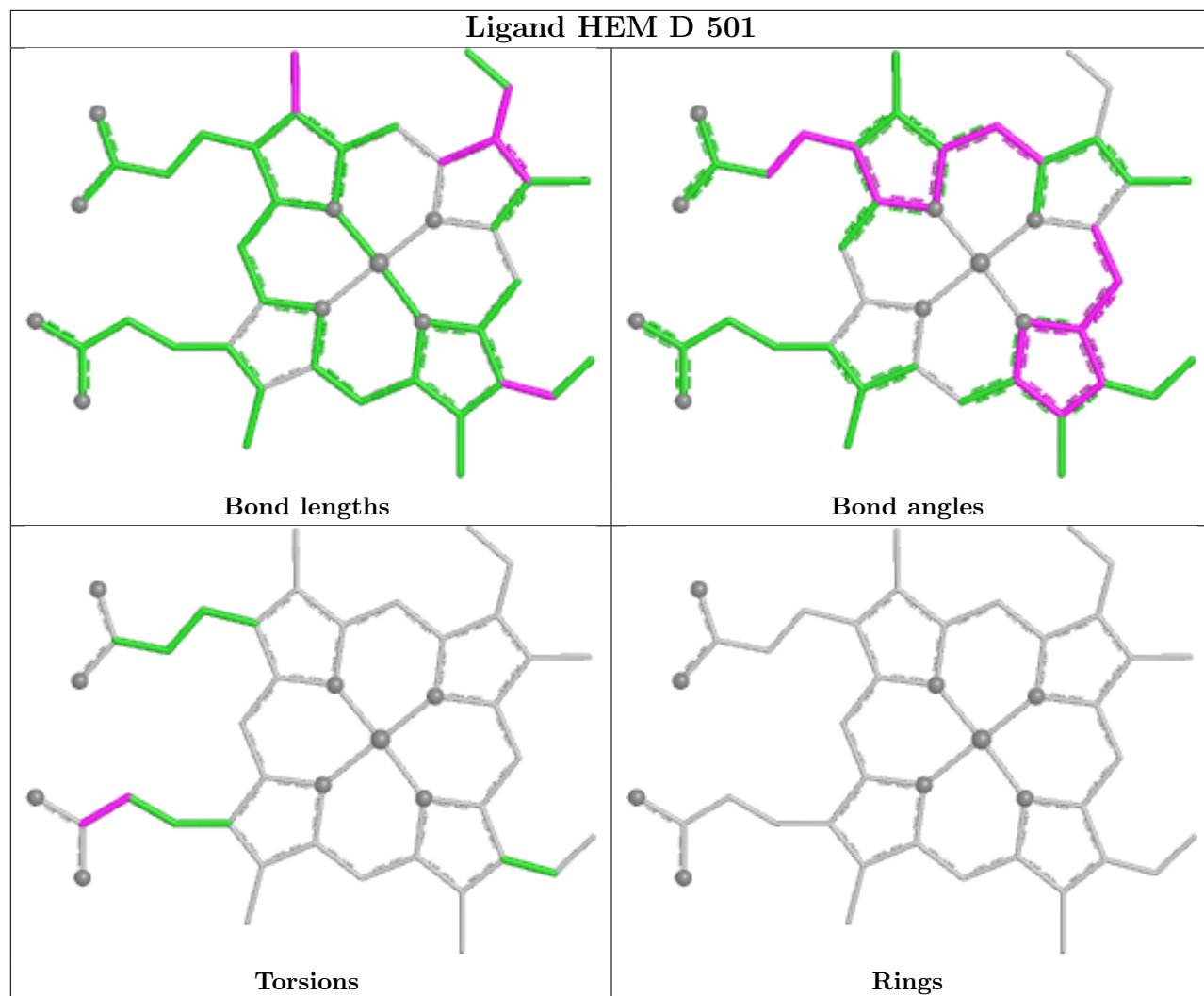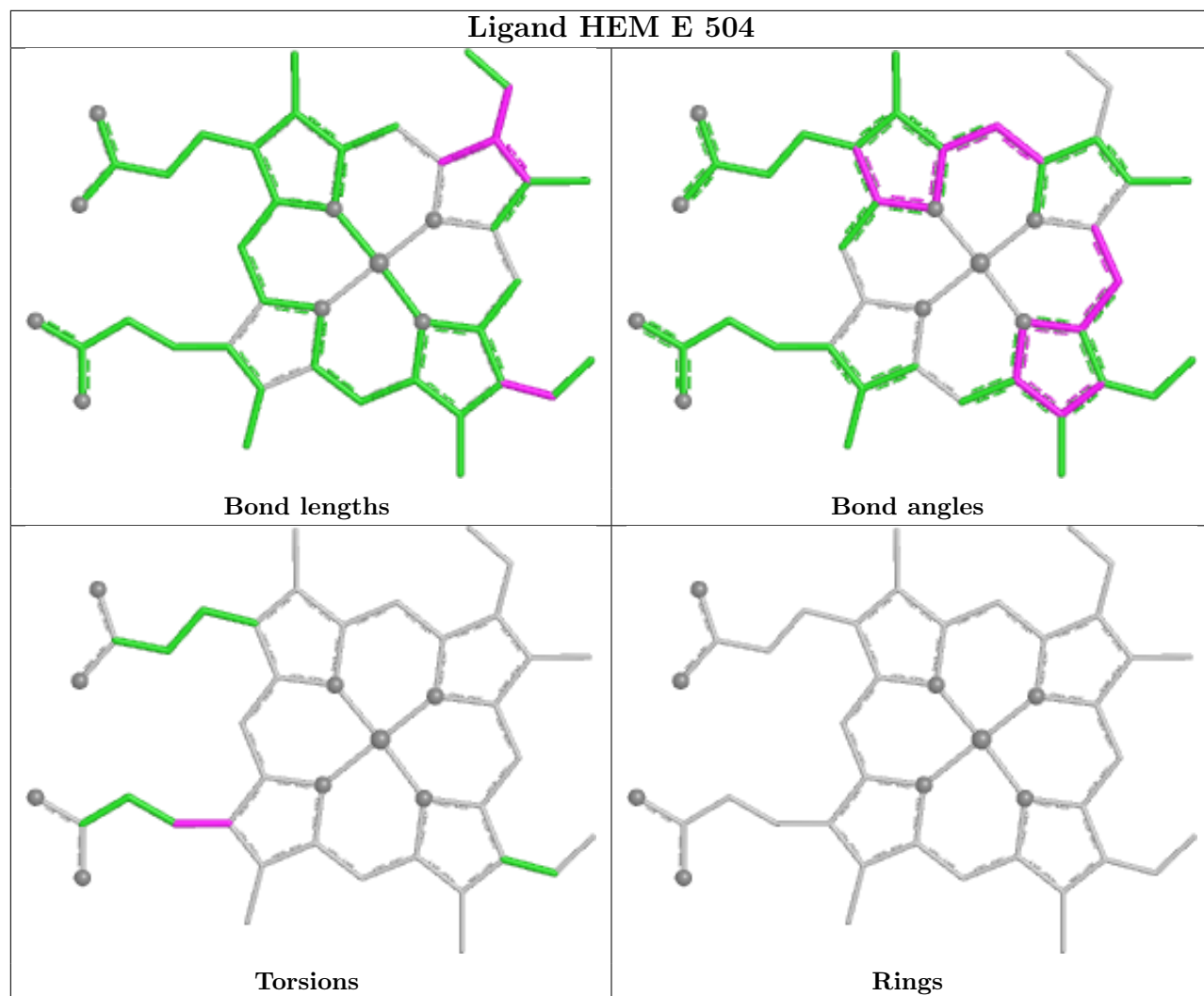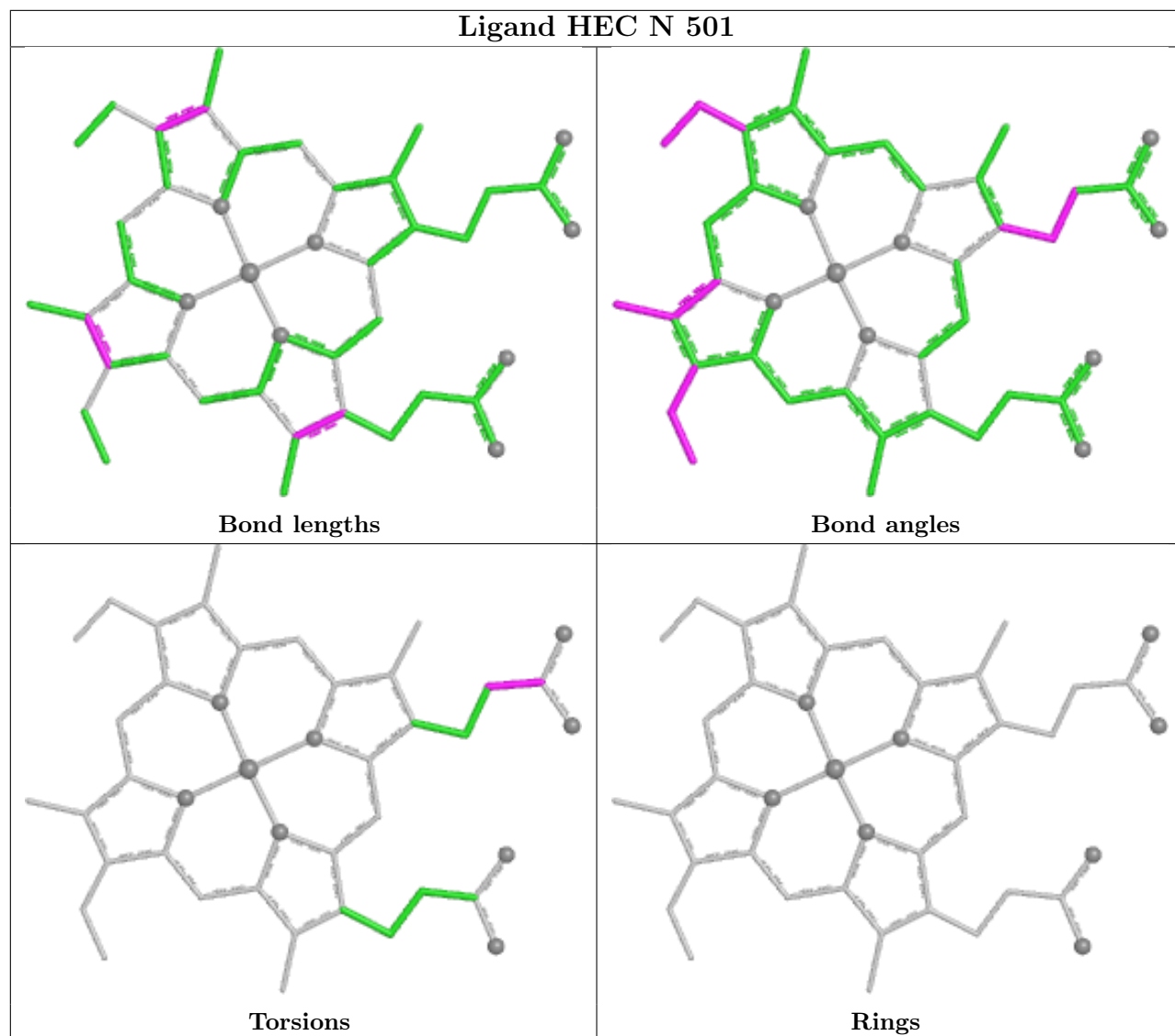