



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 04:50 PM UTC

PDB ID : 8YIO / pdb_00008yio
EMDB ID : EMD-39324
Title : Cryo-EM structure of *Saccharomyces cerevisiae* bc1 complex in azoxystrobin-bound state
Authors : Ye, Y.; Li, Z.W.; Yang, G.F.
Deposited on : 2024-02-29
Resolution : 2.35 Å(reported)
Based on initial model : 6YMX

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

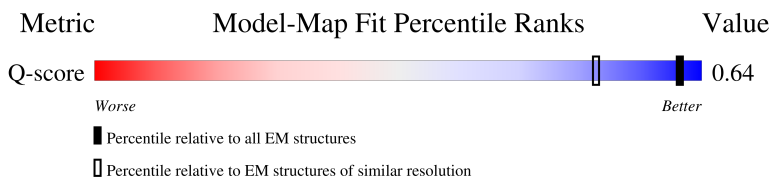
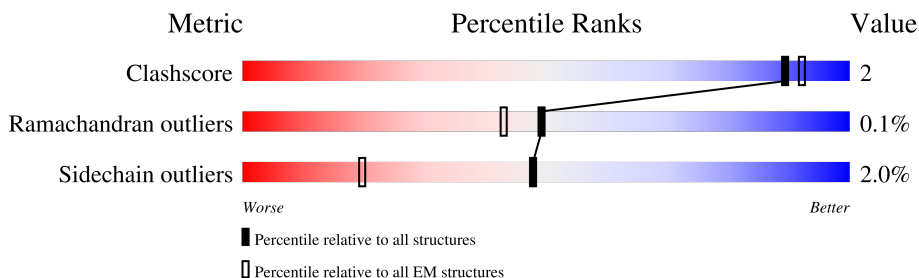
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

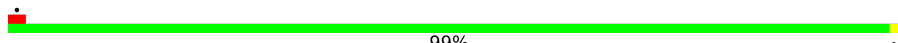
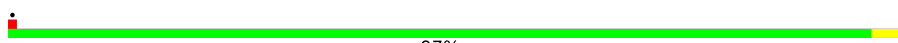
The reported resolution of this entry is 2.35 Å.

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.



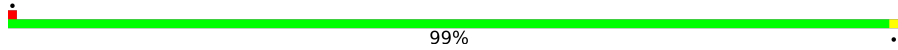
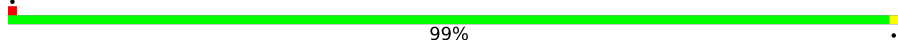
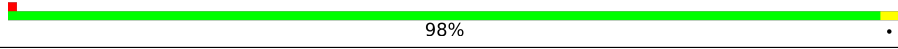
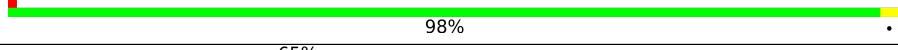
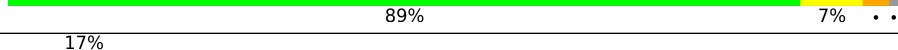
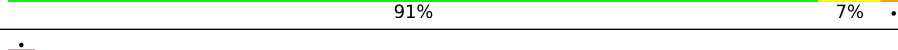
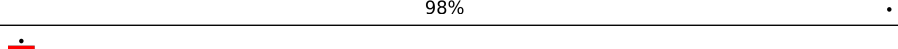
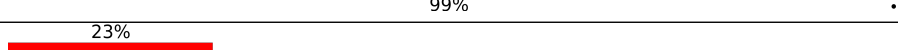
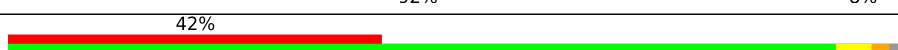
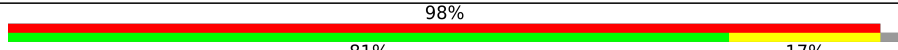
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4607 (1.85 - 2.85)

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	431	 99% .
1	L	431	 99% .
2	C	385	 97% .
2	N	385	 97% .

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Mol	Chain	Length	Quality of chain
3	B	352	
3	M	352	
4	D	248	
4	O	248	
5	E	185	
5	P	185	
6	F	75	
6	Q	75	
7	G	126	
7	R	126	
8	H	93	
8	S	93	
9	I	55	
9	T	55	
10	U	52	
10	V	52	

2 Entry composition [i](#)

There are 18 unique types of molecules in this entry. The entry contains 32370 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 COR1 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	431	Total	C	N	O	S	0	0
			3344	2110	576	652	6		
1	L	431	Total	C	N	O	S	0	0
			3344	2110	576	652	6		

- Molecule 2 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	385	Total	C	N	O	S	0	0
			3090	2082	484	503	21		
2	N	385	Total	C	N	O	S	0	0
			3090	2082	484	503	21		

- Molecule 3 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	352	Total	C	N	O	S	0	0
			2735	1747	453	534	1		
3	M	352	Total	C	N	O	S	0	0
			2735	1747	453	534	1		

- Molecule 4 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	248	Total	C	N	O	S	0	0
			1961	1249	340	363	9		
4	O	248	Total	C	N	O	S	0	0
			1961	1249	340	363	9		

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	185	Total	C	N	O	S	0	0
			1411	893	242	266	10		
5	P	185	Total	C	N	O	S	0	0
			1411	893	242	266	10		

- Molecule 6 is a protein called QCR6 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	74	Total	C	N	O	S	0	0
			624	391	108	123	2		
6	Q	75	Total	C	N	O	S	0	0
			633	396	109	126	2		

- Molecule 7 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	126	Total	C	N	O	S	0	0
			1019	653	173	191	2		
7	R	126	Total	C	N	O	S	0	0
			1019	653	173	191	2		

- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	93	Total	C	N	O	S	0	0
			773	510	131	130	2		
8	S	93	Total	C	N	O	S	0	0
			773	510	131	130	2		

- Molecule 9 is a protein called Cytochrome b-c1 complex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	I	54	Total	C	N	O	0	0
			442	295	74	73		
9	T	54	Total	C	N	O	0	0
			443	295	74	74		

- Molecule 10 is a protein called Cytochrome b-c1 complex subunit 10, mitochondrial.

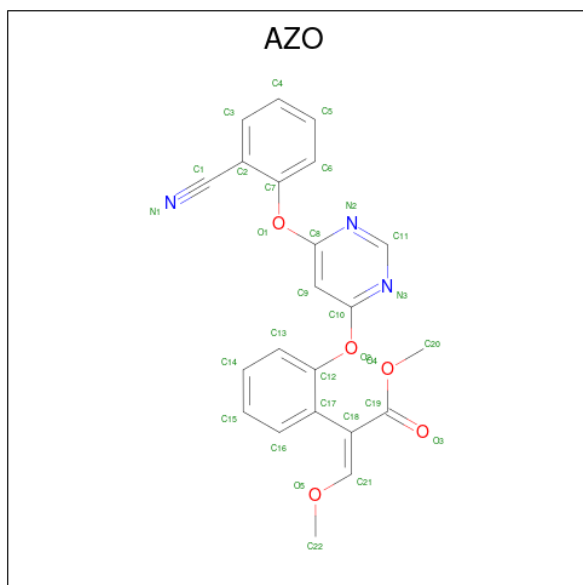
Mol	Chain	Residues	Atoms					AltConf	Trace
10	U	44	Total	C	N	O	S	0	0
			347	230	58	57	2		

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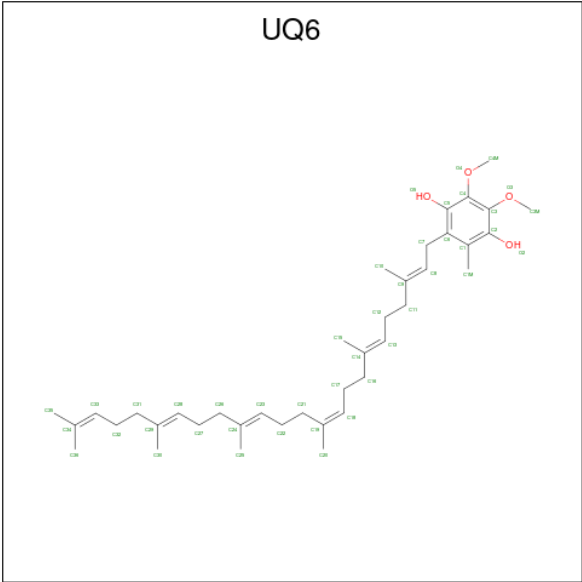
Mol	Chain	Residues	Atoms					AltConf	Trace
10	V	51	Total	C	N	O	S	0	0
			406	272	66	66	2		

- Molecule 11 is METHYL (2Z)-2-(2-([6-(2-CYANOPHENOXY)PYRIMIDIN-4-YL]OXY} PHENYL)-3-METHOXYACRYLATE (CCD ID: AZO) (formula: C₂₂H₁₇N₃O₅) (labeled as "Ligand of Interest" by depositor).



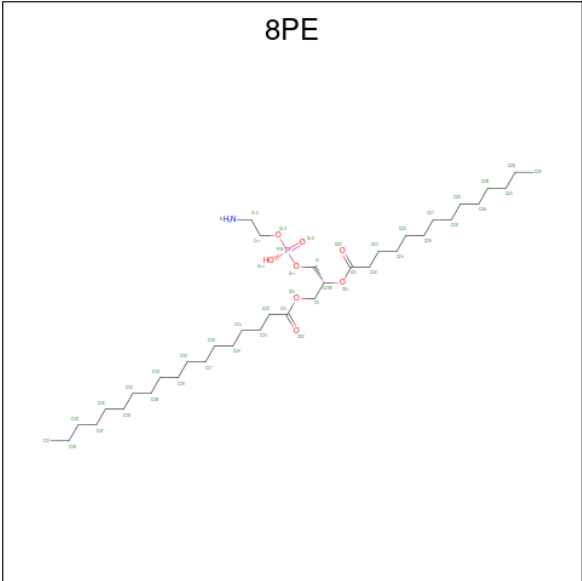
Mol	Chain	Residues	Atoms				AltConf
11	C	1	Total	C	N	O	0
			30	22	3	5	
11	N	1	Total	C	N	O	0
			30	22	3	5	

- Molecule 12 is 5-(3,7,11,15,19,23-HEXAMETHYL-TETRACOSA-2,6,10,14,18,22-HEXA ENYL)-2,3-DIMETHOXY-6-METHYL-BENZENE-1,4-DIOL (CCD ID: UQ6) (formula: C₃₉H₆₀O₄).



Mol	Chain	Residues	Atoms			AltConf
12	C	1	Total	C	O	0
			43	39	4	
12	N	1	Total	C	O	0
			43	39	4	

- Molecule 13 is (2R)-3-{[(S)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-(tetradecanoyloxy)propyl octadecanoate (CCD ID: 8PE) (formula: C₃₇H₇₄NO₈P).



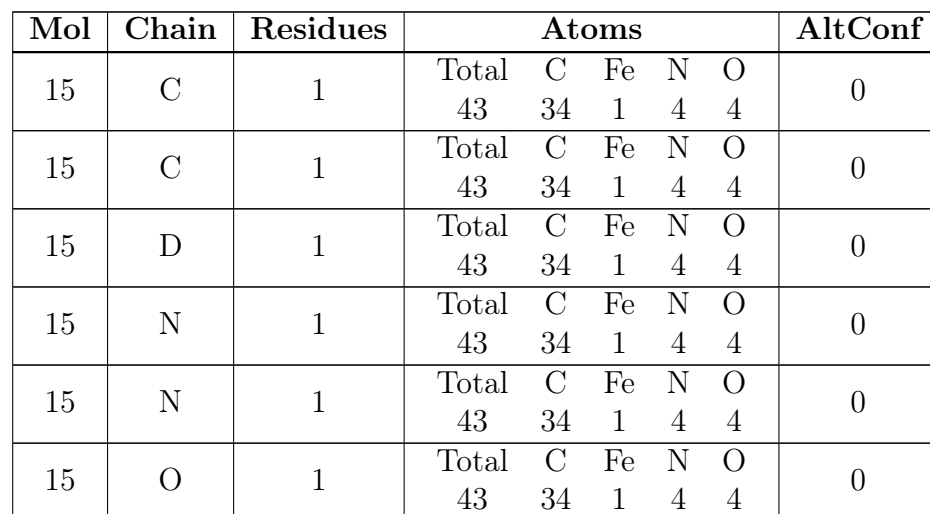
Mol	Chain	Residues	Atoms					AltConf
13	C	1	Total	C	N	O	P	0
			47	37	1	8	1	

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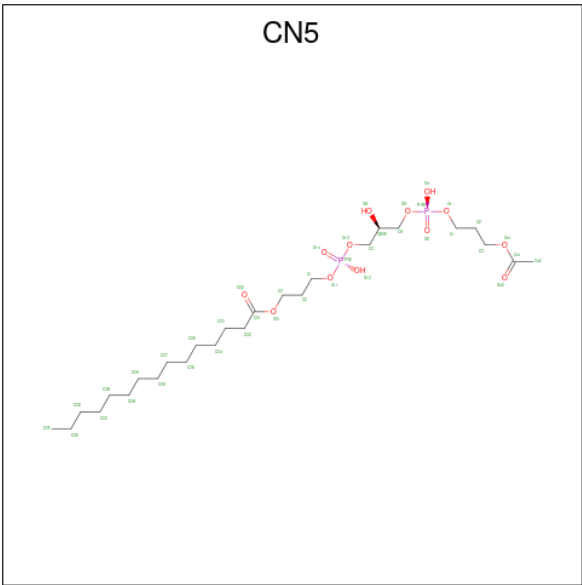
Mol	Chain	Residues	Atoms					AltConf
13	N	1	Total	C	N	O	P	0
			47	37	1	8	1	

- # 9PE

- Molecule 15 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

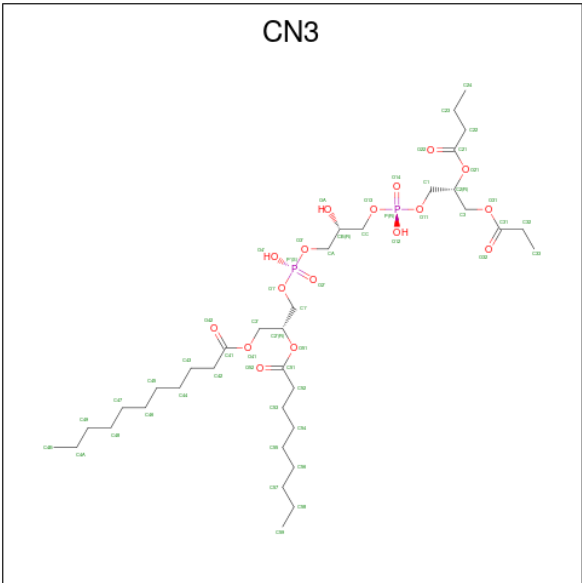


- Molecule 16 is (5S,11R)-5,8,11-trihydroxy-5,11-dioxido-17-oxo-4,6,10,12,16-pentaoxa-5,11-diphosphaoctadec-1-yl pentadecanoate (CCD ID: CN5) (formula: C₂₆H₅₂O₁₃P₂).



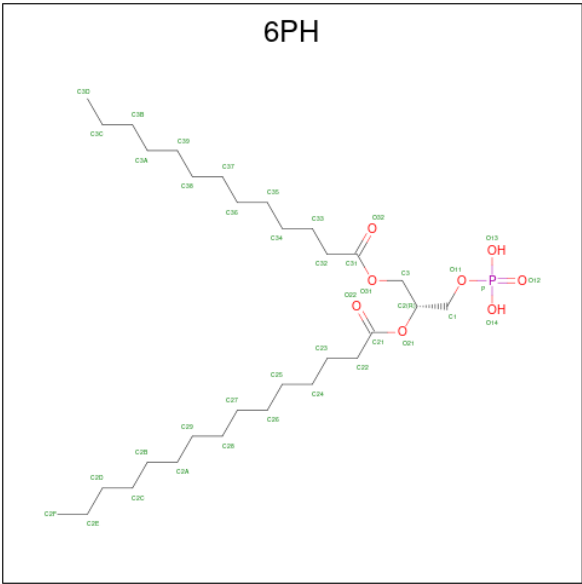
Mol	Chain	Residues	Atoms				AltConf
16	C	1	Total	C	O	P	0
			41	26	13	2	

- Molecule 17 is (2R,5S,11R,14R)-5,8,11-trihydroxy-2-(nonanoyloxy)-5,11-dioxido-16-oxo-14-[(propanoyloxy)methyl]-4,6,10,12,15-pentaoxa-5,11-diphosphanonadec-1-yl undecanoate (CCD ID: CN3) (formula: C₃₆H₆₈O₁₇P₂).



Mol	Chain	Residues	Atoms				AltConf
17	C	1	Total	C	O	P	0
			55	36	17	2	
17	N	1	Total	C	O	P	0
			55	36	17	2	

- Molecule 18 is (1R)-2-(phosphonoxy)-1-[(tridecanoyloxy)methyl]ethyl pentadecanoate (CCD ID: 6PH) (formula: C₃₁H₆₁O₈P).

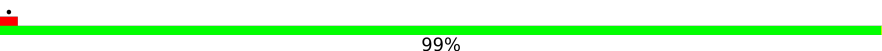


Mol	Chain	Residues	Atoms				AltConf
18	N	1	Total	C	O	P	0
			40	31	8	1	
18	O	1	Total	C	O	P	0
			40	31	8	1	

3 Residue-property plots [i](#)

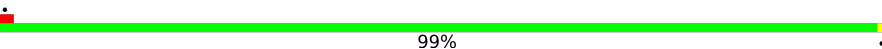
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: COR1 isoform 1

Chain A:  99%

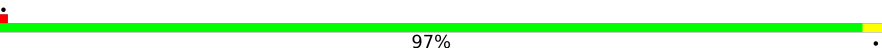


- Molecule 1: COR1 isoform 1

Chain L:  99%

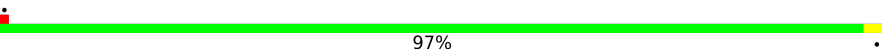


- Molecule 2: Cytochrome b

Chain C:  97%

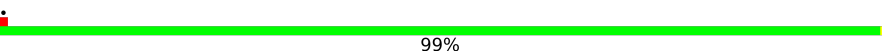


- Molecule 2: Cytochrome b

Chain N:  97%

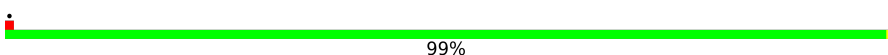


- Molecule 3: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain B:  99%

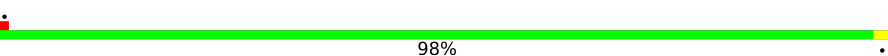


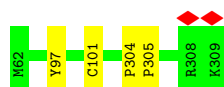
- Molecule 3: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain M:  99%

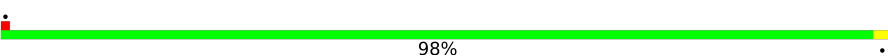


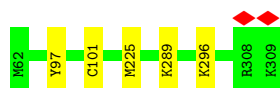
- Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain D:  98%



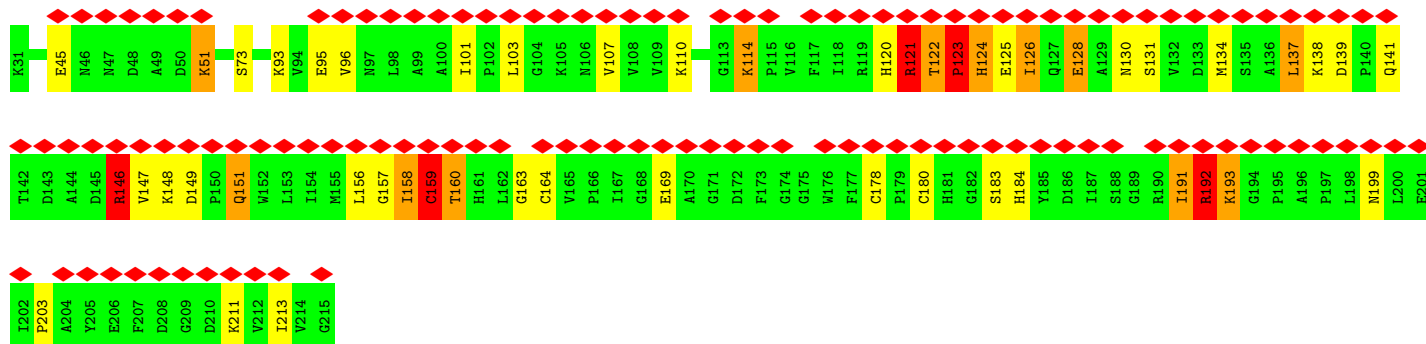
- Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain O:  98%



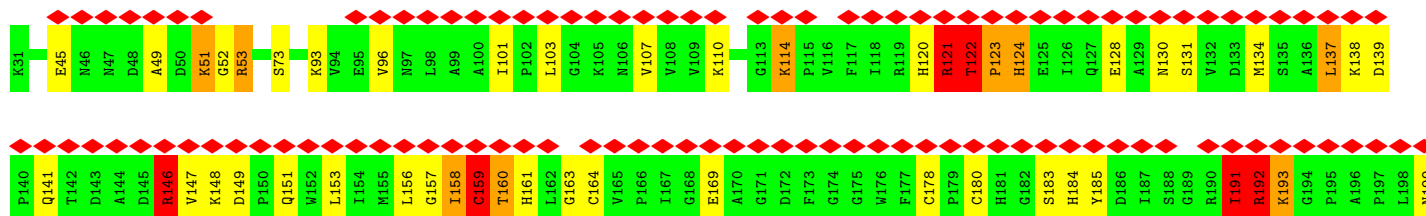
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

