



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 04:39 PM UTC

PDB ID : 8YIL / pdb_00008yil
EMDB ID : EMD-39322
Title : Cryo-EM structure of *Saccharomyces cerevisiae* bc1 complex in YF24228-bound state
Authors : Ye, Y.; Li, Z.W.; Yang, G.F.
Deposited on : 2024-02-29
Resolution : 2.58 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:

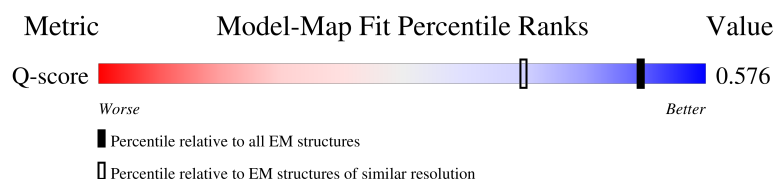
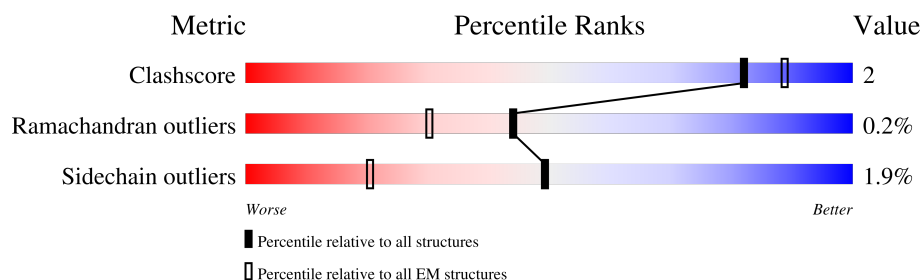
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.58 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



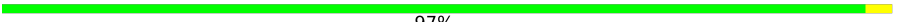
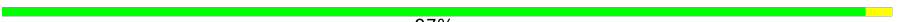
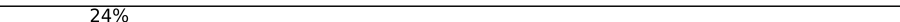
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7675 (2.08 - 3.08)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	431	
1	L	431	
2	C	385	
2	N	385	

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Mol	Chain	Length	Quality of chain
3	B	352	 97% .
3	M	352	 97% .
4	D	248	 97% .
4	O	248	 98% .
5	E	185	 47% 84% 16% .
5	P	185	 48% 84% 16% .
6	F	75	 7% 88% 11% .
6	Q	75	 91% 9% .
7	G	126	 92% 7% .
7	R	126	 92% 7% .
8	H	93	 6% 92% 5% .
8	S	93	 8% 94% . .
9	I	55	 24% 76% 16% 5% .
9	T	55	 24% 85% 9% . .
10	U	52	 81% 67% 10% . . 15%
10	V	52	 94% 62% 27% 10% .

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 32326 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.

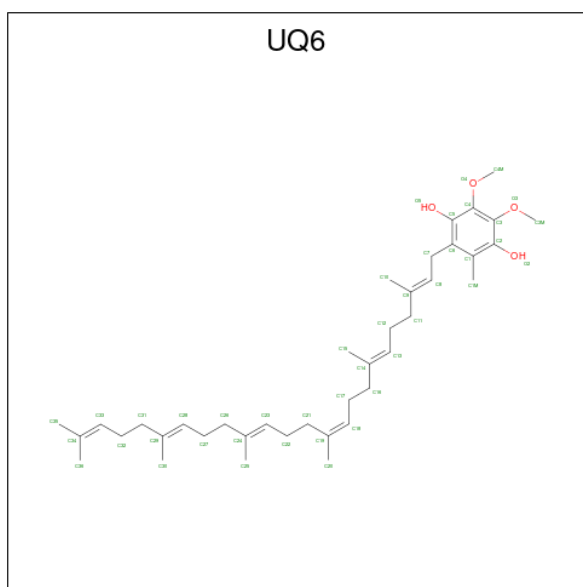
Mol	Chain	Residues	Atoms					AltConf	Trace
10	U	44	Total	C	N	O	S	0	0
			347	230	58	57	2		

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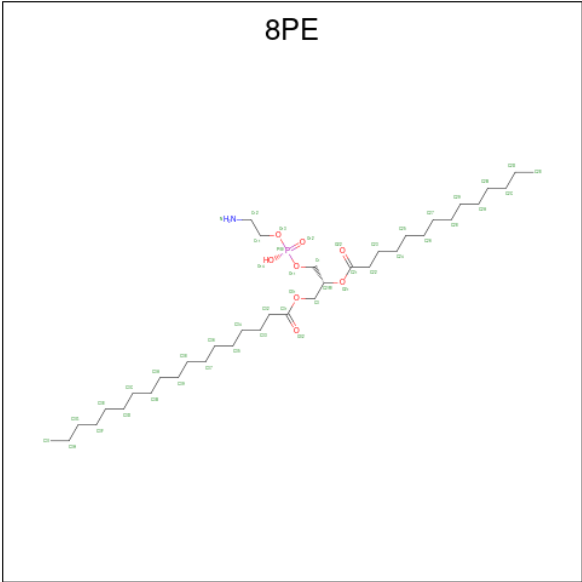
Mol	Chain	Residues	Atoms					AltConf	Trace
10	V	51	Total	C	N	O	S	0	0
			406	272	66	66	2		

- Molecule 11 is 5-(3,7,11,15,19,23-HEXAMETHYL-TETRACOSA-2,6,10,14,18,22-HEXAENYL)-2,3-DIMETHOXY-6-METHYL-BENZENE-1,4-DIOL (CCD ID: UQ6) (formula: $C_{39}H_{60}O_4$).



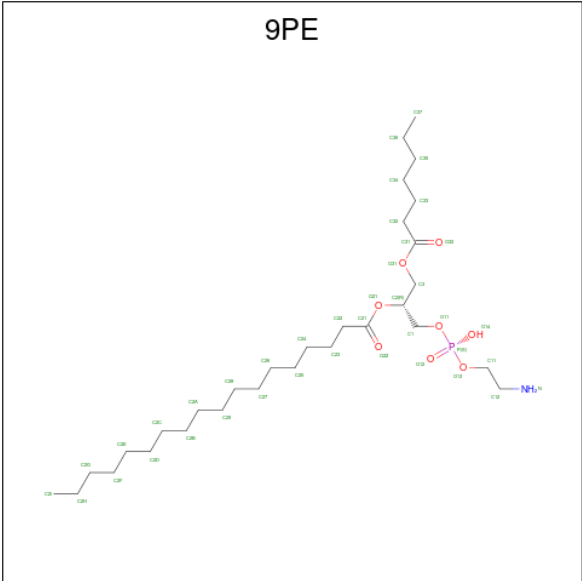
Mol	Chain	Residues	Atoms			AltConf
11	C	1	Total	C	O	0
			43	39	4	
11	N	1	Total	C	O	0
			43	39	4	

- Molecule 12 is (2R)-3-{[(S)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-(tetradecanoyloxy)propyl octadecanoate (CCD ID: 8PE) (formula: $C_{37}H_{74}NO_8P$).



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

- Molecule 13 is (1R)-2-{[(S)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-1-[(heptanoyloxy)methyl]ethyl octadecanoate (CCD ID: 9PE) (formula: C₃₀H₆₀NO₈P).



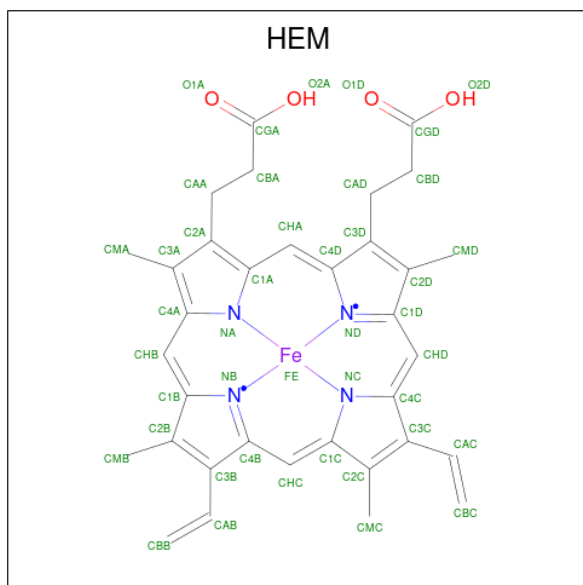
Mol	Chain	Residues	Atoms					AltConf
13	C	1	Total	C	N	O	P	0
			40	30	1	8	1	

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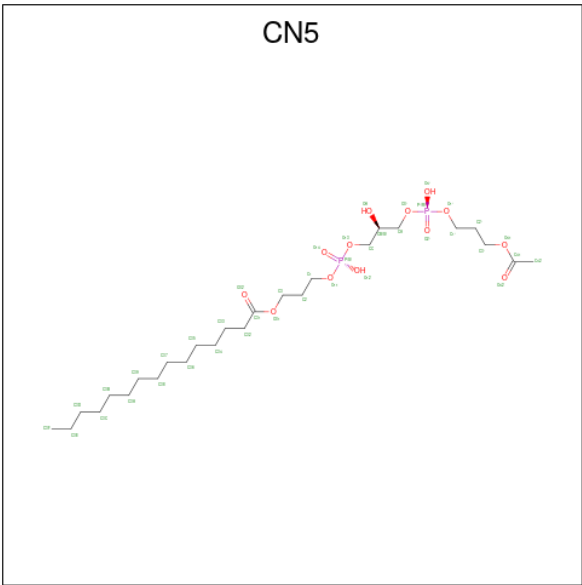
Mol	Chain	Residues	Atoms					AltConf
13	N	1	Total	C	N	O	P	0
			40	30	1	8	1	

- Molecule 14 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



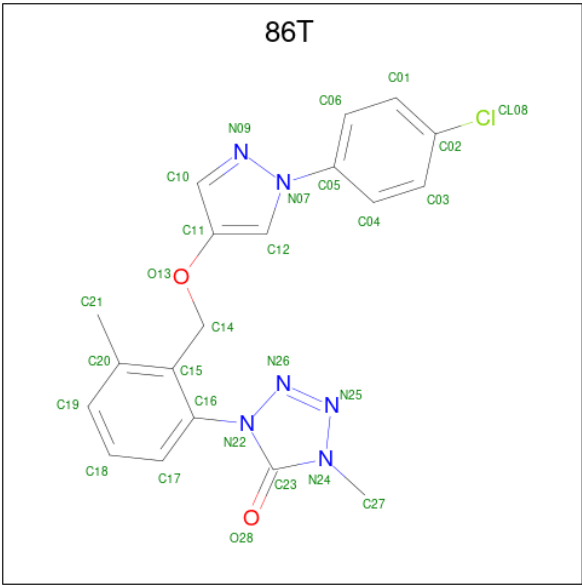
Mol	Chain	Residues	Atoms					AltConf
14	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
14	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
14	D	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
14	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
14	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
14	O	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 15 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: $C_{26}H_{52}O_{13}P_2$).



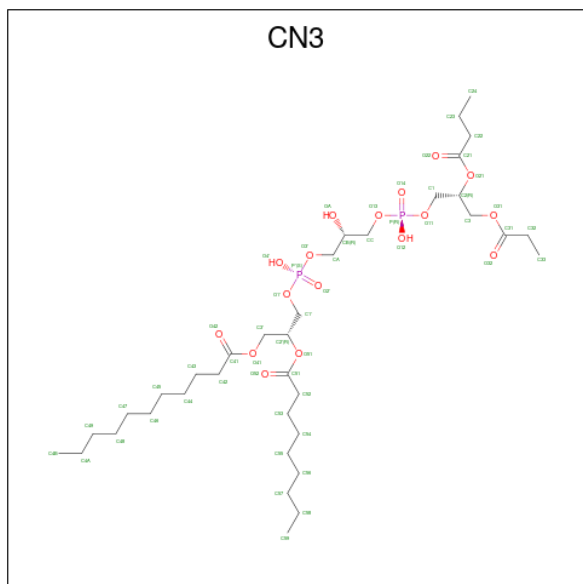
Mol	Chain	Residues	Atoms				AltConf
15	C	1	Total	C	O	P	0
			41	26	13	2	

- Molecule 16 is metyltetraprole (CCD ID: 86T) (formula: C₁₉H₁₇ClN₆O₂) (labeled as "Ligand of Interest" by depositor).



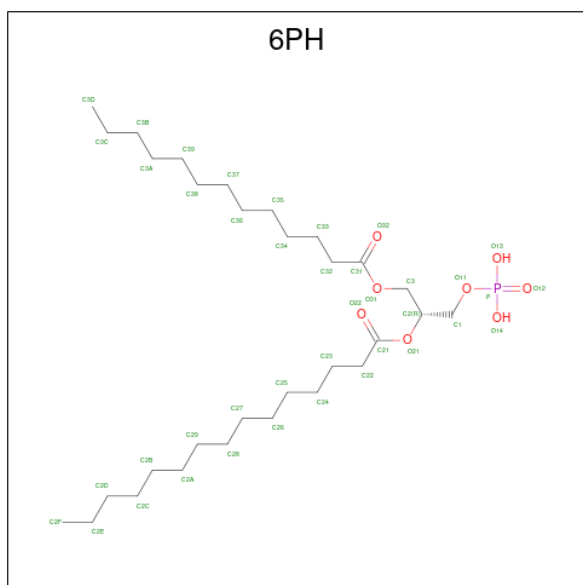
Mol	Chain	Residues	Atoms					AltConf
16	C	1	Total	C	Cl	N	O	0
			28	19	1	6	2	
16	N	1	Total	C	Cl	N	O	0
			28	19	1	6	2	

- 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: $C_{36}H_{68}O_{17}P_2$).



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: $C_{31}H_{61}O_8P$).

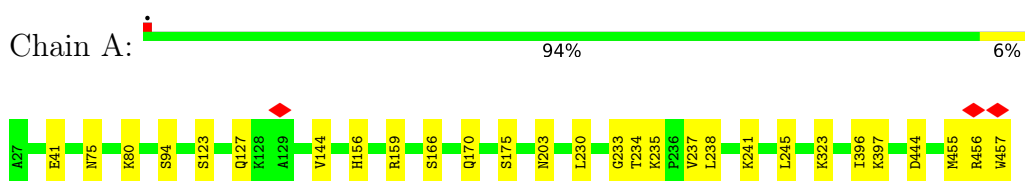


Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
18	O	1	40	31	8	1	0

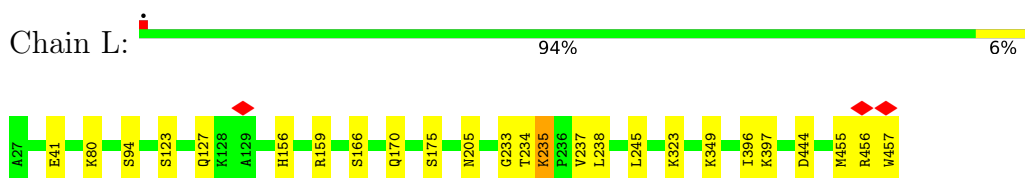
3 Residue-property plots

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

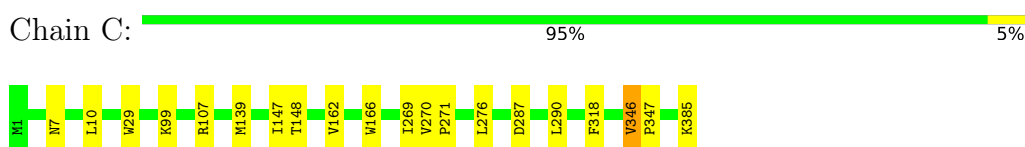
- Molecule 1: COR1 isoform 1



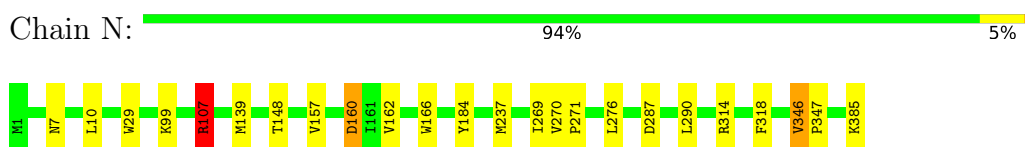
- Molecule 1: COR1 isoform 1



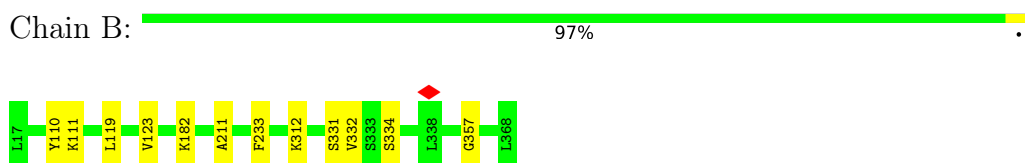
- Molecule 2: Cytochrome b



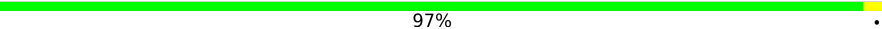
- Molecule 2: Cytochrome b



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

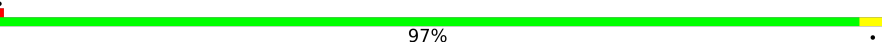


- Molecule 3: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain M:  97% .

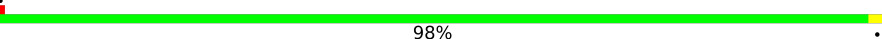


- Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain D:  97% .



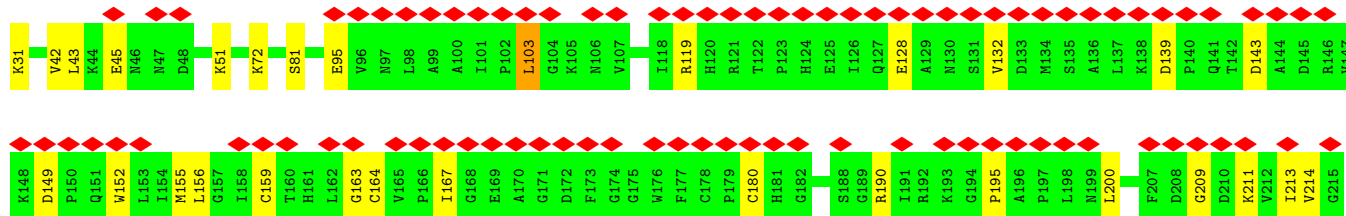
- Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain O:  98% .



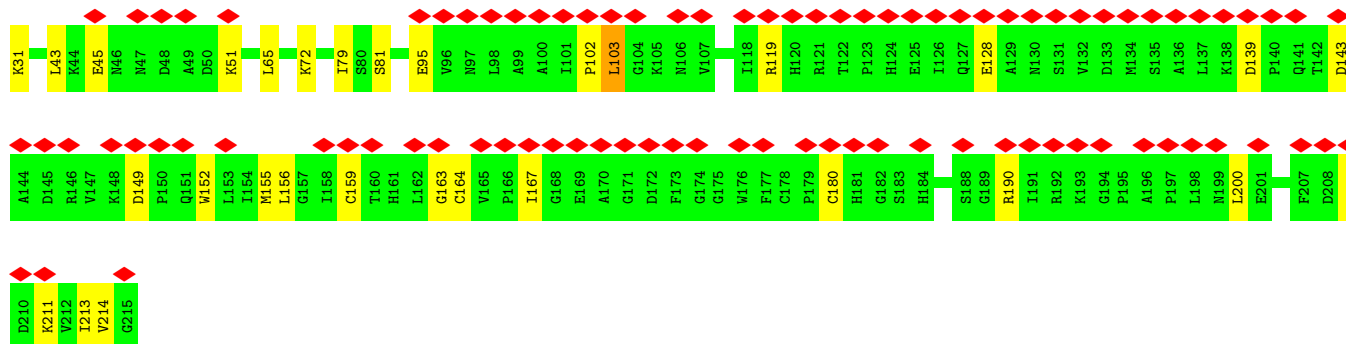
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain E:  47% 84% 16% .



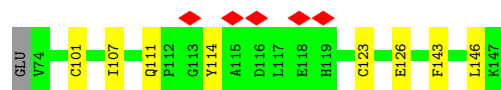
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain P:  48% 84% 16% .

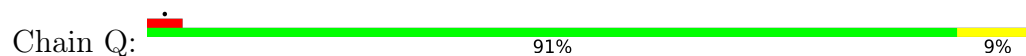


- Molecule 6: QCR6 isoform 1

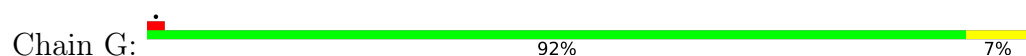
Chain F:  7% 88% 11% .