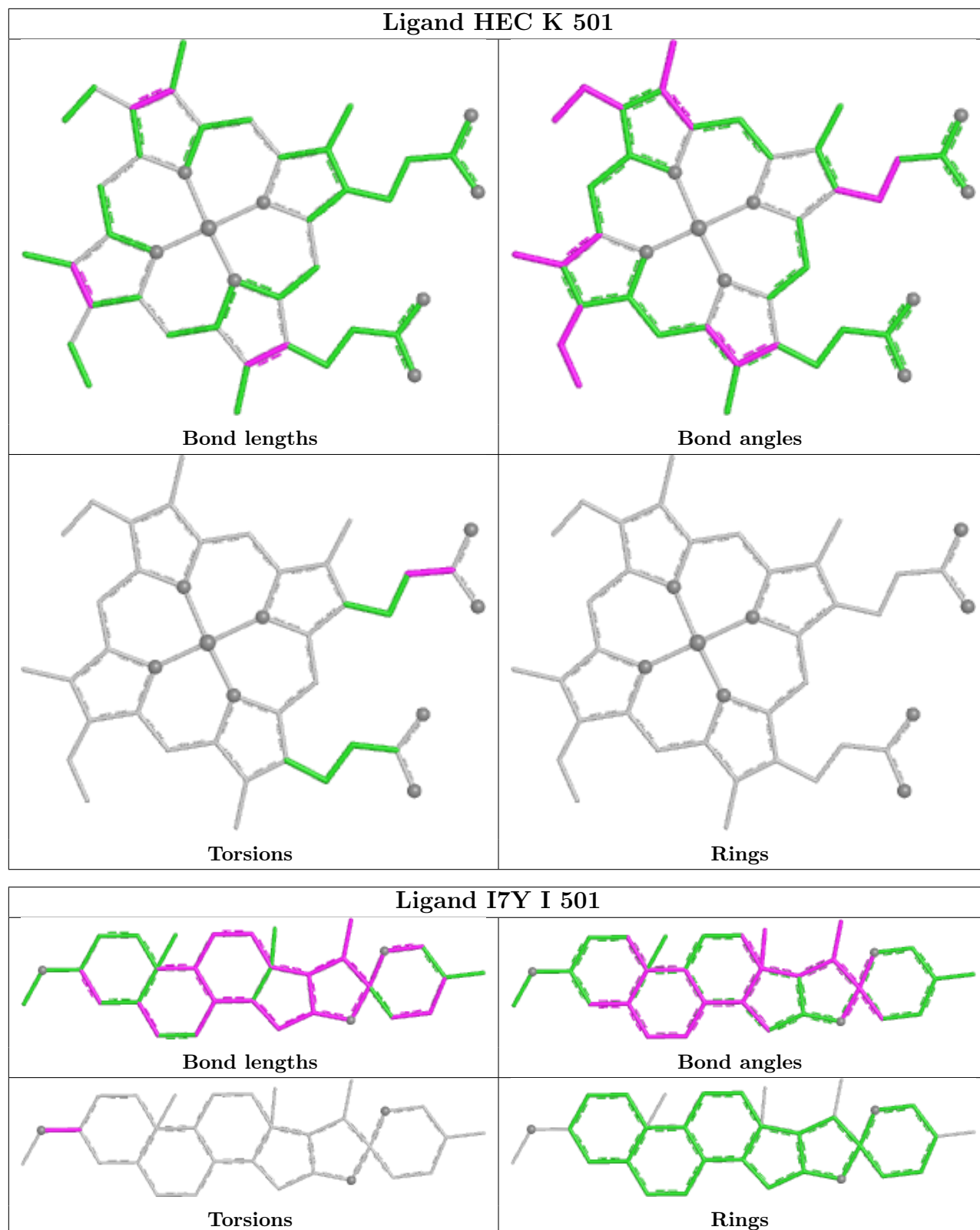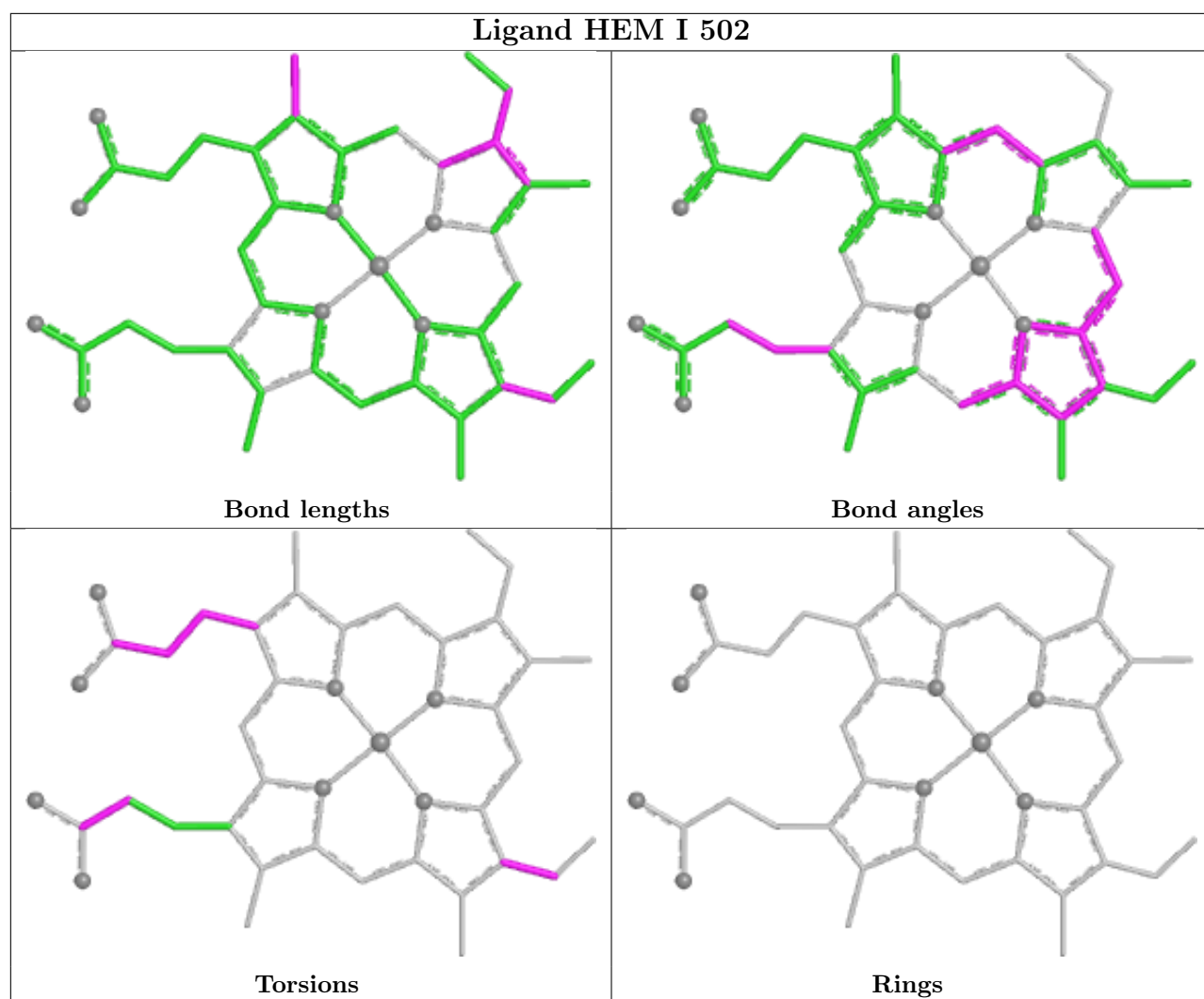
Torsions