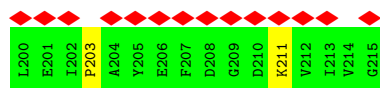
Chain E:  65%
73% 18% 6%



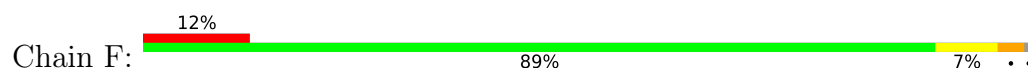
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain P:  65%
72% 20% 5%

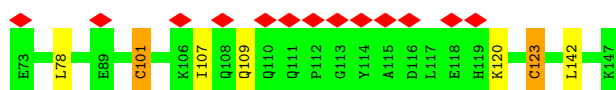
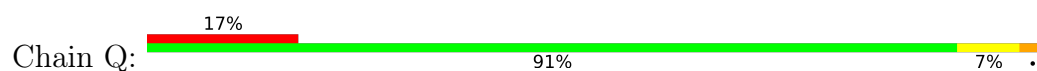




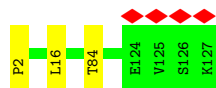
- Molecule 6: QCR6 isoform 1



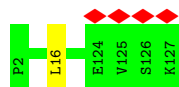
- Molecule 6: QCR6 isoform 1



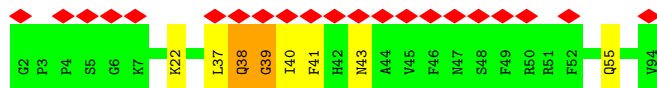
- Molecule 7: Cytochrome b-c1 complex subunit 7



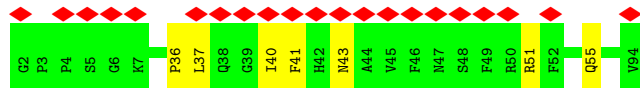
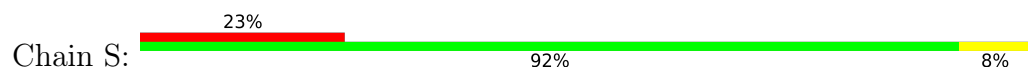
- Molecule 7: Cytochrome b-c1 complex subunit 7



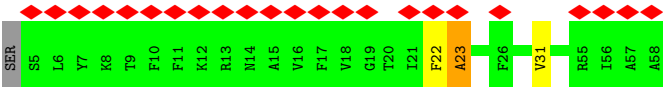
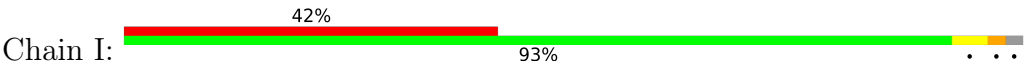
- Molecule 8: Cytochrome b-c1 complex subunit 8



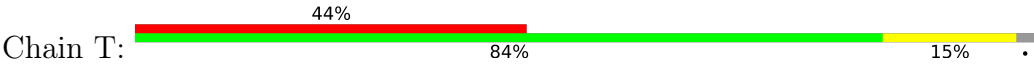
- Molecule 8: Cytochrome b-c1 complex subunit 8



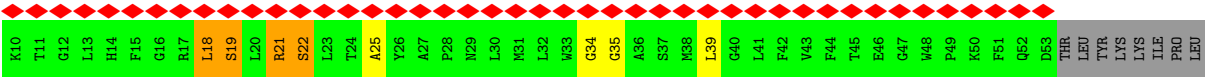
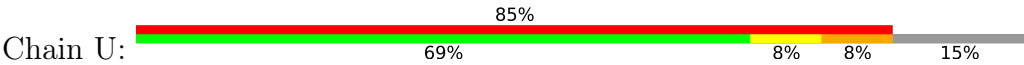
- Molecule 9: Cytochrome b-c1 complex subunit 9, mitochondrial



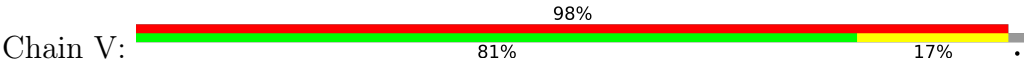
• Molecule 9: Cytochrome b-c1 complex subunit 9, mitochondrial



• Molecule 10: Cytochrome b-c1 complex subunit 10, mitochondrial



• Molecule 10: Cytochrome b-c1 complex subunit 10, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	433970	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 ($e^-/\text{\AA}^2$)	48.80	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	130000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	18.648	Depositor
Minimum map value	-9.340	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.394	Depositor
Recommended contour level	1.2	Depositor
Map size (Å)	307.19998, 307.19998, 307.19998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.9599999, 0.9599999, 0.9599999	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CN5, 6PH, UQ6, AZO, 8PE, 9PE, HEM, CN3

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	0.20	0/3405	0.44	0/4615
1	L	0.20	0/3405	0.44	0/4615
2	C	0.23	0/3192	0.50	2/4354 (0.0%)
2	N	0.23	0/3192	0.50	2/4354 (0.0%)
3	B	0.21	0/2781	0.49	1/3764 (0.0%)
3	M	0.24	1/2781 (0.0%)	0.48	2/3764 (0.1%)
4	D	0.17	0/2022	0.40	0/2751
4	O	0.17	0/2022	0.40	0/2751
5	E	0.59	4/1444 (0.3%)	0.94	9/1957 (0.5%)
5	P	0.84	10/1444 (0.7%)	1.31	16/1957 (0.8%)
6	F	0.37	0/638	0.60	1/858 (0.1%)
6	Q	0.32	0/647	0.62	1/870 (0.1%)
7	G	0.46	1/1040 (0.1%)	0.44	0/1408
7	R	0.20	0/1040	0.42	0/1408
8	H	0.27	0/804	0.69	4/1088 (0.4%)
8	S	0.80	2/804 (0.2%)	0.63	3/1088 (0.3%)
9	I	0.43	1/455 (0.2%)	0.74	2/614 (0.3%)
9	T	0.48	1/456 (0.2%)	0.90	6/615 (1.0%)
10	U	0.71	0/358	1.18	3/483 (0.6%)
10	V	0.48	1/419 (0.2%)	0.90	0/567
All	All	0.35	21/32349 (0.1%)	0.60	52/43881 (0.1%)

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
5	E	0	3
5	P	0	5
6	F	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	9

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	S	36	PRO	C-N	20.56	1.60	1.33
7	G	84	THR	C-N	13.52	1.53	1.33
5	P	53	ARG	C-N	12.45	1.52	1.33
5	P	123	PRO	C-N	12.22	1.50	1.33
5	P	124	HIS	C-N	10.73	1.48	1.33
5	P	191	ILE	C-N	9.25	1.46	1.33
5	P	121	ARG	C-N	9.01	1.52	1.33
9	T	16	VAL	C-N	-8.51	1.22	1.33
5	P	52	GLY	C-N	8.43	1.45	1.34
5	E	157	GLY	C-N	8.17	1.44	1.33
5	E	192	ARG	C-N	-7.98	1.21	1.33
8	S	37	LEU	C-N	7.65	1.44	1.33
5	E	191	ILE	C-N	7.56	1.44	1.33
5	P	157	GLY	C-N	6.43	1.42	1.33
5	P	159	CYS	C-N	6.26	1.42	1.33
5	E	159	CYS	C-O	5.96	1.31	1.24
5	P	192	ARG	C-N	-5.92	1.25	1.33
10	V	59	ILE	C-N	5.71	1.40	1.33
5	P	160	THR	C-N	5.57	1.41	1.33
3	M	332	VAL	C-N	-5.54	1.24	1.33
9	I	22	PHE	C-O	-5.05	1.17	1.24

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	P	122	THR	O-C-N	-21.96	96.06	121.32
5	P	122	THR	CA-C-N	20.54	141.87	119.28
5	P	122	THR	C-N-CA	20.54	141.87	119.28
10	U	21	ARG	N-CA-C	-11.50	98.49	111.71
5	P	157	GLY	O-C-N	-9.54	110.29	122.70
9	T	18	VAL	O-C-N	8.55	130.16	121.87
5	P	124	HIS	CA-C-N	-8.53	107.01	122.54
5	P	124	HIS	C-N-CA	-8.53	107.01	122.54
5	P	123	PRO	O-C-N	-8.53	111.22	122.22
10	U	34	GLY	N-CA-C	-8.52	102.36	115.66
5	P	123	PRO	CA-C-N	8.46	136.72	120.99
5	P	123	PRO	C-N-CA	8.46	136.72	120.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	185	LEU	CA-C-N	8.28	125.45	120.24
2	C	185	LEU	C-N-CA	8.28	125.45	120.24
2	N	185	LEU	CA-C-N	8.25	125.44	120.24
2	N	185	LEU	C-N-CA	8.25	125.44	120.24
5	E	45	GLU	CA-CB-CG	7.93	129.97	114.10
5	P	45	GLU	CA-CB-CG	7.92	129.95	114.10
8	S	36	PRO	CA-C-N	-7.63	111.65	122.63
8	S	36	PRO	C-N-CA	-7.63	111.65	122.63
8	H	37	LEU	O-C-N	7.62	132.73	122.59
5	P	146	ARG	CB-CG-CD	6.78	126.88	111.30
5	E	146	ARG	CB-CG-CD	6.76	126.85	111.30
9	I	22	PHE	CA-C-O	-6.58	111.97	120.00
8	S	36	PRO	O-C-N	6.58	127.40	122.73
9	T	19	GLY	CA-C-N	6.56	130.28	120.31
9	T	19	GLY	C-N-CA	6.56	130.28	120.31
9	T	19	GLY	O-C-N	-6.54	114.19	122.70
8	H	39	GLY	CA-C-N	-6.42	111.48	120.53
8	H	39	GLY	C-N-CA	-6.42	111.48	120.53
5	E	123	PRO	N-CA-CB	-6.39	96.53	103.25
5	E	192	ARG	O-C-N	-6.13	114.25	121.97
5	E	45	GLU	CB-CG-CD	6.03	122.85	112.60
5	P	45	GLU	CB-CG-CD	6.01	122.82	112.60
9	T	15	ALA	CA-C-N	5.98	130.05	121.02
9	T	15	ALA	C-N-CA	5.98	130.05	121.02
10	U	22	SER	O-C-N	-5.95	113.96	122.41
5	E	192	ARG	CA-CB-CG	5.81	125.72	114.10
5	P	192	ARG	CA-CB-CG	5.80	125.70	114.10
5	P	114	LYS	CA-CB-CG	5.67	125.45	114.10
5	E	114	LYS	CA-CB-CG	5.65	125.40	114.10
3	M	151	PHE	CA-C-N	5.64	132.30	121.54
3	M	151	PHE	C-N-CA	5.64	132.30	121.54
6	F	123	CYS	CA-C-O	-5.59	113.77	120.65
5	E	160	THR	CB-CA-C	5.41	120.39	110.11
6	Q	123	CYS	CA-C-O	-5.30	114.13	120.65
5	E	146	ARG	CA-CB-CG	5.28	124.66	114.10
5	P	146	ARG	CA-CB-CG	5.27	124.64	114.10
3	B	332	VAL	O-C-N	-5.26	117.29	122.76
8	H	38	GLN	N-CA-CB	-5.23	103.68	111.43
9	I	23	ALA	CA-C-O	-5.12	113.74	119.79
5	P	122	THR	C-N-CD	-5.04	104.32	125.00

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	E	121	ARG	Sidechain
5	E	191	ILE	Peptide
5	E	192	ARG	Peptide
6	F	116	ASP	Peptide
5	P	121	ARG	Sidechain
5	P	122	THR	Mainchain
5	P	124	HIS	Mainchain
5	P	191	ILE	Peptide
5	P	192	ARG	Peptide

5.2 Too-close contacts [i](#)

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	3344	0	3323	2	0
1	L	3344	0	3323	2	0
2	C	3090	0	3129	10	0
2	N	3090	0	3129	11	0
3	B	2735	0	2774	0	0
3	M	2735	0	2774	0	0
4	D	1961	0	1890	3	0
4	O	1961	0	1890	4	0
5	E	1411	0	1390	23	0
5	P	1411	0	1390	29	0
6	F	624	0	583	3	0
6	Q	633	0	589	3	0
7	G	1019	0	1034	2	0
7	R	1019	0	1034	1	0
8	H	773	0	736	4	0
8	S	773	0	736	3	0
9	I	442	0	440	3	0
9	T	443	0	440	2	0
10	U	347	0	345	4	0
10	V	406	0	414	7	0
11	C	30	0	17	0	0
11	N	30	0	17	0	0
12	C	43	0	60	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	N	43	0	60	2	0
13	C	47	0	73	0	0
13	N	47	0	73	1	0
14	C	40	0	59	0	0
14	N	40	0	59	2	0
15	C	86	0	60	0	0
15	D	43	0	30	0	0
15	N	86	0	60	0	0
15	O	43	0	30	0	0
16	C	41	0	50	10	0
17	C	55	0	66	1	0
17	N	55	0	66	6	0
18	N	40	0	59	0	0
18	O	40	0	59	1	0
All	All	32370	0	32261	112	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 2.

All (112) 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)
5:E:178:CYS:SG	5:E:183:SER:HB2	1.85	1.15
5:P:178:CYS:SG	5:P:183:SER:HB2	1.85	1.15
9:I:23:ALA:HB2	10:V:39:LEU:HD22	1.26	1.12
5:P:178:CYS:SG	5:P:183:SER:CB	2.58	0.91
5:E:178:CYS:SG	5:E:183:SER:CB	2.58	0.90
5:E:164:CYS:SG	5:E:180:CYS:HB2	2.11	0.90
5:P:164:CYS:SG	5:P:180:CYS:HB2	2.11	0.89
6:Q:101:CYS:HG	6:Q:123:CYS:HG	0.84	0.84
5:P:159:CYS:HB2	5:P:163:GLY:CA	2.15	0.76
5:P:159:CYS:HB2	5:P:163:GLY:N	2.04	0.73
5:E:159:CYS:HB2	5:E:163:GLY:HA2	1.72	0.72
5:P:159:CYS:HB2	5:P:163:GLY:HA2	1.73	0.70
10:U:35:GLY:O	10:U:39:LEU:HD23	1.91	0.69
16:C:406:CN5:O4'	2:N:199:MET:HG2	1.92	0.68
6:F:113:GLY:HA2	6:F:116:ASP:HB2	1.77	0.67
5:P:122:THR:HG22	5:P:123:PRO:HD2	1.77	0.66
5:E:159:CYS:HB2	5:E:163:GLY:CA	2.26	0.66
5:P:137:LEU:HB2	5:P:192:ARG:HG3	1.78	0.65
16:C:406:CN5:H1'A	2:N:16:TYR:CZ	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:125:GLU:HA	5:E:128:GLU:HG2	1.80	0.63
2:C:199:MET:HG2	16:C:406:CN5:O12	1.98	0.63
2:N:201:LEU:HD21	12:N:408:UQ6:H3M3	1.81	0.62
1:L:428:ASP:OD2	5:P:53:ARG:HD2	1.99	0.62
6:F:101:CYS:HG	6:F:123:CYS:HG	0.65	0.62
9:I:23:ALA:HB2	10:V:39:LEU:CD2	2.18	0.61
17:N:403:CN3:H22	4:O:289:LYS:HG2	1.84	0.60
5:P:184:HIS:HB3	5:P:193:LYS:HE3	1.86	0.58
8:H:39:GLY:O	8:H:40:ILE:C	2.44	0.58
16:C:406:CN5:O2'	16:C:406:CN5:HC	2.03	0.58
5:E:184:HIS:HB3	5:E:193:LYS:HE3	1.86	0.57
17:N:403:CN3:HCA	8:S:51:ARG:HH12	1.69	0.57
5:E:123:PRO:HD3	5:E:151:GLN:HA	1.85	0.57
5:E:137:LEU:HB2	5:E:192:ARG:HG3	1.86	0.57
2:C:16:TYR:CE2	16:C:406:CN5:H2	2.40	0.56
2:C:16:TYR:CZ	16:C:406:CN5:H2	2.40	0.56
9:T:14:ASN:HA	9:T:17:PHE:HB3	1.88	0.55
5:P:159:CYS:HB2	5:P:163:GLY:H	1.71	0.54
2:C:29:TRP:HB3	2:C:99:LYS:HG3	1.90	0.54
2:N:29:TRP:HB3	2:N:99:LYS:HG3	1.90	0.54
5:P:49:ALA:HB1	5:P:53:ARG:HH22	1.75	0.52
5:P:156:LEU:HB2	5:P:203:PRO:HG3	1.92	0.52
5:P:158:ILE:C	5:P:163:GLY:HA2	2.34	0.52
2:N:32:MET:HE1	17:N:403:CN3:H45	1.92	0.52
5:E:156:LEU:HB2	5:E:203:PRO:HG3	1.92	0.52
6:Q:109:GLN:HE22	6:Q:120:LYS:HE2	1.75	0.52
5:P:159:CYS:C	5:P:161:HIS:H	2.19	0.51
5:E:146:ARG:HB3	5:E:147:VAL:HG23	1.93	0.50
5:E:124:HIS:O	5:E:126:ILE:HD13	2.11	0.50
5:P:146:ARG:HB3	5:P:147:VAL:HG23	1.93	0.50
10:V:13:LEU:HD11	10:V:21:ARG:HB2	1.92	0.50
2:N:385:LYS:HB2	7:R:16:LEU:HD13	1.93	0.49
5:P:49:ALA:HB1	5:P:53:ARG:NH2	2.28	0.49
2:C:17:ILE:HD12	16:C:406:CN5:H3AB	1.94	0.48
2:C:385:LYS:HB2	7:G:16:LEU:HD13	1.95	0.48
16:C:406:CN5:O2'	14:N:404:9PE:H2I	2.14	0.47
17:N:403:CN3:H23	4:O:296:LYS:HE3	1.96	0.47
5:P:159:CYS:C	5:P:161:HIS:N	2.71	0.47
4:O:225:MET:HE3	4:O:225:MET:HB2	1.84	0.47
5:P:159:CYS:O	5:P:161:HIS:N	2.48	0.46
6:Q:78:LEU:HD13	6:Q:142:LEU:HD22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:18:ILE:HD11	16:C:406:CN5:H3F	1.97	0.46
12:N:408:UQ6:H72	12:N:408:UQ6:H111	1.79	0.46
2:N:27:ASN:HB2	17:N:403:CN3:HAA	1.98	0.46
5:E:147:VAL:HG12	5:E:149:ASP:H	1.81	0.46
10:U:18:LEU:H	10:U:18:LEU:HG	1.61	0.46
9:T:20:THR:HA	9:T:23:ALA:HB3	1.98	0.45
5:E:164:CYS:SG	5:E:178:CYS:HB2	2.56	0.45
6:F:78:LEU:HD13	6:F:142:LEU:HD22	1.97	0.45
2:N:237:MET:HE2	18:O:401:6PH:H2B	1.98	0.45
5:P:164:CYS:SG	5:P:178:CYS:HB2	2.55	0.45
10:V:35:GLY:HA2	10:V:38:MET:HB2	1.99	0.45
2:C:17:ILE:HD13	16:C:406:CN5:H36A	1.99	0.45
2:N:8:VAL:H	14:N:404:9PE:H12A	1.82	0.45
5:P:147:VAL:HG12	5:P:149:ASP:H	1.81	0.45
5:E:158:ILE:O	5:E:159:CYS:HB2	2.18	0.44
5:P:159:CYS:CB	5:P:163:GLY:H	2.30	0.44
5:P:146:ARG:HA	5:P:146:ARG:HE	1.83	0.44
5:E:121:ARG:O	5:E:122:THR:C	2.60	0.44
5:E:146:ARG:HA	5:E:146:ARG:HE	1.83	0.43
4:D:304:PRO:HA	4:D:305:PRO:HD3	1.87	0.43
2:N:323:LYS:HD3	8:S:55:GLN:HE22	1.84	0.43
5:E:124:HIS:C	5:E:126:ILE:H	2.27	0.43
5:P:121:ARG:HH22	5:P:153:LEU:HD13	1.84	0.43
2:N:157:VAL:HG12	10:V:50:LYS:HD2	2.01	0.42
2:C:323:LYS:HD3	8:H:55:GLN:HE22	1.84	0.42
17:N:403:CN3:H48	17:N:403:CN3:H45A	1.83	0.42
5:P:51:LYS:HD3	5:P:51:LYS:HA	1.72	0.42
5:P:191:ILE:HG22	5:P:192:ARG:H	1.85	0.42
10:V:13:LEU:HD23	10:V:14:HIS:H	1.84	0.42
13:N:407:8PE:H32A	13:N:407:8PE:H3A	1.71	0.42
5:E:51:LYS:HD3	5:E:51:LYS:HA	1.72	0.41
5:E:95:GLU:HG2	5:E:213:ILE:HG12	2.02	0.41
5:P:101:ILE:HG23	5:P:107:VAL:HG21	2.03	0.41
10:U:22:SER:HA	10:U:25:ALA:HB3	2.02	0.41
5:E:122:THR:O	5:E:123:PRO:C	2.63	0.41
5:P:103:LEU:HB3	5:P:120:HIS:HD2	1.85	0.41
1:A:217:GLU:HA	1:A:220:VAL:HG22	2.03	0.41
12:C:402:UQ6:H301	12:C:402:UQ6:H322	1.77	0.41
17:C:407:CN3:H49A	17:C:407:CN3:H46A	1.80	0.41
8:H:40:ILE:HG23	8:H:41:PHE:CD1	2.56	0.41
1:L:217:GLU:HA	1:L:220:VAL:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:U:18:LEU:O	10:U:19:SER:C	2.64	0.41
4:O:97:TYR:HA	4:O:101:CYS:SG	2.61	0.40
4:D:97:TYR:HA	4:D:101:CYS:SG	2.61	0.40
5:E:101:ILE:HG23	5:E:107:VAL:HG21	2.03	0.40
4:D:305:PRO:HB3	8:H:22:LYS:HE3	2.03	0.40
9:I:31:VAL:HG22	10:V:61:LEU:HG	2.02	0.40
5:P:183:SER:HB3	5:P:185:TYR:HE1	1.86	0.40
8:S:40:ILE:HG23	8:S:41:PHE:CD1	2.56	0.40
1:A:169:PHE:O	1:A:175:SER:HB3	2.22	0.40
2:C:310:ARG:HA	7:G:2:PRO:HB2	2.03	0.40
5:E:103:LEU:HB3	5:E:120:HIS:HD2	1.85	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	L	337/431 (78%)	326 (97%)	11 (3%)	0	100	100
2	N	275/385 (71%)	269 (98%)	6 (2%)	0	100	100
3	M	350/352 (99%)	342 (98%)	8 (2%)	0	100	100
4	D	45/248 (18%)	43 (96%)	2 (4%)	0	100	100
4	O	246/248 (99%)	243 (99%)	3 (1%)	0	100	100
5	E	72/185 (39%)	70 (97%)	2 (3%)	0	100	100
5	P	183/185 (99%)	151 (82%)	30 (16%)	2 (1%)	11	11
6	Q	73/75 (97%)	71 (97%)	2 (3%)	0	100	100
7	R	124/126 (98%)	123 (99%)	1 (1%)	0	100	100
8	S	91/93 (98%)	85 (93%)	6 (7%)	0	100	100
9	I	3/55 (6%)	3 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	T	52/55 (94%)	50 (96%)	2 (4%)	0	100	100
10	U	42/52 (81%)	36 (86%)	6 (14%)	0	100	100
10	V	49/52 (94%)	43 (88%)	6 (12%)	0	100	100
All	All	1942/2542 (76%)	1855 (96%)	85 (4%)	2 (0%)	49	59