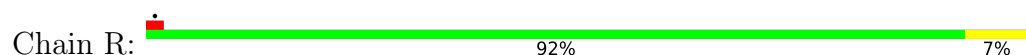
- Molecule 6: QCR6 isoform 1



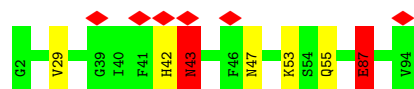
- Molecule 7: Cytochrome b-c1 complex subunit 7



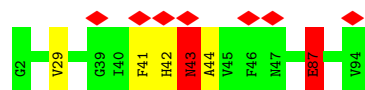
- Molecule 7: Cytochrome b-c1 complex subunit 7



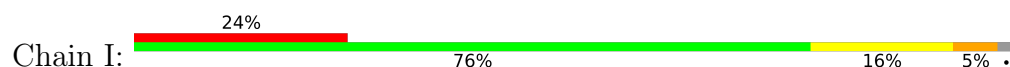
- Molecule 8: Cytochrome b-c1 complex subunit 8



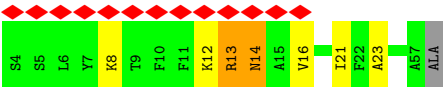
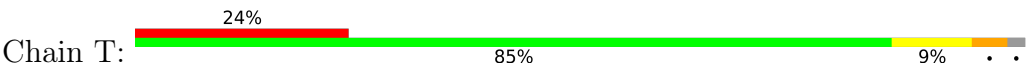
- Molecule 8: Cytochrome b-c1 complex subunit 8



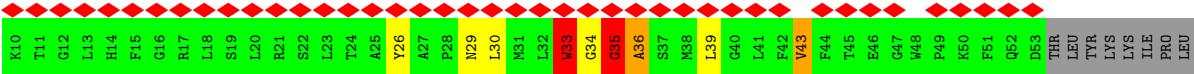
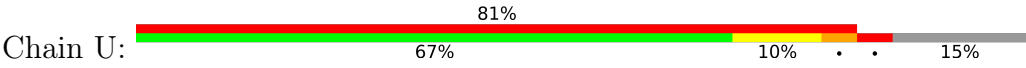
- Molecule 9: Cytochrome b-c1 complex subunit 9, mitochondrial



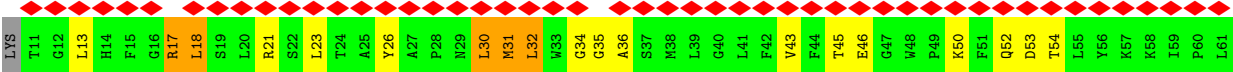
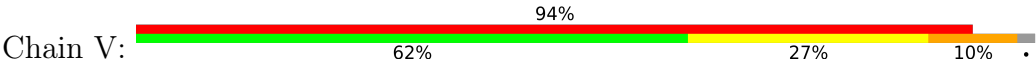
- Molecule 9: Cytochrome b-c1 complex subunit 9, mitochondrial



● 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	105757	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 ($e^-/\text{\AA}^2$)	49.48	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	130000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	5.808	Depositor
Minimum map value	-3.244	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.183	Depositor
Recommended contour level	0.5	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UQ6, 6PH, 9PE, 8PE, CN5, 86T, CN3, 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	A	0.45	3/3405 (0.1%)	0.53	0/4615
1	L	0.49	3/3405 (0.1%)	0.52	0/4615
2	C	0.35	1/3192 (0.0%)	0.49	0/4354
2	N	0.35	1/3192 (0.0%)	0.48	1/4354 (0.0%)
3	B	0.30	1/2781 (0.0%)	0.42	0/3764
3	M	0.30	1/2781 (0.0%)	0.43	0/3764
4	D	0.26	0/2022	0.43	1/2751 (0.0%)
4	O	0.26	0/2022	0.43	1/2751 (0.0%)
5	E	0.41	1/1444 (0.1%)	0.77	4/1957 (0.2%)
5	P	0.63	1/1444 (0.1%)	0.76	3/1957 (0.2%)
6	F	0.27	0/638	0.52	0/858
6	Q	0.25	0/647	0.65	1/870 (0.1%)
7	G	0.51	1/1040 (0.1%)	0.73	6/1408 (0.4%)
7	R	0.42	1/1040 (0.1%)	0.60	2/1408 (0.1%)
8	H	0.58	1/804 (0.1%)	0.92	6/1088 (0.6%)
8	S	0.47	2/804 (0.2%)	0.92	5/1088 (0.5%)
9	I	0.63	1/455 (0.2%)	0.76	3/614 (0.5%)
9	T	0.28	0/456	0.65	1/615 (0.2%)
10	U	0.57	1/358 (0.3%)	1.11	4/483 (0.8%)
10	V	0.72	1/419 (0.2%)	0.94	1/567 (0.2%)
All	All	0.41	20/32349 (0.1%)	0.58	39/43881 (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
1	A	0	1
1	L	0	1
2	C	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	N	0	2
6	Q	0	1
8	H	0	1
8	S	0	1
9	I	0	1
9	T	0	1
10	V	0	1
All	All	0	11

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	233	GLY	C-N	21.12	1.59	1.33
5	P	102	PRO	C-N	19.26	1.58	1.33
1	A	233	GLY	C-N	16.53	1.53	1.33
7	G	2	PRO	C-N	13.58	1.50	1.33
8	H	43	ASN	C-N	13.03	1.51	1.34
9	I	5	SER	C-N	-11.14	1.23	1.33
10	V	53	ASP	C-N	10.83	1.48	1.33
1	A	234	THR	C-N	9.01	1.52	1.33
1	A	238	LEU	C-N	8.19	1.44	1.33
5	E	103	LEU	C-N	8.17	1.45	1.33
7	R	3	GLN	C-N	8.13	1.45	1.33
1	L	238	LEU	C-N	7.70	1.43	1.33
8	S	43	ASN	C-N	7.45	1.44	1.34
2	N	107	ARG	C-O	-6.95	1.14	1.23
2	C	107	ARG	C-O	-6.35	1.15	1.23
3	M	331	SER	C-N	6.09	1.42	1.33
3	B	331	SER	C-N	5.84	1.41	1.33
1	L	234	THR	C-N	5.46	1.44	1.33
10	U	43	VAL	C-N	5.14	1.42	1.33
8	S	44	ALA	C-N	-5.02	1.28	1.34

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	43	ASN	O-C-N	-18.98	97.34	122.59
8	S	43	ASN	CA-C-N	12.45	139.24	120.31
8	S	43	ASN	C-N-CA	12.45	139.24	120.31
8	S	43	ASN	O-C-N	-11.66	107.09	122.59
7	G	2	PRO	CA-C-N	-9.86	106.10	120.89
7	G	2	PRO	C-N-CA	-9.86	106.10	120.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	R	3	GLN	CA-C-N	8.10	137.02	121.54
7	R	3	GLN	C-N-CA	8.10	137.02	121.54
7	G	3	GLN	CA-C-N	7.99	140.55	122.19
7	G	3	GLN	C-N-CA	7.99	140.55	122.19
9	I	5	SER	CA-C-N	7.94	133.98	122.23
9	I	5	SER	C-N-CA	7.94	133.98	122.23
7	G	3	GLN	O-C-N	-7.93	112.75	122.11
8	H	42	HIS	O-C-N	-7.56	113.12	122.57
10	U	35	GLY	CA-C-N	7.53	134.16	122.49
10	U	35	GLY	C-N-CA	7.53	134.16	122.49
5	E	132	VAL	CA-C-N	7.42	136.27	122.84
5	E	132	VAL	C-N-CA	7.42	136.27	122.84
5	P	103	LEU	O-C-N	-7.34	114.10	122.03
10	U	33	TRP	N-CA-C	-7.27	104.22	113.23
8	H	43	ASN	CA-C-N	7.26	130.74	120.28
8	H	43	ASN	C-N-CA	7.26	130.74	120.28
8	S	87	GLU	CA-CB-CG	6.72	127.54	114.10
8	H	87	GLU	CA-CB-CG	6.68	127.45	114.10
5	E	209	GLY	CA-C-N	6.26	133.57	123.93
5	E	209	GLY	C-N-CA	6.26	133.57	123.93
5	P	209	GLY	CA-C-N	6.26	133.57	123.93
5	P	209	GLY	C-N-CA	6.26	133.57	123.93
9	I	16	VAL	N-CA-C	-6.19	105.66	111.48
2	N	157	VAL	O-C-N	-5.87	116.43	122.30
9	T	14	ASN	CB-CA-C	5.83	120.04	110.88
10	V	30	LEU	N-CA-C	-5.81	105.29	112.90
6	Q	108	GLN	N-CA-C	-5.77	98.52	110.80
8	H	87	GLU	CB-CG-CD	5.54	122.02	112.60
8	S	87	GLU	CB-CG-CD	5.54	122.01	112.60
10	U	36	ALA	O-C-N	5.32	128.68	122.24
7	G	2	PRO	O-C-N	5.25	131.40	123.00
4	O	307	PRO	N-CA-C	5.23	119.79	112.26
4	D	307	PRO	N-CA-C	5.21	119.77	112.26

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	456	ARG	Peptide
2	C	346	VAL	Peptide
8	H	43	ASN	Mainchain
9	I	6	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	L	456	ARG	Peptide
2	N	107	ARG	Sidechain
2	N	346	VAL	Peptide
6	Q	114	TYR	Peptide
8	S	43	ASN	Mainchain
9	T	13	ARG	Sidechain
10	V	17	ARG	Sidechain

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	12	0
1	L	3344	0	3323	11	0
2	C	3090	0	3129	12	0
2	N	3090	0	3129	16	0
3	B	2735	0	2774	6	0
3	M	2735	0	2774	5	0
4	D	1961	0	1890	8	0
4	O	1961	0	1890	1	0
5	E	1411	0	1390	13	0
5	P	1411	0	1390	12	0
6	F	624	0	583	10	0
6	Q	633	0	589	5	0
7	G	1019	0	1034	5	0
7	R	1019	0	1034	6	0
8	H	773	0	736	5	0
8	S	773	0	736	3	0
9	I	442	0	440	8	0
9	T	443	0	440	6	0
10	U	347	0	345	12	0
10	V	406	0	414	15	0
11	C	43	0	60	4	0
11	N	43	0	60	4	0
12	C	47	0	73	3	0
12	S	47	0	73	1	0
13	C	40	0	59	1	0
13	N	40	0	59	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	C	86	0	60	0	0
14	D	43	0	30	0	0
14	N	86	0	60	2	0
14	O	43	0	30	1	0
15	C	41	0	50	4	0
16	C	28	0	0	0	0
16	N	28	0	0	0	0
17	C	55	0	66	0	0
17	N	55	0	66	0	0
18	O	40	0	59	2	0
All	All	32326	0	32168	161	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 (161) 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:164:CYS:HB3	5:E:180:CYS:SG	1.89	1.13
5:P:164:CYS:HB3	5:P:180:CYS:SG	1.89	1.13
6:F:101:CYS:HB3	6:F:123:CYS:SG	2.29	0.72
10:V:46:GLU:HA	10:V:52:GLN:HE21	1.54	0.72
1:A:75:ASN:HD22	1:A:144:VAL:CG2	2.04	0.70
2:C:385:LYS:HZ1	7:G:17:LYS:HE3	1.56	0.70
6:Q:101:CYS:HB3	6:Q:123:CYS:SG	2.31	0.70
1:A:75:ASN:ND2	1:A:144:VAL:HG22	2.06	0.69
1:A:170:GLN:HE21	1:A:245:LEU:HD23	1.58	0.69
5:E:159:CYS:H	5:E:163:GLY:HA2	1.58	0.69
1:L:170:GLN:HE21	1:L:245:LEU:HD23	1.58	0.69
9:I:13:ARG:HB3	9:I:16:VAL:HG23	1.76	0.68
5:E:164:CYS:CB	5:E:180:CYS:SG	2.77	0.67
5:P:159:CYS:H	5:P:163:GLY:HA2	1.58	0.67
6:Q:101:CYS:SG	6:Q:126:GLU:HG2	2.36	0.65
10:U:33:TRP:HA	10:U:33:TRP:CE3	2.32	0.64
2:N:385:LYS:HZ1	7:R:17:LYS:HE3	1.62	0.64
6:F:101:CYS:SG	6:F:126:GLU:HG2	2.37	0.64
5:P:164:CYS:CB	5:P:180:CYS:SG	2.77	0.62
1:A:323:LYS:HB3	1:A:396:ILE:HD11	1.82	0.61
11:C:401:UQ6:H103	15:C:405:CN5:H33	1.80	0.61
5:E:164:CYS:SG	5:E:180:CYS:HB3	2.41	0.61
5:P:164:CYS:SG	5:P:180:CYS:HB3	2.41	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:323:LYS:HB3	1:L:396:ILE:HD11	1.82	0.60
5:E:72:LYS:HE2	9:I:29:GLN:HE22	1.67	0.60
1:A:75:ASN:HD22	1:A:144:VAL:HG21	1.66	0.58
10:U:30:LEU:HA	10:U:33:TRP:CB	2.34	0.57
7:G:55:ILE:HD13	7:G:111:GLU:HG2	1.87	0.56
2:N:148:THR:HG22	2:N:162:VAL:HG23	1.87	0.56
10:U:33:TRP:HA	10:U:33:TRP:HE3	1.69	0.56
4:D:249:LYS:HD2	6:F:146:LEU:HD12	1.87	0.56
14:N:404:HEM:HBC2	14:N:404:HEM:HHD	1.88	0.56
7:R:55:ILE:HD13	7:R:111:GLU:HG2	1.87	0.56
2:C:148:THR:HG22	2:C:162:VAL:HG23	1.87	0.55
4:D:249:LYS:HE2	6:F:143:PHE:CE2	2.43	0.54
1:L:205:ASN:ND2	1:L:235:LYS:HE2	2.22	0.54
7:R:51:GLU:HA	7:R:56:MET:HG2	1.90	0.54
10:V:45:THR:HG22	10:V:52:GLN:HA	1.89	0.54
2:N:29:TRP:HB3	2:N:99:LYS:HG3	1.89	0.53
2:C:29:TRP:HB3	2:C:99:LYS:HG3	1.89	0.53
5:E:155:MET:HE3	5:E:200:LEU:HB2	1.90	0.53
10:U:34:GLY:O	10:U:35:GLY:C	2.49	0.52
5:P:155:MET:HE3	5:P:200:LEU:HB2	1.90	0.52
6:Q:101:CYS:SG	6:Q:126:GLU:CD	2.92	0.52
1:L:455:MET:HG2	9:T:14:ASN:OD1	2.10	0.52
11:C:401:UQ6:C10	15:C:405:CN5:H33	2.40	0.52
7:G:51:GLU:HA	7:G:56:MET:HG2	1.90	0.52
2:N:139:MET:HE1	2:N:269:ILE:HA	1.93	0.51
5:E:164:CYS:SG	5:E:180:CYS:CB	2.99	0.51
9:I:13:ARG:NH1	9:I:14:ASN:HB2	2.26	0.51
1:A:123:SER:H	1:A:127:GLN:HG3	1.76	0.51
2:N:287:ASP:HB3	2:N:290:LEU:HB2	1.92	0.51
5:P:164:CYS:SG	5:P:180:CYS:CB	2.99	0.51
5:P:72:LYS:HD2	10:U:43:VAL:O	2.12	0.50
2:N:160:ASP:CG	10:V:50:LYS:HB2	2.36	0.50
2:C:139:MET:HE1	2:C:269:ILE:HA	1.93	0.50
2:C:287:ASP:HB3	2:C:290:LEU:HB2	1.92	0.50
5:E:72:LYS:HD2	10:V:43:VAL:O	2.12	0.50
10:V:32:LEU:O	10:V:36:ALA:N	2.45	0.49
1:L:123:SER:H	1:L:127:GLN:HG3	1.76	0.49
6:Q:101:CYS:SG	6:Q:126:GLU:CG	3.00	0.49
2:C:385:LYS:HB3	7:G:16:LEU:HD13	1.94	0.49
10:V:31:MET:O	10:V:35:GLY:N	2.38	0.49
5:P:65:LEU:HD12	9:T:21:ILE:HA	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:29:TRP:CH2	12:C:402:8PE:H33A	2.48	0.48
2:N:148:THR:HG21	2:N:166:TRP:NE1	2.28	0.48
2:N:385:LYS:HB3	7:R:16:LEU:HD13	1.96	0.48
6:F:101:CYS:SG	6:F:126:GLU:CD	2.96	0.48
1:L:156:HIS:HD2	1:L:159:ARG:HH21	1.62	0.48
2:C:148:THR:HG21	2:C:166:TRP:NE1	2.28	0.48
6:F:101:CYS:SG	6:F:126:GLU:CG	3.01	0.48
1:A:156:HIS:HD2	1:A:159:ARG:HH21	1.62	0.48
4:D:249:LYS:HE2	6:F:143:PHE:CD2	2.49	0.48
10:U:36:ALA:HA	10:U:39:LEU:HB3	1.96	0.47
2:N:237:MET:HE2	18:O:402:6PH:H2B	1.96	0.47
8:H:43:ASN:HA	8:H:47:ASN:HB2	1.96	0.47
5:E:95:GLU:HG2	5:E:213:ILE:HG22	1.96	0.47
3:B:119:LEU:HA	3:B:123:VAL:HB	1.97	0.47
8:H:87:GLU:H	8:H:87:GLU:CD	2.24	0.46
10:U:30:LEU:HA	10:U:33:TRP:HB2	1.97	0.46
10:U:26:TYR:HA	10:U:29:ASN:HB2	1.96	0.46
5:P:95:GLU:HG2	5:P:213:ILE:HG22	1.96	0.46
10:V:18:LEU:HD12	10:V:23:LEU:HB2	1.96	0.46
11:N:406:UQ6:H151	11:N:406:UQ6:H172	1.66	0.46
3:M:119:LEU:HA	3:M:123:VAL:HB	1.97	0.46
15:C:405:CN5:H3AB	15:C:405:CN5:H3DA	1.55	0.46
3:M:110:TYR:HD2	3:M:111:LYS:HG3	1.81	0.46
3:B:110:TYR:HD2	3:B:111:LYS:HG3	1.81	0.46
14:O:401:HEM:HBC2	14:O:401:HEM:HHD	1.97	0.46
10:V:45:THR:O	10:V:52:GLN:HG2	2.15	0.46
1:A:241:LYS:HD3	1:A:241:LYS:HA	1.82	0.45
5:E:43:LEU:HD21	8:H:29:VAL:HG11	1.99	0.45
6:Q:86:LYS:HE3	6:Q:134:LEU:HD21	1.98	0.45
2:N:7:ASN:HA	13:N:403:9PE:H11	1.99	0.45
3:M:182:LYS:HE2	3:M:211:ALA:HB2	1.99	0.45
8:S:87:GLU:H	8:S:87:GLU:CD	2.24	0.44
4:D:249:LYS:HD2	6:F:146:LEU:CD1	2.47	0.44
2:N:184:TYR:CE2	14:N:404:HEM:HBC1	2.53	0.44
1:L:396:ILE:HG23	1:L:397:LYS:HG3	2.00	0.44
4:D:97:TYR:HA	4:D:101:CYS:HB3	1.99	0.44
6:F:111:GLN:HG3	6:F:114:TYR:HB3	2.00	0.44
8:S:29:VAL:HG11	5:P:43:LEU:HD21	2.00	0.44
1:A:396:ILE:HG23	1:A:397:LYS:HG3	2.00	0.44
1:L:205:ASN:HD21	1:L:235:LYS:HE2	1.83	0.44
12:S:101:8PE:H25	12:S:101:8PE:H22A	1.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:182:LYS:HE2	3:B:211:ALA:HB2	1.99	0.43
11:N:406:UQ6:H71	11:N:406:UQ6:H1M1	1.80	0.43
9:T:23:ALA:HA	10:U:39:LEU:HD11	2.01	0.43
9:I:13:ARG:HD3	9:I:15:ALA:H	1.84	0.43
1:A:455:MET:HG2	9:I:14:ASN:HD21	1.83	0.43
11:C:401:UQ6:H301	11:C:401:UQ6:H322	1.86	0.43
4:O:97:TYR:HA	4:O:101:CYS:HB3	1.99	0.43
10:U:30:LEU:HA	10:U:33:TRP:HB3	2.01	0.43
1:L:349:LYS:HD3	1:L:349:LYS:HA	1.84	0.43
10:V:18:LEU:HD13	10:V:18:LEU:HA	1.85	0.43
3:B:332:VAL:HB	3:B:334:SER:H	1.84	0.43
2:C:271:PRO:HG2	2:C:276:LEU:HD23	2.01	0.42
3:B:233:PHE:HB3	3:B:357:GLY:HA2	2.01	0.42
10:V:31:MET:O	10:V:34:GLY:N	2.52	0.42
6:F:101:CYS:CB	6:F:123:CYS:SG	3.06	0.42
9:T:23:ALA:HB2	10:U:39:LEU:HD21	2.02	0.42
12:C:402:8PE:H1A	8:H:55:GLN:HE22	1.84	0.42
13:C:403:9PE:H2B	13:C:403:9PE:H2E	1.69	0.42
10:V:13:LEU:HD12	10:V:13:LEU:HA	1.92	0.42
2:N:160:ASP:OD1	10:V:50:LYS:HB2	2.20	0.42
8:S:41:PHE:C	8:S:43:ASN:H	2.27	0.42
9:I:17:PHE:HD1	9:I:17:PHE:HA	1.75	0.41
2:N:107:ARG:HH21	2:N:314:ARG:HA	1.84	0.41
11:N:406:UQ6:H321	11:N:406:UQ6:H301	1.94	0.41
4:D:62:MET:HE3	4:D:62:MET:HB2	1.94	0.41
2:N:271:PRO:HG2	2:N:276:LEU:HD23	2.01	0.41
11:N:406:UQ6:H251	11:N:406:UQ6:H272	1.82	0.41
9:I:24:GLY:HA2	9:I:27:VAL:HG22	2.01	0.41
2:C:147:ILE:HD13	2:C:147:ILE:HA	1.94	0.41
5:E:164:CYS:HB3	5:E:180:CYS:HG	1.77	0.41
18:O:402:6PH:H38A	18:O:402:6PH:H3B	1.80	0.41
3:M:233:PHE:HB3	3:M:357:GLY:HA2	2.01	0.41
3:M:332:VAL:HB	3:M:334:SER:H	1.84	0.41
10:U:34:GLY:C	10:U:36:ALA:N	2.79	0.41
3:B:312:LYS:HD3	3:B:312:LYS:HA	1.87	0.41
4:D:297:THR:HG21	5:E:42:VAL:HG21	2.02	0.41
5:E:149:ASP:HB3	5:E:152:TRP:HE3	1.86	0.41
2:N:7:ASN:HB3	2:N:10:LEU:HB2	2.03	0.41
2:N:318:PHE:HB3	7:R:36:ALA:HB1	2.03	0.41
1:L:455:MET:O	9:T:14:ASN:ND2	2.54	0.41
5:P:149:ASP:HB3	5:P:152:TRP:HE3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:ASN:HB2	1:A:230:LEU:HB2	2.03	0.41
2:C:7:ASN:HB3	2:C:10:LEU:HB2	2.03	0.41
4:D:306:LYS:HA	4:D:307:PRO:HD3	1.98	0.40
1:L:166:SER:HA	1:L:175:SER:HB2	2.03	0.40
8:H:53:LYS:HA	8:H:53:LYS:HD3	1.95	0.40
7:R:123:ILE:H	10:V:21:ARG:NH2	2.19	0.40
1:A:166:SER:HA	1:A:175:SER:HB2	2.03	0.40
5:P:79:ILE:HD13	5:P:79:ILE:HA	1.96	0.40
10:V:46:GLU:HA	10:V:52:GLN:NE2	2.30	0.40
2:C:318:PHE:HB3	7:G:36:ALA:HB1	2.03	0.40
11:C:401:UQ6:H102	15:C:405:CN5:H35A	2.02	0.40
12:C:402:8PE:H35	12:C:402:8PE:H38A	1.59	0.40
9:I:8:LYS:HA	9:I:12:LYS:HB3	2.03	0.40
9:T:8:LYS:HG2	9:T:12:LYS:HG2	2.03	0.40
10:V:26:TYR:CD2	10:V:30:LEU:HB2	2.56	0.40