Rings

Ligand HEC F 301

Bond lengths

Bond angles

Torsions

Rings

Ligand I7Y Z 202

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM I 503

Bond lengths
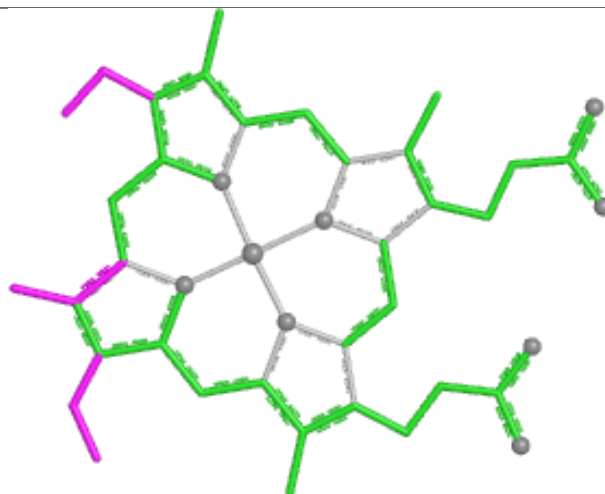
Bond angles
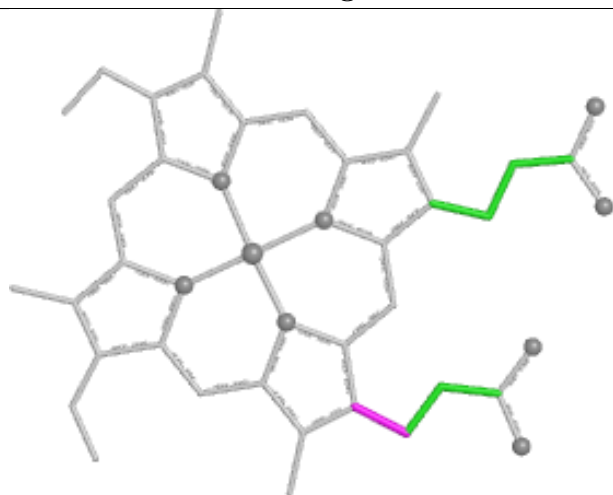
Torsions

Rings
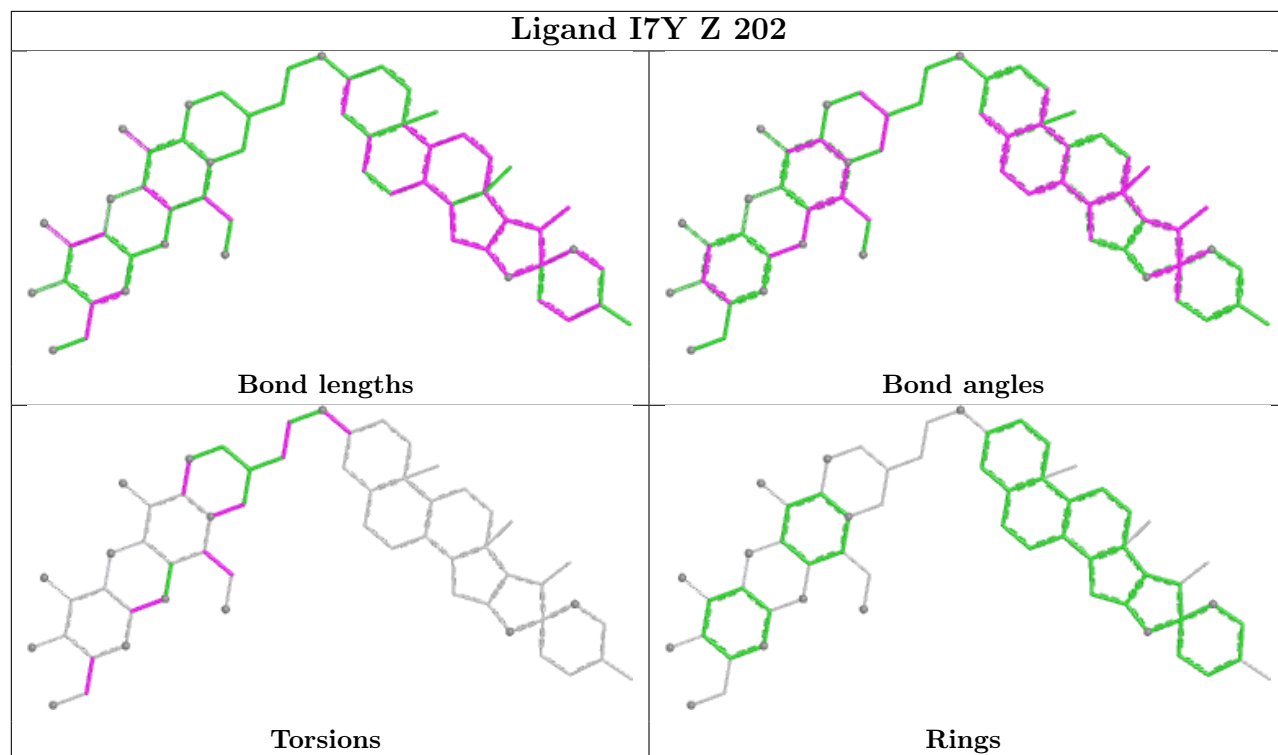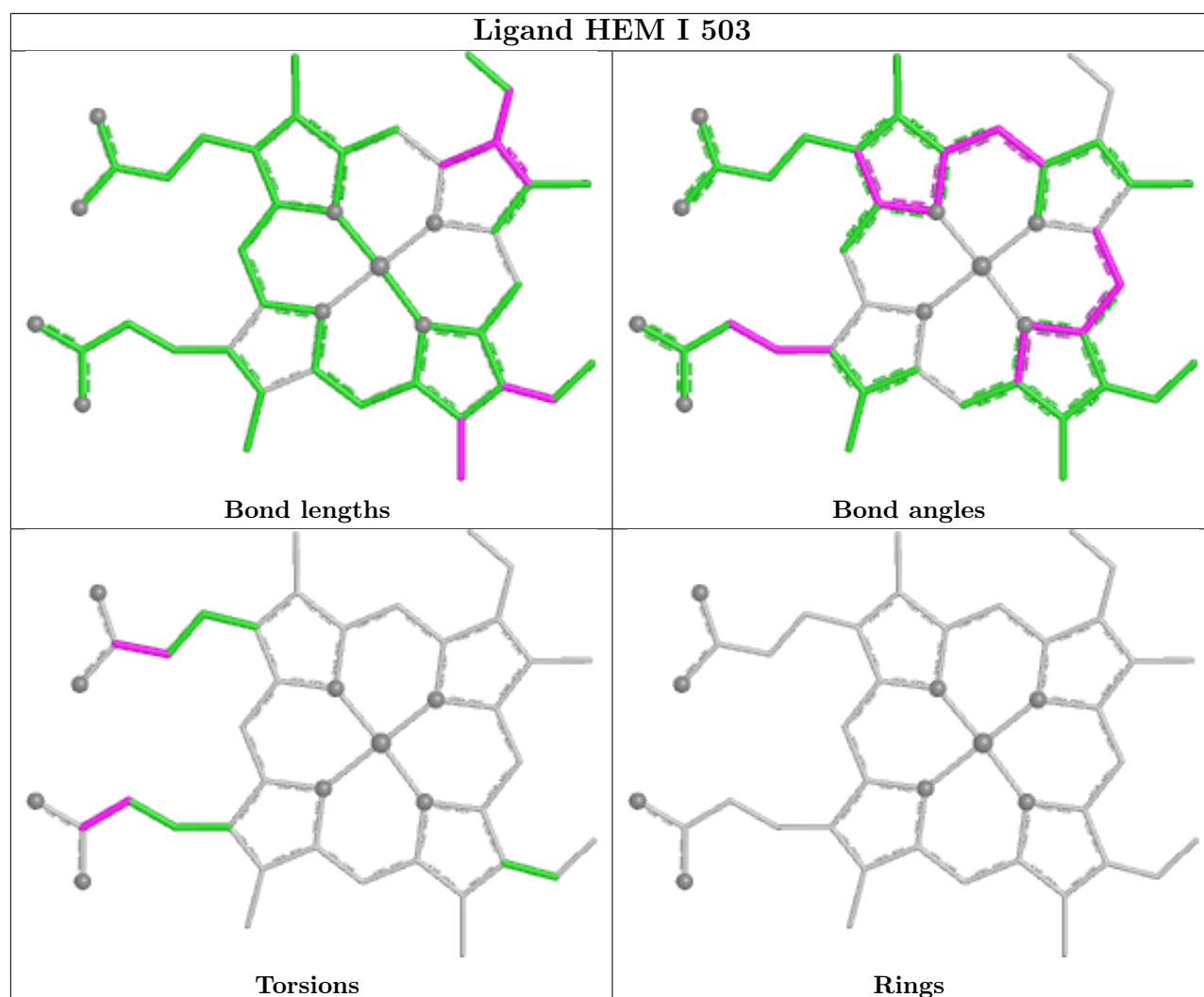
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6   Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-40625. 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 ⓘ
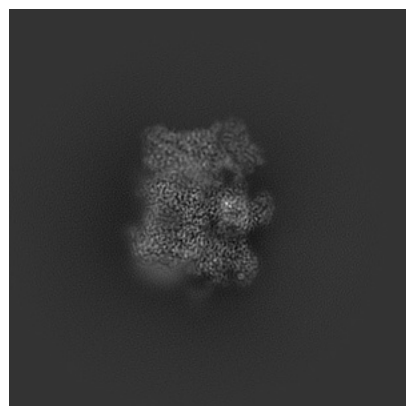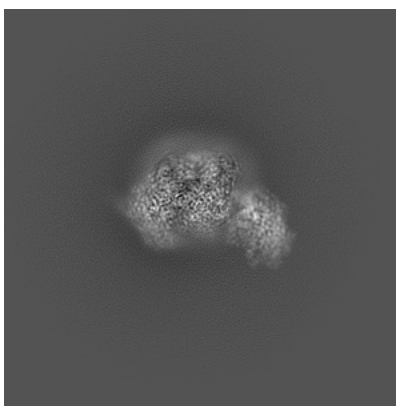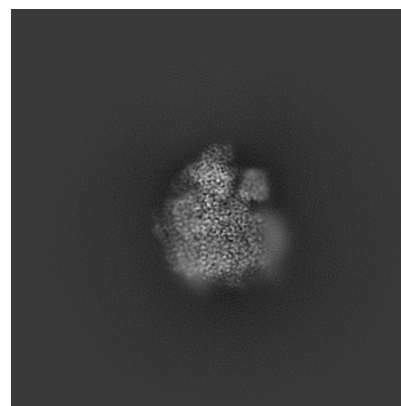
6.1.1   Primary map