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	P	159	CYS
5	P	160	THR

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	370/370 (100%)	369 (100%)	1 (0%)	86	92
1	L	370/370 (100%)	369 (100%)	1 (0%)	86	92
2	C	338/338 (100%)	338 (100%)	0	100	100
2	N	338/338 (100%)	338 (100%)	0	100	100
3	B	301/301 (100%)	300 (100%)	1 (0%)	86	92
3	M	301/301 (100%)	300 (100%)	1 (0%)	86	92
4	D	206/206 (100%)	206 (100%)	0	100	100
4	O	206/206 (100%)	206 (100%)	0	100	100
5	E	151/151 (100%)	121 (80%)	30 (20%)	1	1
5	P	151/151 (100%)	126 (83%)	25 (17%)	2	2
6	F	67/68 (98%)	66 (98%)	1 (2%)	57	72
6	Q	68/68 (100%)	66 (97%)	2 (3%)	37	49
7	G	110/110 (100%)	110 (100%)	0	100	100
7	R	110/110 (100%)	110 (100%)	0	100	100
8	H	77/77 (100%)	75 (97%)	2 (3%)	40	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	S	77/77 (100%)	76 (99%)	1 (1%)	61	76
9	I	44/45 (98%)	44 (100%)	0	100	100
9	T	45/45 (100%)	45 (100%)	0	100	100
10	U	35/43 (81%)	32 (91%)	3 (9%)	10	10
10	V	42/43 (98%)	42 (100%)	0	100	100
All	All	3407/3418 (100%)	3339 (98%)	68 (2%)	48	63

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	172	THR
3	B	183	GLU
5	E	51	LYS
5	E	73	SER
5	E	93	LYS
5	E	96	VAL
5	E	110	LYS
5	E	114	LYS
5	E	121	ARG
5	E	122	THR
5	E	123	PRO
5	E	124	HIS
5	E	126	ILE
5	E	128	GLU
5	E	130	ASN
5	E	131	SER
5	E	134	MET
5	E	137	LEU
5	E	138	LYS
5	E	139	ASP
5	E	141	GLN
5	E	146	ARG
5	E	148	LYS
5	E	151	GLN
5	E	158	ILE
5	E	159	CYS
5	E	160	THR
5	E	169	GLU
5	E	192	ARG
5	E	193	LYS

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Mol	Chain	Res	Type
5	E	199	ASN
5	E	211	LYS
6	F	107	ILE
8	H	38	GLN
8	H	43	ASN
1	L	172	THR
3	M	183	GLU
5	P	51	LYS
5	P	73	SER
5	P	93	LYS
5	P	96	VAL
5	P	110	LYS
5	P	114	LYS
5	P	121	ARG
5	P	128	GLU
5	P	130	ASN
5	P	131	SER
5	P	134	MET
5	P	137	LEU
5	P	138	LYS
5	P	139	ASP
5	P	141	GLN
5	P	146	ARG
5	P	148	LYS
5	P	151	GLN
5	P	158	ILE
5	P	159	CYS
5	P	169	GLU
5	P	192	ARG
5	P	193	LYS
5	P	199	ASN
5	P	211	LYS
6	Q	101	CYS
6	Q	107	ILE
8	S	43	ASN
10	U	18	LEU
10	U	19	SER
10	U	21	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
6	F	132	HIS
8	H	38	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](#)

19 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	$\# Z > 2$
12	UQ6	N	408	-	43,43,43	1.61	9 (20%)	54,55,55	1.59	12 (22%)
17	CN3	N	403	-	54,54,54	1.17	8 (14%)	60,66,66	1.37	6 (10%)
15	HEM	D	401	4	50,50,50	1.43	8 (16%)	67,82,82	1.15	7 (10%)
14	9PE	N	404	-	39,39,39	0.96	4 (10%)	42,44,44	1.11	2 (4%)
15	HEM	O	402	4	50,50,50	1.43	8 (16%)	67,82,82	1.14	7 (10%)
11	AZO	C	401	-	32,32,32	0.84	1 (3%)	42,42,42	1.71	4 (9%)
18	6PH	N	402	-	39,39,39	0.95	4 (10%)	42,44,44	1.17	2 (4%)
13	8PE	C	403	-	46,46,46	0.90	4 (8%)	49,51,51	1.12	2 (4%)
17	CN3	C	407	-	54,54,54	1.18	8 (14%)	60,66,66	1.12	4 (6%)
16	CN5	C	406	-	40,40,40	0.46	0	44,48,48	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	HEM	C	408	2	50,50,50	1.59	9 (18%)	67,82,82	1.28	6 (8%)
15	HEM	C	405	2	50,50,50	1.52	9 (18%)	67,82,82	1.31	7 (10%)
12	UQ6	C	402	-	43,43,43	1.74	9 (20%)	54,55,55	2.00	15 (27%)
18	6PH	O	401	-	39,39,39	0.94	4 (10%)	42,44,44	1.20	2 (4%)
11	AZO	N	401	-	32,32,32	0.84	1 (3%)	42,42,42	1.71	4 (9%)
14	9PE	C	404	-	39,39,39	0.97	4 (10%)	42,44,44	1.08	3 (7%)
13	8PE	N	407	-	46,46,46	0.91	4 (8%)	49,51,51	1.15	2 (4%)
15	HEM	N	406	2	50,50,50	1.59	10 (20%)	67,82,82	1.27	7 (10%)
15	HEM	N	405	2	50,50,50	1.53	9 (18%)	67,82,82	1.30	7 (10%)

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
12	UQ6	N	408	-	-	9/39/39/39	0/1/1/1
17	CN3	N	403	-	-	31/65/65/65	-
15	HEM	D	401	4	-	2/14/54/54	-
14	9PE	N	404	-	-	22/43/43/43	-
15	HEM	O	402	4	-	2/14/54/54	-
11	AZO	C	401	-	-	3/23/23/23	0/3/3/3
18	6PH	N	402	-	-	20/41/41/41	-
13	8PE	C	403	-	-	20/50/50/50	-
17	CN3	C	407	-	-	29/65/65/65	-
16	CN5	C	406	-	-	24/44/44/44	-
15	HEM	C	408	2	-	4/14/54/54	-
15	HEM	C	405	2	-	5/14/54/54	-
12	UQ6	C	402	-	-	13/39/39/39	0/1/1/1
18	6PH	O	401	-	-	16/41/41/41	-
11	AZO	N	401	-	-	3/23/23/23	0/3/3/3
14	9PE	C	404	-	-	18/43/43/43	-
13	8PE	N	407	-	-	15/50/50/50	-
15	HEM	N	406	2	-	4/14/54/54	-
15	HEM	N	405	2	-	5/14/54/54	-

All (113) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	402	UQ6	C7-C6	5.48	1.57	1.51
15	N	406	HEM	FE-ND	4.68	2.09	1.94
15	C	408	HEM	FE-ND	4.66	2.09	1.94
12	N	408	UQ6	C7-C6	4.28	1.56	1.51
15	C	405	HEM	FE-NB	4.01	2.07	1.94
15	N	405	HEM	FE-NB	4.00	2.07	1.94
15	D	401	HEM	FE-NA	3.82	2.07	1.95
15	O	402	HEM	FE-NA	3.82	2.07	1.95
15	C	408	HEM	FE-NC	3.76	2.07	1.95
15	N	406	HEM	FE-NC	3.72	2.07	1.95
15	N	405	HEM	FE-NC	3.64	2.07	1.95
15	C	405	HEM	FE-NC	3.63	2.07	1.95
15	C	408	HEM	FE-NA	3.55	2.06	1.95
15	N	406	HEM	FE-NB	3.54	2.05	1.94
15	C	408	HEM	FE-NB	3.51	2.05	1.94
15	N	406	HEM	FE-NA	3.48	2.06	1.95
15	N	405	HEM	FE-ND	3.41	2.05	1.94
15	C	405	HEM	FE-ND	3.40	2.05	1.94
15	C	408	HEM	CAC-C3C	3.30	1.56	1.47
15	C	405	HEM	FE-NA	3.29	2.06	1.95
15	N	405	HEM	FE-NA	3.28	2.06	1.95
15	N	406	HEM	CAB-C3B	3.28	1.56	1.47
15	N	406	HEM	CAC-C3C	3.27	1.56	1.47
15	O	402	HEM	CAC-C3C	3.26	1.56	1.47
15	C	408	HEM	CAB-C3B	3.25	1.56	1.47
15	D	401	HEM	CAC-C3C	3.23	1.56	1.47
15	O	402	HEM	FE-ND	3.15	2.04	1.94
15	C	405	HEM	CAB-C3B	3.15	1.55	1.47
15	D	401	HEM	FE-ND	3.14	2.04	1.94
15	N	405	HEM	CAB-C3B	3.11	1.55	1.47
15	C	405	HEM	CAC-C3C	3.10	1.55	1.47
15	N	405	HEM	CAC-C3C	3.10	1.55	1.47
15	D	401	HEM	CAB-C3B	3.07	1.55	1.47
15	O	402	HEM	CAB-C3B	3.02	1.55	1.47
11	C	401	AZO	O5-C22	-3.00	1.38	1.43
11	N	401	AZO	O5-C22	-3.00	1.38	1.43
12	C	402	UQ6	O3-C3	2.80	1.43	1.38
13	N	407	8PE	O21-C2	-2.79	1.40	1.46
17	C	407	CN3	O51-C2'	-2.77	1.40	1.46
12	N	408	UQ6	C26-C24	2.75	1.57	1.51
18	N	402	6PH	O21-C2	-2.74	1.40	1.46
17	C	407	CN3	O21-C2	-2.72	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	D	401	HEM	FE-NB	2.69	2.03	1.94
15	O	402	HEM	FE-NC	2.69	2.04	1.95
15	O	402	HEM	FE-NB	2.68	2.03	1.94
15	D	401	HEM	FE-NC	2.68	2.04	1.95
12	N	408	UQ6	O3-C3	2.67	1.43	1.38
17	N	403	CN3	O51-C2'	-2.67	1.40	1.46
13	C	403	8PE	O21-C2	-2.66	1.40	1.46
12	C	402	UQ6	C26-C24	2.64	1.56	1.51
14	C	404	9PE	O21-C21	2.59	1.41	1.34
17	N	403	CN3	O41-C3'	-2.55	1.39	1.45
18	O	401	6PH	O21-C2	-2.54	1.40	1.46
17	N	403	CN3	O21-C21	2.53	1.41	1.34
14	N	404	9PE	O21-C21	2.52	1.41	1.34
18	N	402	6PH	O31-C31	2.49	1.40	1.33
18	O	401	6PH	O31-C31	2.43	1.40	1.33
15	N	405	HEM	CMC-C2C	2.42	1.55	1.50
13	C	403	8PE	O31-C3	-2.41	1.39	1.45
12	C	402	UQ6	C13-C14	2.41	1.38	1.33
12	C	402	UQ6	C11-C9	2.40	1.56	1.51
13	N	407	8PE	O31-C31	2.39	1.40	1.33
17	N	403	CN3	O21-C2	-2.39	1.41	1.46
12	N	408	UQ6	C11-C9	2.39	1.56	1.51
14	C	404	9PE	O31-C31	2.38	1.40	1.33
15	C	405	HEM	CMC-C2C	2.38	1.55	1.50
17	C	407	CN3	O41-C3'	-2.35	1.39	1.45
12	C	402	UQ6	C21-C19	2.35	1.56	1.51
15	C	405	HEM	CMB-C2B	2.34	1.55	1.50
15	N	405	HEM	CMB-C2B	2.34	1.55	1.50
12	C	402	UQ6	C16-C14	2.33	1.56	1.51
17	C	407	CN3	O31-C3	-2.31	1.40	1.45
17	C	407	CN3	O41-C41	2.30	1.40	1.33
17	C	407	CN3	O31-C31	2.28	1.40	1.33
14	N	404	9PE	O31-C31	2.28	1.40	1.33
18	N	402	6PH	O31-C3	-2.28	1.40	1.45
13	N	407	8PE	O31-C3	-2.27	1.40	1.45
17	N	403	CN3	O31-C31	2.26	1.40	1.33
17	N	403	CN3	O41-C41	2.26	1.39	1.33
13	C	403	8PE	O31-C31	2.26	1.39	1.33
15	N	406	HEM	CMB-C2B	2.25	1.55	1.50
12	C	402	UQ6	C12-C13	2.24	1.57	1.50
17	C	407	CN3	O51-C51	2.24	1.40	1.34
15	C	408	HEM	CMB-C2B	2.24	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	C	408	HEM	CMC-C2C	2.22	1.55	1.50
18	O	401	6PH	O31-C3	-2.22	1.40	1.45
15	D	401	HEM	CMC-C2C	2.21	1.55	1.50
12	N	408	UQ6	C21-C19	2.21	1.55	1.51
15	N	406	HEM	CMC-C2C	2.20	1.55	1.50
14	N	404	9PE	O31-C3	-2.20	1.40	1.45
17	N	403	CN3	O51-C51	2.20	1.40	1.34
15	O	402	HEM	CMC-C2C	2.20	1.55	1.50
12	N	408	UQ6	C12-C13	2.19	1.57	1.50
15	N	406	HEM	CMA-C3A	2.18	1.55	1.50
12	N	408	UQ6	C13-C14	2.15	1.38	1.33
13	N	407	8PE	O21-C21	2.13	1.40	1.34
18	O	401	6PH	O21-C21	2.13	1.40	1.34
18	N	402	6PH	O21-C21	2.12	1.40	1.34
17	N	403	CN3	O31-C3	-2.12	1.40	1.45
15	D	401	HEM	CMB-C2B	2.11	1.55	1.50
15	C	408	HEM	CMA-C3A	2.10	1.55	1.50
17	C	407	CN3	O21-C21	2.08	1.40	1.34
15	N	405	HEM	CMD-C2D	2.08	1.55	1.50
13	C	403	8PE	O21-C21	2.08	1.40	1.34
15	O	402	HEM	CMB-C2B	2.07	1.55	1.50
12	C	402	UQ6	C7-C8	2.07	1.55	1.50
12	N	408	UQ6	C16-C14	2.07	1.55	1.51
14	C	404	9PE	O31-C3	-2.06	1.40	1.45
15	C	405	HEM	CMD-C2D	2.05	1.55	1.50
12	N	408	UQ6	O4-C4	2.04	1.42	1.38
14	N	404	9PE	O21-C2	-2.04	1.41	1.46
14	C	404	9PE	O21-C2	-2.03	1.41	1.46
15	N	406	HEM	CMD-C2D	2.01	1.54	1.50

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	N	401	AZO	C12-O2-C10	7.28	133.19	118.43
11	C	401	AZO	C12-O2-C10	7.27	133.16	118.43
12	C	402	UQ6	C6-C7-C8	6.58	123.30	112.06
11	C	401	AZO	C7-O1-C8	5.78	130.13	118.43
11	N	401	AZO	C7-O1-C8	5.77	130.13	118.43
12	C	402	UQ6	C7-C8-C9	-4.82	120.51	127.42
17	N	403	CN3	O51-C51-C52	4.67	121.58	111.48
17	N	403	CN3	O21-C21-C22	4.44	121.09	111.48
12	C	402	UQ6	C7-C6-C5	4.20	127.48	120.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	C	403	8PE	O21-C21-C22	3.91	119.94	111.48
18	O	401	6PH	O21-C21-C22	3.80	119.71	111.48
17	C	407	CN3	O21-C21-C22	3.77	119.65	111.48
12	N	408	UQ6	C10-C9-C11	3.77	121.78	115.23
13	N	407	8PE	O21-C21-C22	3.75	119.60	111.48
18	N	402	6PH	O21-C21-C22	3.64	119.35	111.48
12	C	402	UQ6	C7-C6-C1	-3.64	115.24	120.79
17	C	407	CN3	O51-C51-C52	3.35	118.73	111.48
15	C	408	HEM	C4D-ND-C1D	3.26	109.07	105.21
14	N	404	9PE	O21-C21-C22	3.21	118.43	111.48
15	N	406	HEM	C4D-ND-C1D	3.19	108.99	105.21
13	N	407	8PE	O31-C31-C32	3.18	121.54	111.83
17	N	403	CN3	O31-C31-C32	3.12	120.62	111.15
18	O	401	6PH	O31-C31-C32	3.07	121.18	111.83
12	N	408	UQ6	C12-C13-C14	-3.06	120.62	127.62
12	C	402	UQ6	C27-C28-C29	-3.06	120.63	127.62
15	C	405	HEM	C4D-ND-C1D	3.03	108.80	105.21
15	N	405	HEM	C4D-ND-C1D	3.00	108.76	105.21
15	N	405	HEM	CBA-CAA-C2A	-3.00	104.24	112.53
15	C	405	HEM	CBA-CAA-C2A	-3.00	104.25	112.53
12	C	402	UQ6	C20-C19-C21	2.98	120.40	115.23
12	N	408	UQ6	C25-C24-C26	2.98	120.40	115.23
12	C	402	UQ6	C2-C1-C6	2.97	122.17	118.59
12	C	402	UQ6	C30-C29-C31	2.94	120.33	115.23
15	N	406	HEM	C1B-NB-C4B	2.92	108.67	105.21
15	C	408	HEM	C1B-NB-C4B	2.91	108.65	105.21
12	C	402	UQ6	C22-C23-C24	-2.91	120.97	127.62
12	N	408	UQ6	C7-C8-C9	-2.90	123.27	127.42
17	C	407	CN3	O31-C31-C32	2.89	119.92	111.15
14	C	404	9PE	O21-C21-C22	2.84	117.64	111.48
12	N	408	UQ6	C17-C18-C19	-2.83	121.14	127.62
13	C	403	8PE	O31-C31-C32	2.81	120.39	111.83
12	N	408	UQ6	C27-C28-C29	-2.80	121.22	127.62
15	N	405	HEM	C2A-C1A-NA	-2.78	107.06	110.15
15	C	405	HEM	C2A-C1A-NA	-2.78	107.07	110.15
11	C	401	AZO	C11-N3-C10	2.77	116.61	114.50
15	N	405	HEM	C3D-C4D-ND	-2.74	107.17	110.17
12	N	408	UQ6	C20-C19-C21	2.73	119.97	115.23
12	N	408	UQ6	C15-C14-C16	2.72	119.94	115.23
15	C	405	HEM	C3D-C4D-ND	-2.71	107.20	110.17
14	C	404	9PE	O31-C31-C32	2.71	120.09	111.83
11	N	401	AZO	C11-N3-C10	2.69	116.55	114.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	C	407	CN3	O41-C41-C42	2.69	120.03	111.83
12	C	402	UQ6	C1M-C1-C2	-2.69	116.04	120.52
15	C	408	HEM	C3D-C4D-ND	-2.69	107.22	110.17
12	C	402	UQ6	C15-C14-C16	2.68	119.88	115.23
14	N	404	9PE	O31-C31-C32	2.68	120.00	111.83
15	N	406	HEM	C2A-C1A-NA	-2.67	107.19	110.15
15	N	406	HEM	C3D-C4D-ND	-2.61	107.31	110.17
18	N	402	6PH	O31-C31-C32	2.56	119.65	111.83
12	N	408	UQ6	C30-C29-C31	2.55	119.65	115.23
17	N	403	CN3	O41-C41-C42	2.54	119.57	111.83
12	C	402	UQ6	C12-C13-C14	-2.53	121.84	127.62
14	C	404	9PE	C2-O21-C21	2.52	123.83	117.80
15	C	408	HEM	C2A-C1A-NA	-2.50	107.38	110.15
15	C	405	HEM	CAC-C3C-C4C	-2.47	118.93	124.82
15	N	405	HEM	CAC-C3C-C4C	-2.45	118.96	124.82
12	C	402	UQ6	C17-C18-C19	-2.45	122.02	127.62
15	C	408	HEM	C2D-C1D-ND	-2.44	107.08	109.90
12	N	408	UQ6	C10-C9-C8	-2.43	117.37	123.63
12	C	402	UQ6	C25-C24-C26	2.43	119.45	115.23
15	N	406	HEM	C2D-C1D-ND	-2.42	107.10	109.90
12	N	408	UQ6	C22-C23-C24	-2.38	122.17	127.62
15	N	405	HEM	C1B-NB-C4B	2.36	108.01	105.21
15	C	405	HEM	C1B-NB-C4B	2.34	107.97	105.21
17	N	403	CN3	CC-CB-CA	-2.32	105.98	112.65
12	N	408	UQ6	C1M-C1-C2	-2.30	116.69	120.52
15	D	401	HEM	C4D-ND-C1D	2.27	107.89	105.21
15	O	402	HEM	C4D-ND-C1D	2.27	107.89	105.21
15	D	401	HEM	CAA-CBA-CGA	-2.21	107.79	113.67
15	O	402	HEM	CAA-CBA-CGA	-2.21	107.81	113.67
15	D	401	HEM	C3D-C4D-ND	-2.19	107.77	110.17
11	N	401	AZO	O4-C19-C18	2.15	114.98	112.05
17	N	403	CN3	O51-C51-O52	-2.14	118.71	123.70
15	O	402	HEM	C1B-NB-C4B	2.13	107.73	105.21
15	O	402	HEM	C3D-C4D-ND	-2.13	107.83	110.17
11	C	401	AZO	O4-C19-C18	2.12	114.94	112.05
15	D	401	HEM	C1B-NB-C4B	2.12	107.72	105.21
15	D	401	HEM	C2A-C1A-NA	-2.11	107.81	110.15
15	N	406	HEM	CMB-C2B-C1B	-2.10	121.75	125.03
15	C	405	HEM	C2D-C1D-ND	-2.10	107.47	109.90
15	N	405	HEM	C2D-C1D-ND	-2.08	107.50	109.90
15	O	402	HEM	C2A-C1A-NA	-2.08	107.85	110.15
15	D	401	HEM	CMB-C2B-C1B	-2.05	121.83	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	C	408	HEM	CMB-C2B-C1B	-2.05	121.83	125.03
15	N	406	HEM	C3B-C2B-C1B	2.04	107.94	106.41
15	O	402	HEM	CHC-C4B-NB	2.03	126.60	124.42
12	C	402	UQ6	C32-C33-C34	-2.01	120.93	127.64
15	D	401	HEM	CHC-C4B-NB	2.01	126.59	124.42
15	O	402	HEM	CMB-C2B-C1B	-2.01	121.90	125.03

