



Full wwPDB EM Validation Report ⓘ

Dec 16, 2024 – 06:21 PM JST

PDB ID : 8YHQ
EMDB ID : EMD-39291
Title : Cryo-EM structure of *Saccharomyces cerevisiae* bc1 complex in pyraclostrobin-bound state
Authors : Ye, Y.; Li, Z.W.; Yang, G.F.
Deposited on : 2024-02-28
Resolution : 2.42 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:

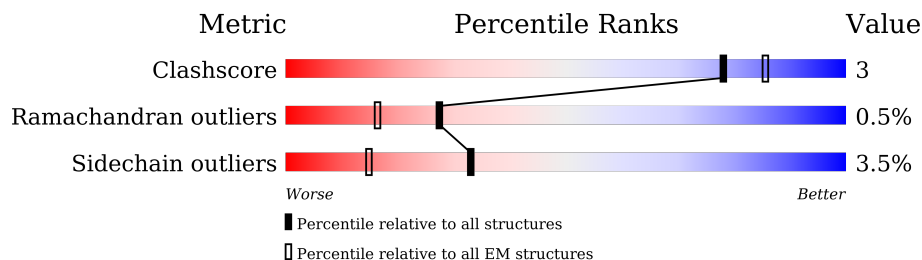
EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

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 2.42 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	J	431	
2	C	385	
2	L	385	
3	B	352	
3	K	352	
4	D	248	
4	M	248	

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Mol	Chain	Length	Quality of chain
5	E	185	
5	N	185	
6	F	75	
6	O	75	
7	G	126	
7	P	126	
8	H	93	
8	Q	93	
9	I	55	
9	R	55	
10	S	52	
10	T	52	

2 Entry composition [i](#)

There are 19 unique types of molecules in this entry. The entry contains 32385 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
			Total	C	N	O	S		
1	A	431	Total	C	N	O	S	0	0
			3344	2110	576	652	6		
1	J	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
			Total	C	N	O	S		
2	C	385	Total	C	N	O	S	0	0
			3090	2082	484	503	21		
2	L	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
			Total	C	N	O	S		
3	B	352	Total	C	N	O	S	0	0
			2735	1747	453	534	1		
3	K	352	Total	C	N	O	S	0	0
			2735	1747	453	534	1		

- Molecule 4 is a protein called quinol-cytochrome-c reductase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	248	Total	C	N	O	S	0	0
			1961	1249	340	363	9		
4	M	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
			Total	C	N	O	S		
5	E	185	1411	893	242	266	10	0	0
5	N	185	1411	893	242	266	10	0	0

- Molecule 6 is a protein called QCR6 isoform 1.

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

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

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

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

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

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

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

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

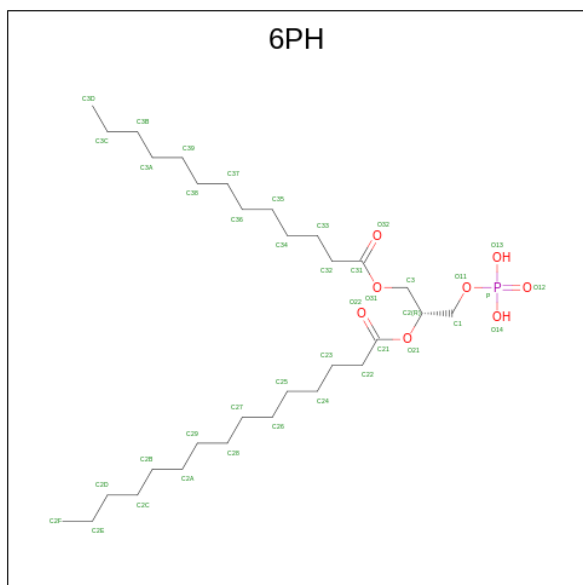
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	S	44	347	230	58	57	2	0	0

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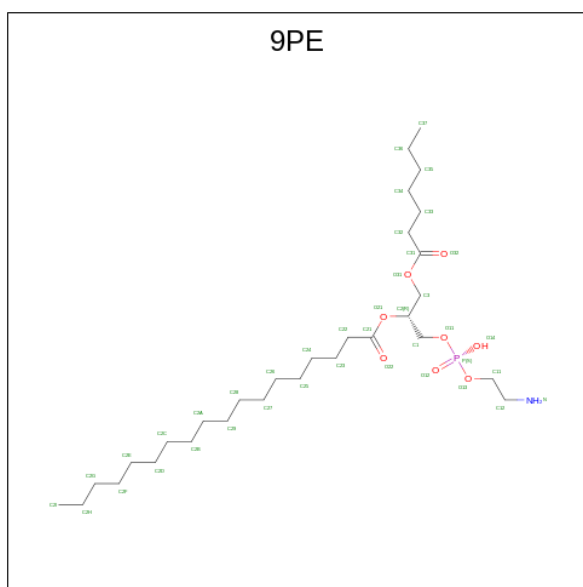
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	T	51	406	272	66	66	2	0	0

- Molecule 11 is (1R)-2-(phosphonoxy)-1-[(tridecanoyloxy)methyl]ethyl pentadecanoate (three-letter code: 6PH) (formula: C₃₁H₆₁O₈P).



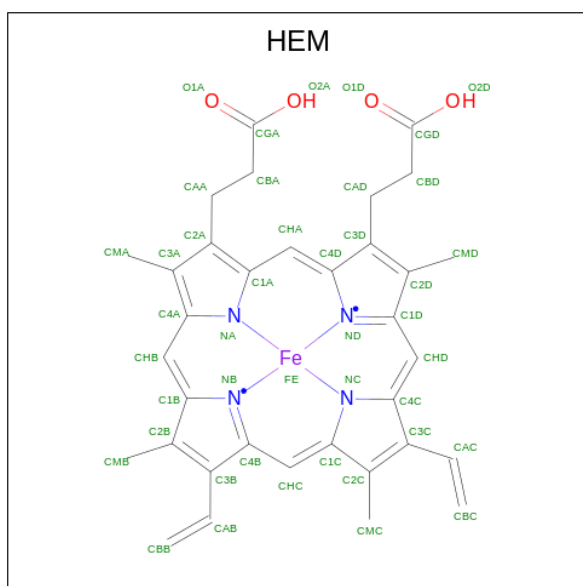
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
11	C	1	40	31	8	1	0
11	N	1	40	31	8	1	0

- Molecule 12 is (1R)-2-[(S)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy-1-[(heptanoyloxy)methyl]ethyl octadecanoate (three-letter code: 9PE) (formula: C₃₀H₆₀NO₈P).



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

- Molecule 13 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



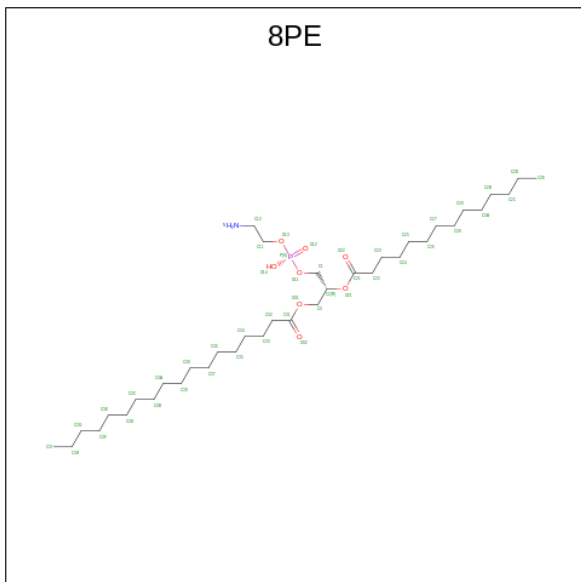
Mol	Chain	Residues	Atoms					AltConf
13	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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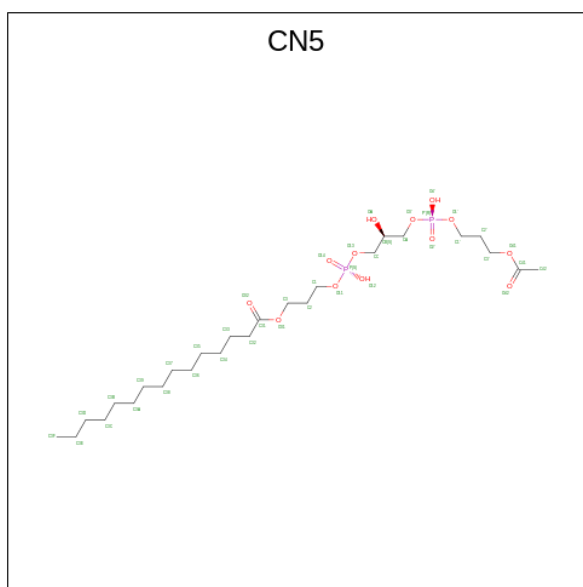
Mol	Chain	Residues	Atoms				AltConf	
13	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
13	D	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
13	L	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
13	L	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
13	M	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 14 is (2R)-3-[[[(S)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy]-2-(tetradecanoyloxy)propyl octadecanoate (three-letter code: 8PE) (formula: C₃₇H₇₄NO₈P).



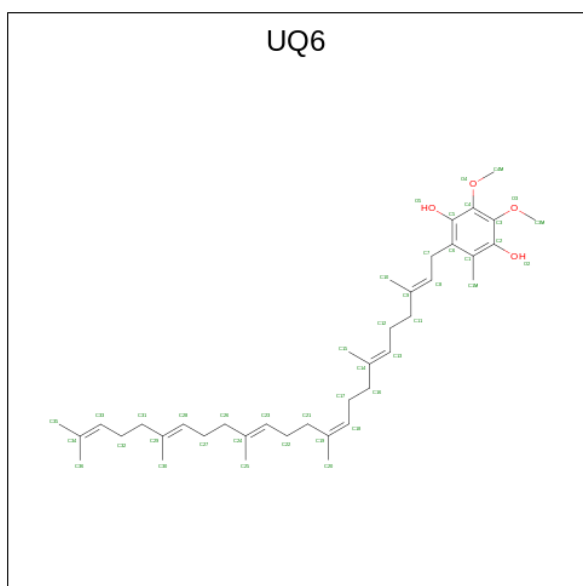
Mol	Chain	Residues	Atoms				AltConf	
14	C	1	Total	C	N	O	P	0
			47	37	1	8	1	
14	Q	1	Total	C	N	O	P	0
			47	37	1	8	1	

- 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 (three-letter code: CN5) (formula: C₂₆H₅₂O₁₃P₂).



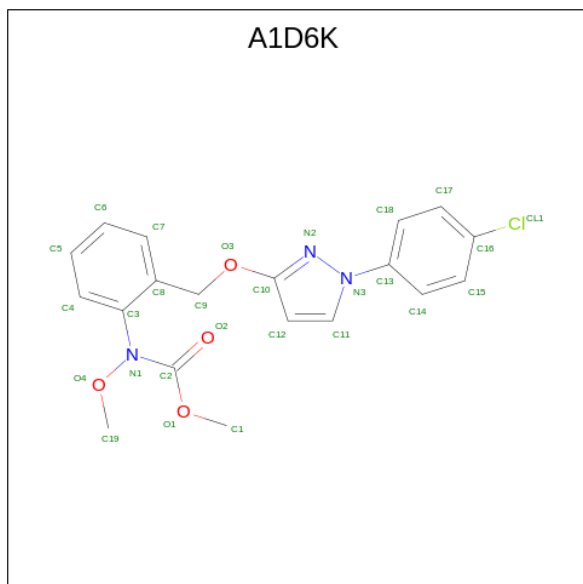
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
15	C	1	41	26	13	2	0

- Molecule 16 is 5-(3,7,11,15,19,23-HEXAMETHYL-TETRACOSA-2,6,10,14,18,22-HEX AENYL)-2,3-DIMETHOXY-6-METHYL-BENZENE-1,4-DIOL (three-letter code: UQ6) (formula: C₃₉H₆₀O₄).



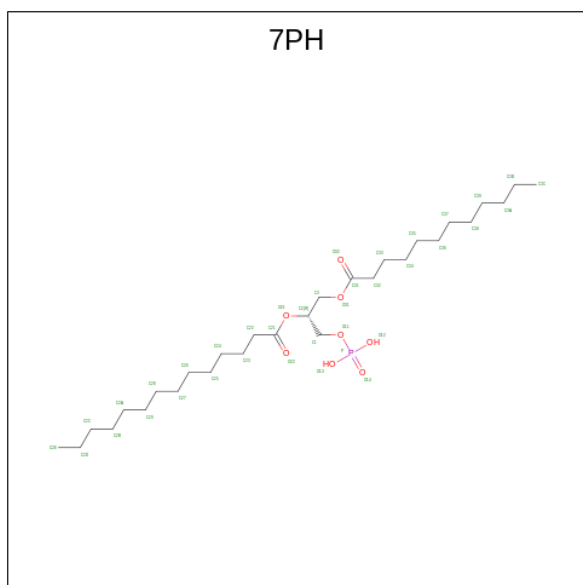
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
16	C	1	43	39	4	0
16	L	1	43	39	4	0

- Molecule 17 is methyl {N}-[2-[[1-(4-chlorophenyl)pyrazol-3-yl]oxymethyl]phenyl]- {N}-methoxy-carbamate (three-letter code: A1D6K) (formula: C₁₉H₁₈ClN₃O₄) (labeled as "Ligand of Interest" by depositor).



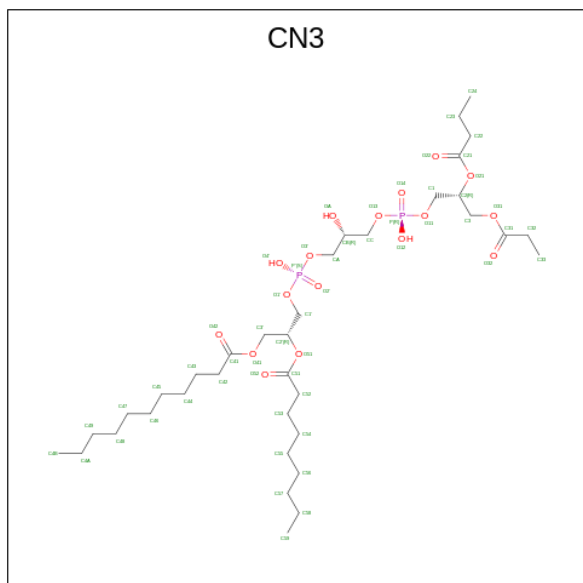
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Cl	N	O	
17	C	1	Total	C	Cl	N	O	0
				27	19	1	3	
17	L	1	Total	C	Cl	N	O	0
				27	19	1	3	

- Molecule 18 is (1R)-2-(dodecanoyloxy)-1-[(phosphonoxy)methyl]ethyl tetradecanoate (three-letter code: 7PH) (formula: C₂₉H₅₇O₈P).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
18	D	1	38	29	8	1	0
18	N	1	38	29	8	1	0

- Molecule 19 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-diphosphanadec-1-yl undecanoate (three-letter code: CN3) (formula: C₃₆H₆₈O₁₇P₂).

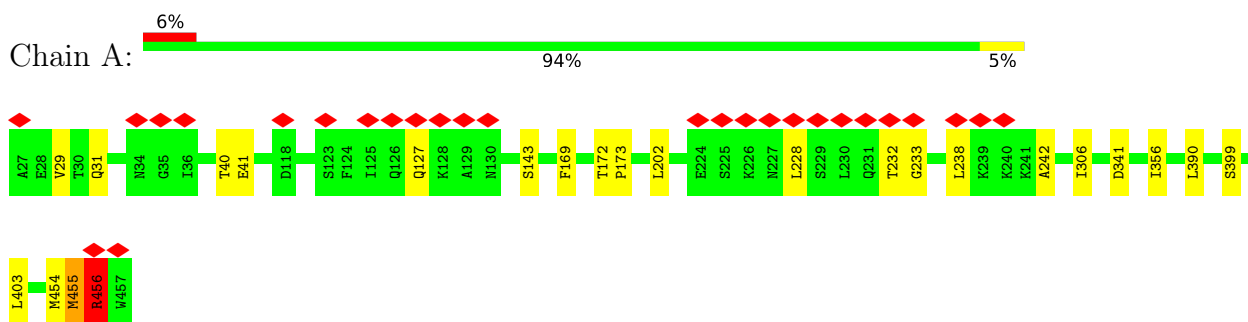


Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
19	L	1	55	36	17	2	0

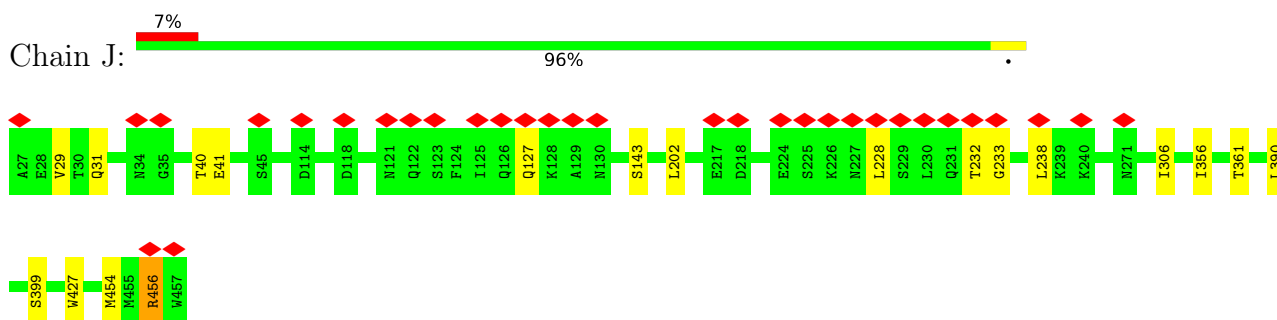
3 Residue-property plots [i](#)

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.

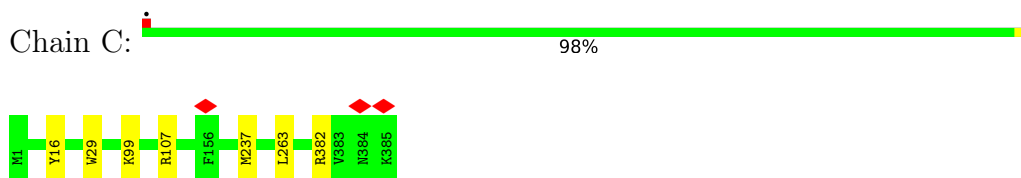
- Molecule 1: COR1 isoform 1



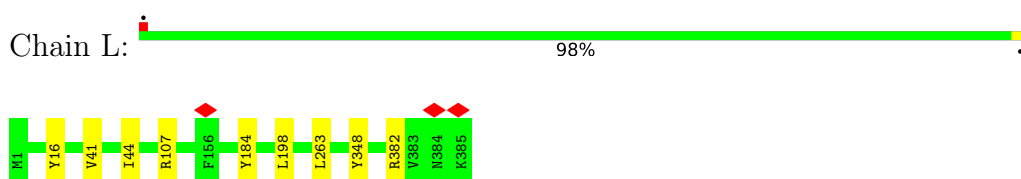
- Molecule 1: COR1 isoform 1



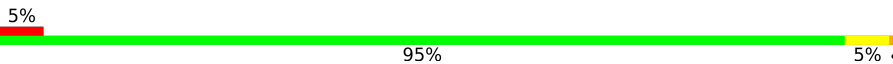
- Molecule 2: Cytochrome b

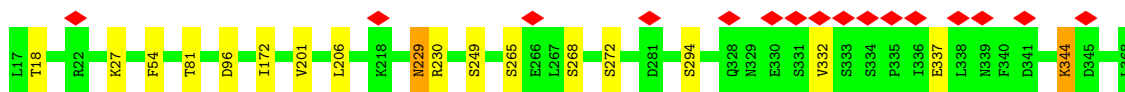


- Molecule 2: Cytochrome b



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

Chain B: 



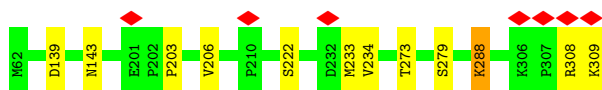
- Molecule 3: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain K: 



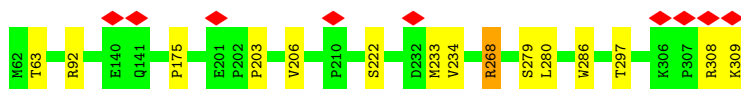
- Molecule 4: quinol-cytochrome-c reductase

Chain D: 




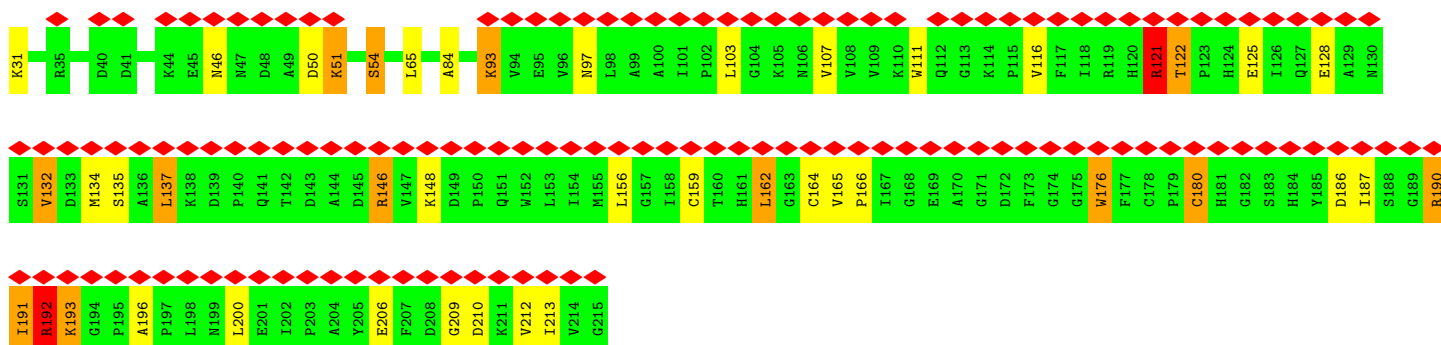
- Molecule 4: quinol-cytochrome-c reductase

Chain M: 




