



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 11:37 PM UTC

PDB ID : 8ZOM / pdb_00008zom
EMDB ID : EMD-60307
Title : Cryo-EM structure of pyraclostrobin-bound *Arachis hypogaea* bc1 complex
Authors : Cui, G.R.; Wang, Y.X.; Yang, G.F.
Deposited on : 2024-05-28
Resolution : 2.74 Å(reported)

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:

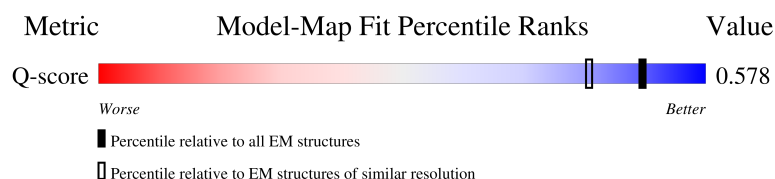
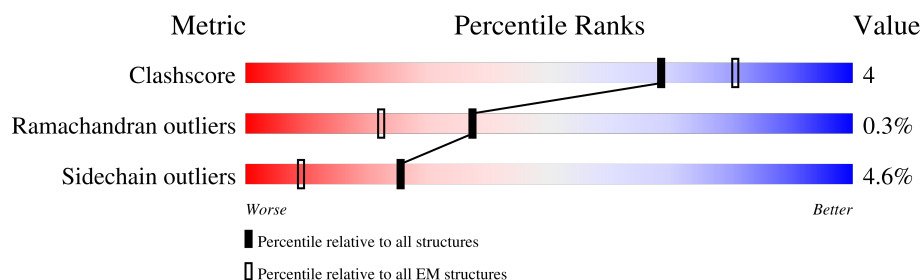
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.74 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.



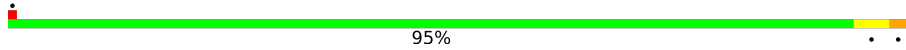
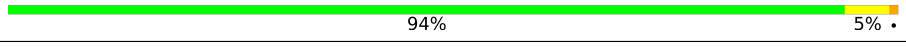
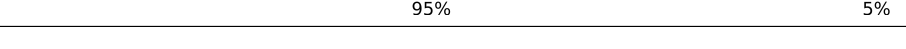
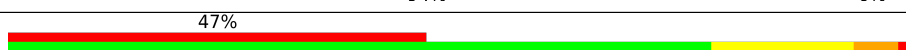
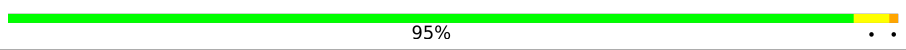
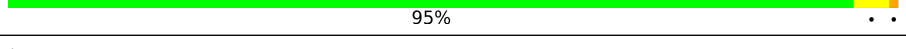
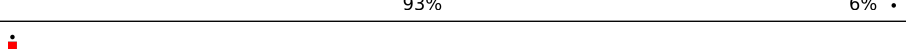
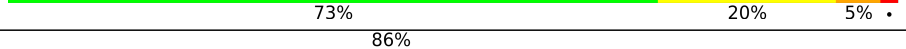
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10492 (2.24 - 3.24)

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	460	 85% 12% •
1	M	460	 86% 10% ••
2	B	487	 91% 8% •
2	N	487	 91% 7% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	386	
3	O	386	
4	D	242	
4	P	242	
5	E	196	
5	Q	196	
6	F	117	
6	R	117	
7	G	70	
7	S	70	
8	H	64	
8	T	64	
9	J	60	
9	V	60	
10	K	29	
10	W	29	

2 Entry composition [i](#)

There are 18 unique types of molecules in this entry. The entry contains 34466 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 Mitochondrial-processing peptidase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	460	Total	C	N	O	S	0	0
			3502	2220	591	679	12		
1	M	460	Total	C	N	O	S	0	0
			3502	2220	591	679	12		

- Molecule 2 is a protein called Mitochondrial-processing peptidase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	487	Total	C	N	O	S	0	0
			3855	2426	676	738	15		
2	N	487	Total	C	N	O	S	0	0
			3855	2426	676	738	15		