There are no chirality outliers.

All (245) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	C	401	AZO	N1-C1-C2-C7
11	C	401	AZO	C17-C18-C21-O5
11	C	401	AZO	C19-C18-C21-O5
11	N	401	AZO	N1-C1-C2-C7
11	N	401	AZO	C17-C18-C21-O5
11	N	401	AZO	C19-C18-C21-O5
12	C	402	UQ6	C1-C6-C7-C8
12	C	402	UQ6	C5-C6-C7-C8
13	C	403	8PE	C11-O13-P-O11
13	C	403	8PE	C11-O13-P-O12
13	C	403	8PE	C11-O13-P-O14
13	C	403	8PE	O11-C1-C2-O21
13	C	403	8PE	C22-C21-O21-C2
13	N	407	8PE	C1-O11-P-O13
13	N	407	8PE	O32-C31-O31-C3
13	N	407	8PE	C32-C31-O31-C3
14	C	404	9PE	C1-O11-P-O12
14	C	404	9PE	C1-O11-P-O14
14	N	404	9PE	C1-O11-P-O12
14	N	404	9PE	C1-O11-P-O13
14	N	404	9PE	C11-O13-P-O11
14	N	404	9PE	C11-O13-P-O12
16	C	406	CN5	CC-O13-P-O11
16	C	406	CN5	CC-O13-P-O12
16	C	406	CN5	CB-CC-O13-P
16	C	406	CN5	C1'-O1'-P'-O3'
17	C	407	CN3	CC-O13-P-O11
17	C	407	CN3	CC-O13-P-O12
17	C	407	CN3	CC-O13-P-O14
17	C	407	CN3	C1'-O1'-P'-O3'
17	C	407	CN3	C1'-O1'-P'-O4'

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Mol	Chain	Res	Type	Atoms
17	C	407	CN3	CA-O3'-P'-O1'
17	C	407	CN3	CA-O3'-P'-O2'
17	C	407	CN3	CA-O3'-P'-O4'
17	N	403	CN3	O22-C21-O21-C2
17	N	403	CN3	O52-C51-O51-C2'
17	N	403	CN3	C52-C51-O51-C2'
17	C	407	CN3	O42-C41-O41-C3'
18	O	401	6PH	O32-C31-O31-C3
13	C	403	8PE	O22-C21-O21-C2
17	C	407	CN3	C42-C41-O41-C3'
17	N	403	CN3	C22-C21-O21-C2
12	C	402	UQ6	C20-C19-C21-C22
12	C	402	UQ6	C30-C29-C31-C32
12	C	402	UQ6	C28-C29-C31-C32
14	C	404	9PE	C32-C31-O31-C3
18	O	401	6PH	C32-C31-O31-C3
14	N	404	9PE	O32-C31-O31-C3
16	C	406	CN5	O32-C31-O31-C3
17	N	403	CN3	O3'-CA-CB-OA
13	C	403	8PE	C32-C31-O31-C3
14	N	404	9PE	C32-C31-O31-C3
16	C	406	CN5	C32-C31-O31-C3
12	C	402	UQ6	C9-C11-C12-C13
12	C	402	UQ6	C19-C21-C22-C23
12	C	402	UQ6	C29-C31-C32-C33
12	N	408	UQ6	C14-C16-C17-C18
12	N	408	UQ6	C19-C21-C22-C23
12	N	408	UQ6	C24-C26-C27-C28
12	N	408	UQ6	C29-C31-C32-C33
13	C	403	8PE	O32-C31-O31-C3
14	C	404	9PE	O32-C31-O31-C3
16	C	406	CN5	C39-C3A-C3B-C3C
12	C	402	UQ6	C15-C14-C16-C17
12	C	402	UQ6	C13-C14-C16-C17
12	C	402	UQ6	C18-C19-C21-C22
16	C	406	CN5	C3B-C3C-C3D-C3E
16	C	406	CN5	O42-C41-O41-C3'
17	N	403	CN3	C32-C31-O31-C3
13	N	407	8PE	C31-C32-C33-C34
17	N	403	CN3	C51-C52-C53-C54
16	C	406	CN5	C42-C41-O41-C3'
17	C	407	CN3	C51-C52-C53-C54

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Mol	Chain	Res	Type	Atoms
17	N	403	CN3	O32-C31-O31-C3
17	N	403	CN3	O3'-CA-CB-CC
16	C	406	CN5	O3'-CA-CB-OA
16	C	406	CN5	O11-C1-C2-C3
16	C	406	CN5	O1'-C1'-C2'-C3'
18	N	402	6PH	C21-C22-C23-C24
13	C	403	8PE	C32-C33-C34-C35
14	N	404	9PE	C26-C27-C28-C29
18	O	401	6PH	C26-C27-C28-C29
14	C	404	9PE	C21-C22-C23-C24
16	C	406	CN5	C34-C35-C36-C37
18	N	402	6PH	C22-C21-O21-C2
13	C	403	8PE	C21-C22-C23-C24
13	N	407	8PE	C33-C34-C35-C36
13	N	407	8PE	C36-C37-C38-C39
18	O	401	6PH	C27-C28-C29-C2A
13	C	403	8PE	C39-C3A-C3B-C3C
14	C	404	9PE	C32-C33-C34-C35
18	O	401	6PH	C31-C32-C33-C34
18	N	402	6PH	C25-C26-C27-C28
18	N	402	6PH	C27-C28-C29-C2A
14	N	404	9PE	C2E-C2F-C2G-C2H
18	N	402	6PH	C38-C39-C3A-C3B
14	C	404	9PE	C2B-C2C-C2D-C2E
17	N	403	CN3	C52-C53-C54-C55
17	C	407	CN3	C22-C21-O21-C2
18	N	402	6PH	O22-C21-O21-C2
13	C	403	8PE	C3A-C3B-C3C-C3D
17	C	407	CN3	C45-C46-C47-C48
14	C	404	9PE	C23-C24-C25-C26
14	C	404	9PE	C29-C2A-C2B-C2C
16	C	406	CN5	C36-C37-C38-C39
14	N	404	9PE	C22-C21-O21-C2
18	O	401	6PH	C22-C21-O21-C2
18	O	401	6PH	O22-C21-O21-C2
13	N	407	8PE	C3C-C3D-C3E-C3F
13	N	407	8PE	C22-C23-C24-C25
14	N	404	9PE	O22-C21-O21-C2
14	N	404	9PE	C27-C28-C29-C2A
14	C	404	9PE	C31-C32-C33-C34
18	N	402	6PH	C26-C27-C28-C29
13	N	407	8PE	C39-C3A-C3B-C3C

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Mol	Chain	Res	Type	Atoms
17	N	403	CN3	C41-C42-C43-C44
17	C	407	CN3	C54-C55-C56-C57
14	N	404	9PE	C22-C23-C24-C25
13	C	403	8PE	O11-C1-C2-C3
18	O	401	6PH	O11-C1-C2-C3
17	C	407	CN3	O22-C21-O21-C2
17	C	407	CN3	C41-C42-C43-C44
18	N	402	6PH	C32-C33-C34-C35
18	N	402	6PH	C31-C32-C33-C34
17	C	407	CN3	C1'-C2'-C3'-O41
17	N	403	CN3	C1'-C2'-C3'-O41
18	N	402	6PH	C32-C31-O31-C3
18	N	402	6PH	C39-C3A-C3B-C3C
14	N	404	9PE	O11-C1-C2-O21
17	N	403	CN3	O1'-C1'-C2'-O51
17	N	403	CN3	O51-C2'-C3'-O41
13	C	403	8PE	C36-C37-C38-C39
18	N	402	6PH	C36-C37-C38-C39
12	N	408	UQ6	C9-C11-C12-C13
18	O	401	6PH	C3A-C3B-C3C-C3D
17	C	407	CN3	C48-C49-C4A-C4B
18	O	401	6PH	C39-C3A-C3B-C3C
17	N	403	CN3	O1'-C1'-C2'-C3'
17	N	403	CN3	C21-C22-C23-C24
17	N	403	CN3	C54-C55-C56-C57
14	N	404	9PE	C1-C2-C3-O31
18	O	401	6PH	C28-C29-C2A-C2B
18	N	402	6PH	O32-C31-O31-C3
12	N	408	UQ6	C20-C19-C21-C22
16	C	406	CN5	C35-C36-C37-C38
14	C	404	9PE	C2-C1-O11-P
14	C	404	9PE	C25-C26-C27-C28
17	N	403	CN3	C46-C47-C48-C49
18	N	402	6PH	C2A-C2B-C2C-C2D
13	N	407	8PE	C35-C36-C37-C38
17	C	407	CN3	C55-C56-C57-C58
13	N	407	8PE	C22-C21-O21-C2
16	C	406	CN5	C1'-C2'-C3'-O41
18	N	402	6PH	C2C-C2D-C2E-C2F
16	C	406	CN5	C3A-C3B-C3C-C3D
18	O	401	6PH	O11-C1-C2-O21
14	N	404	9PE	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
18	O	401	6PH	C2A-C2B-C2C-C2D
13	C	403	8PE	C23-C24-C25-C26
12	C	402	UQ6	C25-C24-C26-C27
17	C	407	CN3	C46-C47-C48-C49
17	C	407	CN3	CA-CB-CC-O13
17	N	403	CN3	C44-C45-C46-C47
18	N	402	6PH	C24-C25-C26-C27
18	N	402	6PH	C35-C36-C37-C38
13	C	403	8PE	C3C-C3D-C3E-C3F
13	C	403	8PE	C37-C38-C39-C3A
17	C	407	CN3	C42-C43-C44-C45
13	N	407	8PE	O22-C21-O21-C2
14	C	404	9PE	O22-C21-O21-C2
14	C	404	9PE	O11-C1-C2-O21
13	C	403	8PE	C24-C25-C26-C27
17	C	407	CN3	O51-C2'-C3'-O41
13	N	407	8PE	C23-C24-C25-C26
18	N	402	6PH	O31-C31-C32-C33
18	O	401	6PH	C37-C38-C39-C3A
14	C	404	9PE	C1-O11-P-O13
14	C	404	9PE	C11-O13-P-O12
16	C	406	CN5	C1'-O1'-P'-O2'
17	N	403	CN3	C1-O11-P-O14
17	N	403	CN3	C1'-O1'-P'-O2'
17	N	403	CN3	C1'-O1'-P'-O3'
17	N	403	CN3	C1'-O1'-P'-O4'
14	N	404	9PE	C2-C1-O11-P
16	C	406	CN5	CB-CA-O3'-P'
17	N	403	CN3	C2-C1-O11-P
14	N	404	9PE	C34-C35-C36-C37
14	C	404	9PE	C1-C2-O21-C21
14	N	404	9PE	C3-C2-O21-C21
17	C	407	CN3	O51-C51-C52-C53
13	N	407	8PE	C26-C27-C28-C29
16	C	406	CN5	O3'-CA-CB-CC
14	C	404	9PE	C22-C21-O21-C2
15	C	405	HEM	C3D-CAD-CBD-CGD
13	C	403	8PE	C31-C32-C33-C34
18	O	401	6PH	C29-C2A-C2B-C2C
15	N	405	HEM	C3D-CAD-CBD-CGD
15	C	408	HEM	CAA-CBA-CGA-O1A
15	C	405	HEM	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
15	C	405	HEM	CAA-CBA-CGA-O2A
17	C	407	CN3	OA-CB-CC-O13
16	C	406	CN5	C32-C33-C34-C35
15	O	402	HEM	CAA-CBA-CGA-O1A
14	N	404	9PE	O11-C1-C2-C3
15	C	405	HEM	CAD-CBD-CGD-O1D
12	N	408	UQ6	C18-C19-C21-C22
15	N	405	HEM	CAA-CBA-CGA-O2A
13	N	407	8PE	C28-C29-C2A-C2B
12	C	402	UQ6	C23-C24-C26-C27
15	C	405	HEM	CAD-CBD-CGD-O2D
15	O	402	HEM	CAA-CBA-CGA-O2A
15	N	405	HEM	CAA-CBA-CGA-O1A
15	C	408	HEM	CAA-CBA-CGA-O2A
15	D	401	HEM	CAA-CBA-CGA-O2A
17	C	407	CN3	O1'-C1'-C2'-O51
17	N	403	CN3	O11-C1-C2-O21
15	N	405	HEM	CAD-CBD-CGD-O2D
17	C	407	CN3	O1'-C1'-C2'-C3'
15	N	406	HEM	CAA-CBA-CGA-O2A
18	O	401	6PH	O21-C21-C22-C23
17	N	403	CN3	C1-C2-O21-C21
15	D	401	HEM	CAA-CBA-CGA-O1A
15	N	406	HEM	CAA-CBA-CGA-O1A
15	N	405	HEM	CAD-CBD-CGD-O1D
17	C	407	CN3	C32-C31-O31-C3
17	C	407	CN3	O32-C31-O31-C3
16	C	406	CN5	C3C-C3D-C3E-C3F
12	N	408	UQ6	C25-C24-C26-C27
13	C	403	8PE	C3B-C3C-C3D-C3E
14	N	404	9PE	C23-C24-C25-C26
17	N	403	CN3	O21-C21-C22-C23
18	N	402	6PH	O21-C21-C22-C23
12	N	408	UQ6	C15-C14-C16-C17
17	N	403	CN3	O51-C51-C52-C53
14	N	404	9PE	C25-C26-C27-C28
14	N	404	9PE	C2B-C2C-C2D-C2E
17	N	403	CN3	C55-C56-C57-C58
17	N	403	CN3	O52-C51-C52-C53
17	N	403	CN3	O22-C21-C22-C23
15	C	408	HEM	CAD-CBD-CGD-O2D
18	N	402	6PH	O22-C21-C22-C23

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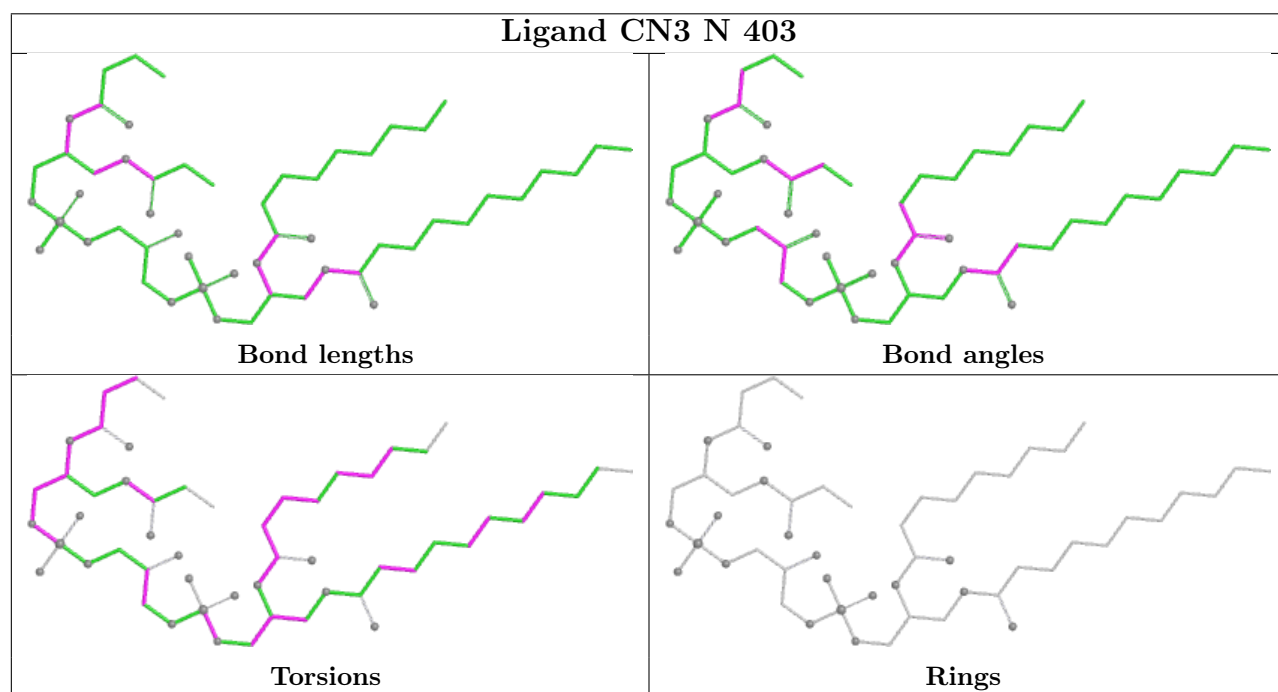
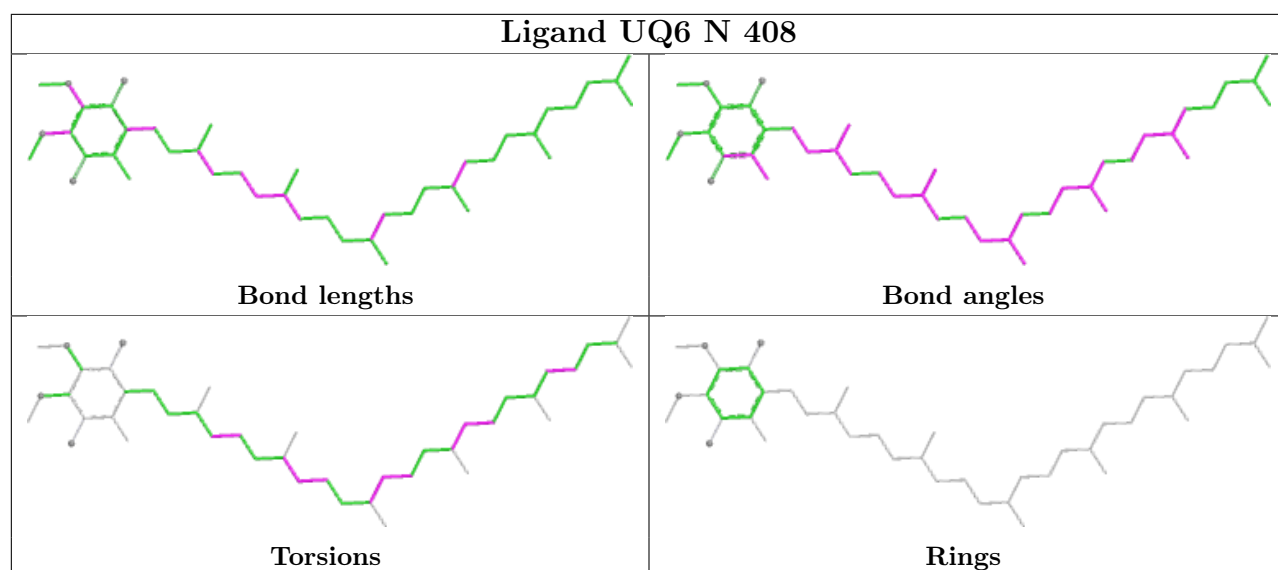
Mol	Chain	Res	Type	Atoms
15	C	408	HEM	CAD-CBD-CGD-O1D
15	N	406	HEM	CAD-CBD-CGD-O1D
15	N	406	HEM	CAD-CBD-CGD-O2D
16	C	406	CN5	C38-C39-C3A-C3B