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	A	429/431 (100%)	396 (92%)	33 (8%)	0	100	100
1	L	429/431 (100%)	396 (92%)	33 (8%)	0	100	100
2	C	383/385 (100%)	368 (96%)	14 (4%)	1 (0%)	36	56
2	N	383/385 (100%)	369 (96%)	13 (3%)	1 (0%)	36	56
3	B	350/352 (99%)	336 (96%)	14 (4%)	0	100	100
3	M	350/352 (99%)	336 (96%)	14 (4%)	0	100	100
4	D	246/248 (99%)	236 (96%)	10 (4%)	0	100	100
4	O	246/248 (99%)	236 (96%)	10 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	183/185 (99%)	152 (83%)	30 (16%)	1 (0%)	24	44
5	P	183/185 (99%)	154 (84%)	29 (16%)	0	100	100
6	F	72/75 (96%)	68 (94%)	4 (6%)	0	100	100
6	Q	73/75 (97%)	68 (93%)	5 (7%)	0	100	100
7	G	124/126 (98%)	119 (96%)	5 (4%)	0	100	100
7	R	124/126 (98%)	119 (96%)	5 (4%)	0	100	100
8	H	91/93 (98%)	79 (87%)	12 (13%)	0	100	100
8	S	91/93 (98%)	80 (88%)	11 (12%)	0	100	100
9	I	52/55 (94%)	48 (92%)	4 (8%)	0	100	100
9	T	52/55 (94%)	49 (94%)	3 (6%)	0	100	100
10	U	42/52 (81%)	32 (76%)	9 (21%)	1 (2%)	4	8
10	V	49/52 (94%)	36 (74%)	11 (22%)	2 (4%)	2	2
All	All	3952/4004 (99%)	3677 (93%)	269 (7%)	6 (0%)	44	63

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	V	17	ARG
10	V	54	THR
2	N	347	PRO
10	U	35	GLY
2	C	347	PRO
5	E	195	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	370/370 (100%)	363 (98%)	7 (2%)	50	73
1	L	370/370 (100%)	363 (98%)	7 (2%)	50	73
2	C	338/338 (100%)	336 (99%)	2 (1%)	78	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	N	338/338 (100%)	335 (99%)	3 (1%)	70	85
3	B	301/301 (100%)	301 (100%)	0	100	100
3	M	301/301 (100%)	301 (100%)	0	100	100
4	D	206/206 (100%)	205 (100%)	1 (0%)	81	91
4	O	206/206 (100%)	205 (100%)	1 (0%)	81	91
5	E	151/151 (100%)	137 (91%)	14 (9%)	8	18
5	P	151/151 (100%)	137 (91%)	14 (9%)	8	18
6	F	67/68 (98%)	66 (98%)	1 (2%)	57	78
6	Q	68/68 (100%)	68 (100%)	0	100	100
7	G	110/110 (100%)	108 (98%)	2 (2%)	51	74
7	R	110/110 (100%)	108 (98%)	2 (2%)	51	74
8	H	77/77 (100%)	76 (99%)	1 (1%)	61	81
8	S	77/77 (100%)	75 (97%)	2 (3%)	40	66
9	I	44/45 (98%)	42 (96%)	2 (4%)	24	47
9	T	45/45 (100%)	43 (96%)	2 (4%)	25	48
10	U	35/43 (81%)	34 (97%)	1 (3%)	37	63
10	V	42/43 (98%)	39 (93%)	3 (7%)	13	29
All	All	3407/3418 (100%)	3342 (98%)	65 (2%)	49	73

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	GLU
1	A	80	LYS
1	A	94	SER
1	A	235	LYS
1	A	237	VAL
1	A	444	ASP
1	A	457	TRP
2	C	270	VAL
2	C	346	VAL
4	D	63	THR
5	E	31	LYS
5	E	45	GLU
5	E	51	LYS
5	E	81	SER

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Mol	Chain	Res	Type
5	E	103	LEU
5	E	119	ARG
5	E	128	GLU
5	E	139	ASP
5	E	143	ASP
5	E	156	LEU
5	E	167	ILE
5	E	190	ARG
5	E	211	LYS
5	E	214	VAL
2	N	160	ASP
2	N	270	VAL
2	N	346	VAL
6	F	107	ILE
7	G	17	LYS
7	G	100	VAL
8	H	87	GLU
9	I	13	ARG
9	I	17	PHE
1	L	41	GLU
1	L	80	LYS
1	L	94	SER
1	L	235	LYS
1	L	237	VAL
1	L	444	ASP
1	L	457	TRP
4	O	63	THR
8	S	42	HIS
8	S	87	GLU
5	P	31	LYS
5	P	45	GLU
5	P	51	LYS
5	P	81	SER
5	P	103	LEU
5	P	119	ARG
5	P	128	GLU
5	P	139	ASP
5	P	143	ASP
5	P	156	LEU
5	P	167	ILE
5	P	190	ARG
5	P	211	LYS

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Mol	Chain	Res	Type
5	P	214	VAL
7	R	17	LYS
7	R	100	VAL
9	T	13	ARG
9	T	16	VAL
10	U	33	TRP
10	V	18	LEU
10	V	31	MET
10	V	32	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	75	ASN
1	A	122	GLN
1	A	149	GLN
1	A	156	HIS
1	A	170	GLN
1	A	199	ASN
1	A	274	ASN
1	A	283	GLN
1	A	298	GLN
1	A	317	HIS
1	A	350	GLN
1	A	352	ASN
1	A	376	GLN
1	A	388	ASN
2	C	332	ASN
3	B	57	GLN
3	B	58	ASN
3	B	328	GLN
4	D	79	ASN
4	D	127	ASN
4	D	143	ASN
4	D	185	HIS
2	N	73	HIS
2	N	253	HIS
6	F	87	ASN
6	F	96	HIS
7	G	3	GLN
7	G	57	GLN

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Mol	Chain	Res	Type
8	H	21	GLN
9	I	14	ASN
9	I	29	GLN
9	I	44	ASN
1	L	34	ASN
1	L	122	GLN
1	L	149	GLN
1	L	156	HIS
1	L	170	GLN
1	L	199	ASN
1	L	274	ASN
1	L	283	GLN
1	L	298	GLN
1	L	310	GLN
1	L	317	HIS
1	L	350	GLN
1	L	352	ASN
1	L	376	GLN
1	L	388	ASN
4	O	79	ASN
4	O	127	ASN
4	O	185	HIS
3	M	57	GLN
3	M	58	ASN
3	M	328	GLN
8	S	21	GLN
6	Q	87	ASN
7	R	3	GLN
7	R	85	HIS
9	T	14	ASN
10	U	14	HIS
10	V	52	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

18 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$
11	UQ6	C	401	-	43,43,43	1.60	8 (18%)	54,55,55	1.51	10 (18%)
14	HEM	C	408	2	50,50,50	1.36	6 (12%)	67,82,82	1.11	3 (4%)
13	9PE	N	403	-	39,39,39	0.95	4 (10%)	42,44,44	1.12	2 (4%)
16	86T	N	401	-	31,31,31	0.59	0	37,44,44	2.08	4 (10%)
17	CN3	N	402	-	54,54,54	1.18	7 (12%)	60,66,66	1.26	4 (6%)
14	HEM	C	404	2	50,50,50	1.47	9 (18%)	67,82,82	1.61	11 (16%)
11	UQ6	N	406	-	43,43,43	1.70	12 (27%)	54,55,55	1.46	9 (16%)
14	HEM	D	401	4	50,50,50	1.29	6 (12%)	67,82,82	1.17	3 (4%)
18	6PH	O	402	-	39,39,39	0.95	3 (7%)	42,44,44	1.18	2 (4%)
14	HEM	N	404	2	50,50,50	1.49	9 (18%)	67,82,82	1.63	12 (17%)
12	8PE	S	101	-	46,46,46	0.92	4 (8%)	49,51,51	1.08	2 (4%)
15	CN5	C	405	-	40,40,40	0.35	0	44,48,48	0.43	0
13	9PE	C	403	-	39,39,39	0.94	4 (10%)	42,44,44	1.03	2 (4%)
16	86T	C	406	-	31,31,31	0.58	0	37,44,44	2.08	4 (10%)
14	HEM	O	401	4	50,50,50	1.36	6 (12%)	67,82,82	1.38	10 (14%)
12	8PE	C	402	-	46,46,46	0.51	0	49,51,51	0.50	0
14	HEM	N	405	2	50,50,50	1.40	6 (12%)	67,82,82	1.17	3 (4%)
17	CN3	C	407	-	54,54,54	1.17	8 (14%)	60,66,66	1.18	4 (6%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	UQ6	C	401	-	-	6/39/39/39	0/1/1/1
14	HEM	C	408	2	-	3/14/54/54	-
13	9PE	N	403	-	-	23/43/43/43	-
16	86T	N	401	-	-	0/13/13/13	0/4/4/4
17	CN3	N	402	-	-	36/65/65/65	-
14	HEM	C	404	2	-	3/14/54/54	-
11	UQ6	N	406	-	-	13/39/39/39	0/1/1/1
14	HEM	D	401	4	-	0/14/54/54	-
18	6PH	O	402	-	-	26/41/41/41	-
14	HEM	N	404	2	-	5/14/54/54	-
12	8PE	S	101	-	-	16/50/50/50	-
15	CN5	C	405	-	-	26/44/44/44	-
13	9PE	C	403	-	-	18/43/43/43	-
16	86T	C	406	-	-	0/13/13/13	0/4/4/4
14	HEM	O	401	4	-	2/14/54/54	-
12	8PE	C	402	-	-	31/50/50/50	-
14	HEM	N	405	2	-	4/14/54/54	-
17	CN3	C	407	-	-	25/65/65/65	-

All (92) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	N	406	UQ6	C7-C6	5.15	1.57	1.51
11	C	401	UQ6	C7-C6	4.68	1.56	1.51
14	C	404	HEM	FE-ND	4.04	2.07	1.94
14	N	404	HEM	FE-ND	3.76	2.06	1.94
11	N	406	UQ6	C16-C14	3.73	1.59	1.51
14	C	408	HEM	FE-ND	3.64	2.06	1.94
14	N	405	HEM	FE-ND	3.61	2.06	1.94
14	N	404	HEM	FE-NC	3.45	2.06	1.95
14	C	404	HEM	FE-NB	3.40	2.05	1.94
11	C	401	UQ6	C16-C14	3.38	1.58	1.51
14	O	401	HEM	FE-NB	3.30	2.05	1.94
14	N	404	HEM	FE-NB	3.25	2.04	1.94
14	N	405	HEM	CAB-C3B	3.22	1.56	1.47
14	C	408	HEM	CAB-C3B	3.20	1.55	1.47
14	N	405	HEM	FE-NC	3.08	2.05	1.95
14	D	401	HEM	CAC-C3C	3.07	1.55	1.47
14	C	404	HEM	CAB-C3B	3.07	1.55	1.47
14	N	404	HEM	CAB-C3B	3.07	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	C	408	HEM	CAC-C3C	3.04	1.55	1.47
14	N	405	HEM	CAC-C3C	3.02	1.55	1.47
14	N	405	HEM	FE-NA	2.99	2.05	1.95
14	O	401	HEM	CAC-C3C	2.99	1.55	1.47
12	S	101	8PE	O21-C2	-2.98	1.39	1.46
17	N	402	CN3	O21-C2	-2.94	1.39	1.46
14	D	401	HEM	CAB-C3B	2.90	1.55	1.47
14	C	408	HEM	FE-NC	2.89	2.04	1.95
11	N	406	UQ6	C12-C13	2.85	1.59	1.50
14	O	401	HEM	FE-NA	2.83	2.04	1.95
14	C	404	HEM	CAC-C3C	2.81	1.54	1.47
14	C	404	HEM	FE-NC	2.80	2.04	1.95
14	O	401	HEM	CAB-C3B	2.79	1.54	1.47
17	C	407	CN3	O21-C2	-2.75	1.40	1.46
11	C	401	UQ6	O3-C3	2.74	1.43	1.38
18	O	402	6PH	O21-C2	-2.72	1.40	1.46
17	N	402	CN3	O51-C2'	-2.69	1.40	1.46
11	N	406	UQ6	C11-C9	2.68	1.56	1.51
17	C	407	CN3	O51-C2'	-2.64	1.40	1.46
11	C	401	UQ6	C12-C13	2.60	1.58	1.50
14	D	401	HEM	FE-NB	2.59	2.02	1.94
14	N	404	HEM	CAC-C3C	2.59	1.54	1.47
14	C	408	HEM	FE-NA	2.58	2.03	1.95
11	N	406	UQ6	C7-C8	2.58	1.56	1.50
17	C	407	CN3	O41-C3'	-2.52	1.39	1.45
14	D	401	HEM	FE-NA	2.46	2.03	1.95
11	C	401	UQ6	C7-C8	2.45	1.56	1.50
12	S	101	8PE	O31-C3	-2.42	1.39	1.45
11	C	401	UQ6	C11-C9	2.42	1.56	1.51
11	N	406	UQ6	O3-C3	2.42	1.42	1.38
17	C	407	CN3	O31-C3	-2.39	1.39	1.45
14	N	404	HEM	FE-NA	2.38	2.03	1.95
17	N	402	CN3	O31-C3	-2.38	1.39	1.45
11	N	406	UQ6	C17-C18	2.35	1.57	1.50
13	N	403	9PE	O31-C31	2.34	1.40	1.33
18	O	402	6PH	O31-C31	2.32	1.40	1.33
17	C	407	CN3	O51-C51	2.31	1.40	1.34
14	N	405	HEM	C2A-C3A	-2.30	1.32	1.38
17	N	402	CN3	O41-C3'	-2.29	1.40	1.45
14	C	404	HEM	C2A-C3A	-2.27	1.33	1.38
17	N	402	CN3	O41-C41	2.27	1.40	1.33
13	C	403	9PE	O21-C21	2.27	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	404	HEM	C2A-C3A	-2.26	1.33	1.38
12	S	101	8PE	O31-C31	2.26	1.39	1.33
17	C	407	CN3	O41-C41	2.26	1.39	1.33
18	O	402	6PH	O31-C3	-2.26	1.40	1.45
14	N	404	HEM	C3C-C2C	-2.25	1.32	1.37
13	N	403	9PE	O21-C21	2.25	1.40	1.34
13	N	403	9PE	O21-C2	-2.25	1.41	1.46
17	N	402	CN3	O31-C31	2.25	1.39	1.33
11	N	406	UQ6	C26-C24	2.23	1.55	1.51
13	C	403	9PE	O21-C2	-2.20	1.41	1.46
13	C	403	9PE	O31-C31	2.20	1.39	1.33
17	N	402	CN3	O51-C51	2.20	1.40	1.34
11	C	401	UQ6	C17-C18	2.19	1.57	1.50
13	C	403	9PE	O31-C3	-2.18	1.40	1.45
17	C	407	CN3	O31-C31	2.18	1.39	1.33
11	N	406	UQ6	C31-C29	2.18	1.55	1.51
13	N	403	9PE	O31-C3	-2.16	1.40	1.45
11	N	406	UQ6	C21-C19	2.15	1.55	1.51
14	C	408	HEM	C2A-C3A	-2.14	1.33	1.38
17	C	407	CN3	O21-C21	2.12	1.40	1.34
14	D	401	HEM	C2A-C3A	-2.11	1.33	1.38
11	C	401	UQ6	C26-C24	2.10	1.55	1.51
14	O	401	HEM	C2A-C3A	-2.09	1.33	1.38
14	C	404	HEM	CMC-C2C	2.09	1.55	1.50
14	C	404	HEM	FE-NA	2.09	2.02	1.95
12	S	101	8PE	O21-C21	2.08	1.40	1.34
14	N	404	HEM	CMB-C2B	2.07	1.55	1.50
11	N	406	UQ6	O4-C4	2.07	1.42	1.38
11	N	406	UQ6	C22-C23	2.06	1.56	1.50
14	D	401	HEM	CMC-C2C	2.04	1.55	1.50
14	O	401	HEM	C3C-C2C	-2.01	1.33	1.37
14	C	404	HEM	CMB-C2B	2.01	1.54	1.50