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	386	Total	C	N	O	S	0	0
			3076	2059	501	502	14		
3	O	385	Total	C	N	O	S	0	0
			3068	2055	500	499	14		

- Molecule 4 is a protein called Cytochrome c domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	242	Total	C	N	O	S	0	0
			1893	1205	323	354	11		
4	P	242	Total	C	N	O	S	0	0
			1893	1205	323	354	11		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	81	GLN	ASN	conflict	UNP A0A445B1W5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	125	GLU	ASP	conflict	UNP A0A445B1W5
D	186	PRO	ARG	conflict	UNP A0A445B1W5
D	246	SER	ALA	conflict	UNP A0A445B1W5
P	81	GLN	ASN	conflict	UNP A0A445B1W5
P	125	GLU	ASP	conflict	UNP A0A445B1W5
P	186	PRO	ARG	conflict	UNP A0A445B1W5
P	246	SER	ALA	conflict	UNP A0A445B1W5

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	196	Total	C	N	O	S	0	0
			1536	986	265	280	5		
5	Q	196	Total	C	N	O	S	0	0
			1536	986	265	280	5		

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	117	Total	C	N	O	S	0	0
			986	628	179	174	5		
6	R	117	Total	C	N	O	S	0	0
			986	628	179	174	5		

- Molecule 7 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	70	Total	C	N	O	S	0	0
			573	378	95	98	2		
7	S	70	Total	C	N	O	S	0	0
			573	378	95	98	2		

- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	64	Total	C	N	O	S	0	0
			519	330	87	96	6		
8	T	64	Total	C	N	O	S	0	0
			519	330	87	96	6		

- Molecule 9 is a protein called Complex III subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	60	Total	C	N	O	S	0	0
			486	312	88	85	1		
9	V	60	Total	C	N	O	S	0	0
			486	312	88	85	1		

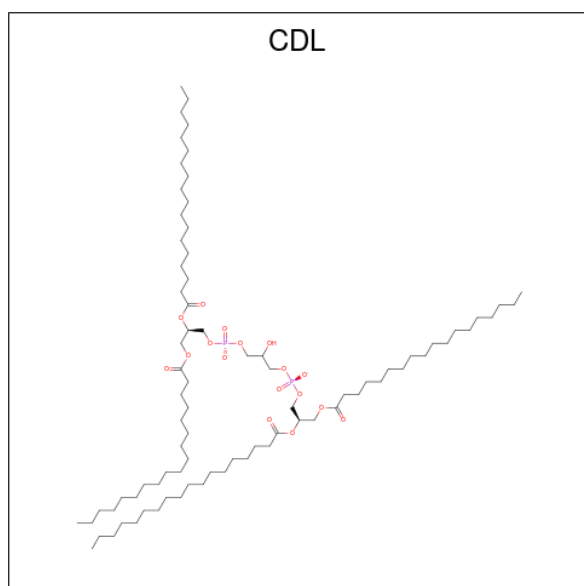
- Molecule 10 is a protein called Ubiquinol-cytochrome c reductase complex 6.7 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	29	Total	C	N	O	S	0	0
			218	145	35	37	1		
10	W	29	Total	C	N	O	S	0	0
			218	145	35	37	1		

- Molecule 11 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

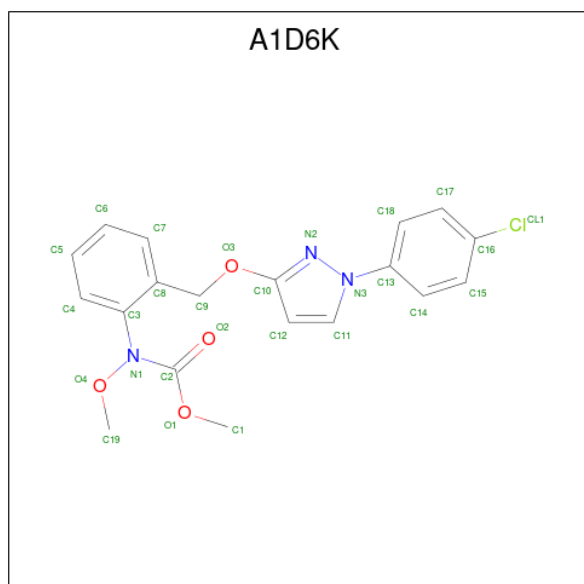
Mol	Chain	Residues	Atoms		AltConf
11	B	1	Total	Zn	0
			1	1	
11	N	1	Total	Zn	0
			1	1	