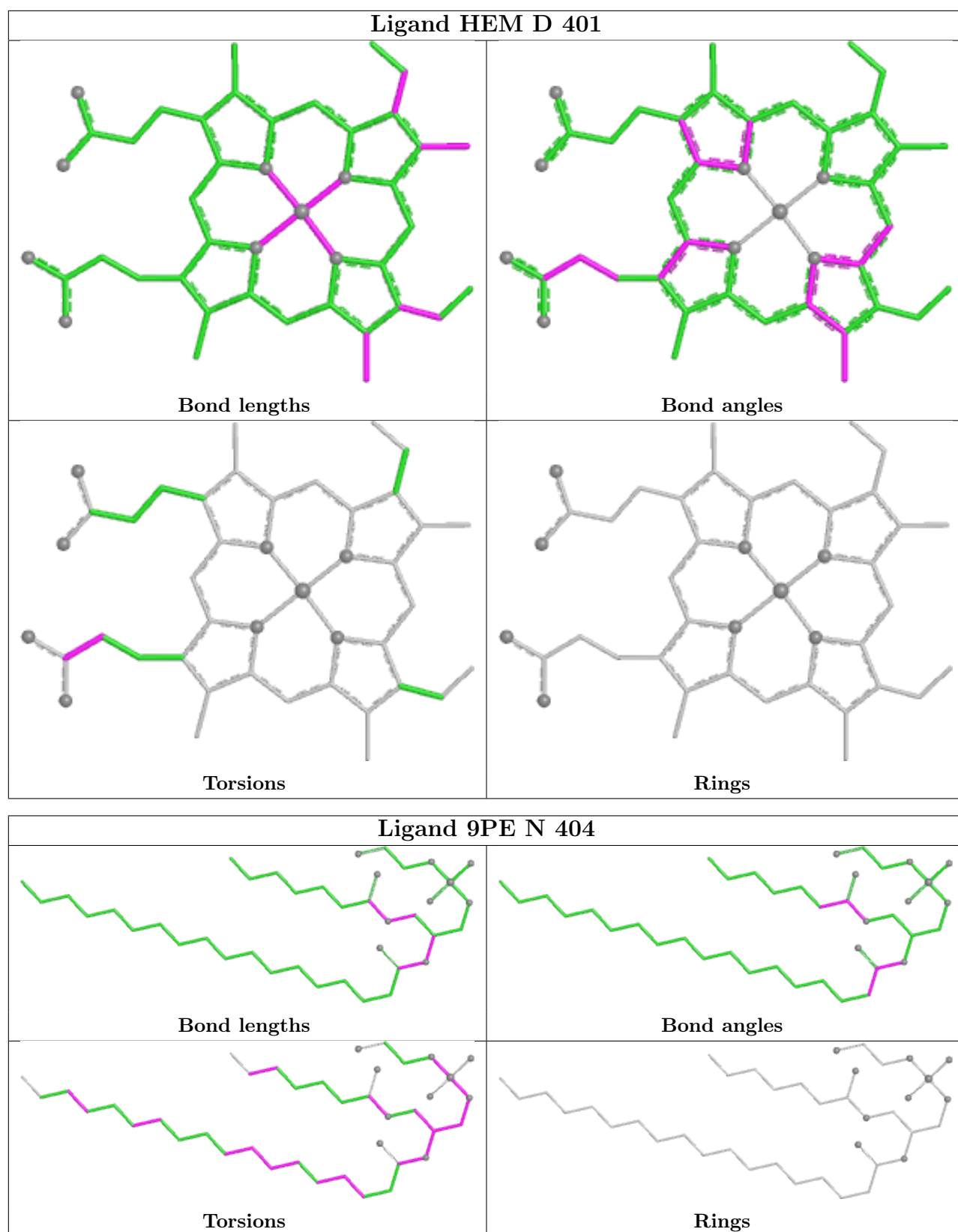
There are no ring outliers.

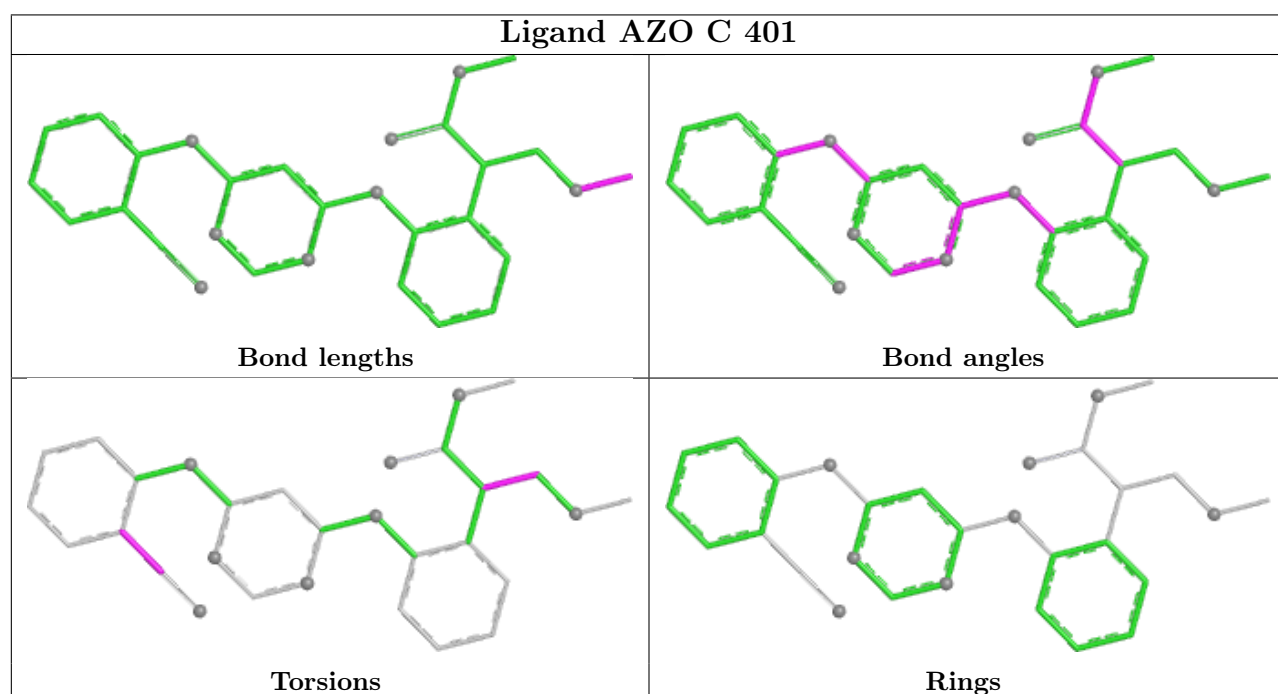
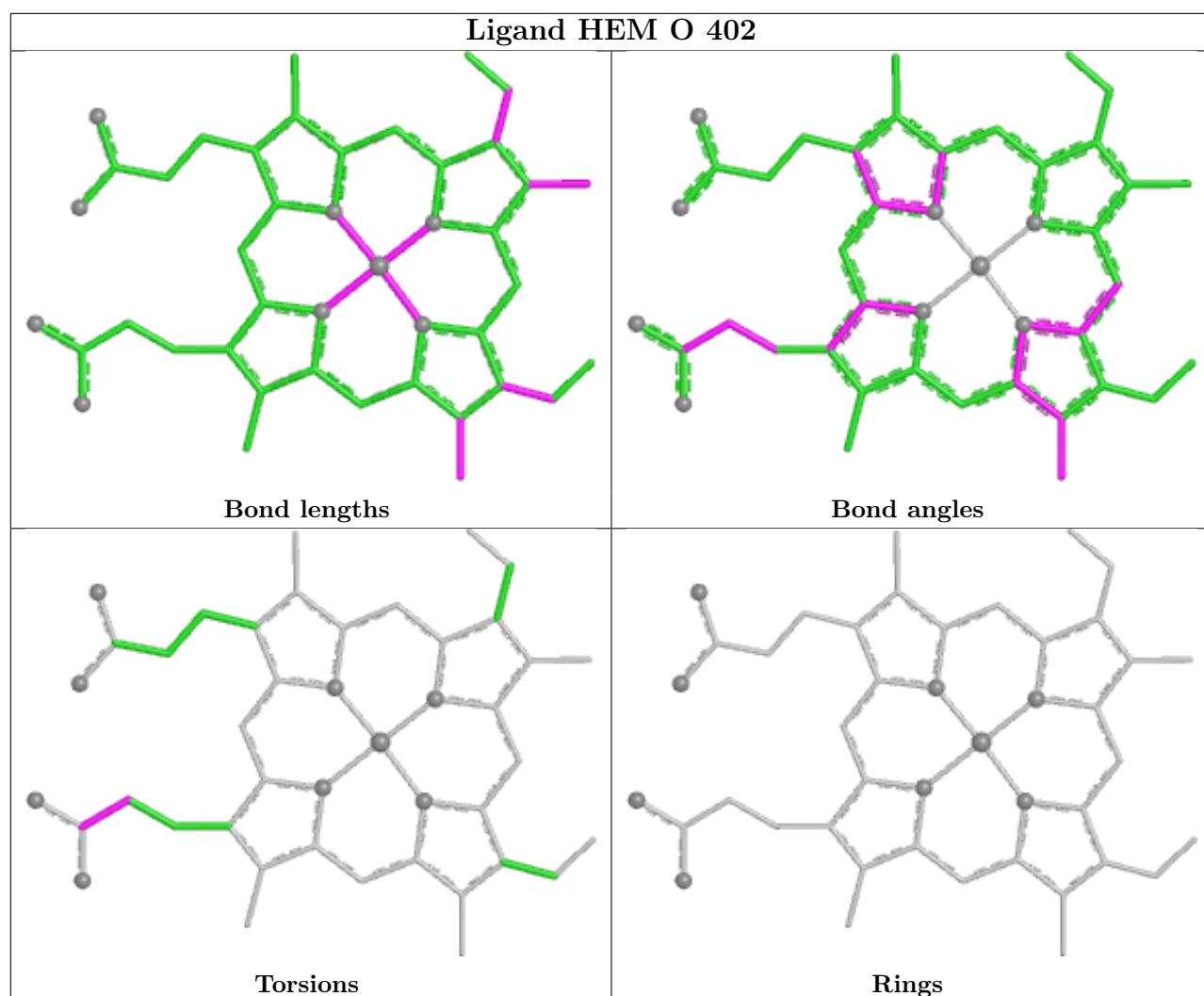
8 monomers are involved in 23 short contacts:

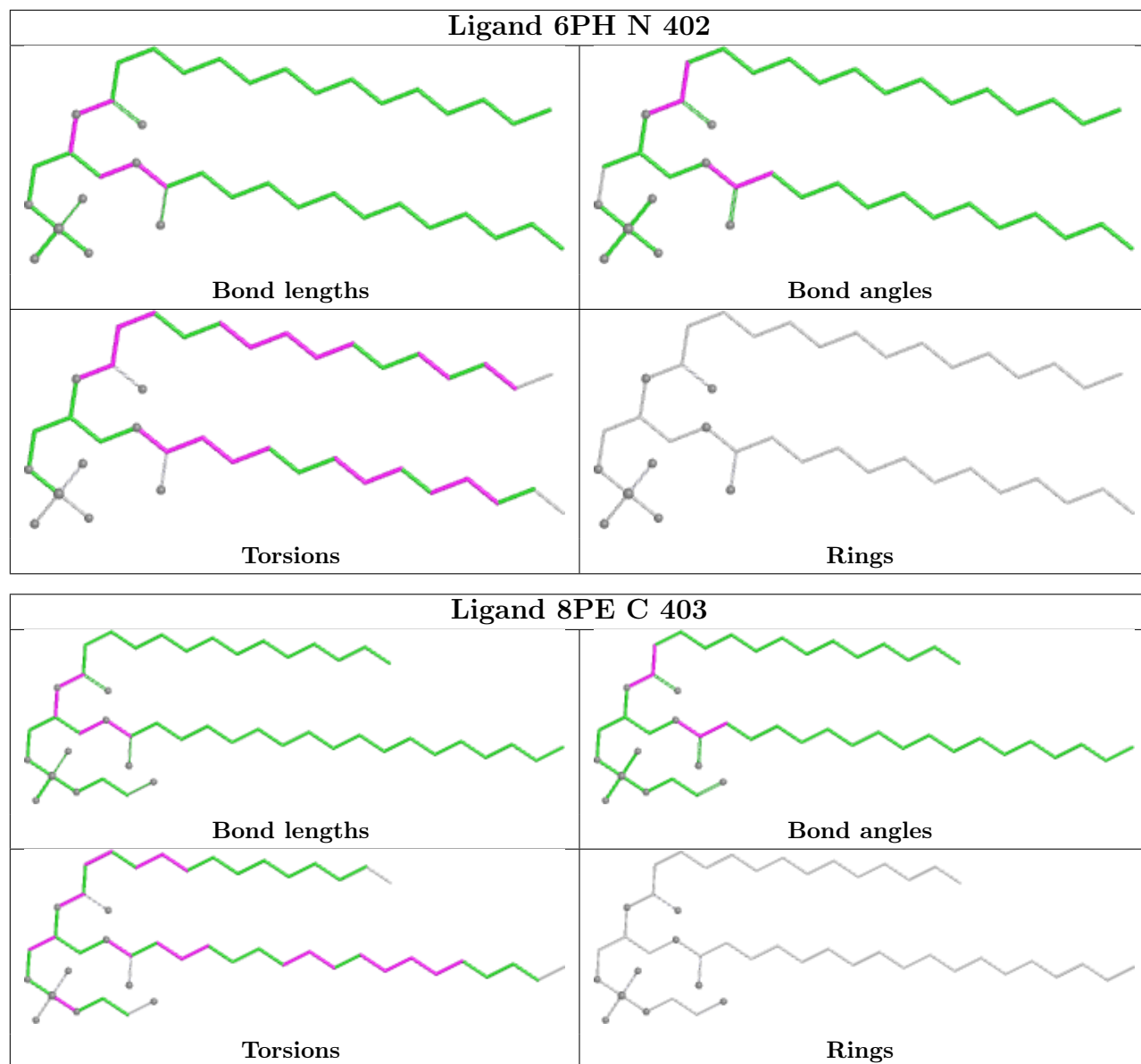
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	N	408	UQ6	2	0
17	N	403	CN3	6	0
14	N	404	9PE	2	0
17	C	407	CN3	1	0
16	C	406	CN5	10	0
12	C	402	UQ6	1	0
18	O	401	6PH	1	0
13	N	407	8PE	1	0

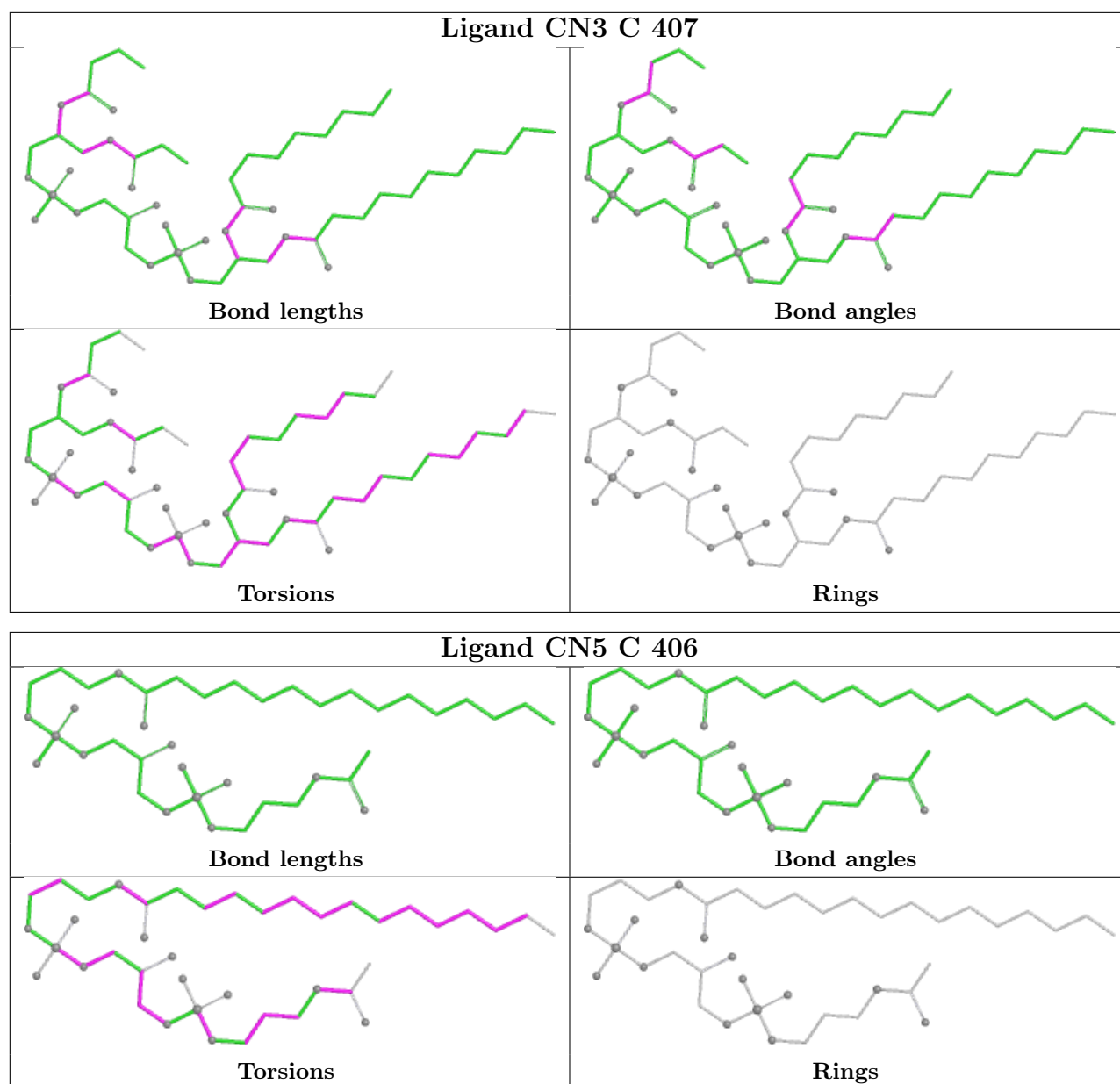
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