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	C	406	86T	N22-C23-N24	9.78	105.93	101.46
16	N	401	86T	N22-C23-N24	9.73	105.90	101.46
14	C	404	HEM	CAD-C3D-C4D	5.76	134.73	124.70
14	N	404	HEM	CAD-C3D-C4D	5.36	134.03	124.70
14	C	404	HEM	CAD-C3D-C2D	-5.07	118.37	127.87
11	C	401	UQ6	C7-C8-C9	-4.89	120.41	127.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	404	HEM	CAD-C3D-C2D	-4.72	119.03	127.87
16	N	401	86T	C05-N07-C12	-4.39	122.78	129.12
16	C	406	86T	C05-N07-C12	-4.39	122.78	129.12
17	N	402	CN3	O21-C21-C22	3.96	120.06	111.48
17	C	407	CN3	O51-C51-C52	3.96	120.04	111.48
17	N	402	CN3	O51-C51-C52	3.93	119.98	111.48
18	O	402	6PH	O21-C21-C22	3.88	119.88	111.48
17	C	407	CN3	O21-C21-C22	3.74	119.58	111.48
16	N	401	86T	C23-N22-N26	-3.69	108.08	110.53
16	C	406	86T	C23-N22-N26	-3.68	108.09	110.53
14	O	401	HEM	C3B-C2B-C1B	3.51	109.04	106.41
12	S	101	8PE	O21-C21-C22	3.40	118.83	111.48
13	N	403	9PE	O21-C21-C22	3.36	118.75	111.48
13	C	403	9PE	O21-C21-C22	3.27	118.55	111.48
17	N	402	CN3	O31-C31-C32	3.23	120.95	111.15
14	C	404	HEM	CHA-C4D-C3D	3.14	131.02	125.23
11	C	401	UQ6	C12-C13-C14	-3.11	120.50	127.62
11	N	406	UQ6	C10-C9-C11	2.97	120.39	115.23
14	N	404	HEM	CBD-CAD-C3D	2.94	120.67	112.53
14	D	401	HEM	CAA-CBA-CGA	-2.94	105.86	113.67
17	C	407	CN3	O31-C31-C32	2.94	120.07	111.15
11	N	406	UQ6	C15-C14-C16	2.91	120.28	115.23
14	O	401	HEM	C3B-C4B-NB	-2.91	107.38	109.47
11	C	401	UQ6	C17-C18-C19	-2.90	120.98	127.62
14	D	401	HEM	CMB-C2B-C1B	-2.90	120.50	125.03
14	N	404	HEM	CHA-C4D-C3D	2.89	130.55	125.23
18	O	402	6PH	O31-C31-C32	2.89	120.64	111.83
14	O	401	HEM	CAA-CBA-CGA	-2.87	106.06	113.67
14	C	404	HEM	CBD-CAD-C3D	2.85	120.42	112.53
13	N	403	9PE	O31-C31-C32	2.85	120.52	111.83
16	C	406	86T	C05-N07-N09	2.83	125.92	121.08
11	N	406	UQ6	C27-C28-C29	-2.83	121.15	127.62
16	N	401	86T	C05-N07-N09	2.82	125.90	121.08
11	N	406	UQ6	C30-C29-C31	2.82	120.11	115.23
12	S	101	8PE	O31-C31-C32	2.77	120.28	111.83
11	C	401	UQ6	C22-C23-C24	-2.77	121.28	127.62
11	N	406	UQ6	C2-C1-C6	2.77	121.93	118.59
11	N	406	UQ6	C22-C23-C24	-2.75	121.33	127.62
14	C	408	HEM	CMB-C2B-C1B	-2.70	120.81	125.03
14	O	401	HEM	CHB-C1B-NB	2.70	127.70	124.37
14	O	401	HEM	CAC-C3C-C4C	2.69	131.24	124.82
11	N	406	UQ6	C17-C18-C19	-2.68	121.48	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	C	404	HEM	CHD-C1D-ND	2.65	127.28	124.42
14	O	401	HEM	C3C-C2C-C1C	2.64	109.54	107.05
11	C	401	UQ6	C20-C19-C21	2.64	119.80	115.23
14	N	404	HEM	CAC-C3C-C4C	2.62	131.08	124.82
14	N	405	HEM	CMB-C2B-C1B	-2.60	120.97	125.03
11	C	401	UQ6	C25-C24-C26	2.60	119.74	115.23
11	N	406	UQ6	C25-C24-C26	2.60	119.74	115.23
14	N	405	HEM	CAA-C2A-C1A	2.59	129.99	124.94
14	C	404	HEM	C2A-C1A-NA	-2.55	107.32	110.15
14	D	401	HEM	CAC-C3C-C4C	-2.52	118.81	124.82
14	N	404	HEM	CHD-C1D-ND	2.51	127.12	124.42
17	C	407	CN3	O41-C41-C42	2.50	119.46	111.83
17	N	402	CN3	O41-C41-C42	2.50	119.45	111.83
14	N	404	HEM	C2A-C1A-NA	-2.49	107.39	110.15
14	C	404	HEM	C4D-ND-C1D	2.43	108.08	105.21
14	C	404	HEM	C3D-C4D-ND	-2.43	107.51	110.17
11	C	401	UQ6	C10-C9-C11	2.42	119.43	115.23
14	O	401	HEM	C1B-NB-C4B	2.41	108.06	105.21
14	N	404	HEM	CAC-C3C-C2C	-2.40	120.62	128.43
14	C	408	HEM	C4D-ND-C1D	2.39	108.04	105.21
14	O	401	HEM	CHC-C1C-NC	2.38	127.05	124.45
14	N	404	HEM	CHD-C4C-C3C	2.37	129.21	125.21
14	C	404	HEM	CHA-C4D-ND	-2.34	121.47	124.37
11	C	401	UQ6	C15-C14-C16	2.33	119.28	115.23
11	C	401	UQ6	C36-C34-C35	2.29	119.87	114.59
14	C	404	HEM	C1D-C2D-C3D	2.20	109.30	106.98
14	O	401	HEM	CAC-C3C-C2C	-2.19	121.30	128.43
14	N	404	HEM	C4D-ND-C1D	2.19	107.80	105.21
14	N	404	HEM	C3D-C4D-ND	-2.18	107.78	110.17
14	N	404	HEM	CHA-C4D-ND	-2.18	121.67	124.37
14	C	408	HEM	C3D-C4D-ND	-2.15	107.82	110.17
11	C	401	UQ6	C30-C29-C31	2.14	118.95	115.23
14	O	401	HEM	CAB-C3B-C2B	-2.14	121.49	128.43
14	N	405	HEM	C4D-ND-C1D	2.13	107.72	105.21
13	C	403	9PE	O31-C31-C32	2.10	118.24	111.83
11	N	406	UQ6	C12-C13-C14	-2.06	122.92	127.62
14	C	404	HEM	CHD-C4C-NC	2.05	126.68	124.45

There are no chirality outliers.

All (237) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	C	401	UQ6	C9-C11-C12-C13
11	N	406	UQ6	C1-C6-C7-C8
11	N	406	UQ6	C25-C24-C26-C27
11	N	406	UQ6	C28-C29-C31-C32
11	N	406	UQ6	C30-C29-C31-C32
12	C	402	8PE	C1-O11-P-O13
12	C	402	8PE	C1-O11-P-O14
12	C	402	8PE	C11-O13-P-O11
12	C	402	8PE	C11-O13-P-O12
12	C	402	8PE	C11-O13-P-O14
12	C	402	8PE	O11-C1-C2-O21
12	C	402	8PE	O22-C21-O21-C2
12	S	101	8PE	C1-O11-P-O12
12	S	101	8PE	C1-O11-P-O13
12	S	101	8PE	C11-O13-P-O11
13	C	403	9PE	C1-O11-P-O12
13	C	403	9PE	C1-O11-P-O13
13	C	403	9PE	C1-O11-P-O14
13	C	403	9PE	O13-C11-C12-N
13	N	403	9PE	C11-O13-P-O11
13	N	403	9PE	C11-O13-P-O14
14	C	404	HEM	C2D-C3D-CAD-CBD
14	C	404	HEM	C4D-C3D-CAD-CBD
14	N	404	HEM	C2D-C3D-CAD-CBD
14	N	404	HEM	C4D-C3D-CAD-CBD
15	C	405	CN5	C1-O11-P-O14
15	C	405	CN5	CC-O13-P-O11
15	C	405	CN5	C2-C1-O11-P
15	C	405	CN5	C1'-O1'-P'-O3'
15	C	405	CN5	C1'-O1'-P'-O4'
15	C	405	CN5	CB-CA-O3'-P'
17	C	407	CN3	CC-O13-P-O11
17	C	407	CN3	CC-O13-P-O12
17	C	407	CN3	O3'-CA-CB-OA
17	C	407	CN3	O3'-CA-CB-CC
17	N	402	CN3	C1-O11-P-O12
17	N	402	CN3	C1-O11-P-O13
17	N	402	CN3	C1-O11-P-O14
17	N	402	CN3	CC-O13-P-O11
17	N	402	CN3	CC-O13-P-O12
17	N	402	CN3	C1'-O1'-P'-O2'
17	N	402	CN3	C1'-O1'-P'-O3'
17	N	402	CN3	C1'-O1'-P'-O4'

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Mol	Chain	Res	Type	Atoms
17	N	402	CN3	CA-O3'-P'-O1'
17	N	402	CN3	CA-O3'-P'-O2'
17	N	402	CN3	O3'-CA-CB-CC
18	O	402	6PH	C1-O11-P-O13
18	O	402	6PH	C1-O11-P-O14
12	S	101	8PE	C32-C31-O31-C3
12	S	101	8PE	O32-C31-O31-C3
13	N	403	9PE	O32-C31-O31-C3
13	N	403	9PE	O22-C21-O21-C2
13	N	403	9PE	C32-C31-O31-C3
12	C	402	8PE	C22-C21-O21-C2
11	C	401	UQ6	C12-C11-C9-C10
11	C	401	UQ6	C12-C11-C9-C8
11	N	406	UQ6	C23-C24-C26-C27
15	C	405	CN5	C42-C41-O41-C3'
17	N	402	CN3	O3'-CA-CB-OA
13	C	403	9PE	C22-C21-O21-C2
13	N	403	9PE	C22-C21-O21-C2
13	C	403	9PE	O22-C21-O21-C2
11	C	401	UQ6	C19-C21-C22-C23
11	N	406	UQ6	C9-C11-C12-C13
12	C	402	8PE	C3B-C3C-C3D-C3E
18	O	402	6PH	C32-C31-O31-C3
17	N	402	CN3	C32-C31-O31-C3
15	C	405	CN5	C3A-C3B-C3C-C3D
11	N	406	UQ6	C15-C14-C16-C17
11	N	406	UQ6	C13-C14-C16-C17
15	C	405	CN5	O11-C1-C2-C3
17	C	407	CN3	O51-C2'-C3'-O41
17	C	407	CN3	C42-C41-O41-C3'
15	C	405	CN5	C31-C32-C33-C34
15	C	405	CN5	O42-C41-O41-C3'
18	O	402	6PH	C31-C32-C33-C34
11	N	406	UQ6	C19-C21-C22-C23
17	N	402	CN3	C51-C52-C53-C54
17	N	402	CN3	O32-C31-O31-C3
12	C	402	8PE	C35-C36-C37-C38
15	C	405	CN5	C1-C2-C3-O31
18	O	402	6PH	O32-C31-O31-C3
15	C	405	CN5	C32-C31-O31-C3
17	N	402	CN3	C22-C21-O21-C2
11	N	406	UQ6	C14-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
12	C	402	8PE	C31-C32-C33-C34
14	N	405	HEM	C1A-C2A-CAA-CBA
17	C	407	CN3	O42-C41-O41-C3'
17	N	402	CN3	C52-C51-O51-C2'
15	C	405	CN5	O32-C31-O31-C3
17	N	402	CN3	C52-C53-C54-C55
18	O	402	6PH	C23-C24-C25-C26
15	C	405	CN5	C39-C3A-C3B-C3C
18	O	402	6PH	C26-C27-C28-C29
12	C	402	8PE	C38-C39-C3A-C3B
12	C	402	8PE	C34-C35-C36-C37
17	N	402	CN3	O22-C21-O21-C2
17	N	402	CN3	C41-C42-C43-C44
12	S	101	8PE	C36-C37-C38-C39
13	C	403	9PE	C2E-C2F-C2G-C2H
15	C	405	CN5	C34-C35-C36-C37
12	C	402	8PE	C27-C28-C29-C2A
17	C	407	CN3	C51-C52-C53-C54
12	C	402	8PE	C22-C23-C24-C25
12	C	402	8PE	C2A-C2B-C2C-C2D
18	O	402	6PH	C25-C26-C27-C28
17	N	402	CN3	O52-C51-O51-C2'
11	N	406	UQ6	C12-C11-C9-C8
13	N	403	9PE	C2D-C2E-C2F-C2G
15	C	405	CN5	C33-C34-C35-C36
12	C	402	8PE	C23-C24-C25-C26
12	S	101	8PE	C38-C39-C3A-C3B
12	S	101	8PE	C3A-C3B-C3C-C3D
18	O	402	6PH	C33-C34-C35-C36
12	S	101	8PE	C3E-C3F-C3G-C3H
12	C	402	8PE	C21-C22-C23-C24
15	C	405	CN5	C32-C33-C34-C35
12	S	101	8PE	C35-C36-C37-C38
11	N	406	UQ6	C12-C11-C9-C10
18	O	402	6PH	C36-C37-C38-C39
15	C	405	CN5	C3C-C3D-C3E-C3F
14	N	404	HEM	C4C-C3C-CAC-CBC
13	N	403	9PE	C2E-C2F-C2G-C2H
18	O	402	6PH	C22-C23-C24-C25
13	C	403	9PE	C24-C25-C26-C27
18	O	402	6PH	C27-C28-C29-C2A
18	O	402	6PH	C37-C38-C39-C3A

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Mol	Chain	Res	Type	Atoms
17	C	407	CN3	C47-C48-C49-C4A
13	N	403	9PE	C26-C27-C28-C29
17	C	407	CN3	C32-C31-O31-C3
13	N	403	9PE	C1-C2-C3-O31
17	C	407	CN3	C1'-C2'-C3'-O41
12	S	101	8PE	C28-C29-C2A-C2B
15	C	405	CN5	O1'-C1'-C2'-C3'
18	O	402	6PH	C24-C25-C26-C27
18	O	402	6PH	C1-O11-P-O12
13	C	403	9PE	C28-C29-C2A-C2B
13	N	403	9PE	C3-C2-O21-C21
12	C	402	8PE	C24-C25-C26-C27
12	C	402	8PE	C3C-C3D-C3E-C3F
17	C	407	CN3	C43-C44-C45-C46
17	N	402	CN3	C42-C43-C44-C45
18	O	402	6PH	C35-C36-C37-C38
18	O	402	6PH	C29-C2A-C2B-C2C
12	C	402	8PE	C29-C2A-C2B-C2C
13	N	403	9PE	C21-C22-C23-C24
17	C	407	CN3	C45-C46-C47-C48
12	S	101	8PE	O11-C1-C2-C3
13	C	403	9PE	O11-C1-C2-C3
13	N	403	9PE	O11-C1-C2-C3
17	C	407	CN3	O32-C31-O31-C3
12	C	402	8PE	C39-C3A-C3B-C3C
13	N	403	9PE	C25-C26-C27-C28
17	N	402	CN3	C56-C57-C58-C59
13	C	403	9PE	C23-C24-C25-C26
17	C	407	CN3	C1-C2-C3-O31
17	N	402	CN3	C1'-C2'-C3'-O41
18	O	402	6PH	C32-C33-C34-C35
18	O	402	6PH	O11-C1-C2-O21
15	C	405	CN5	C1'-C2'-C3'-O41
17	N	402	CN3	O51-C2'-C3'-O41
13	C	403	9PE	C31-C32-C33-C34
11	C	401	UQ6	C24-C26-C27-C28
17	C	407	CN3	O51-C51-C52-C53
12	C	402	8PE	O11-C1-C2-C3
18	O	402	6PH	O11-C1-C2-C3
14	N	405	HEM	C3A-C2A-CAA-CBA
13	N	403	9PE	C2A-C2B-C2C-C2D
15	C	405	CN5	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
18	O	402	6PH	C22-C21-O21-C2
13	N	403	9PE	C24-C25-C26-C27
13	C	403	9PE	C3-C2-O21-C21
13	N	403	9PE	C29-C2A-C2B-C2C
13	C	403	9PE	O11-C1-C2-O21
13	N	403	9PE	O11-C1-C2-O21
12	C	402	8PE	C32-C33-C34-C35
14	O	401	HEM	C4C-C3C-CAC-CBC
17	C	407	CN3	C52-C53-C54-C55
17	N	402	CN3	C55-C56-C57-C58
11	N	406	UQ6	C5-C6-C7-C8
18	O	402	6PH	C2A-C2B-C2C-C2D
17	N	402	CN3	C2-C1-O11-P
18	O	402	6PH	O22-C21-O21-C2
12	S	101	8PE	O11-C1-C2-O21
13	C	403	9PE	C2A-C2B-C2C-C2D
17	N	402	CN3	C45-C46-C47-C48
13	N	403	9PE	O21-C2-C3-O31
17	C	407	CN3	O21-C2-C3-O31
17	C	407	CN3	C42-C43-C44-C45
18	O	402	6PH	C34-C35-C36-C37
12	C	402	8PE	C1-O11-P-O12
12	C	402	8PE	O13-C11-C12-N
13	N	403	9PE	C11-O13-P-O12
15	C	405	CN5	C1-O11-P-O13
15	C	405	CN5	CC-O13-P-O14
17	N	402	CN3	CC-O13-P-O14
17	N	402	CN3	CA-O3'-P'-O4'
17	C	407	CN3	C41-C42-C43-C44
17	N	402	CN3	O42-C41-O41-C3'
17	N	402	CN3	C46-C47-C48-C49
12	C	402	8PE	C2B-C2C-C2D-C2E
15	C	405	CN5	C38-C39-C3A-C3B
15	C	405	CN5	C3B-C3C-C3D-C3E
17	N	402	CN3	C42-C41-O41-C3'
12	S	101	8PE	C34-C35-C36-C37
18	O	402	6PH	O21-C2-C3-O31
13	N	403	9PE	C28-C29-C2A-C2B
13	N	403	9PE	C2F-C2G-C2H-C2I
13	C	403	9PE	C32-C33-C34-C35
17	C	407	CN3	C44-C45-C46-C47
17	C	407	CN3	C2-C1-O11-P

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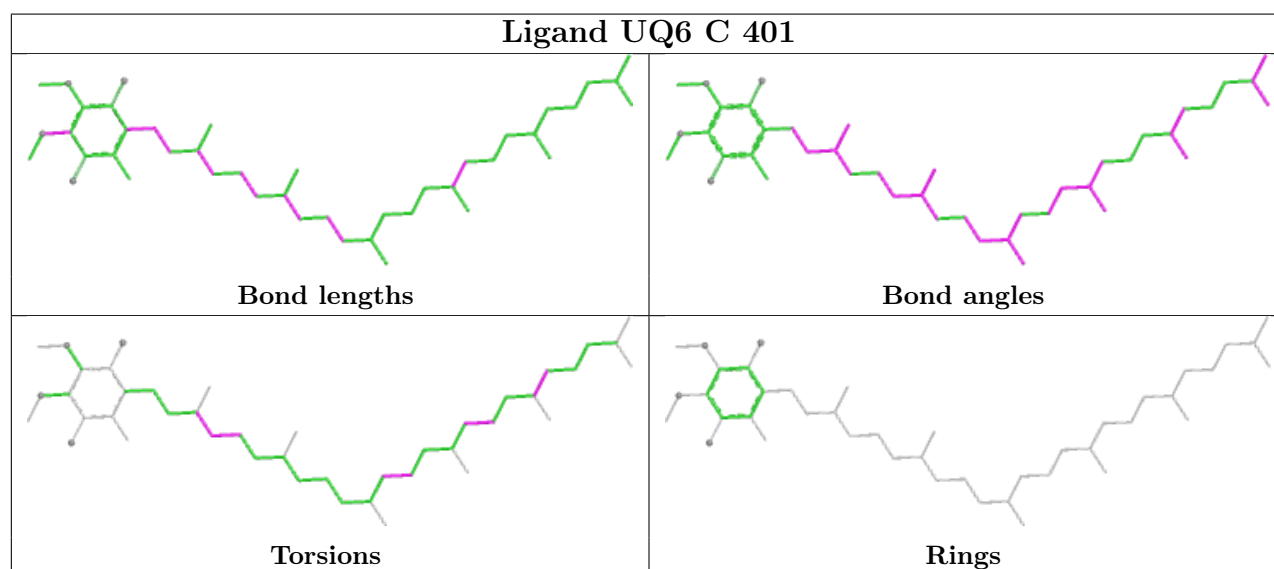
Mol	Chain	Res	Type	Atoms
12	C	402	8PE	C3F-C3G-C3H-C3I
11	C	401	UQ6	C30-C29-C31-C32
14	N	405	HEM	CAA-CBA-CGA-O1A
12	C	402	8PE	C36-C37-C38-C39
17	N	402	CN3	C53-C54-C55-C56
12	S	101	8PE	O21-C2-C3-O31
17	C	407	CN3	O41-C41-C42-C43
17	C	407	CN3	O52-C51-C52-C53
13	C	403	9PE	O31-C31-C32-C33
14	N	405	HEM	CAA-CBA-CGA-O2A
14	C	408	HEM	CAA-CBA-CGA-O2A
17	N	402	CN3	O41-C41-C42-C43
12	C	402	8PE	O21-C2-C3-O31
12	S	101	8PE	C37-C38-C39-C3A
14	C	404	HEM	CAA-CBA-CGA-O1A
14	O	401	HEM	CAA-CBA-CGA-O1A
14	C	408	HEM	CAA-CBA-CGA-O1A
14	C	408	HEM	CAD-CBD-CGD-O2D
13	N	403	9PE	C23-C24-C25-C26
18	O	402	6PH	C38-C39-C3A-C3B
17	C	407	CN3	O42-C41-C42-C43
17	N	402	CN3	O42-C41-C42-C43
13	C	403	9PE	C2B-C2C-C2D-C2E
14	N	404	HEM	CAD-CBD-CGD-O1D
14	N	404	HEM	CAD-CBD-CGD-O2D
12	C	402	8PE	C3E-C3F-C3G-C3H

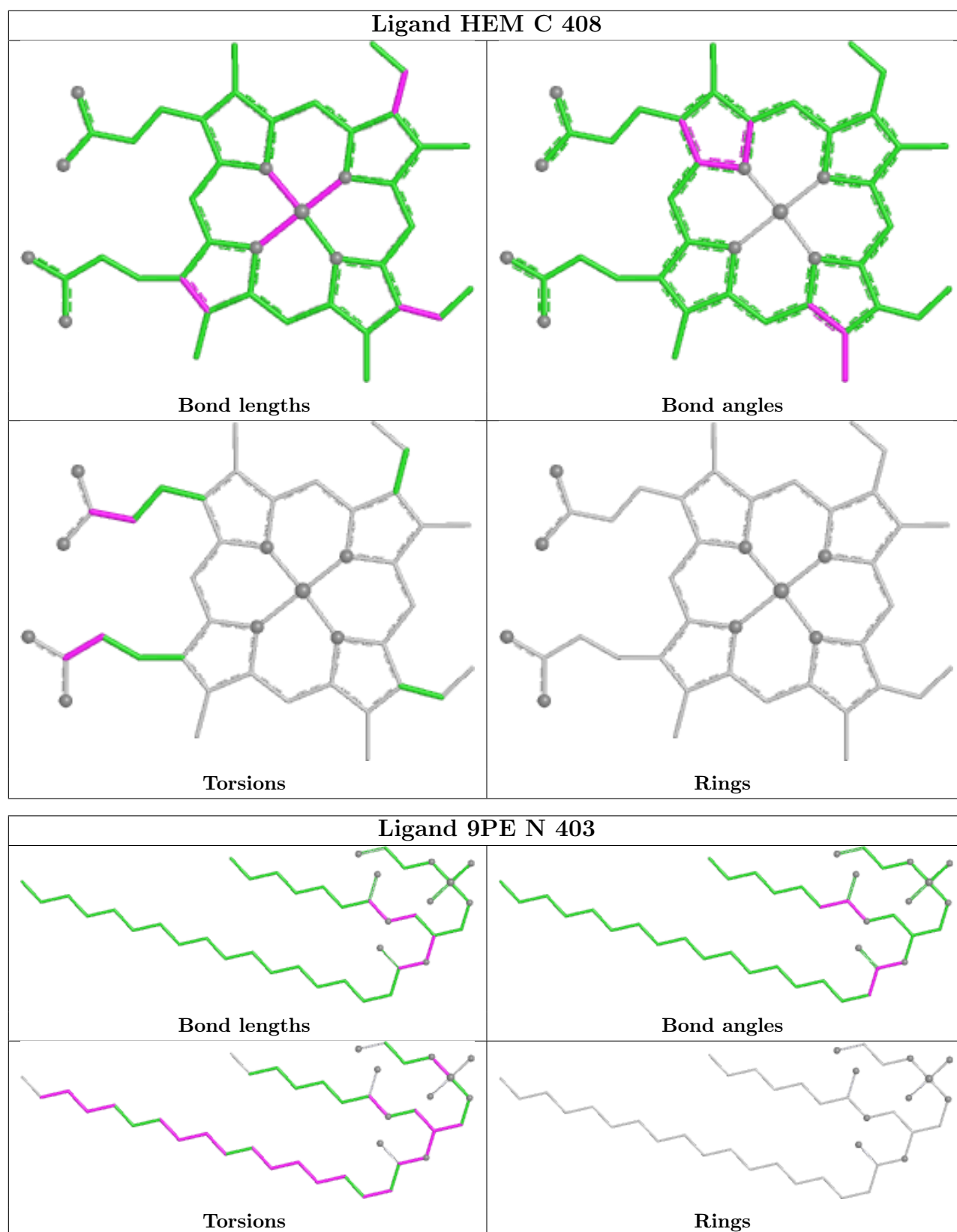
There are no ring outliers.