X   Y   Z

6.1.2   Raw map

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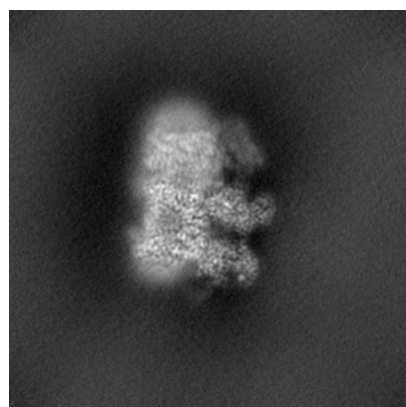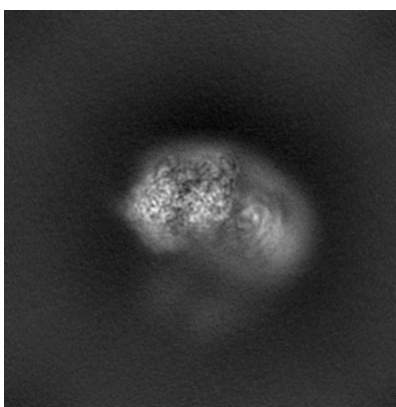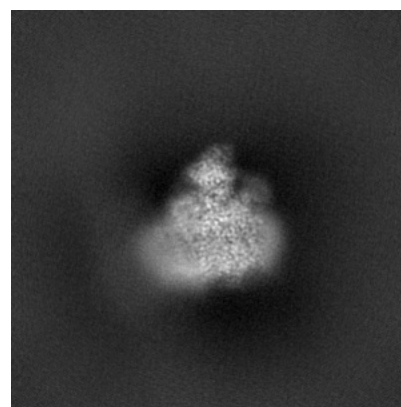
The images above show the map projected in three orthogonal directions.

6.2   Central slices ⓘ
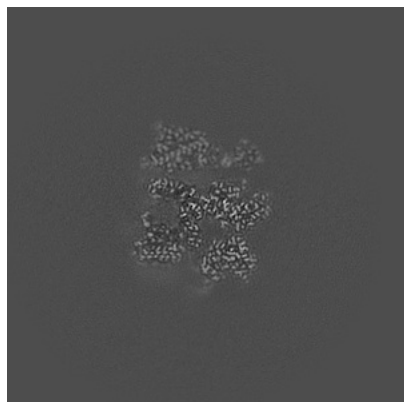
6.2.1   Primary map
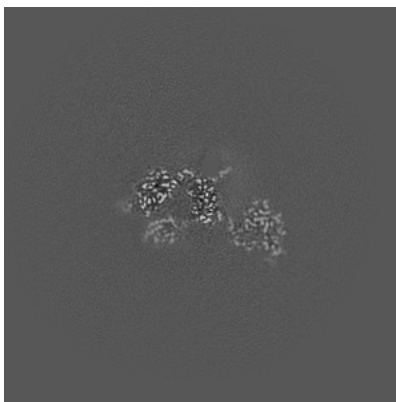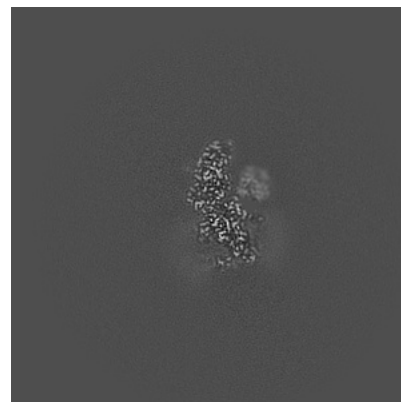
X Index: 166   Y Index: 166   Z Index: 166

6.2.2   Raw map
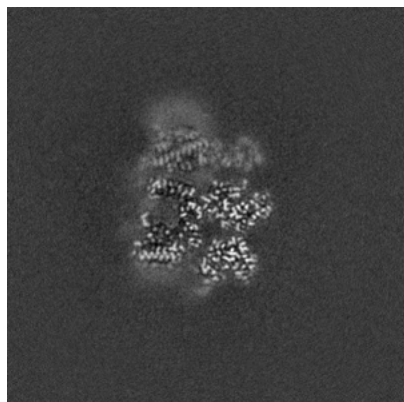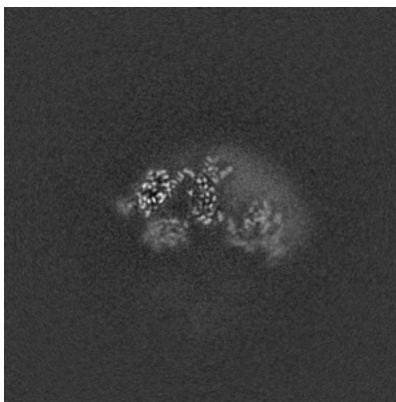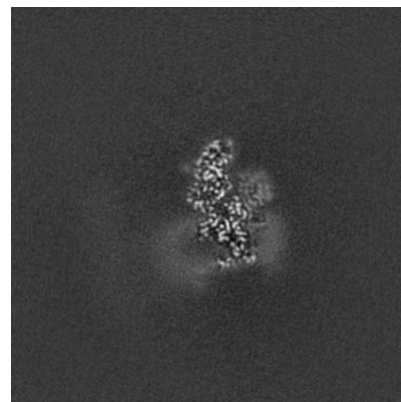
X Index: 166   Y Index: 166   Z Index: 166