- Molecule 12 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



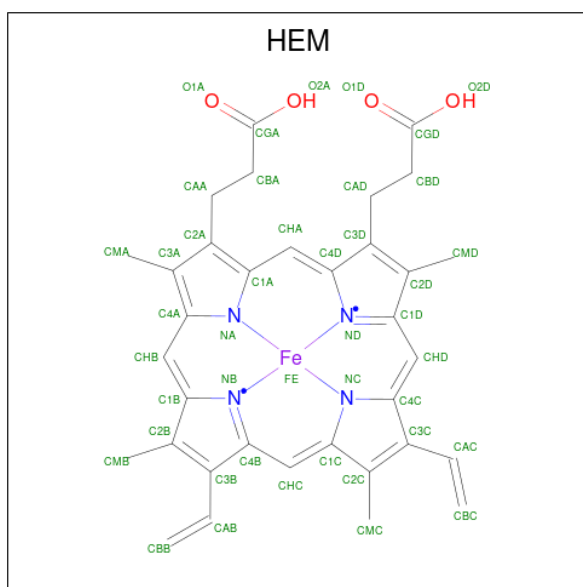
Mol	Chain	Residues	Atoms				AltConf
12	B	1	Total	C	O	P	0
			64	45	17	2	
12	C	1	Total	C	O	P	0
			64	45	17	2	
12	N	1	Total	C	O	P	0
			81	62	17	2	
12	N	1	Total	C	O	P	0
			70	51	17	2	
12	O	1	Total	C	O	P	0
			58	39	17	2	
12	O	1	Total	C	O	P	0
			63	44	17	2	

- Molecule 13 is methyl {N}-[2-[[1-(4-chlorophenyl)pyrazol-3-yl]oxymethyl]phenyl]- {N}-methoxy-carbamate (CCD ID: A1D6K) (formula: C₁₉H₁₈ClN₃O₄).



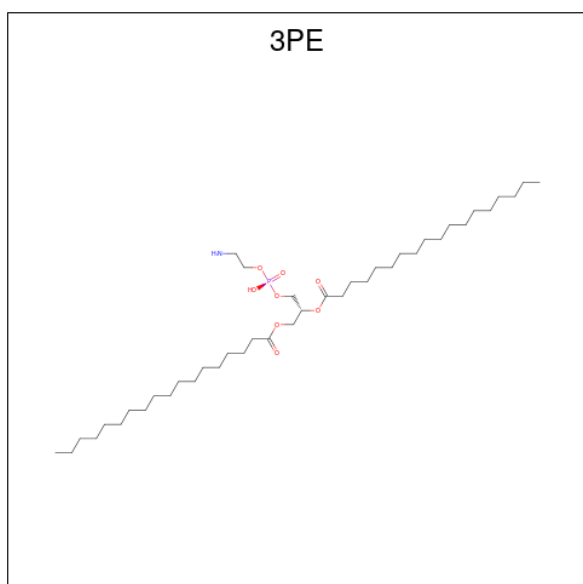
Mol	Chain	Residues	Atoms					AltConf
13	C	1	Total	C	Cl	N	O	0
			27	19	1	3	4	
13	O	1	Total	C	Cl	N	O	0
			27	19	1	3	4	

- Molecule 14 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄) (labeled as "Ligand of Interest" by depositor).