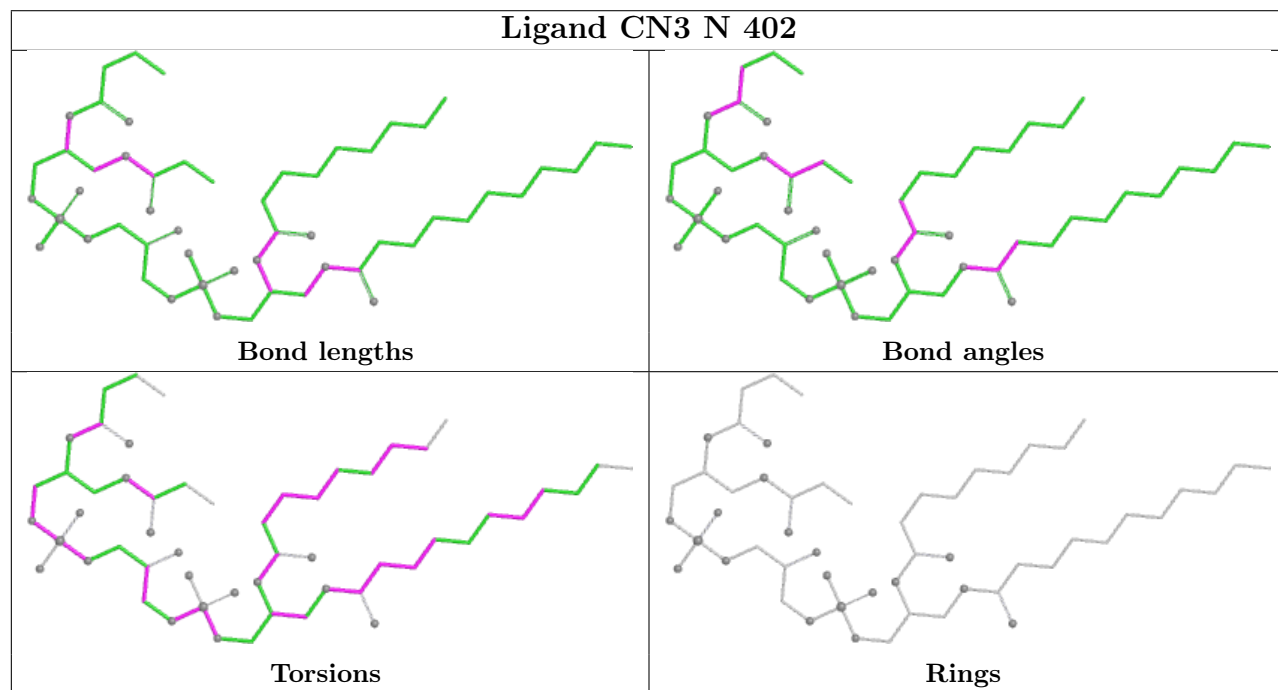
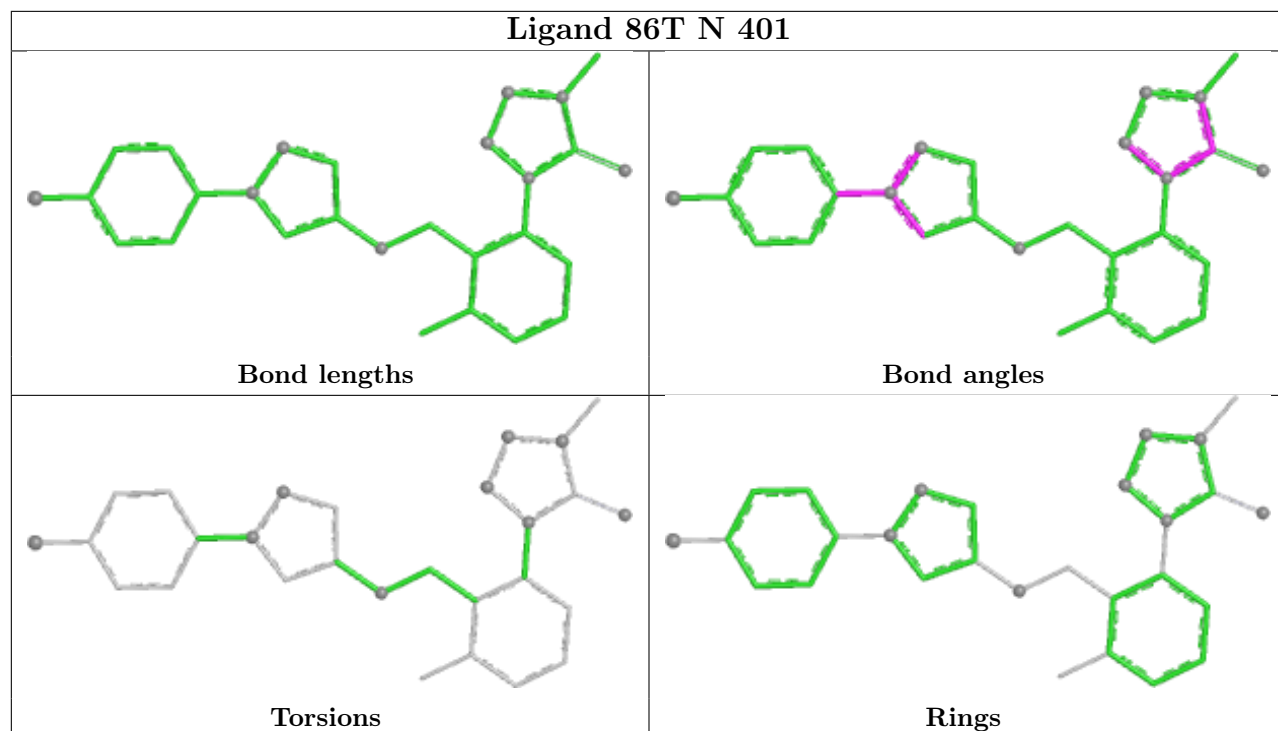
10 monomers are involved in 20 short contacts:

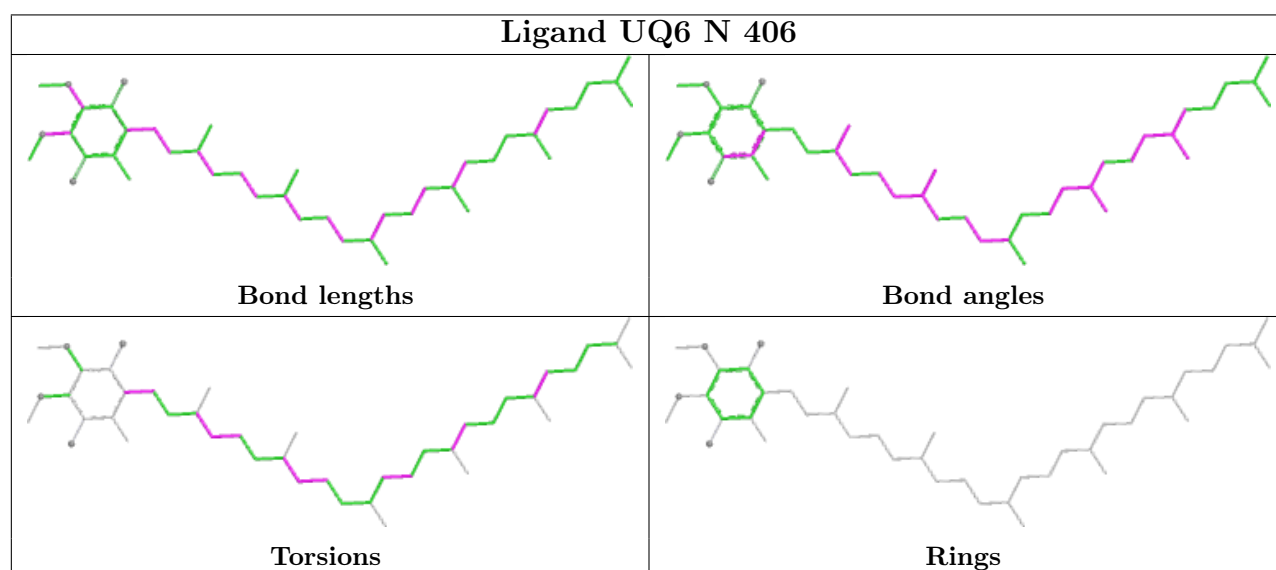
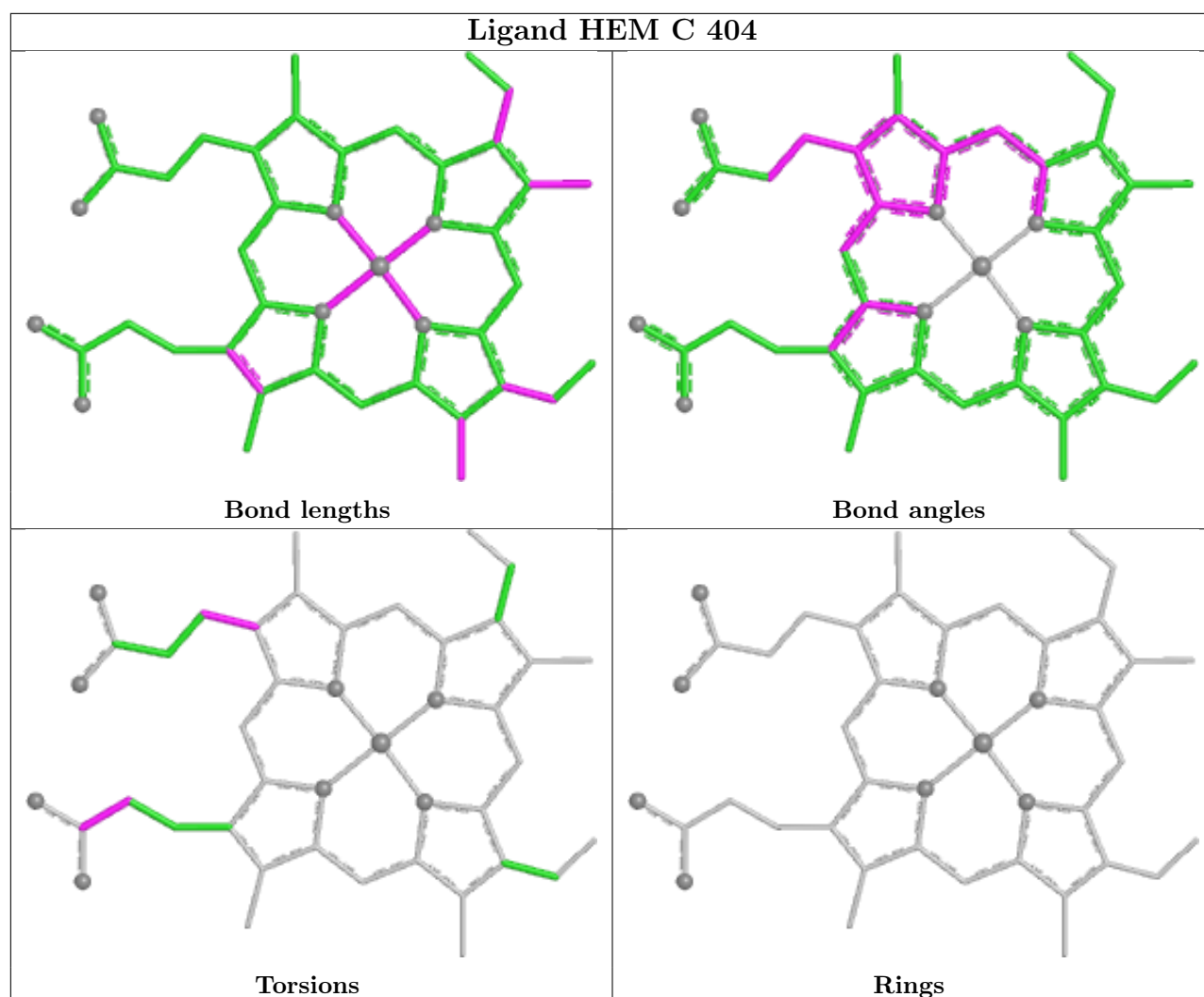
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	C	401	UQ6	4	0
13	N	403	9PE	1	0
11	N	406	UQ6	4	0
18	O	402	6PH	2	0
14	N	404	HEM	2	0
12	S	101	8PE	1	0
15	C	405	CN5	4	0
13	C	403	9PE	1	0
14	O	401	HEM	1	0
12	C	402	8PE	3	0

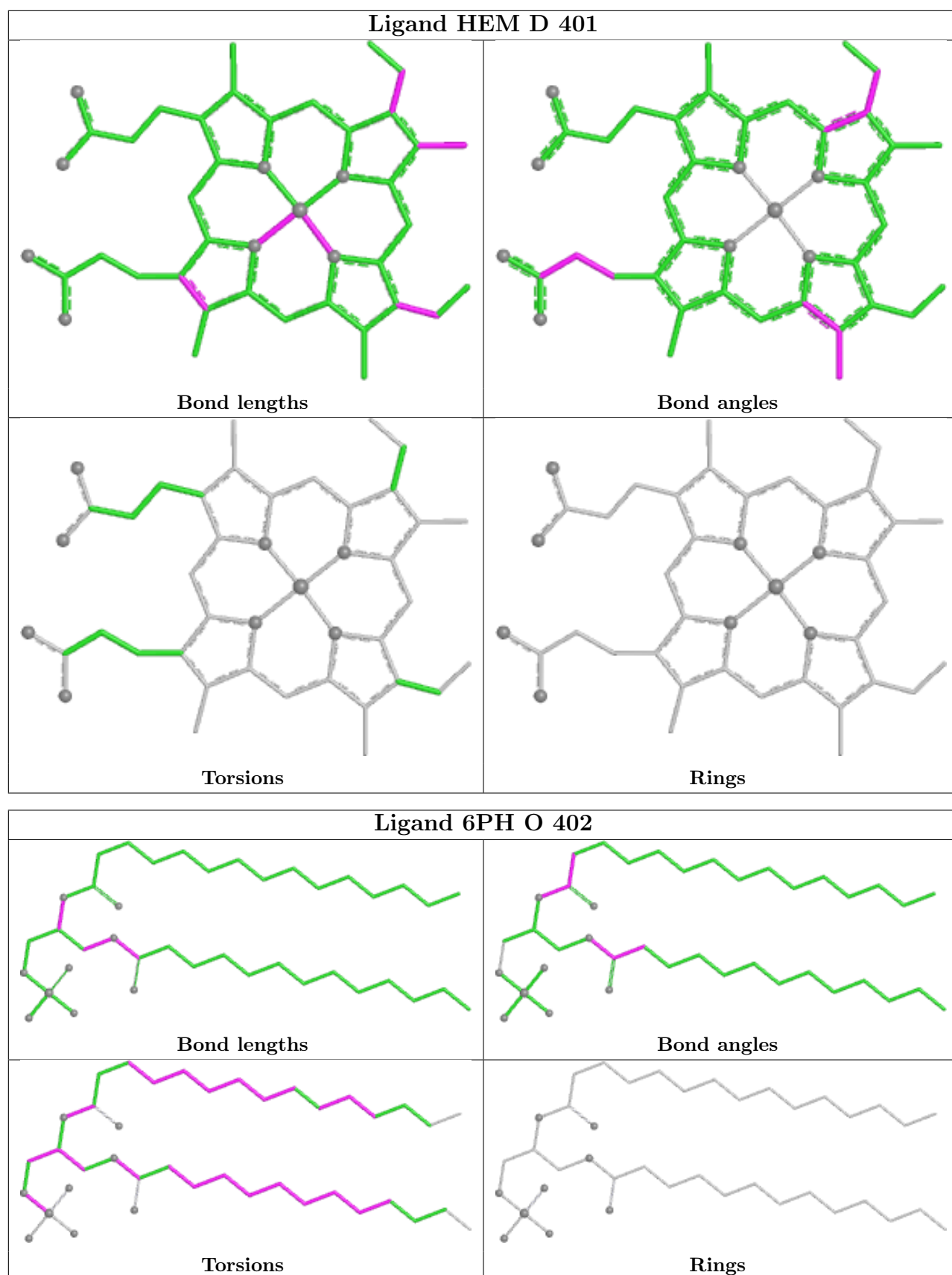
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

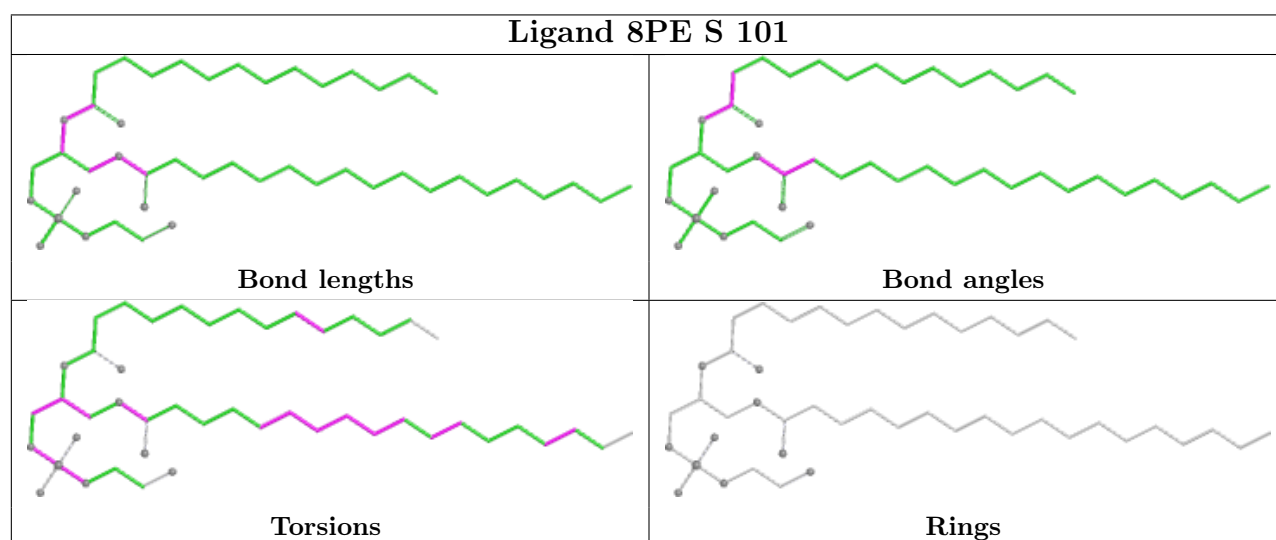
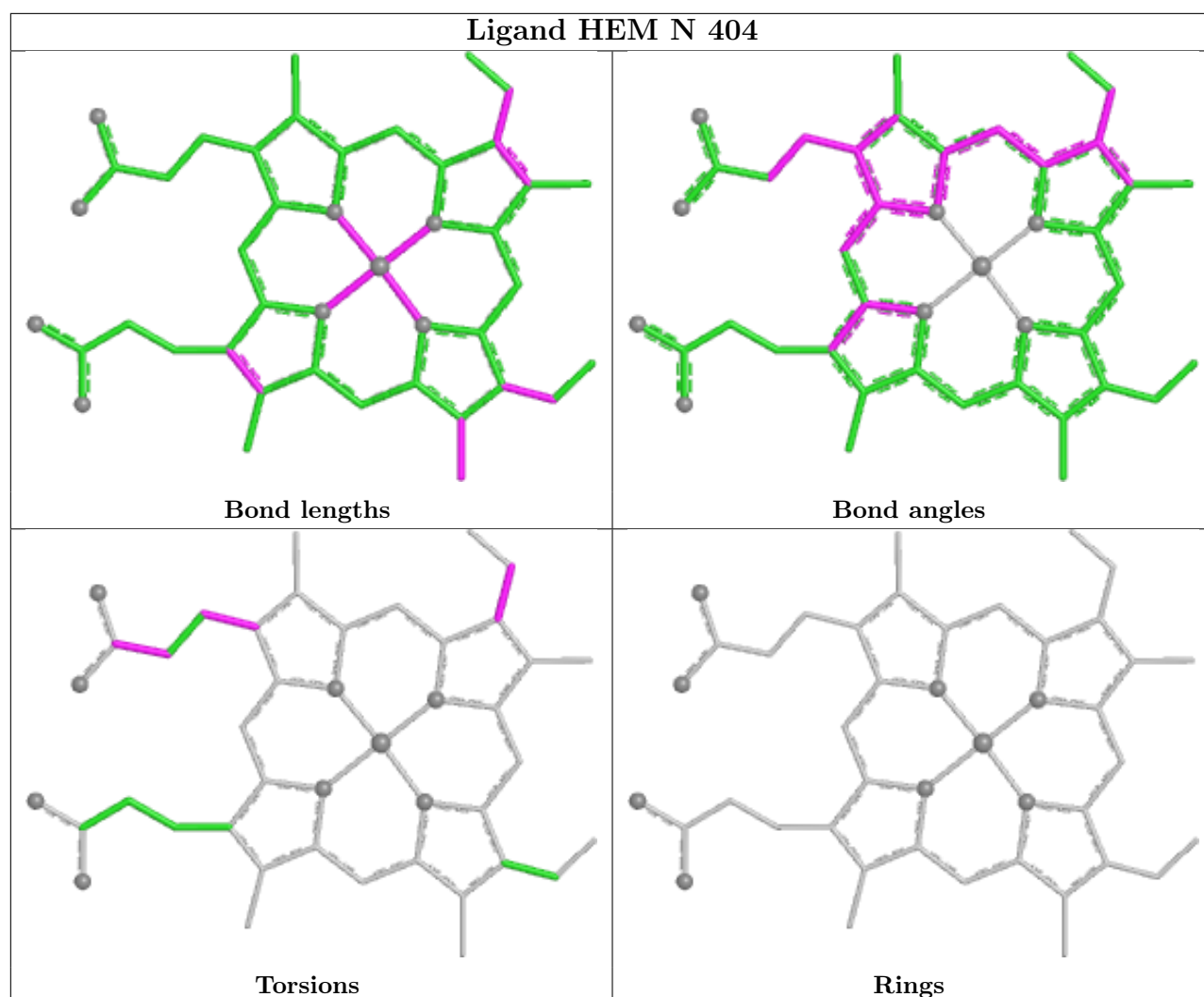