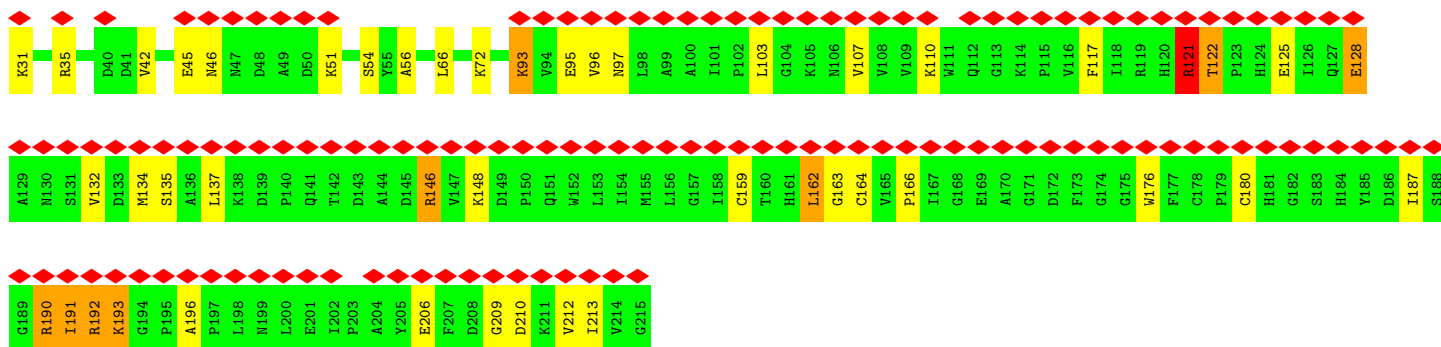
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain E: 

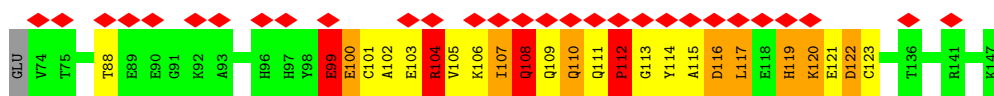
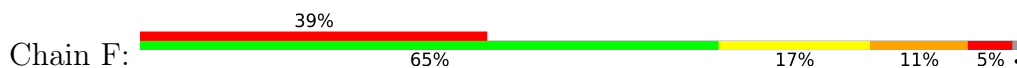


- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

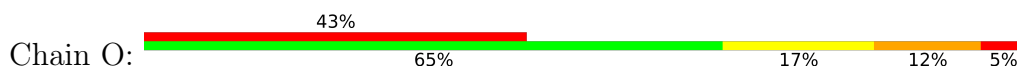
Chain N: 



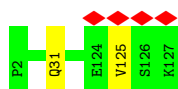
- Molecule 6: QCR6 isoform 1



- Molecule 6: QCR6 isoform 1



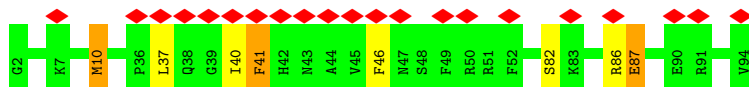
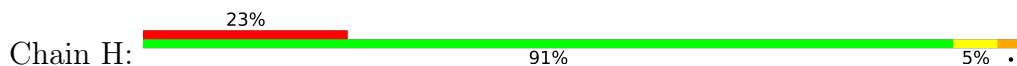
- Molecule 7: Cytochrome b-c1 complex subunit 7



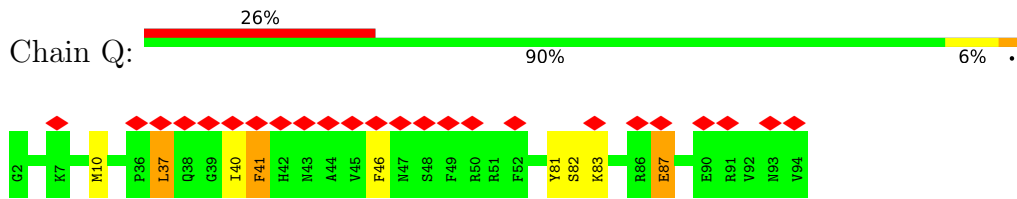
- Molecule 7: Cytochrome b-c1 complex subunit 7



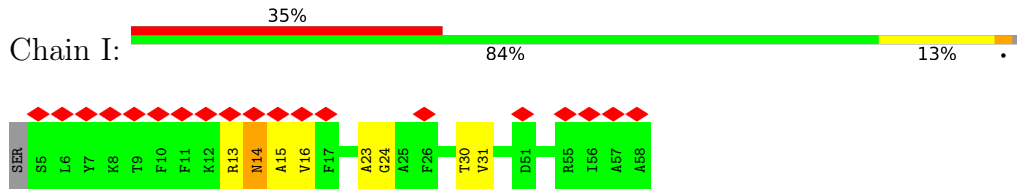
- Molecule 8: Cytochrome b-c1 complex subunit 8



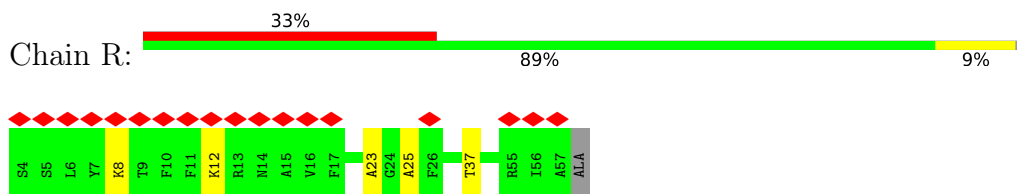
- Molecule 8: Cytochrome b-c1 complex subunit 8



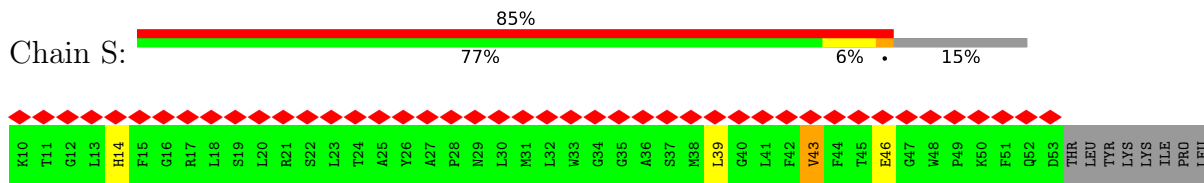
• Molecule 9: Cytochrome b-c1 complex subunit 9, mitochondrial



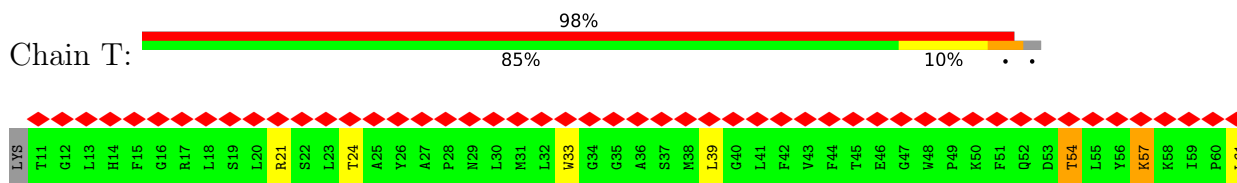
• Molecule 9: Cytochrome b-c1 complex subunit 9, mitochondrial



• 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	495602	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 ($e^-/\text{\AA}^2$)	49.04	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	8.742	Depositor
Minimum map value	-5.712	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.278	Depositor
Recommended contour level	1	Depositor
Map size (Å)	268.8, 268.8, 268.8	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.96, 0.96, 0.96	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: 9PE, 7PH, HEM, A1D6K, 6PH, CN5, 8PE, UQ6, 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	0.40	1/3405 (0.0%)	0.65	4/4615 (0.1%)
1	J	0.36	0/3405	0.61	0/4615
2	C	0.49	1/3192 (0.0%)	0.60	2/4354 (0.0%)
2	L	0.46	0/3192	0.60	3/4354 (0.1%)
3	B	0.39	0/2781	0.63	2/3764 (0.1%)
3	K	0.40	0/2781	0.62	1/3764 (0.0%)
4	D	0.45	1/2022 (0.0%)	0.61	0/2751
4	M	0.46	1/2022 (0.0%)	0.61	1/2751 (0.0%)
5	E	0.50	1/1444 (0.1%)	1.05	11/1957 (0.6%)
5	N	0.48	0/1444	1.02	11/1957 (0.6%)
6	F	0.52	0/638	0.96	5/858 (0.6%)
6	O	0.52	0/647	0.99	4/870 (0.5%)
7	G	0.40	0/1040	0.67	0/1408
7	P	0.40	0/1040	0.65	0/1408
8	H	0.56	1/804 (0.1%)	0.72	1/1088 (0.1%)
8	Q	0.52	1/804 (0.1%)	0.70	1/1088 (0.1%)
9	I	0.41	0/455	0.63	0/614
9	R	0.35	0/456	0.59	0/615
10	S	0.37	0/358	0.73	0/483
10	T	0.40	0/419	0.69	0/567
All	All	0.44	7/32349 (0.0%)	0.69	46/43881 (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	J	0	1
3	B	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	K	0	1
4	M	0	1
5	E	0	4
5	N	0	4
6	F	0	2
6	O	0	2
8	H	0	3
8	Q	0	2
All	All	0	22

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	10	MET	C-O	-7.96	1.08	1.23
4	M	175	PRO	C-O	-7.27	1.08	1.23
8	Q	10	MET	C-O	-6.24	1.11	1.23
1	A	173	PRO	N-CD	6.24	1.56	1.47
2	C	237	MET	C-O	-5.85	1.12	1.23
4	D	288	LYS	C-O	-5.80	1.12	1.23
5	E	84	ALA	C-O	-5.66	1.12	1.23

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	93	LYS	CD-CE-NZ	12.38	140.16	111.70
5	N	93	LYS	CD-CE-NZ	12.36	140.13	111.70
5	N	121	ARG	NE-CZ-NH1	-8.83	115.89	120.30
5	E	121	ARG	NE-CZ-NH1	-8.83	115.89	120.30
5	N	51	LYS	CB-CA-C	-8.26	93.88	110.40
5	E	180	CYS	CA-CB-SG	-7.87	99.84	114.00
5	N	162	LEU	CA-CB-CG	7.24	131.94	115.30
5	E	162	LEU	CA-CB-CG	7.24	131.94	115.30
5	E	121	ARG	NE-CZ-NH2	6.72	123.66	120.30
5	N	121	ARG	NE-CZ-NH2	6.68	123.64	120.30
5	E	146	ARG	CB-CG-CD	6.57	128.69	111.60
5	N	146	ARG	CB-CG-CD	6.56	128.66	111.60
6	F	122	ASP	CB-CA-C	-6.42	97.55	110.40
6	F	100	GLU	N-CA-CB	-6.34	99.19	110.60
6	F	104	ARG	CB-CA-C	6.30	123.01	110.40
5	E	31	LYS	CD-CE-NZ	6.27	126.13	111.70
5	N	31	LYS	CD-CE-NZ	6.26	126.09	111.70
6	F	99	GLU	CA-C-N	-6.22	103.52	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	O	122	ASP	CB-CA-C	-6.21	97.97	110.40
3	B	229	ASN	CB-CA-C	5.94	122.28	110.40
1	A	456	ARG	CA-C-O	-5.75	108.04	120.10
6	F	112	PRO	N-CA-C	5.71	126.95	112.10
6	O	111	GLN	CB-CA-C	-5.70	99.00	110.40
5	N	146	ARG	CA-CB-CG	5.67	125.88	113.40
5	E	46	ASN	N-CA-C	-5.65	95.73	111.00
5	E	146	ARG	CA-CB-CG	5.64	125.81	113.40
1	A	455	MET	N-CA-CB	5.56	120.60	110.60
6	O	100	GLU	CB-CA-C	5.55	121.51	110.40
1	A	455	MET	CB-CA-C	-5.43	99.53	110.40
1	A	456	ARG	N-CA-C	-5.42	96.36	111.00
5	E	146	ARG	CG-CD-NE	5.39	123.12	111.80
6	O	118	GLU	CB-CA-C	5.39	121.18	110.40
5	N	146	ARG	CG-CD-NE	5.38	123.09	111.80
8	Q	87	GLU	CA-CB-CG	5.24	124.93	113.40
8	H	87	GLU	CA-CB-CG	5.24	124.93	113.40
3	B	344	LYS	CG-CD-CE	5.22	127.55	111.90
2	C	382	ARG	NE-CZ-NH1	5.21	122.91	120.30
3	K	344	LYS	CG-CD-CE	5.20	127.49	111.90
2	C	107	ARG	NE-CZ-NH1	5.18	122.89	120.30
2	L	107	ARG	NE-CZ-NH1	5.10	122.85	120.30
5	E	103	LEU	CA-CB-CG	5.10	127.03	115.30
5	N	103	LEU	CA-CB-CG	5.08	126.99	115.30
4	M	92	ARG	NE-CZ-NH2	5.08	122.84	120.30
2	L	382	ARG	NE-CZ-NH1	5.08	122.84	120.30
2	L	348	TYR	CB-CG-CD2	-5.04	117.97	121.00
5	N	35	ARG	NE-CZ-NH2	5.01	122.81	120.30

There are no chirality outliers.

All (22) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	456	ARG	Sidechain
3	B	230	ARG	Sidechain
5	E	190	ARG	Sidechain
5	E	192	ARG	Sidechain
5	E	209	GLY	Peptide
5	E	97	ASN	Peptide
6	F	104	ARG	Sidechain
6	F	99	GLU	Mainchain
8	H	10	MET	Mainchain

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Mol	Chain	Res	Type	Group
8	H	40	ILE	Peptide
8	H	41	PHE	Peptide
1	J	456	ARG	Sidechain
3	K	166	ARG	Sidechain
4	M	268	ARG	Sidechain
5	N	190	ARG	Sidechain
5	N	192	ARG	Sidechain
5	N	209	GLY	Peptide
5	N	97	ASN	Peptide
6	O	104	ARG	Sidechain
6	O	99	GLU	Mainchain
8	Q	40	ILE	Peptide
8	Q	41	PHE	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	12	0
1	J	3344	0	3323	7	0
2	C	3090	0	3129	3	0
2	L	3090	0	3129	7	0
3	B	2735	0	2774	3	0
3	K	2735	0	2774	3	0
4	D	1961	0	1890	4	0
4	M	1961	0	1890	7	0
5	E	1411	0	1390	20	0
5	N	1411	0	1390	29	0
6	F	624	0	583	20	0
6	O	633	0	589	38	0
7	G	1019	0	1034	1	0
7	P	1019	0	1034	0	0
8	H	773	0	736	2	0
8	Q	773	0	736	3	0
9	I	442	0	440	9	0
9	R	443	0	440	3	0
10	S	347	0	345	3	0
10	T	406	0	414	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	C	40	0	59	1	0
11	N	40	0	59	0	0
12	C	40	0	59	0	0
12	L	40	0	59	0	0
13	C	86	0	60	2	0
13	D	43	0	30	2	0
13	L	86	0	60	3	0
13	M	43	0	30	1	0
14	C	47	0	73	0	0
14	Q	47	0	73	0	0
15	C	41	0	50	2	0
16	C	43	0	60	1	0
16	L	43	0	60	4	0
17	C	27	0	0	0	0
17	L	27	0	0	0	0
18	D	38	0	55	2	0
18	N	38	0	55	0	0
19	L	55	0	66	0	0
All	All	32385	0	32271	168	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 3.

All (168) 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:N:162:LEU:HD12	5:N:164:CYS:SG	1.79	1.22
5:N:162:LEU:CD1	5:N:164:CYS:SG	2.40	1.08
6:O:111:GLN:HB3	6:O:112:PRO:HD2	1.39	1.04
5:N:162:LEU:CG	5:N:164:CYS:SG	2.46	1.04
5:N:162:LEU:HG	5:N:164:CYS:SG	2.01	1.00
6:O:99:GLU:HG2	6:O:100:GLU:N	1.93	0.83
6:O:109:GLN:HE21	6:O:114:TYR:HB2	1.41	0.83
6:O:111:GLN:HB3	6:O:112:PRO:CD	2.12	0.80
5:E:191:ILE:HD12	5:E:196:ALA:HB3	1.64	0.78
5:N:191:ILE:HD12	5:N:196:ALA:HB3	1.64	0.78
6:O:99:GLU:CG	6:O:100:GLU:N	2.48	0.76
9:R:23:ALA:HB2	10:S:39:LEU:HD22	1.68	0.75
5:N:162:LEU:HB3	5:N:164:CYS:SG	2.28	0.74
6:F:105:VAL:O	6:F:109:GLN:HG3	1.91	0.71
4:M:297:THR:HG21	5:N:42:VAL:HG11	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:198:LEU:HD22	16:L:401:UQ6:H4M3	1.72	0.69
5:N:190:ARG:HD2	5:N:192:ARG:HH11	1.57	0.69
6:O:103:GLU:O	6:O:105:VAL:N	2.26	0.68
5:N:128:GLU:OE2	5:N:187:ILE:HG21	1.94	0.68
15:C:406:CN5:H2	2:L:16:TYR:CE2	2.29	0.67
6:O:114:TYR:HA	6:O:117:LEU:HD23	1.77	0.66
5:E:132:VAL:HG21	5:E:192:ARG:HH12	1.61	0.65
6:F:99:GLU:O	6:F:102:ALA:N	2.30	0.64
2:C:16:TYR:O	16:C:407:UQ6:H4M2	1.96	0.64
6:O:101:CYS:HG	6:O:123:CYS:HG	0.65	0.64
6:F:106:LYS:C	6:F:108:GLN:H	1.99	0.64
5:N:162:LEU:CB	5:N:164:CYS:SG	2.86	0.64
6:O:99:GLU:C	6:O:101:CYS:N	2.52	0.62
6:O:105:VAL:O	6:O:107:ILE:N	2.32	0.62
5:E:165:VAL:HG21	2:L:263:LEU:O	1.99	0.62
6:F:114:TYR:C	6:F:116:ASP:N	2.52	0.62
6:O:121:GLU:HG2	6:O:122:ASP:N	2.14	0.62
6:F:121:GLU:HG2	6:F:122:ASP:N	2.14	0.61
6:O:99:GLU:C	6:O:102:ALA:H	2.06	0.59
6:O:97:HIS:HA	6:O:100:GLU:OE1	2.02	0.59
6:O:116:ASP:N	6:O:116:ASP:OD1	2.35	0.59
10:T:54:THR:HG22	10:T:57:LYS:HG2	1.85	0.58
6:F:114:TYR:CE2	6:F:120:LYS:HD3	2.38	0.58
9:I:15:ALA:HB2	10:T:33:TRP:CD1	2.39	0.58
6:F:112:PRO:O	6:F:114:TYR:N	2.37	0.58
7:G:125:VAL:HG11	1:J:361:THR:HG23	1.87	0.57
6:O:114:TYR:C	6:O:116:ASP:N	2.57	0.57
2:L:16:TYR:HD2	16:L:401:UQ6:H4M1	1.69	0.57
1:J:202:LEU:HD13	1:J:233:GLY:O	2.05	0.56
6:O:114:TYR:CG	6:O:115:ALA:N	2.72	0.56
5:N:128:GLU:CD	5:N:187:ILE:HG21	2.25	0.56
13:D:401:HEM:HMB1	13:D:401:HEM:HBB2	1.88	0.55
4:M:233:MET:HG3	4:M:234:VAL:HG23	1.88	0.55
1:A:202:LEU:HD13	1:A:233:GLY:O	2.05	0.55
4:D:233:MET:HG3	4:D:234:VAL:HG23	1.88	0.55
5:E:186:ASP:HB2	5:E:192:ARG:NE	2.22	0.55
6:O:99:GLU:HG2	6:O:100:GLU:H	1.71	0.54
6:O:99:GLU:O	6:O:102:ALA:N	2.40	0.54
6:O:112:PRO:O	6:O:114:TYR:N	2.41	0.54
3:K:54:PHE:CE2	3:K:172:ILE:HD13	2.43	0.54
6:F:114:TYR:O	6:F:115:ALA:C	2.46	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:114:TYR:O	6:F:116:ASP:N	2.41	0.53
13:M:401:HEM:HMB1	13:M:401:HEM:HBB2	1.90	0.53
5:N:166:PRO:HB2	5:N:176:TRP:CE3	2.44	0.53
13:L:405:HEM:HBB2	13:L:405:HEM:HHC	1.89	0.53
6:O:105:VAL:HG23	6:O:108:GLN:HG3	1.90	0.53
6:O:99:GLU:O	6:O:102:ALA:HB3	2.09	0.53
3:B:54:PHE:CE2	3:B:172:ILE:HD13	2.43	0.53
1:A:455:MET:O	9:I:14:ASN:HB3	2.09	0.53
6:O:105:VAL:HA	6:O:108:GLN:CG	2.39	0.53
5:E:128:GLU:OE1	5:E:187:ILE:HG21	2.09	0.52
13:C:403:HEM:HHA	13:C:403:HEM:HBD2	1.92	0.52
5:E:122:THR:HG22	5:E:125:GLU:HG3	1.91	0.52
5:N:122:THR:HG22	5:N:125:GLU:HG3	1.91	0.52
1:A:29:VAL:HG21	1:A:390:LEU:HD11	1.92	0.52
6:F:106:LYS:C	6:F:108:GLN:N	2.64	0.51
6:O:105:VAL:O	6:O:106:LYS:C	2.49	0.51
9:I:23:ALA:HB2	10:T:39:LEU:CD1	2.41	0.51
5:N:72:LYS:HG3	10:S:43:VAL:O	2.11	0.51
6:F:119:HIS:ND1	6:F:119:HIS:N	2.58	0.50
8:Q:83:LYS:NZ	6:O:121:GLU:OE2	2.41	0.50
6:O:105:VAL:HG13	6:O:106:LYS:H	1.76	0.50
13:L:403:HEM:HHA	13:L:403:HEM:HBD2	1.92	0.50
1:J:29:VAL:HG21	1:J:390:LEU:HD11	1.92	0.50
5:N:122:THR:HG22	5:N:125:GLU:CG	2.42	0.49
5:E:122:THR:HG22	5:E:125:GLU:CG	2.42	0.49
4:D:273:THR:HG23	18:D:402:7PH:H32A	1.94	0.49
13:D:401:HEM:HHA	13:D:401:HEM:HBA1	1.93	0.49
1:A:455:MET:HB3	1:A:456:ARG:HD3	1.94	0.49
5:N:162:LEU:HG	5:N:180:CYS:SG	2.53	0.49
9:R:25:ALA:HB3	10:S:43:VAL:HG21	1.95	0.48
6:O:110:GLN:OE1	6:O:111:GLN:N	2.47	0.48
13:C:404:HEM:HBA1	13:C:404:HEM:HHA	1.96	0.47
5:E:121:ARG:HH12	5:E:187:ILE:HG22	1.79	0.47
9:I:30:THR:HG22	10:T:61:LEU:HD22	1.96	0.47
3:B:201:VAL:HG13	3:B:206:LEU:HD11	1.96	0.47
4:M:280:LEU:HD21	5:N:66:LEU:HB2	1.96	0.47
5:N:121:ARG:HH12	5:N:187:ILE:HG22	1.79	0.47
6:F:99:GLU:C	6:F:101:CYS:N	2.68	0.47
6:O:105:VAL:HA	6:O:108:GLN:HG3	1.96	0.47
9:I:31:VAL:HG22	10:T:61:LEU:HD21	1.96	0.47
5:E:128:GLU:CD	5:E:187:ILE:HG21	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:O:99:GLU:C	6:O:101:CYS:H	2.16	0.46
1:A:169:PHE:O	1:A:172:THR:HB	2.16	0.46
2:L:44:ILE:HD12	16:L:401:UQ6:H202	1.98	0.46
6:F:104:ARG:HA	6:F:107:ILE:HG12	1.96	0.46
5:E:51:LYS:HA	5:E:54:SER:HB2	1.97	0.46
2:L:41:VAL:HA	16:L:401:UQ6:H203	1.97	0.46
3:K:201:VAL:HG13	3:K:206:LEU:HD11	1.97	0.46
6:F:105:VAL:O	6:F:105:VAL:HG12	2.15	0.46
5:E:111:TRP:HB3	5:E:116:VAL:HG21	1.98	0.46
5:E:162:LEU:HG	5:E:164:CYS:SG	2.56	0.46
1:A:356:ILE:HD12	1:A:454:MET:CE	2.46	0.46
5:N:95:GLU:HG2	5:N:95:GLU:O	2.16	0.46
5:E:137:LEU:HD21	5:E:192:ARG:HH11	1.81	0.45
6:F:119:HIS:HD2	8:H:86:ARG:HH12	1.65	0.45
6:O:103:GLU:O	6:O:104:ARG:C	2.54	0.45
9:I:23:ALA:HB2	10:T:39:LEU:HD12	1.98	0.45
1:A:172:THR:CG2	1:A:242:ALA:HA	2.47	0.45
6:O:103:GLU:HB3	6:O:104:ARG:H	1.69	0.45
9:R:8:LYS:HA	9:R:12:LYS:HB3	1.99	0.45
5:N:117:PHE:CG	5:N:176:TRP:HH2	2.35	0.45
6:O:94:LEU:HD23	6:O:130:LEU:HA	1.99	0.44
15:C:406:CN5:H32A	15:C:406:CN5:H3A	1.87	0.44
5:E:166:PRO:HB2	5:E:176:TRP:CE3	2.53	0.44
9:I:13:ARG:HG2	9:I:16:VAL:HG22	2.00	0.44
4:M:63:THR:HG22	8:Q:81:TYR:O	2.17	0.44
6:O:114:TYR:C	6:O:116:ASP:H	2.21	0.44
5:E:111:TRP:HZ3	5:E:156:LEU:HD21	1.83	0.44
6:O:109:GLN:NE2	6:O:114:TYR:HD1	2.16	0.44
3:K:166:ARG:HH12	3:K:168:SER:HB3	1.82	0.43
5:N:166:PRO:HB2	5:N:176:TRP:CZ3	2.53	0.43
1:A:29:VAL:HG23	1:A:40:THR:O	2.18	0.43
6:F:106:LYS:O	6:F:108:GLN:N	2.47	0.43
6:O:111:GLN:CB	6:O:112:PRO:CD	2.88	0.43
6:F:103:GLU:O	6:F:103:GLU:HG3	2.17	0.43
6:F:119:HIS:HD2	8:H:86:ARG:NH1	2.16	0.43
4:M:203:PRO:O	4:M:206:VAL:HG12	2.18	0.43
2:C:263:LEU:HD21	5:N:110:LYS:HD3	2.00	0.43
10:T:21:ARG:HA	10:T:24:THR:HG22	2.01	0.43
5:N:159:CYS:HB2	5:N:163:GLY:H	1.83	0.43
1:A:172:THR:HG23	1:A:242:ALA:HA	2.01	0.43
4:M:286:TRP:CD1	8:Q:37:LEU:HD22	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:29:VAL:HG23	1:J:40:THR:O	2.18	0.42
6:O:104:ARG:O	6:O:105:VAL:O	2.36	0.42
1:J:41:GLU:HG3	1:J:390:LEU:HD22	2.02	0.42
1:A:41:GLU:HG3	1:A:390:LEU:HD22	2.02	0.42
1:A:29:VAL:HG22	1:A:31:GLN:OE1	2.19	0.42
4:D:139:ASP:OD1	4:D:143:ASN:N	2.52	0.42
1:J:29:VAL:HG22	1:J:31:GLN:OE1	2.19	0.42
5:N:45:GLU:HG2	5:N:46:ASN:OD1	2.19	0.42
5:E:166:PRO:HB2	5:E:176:TRP:HE3	1.85	0.42
6:O:105:VAL:HG23	6:O:108:GLN:HE21	1.85	0.41
1:J:356:ILE:HD11	1:J:427:TRP:CH2	2.55	0.41
5:N:93:LYS:HD3	5:N:213:ILE:CG2	2.50	0.41
5:N:162:LEU:HG	5:N:164:CYS:HG	1.82	0.41
4:D:203:PRO:O	4:D:206:VAL:HG12	2.18	0.41
5:E:93:LYS:HD3	5:E:213:ILE:CG2	2.50	0.41
5:E:212:VAL:O	5:E:212:VAL:HG23	2.21	0.41
9:I:15:ALA:HB2	10:T:33:TRP:NE1	2.35	0.41
5:N:212:VAL:O	5:N:212:VAL:HG23	2.21	0.41
6:O:105:VAL:HG13	6:O:106:LYS:N	2.36	0.41
11:C:401:6PH:H3C	18:D:402:7PH:H38A	2.02	0.41
6:F:122:ASP:HB3	6:F:123:CYS:H	1.58	0.40
6:O:105:VAL:HG22	6:O:106:LYS:N	2.36	0.40
1:A:403:LEU:HD23	3:B:27:LYS:HG3	2.03	0.40
2:C:29:TRP:HB3	2:C:99:LYS:HG3	2.04	0.40
5:E:65:LEU:HD11	9:I:24:GLY:HA3	2.04	0.40
5:N:95:GLU:HB2	5:N:212:VAL:O	2.22	0.40
5:E:159:CYS:HA	5:E:200:LEU:HD11	2.04	0.40
6:F:117:LEU:HD22	6:F:117:LEU:HA	1.68	0.40
2:L:184:TYR:CE2	13:L:403:HEM:HBC1	2.57	0.40
4:M:286:TRP:CH2	5:N:56:ALA:HA	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	429/431 (100%)	410 (96%)	19 (4%)	0	100	100
1	J	429/431 (100%)	411 (96%)	18 (4%)	0	100	100
2	C	383/385 (100%)	375 (98%)	8 (2%)	0	100	100
2	L	383/385 (100%)	375 (98%)	8 (2%)	0	100	100
3	B	350/352 (99%)	337 (96%)	13 (4%)	0	100	100
3	K	350/352 (99%)	337 (96%)	13 (4%)	0	100	100
4	D	246/248 (99%)	240 (98%)	6 (2%)	0	100	100
4	M	246/248 (99%)	240 (98%)	6 (2%)	0	100	100
5	E	183/185 (99%)	156 (85%)	25 (14%)	2 (1%)	12	17
5	N	183/185 (99%)	156 (85%)	25 (14%)	2 (1%)	12	17
6	F	72/75 (96%)	56 (78%)	8 (11%)	8 (11%)	0	0
6	O	73/75 (97%)	58 (80%)	8 (11%)	7 (10%)	0	0
7	G	124/126 (98%)	123 (99%)	1 (1%)	0	100	100
7	P	124/126 (98%)	122 (98%)	2 (2%)	0	100	100
8	H	91/93 (98%)	83 (91%)	8 (9%)	0	100	100
8	Q	91/93 (98%)	83 (91%)	8 (9%)	0	100	100
9	I	52/55 (94%)	49 (94%)	3 (6%)	0	100	100
9	R	52/55 (94%)	46 (88%)	6 (12%)	0	100	100
10	S	42/52 (81%)	38 (90%)	4 (10%)	0	100	100
10	T	49/52 (94%)	41 (84%)	8 (16%)	0	100	100
All	All	3952/4004 (99%)	3736 (94%)	197 (5%)	19 (0%)	27	36