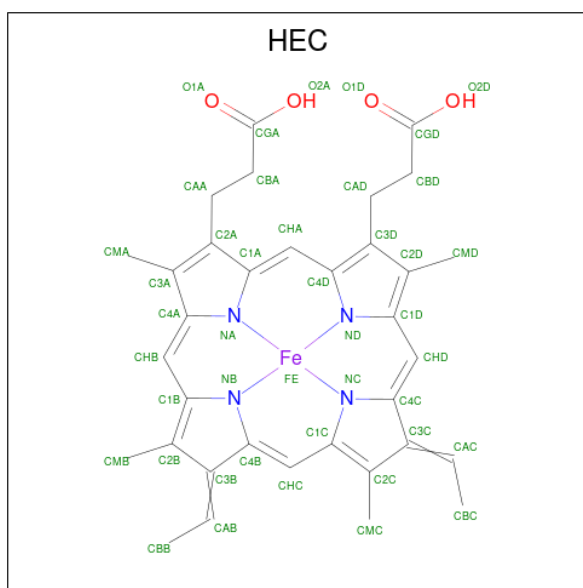
Mol	Chain	Residues	Atoms					AltConf
14	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
14	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
14	O	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
14	O	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 15 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).



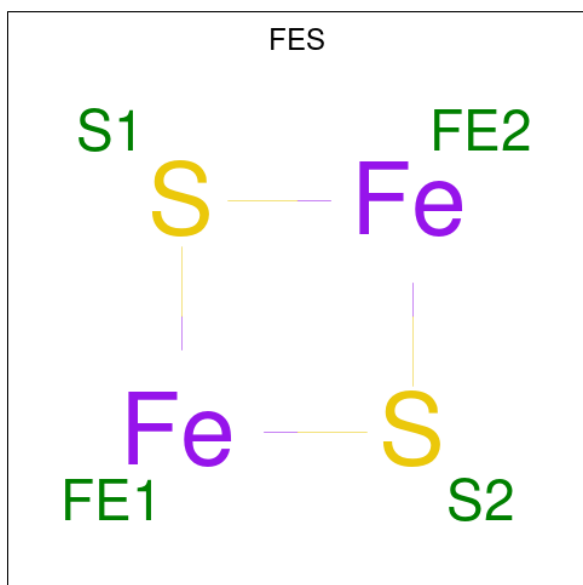
Mol	Chain	Residues	Atoms					AltConf
15	C	1	Total 28	C 18	N 1	O 8	P 1	0
15	C	1	Total 32	C 22	N 1	O 8	P 1	0
15	C	1	Total 51	C 41	N 1	O 8	P 1	0
15	C	1	Total 37	C 27	N 1	O 8	P 1	0
15	C	1	Total 33	C 23	N 1	O 8	P 1	0
15	C	1	Total 34	C 24	N 1	O 8	P 1	0
15	C	1	Total 36	C 26	N 1	O 8	P 1	0
15	K	1	Total 30	C 20	N 1	O 8	P 1	0
15	O	1	Total 39	C 29	N 1	O 8	P 1	0
15	O	1	Total 33	C 23	N 1	O 8	P 1	0
15	R	1	Total 38	C 28	N 1	O 8	P 1	0
15	R	1	Total 48	C 38	N 1	O 8	P 1	0

- Molecule 16 is HEME C (CCD ID: HEC) (formula: $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$) (labeled as "Ligand of Interest" by depositor).



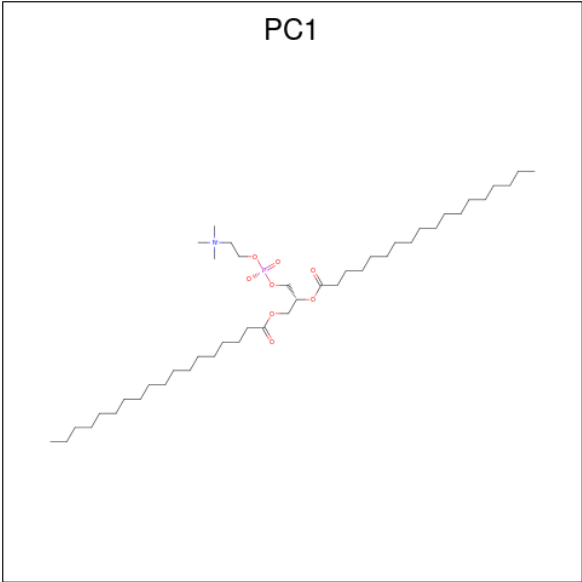
Mol	Chain	Residues	Atoms					AltConf
16	D	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
16	P	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 17 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
17	E	1	Total	Fe	S	0
			4	2	2	
17	Q	1	Total	Fe	S	0
			4	2	2	

- Molecule 18 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $\text{C}_{44}\text{H}_{88}\text{NO}_8\text{P}$) (labeled as "Ligand of Interest" by depositor).