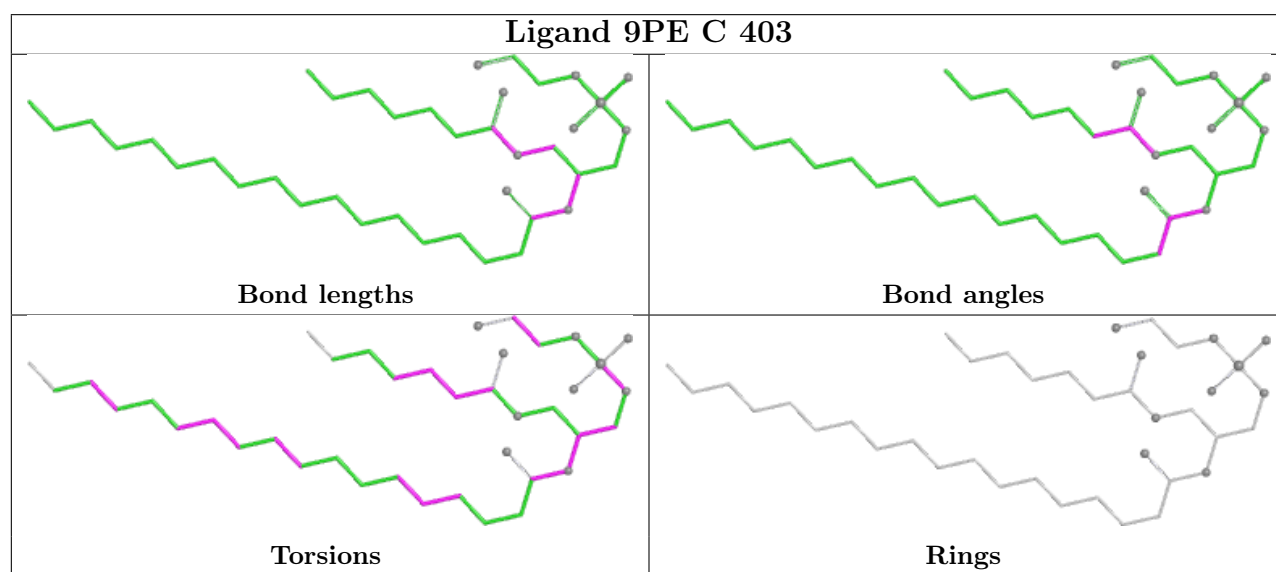
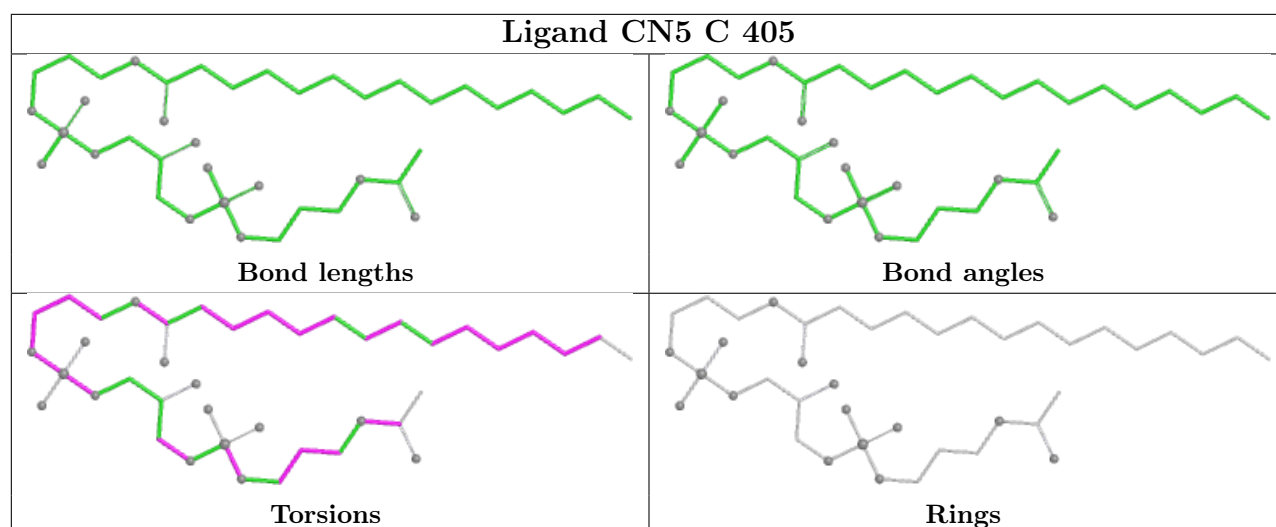




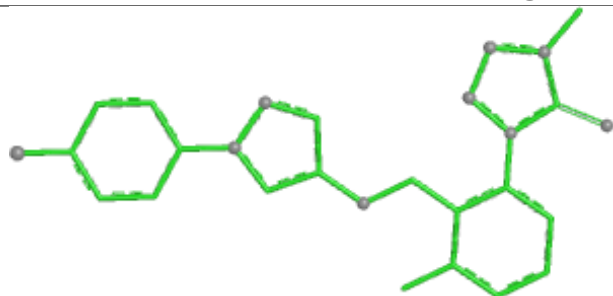




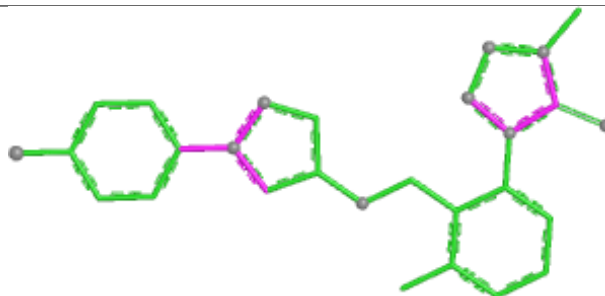




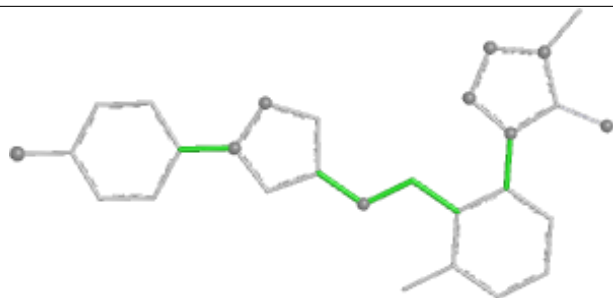
Ligand 86T C 406



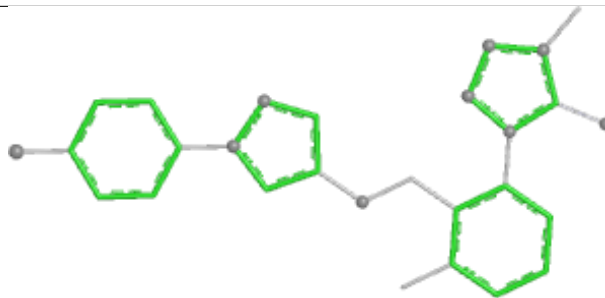
Bond lengths



Bond angles

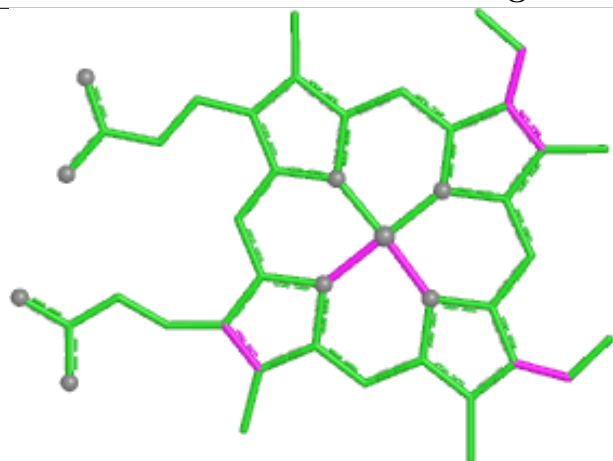


Torsions

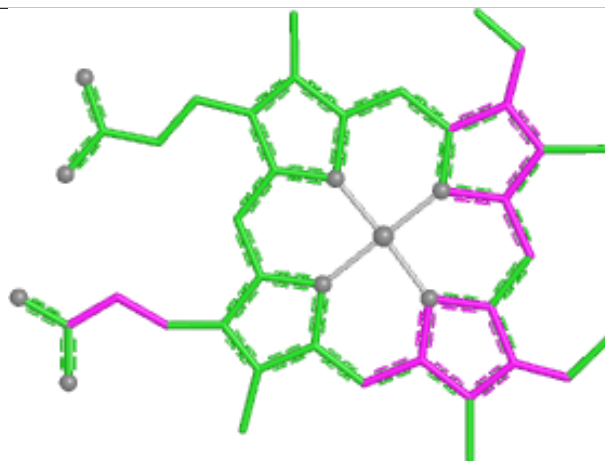


Rings

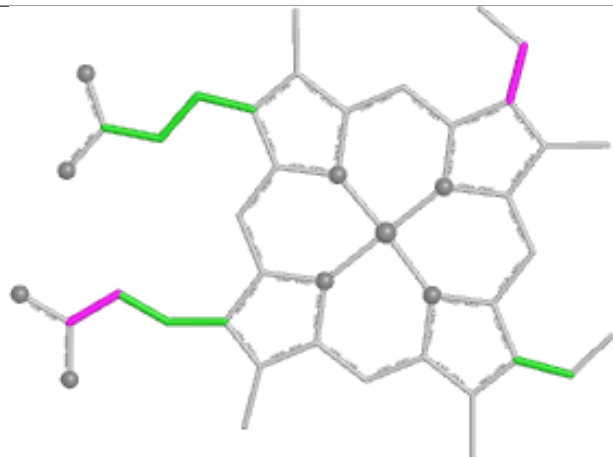
Ligand HEM O 401



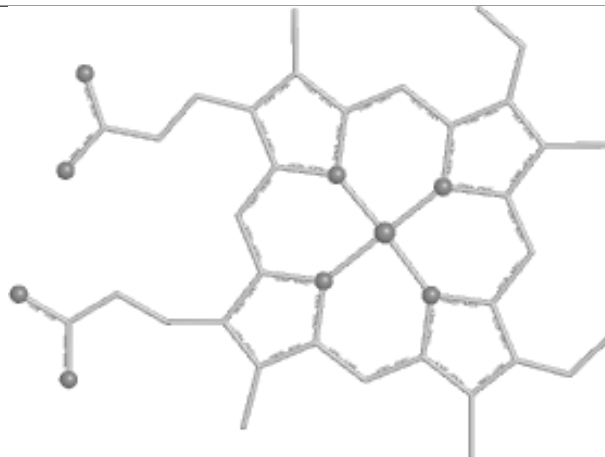
Bond lengths



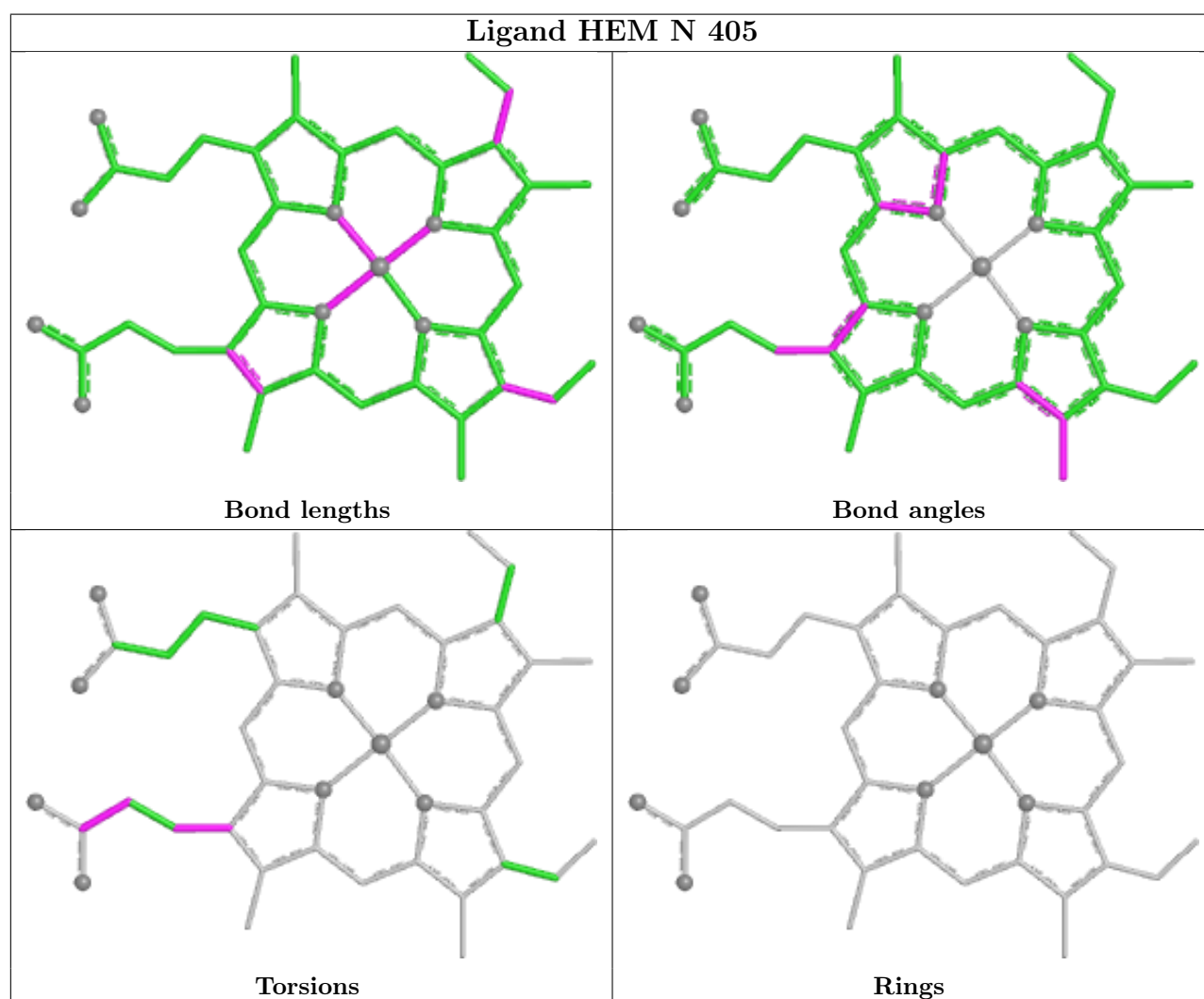
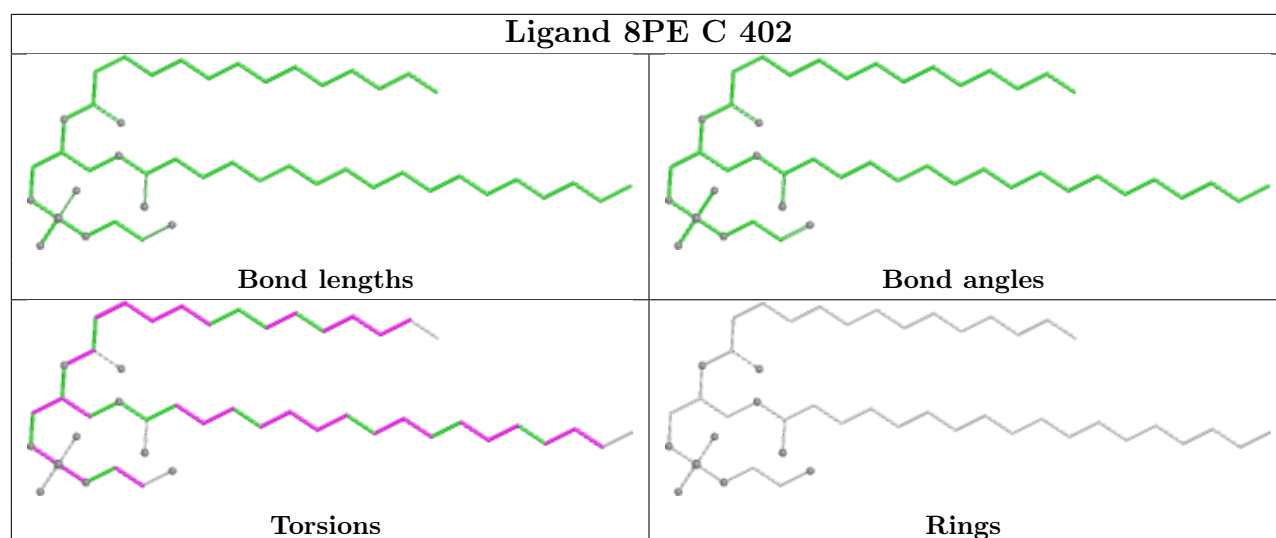
Bond angles

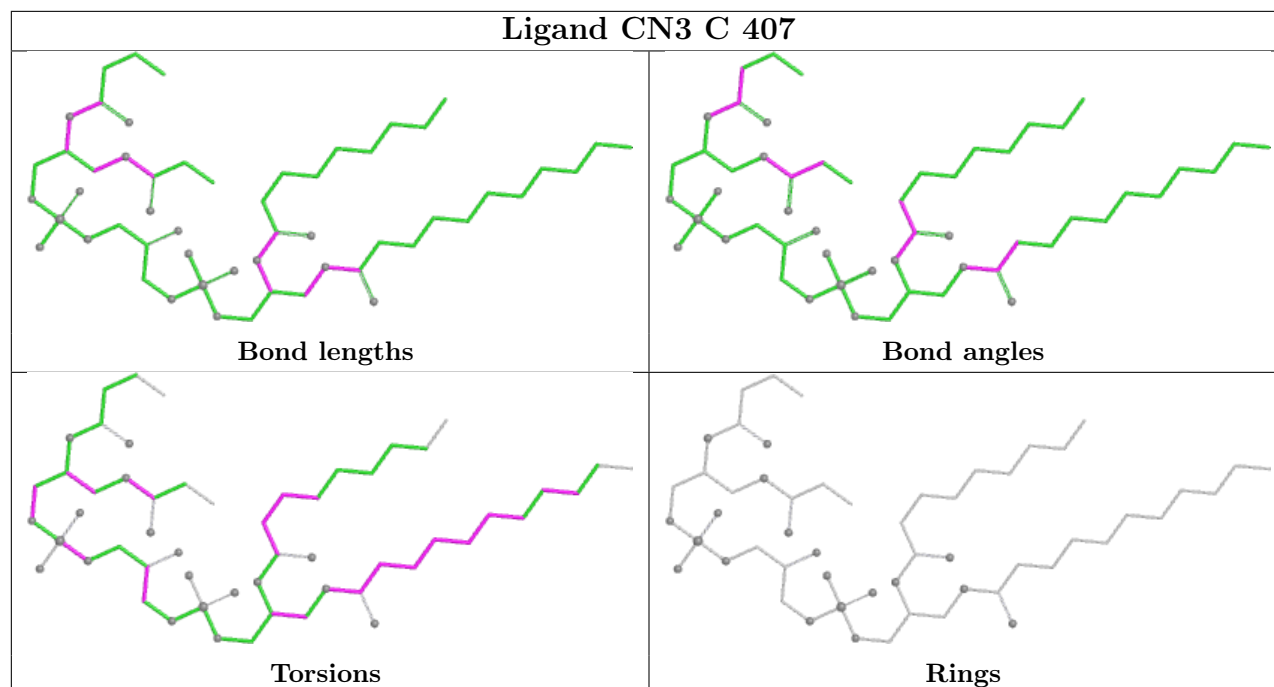


Torsions



Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

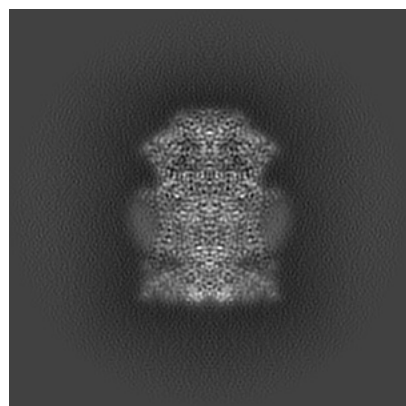
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39322. These allow visual inspection of the internal detail of the map and identification of artifacts.