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	180	CYS
5	E	193	LYS
6	F	113	GLY
6	O	104	ARG
6	O	105	VAL
6	O	110	GLN
6	O	111	GLN
6	O	113	GLY

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Mol	Chain	Res	Type
6	F	99	GLU
6	F	100	GLU
6	F	107	ILE
6	F	110	GLN
6	F	108	GLN
5	N	193	LYS
6	O	103	GLU
6	O	106	LYS
6	F	111	GLN
6	F	112	PRO
5	N	96	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	370/370 (100%)	361 (98%)	9 (2%)	44	63
1	J	370/370 (100%)	361 (98%)	9 (2%)	44	63
2	C	338/338 (100%)	338 (100%)	0	100	100
2	L	338/338 (100%)	338 (100%)	0	100	100
3	B	301/301 (100%)	289 (96%)	12 (4%)	27	43
3	K	301/301 (100%)	290 (96%)	11 (4%)	29	46
4	D	206/206 (100%)	201 (98%)	5 (2%)	44	63
4	M	206/206 (100%)	201 (98%)	5 (2%)	44	63
5	E	151/151 (100%)	132 (87%)	19 (13%)	3	4
5	N	151/151 (100%)	136 (90%)	15 (10%)	6	9
6	F	67/68 (98%)	59 (88%)	8 (12%)	4	5
6	O	68/68 (100%)	62 (91%)	6 (9%)	8	12
7	G	110/110 (100%)	109 (99%)	1 (1%)	75	87
7	P	110/110 (100%)	109 (99%)	1 (1%)	75	87
8	H	77/77 (100%)	72 (94%)	5 (6%)	14	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	Q	77/77 (100%)	72 (94%)	5 (6%)	14	22
9	I	44/45 (98%)	43 (98%)	1 (2%)	45	64
9	R	45/45 (100%)	44 (98%)	1 (2%)	47	65
10	S	35/43 (81%)	32 (91%)	3 (9%)	8	13
10	T	42/43 (98%)	40 (95%)	2 (5%)	21	35
All	All	3407/3418 (100%)	3289 (96%)	118 (4%)	33	49

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	GLN
1	A	143	SER
1	A	228	LEU
1	A	232	THR
1	A	238	LEU
1	A	306	ILE
1	A	341	ASP
1	A	399	SER
1	A	456	ARG
3	B	18	THR
3	B	81	THR
3	B	96	ASP
3	B	229	ASN
3	B	249	SER
3	B	265	SER
3	B	268	SER
3	B	272	SER
3	B	294	SER
3	B	332	VAL
3	B	337	GLU
3	B	344	LYS
4	D	222	SER
4	D	279	SER
4	D	288	LYS
4	D	308	ARG
4	D	309	LYS
5	E	50	ASP
5	E	51	LYS
5	E	54	SER
5	E	107	VAL

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Mol	Chain	Res	Type
5	E	121	ARG
5	E	122	THR
5	E	132	VAL
5	E	134	MET
5	E	135	SER
5	E	137	LEU
5	E	146	ARG
5	E	148	LYS
5	E	176	TRP
5	E	190	ARG
5	E	191	ILE
5	E	192	ARG
5	E	193	LYS
5	E	206	GLU
5	E	210	ASP
6	F	88	THR
6	F	104	ARG
6	F	108	GLN
6	F	110	GLN
6	F	116	ASP
6	F	117	LEU
6	F	119	HIS
6	F	120	LYS
7	G	31	GLN
8	H	37	LEU
8	H	41	PHE
8	H	46	PHE
8	H	82	SER
8	H	87	GLU
9	I	14	ASN
1	J	127	GLN
1	J	143	SER
1	J	228	LEU
1	J	232	THR
1	J	238	LEU
1	J	306	ILE
1	J	399	SER
1	J	454	MET
1	J	456	ARG
3	K	18	THR
3	K	81	THR
3	K	96	ASP

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Mol	Chain	Res	Type
3	K	166	ARG
3	K	249	SER
3	K	265	SER
3	K	268	SER
3	K	272	SER
3	K	294	SER
3	K	332	VAL
3	K	344	LYS
4	M	222	SER
4	M	268	ARG
4	M	279	SER
4	M	308	ARG
4	M	309	LYS
5	N	54	SER
5	N	107	VAL
5	N	121	ARG
5	N	122	THR
5	N	128	GLU
5	N	132	VAL
5	N	134	MET
5	N	135	SER
5	N	137	LEU
5	N	146	ARG
5	N	148	LYS
5	N	191	ILE
5	N	193	LYS
5	N	206	GLU
5	N	210	ASP
8	Q	37	LEU
8	Q	41	PHE
8	Q	46	PHE
8	Q	82	SER
8	Q	87	GLU
6	O	99	GLU
6	O	103	GLU
6	O	109	GLN
6	O	116	ASP
6	O	117	LEU
6	O	118	GLU
7	P	31	GLN
9	R	37	THR
10	S	14	HIS

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Mol	Chain	Res	Type
10	S	43	VAL
10	S	46	GLU
10	T	54	THR
10	T	57	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	199	ASN
1	A	221	ASN
7	G	86	HIS
7	G	122	ASN
8	H	47	ASN
1	J	199	ASN
1	J	221	ASN
5	N	141	GLN
8	Q	47	ASN
6	O	109	GLN
7	P	86	HIS
9	R	29	GLN
10	S	14	HIS

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](#)

20 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
15	CN5	C	406	-	40,40,40	0.43	0	44,48,48	0.60	0
13	HEM	D	401	4	41,50,50	1.47	5 (12%)	45,82,82	1.59	8 (17%)
13	HEM	C	403	2	41,50,50	1.53	4 (9%)	45,82,82	1.54	10 (22%)
14	8PE	Q	101	-	46,46,46	0.91	3 (6%)	49,51,51	0.90	2 (4%)
17	A1D6K	L	406	-	26,29,29	4.51	17 (65%)	27,39,39	1.87	7 (25%)
13	HEM	C	404	2	41,50,50	1.47	5 (12%)	45,82,82	1.32	7 (15%)
18	7PH	N	402	-	37,37,37	0.96	4 (10%)	41,42,42	0.93	2 (4%)
11	6PH	C	401	-	39,39,39	0.95	4 (10%)	43,44,44	1.05	2 (4%)
11	6PH	N	401	-	39,39,39	0.99	4 (10%)	43,44,44	1.17	3 (6%)
17	A1D6K	C	408	-	26,29,29	4.50	18 (69%)	27,39,39	1.88	7 (25%)
19	CN3	L	404	-	54,54,54	1.15	8 (14%)	60,66,66	1.01	4 (6%)
13	HEM	L	403	2	41,50,50	1.54	4 (9%)	45,82,82	1.57	10 (22%)
16	UQ6	L	401	-	43,43,43	1.87	11 (25%)	51,55,55	2.35	15 (29%)
12	9PE	C	402	-	39,39,39	0.96	4 (10%)	42,44,44	0.87	2 (4%)
12	9PE	L	402	-	39,39,39	0.95	4 (10%)	42,44,44	0.85	2 (4%)
14	8PE	C	405	-	46,46,46	0.92	4 (8%)	49,51,51	1.00	2 (4%)
18	7PH	D	402	-	37,37,37	0.61	1 (2%)	41,42,42	0.68	2 (4%)
16	UQ6	C	407	-	43,43,43	1.70	10 (23%)	51,55,55	1.73	14 (27%)
13	HEM	M	401	4	41,50,50	1.44	4 (9%)	45,82,82	1.40	6 (13%)
13	HEM	L	405	2	41,50,50	1.49	4 (9%)	45,82,82	1.42	5 (11%)

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
15	CN5	C	406	-	-	26/44/44/44	-
13	HEM	D	401	4	-	5/12/54/54	-
13	HEM	C	403	2	-	6/12/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	8PE	Q	101	-	-	24/50/50/50	-
17	A1D6K	L	406	-	-	3/16/21/21	0/3/3/3
13	HEM	C	404	2	-	7/12/54/54	-
18	7PH	N	402	-	-	22/39/39/39	-
11	6PH	C	401	-	-	21/41/41/41	-
11	6PH	N	401	-	-	19/41/41/41	-
17	A1D6K	C	408	-	-	3/16/21/21	0/3/3/3
19	CN3	L	404	-	-	28/65/65/65	-
13	HEM	L	403	2	-	4/12/54/54	-
16	UQ6	L	401	-	-	12/39/39/39	0/1/1/1
12	9PE	C	402	-	-	22/43/43/43	-
12	9PE	L	402	-	-	17/43/43/43	-
14	8PE	C	405	-	-	25/50/50/50	-
18	7PH	D	402	-	-	21/39/39/39	-
16	UQ6	C	407	-	-	9/39/39/39	0/1/1/1
13	HEM	M	401	4	-	0/12/54/54	-
13	HEM	L	405	2	-	3/12/54/54	-

All (118) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	C	408	A1D6K	C3-C8	8.97	1.52	1.40
17	L	406	A1D6K	C3-C8	8.95	1.52	1.40
17	L	406	A1D6K	C15-C16	7.73	1.52	1.38
17	L	406	A1D6K	C18-C17	7.73	1.52	1.38
17	C	408	A1D6K	C18-C17	7.71	1.52	1.38
17	C	408	A1D6K	C15-C16	7.69	1.52	1.38
17	C	408	A1D6K	C14-C13	7.23	1.52	1.38
17	L	406	A1D6K	C14-C13	7.19	1.52	1.38
17	C	408	A1D6K	C12-C10	6.59	1.50	1.39
17	L	406	A1D6K	C12-C10	6.58	1.50	1.39
17	L	406	A1D6K	C5-C4	6.37	1.52	1.38
17	C	408	A1D6K	C5-C4	6.34	1.52	1.38
17	L	406	A1D6K	C6-C7	6.32	1.52	1.38
17	C	408	A1D6K	C6-C7	6.29	1.52	1.38
16	L	401	UQ6	C7-C6	6.20	1.58	1.51
16	C	407	UQ6	C7-C6	4.98	1.57	1.51
17	C	408	A1D6K	C4-C3	-4.91	1.31	1.39
13	L	403	HEM	C3C-C2C	-4.87	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	L	406	A1D6K	C4-C3	-4.86	1.31	1.39
13	C	403	HEM	C3C-C2C	-4.76	1.33	1.40
17	L	406	A1D6K	C7-C8	-4.71	1.31	1.39
17	C	408	A1D6K	C7-C8	-4.67	1.31	1.39
13	C	404	HEM	C3C-C2C	-4.30	1.34	1.40
13	L	405	HEM	C3C-C2C	-4.26	1.34	1.40
13	D	401	HEM	C3C-C2C	-4.13	1.34	1.40
13	M	401	HEM	C3C-C2C	-4.08	1.34	1.40
17	L	406	A1D6K	C10-N2	4.06	1.39	1.34
17	C	408	A1D6K	C10-N2	3.99	1.39	1.34
17	C	408	A1D6K	C14-C15	-3.87	1.31	1.38
17	L	406	A1D6K	C14-C15	-3.85	1.31	1.38
13	L	405	HEM	C3C-CAC	3.60	1.55	1.47
16	L	401	UQ6	C16-C14	3.58	1.58	1.51
13	D	401	HEM	C3C-CAC	3.52	1.55	1.47
13	M	401	HEM	C3C-CAC	3.50	1.55	1.47
13	C	404	HEM	C3C-CAC	3.47	1.54	1.47
17	L	406	A1D6K	C18-C13	-3.46	1.31	1.38
17	L	406	A1D6K	C17-C16	-3.42	1.31	1.38
17	C	408	A1D6K	C18-C13	-3.41	1.31	1.38
17	C	408	A1D6K	C17-C16	-3.39	1.31	1.38
16	C	407	UQ6	C16-C14	3.38	1.58	1.51
17	C	408	A1D6K	N2-N3	-3.36	1.33	1.39
17	L	406	A1D6K	N2-N3	-3.35	1.33	1.39
17	C	408	A1D6K	O1-C2	3.31	1.39	1.34
17	L	406	A1D6K	O1-C2	3.28	1.39	1.34
16	L	401	UQ6	C11-C9	3.20	1.57	1.51
13	L	403	HEM	C3C-CAC	3.07	1.54	1.47
13	C	403	HEM	C3C-CAC	3.02	1.54	1.47
16	C	407	UQ6	C26-C24	2.93	1.57	1.51
13	D	401	HEM	CAB-C3B	2.93	1.55	1.47
16	L	401	UQ6	C21-C19	2.92	1.57	1.51
13	M	401	HEM	CAB-C3B	2.90	1.55	1.47
13	C	404	HEM	CAB-C3B	2.86	1.55	1.47
16	L	401	UQ6	C26-C24	2.84	1.57	1.51
13	L	405	HEM	CAB-C3B	2.84	1.55	1.47
16	C	407	UQ6	C12-C13	2.82	1.59	1.50
14	Q	101	8PE	O21-C2	-2.78	1.39	1.46
13	L	403	HEM	CAB-C3B	2.75	1.54	1.47
13	C	403	HEM	CAB-C3B	2.72	1.54	1.47
16	L	401	UQ6	C12-C13	2.69	1.59	1.50
16	C	407	UQ6	O3-C3	2.69	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	N	401	6PH	O21-C21	2.62	1.41	1.34
16	C	407	UQ6	C11-C9	2.61	1.56	1.51
16	L	401	UQ6	C31-C29	2.59	1.56	1.51
19	L	404	CN3	O51-C2'	-2.58	1.40	1.46
16	C	407	UQ6	C21-C19	2.58	1.56	1.51
14	C	405	8PE	O21-C2	-2.58	1.40	1.46
17	L	406	A1D6K	C6-C5	-2.58	1.31	1.38
17	C	408	A1D6K	C6-C5	-2.56	1.31	1.38
16	L	401	UQ6	C7-C8	2.50	1.56	1.50
13	L	405	HEM	FE-ND	2.49	2.09	1.96
14	Q	101	8PE	O31-C3	-2.49	1.39	1.45
13	L	403	HEM	FE-ND	2.49	2.09	1.96
13	C	403	HEM	FE-ND	2.48	2.09	1.96
19	L	404	CN3	O21-C2	-2.48	1.40	1.46
16	L	401	UQ6	O3-C3	2.45	1.42	1.38
14	C	405	8PE	O31-C31	2.45	1.40	1.33
11	N	401	6PH	O31-C31	2.43	1.40	1.33
19	L	404	CN3	O31-C3	-2.42	1.39	1.45
18	N	402	7PH	O31-C31	2.40	1.40	1.33
12	C	402	9PE	O31-C31	2.36	1.40	1.33
13	C	404	HEM	CAA-C2A	2.35	1.55	1.52
18	N	402	7PH	O21-C2	-2.35	1.40	1.46
17	C	408	A1D6K	O1-C1	-2.35	1.39	1.45
14	C	405	8PE	O31-C3	-2.35	1.39	1.45
11	C	401	6PH	O21-C2	-2.34	1.40	1.46
13	D	401	HEM	CAA-C2A	2.33	1.55	1.52
12	L	402	9PE	O31-C31	2.32	1.40	1.33
17	L	406	A1D6K	O1-C1	-2.32	1.39	1.45
16	C	407	UQ6	O4-C4	2.30	1.42	1.38
11	C	401	6PH	O31-C3	-2.30	1.39	1.45
19	L	404	CN3	O31-C31	2.28	1.40	1.33
11	C	401	6PH	O31-C31	2.26	1.39	1.33
12	C	402	9PE	O21-C2	-2.25	1.41	1.46
11	N	401	6PH	O31-C3	-2.25	1.40	1.45
19	L	404	CN3	O41-C3'	-2.25	1.40	1.45
11	C	401	6PH	O21-C21	2.25	1.40	1.34
19	L	404	CN3	O51-C51	2.24	1.40	1.34
18	N	402	7PH	O21-C21	2.23	1.40	1.34
16	L	401	UQ6	C17-C18	2.23	1.57	1.50
18	D	402	7PH	P-O13	-2.22	1.46	1.54
19	L	404	CN3	O41-C41	2.21	1.39	1.33
12	C	402	9PE	O31-C3	-2.21	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	L	402	9PE	O21-C2	-2.19	1.41	1.46
19	L	404	CN3	O21-C21	2.19	1.40	1.34
12	L	402	9PE	O21-C21	2.15	1.40	1.34
13	C	404	HEM	FE-ND	2.14	2.07	1.96
14	Q	101	8PE	O31-C31	2.12	1.39	1.33
12	L	402	9PE	O31-C3	-2.12	1.40	1.45
14	C	405	8PE	O21-C21	2.11	1.40	1.34
11	N	401	6PH	O21-C2	-2.11	1.41	1.46
18	N	402	7PH	O31-C3	-2.10	1.40	1.45
16	C	407	UQ6	C7-C8	2.10	1.55	1.50
16	L	401	UQ6	C27-C28	2.08	1.57	1.50
16	C	407	UQ6	C17-C18	2.06	1.57	1.50
12	C	402	9PE	O21-C21	2.05	1.40	1.34
13	D	401	HEM	CMB-C2B	2.02	1.55	1.50
13	M	401	HEM	CAA-C2A	2.02	1.55	1.52
17	C	408	A1D6K	C16-CL1	2.00	1.78	1.74