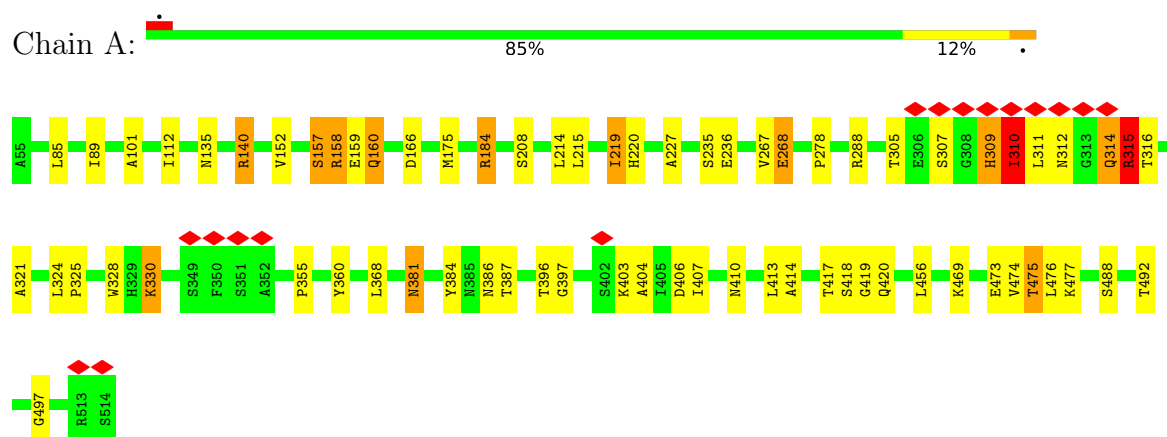


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
18	Q	1	25	17	1	6	1	0

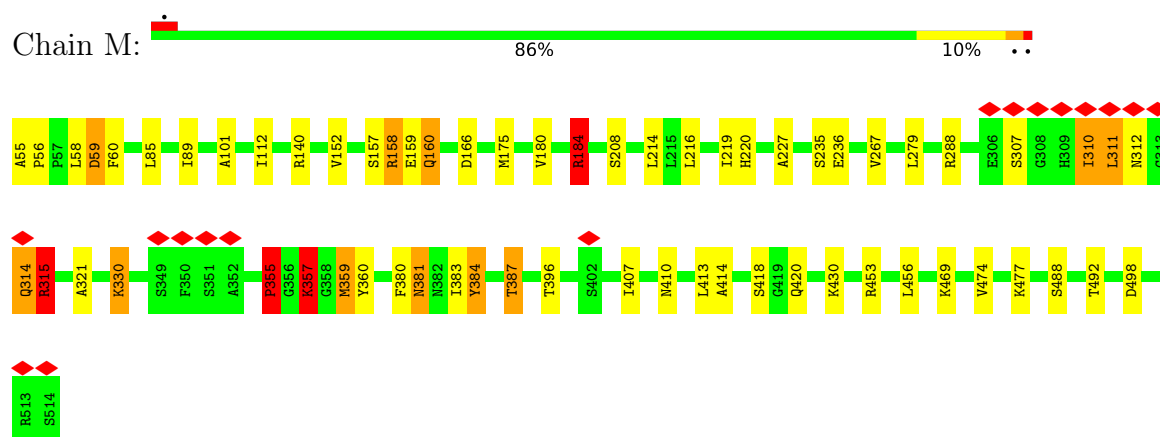
3 Residue-property plots

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.