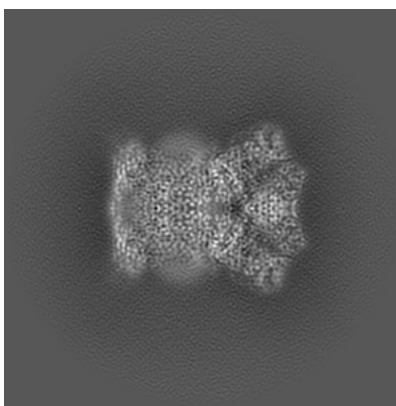
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

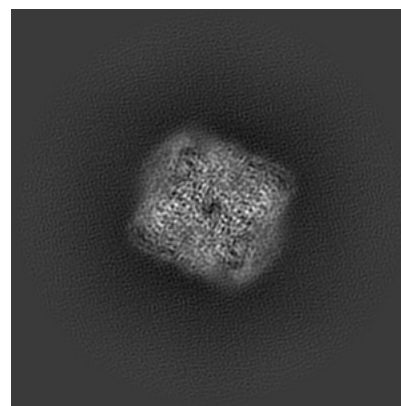
6.1.1 Primary map



X

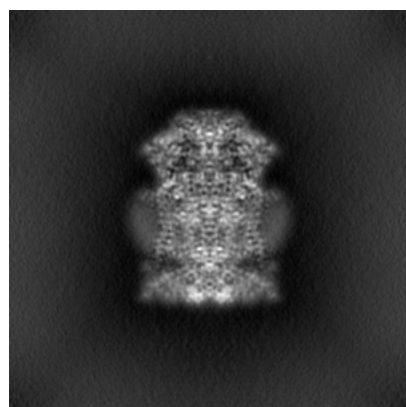


Y

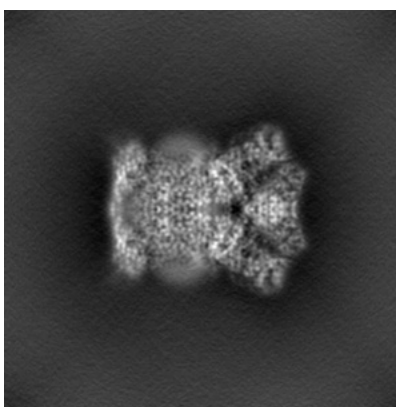


Z

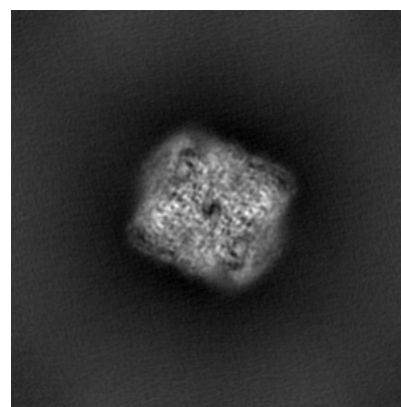
6.1.2 Raw map



X



Y

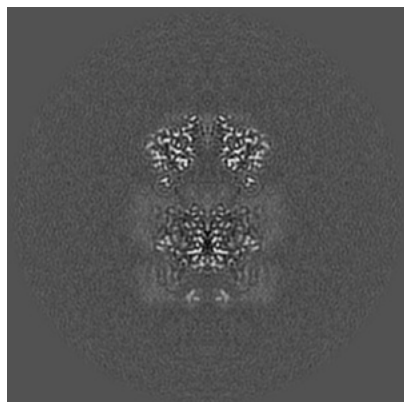


Z

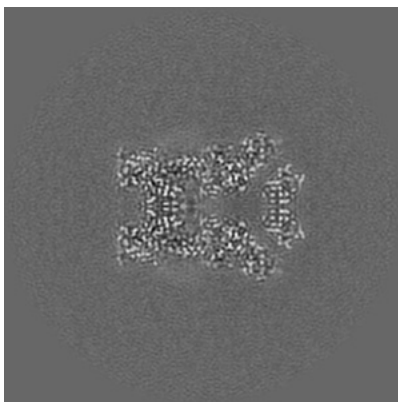
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

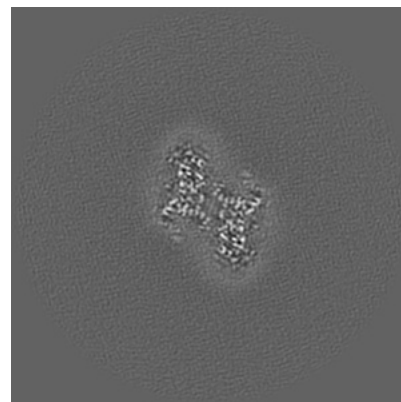
6.2.1 Primary map



X Index: 160

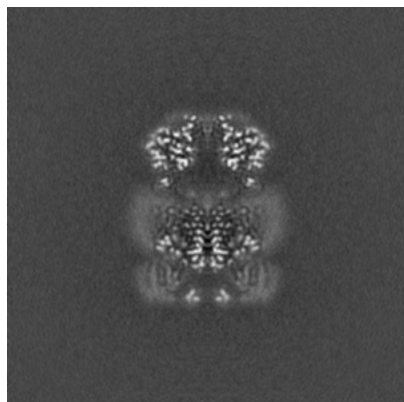


Y Index: 160

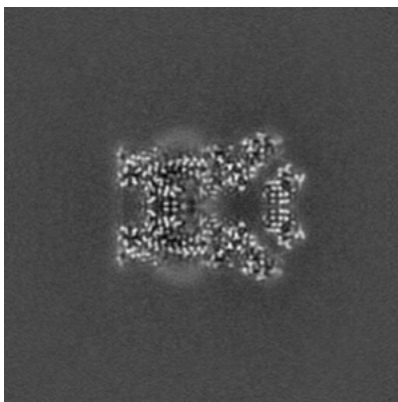


Z Index: 160

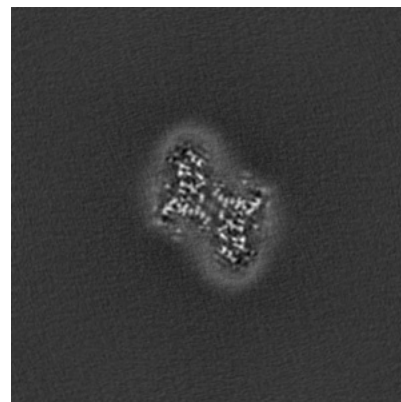
6.2.2 Raw map



X Index: 160



Y Index: 160

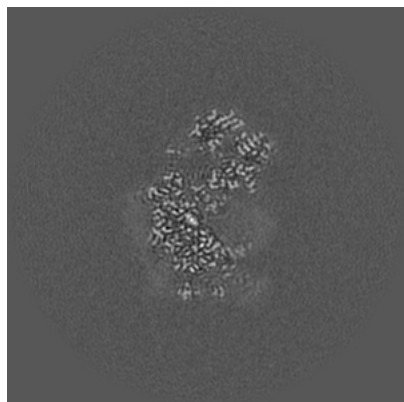


Z Index: 160

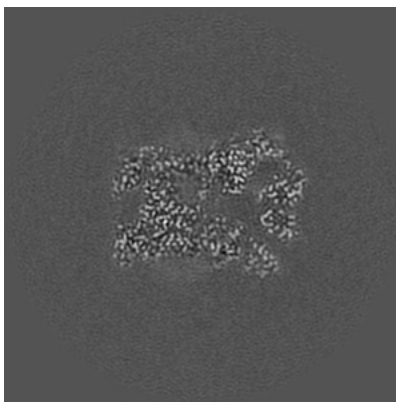
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

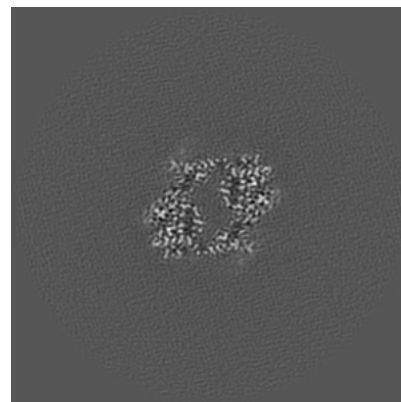
6.3.1 Primary map



X Index: 172

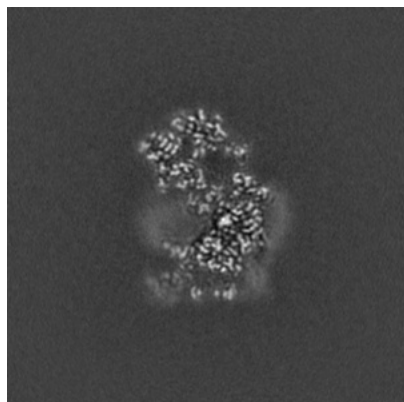


Y Index: 165

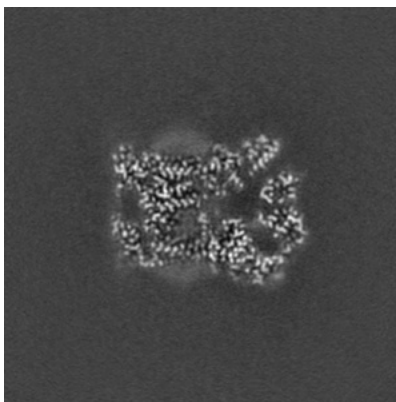


Z Index: 181

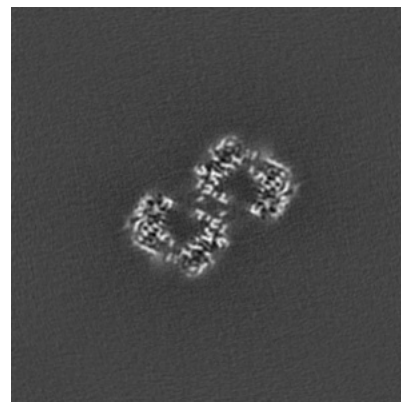
6.3.2 Raw map



X Index: 149



Y Index: 155

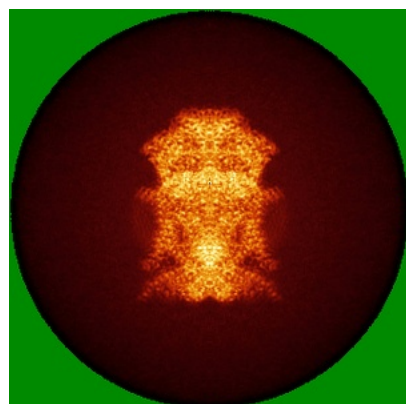


Z Index: 205

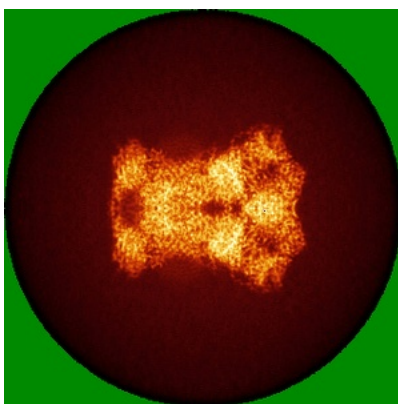
The images above show the largest variance slices of the map in three orthogonal directions.

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

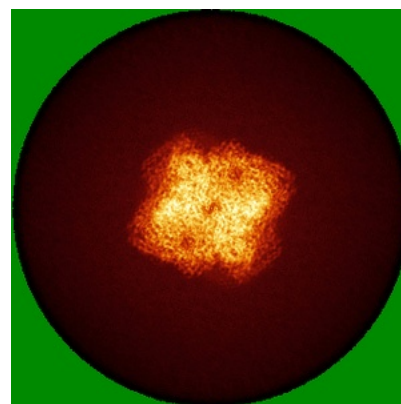
6.4.1 Primary map



X

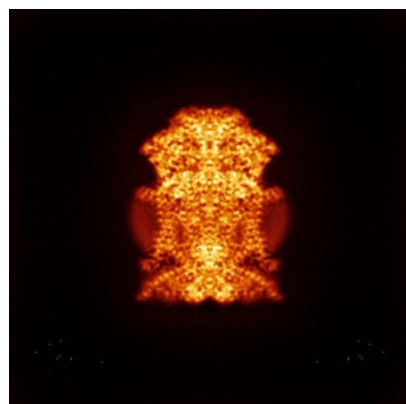


Y

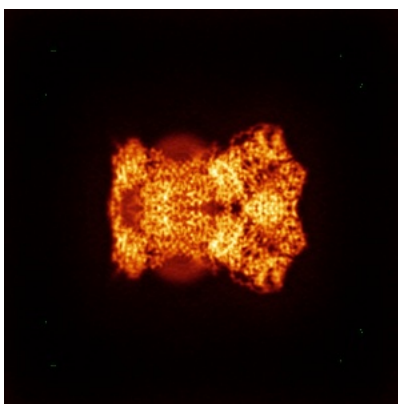


Z

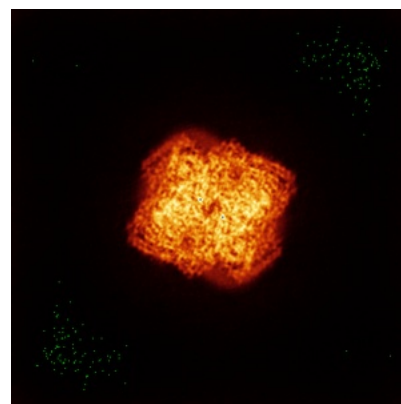
6.4.2 Raw map



X



Y

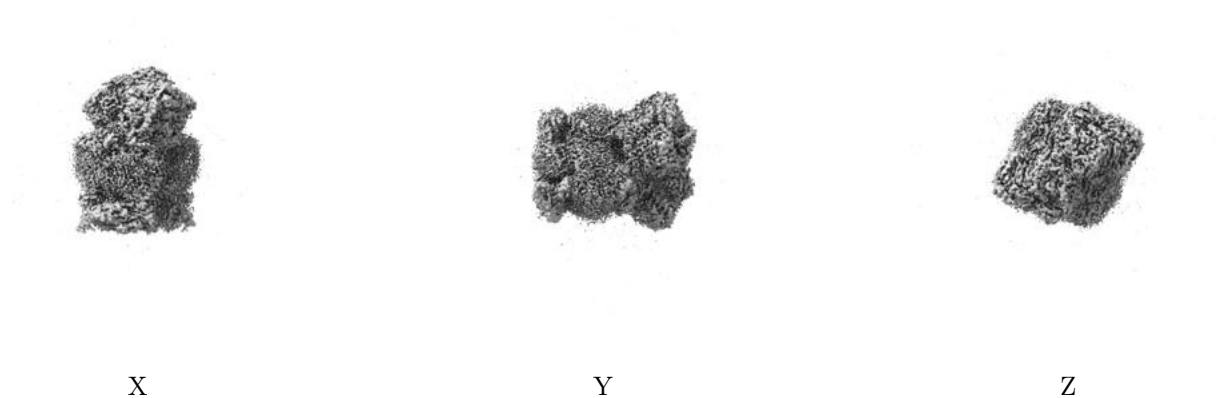


Z

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

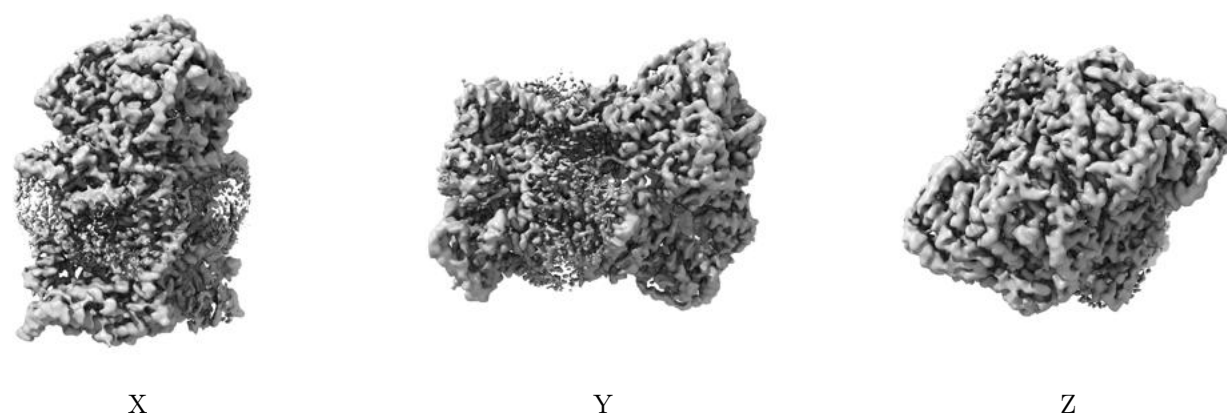
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

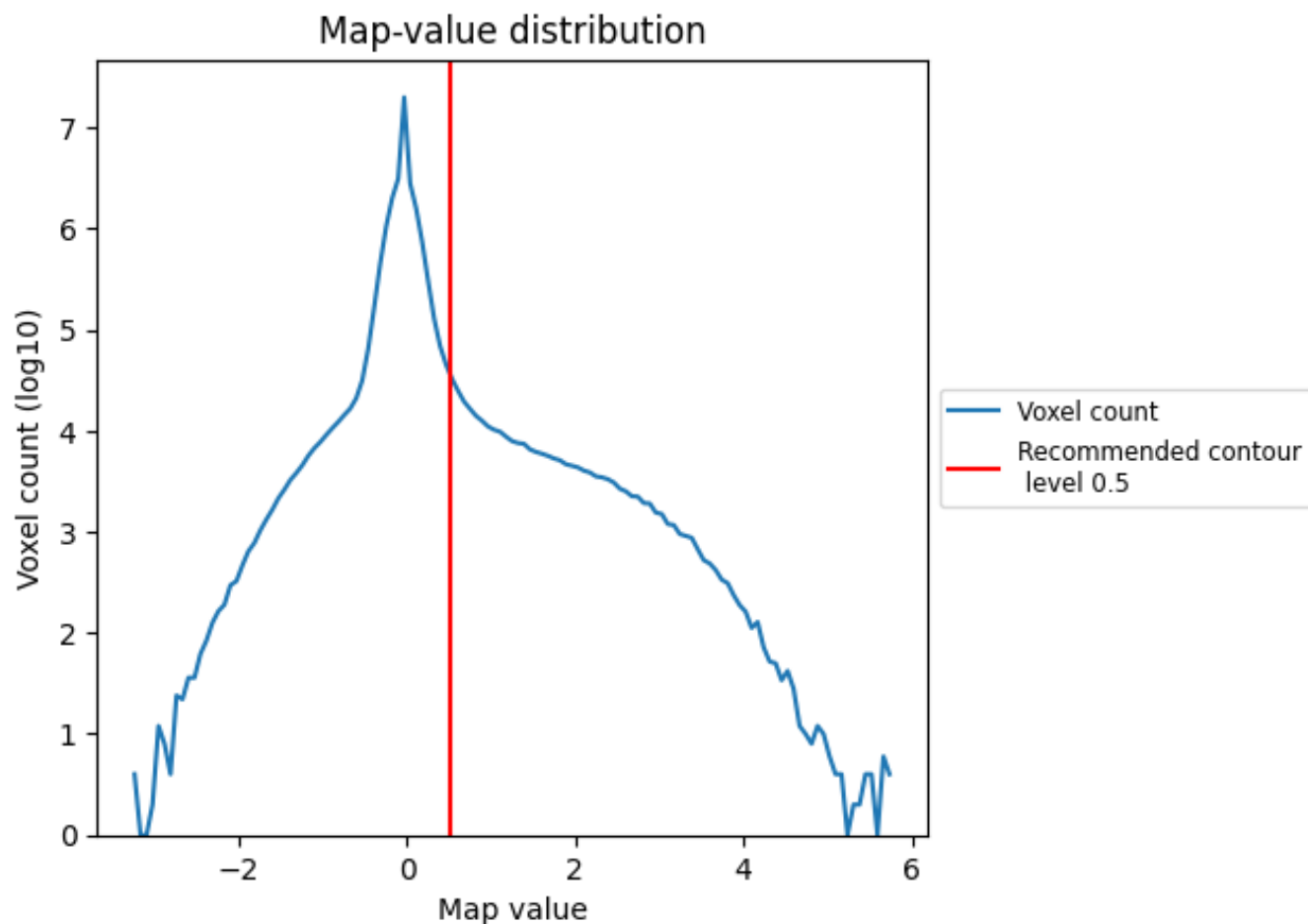
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