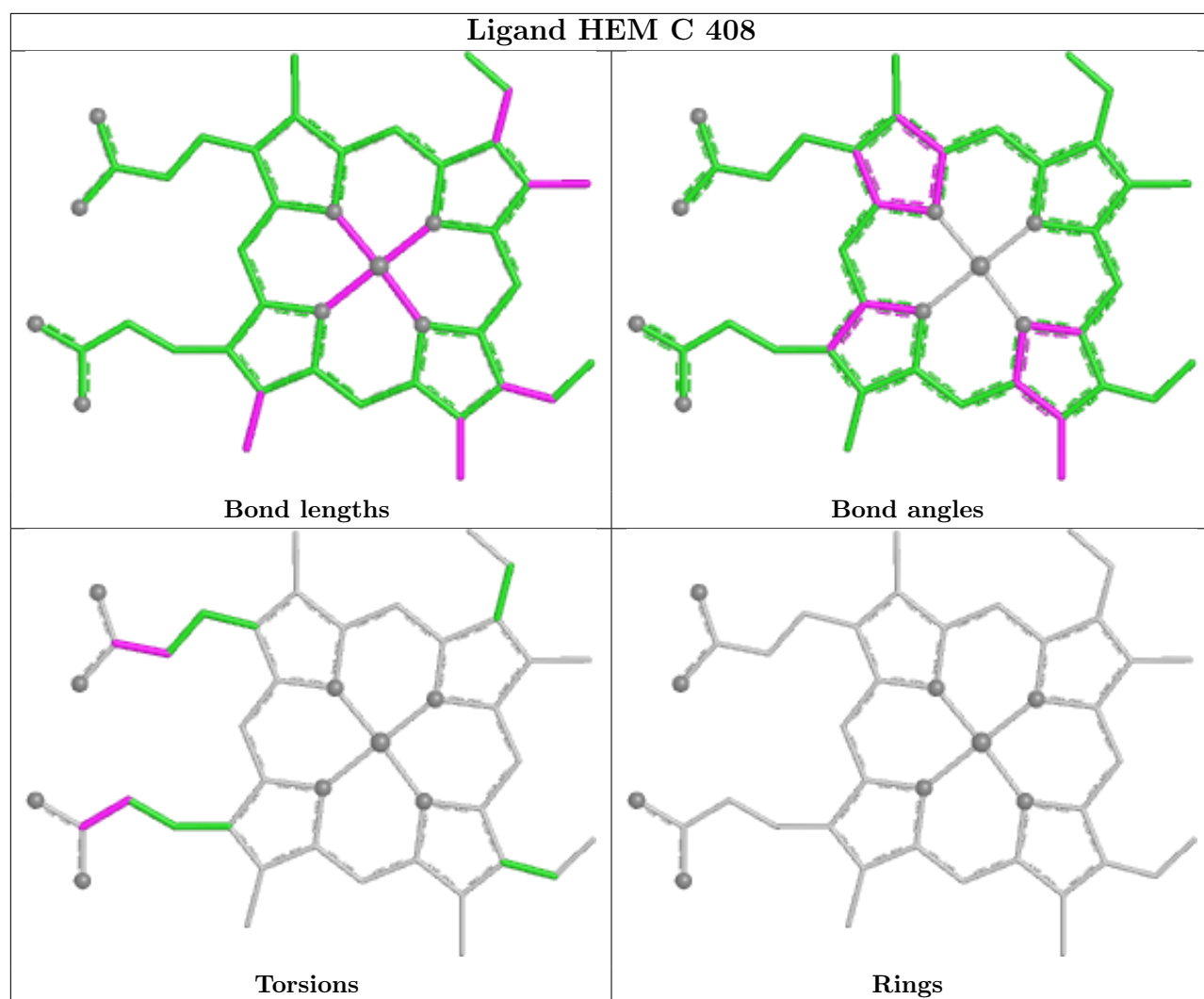


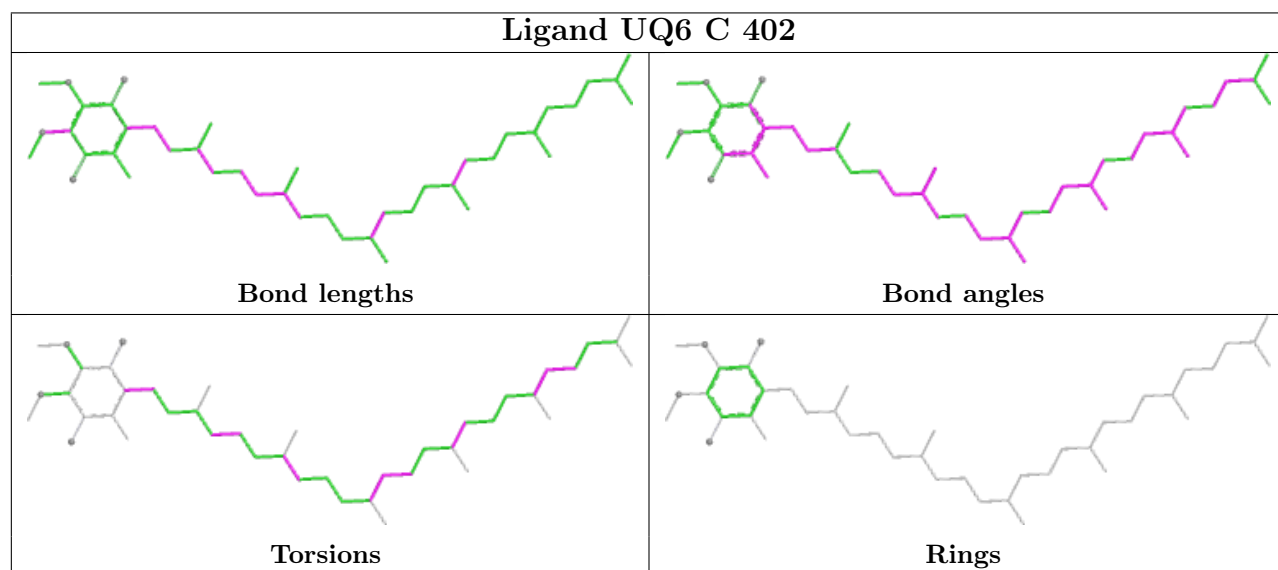
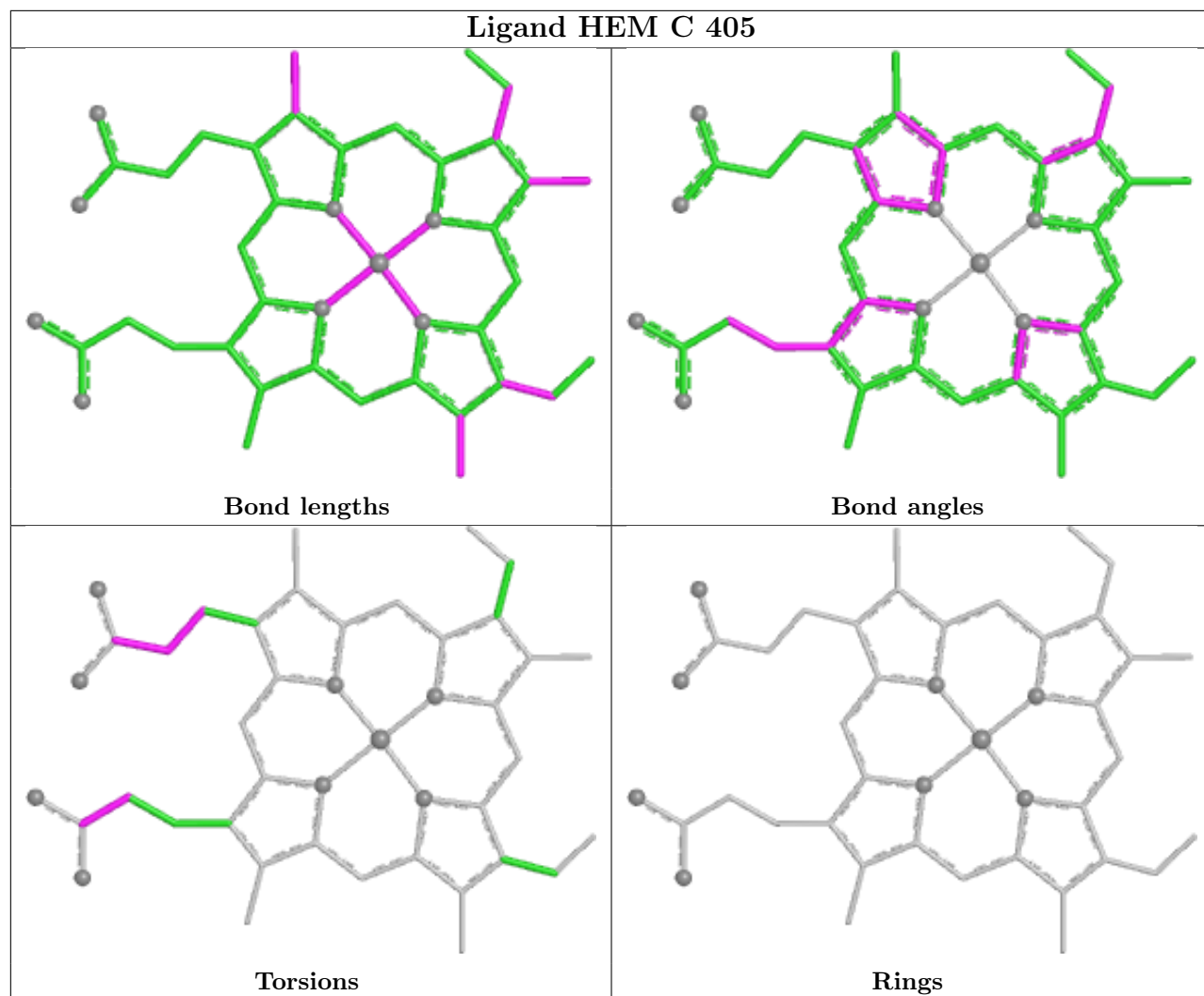


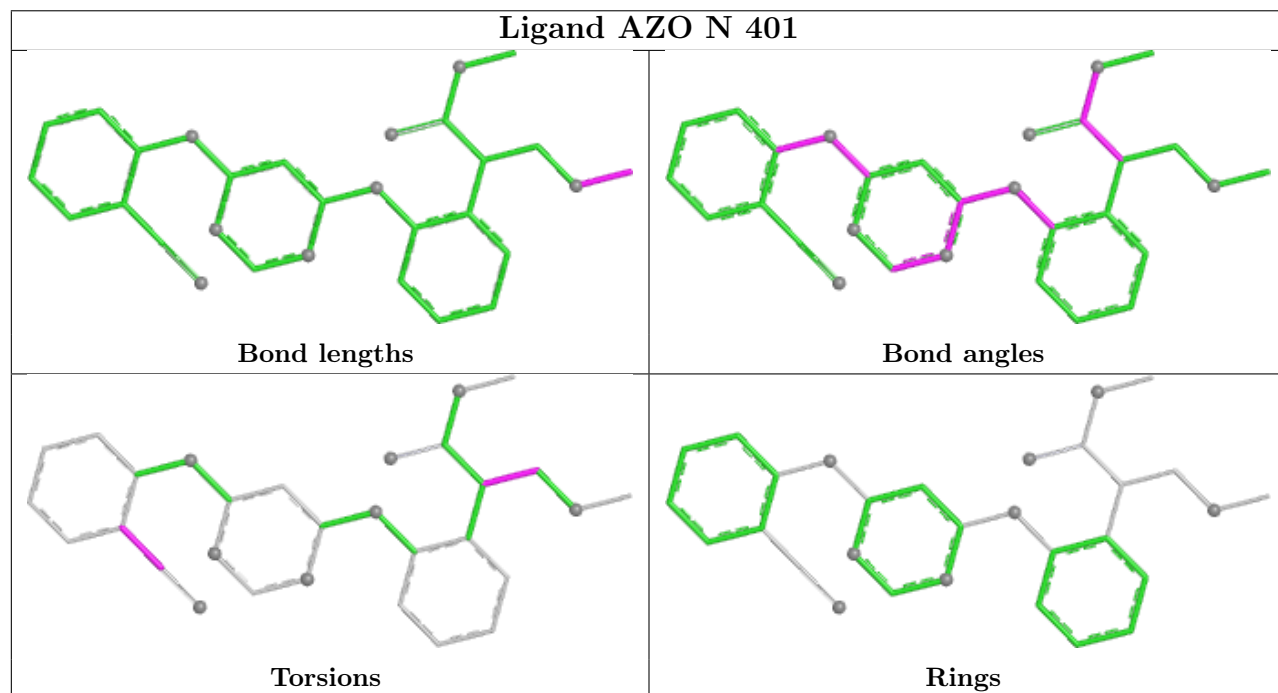
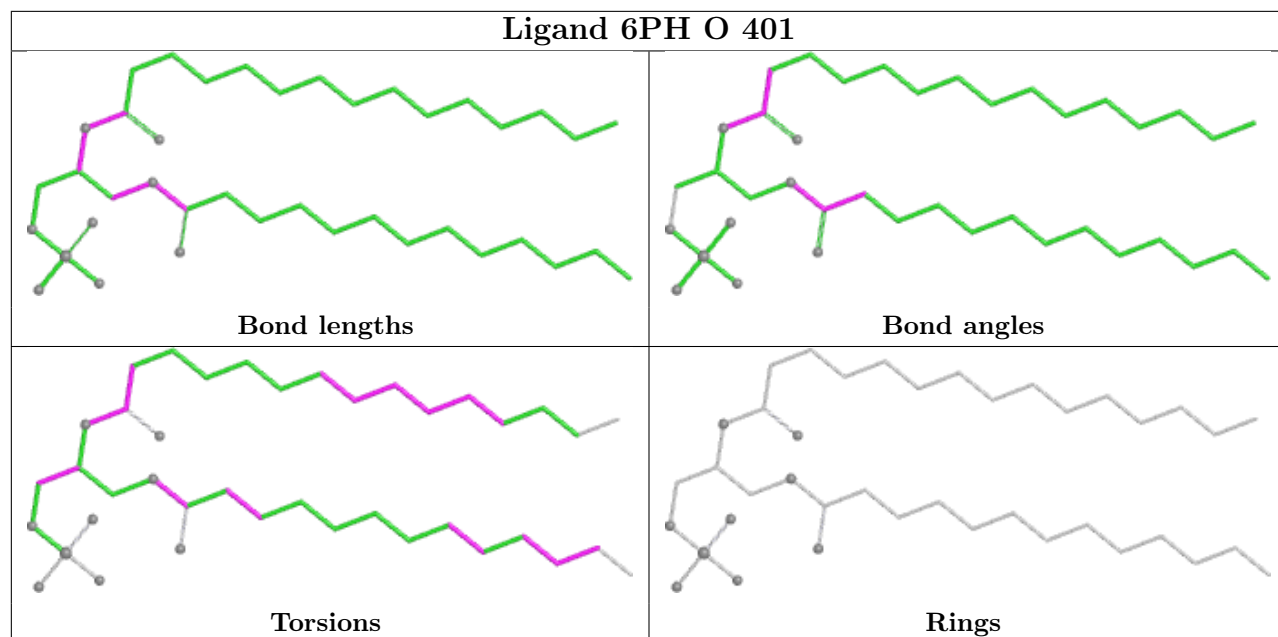


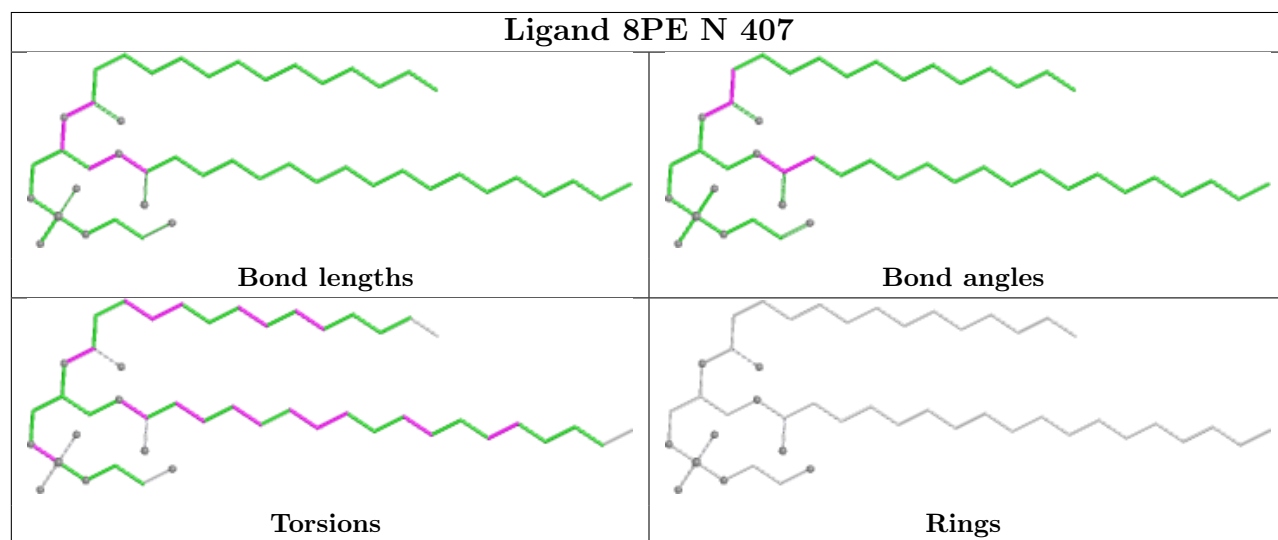
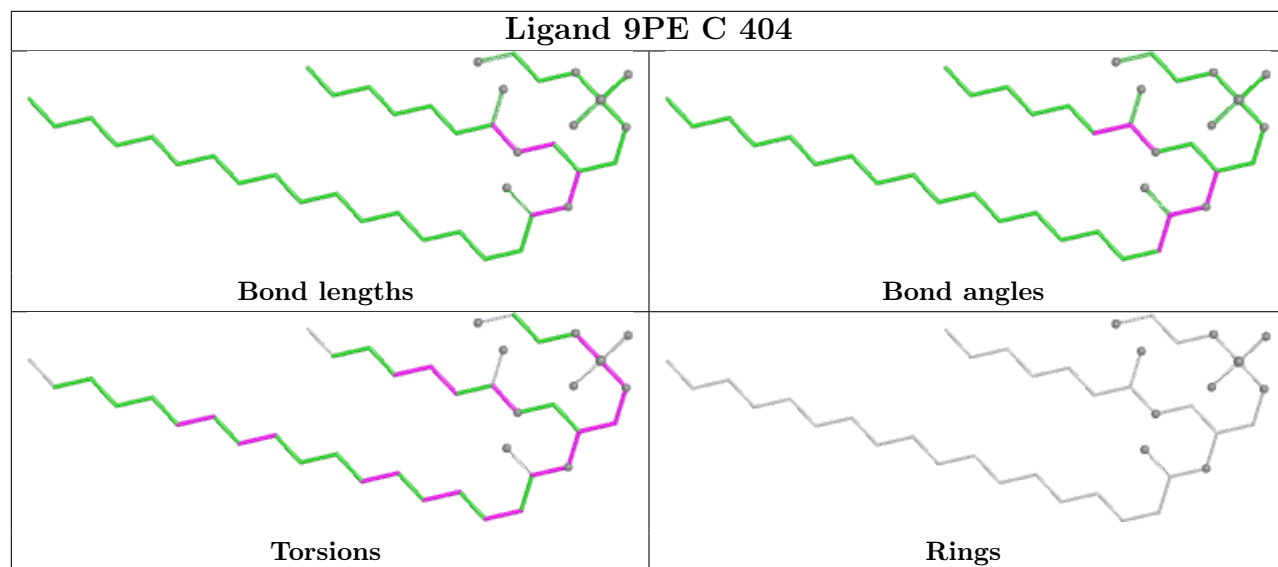