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

6.3   Largest variance slices ⓘ

6.3.1   Primary map
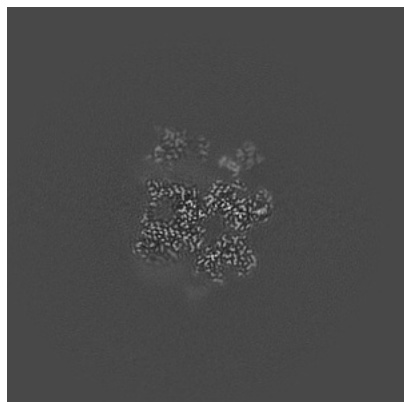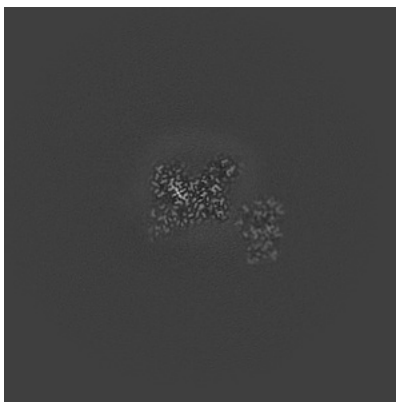
X Index: 171   Y Index: 145   Z Index: 164
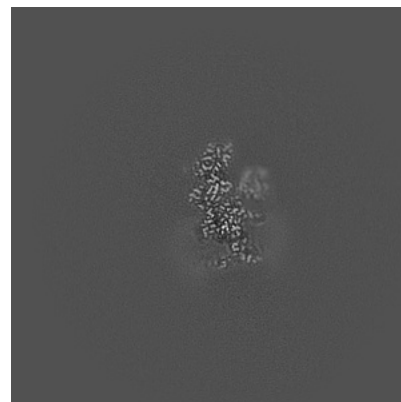
6.3.2   Raw map
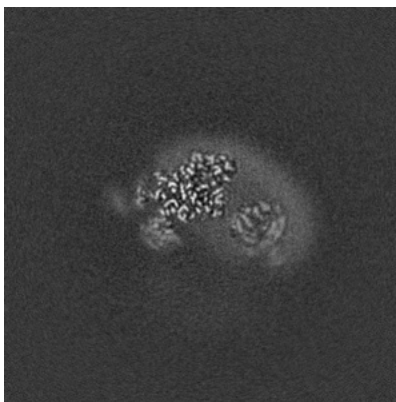
X Index: 171   Y Index: 156   Z Index: 131
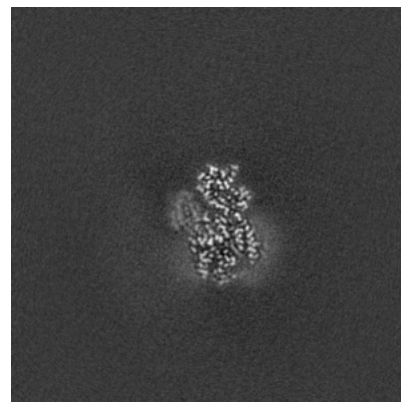
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1　Primary map
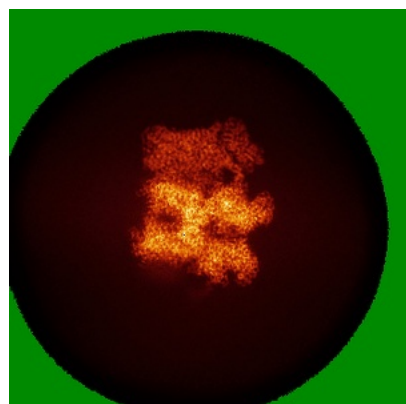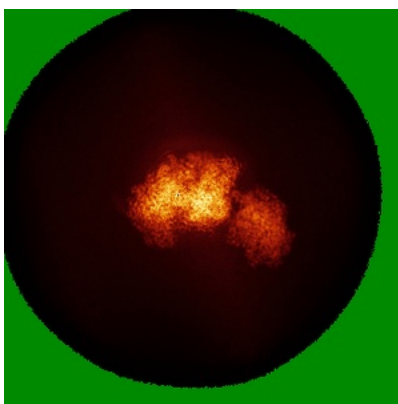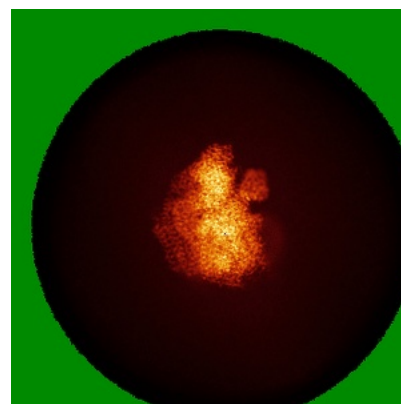
X　　　　　　　　　　Y　　　　　　　　　　Z

6.4.2　Raw map

X　　　　　　　　　　Y　　　　　　　　　　Z
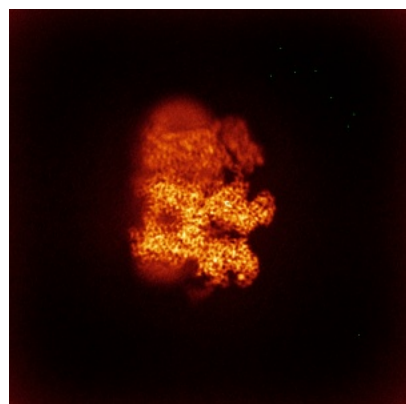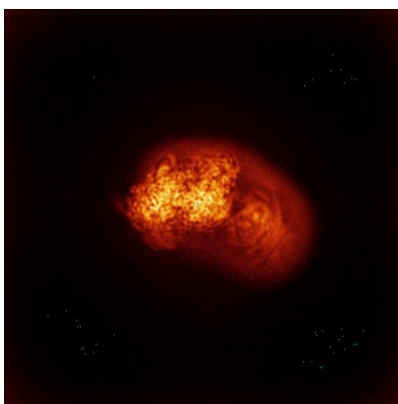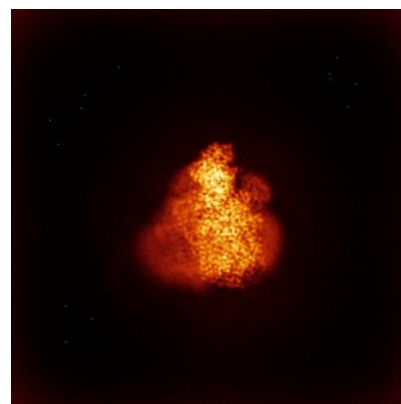
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X	Y	Z
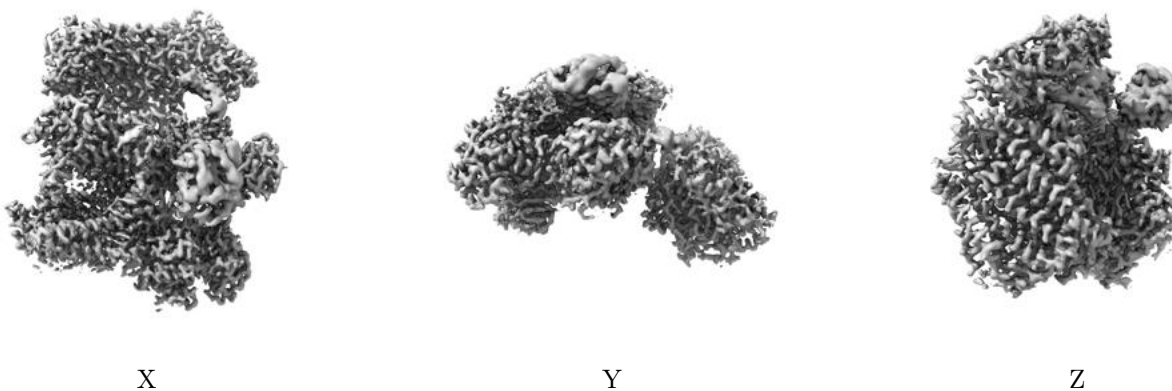
The images above show the 3D surface view of the map at the recommended contour level 1.24. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