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	L	401	UQ6	C6-C7-C8	9.29	126.88	112.17
16	L	401	UQ6	C1M-C1-C2	-5.10	111.85	120.50
11	N	401	6PH	O21-C21-C22	4.90	122.05	111.50
17	C	408	A1D6K	C12-C10-N2	-4.57	105.64	110.44
13	D	401	HEM	CBA-CAA-C2A	4.55	120.38	112.62
17	C	408	A1D6K	C19-O4-N1	4.55	114.91	109.99
17	L	406	A1D6K	C12-C10-N2	-4.54	105.68	110.44
17	L	406	A1D6K	C19-O4-N1	4.46	114.82	109.99
17	L	406	A1D6K	C11-N3-N2	4.29	117.10	112.72
16	C	407	UQ6	C6-C7-C8	-4.27	105.39	112.17
16	C	407	UQ6	C20-C19-C21	4.22	122.38	115.27
17	C	408	A1D6K	C11-N3-N2	4.20	117.01	112.72
11	C	401	6PH	O21-C21-C22	4.08	120.28	111.50
16	L	401	UQ6	C26-C27-C28	3.95	124.88	111.88
13	L	403	HEM	C4C-CHD-C1D	3.84	127.62	122.56
13	C	403	HEM	C4C-CHD-C1D	3.82	127.60	122.56
16	L	401	UQ6	C15-C14-C16	3.70	121.49	115.27
16	C	407	UQ6	C1M-C1-C2	-3.67	114.28	120.50
16	L	401	UQ6	C1M-C1-C6	3.63	125.69	120.42
16	L	401	UQ6	C20-C19-C18	-3.59	114.47	123.68
13	L	405	HEM	C1B-NB-C4B	3.46	108.65	105.07
14	C	405	8PE	O21-C21-C22	3.45	118.94	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	L	401	UQ6	C2-C1-C6	3.39	122.43	118.75
16	L	401	UQ6	C16-C17-C18	-3.36	100.84	111.88
16	L	401	UQ6	C16-C14-C13	-3.28	114.48	121.12
13	C	403	HEM	CAD-C3D-C4D	3.21	130.26	124.66
13	L	403	HEM	CAD-C3D-C4D	3.21	130.26	124.66
16	C	407	UQ6	C25-C24-C26	3.19	120.64	115.27
13	L	405	HEM	C4B-CHC-C1C	3.18	126.75	122.56
12	L	402	9PE	O21-C21-C22	3.17	118.33	111.50
18	N	402	7PH	O21-C21-C22	3.10	118.18	111.50
19	L	404	CN3	O21-C21-C22	3.09	118.15	111.50
14	Q	101	8PE	O21-C21-C22	3.04	118.05	111.50
16	L	401	UQ6	C21-C19-C18	3.01	127.22	121.12
16	C	407	UQ6	C1M-C1-C6	2.99	124.76	120.42
13	L	405	HEM	CHC-C4B-C3B	2.96	129.10	124.57
13	L	405	HEM	C3B-C2B-C1B	2.95	108.68	106.49
13	D	401	HEM	C4C-CHD-C1D	2.95	126.45	122.56
13	D	401	HEM	CAA-C2A-C3A	-2.95	118.78	127.25
16	C	407	UQ6	C11-C9-C8	2.94	127.06	121.12
13	M	401	HEM	C4D-ND-C1D	2.94	108.11	105.07
18	D	402	7PH	O21-C21-C22	2.93	117.81	111.50
13	C	404	HEM	C1B-NB-C4B	2.92	108.09	105.07
13	D	401	HEM	C4D-ND-C1D	2.90	108.07	105.07
13	D	401	HEM	C4A-C3A-C2A	2.84	108.97	107.00
13	C	404	HEM	C4B-CHC-C1C	2.84	126.30	122.56
11	N	401	6PH	O21-C21-O22	-2.84	116.85	123.70
19	L	404	CN3	O51-C51-C52	2.83	117.60	111.50
16	C	407	UQ6	C10-C9-C8	-2.83	116.42	123.68
16	L	401	UQ6	C17-C16-C14	2.79	122.17	112.98
17	L	406	A1D6K	C9-C8-C3	-2.75	120.73	123.63
13	L	403	HEM	C1B-NB-C4B	2.71	107.88	105.07
17	C	408	A1D6K	C9-C8-C3	-2.71	120.77	123.63
13	M	401	HEM	CMC-C2C-C3C	2.67	129.68	124.68
13	C	403	HEM	C1B-NB-C4B	2.67	107.83	105.07
14	C	405	8PE	O31-C31-C32	2.66	120.27	111.91
13	M	401	HEM	C4C-CHD-C1D	2.66	126.06	122.56
17	C	408	A1D6K	C3-N1-C2	-2.65	120.95	127.60
17	L	406	A1D6K	C3-N1-C2	-2.63	121.00	127.60
19	L	404	CN3	O31-C31-C32	2.59	118.18	111.38
16	L	401	UQ6	C26-C24-C23	2.58	126.33	121.12
16	L	401	UQ6	C25-C24-C23	-2.54	117.17	123.68
13	D	401	HEM	CMC-C2C-C3C	2.51	129.37	124.68
16	C	407	UQ6	C20-C19-C18	-2.49	117.30	123.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	L	403	HEM	C4D-ND-C1D	2.46	107.62	105.07
16	L	401	UQ6	C27-C28-C29	2.46	133.59	127.66
12	C	402	9PE	O31-C31-C32	2.44	119.57	111.91
13	C	403	HEM	C4A-C3A-C2A	2.43	108.69	107.00
13	M	401	HEM	CMA-C3A-C4A	-2.43	124.73	128.46
13	L	403	HEM	C4A-C3A-C2A	2.43	108.69	107.00
13	C	404	HEM	C4D-ND-C1D	2.43	107.58	105.07
11	C	401	6PH	O31-C31-C32	2.42	119.51	111.91
16	L	401	UQ6	C22-C23-C24	-2.42	121.83	127.66
13	C	403	HEM	C4D-ND-C1D	2.42	107.57	105.07
13	C	403	HEM	CAD-C3D-C2D	-2.41	123.39	127.88
16	C	407	UQ6	C25-C24-C23	-2.40	117.52	123.68
13	L	403	HEM	CAD-C3D-C2D	-2.40	123.41	127.88
18	N	402	7PH	O31-C31-C32	2.35	119.27	111.91
13	C	404	HEM	C4A-C3A-C2A	2.33	108.61	107.00
13	C	403	HEM	C4B-CHC-C1C	2.31	125.61	122.56
13	L	403	HEM	CBA-CAA-C2A	-2.30	108.70	112.62
13	L	403	HEM	C2C-C3C-C4C	2.29	108.50	106.90
12	C	402	9PE	O21-C21-C22	2.29	116.43	111.50
13	L	403	HEM	C4B-CHC-C1C	2.27	125.55	122.56
13	C	403	HEM	CBA-CAA-C2A	-2.27	108.75	112.62
19	L	404	CN3	O41-C41-C42	2.24	118.94	111.91
13	M	401	HEM	C4A-C3A-C2A	2.23	108.55	107.00
18	D	402	7PH	O11-P-O14	2.23	112.72	106.47
13	C	404	HEM	CBA-CAA-C2A	2.22	116.40	112.62
13	C	404	HEM	CMC-C2C-C3C	2.21	128.81	124.68
14	Q	101	8PE	O31-C31-C32	2.20	118.83	111.91
16	C	407	UQ6	O3-C3-C2	2.18	123.69	119.00
13	L	405	HEM	C4D-ND-C1D	2.17	107.32	105.07
16	C	407	UQ6	C3M-O3-C3	2.16	120.69	114.78
13	D	401	HEM	CAA-CBA-CGA	-2.15	107.73	113.76
13	D	401	HEM	CMB-C2B-C1B	-2.10	121.84	125.04
13	C	403	HEM	C2C-C3C-C4C	2.10	108.36	106.90
12	L	402	9PE	O31-C31-C32	2.10	118.49	111.91
17	C	408	A1D6K	C14-C13-N3	2.10	120.99	119.15
16	C	407	UQ6	C4M-O4-C4	2.08	120.47	114.78
17	L	406	A1D6K	C14-C13-N3	2.08	120.97	119.15
13	L	403	HEM	C1D-C2D-C3D	2.06	109.13	106.96
13	M	401	HEM	CAA-CBA-CGA	-2.06	107.98	113.76
11	N	401	6PH	C33-C32-C31	-2.06	106.13	113.62
13	C	404	HEM	CMA-C3A-C4A	-2.05	125.32	128.46
16	C	407	UQ6	C2-C1-C6	2.04	120.96	118.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	C	408	A1D6K	O1-C2-O2	-2.03	120.81	124.63
16	C	407	UQ6	C22-C23-C24	-2.02	122.79	127.66
17	L	406	A1D6K	O1-C2-O2	-2.02	120.83	124.63
13	C	403	HEM	C1D-C2D-C3D	2.01	109.07	106.96

There are no chirality outliers.

All (277) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	C	401	6PH	C22-C21-O21-C2
11	N	401	6PH	O22-C21-O21-C2
11	N	401	6PH	C22-C21-O21-C2
12	C	402	9PE	C1-O11-P-O12
12	C	402	9PE	O13-C11-C12-N
13	C	403	HEM	C2D-C3D-CAD-CBD
13	C	404	HEM	C1A-C2A-CAA-CBA
13	C	404	HEM	C3A-C2A-CAA-CBA
13	D	401	HEM	C1A-C2A-CAA-CBA
13	D	401	HEM	C3A-C2A-CAA-CBA
13	L	403	HEM	C2D-C3D-CAD-CBD
14	C	405	8PE	C1-O11-P-O12
14	C	405	8PE	C1-O11-P-O13
14	C	405	8PE	C1-O11-P-O14
14	Q	101	8PE	C1-O11-P-O14
15	C	406	CN5	C1-O11-P-O12
15	C	406	CN5	C1-O11-P-O14
15	C	406	CN5	CC-O13-P-O11
15	C	406	CN5	CC-O13-P-O12
15	C	406	CN5	CC-O13-P-O14
15	C	406	CN5	C32-C31-O31-C3
15	C	406	CN5	CA-O3'-P'-O1'
15	C	406	CN5	CA-O3'-P'-O2'
16	L	401	UQ6	C1-C6-C7-C8
16	L	401	UQ6	C6-C7-C8-C9
16	L	401	UQ6	C13-C14-C16-C17
16	L	401	UQ6	C15-C14-C16-C17
16	L	401	UQ6	C24-C26-C27-C28
16	L	401	UQ6	C26-C27-C28-C29
16	L	401	UQ6	C29-C31-C32-C33
18	D	402	7PH	O22-C21-O21-C2
18	N	402	7PH	C1-O11-P-O12
18	N	402	7PH	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
18	N	402	7PH	C1-O11-P-O14
19	L	404	CN3	CA-O3'-P'-O2'
15	C	406	CN5	O32-C31-O31-C3
19	L	404	CN3	C42-C41-O41-C3'
11	C	401	6PH	O32-C31-O31-C3
14	C	405	8PE	O32-C31-O31-C3
18	D	402	7PH	O32-C31-O31-C3
19	L	404	CN3	O42-C41-O41-C3'
11	C	401	6PH	O22-C21-O21-C2
11	C	401	6PH	C32-C31-O31-C3
14	C	405	8PE	C32-C31-O31-C3
18	D	402	7PH	C32-C31-O31-C3
18	D	402	7PH	C22-C21-O21-C2
12	C	402	9PE	C32-C31-O31-C3
13	C	403	HEM	C4D-C3D-CAD-CBD
13	L	403	HEM	C4D-C3D-CAD-CBD
12	C	402	9PE	O32-C31-O31-C3
15	C	406	CN5	O42-C41-O41-C3'
15	C	406	CN5	C42-C41-O41-C3'
11	C	401	6PH	C36-C37-C38-C39
11	N	401	6PH	C32-C33-C34-C35
16	C	407	UQ6	C20-C19-C21-C22
16	C	407	UQ6	C25-C24-C26-C27
16	L	401	UQ6	C20-C19-C21-C22
16	C	407	UQ6	C18-C19-C21-C22
16	C	407	UQ6	C23-C24-C26-C27
16	L	401	UQ6	C18-C19-C21-C22
16	C	407	UQ6	C9-C11-C12-C13
19	L	404	CN3	C46-C47-C48-C49
14	Q	101	8PE	C28-C29-C2A-C2B
14	Q	101	8PE	C32-C31-O31-C3
16	C	407	UQ6	C4-C3-O3-C3M
11	C	401	6PH	C38-C39-C3A-C3B
15	C	406	CN5	O3'-CA-CB-OA
19	L	404	CN3	OA-CB-CC-O13
11	N	401	6PH	C21-C22-C23-C24
14	Q	101	8PE	O32-C31-O31-C3
16	C	407	UQ6	C19-C21-C22-C23
16	L	401	UQ6	C9-C11-C12-C13
11	C	401	6PH	C21-C22-C23-C24
14	C	405	8PE	C22-C21-O21-C2
14	Q	101	8PE	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
15	C	406	CN5	C1-O11-P-O13
15	C	406	CN5	C1'-O1'-P'-O3'
19	L	404	CN3	CC-O13-P-O11
12	C	402	9PE	C24-C25-C26-C27
18	D	402	7PH	C31-C32-C33-C34
15	C	406	CN5	O3'-CA-CB-CC
19	L	404	CN3	CA-CB-CC-O13
14	C	405	8PE	O22-C21-O21-C2
14	Q	101	8PE	C32-C33-C34-C35
14	C	405	8PE	C28-C29-C2A-C2B
11	C	401	6PH	C32-C33-C34-C35
18	D	402	7PH	C26-C27-C28-C29
19	L	404	CN3	C47-C48-C49-C4A
11	N	401	6PH	C27-C28-C29-C2A
14	C	405	8PE	C3E-C3F-C3G-C3H
14	Q	101	8PE	C22-C23-C24-C25
11	N	401	6PH	C34-C35-C36-C37
12	L	402	9PE	C25-C26-C27-C28
14	C	405	8PE	C25-C26-C27-C28
11	C	401	6PH	C22-C23-C24-C25
14	Q	101	8PE	C25-C26-C27-C28
12	L	402	9PE	C2A-C2B-C2C-C2D
18	D	402	7PH	C24-C25-C26-C27
15	C	406	CN5	O1'-C1'-C2'-C3'
14	Q	101	8PE	C36-C37-C38-C39
15	C	406	CN5	C38-C39-C3A-C3B
11	N	401	6PH	C33-C34-C35-C36
14	C	405	8PE	C22-C23-C24-C25
11	N	401	6PH	C22-C23-C24-C25
18	N	402	7PH	C32-C31-O31-C3
11	C	401	6PH	C33-C34-C35-C36
18	N	402	7PH	C36-C37-C38-C39
12	L	402	9PE	C2C-C2D-C2E-C2F
15	C	406	CN5	C31-C32-C33-C34
15	C	406	CN5	C32-C33-C34-C35
12	C	402	9PE	C27-C28-C29-C2A
12	C	402	9PE	C2F-C2G-C2H-C2I
12	L	402	9PE	C21-C22-C23-C24
18	N	402	7PH	O32-C31-O31-C3
11	C	401	6PH	C24-C25-C26-C27
18	N	402	7PH	C26-C27-C28-C29
12	L	402	9PE	C28-C29-C2A-C2B

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Mol	Chain	Res	Type	Atoms
14	Q	101	8PE	C39-C3A-C3B-C3C
14	Q	101	8PE	C3C-C3D-C3E-C3F
18	N	402	7PH	C28-C29-C2A-C2B
12	C	402	9PE	C22-C21-O21-C2
19	L	404	CN3	C52-C51-O51-C2'
11	N	401	6PH	C28-C29-C2A-C2B
16	L	401	UQ6	C12-C11-C9-C8
18	D	402	7PH	C36-C37-C38-C39
18	D	402	7PH	C22-C23-C24-C25
19	L	404	CN3	O52-C51-O51-C2'
18	D	402	7PH	C27-C28-C29-C2A
12	C	402	9PE	C1-O11-P-O13
12	L	402	9PE	O11-C1-C2-C3
14	C	405	8PE	O11-C1-C2-C3
11	C	401	6PH	C29-C2A-C2B-C2C
18	N	402	7PH	C33-C34-C35-C36
18	D	402	7PH	C33-C34-C35-C36
18	N	402	7PH	C27-C28-C29-C2A
14	C	405	8PE	C39-C3A-C3B-C3C
12	C	402	9PE	O22-C21-O21-C2
16	L	401	UQ6	C12-C11-C9-C10
12	L	402	9PE	C2D-C2E-C2F-C2G
16	C	407	UQ6	C2-C3-O3-C3M
15	C	406	CN5	C34-C35-C36-C37
11	C	401	6PH	C1-C2-C3-O31
14	Q	101	8PE	C1-C2-C3-O31
19	L	404	CN3	C1-C2-C3-O31
19	L	404	CN3	C1'-C2'-C3'-O41
19	L	404	CN3	C43-C44-C45-C46
11	N	401	6PH	C26-C27-C28-C29
18	D	402	7PH	C2B-C2C-C2D-C2E
12	L	402	9PE	C2F-C2G-C2H-C2I
14	Q	101	8PE	C3A-C3B-C3C-C3D
14	C	405	8PE	C27-C28-C29-C2A
12	C	402	9PE	O11-C1-C2-O21
14	Q	101	8PE	C3B-C3C-C3D-C3E
18	D	402	7PH	C38-C39-C3A-C3B
18	N	402	7PH	C32-C33-C34-C35
14	C	405	8PE	C31-C32-C33-C34
14	Q	101	8PE	C33-C34-C35-C36
14	C	405	8PE	C3B-C3C-C3D-C3E
14	Q	101	8PE	C37-C38-C39-C3A

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Mol	Chain	Res	Type	Atoms
11	C	401	6PH	C31-C32-C33-C34
12	C	402	9PE	C2E-C2F-C2G-C2H
14	C	405	8PE	C38-C39-C3A-C3B
12	C	402	9PE	C1-C2-C3-O31
18	N	402	7PH	C1-C2-C3-O31
15	C	406	CN5	C33-C34-C35-C36
18	N	402	7PH	C22-C23-C24-C25
19	L	404	CN3	CA-O3'-P'-O1'
11	N	401	6PH	O11-C1-C2-O21
12	L	402	9PE	O11-C1-C2-O21
14	C	405	8PE	O11-C1-C2-O21
15	C	406	CN5	C39-C3A-C3B-C3C
12	C	402	9PE	C2A-C2B-C2C-C2D
12	L	402	9PE	C23-C24-C25-C26
19	L	404	CN3	C55-C56-C57-C58
12	C	402	9PE	C2-C1-O11-P
12	C	402	9PE	C33-C34-C35-C36
14	Q	101	8PE	C24-C25-C26-C27
18	D	402	7PH	C34-C35-C36-C37
12	C	402	9PE	C29-C2A-C2B-C2C
11	N	401	6PH	O11-C1-C2-C3
15	C	406	CN5	C3B-C3C-C3D-C3E
12	L	402	9PE	C22-C21-O21-C2
12	L	402	9PE	C3-C2-O21-C21
11	N	401	6PH	C1-C2-C3-O31
14	C	405	8PE	C3A-C3B-C3C-C3D
19	L	404	CN3	C54-C55-C56-C57
11	N	401	6PH	O21-C2-C3-O31
19	L	404	CN3	O21-C2-C3-O31
19	L	404	CN3	O51-C2'-C3'-O41
18	D	402	7PH	C35-C36-C37-C38
14	Q	101	8PE	C22-C21-O21-C2
14	C	405	8PE	C3F-C3G-C3H-C3I
12	L	402	9PE	O22-C21-O21-C2
19	L	404	CN3	C41-C42-C43-C44
11	C	401	6PH	C2B-C2C-C2D-C2E
14	C	405	8PE	C35-C36-C37-C38
12	C	402	9PE	C11-O13-P-O11
11	C	401	6PH	C2-C1-O11-P
14	Q	101	8PE	C2-C1-O11-P
15	C	406	CN5	CB-CC-O13-P
15	C	406	CN5	C1'-O1'-P'-O4'