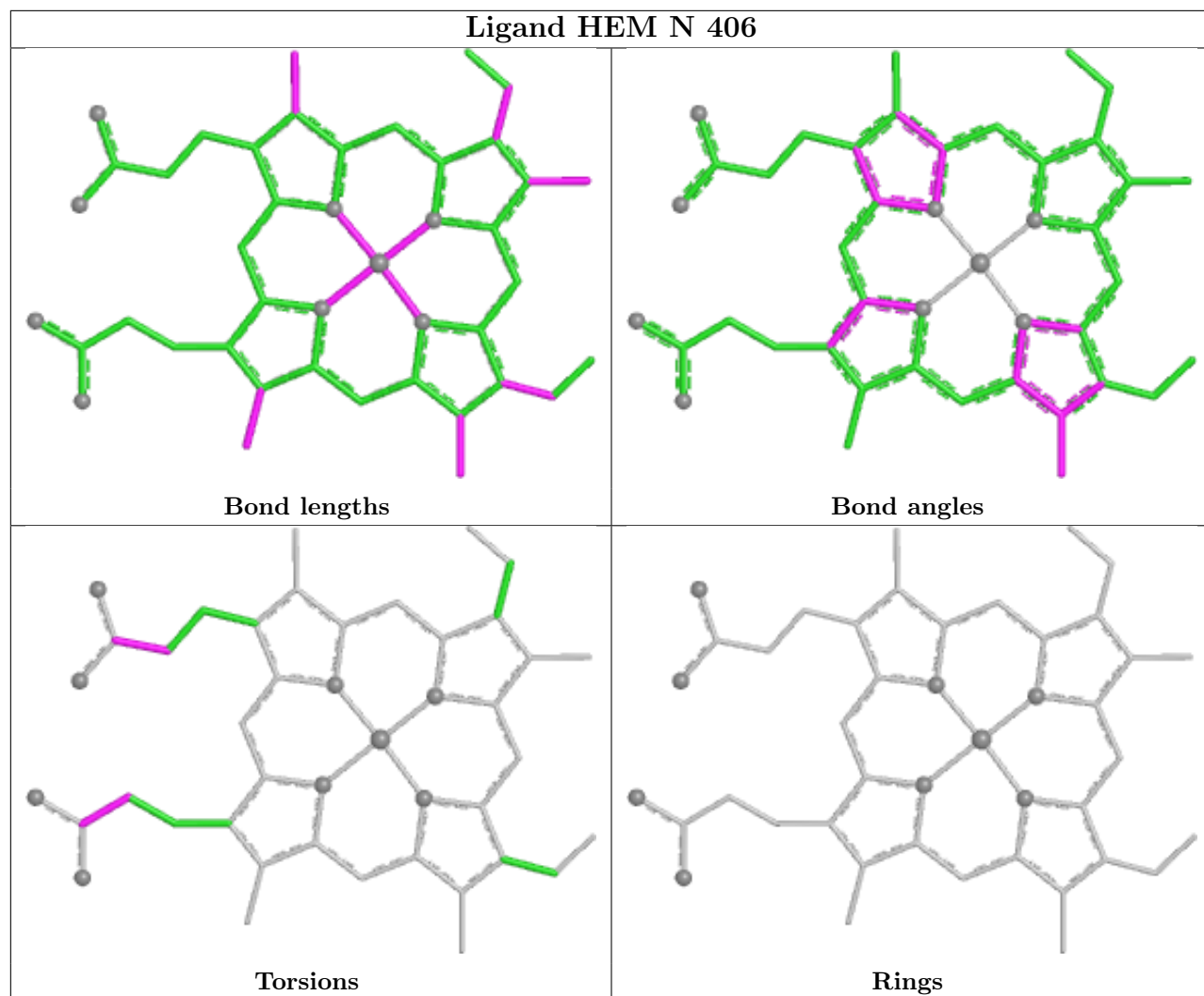


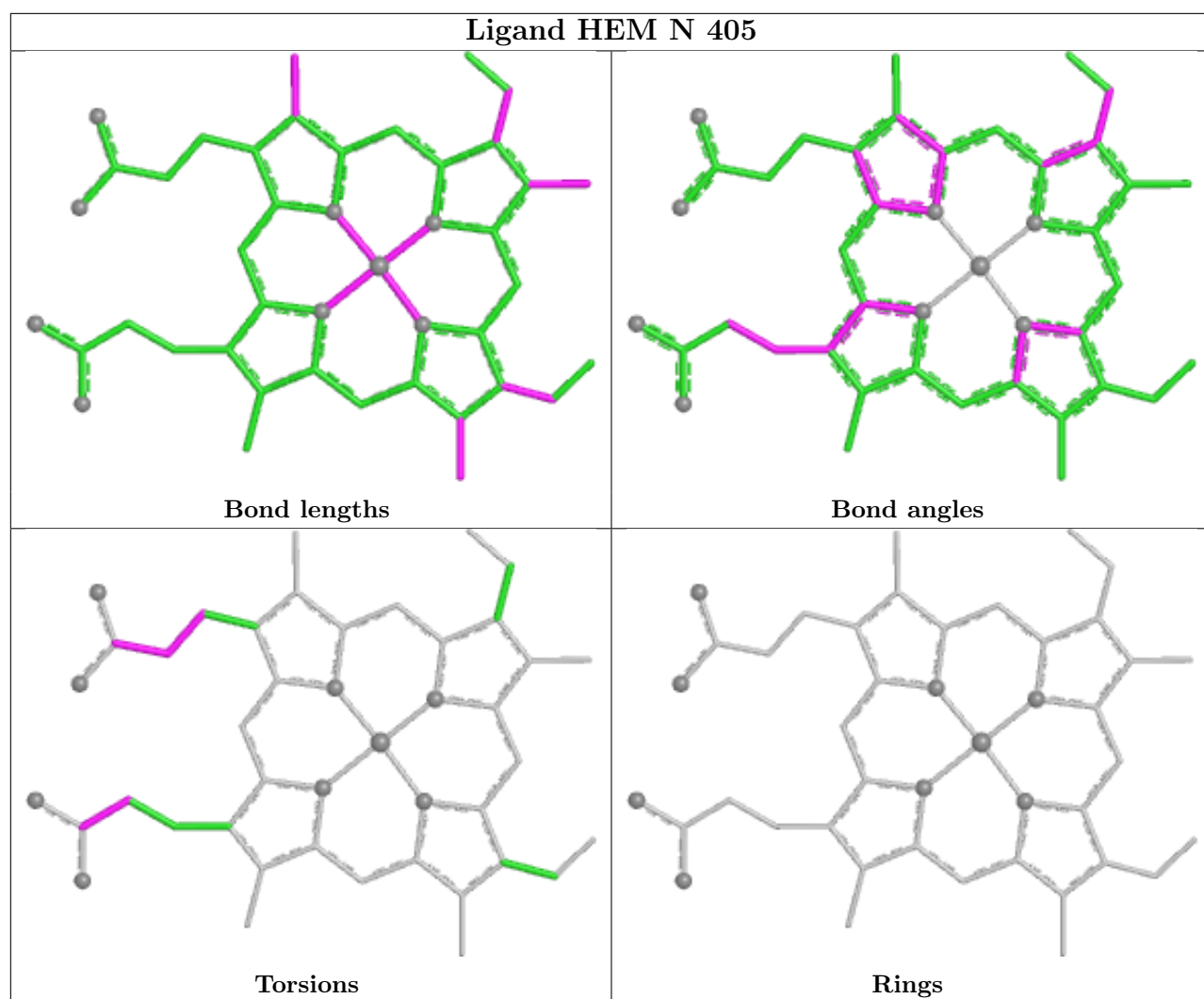












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

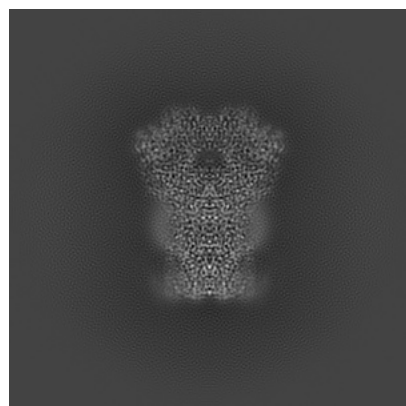
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39324. These allow visual inspection of the internal detail of the map and identification of artifacts.

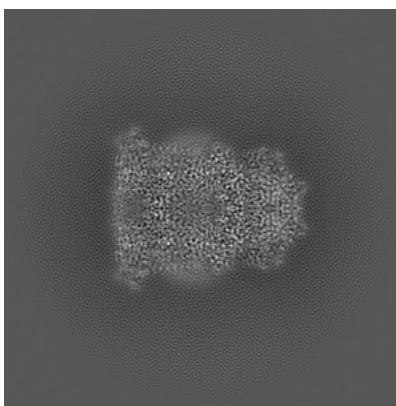
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

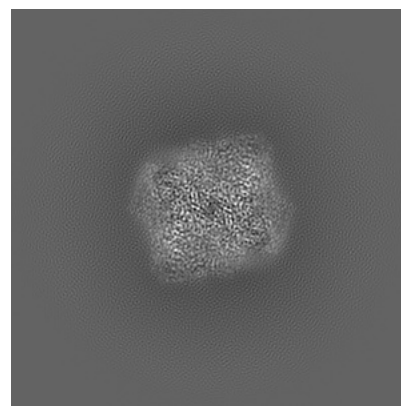
6.1.1 Primary map



X

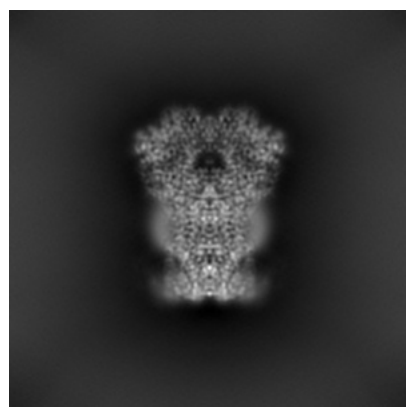


Y

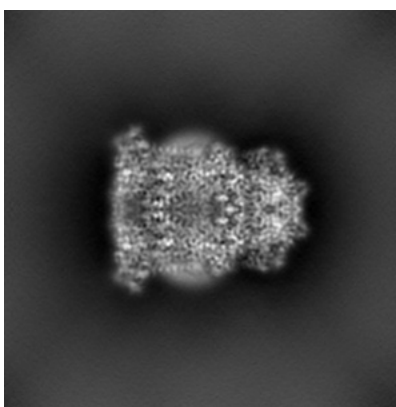


Z

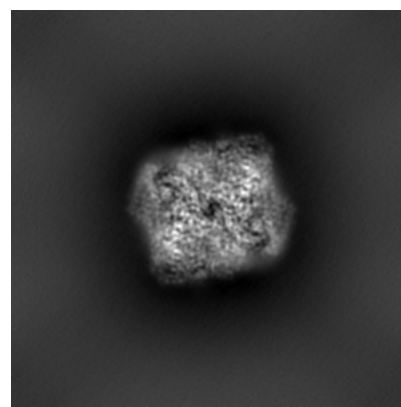
6.1.2 Raw map



X



Y

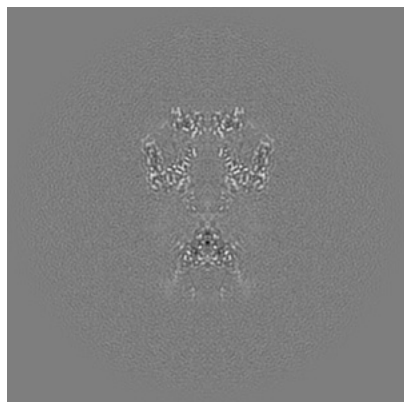


Z

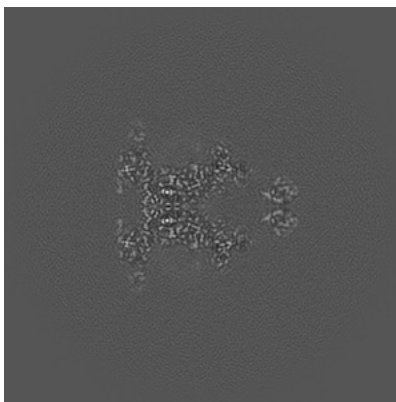
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

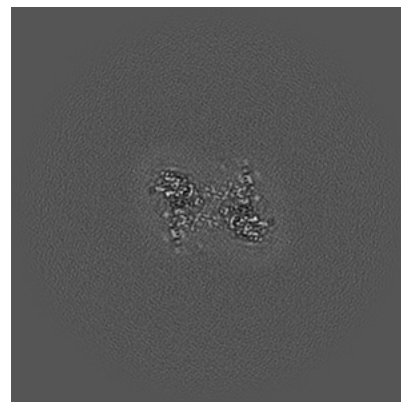
6.2.1 Primary map



X Index: 160

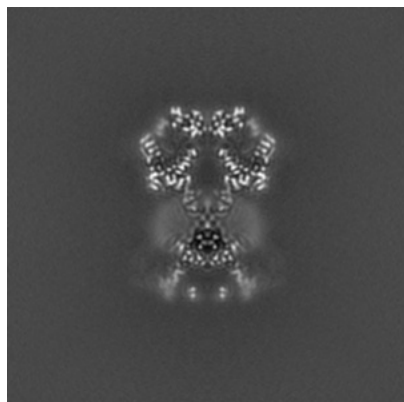


Y Index: 160

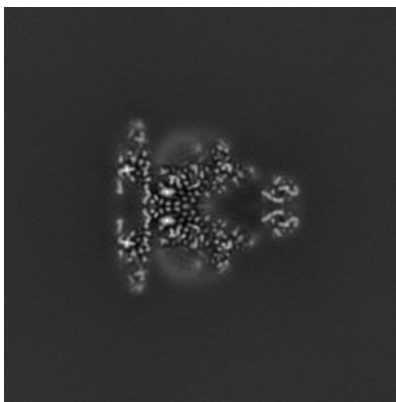


Z Index: 160

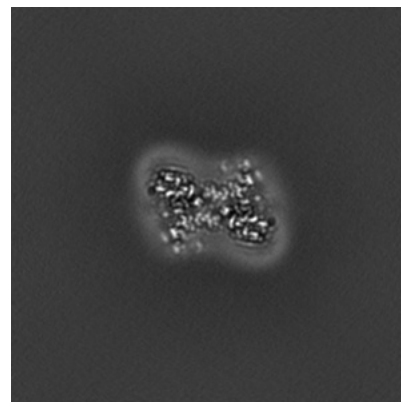
6.2.2 Raw map



X Index: 160



Y Index: 160

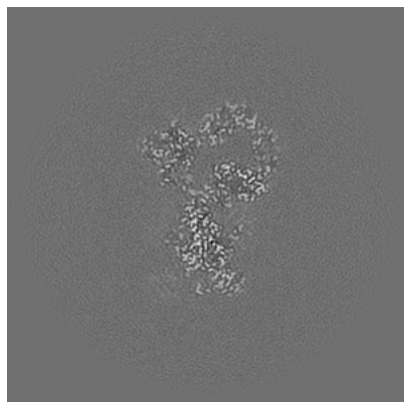


Z Index: 160

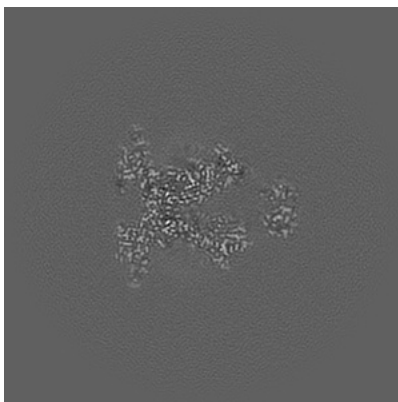
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

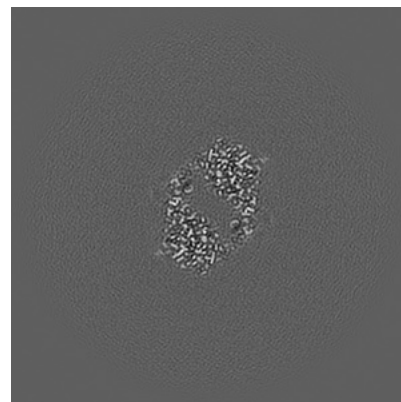
6.3.1 Primary map



X Index: 175

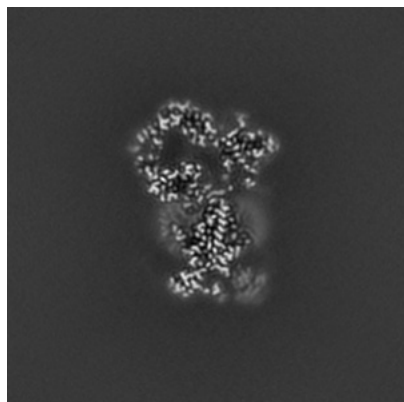


Y Index: 157

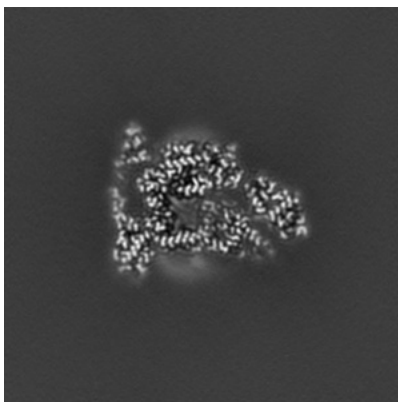


Z Index: 185

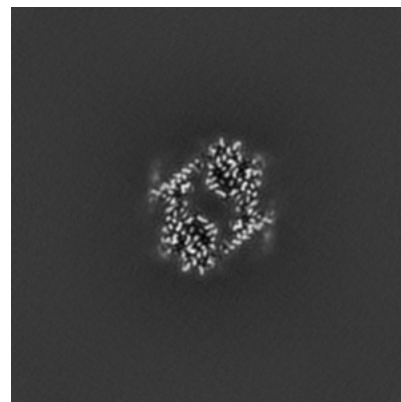
6.3.2 Raw map



X Index: 145



Y Index: 147

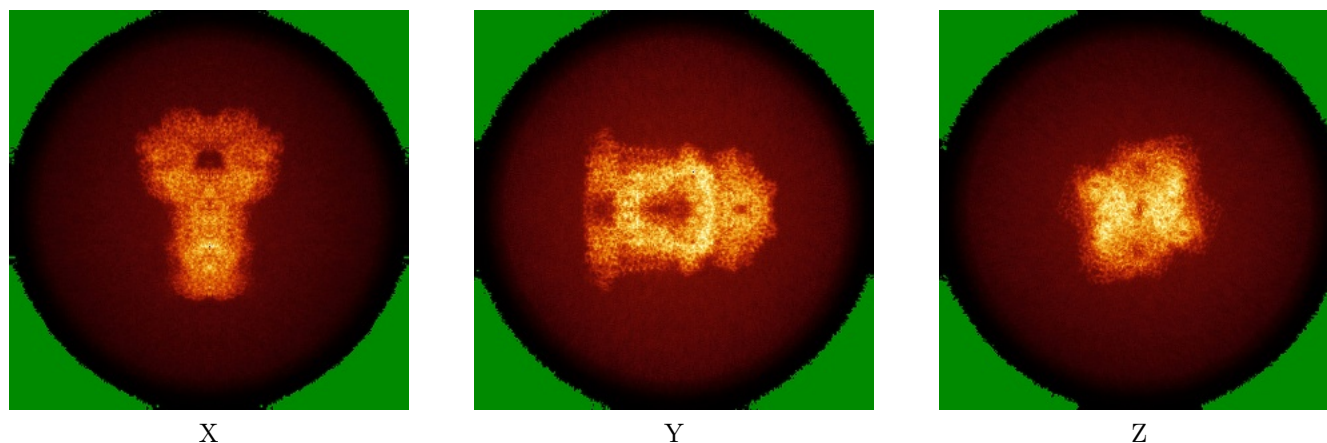


Z Index: 182

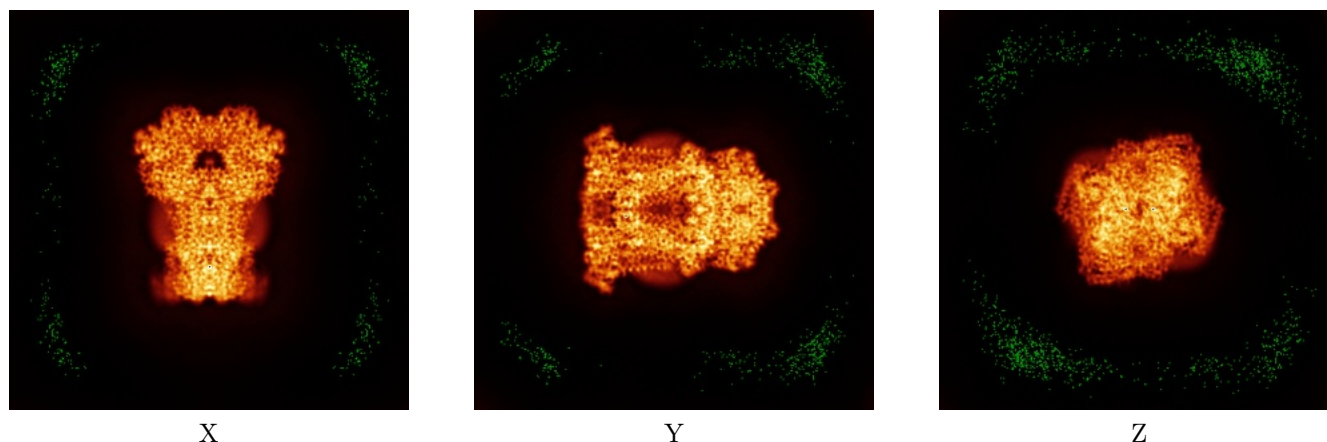
The images above show the largest variance slices of the map in three orthogonal directions.

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.