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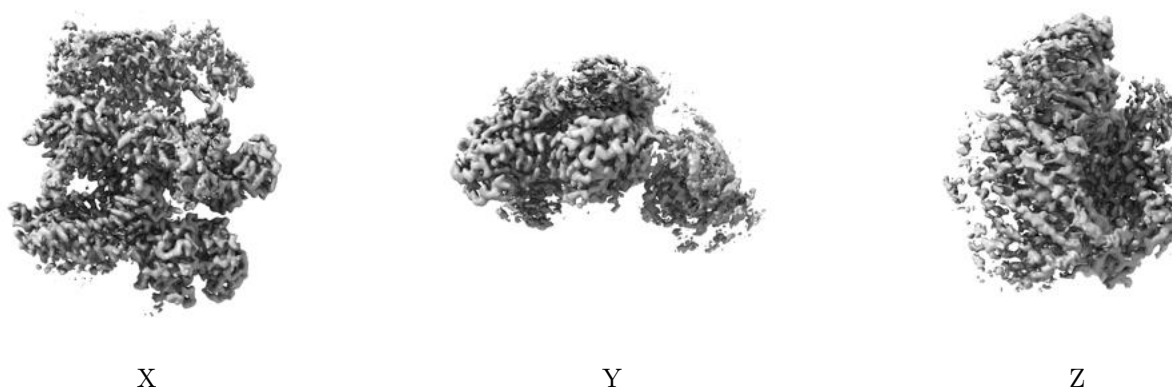
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation (i)

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

7   Map analysis ⓘ

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

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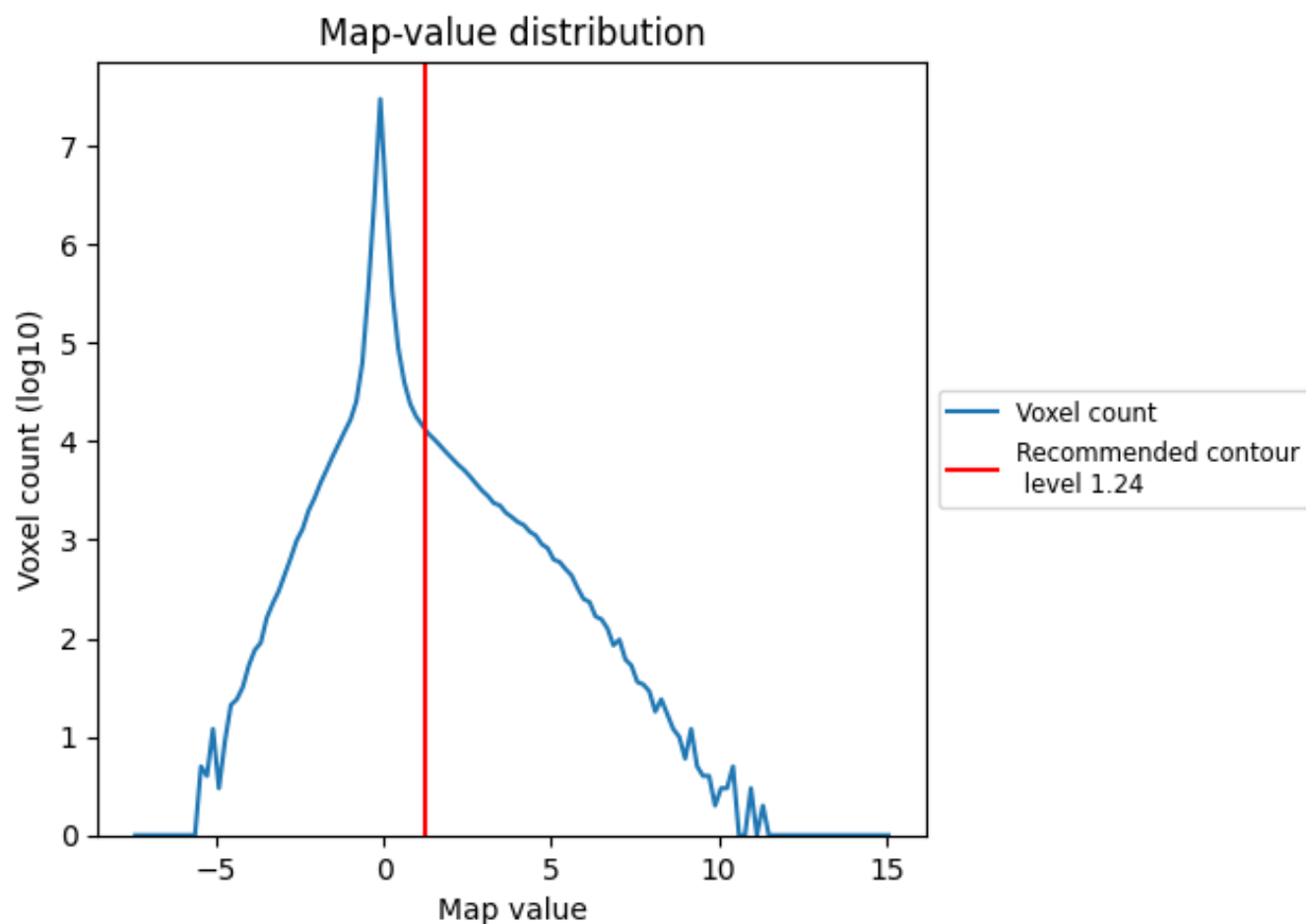
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2　Volume estimate ⓘ
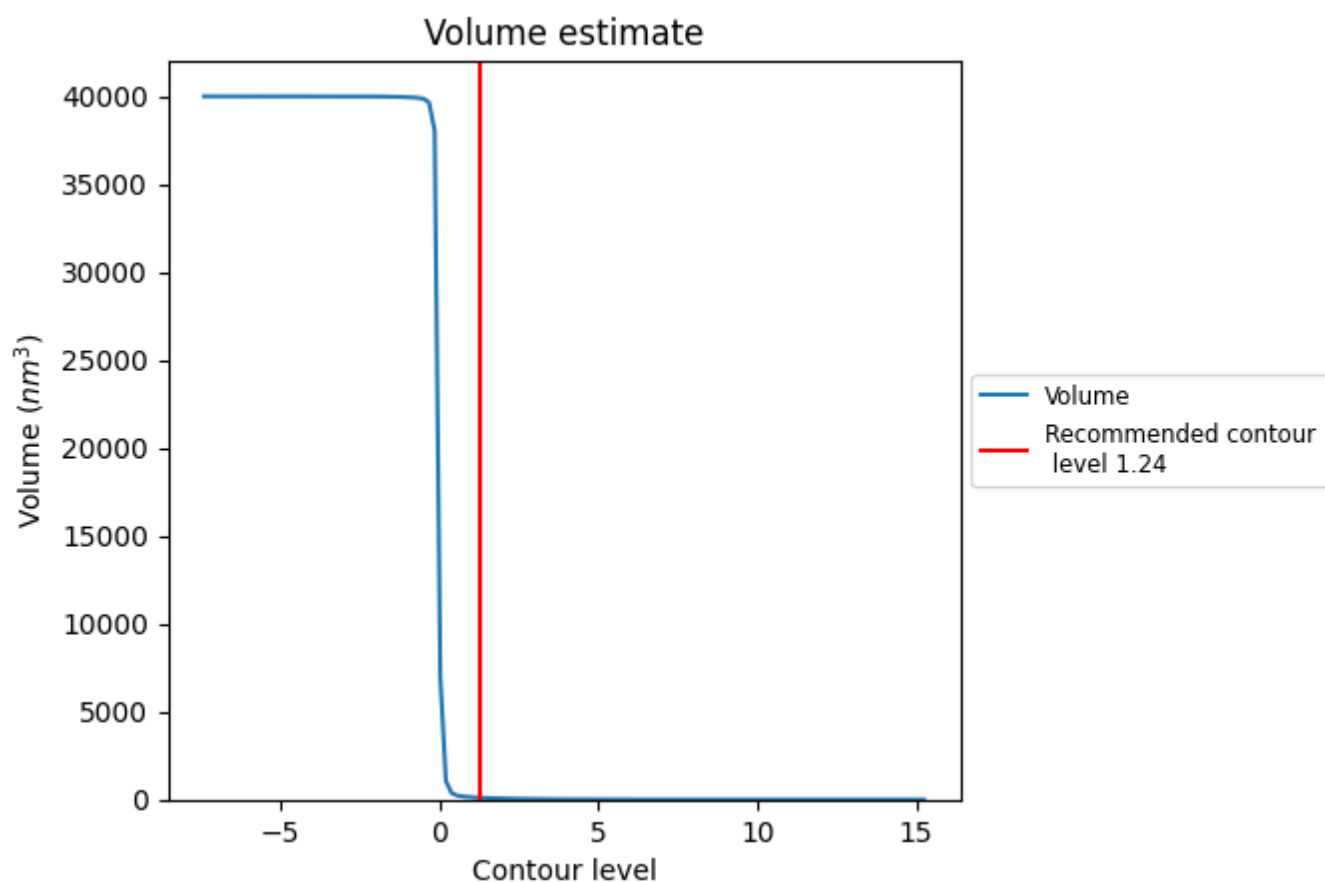
The volume at the recommended contour level is 106 nm^3; this corresponds to an approximate mass of 96 kDa.