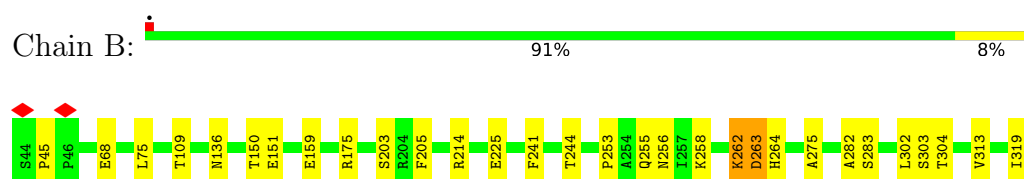
- Molecule 1: Mitochondrial-processing peptidase subunit alpha



- Molecule 1: Mitochondrial-processing peptidase subunit alpha



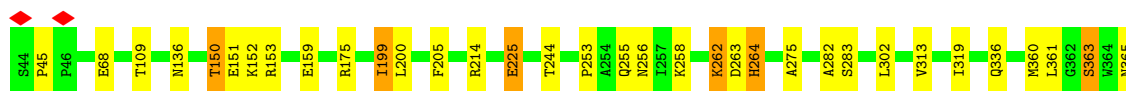
- Molecule 2: Mitochondrial-processing peptidase subunit beta





- Molecule 2: Mitochondrial-processing peptidase subunit beta

Chain N: 91% 7% .



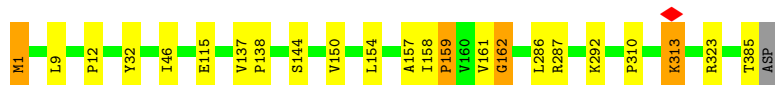
- Molecule 3: Cytochrome b

Chain C: 95% . .



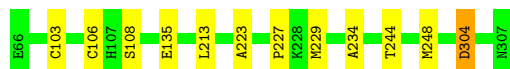
- Molecule 3: Cytochrome b

Chain O: 94% 5% .



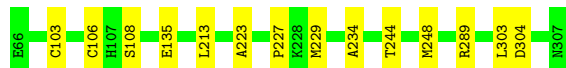
- Molecule 4: Cytochrome c domain-containing protein

Chain D: 95% 5%



- Molecule 4: Cytochrome c domain-containing protein

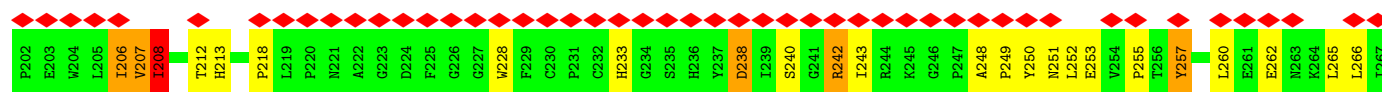
Chain P: 94% 6%



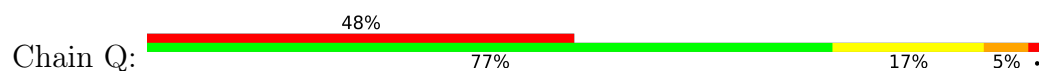
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain E: 47% 79% 16% 5% .

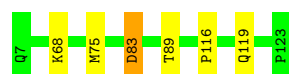




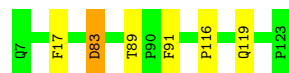
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



- Molecule 6: Cytochrome b-c1 complex subunit 7



- Molecule 6: Cytochrome b-c1 complex subunit 7



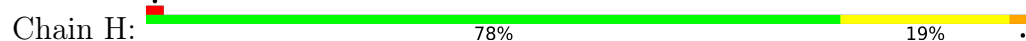
- Molecule 7: Cytochrome b-c1 complex subunit 8

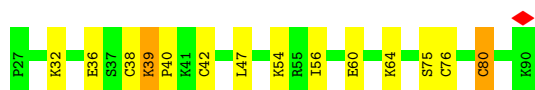


- Molecule 7: Cytochrome b-c1 complex subunit 8

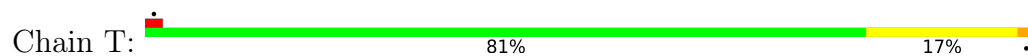


- Molecule 8: Cytochrome b-c1 complex subunit 6

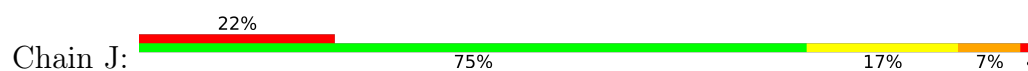




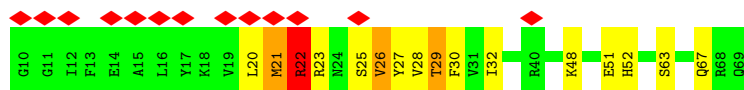
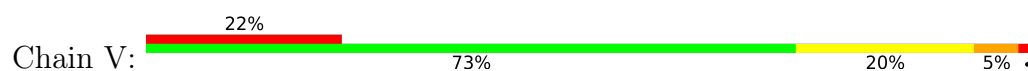
- Molecule 8: Cytochrome b-c1 complex subunit 6