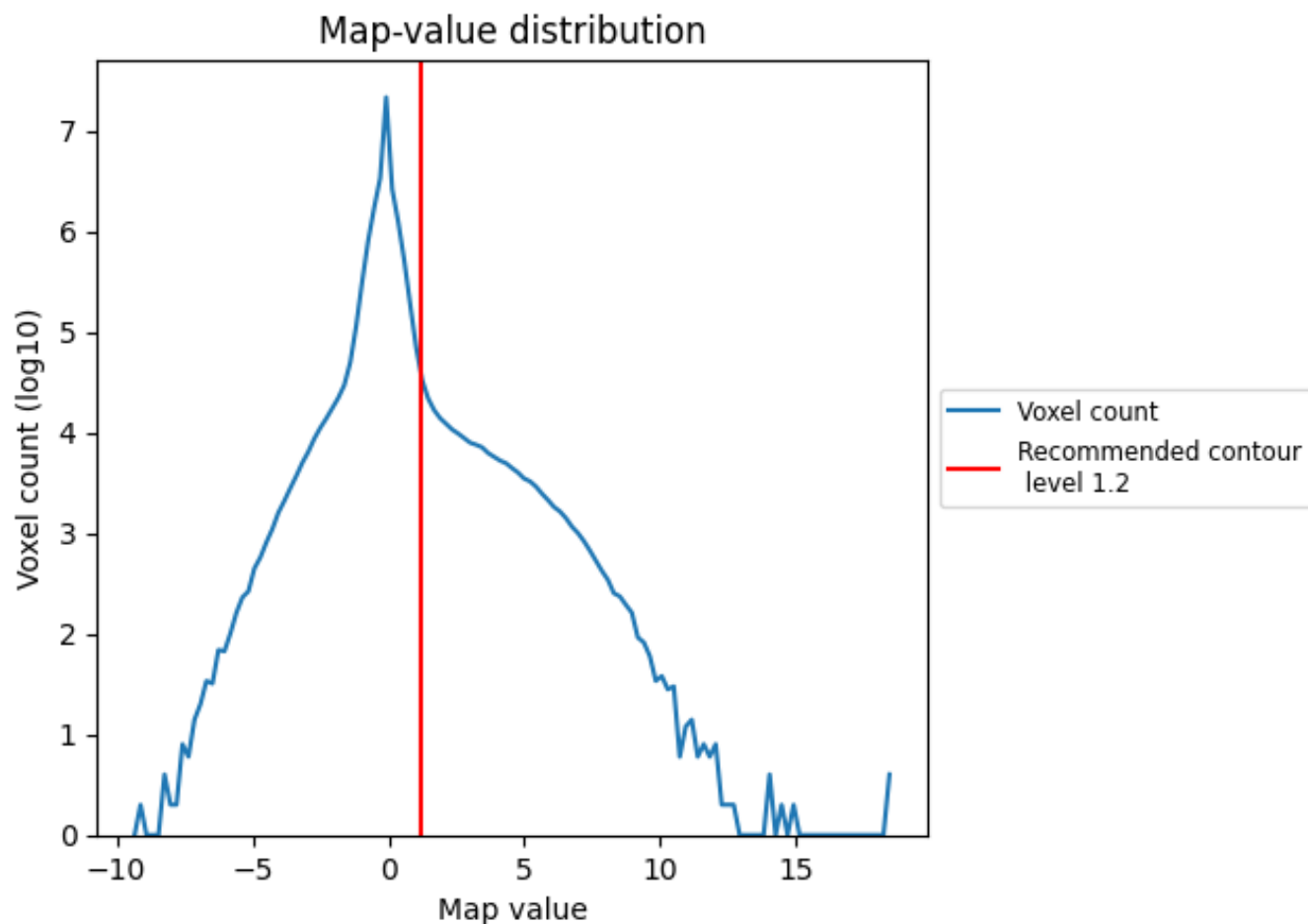
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

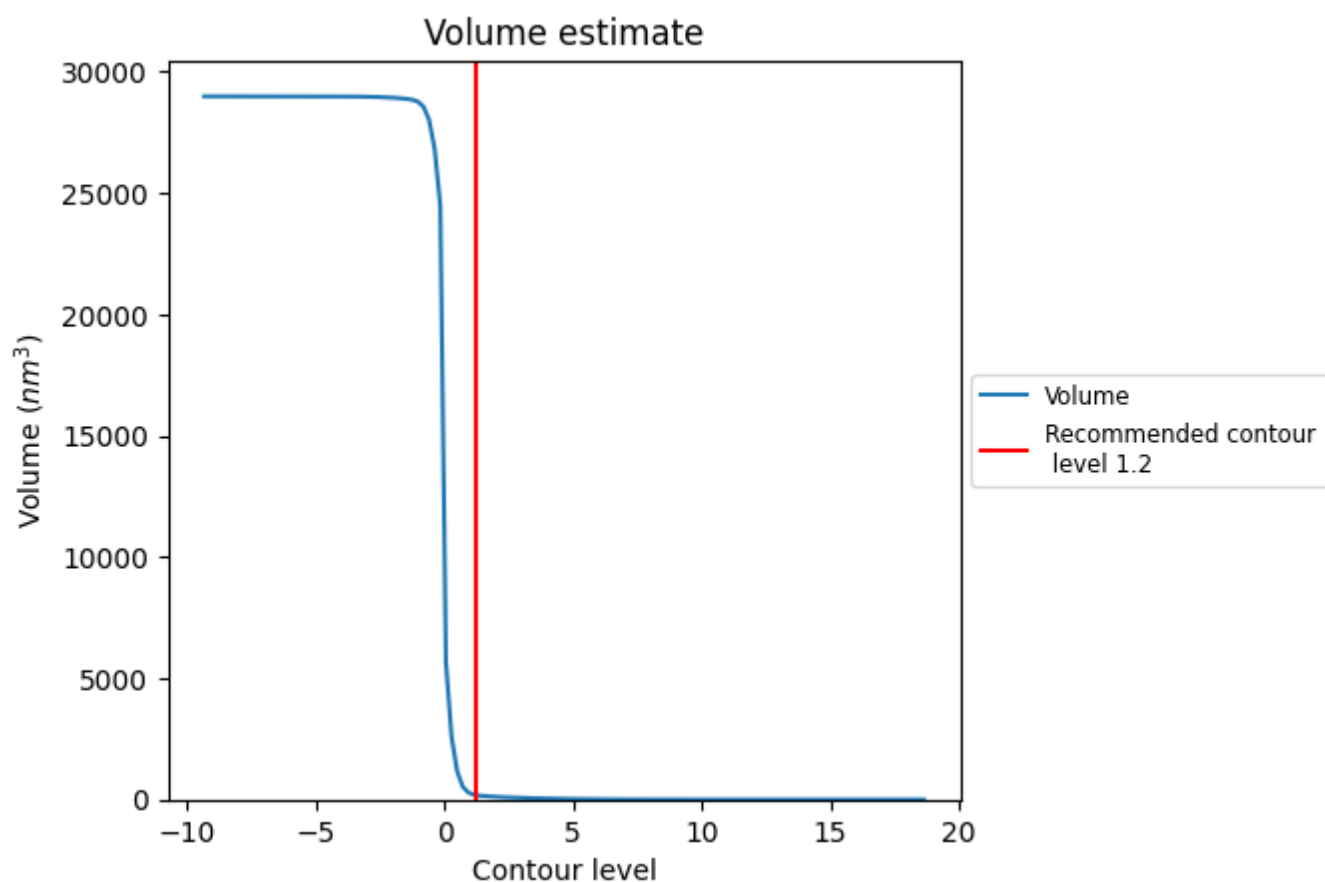
This section contains the results of statistical analysis of the map.

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.

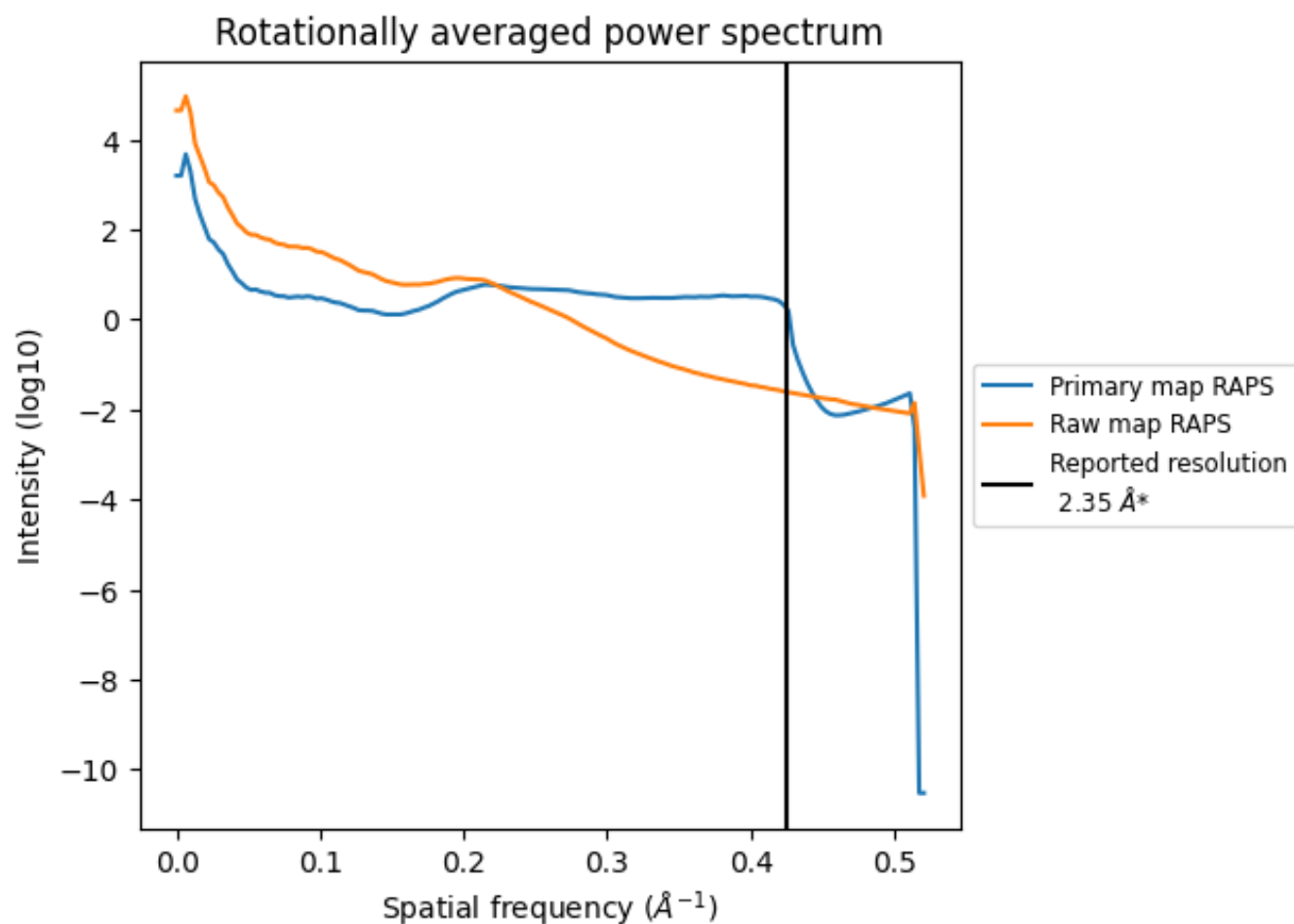
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 191 nm³; this corresponds to an approximate mass of 173 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 ⓘ

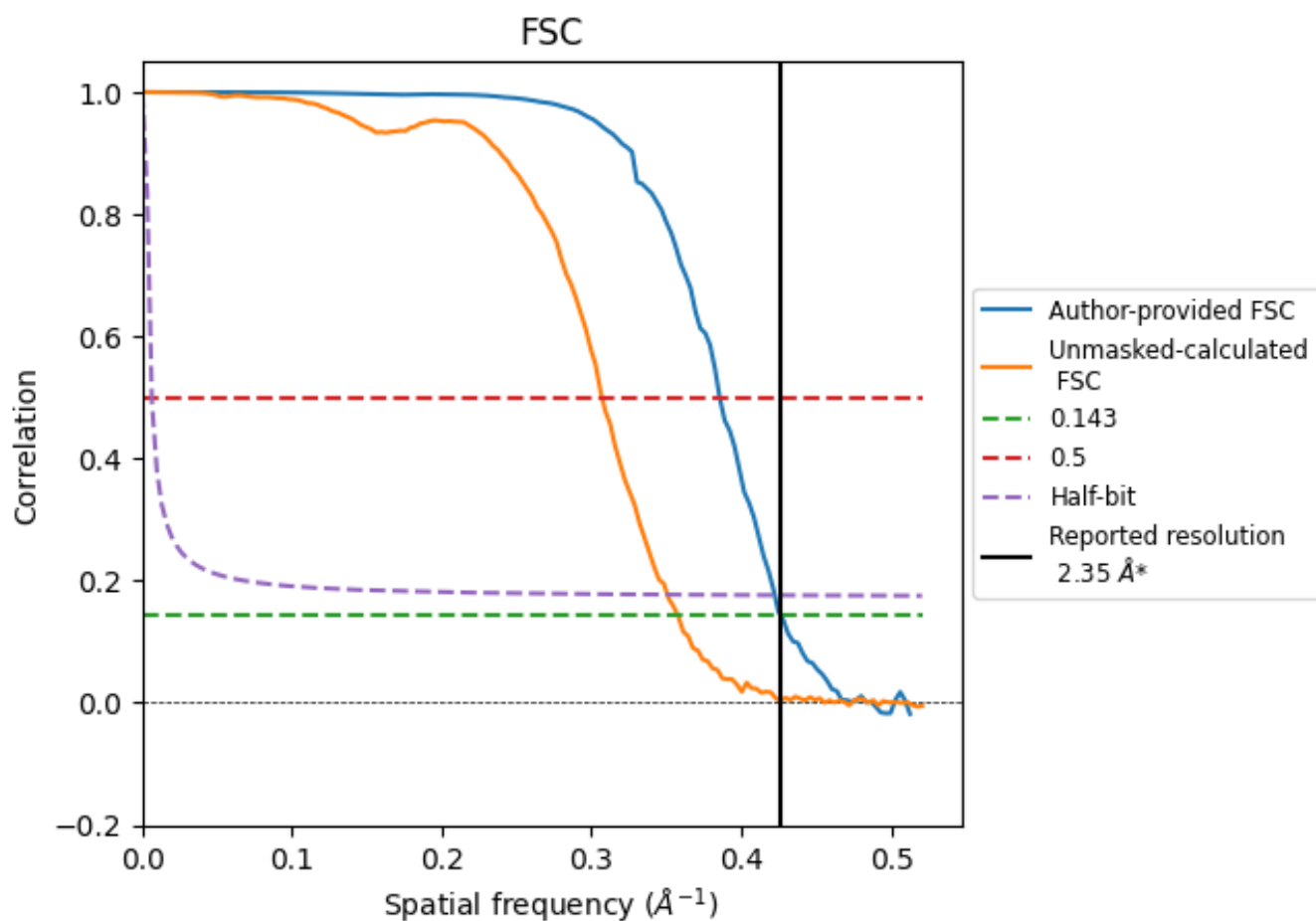


*Reported resolution corresponds to spatial frequency of 0.426 Å⁻¹

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 0.426 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.35	-	-
Author-provided FSC curve	2.35	2.59	2.37
Unmasked-calculated*	2.80	3.26	2.85

*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 2.80 differs from the reported value 2.35 by more than 10 %

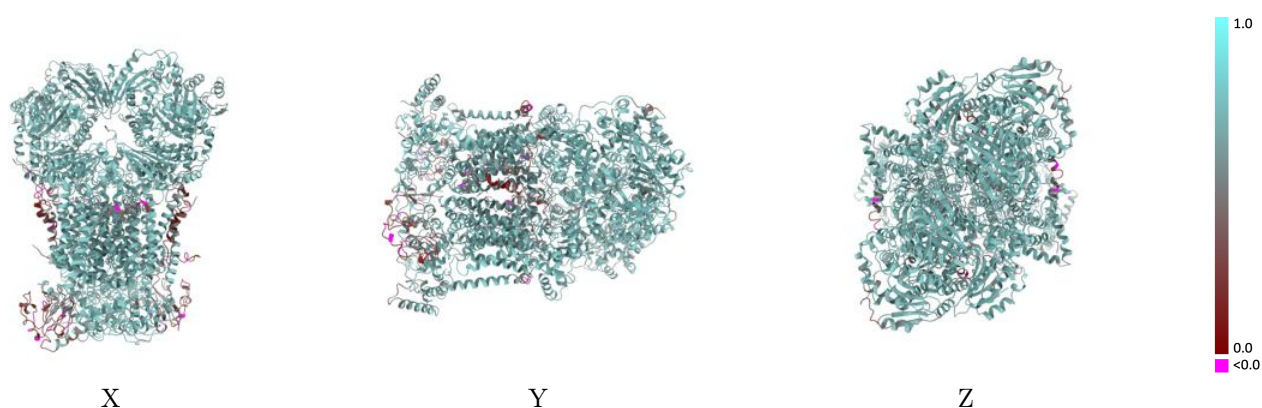
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-39324 and PDB model 8YIO. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)

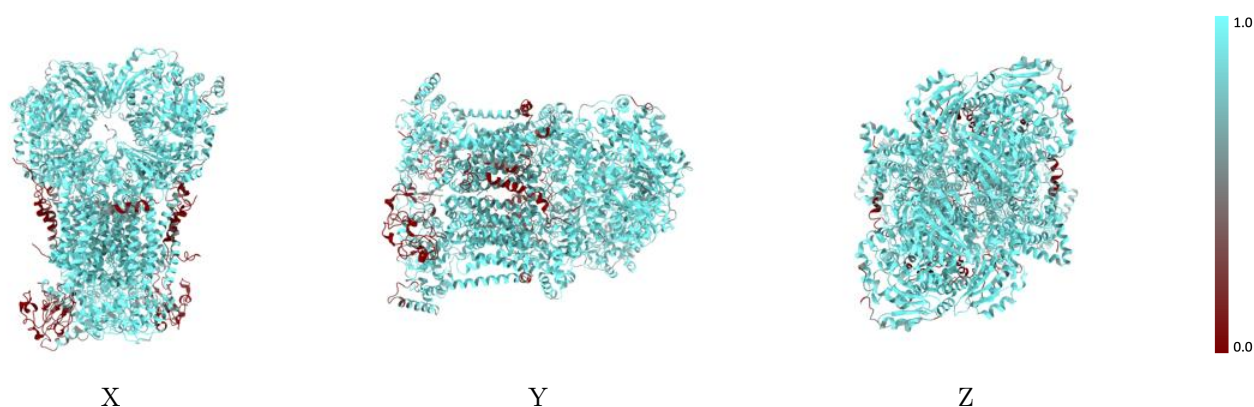
This section was not generated.

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



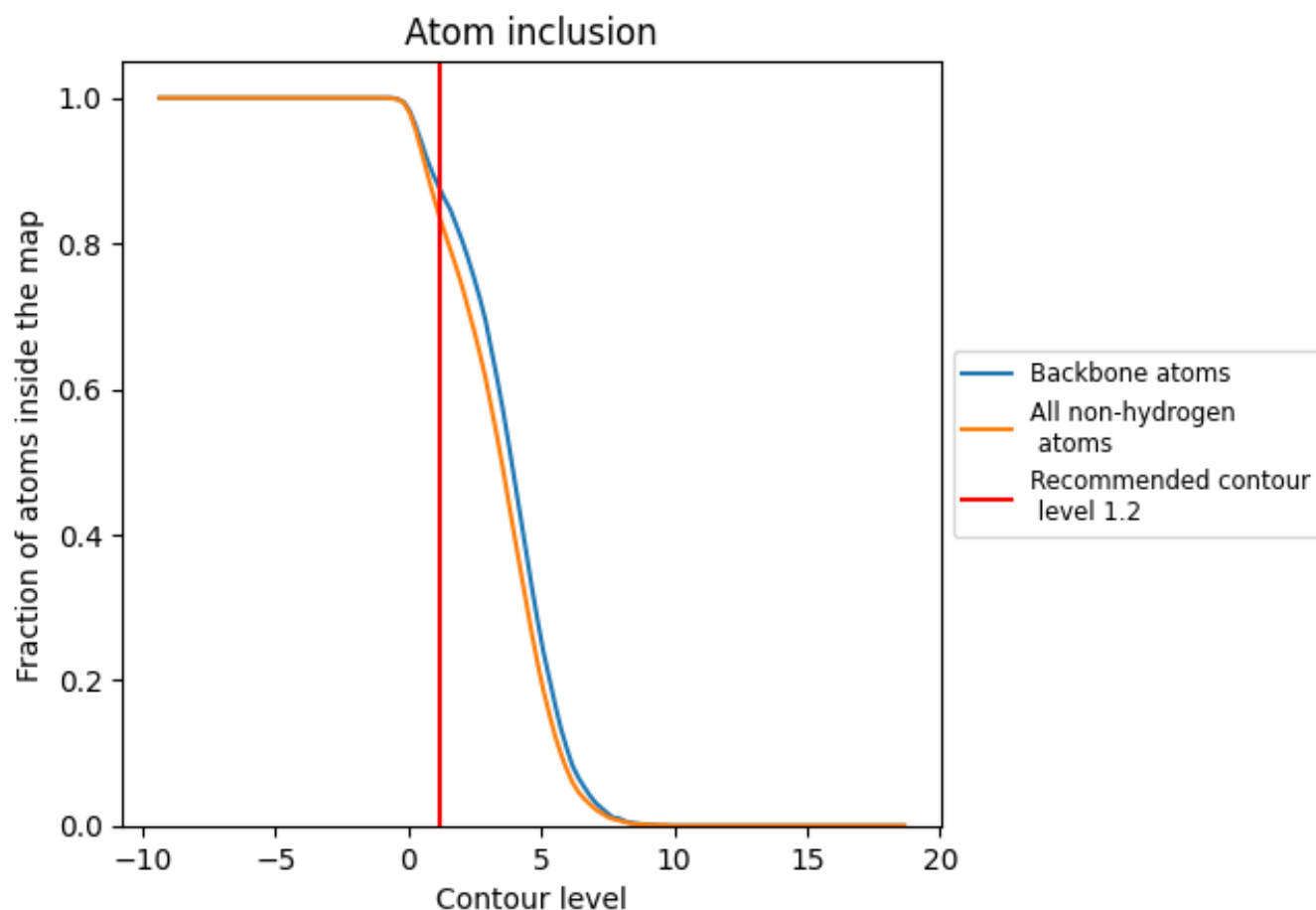
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 83% 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 (1.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8340	 0.6400
A	 0.9200	 0.6820
B	 0.9360	 0.6870
C	 0.9580	 0.7080
D	 0.9470	 0.6900
E	 0.3460	 0.3900
F	 0.7270	 0.5780
G	 0.9180	 0.6880
H	 0.7270	 0.5910
I	 0.5300	 0.5150
L	 0.9200	 0.6810
M	 0.9370	 0.6860
N	 0.9560	 0.7060
O	 0.9410	 0.6860
P	 0.3410	 0.3790
Q	 0.7130	 0.5850
R	 0.9180	 0.6860
S	 0.7270	 0.5880
T	 0.5240	 0.4970
U	 0.0180	 0.2440
V	 0.0100	 0.2390