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 ⓘ
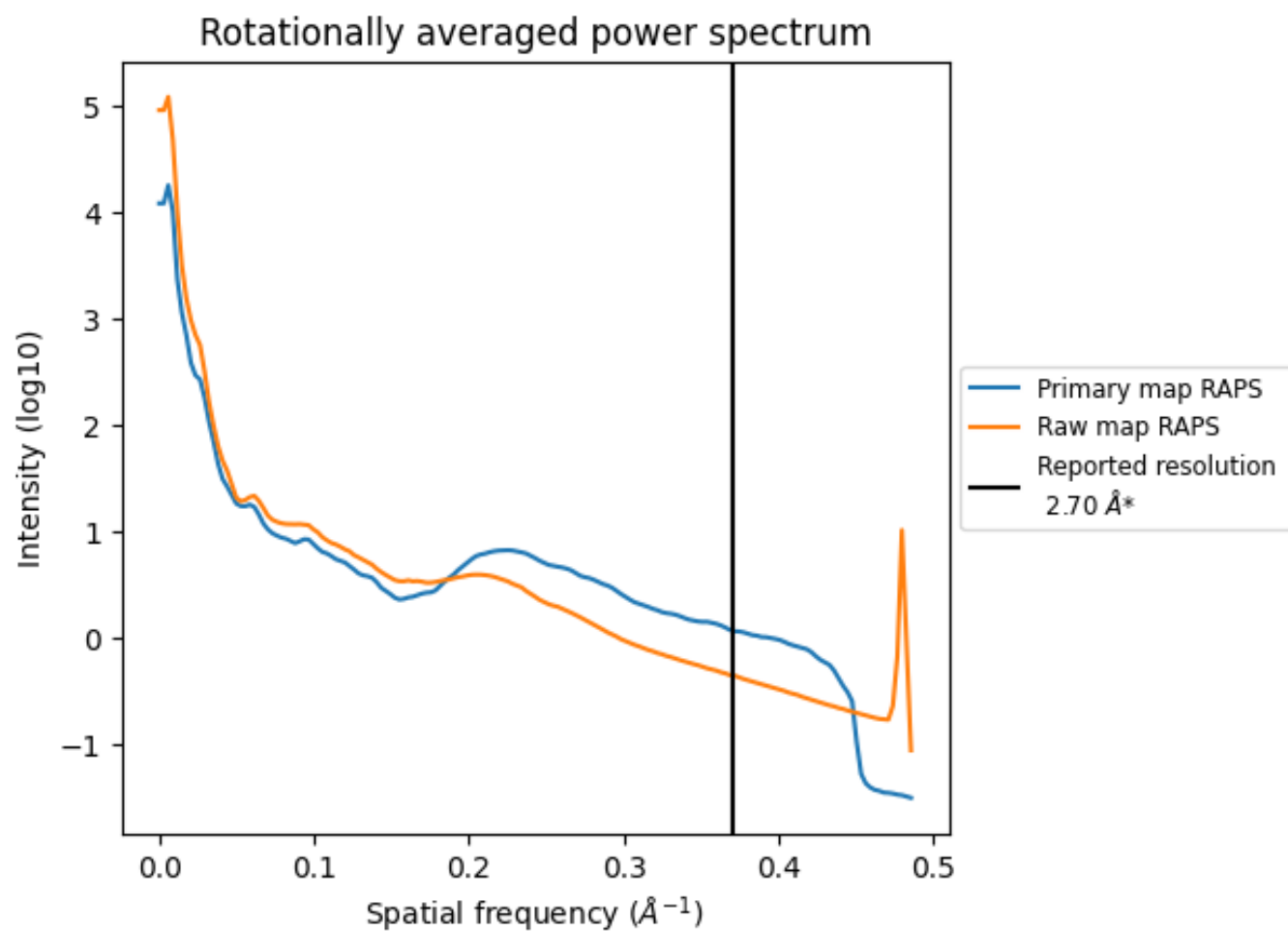
*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

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)
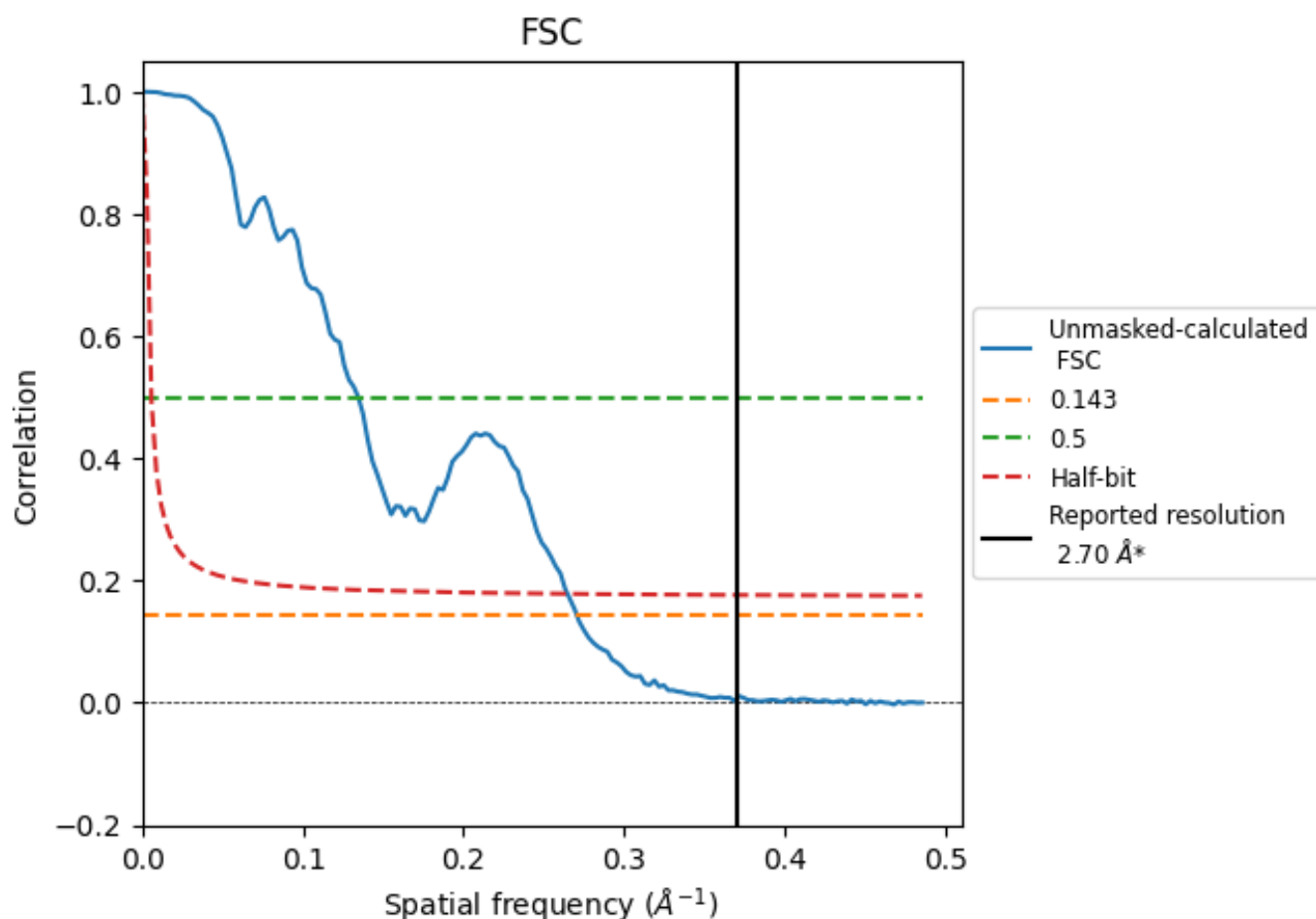
*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