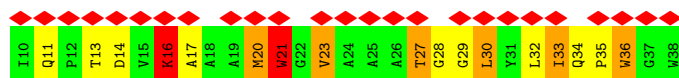
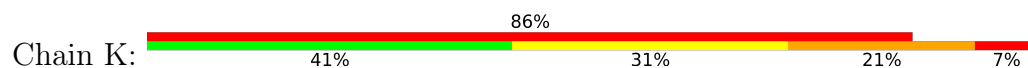
- Molecule 9: Complex III subunit 9



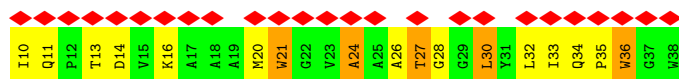
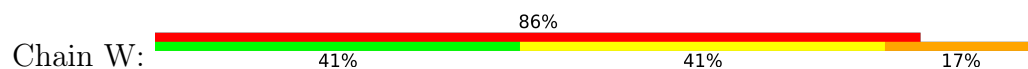
- Molecule 9: Complex III subunit 9



- Molecule 10: Ubiquinol-cytochrome c reductase complex 6.7 kDa protein



- Molecule 10: Ubiquinol-cytochrome c reductase complex 6.7 kDa protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	95092	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)	1600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	FEI EAGLE (4k x 4k)	Depositor
Maximum map value	8.780	Depositor
Minimum map value	-4.329	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.230	Depositor
Recommended contour level	0.586	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: CDL, A1D6K, ZN, HEC, PC1, HEM, FES, 3PE

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	0.59	7/3574 (0.2%)	0.85	5/4860 (0.1%)
1	M	0.65	13/3574 (0.4%)	0.92	14/4860 (0.3%)
2	B	0.56	6/3933 (0.2%)	0.74	10/5332 (0.2%)
2	N	0.57	6/3933 (0.2%)	0.80	12/5332 (0.2%)
3	C	0.51	2/3194 (0.1%)	0.80	8/4379 (0.2%)
3	O	0.51	1/3186 (0.0%)	0.77	5/4368 (0.1%)
4	D	0.47	0/1946	0.62	1/2644 (0.0%)
4	P	0.52	3/1946 (0.2%)	0.70	7/2644 (0.3%)
5	E	0.48	1/1576 (0.1%)	0.84	6/2144 (0.3%)
5	Q	0.56	1/1576 (0.1%)	0.94	7/2144 (0.3%)
6	F	0.49	0/1008	0.69	1/1352 (0.1%)
6	R	0.49	0/1008	0.72	1/1352 (0.1%)
7	G	0.56	0/591	0.87	3/799 (0.4%)
7	S	0.56	0/591	0.87	3/799 (0.4%)
8	H	0.44	0/529	0.79	2/705 (0.3%)
8	T	0.41	0/529	0.73	1/705 (0.1%)
9	J	0.58	0/496	1.20	4/666 (0.6%)
9	V	0.60	0/496	1.27	9/666 (1.4%)
10	K	0.99	0/226	2.02	9/310 (2.9%)
10	W	0.67	0/226	1.80	7/310 (2.3%)
All	All	0.55	40/34138 (0.1%)	0.84	115/46371 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	M	0	5
2	B	0	3

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
2	N	0	4
3	C	0	2
3	O	0	1
5	E	0	2
5	Q	0	4
9	J	0	2
9	V	0	1
All	All	0	29