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Mol	Chain	Res	Type	Atoms
19	L	404	CN3	CC-O13-P-O12
19	L	404	CN3	CA-O3'-P'-O4'
18	D	402	7PH	C28-C29-C2A-C2B
18	N	402	7PH	C25-C26-C27-C28
12	C	402	9PE	O11-C1-C2-C3
18	D	402	7PH	O11-C1-C2-C3
12	L	402	9PE	O13-C11-C12-N
14	Q	101	8PE	C12-C11-O13-P
14	Q	101	8PE	O22-C21-O21-C2
13	D	401	HEM	C2A-CAA-CBA-CGA
18	D	402	7PH	O11-C1-C2-O21
19	L	404	CN3	C42-C43-C44-C45
11	C	401	6PH	O21-C2-C3-O31
14	Q	101	8PE	O21-C2-C3-O31
11	C	401	6PH	C2C-C2D-C2E-C2F
12	C	402	9PE	C34-C35-C36-C37
19	L	404	CN3	C21-C22-C23-C24
11	C	401	6PH	C25-C26-C27-C28
11	N	401	6PH	C38-C39-C3A-C3B
12	C	402	9PE	C3-C2-O21-C21
15	C	406	CN5	C3A-C3B-C3C-C3D
11	N	401	6PH	C2-C1-O11-P
14	C	405	8PE	C36-C37-C38-C39
19	L	404	CN3	O51-C51-C52-C53
13	C	404	HEM	C2A-CAA-CBA-CGA
11	N	401	6PH	C2-C3-O31-C31
18	N	402	7PH	O21-C2-C3-O31
18	N	402	7PH	C38-C39-C3A-C3B
19	L	404	CN3	C52-C53-C54-C55
18	D	402	7PH	C25-C26-C27-C28
13	L	405	HEM	CAA-CBA-CGA-O1A
11	N	401	6PH	C3A-C3B-C3C-C3D
19	L	404	CN3	C2-C1-O11-P
12	L	402	9PE	O31-C31-C32-C33
18	N	402	7PH	C31-C32-C33-C34
13	C	403	HEM	CAA-CBA-CGA-O2A
13	L	403	HEM	CAA-CBA-CGA-O2A
12	C	402	9PE	O21-C2-C3-O31
13	L	405	HEM	CAA-CBA-CGA-O2A
13	C	403	HEM	CAA-CBA-CGA-O1A
14	Q	101	8PE	O13-C11-C12-N
17	C	408	A1D6K	C18-C13-N3-C11

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Mol	Chain	Res	Type	Atoms
17	L	406	A1D6K	C18-C13-N3-C11
13	L	403	HEM	CAA-CBA-CGA-O1A
11	C	401	6PH	C26-C27-C28-C29
18	N	402	7PH	C37-C38-C39-C3A
13	C	404	HEM	CAA-CBA-CGA-O1A
18	D	402	7PH	C3-C2-O21-C21
18	N	402	7PH	C39-C3A-C3B-C3C
19	L	404	CN3	C53-C54-C55-C56
18	N	402	7PH	O11-C1-C2-O21
16	C	407	UQ6	C5-C4-O4-C4M
13	D	401	HEM	CAA-CBA-CGA-O1A
13	D	401	HEM	CAA-CBA-CGA-O2A
12	L	402	9PE	O21-C2-C3-O31
13	C	403	HEM	CAD-CBD-CGD-O1D
13	C	404	HEM	CAA-CBA-CGA-O2A
19	L	404	CN3	C32-C31-O31-C3
17	C	408	A1D6K	C14-C13-N3-C11
17	L	406	A1D6K	C14-C13-N3-C11
13	L	405	HEM	CAD-CBD-CGD-O2D
11	C	401	6PH	C3A-C3B-C3C-C3D
12	L	402	9PE	C1-O11-P-O12
14	Q	101	8PE	C1-O11-P-O12
14	C	405	8PE	C23-C24-C25-C26
14	C	405	8PE	O13-C11-C12-N
13	C	404	HEM	CAD-CBD-CGD-O2D
18	N	402	7PH	C2B-C2C-C2D-C2E
11	N	401	6PH	C3-C2-O21-C21
17	C	408	A1D6K	C7-C8-C9-O3
17	L	406	A1D6K	C7-C8-C9-O3
13	C	403	HEM	CAD-CBD-CGD-O2D
14	C	405	8PE	C2B-C2C-C2D-C2E
18	N	402	7PH	C2A-C2B-C2C-C2D
13	C	404	HEM	CAD-CBD-CGD-O1D
18	D	402	7PH	O31-C31-C32-C33

There are no ring outliers.

11 monomers are involved in 17 short contacts:

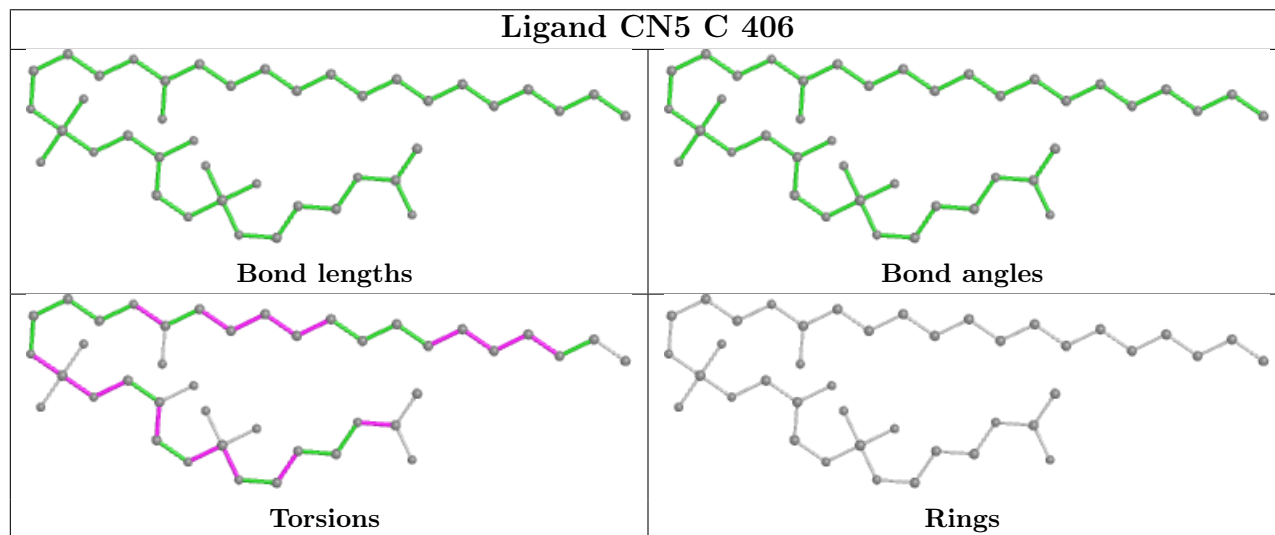
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	C	406	CN5	2	0
13	D	401	HEM	2	0
13	C	403	HEM	1	0

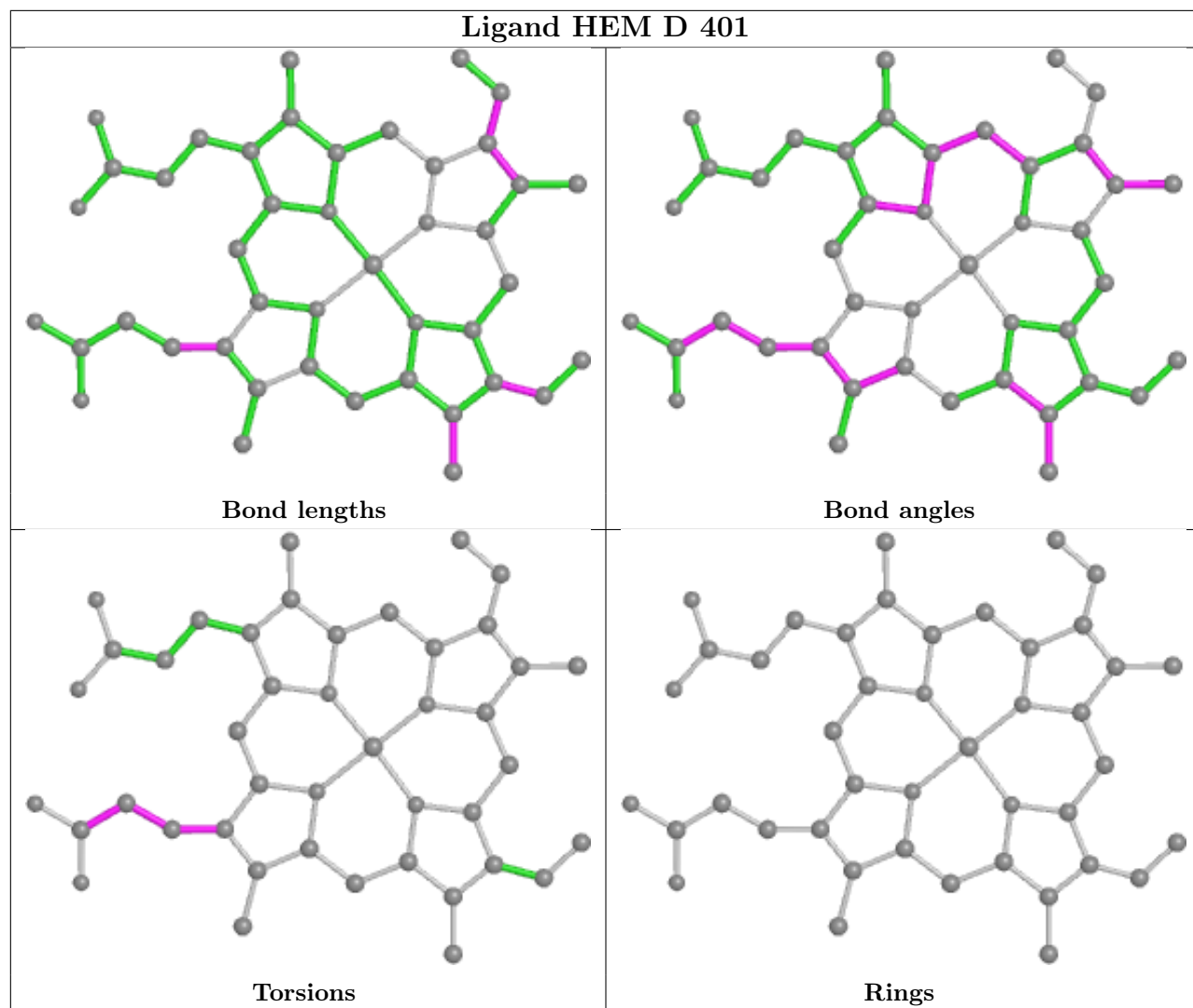
Continued on next page...

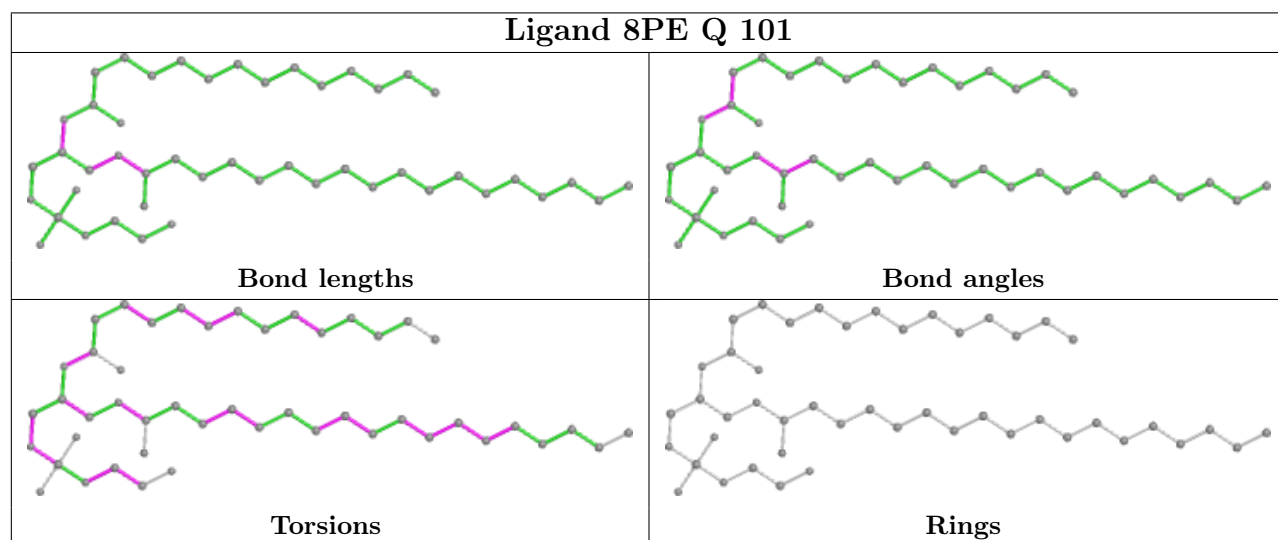
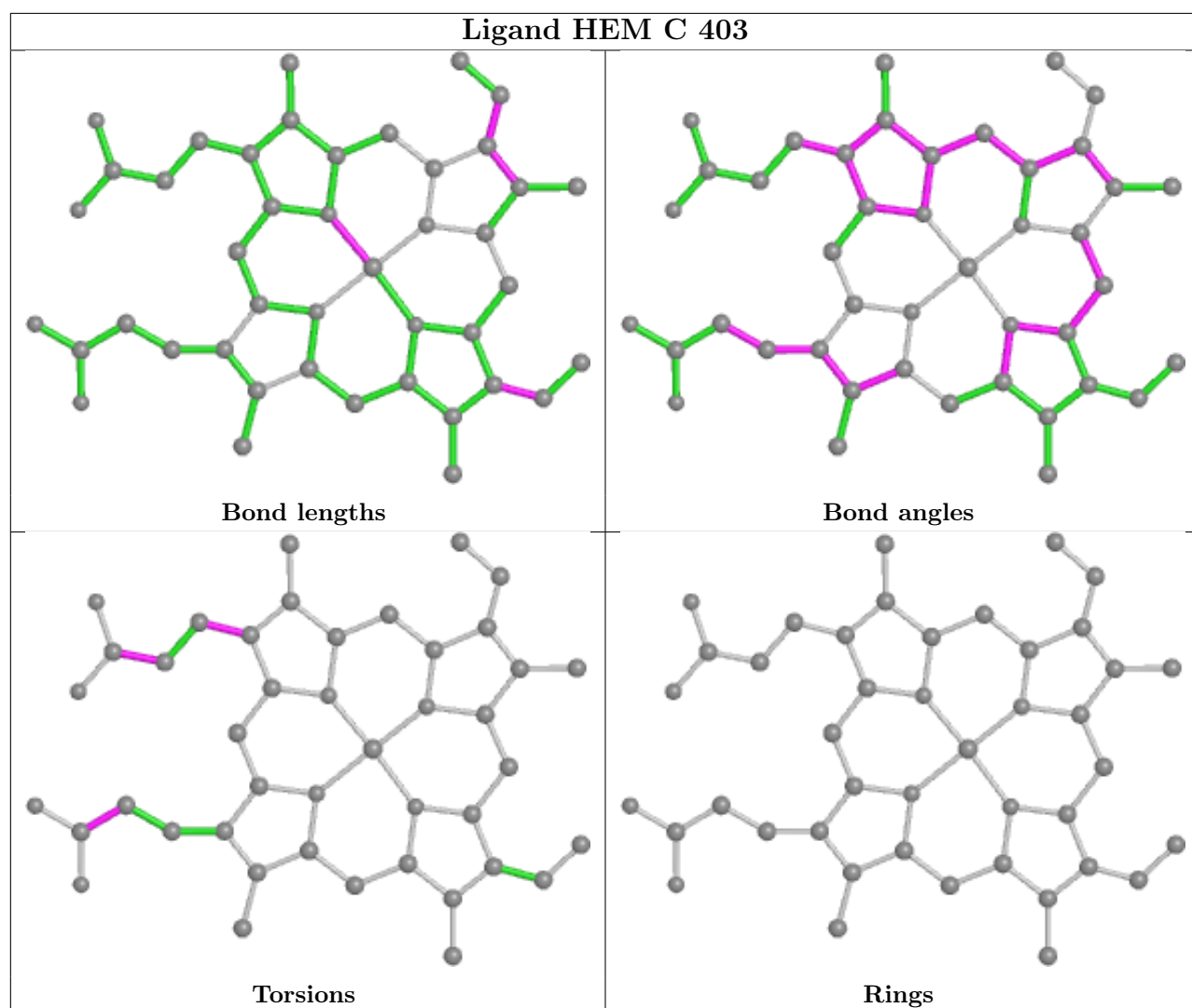
Continued from previous page...

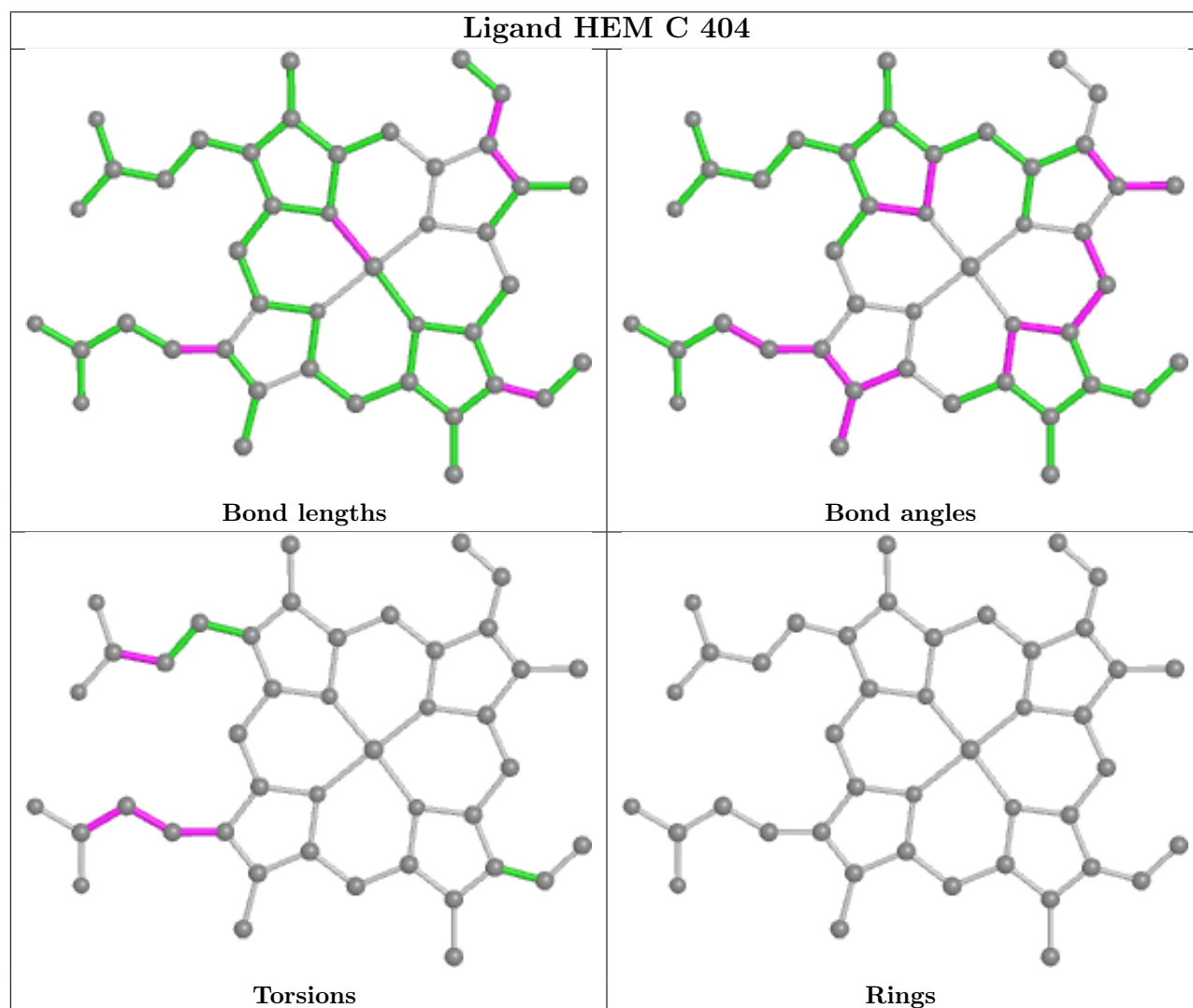
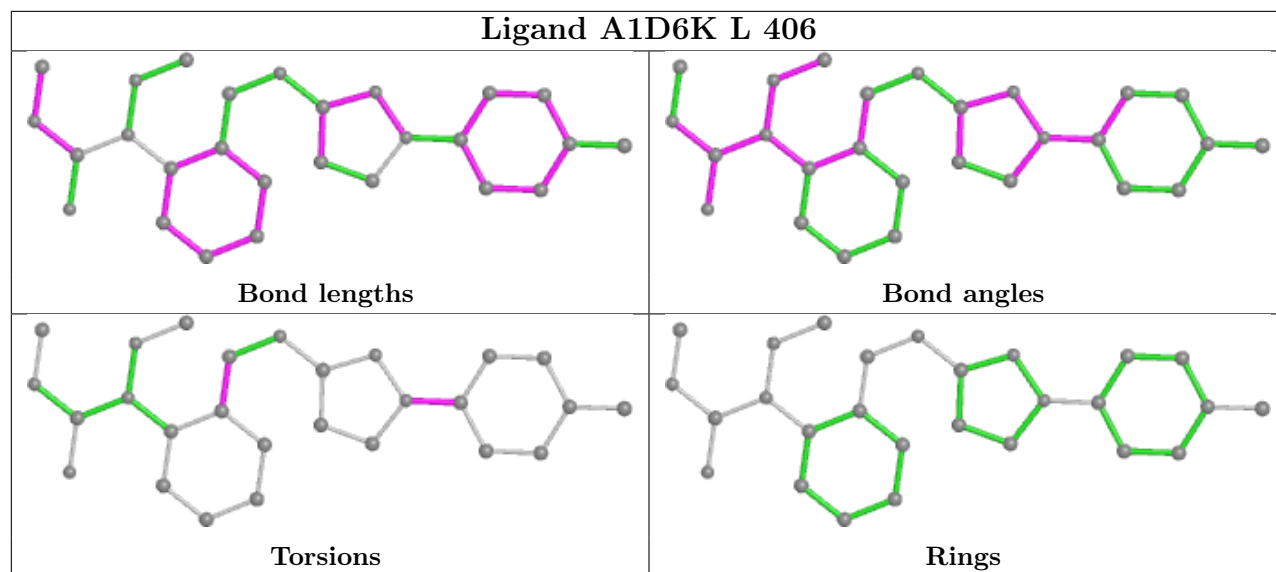
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	C	404	HEM	1	0
11	C	401	6PH	1	0
13	L	403	HEM	2	0
16	L	401	UQ6	4	0
18	D	402	7PH	2	0
16	C	407	UQ6	1	0
13	M	401	HEM	1	0
13	L	405	HEM	1	0