8.2   Resolution estimates ⓘ

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.70	7.43	3.78

*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 3.70 differs from the reported value 2.7 by more than 10 %
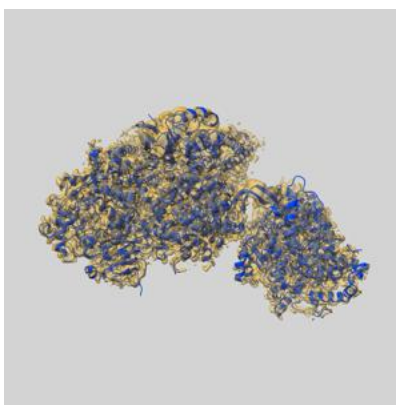
9   Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-40625 and PDB model 8SNH. Per-residue inclusion information can be found in section 3 on page 10.
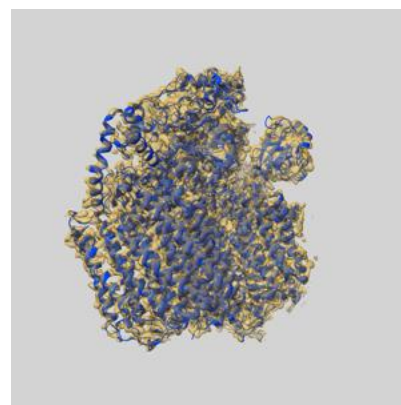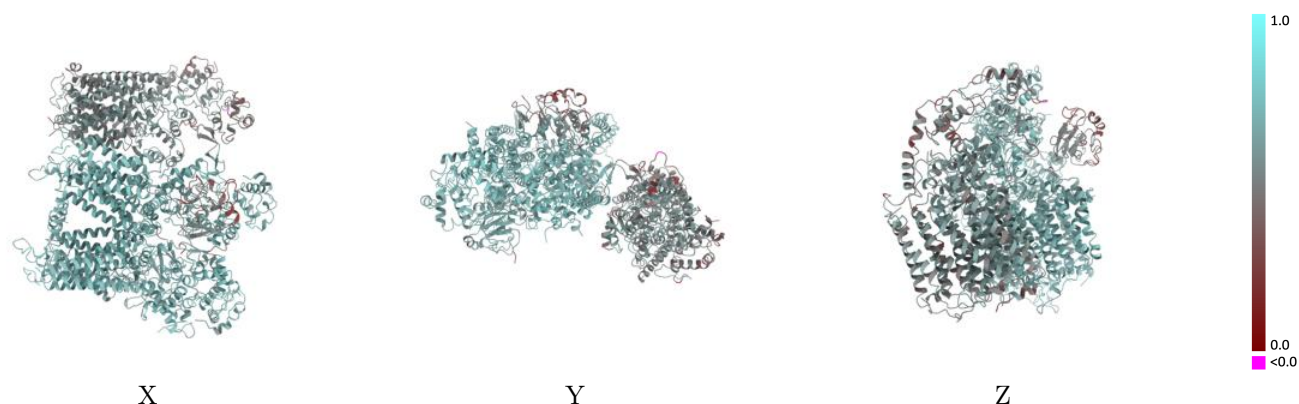
9.1   Map-model overlay (i)
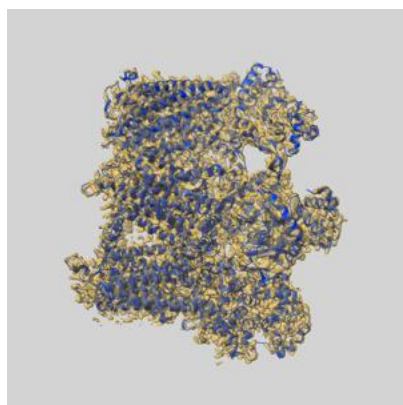
| X | Y | Z |

The images above show the 3D surface view of the map at the recommended contour level 1.24 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 ⓘ

X	Y	Z

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 ⓘ

X	Y	Z
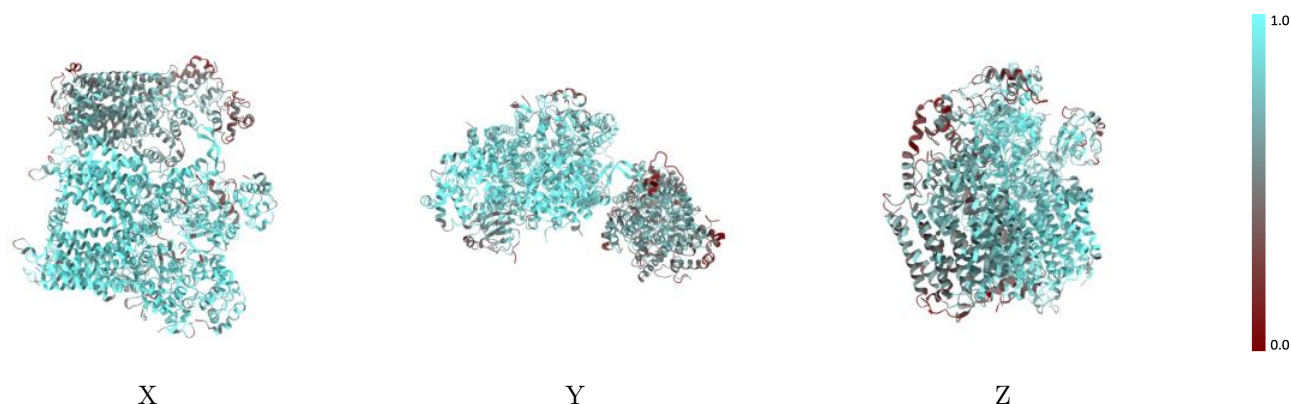
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.24).

9.4   Atom inclusion ⓘ
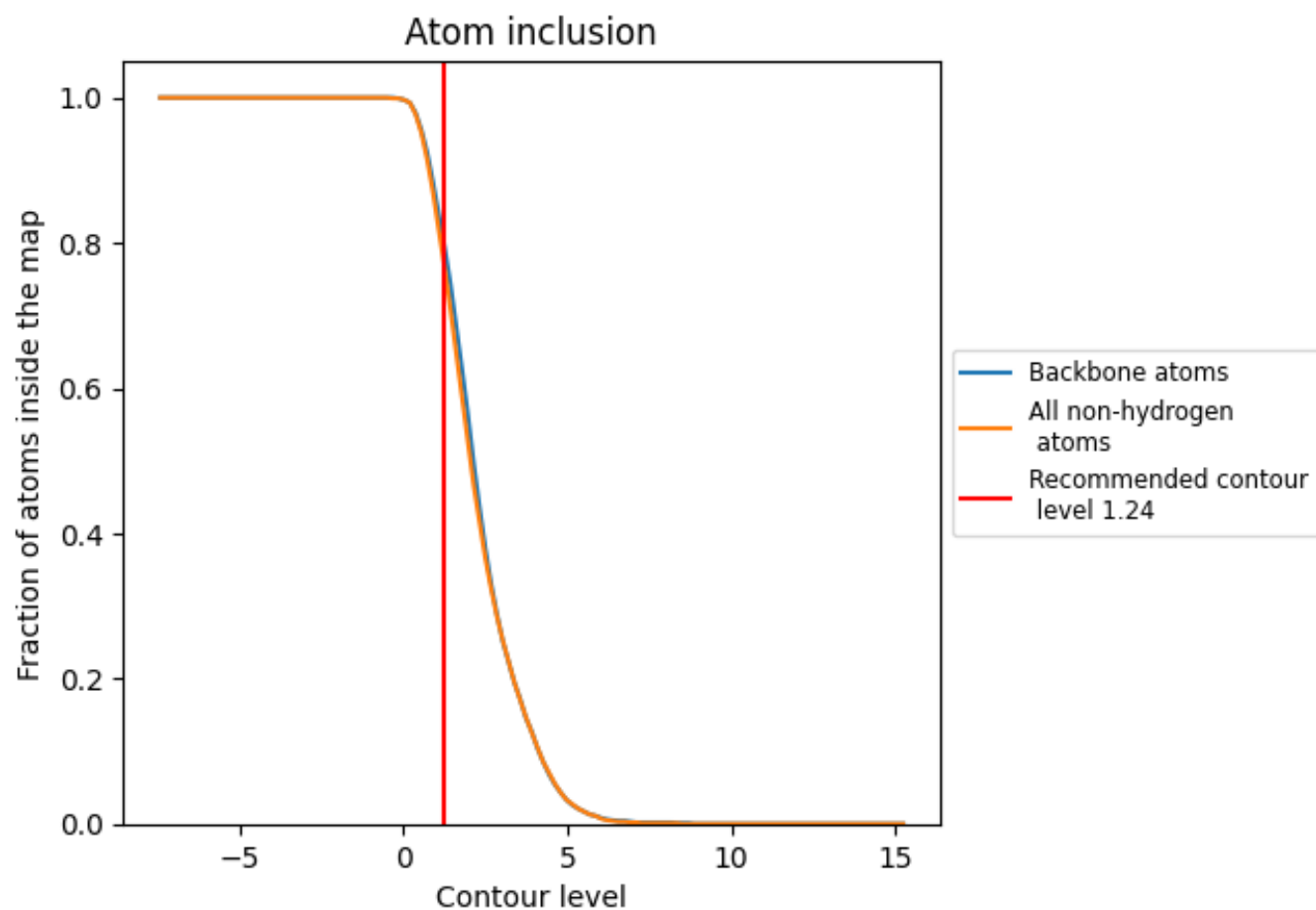
At the recommended contour level, 80% of all backbone atoms, 77% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (1.24) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7730	0.6130
C	0.7460	0.4780
D	0.9120	0.6830
E	0.6740	0.5390
F	0.6240	0.5550
G	0.4870	0.4880
I	0.9070	0.6830
J	0.9110	0.6560
K	0.9170	0.6790
L	0.7790	0.6590
M	0.9070	0.6820
N	0.8930	0.6740
O	0.7260	0.6500
Z	0.6850	0.6250

1.0

0.0
<0.0