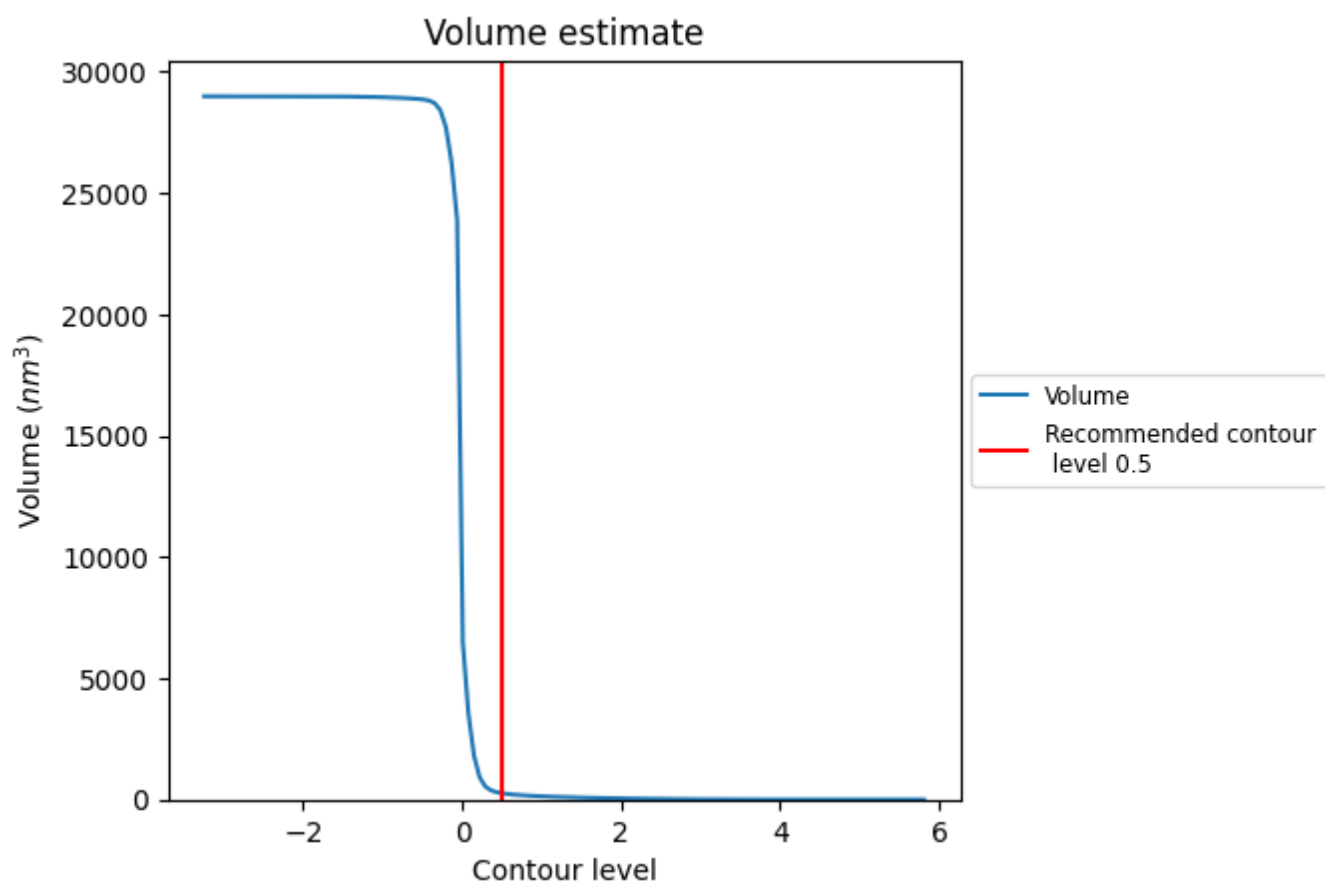
This section contains the results of statistical analysis of the map.

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.

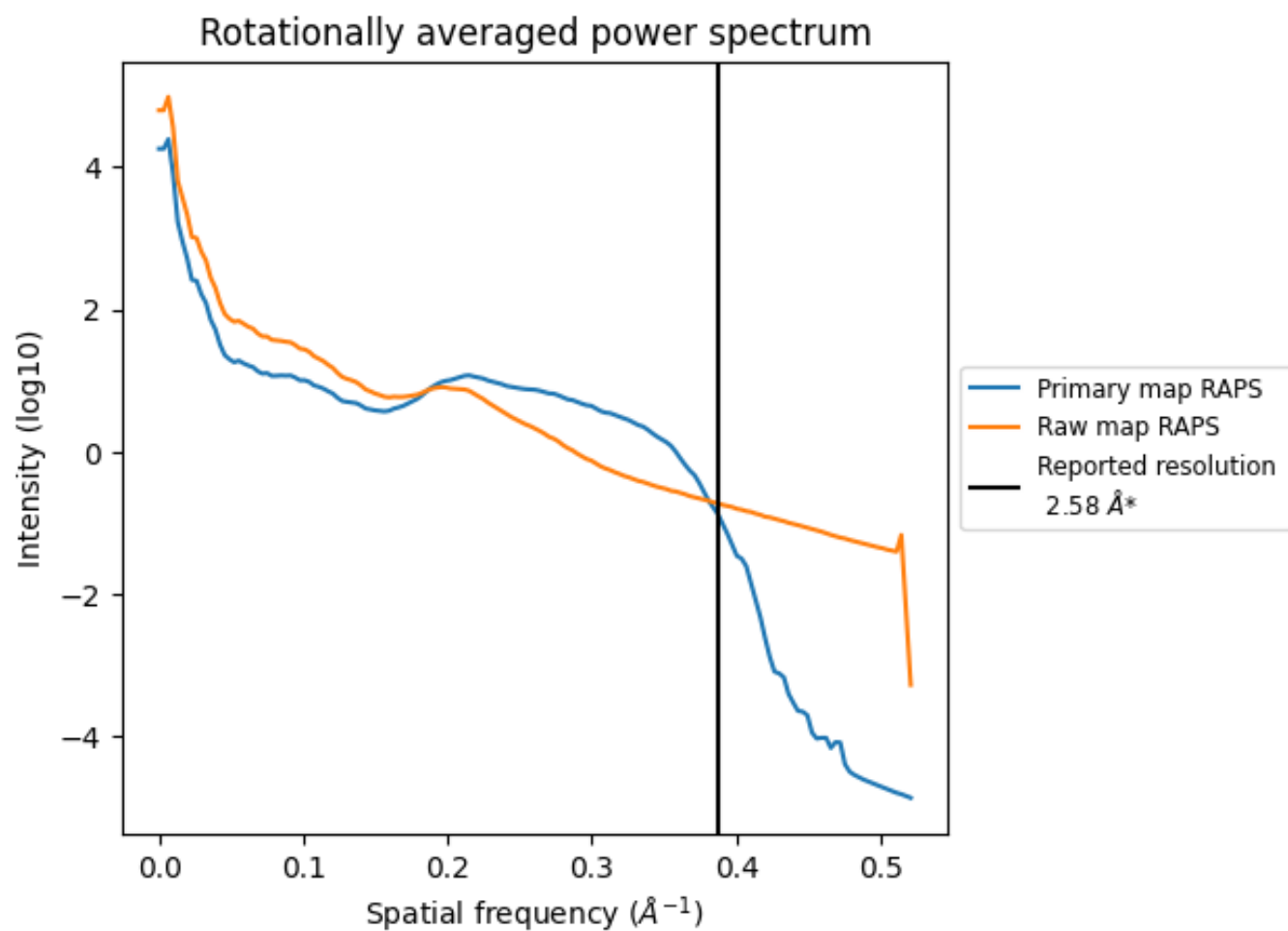
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 262 nm³; this corresponds to an approximate mass of 237 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

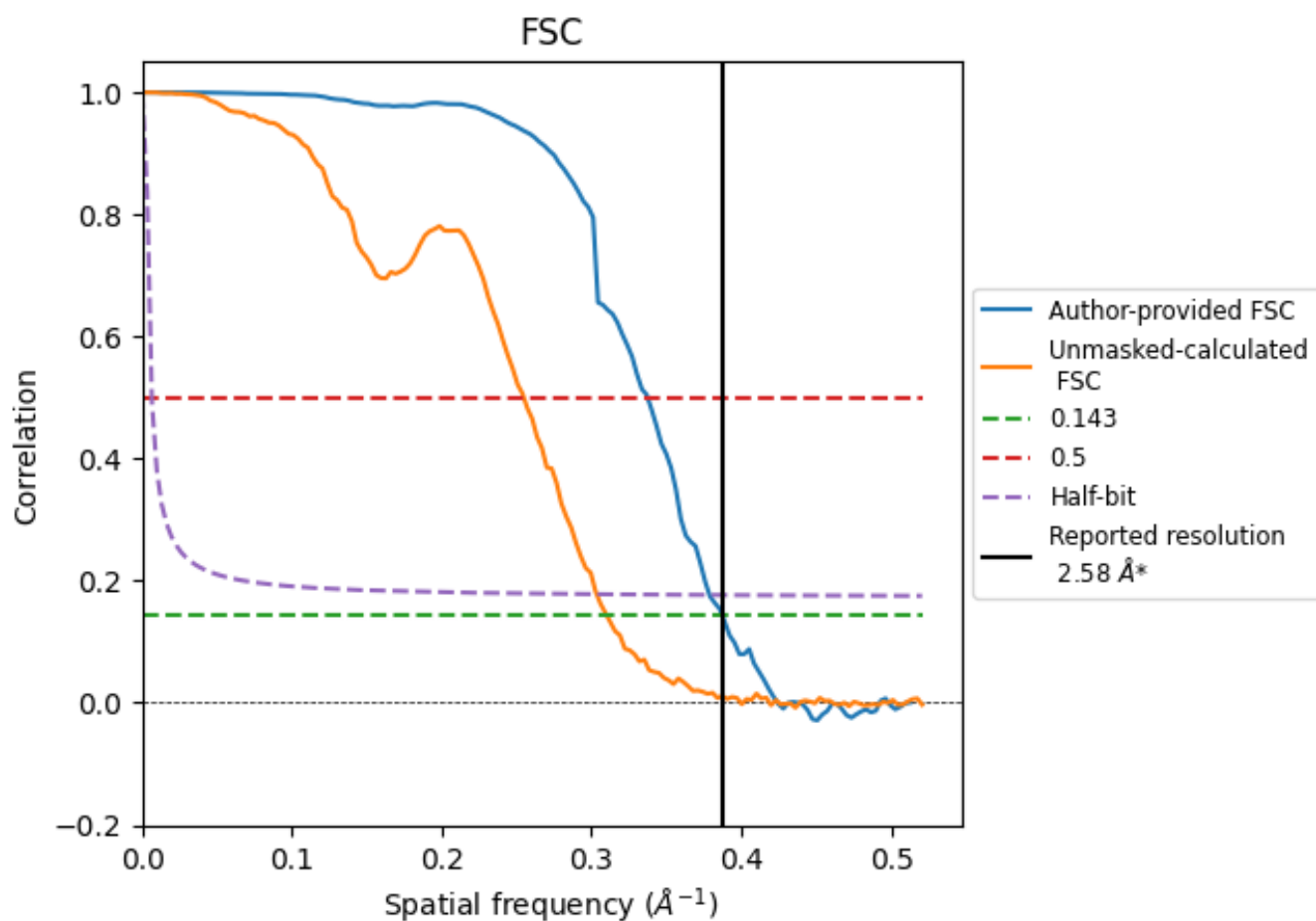


*Reported resolution corresponds to spatial frequency of 0.388 Å⁻¹

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

8.2 Resolution estimates [i](#)

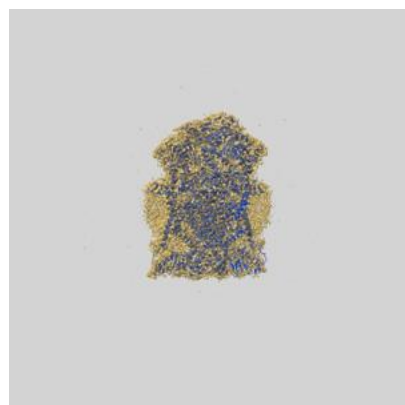
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.58	-	-
Author-provided FSC curve	2.58	2.96	2.64
Unmasked-calculated*	3.22	3.92	3.29

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

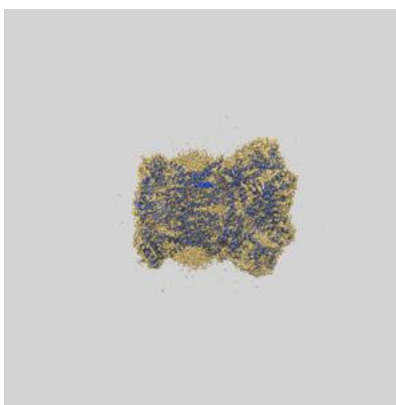
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-39322 and PDB model 8YIL. Per-residue inclusion information can be found in section [3](#) on page [12](#).

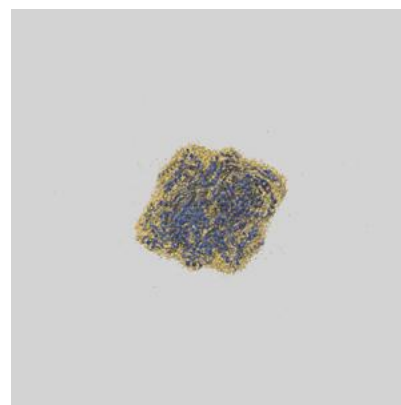
9.1 Map-model overlay [i](#)



X



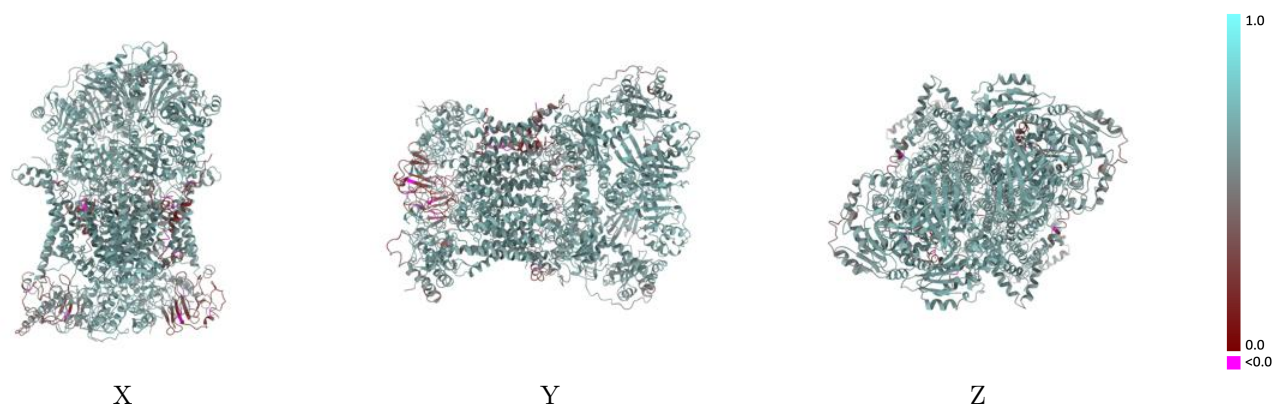
Y



Z

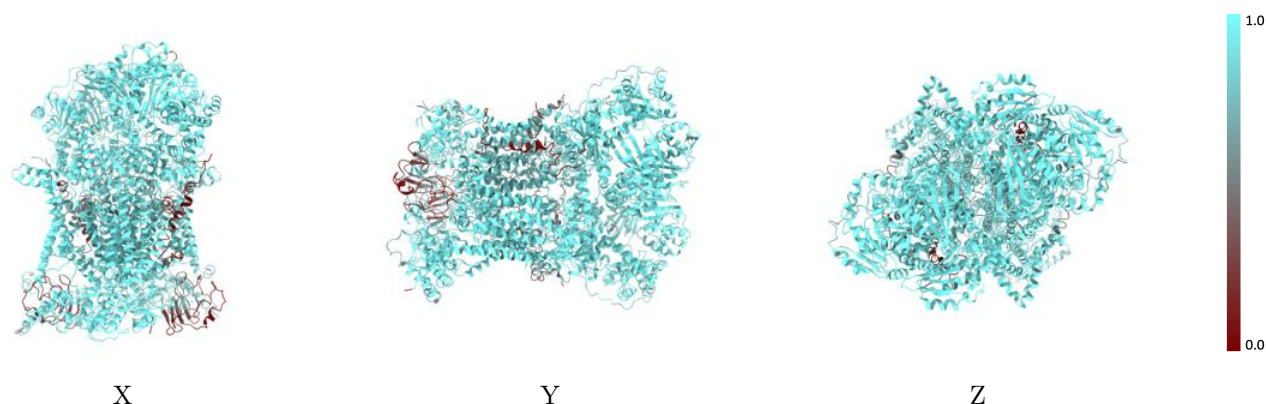
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



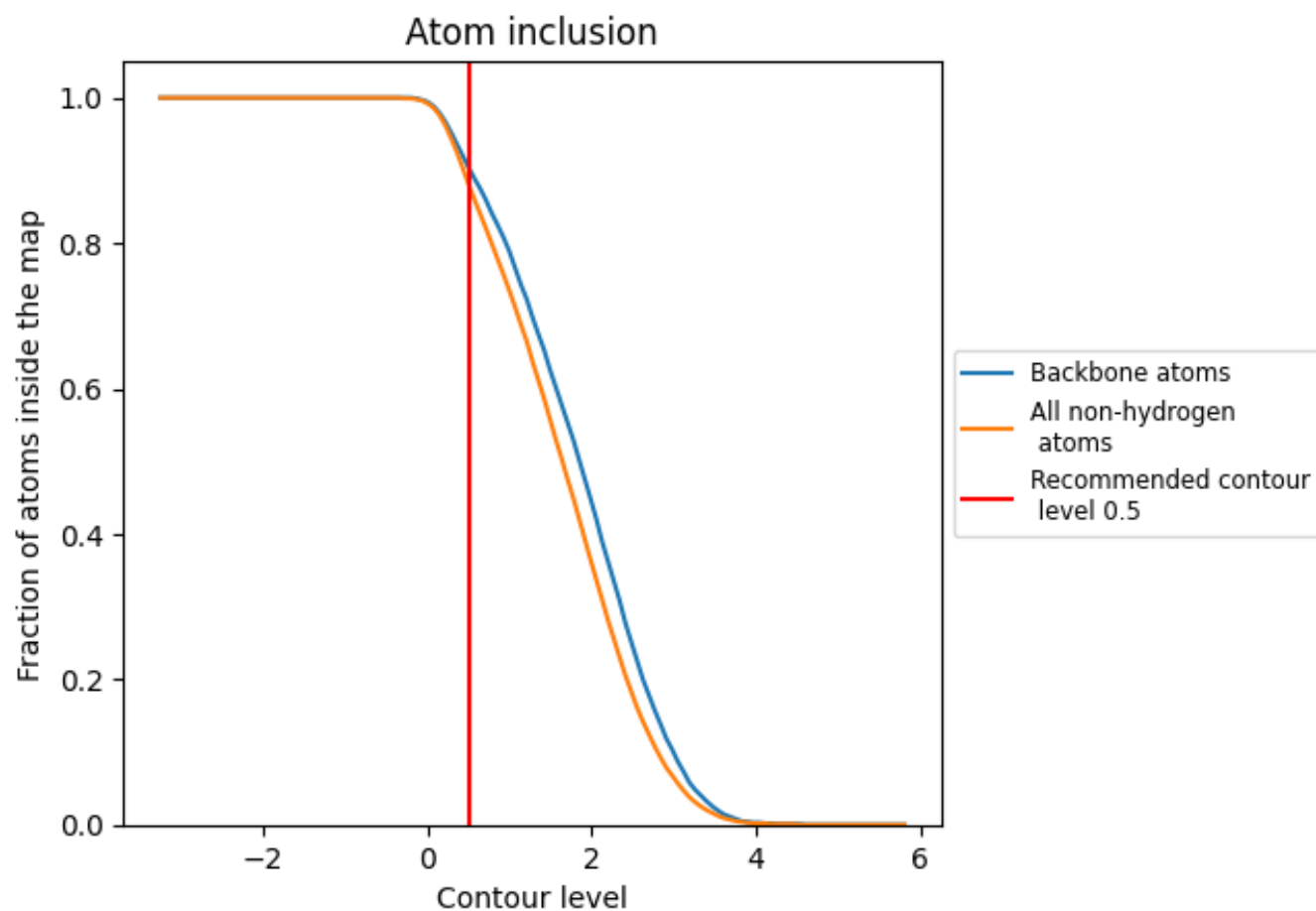
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8820	 0.5760
A	 0.9560	 0.6000
B	 0.9720	 0.6290
C	 0.9720	 0.6370
D	 0.9650	 0.6160
E	 0.4880	 0.3830
F	 0.8210	 0.5030
G	 0.9370	 0.6040
H	 0.8440	 0.5370
I	 0.6700	 0.4430
L	 0.9560	 0.6010
M	 0.9710	 0.6290
N	 0.9740	 0.6390
O	 0.9660	 0.6190
P	 0.4760	 0.3770
Q	 0.8290	 0.4980
R	 0.9380	 0.6030
S	 0.8400	 0.5340
T	 0.6690	 0.4720
U	 0.1030	 0.2300
V	 0.0850	 0.1980