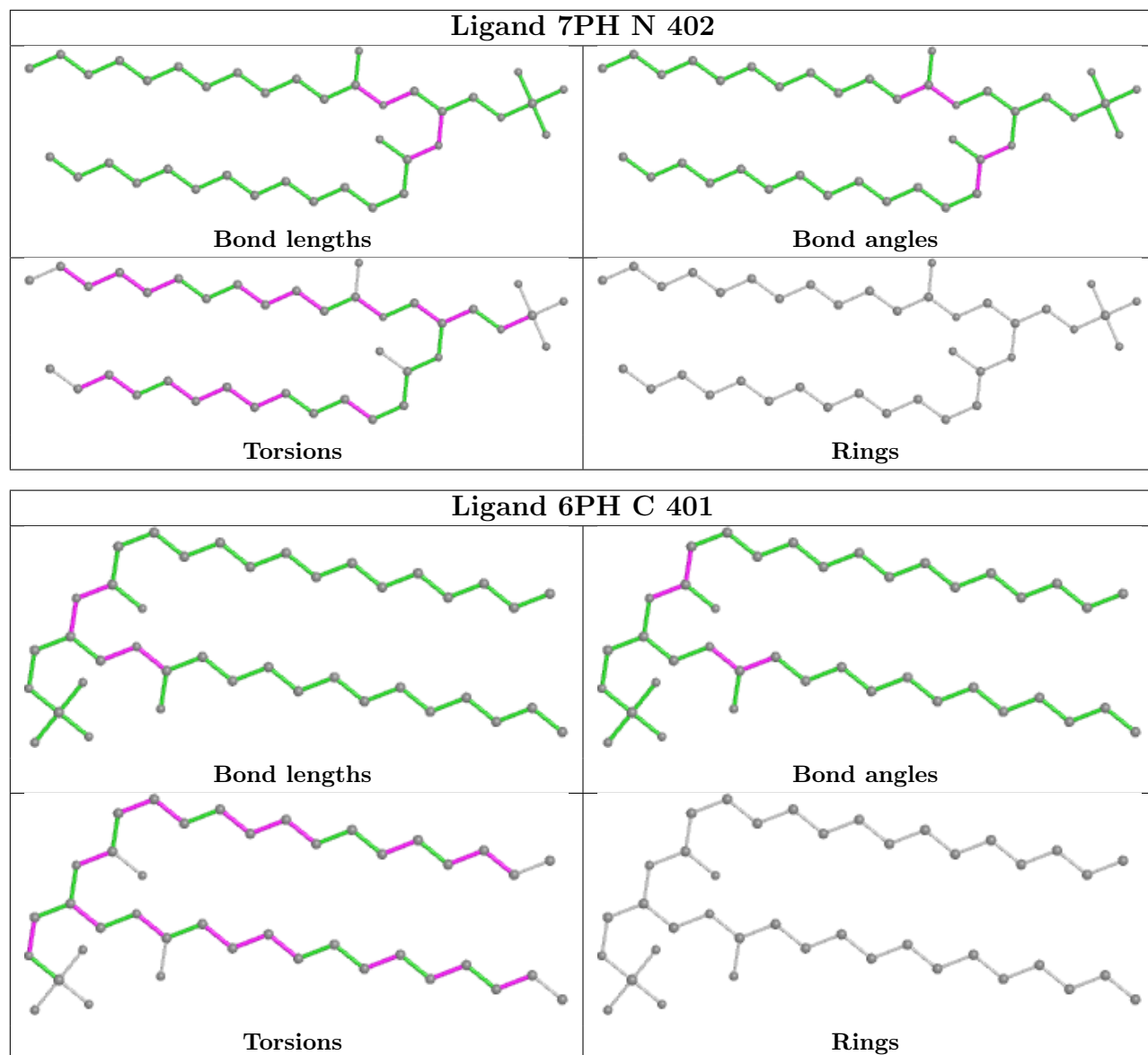
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

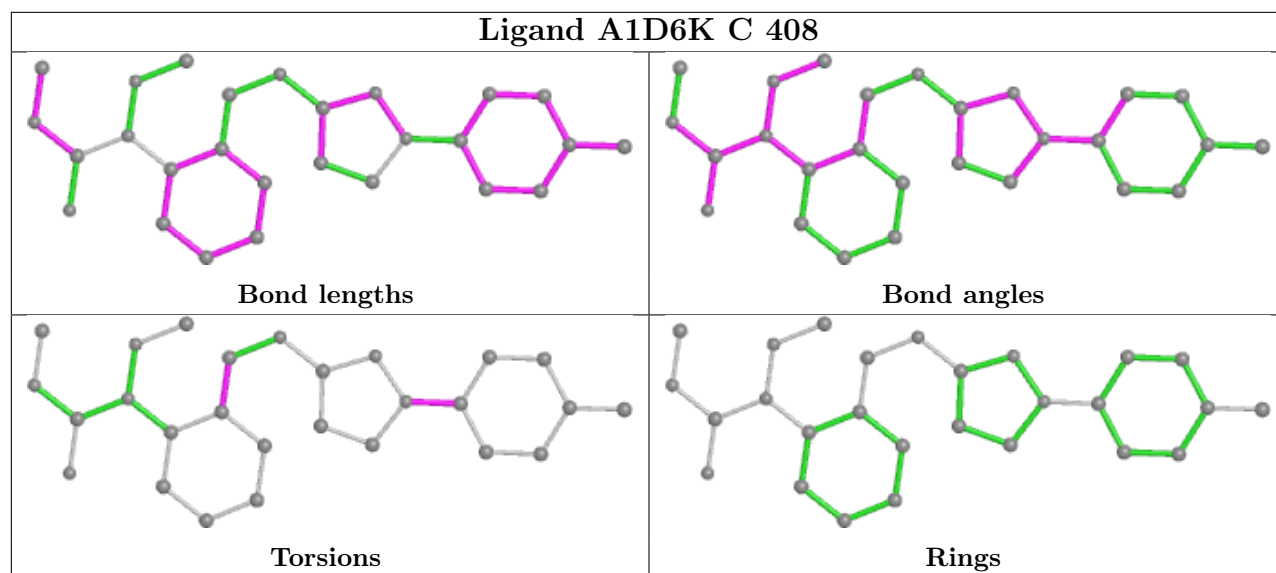
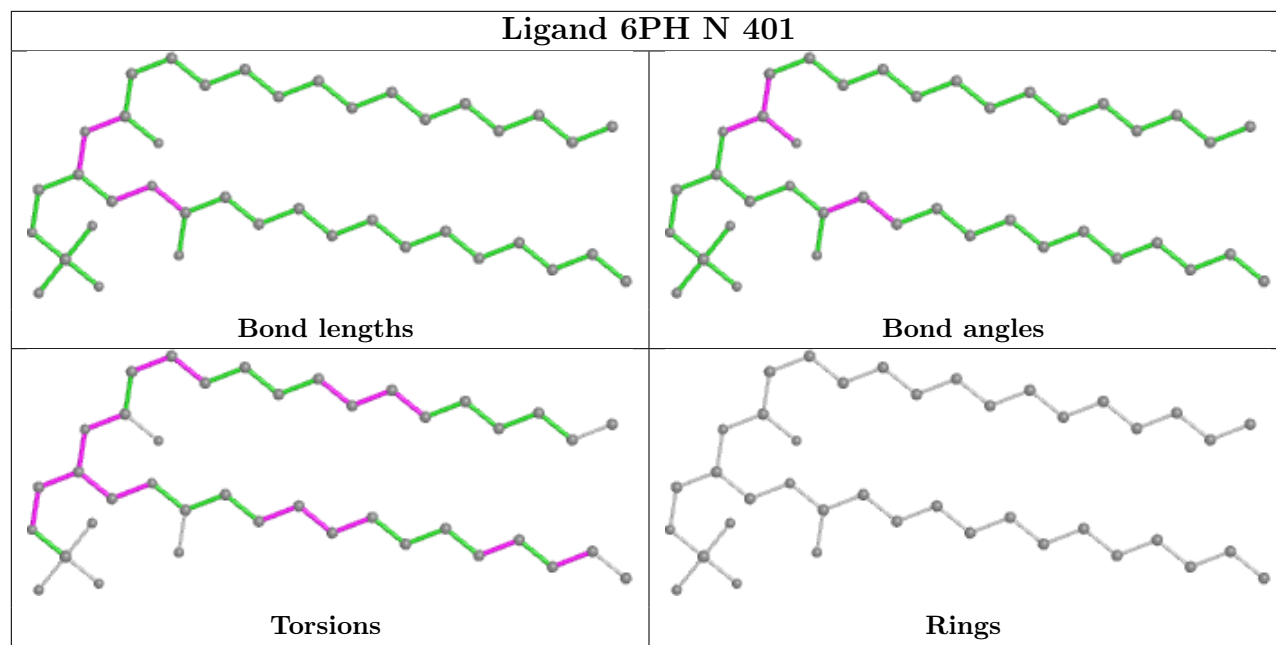


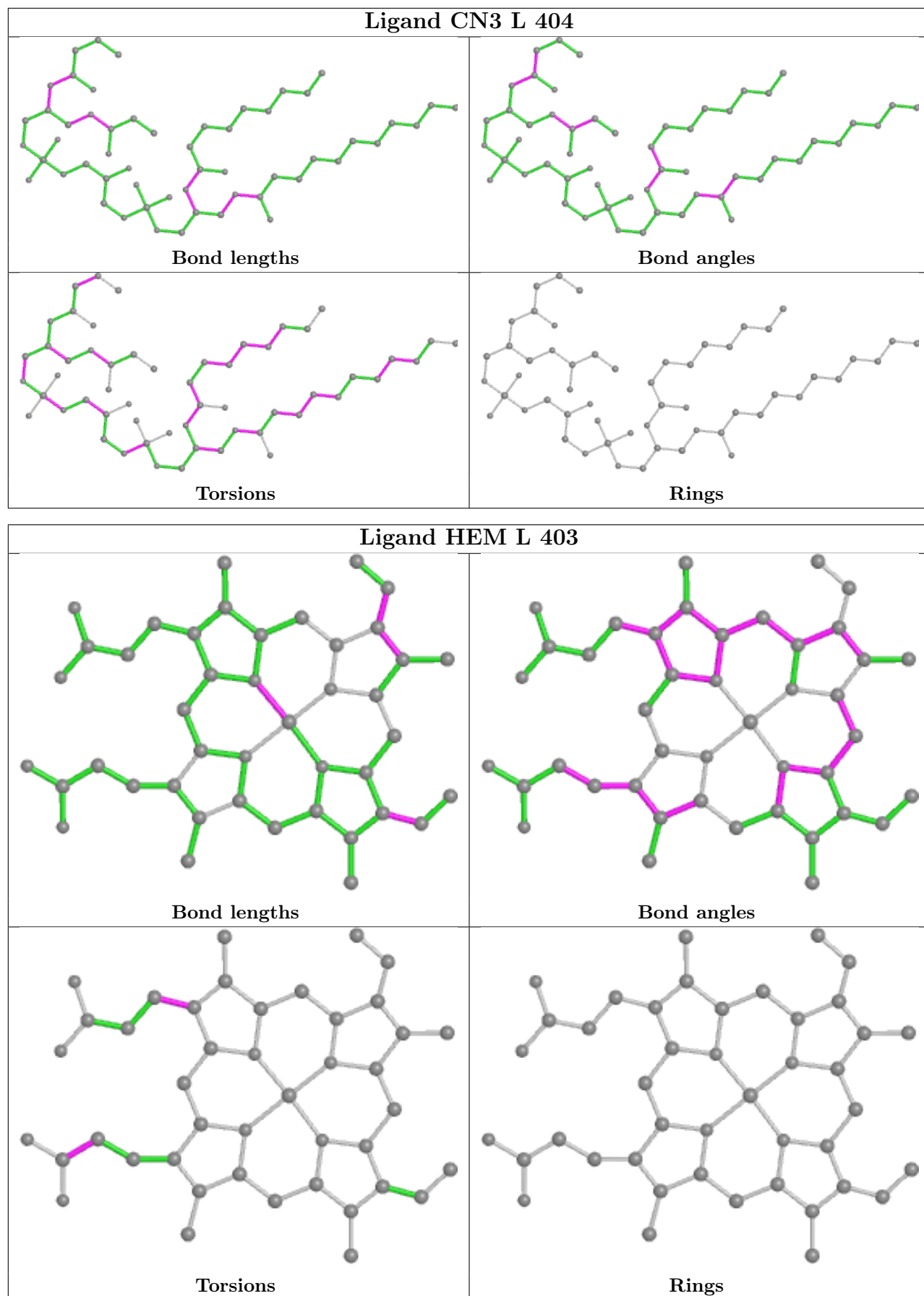


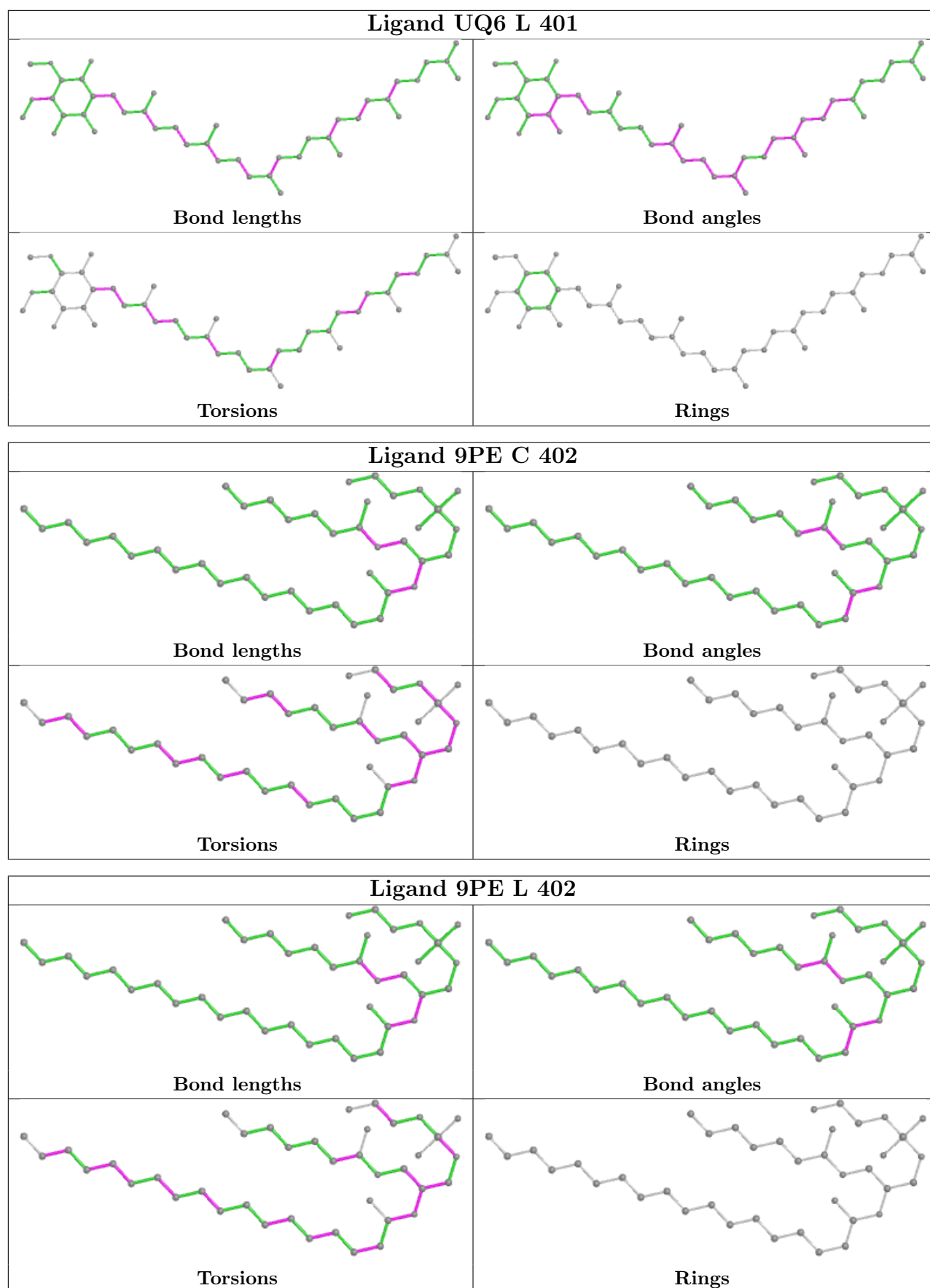


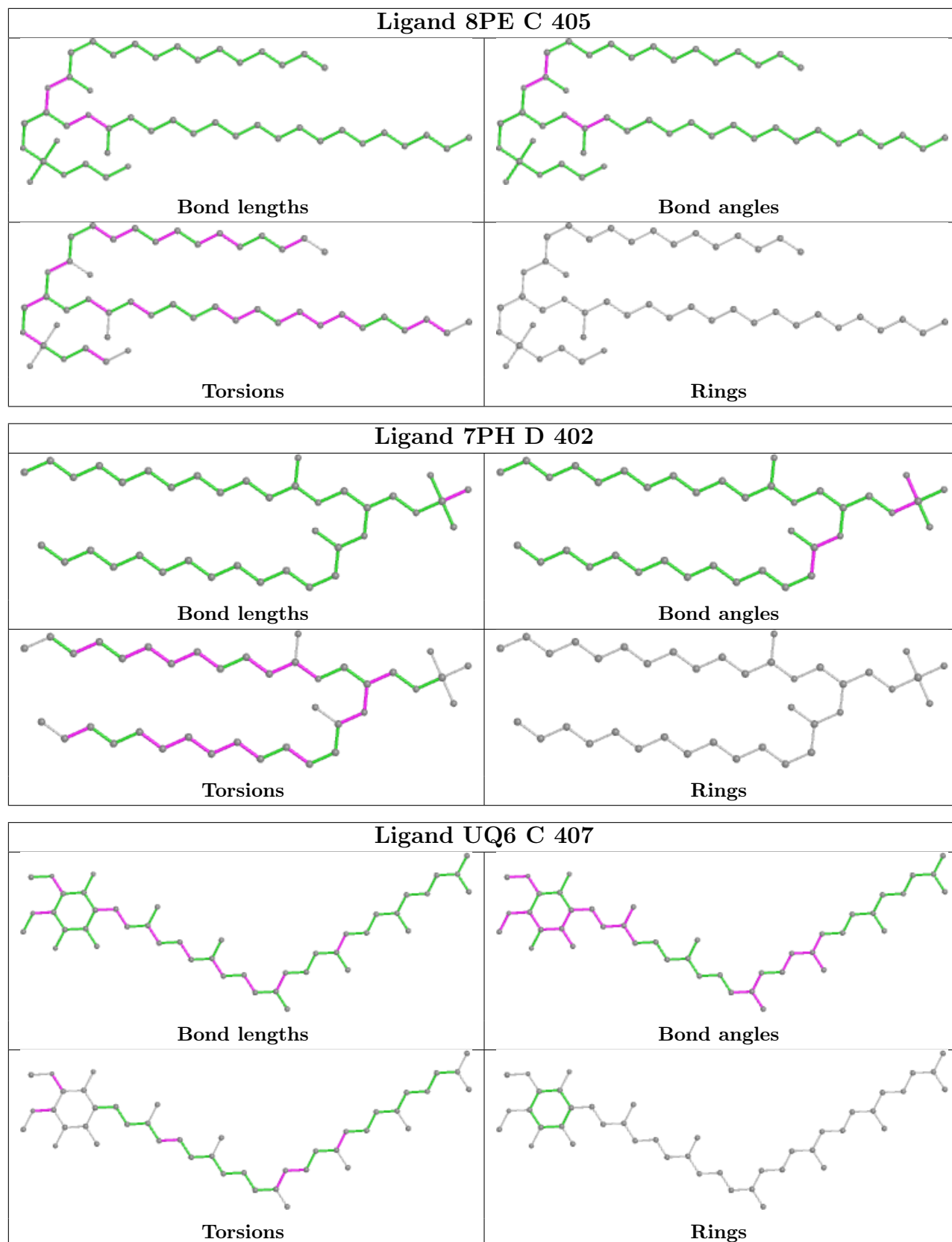


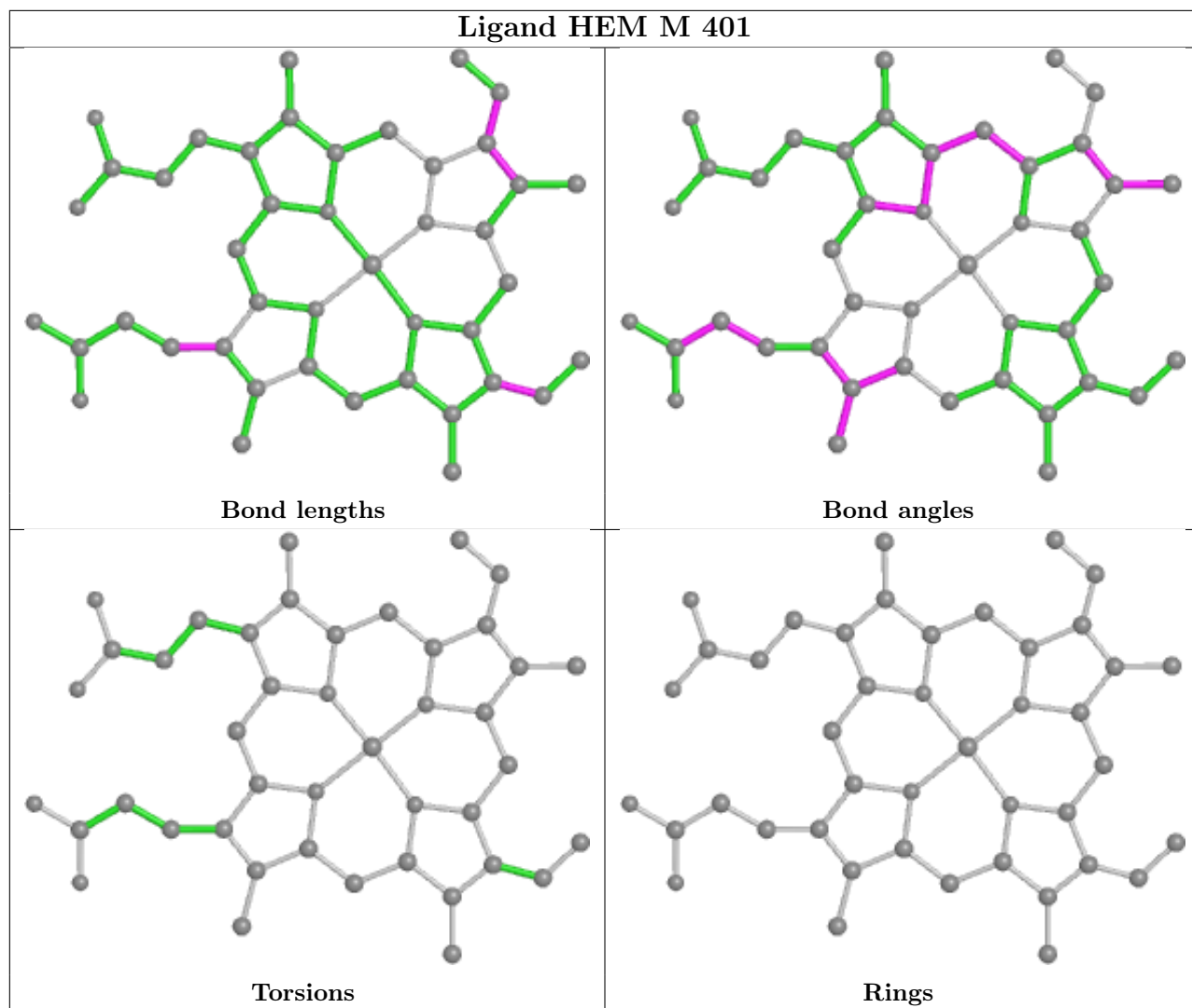


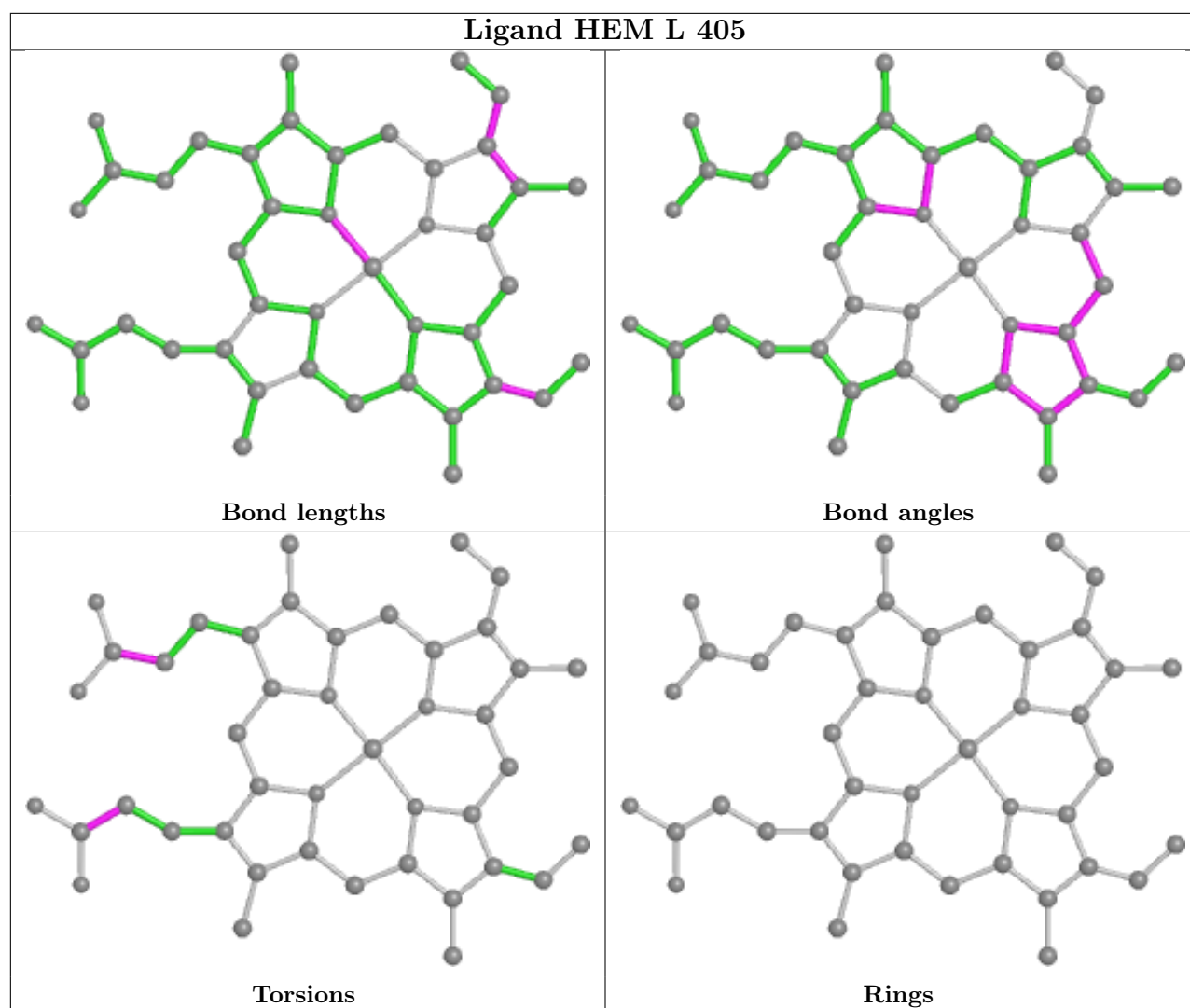












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

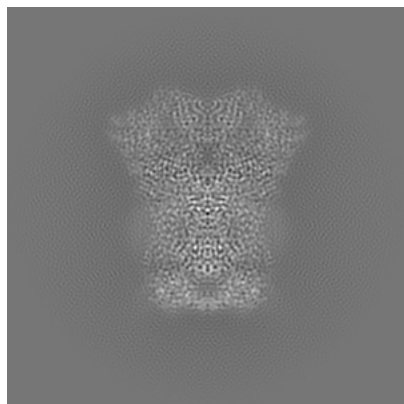
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39291. These allow visual inspection of the internal detail of the map and identification of artifacts.

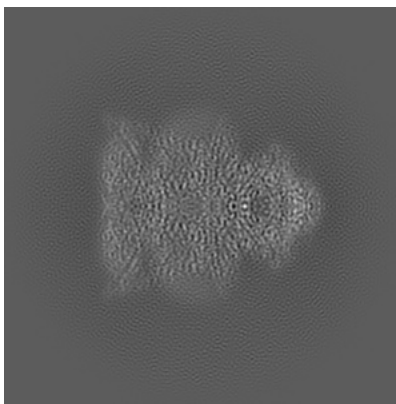
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

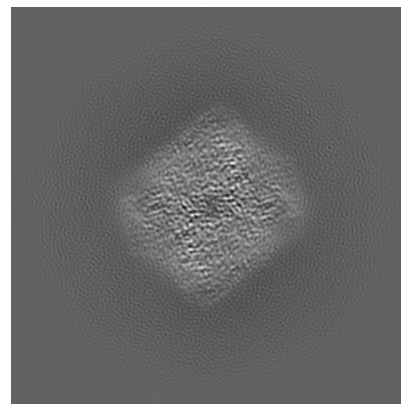
6.1.1 Primary map



X

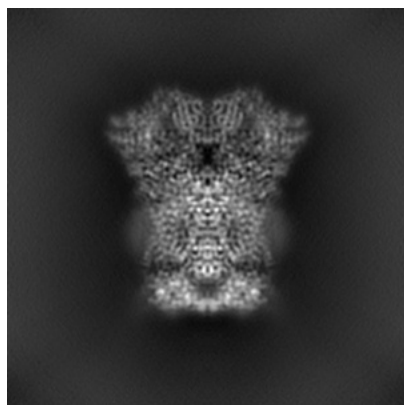


Y

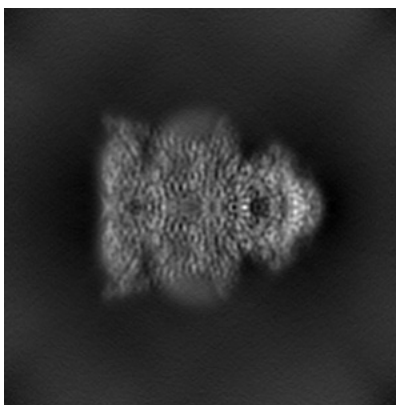


Z

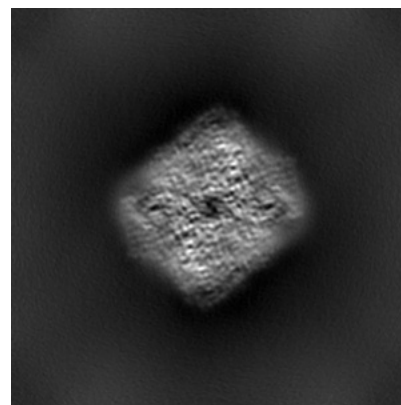
6.1.2 Raw map



X



Y

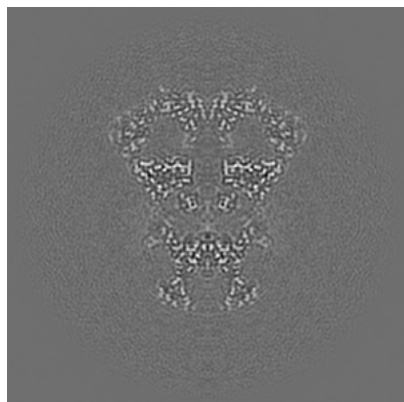


Z

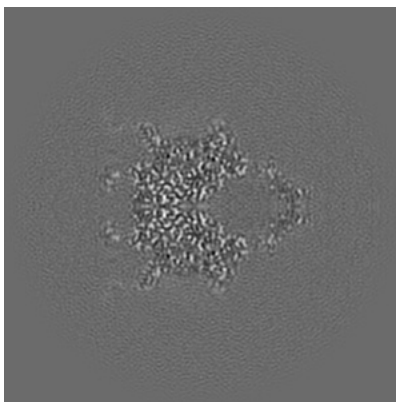
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

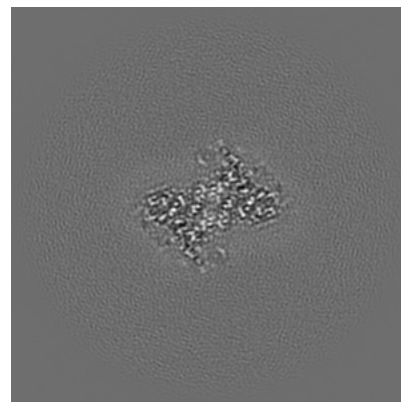
6.2.1 Primary map



X Index: 140

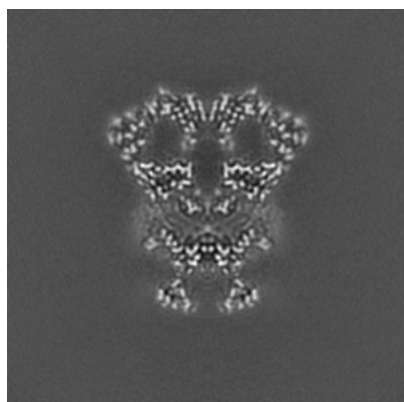


Y Index: 140

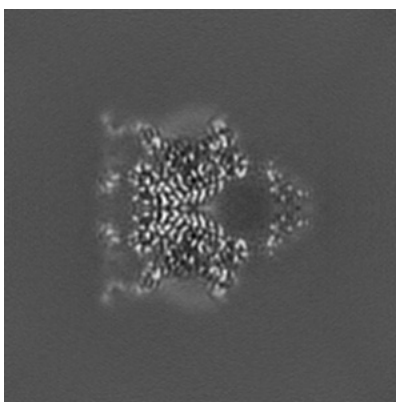


Z Index: 140

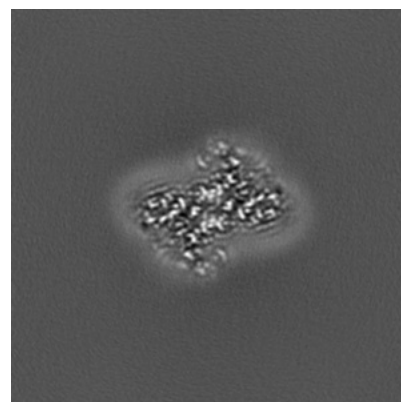
6.2.2 Raw map



X Index: 140



Y Index: 140

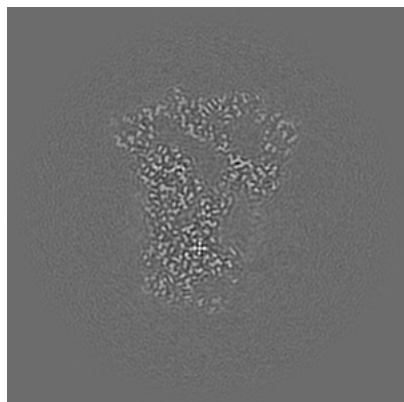


Z Index: 140

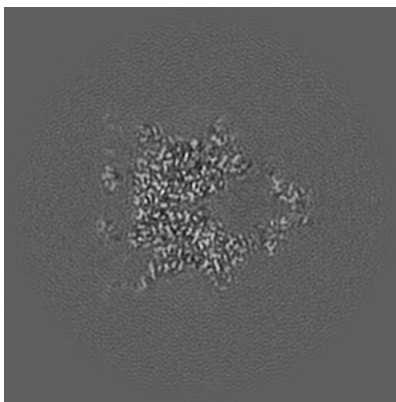
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

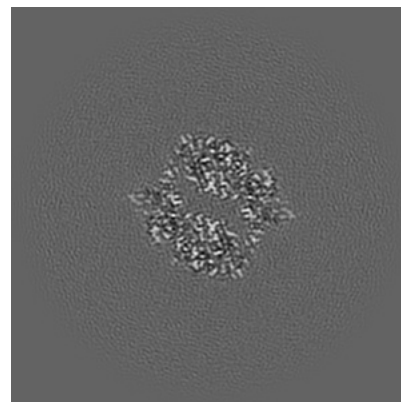
6.3.1 Primary map



X Index: 130

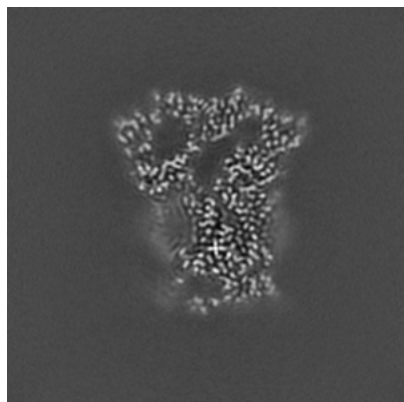


Y Index: 142

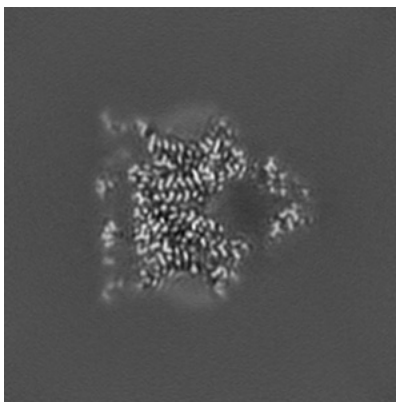


Z Index: 158

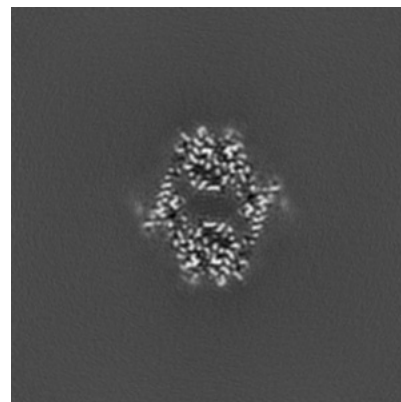
6.3.2 Raw map



X Index: 150



Y Index: 138

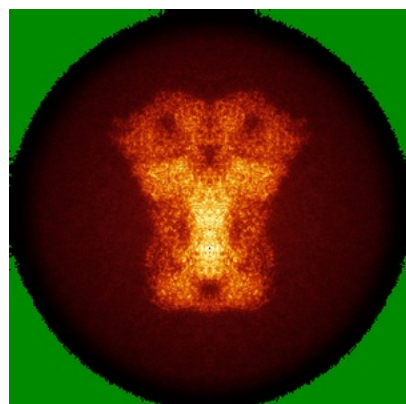


Z Index: 163

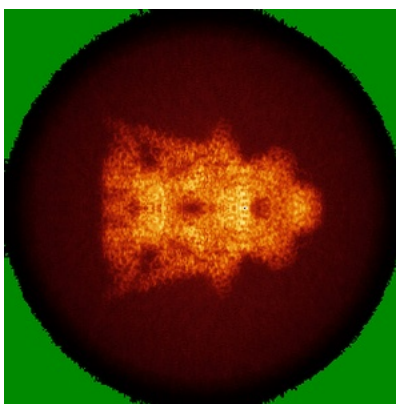
The images above show the largest variance slices of the map in three orthogonal directions.

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

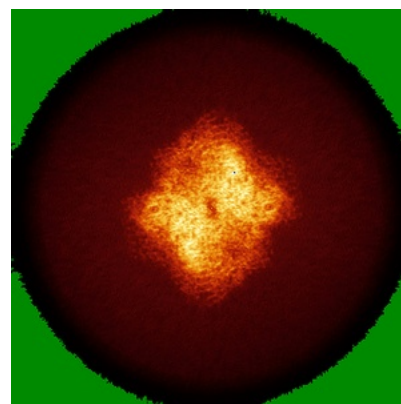
6.4.1 Primary map



X

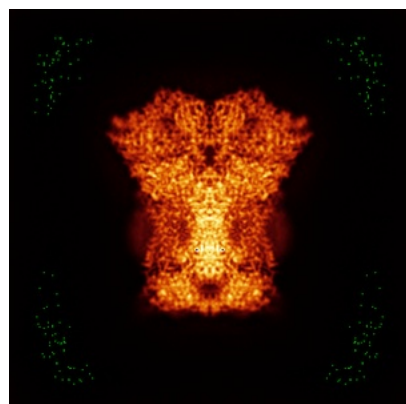


Y

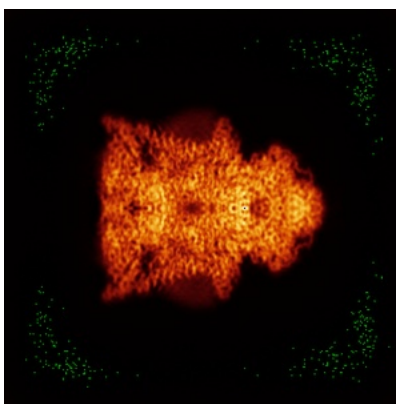


Z

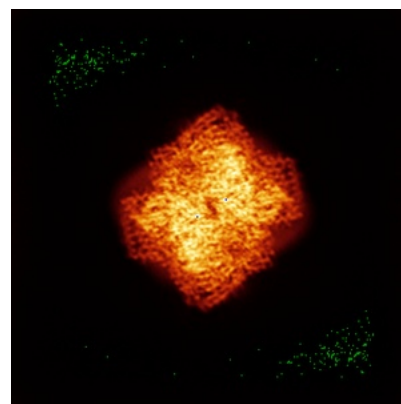
6.4.2 Raw map



X



Y

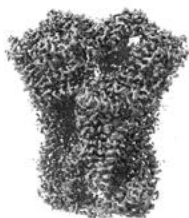


Z

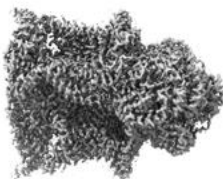
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



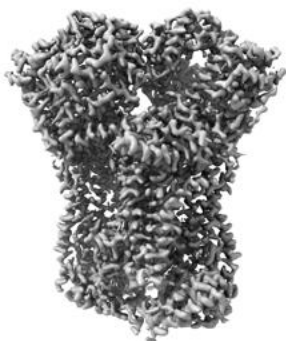
Y



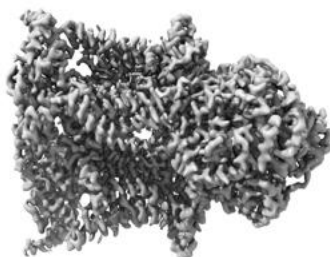
Z

The images above show the 3D surface view of the map at the recommended contour level 1.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

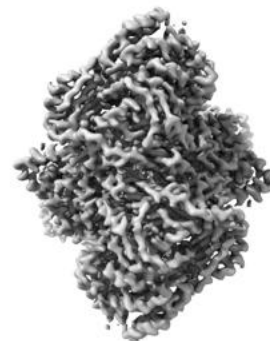
6.5.2 Raw map



X



Y



Z

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

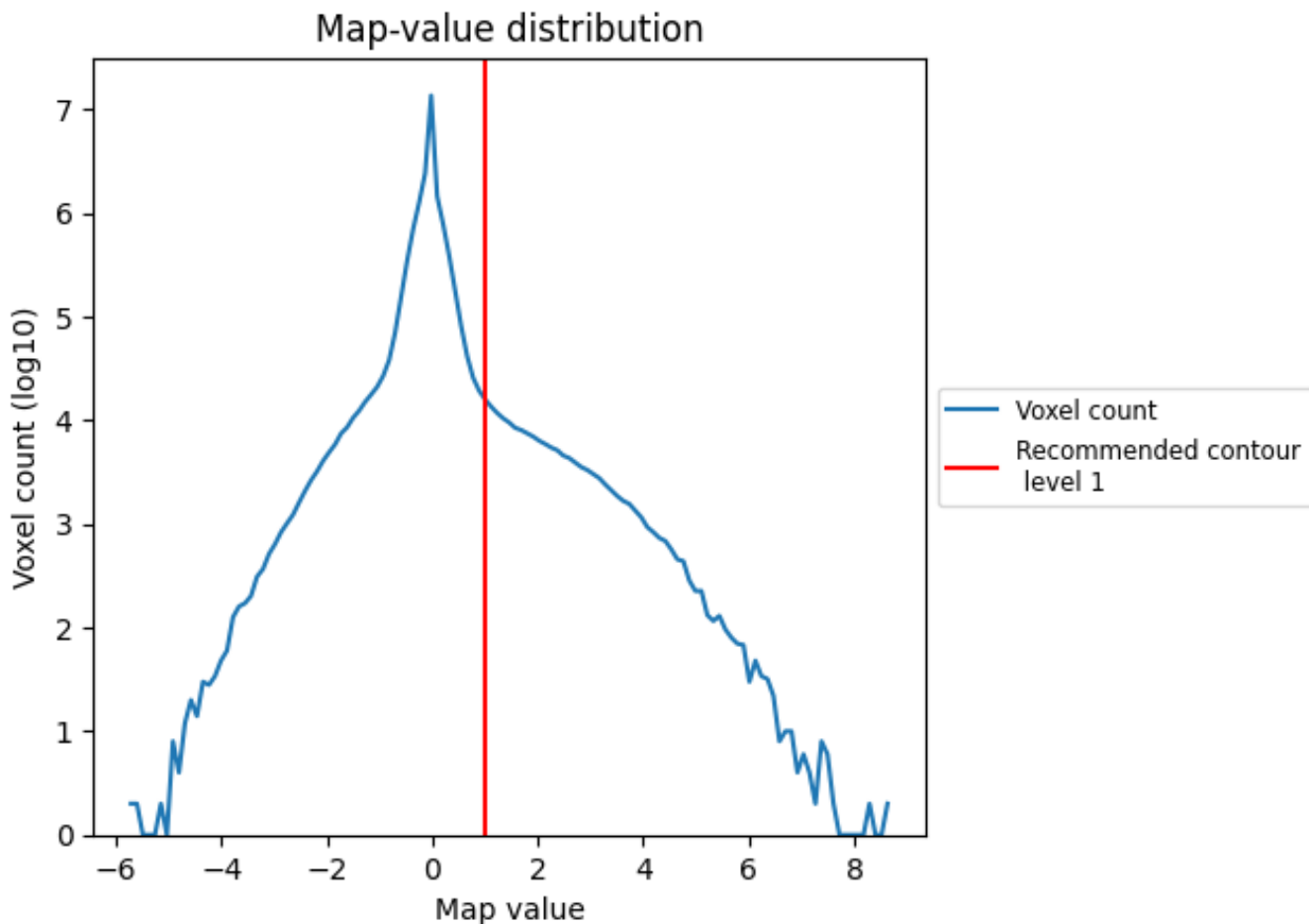
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

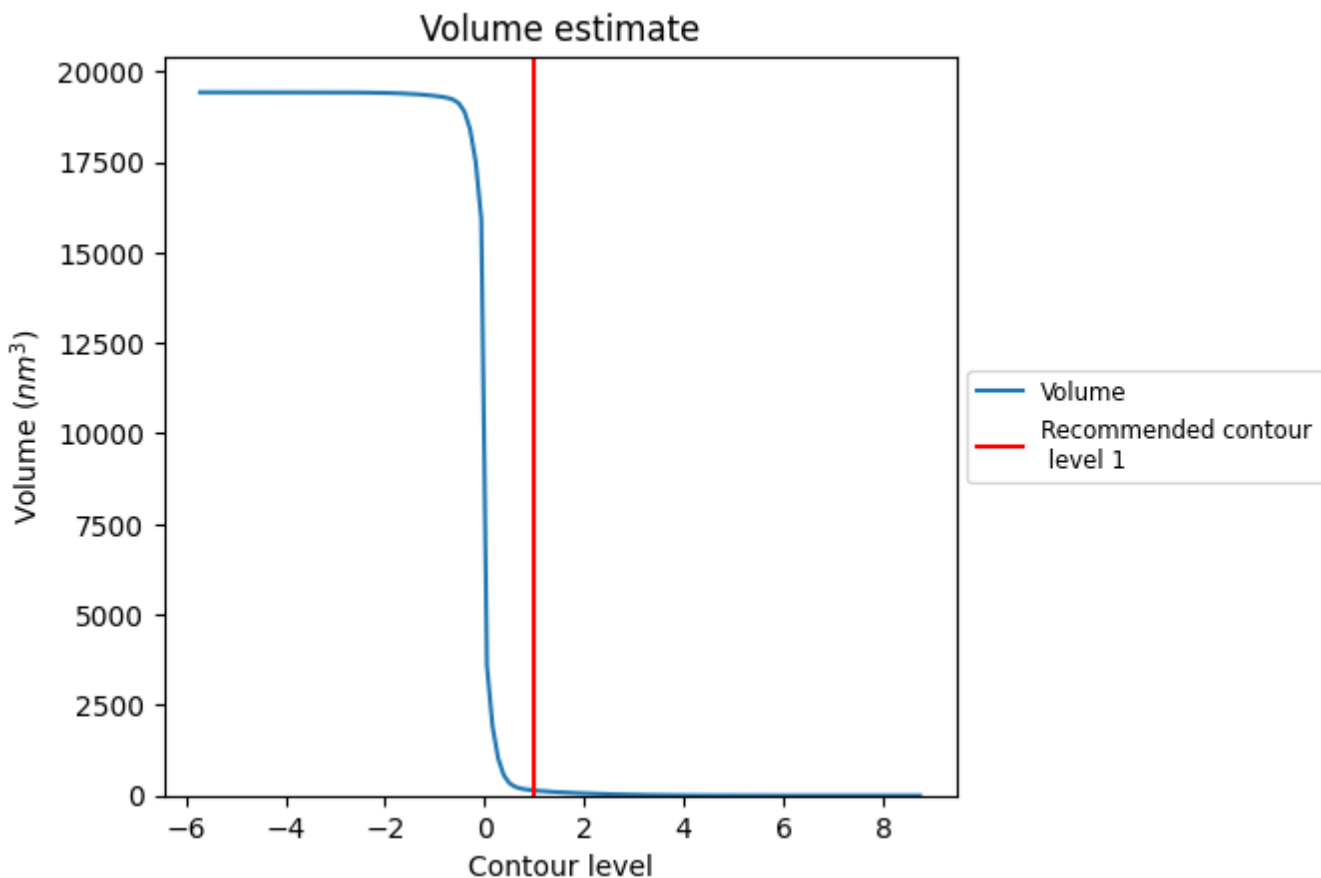
This section contains the results of statistical analysis of the map.

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.

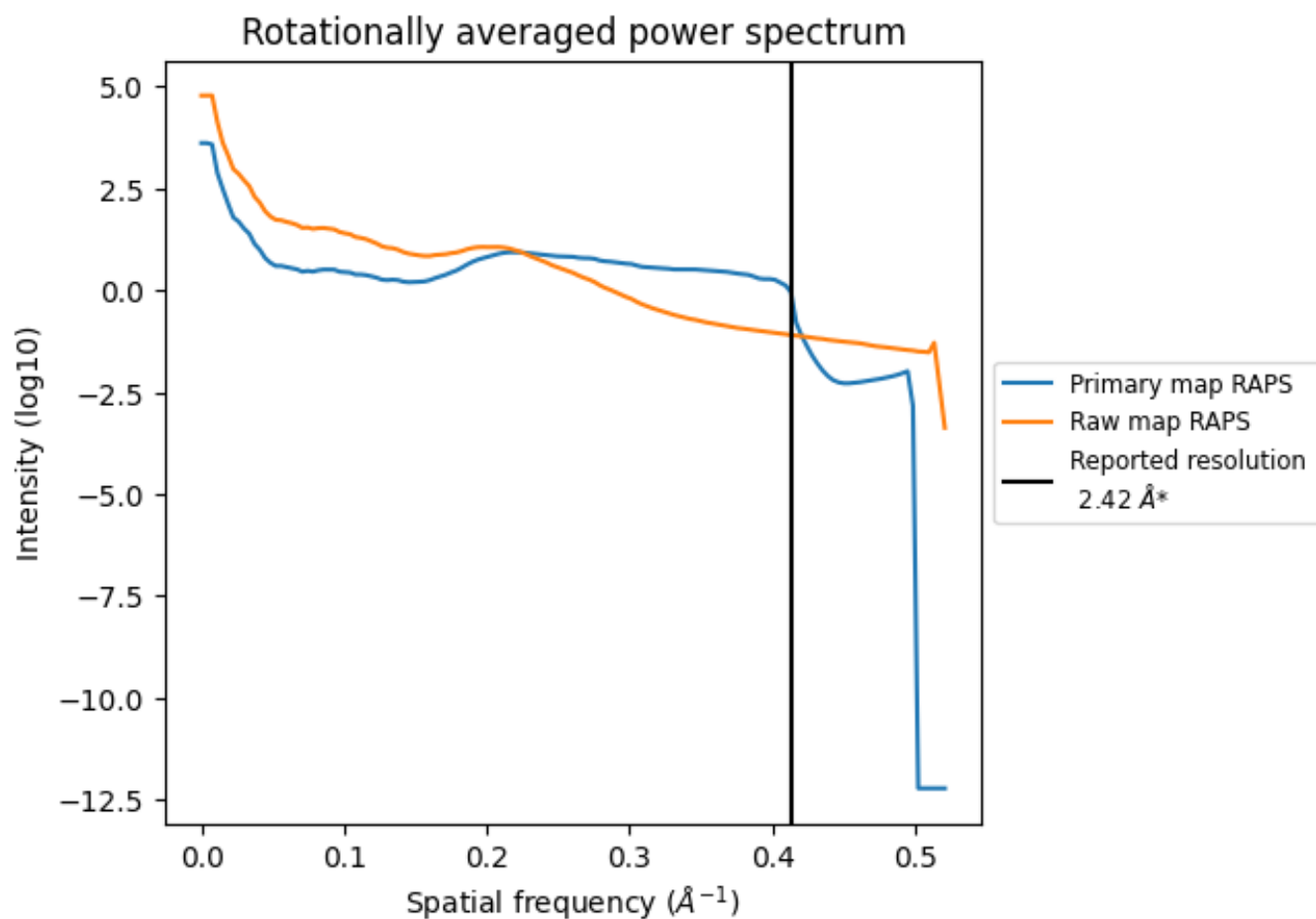
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 141 nm³; this corresponds to an approximate mass of 128 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 [i](#)

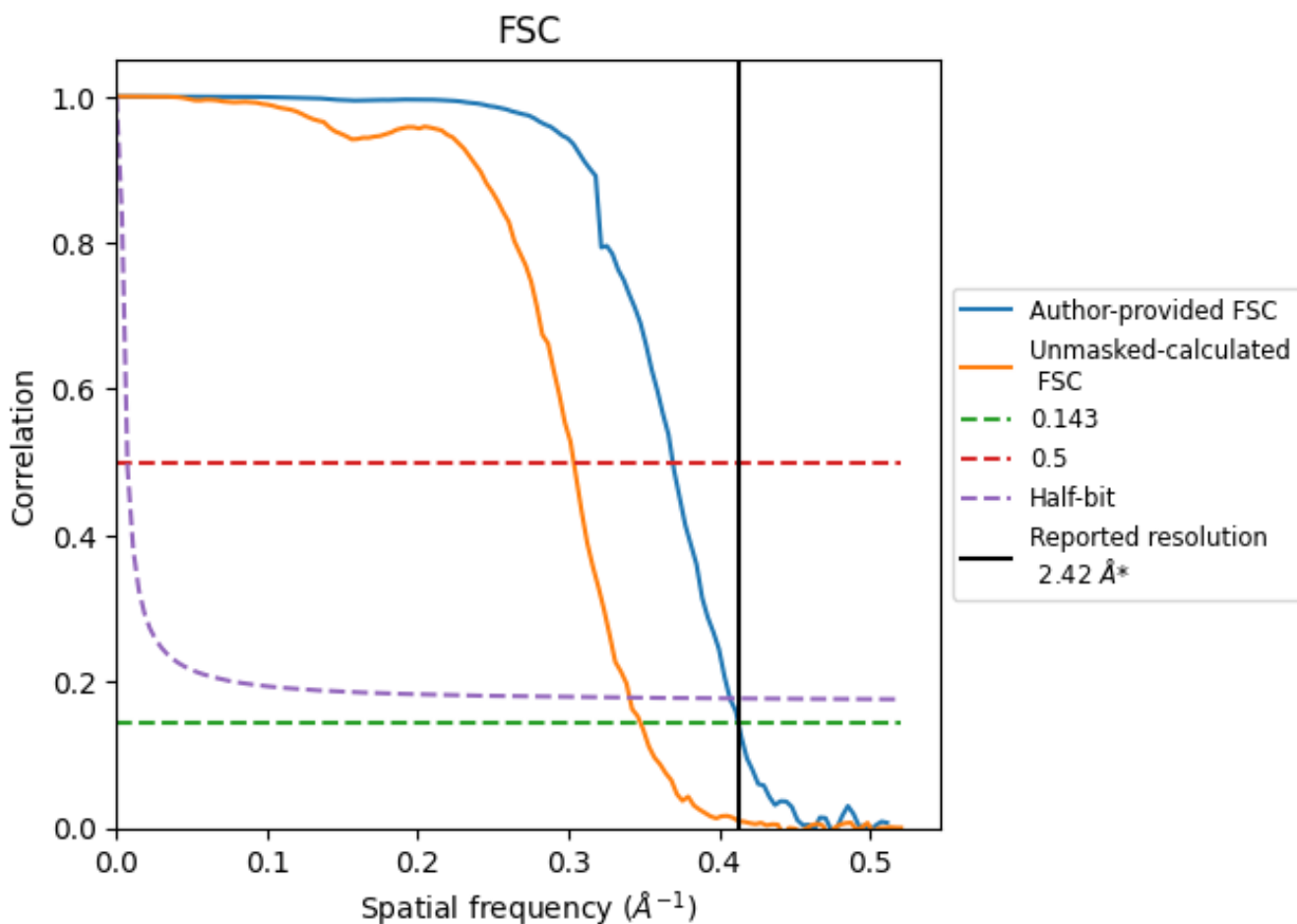


*Reported resolution corresponds to spatial frequency of 0.413 Å⁻¹

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 0.413 Å⁻¹

8.2 Resolution estimates [i](#)

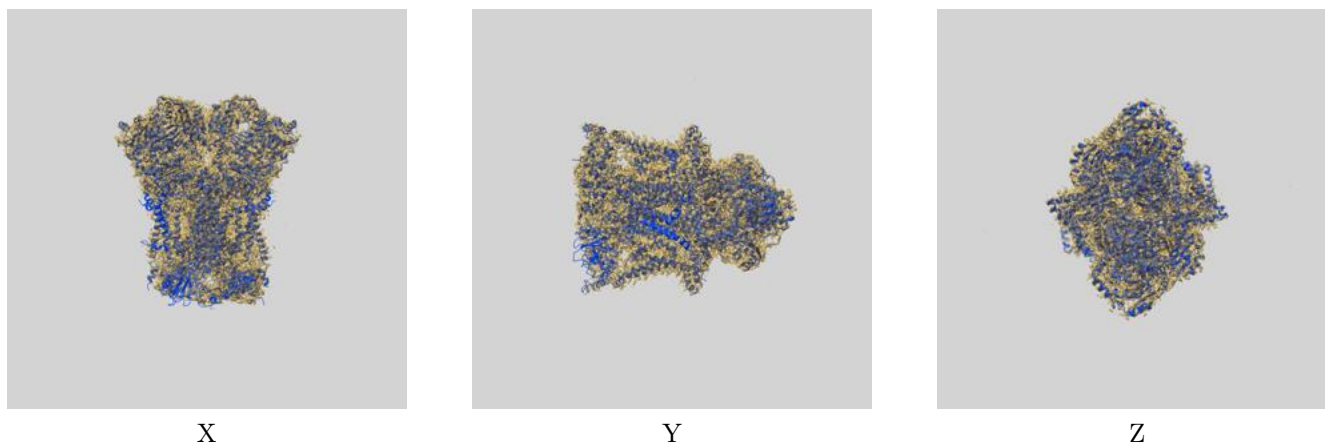
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.42	-	-
Author-provided FSC curve	2.42	2.71	2.46
Unmasked-calculated*	2.87	3.29	2.94

*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 2.87 differs from the reported value 2.42 by more than 10 %

9 Map-model fit [i](#)

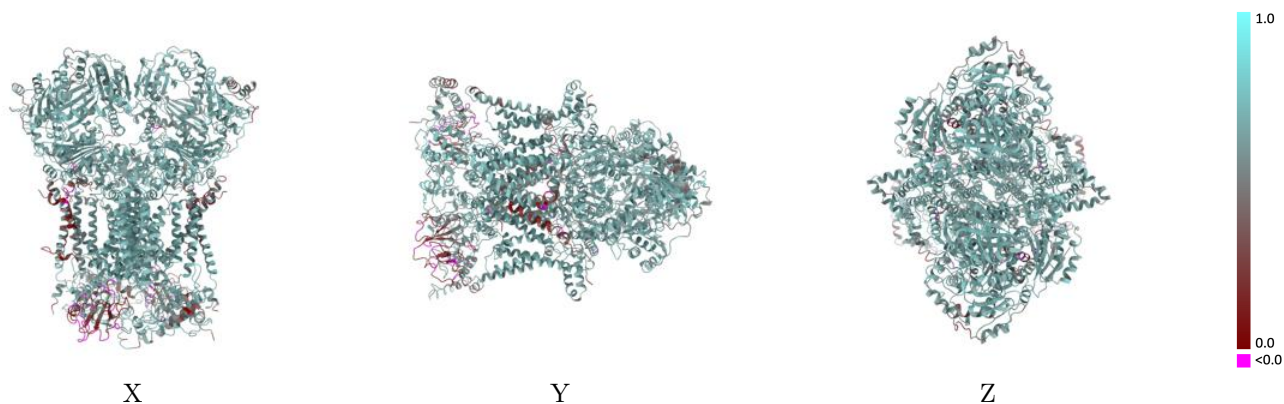
This section contains information regarding the fit between EMDB map EMD-39291 and PDB model 8YHQ. Per-residue inclusion information can be found in section [3](#) on page [12](#).

9.1 Map-model overlay [i](#)



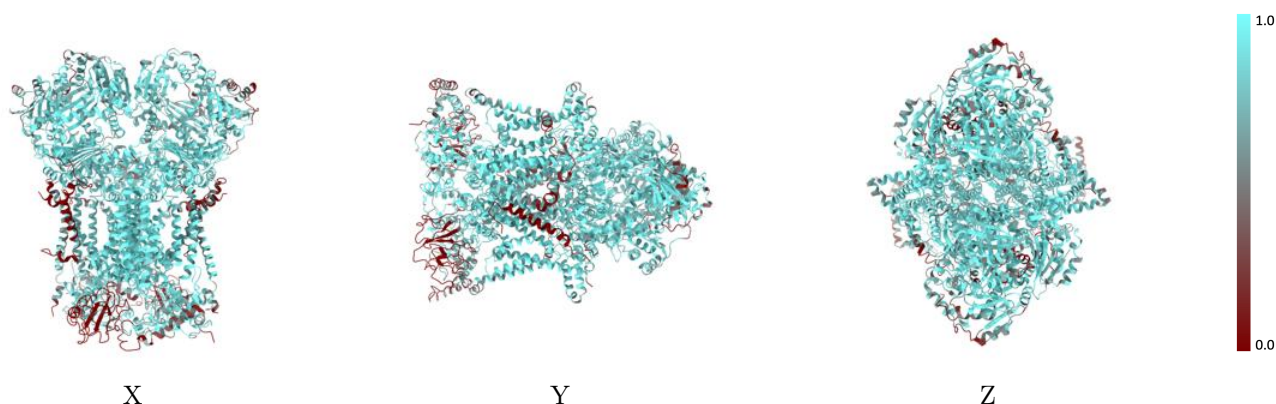
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



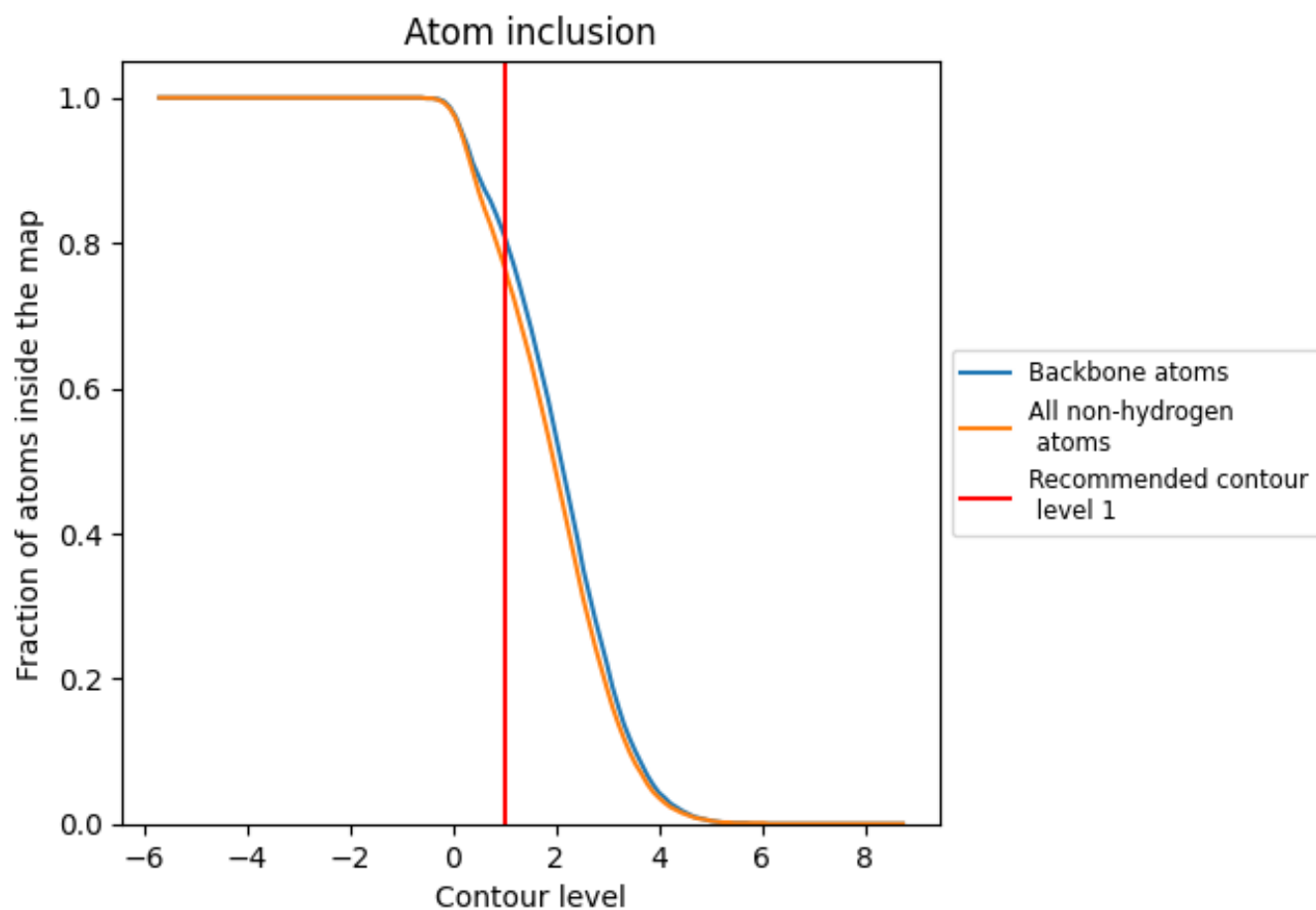
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1).











































9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 77% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7660	 0.5990
A	 0.8390	 0.6440
B	 0.8350	 0.6420
C	 0.9420	 0.6750
D	 0.8900	 0.6510
E	 0.2420	 0.2940
F	 0.4940	 0.5450
G	 0.8600	 0.6420
H	 0.6730	 0.5580
I	 0.5280	 0.5050
J	 0.8340	 0.6430
K	 0.8390	 0.6400
L	 0.9510	 0.6760
M	 0.8940	 0.6520
N	 0.2680	 0.3350
O	 0.4660	 0.5190
P	 0.8620	 0.6430
Q	 0.6690	 0.5650
R	 0.5310	 0.4950
S	 0.0060	 0.2200
T	 0.0070	 0.2030