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	P	303	LEU	C-N	11.20	1.48	1.33
1	M	384	TYR	CA-C	-9.97	1.43	1.53
1	A	386	ASN	C-O	-9.35	1.12	1.24
2	N	363	SER	C-O	-9.22	1.12	1.23
2	B	363	SER	C-O	-9.13	1.12	1.24
2	B	264	HIS	C-N	-8.99	1.22	1.34
1	M	383	ILE	C-N	-7.66	1.26	1.33
3	O	323	ARG	C-O	-7.36	1.15	1.24
3	C	323	ARG	C-O	-7.31	1.15	1.24
5	Q	167	PRO	C-N	6.74	1.42	1.33
1	M	384	TYR	C-O	-6.72	1.17	1.24
1	M	387	THR	C-O	-6.58	1.17	1.23
1	M	267	VAL	C-O	-6.55	1.17	1.24
1	A	140	ARG	C-O	-6.51	1.15	1.24
1	A	267	VAL	C-O	-6.46	1.17	1.24
1	M	140	ARG	C-O	-6.45	1.15	1.24
2	N	365	ASN	C-N	-6.42	1.24	1.33
1	A	330	LYS	CA-CB	6.32	1.61	1.53
1	M	330	LYS	CA-CB	6.32	1.61	1.53
1	A	278	PRO	C-O	-6.12	1.16	1.24
5	E	166	LYS	N-CA	6.11	1.50	1.46
2	B	263	ASP	C-N	6.09	1.41	1.33
2	B	365	ASN	C-N	-6.05	1.24	1.33
2	N	199	ILE	C-O	-5.90	1.17	1.24
1	M	355	PRO	C-O	-5.84	1.16	1.23
1	M	311	LEU	C-N	5.74	1.41	1.33
1	A	158	ARG	C-O	-5.49	1.16	1.24
2	B	400	ASP	C-O	-5.48	1.17	1.23
1	M	158	ARG	C-O	-5.48	1.16	1.24
4	P	304	ASP	C-N	-5.48	1.20	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	400	ASP	C-O	-5.37	1.17	1.23
1	M	310	ILE	C-N	5.33	1.40	1.34
2	B	365	ASN	C-O	-5.28	1.17	1.23
2	N	365	ASN	C-O	-5.24	1.17	1.23
1	A	157	SER	CA-CB	-5.22	1.45	1.53
2	N	386	GLU	C-N	-5.12	1.27	1.33
4	P	304	ASP	N-CA	5.11	1.52	1.46
1	M	279	LEU	C-O	-5.08	1.17	1.24
1	M	380	PHE	C-O	-5.06	1.17	1.23
3	C	5	ARG	C-N	-5.01	1.28	1.33

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	J	22	ARG	N-CA-C	-12.63	96.58	112.88
2	N	225	GLU	N-CA-C	-12.51	95.64	114.16
6	R	83	ASP	CB-CA-C	-11.73	91.08	110.79
10	K	33	ILE	CA-C-N	-10.50	112.61	122.37
10	K	33	ILE	C-N-CA	-10.50	112.61	122.37
1	M	311	LEU	O-C-N	10.28	128.44	120.83
6	F	83	ASP	CB-CA-C	-10.20	94.78	110.90
5	Q	167	PRO	CB-CA-C	-9.69	95.58	111.56
2	N	365	ASN	CB-CA-C	-9.43	90.47	109.79
2	B	225	GLU	N-CA-C	-8.99	100.15	114.09
2	B	365	ASN	CB-CA-C	-8.93	90.42	110.07
4	P	304	ASP	N-CA-CB	8.82	124.22	114.17
2	N	386	GLU	CA-CB-CG	8.78	131.65	114.10
5	Q	167	PRO	N-CA-CB	-8.75	94.06	103.25
7	S	61	ILE	N-CA-C	-8.64	104.72	113.10
9	V	29	THR	N-CA-C	-8.64	104.77	114.62
10	W	21	TRP	N-CA-C	-8.64	102.52	113.23
7	G	61	ILE	N-CA-C	-8.59	104.77	113.10
5	Q	167	PRO	N-CA-C	8.32	129.61	112.47
9	J	26	VAL	N-CA-C	-8.31	102.72	110.53
4	P	304	ASP	CB-CA-C	-8.23	98.20	110.06
4	P	304	ASP	O-C-N	-8.15	113.82	121.56
10	W	27	THR	N-CA-C	-8.10	102.39	111.71
10	W	26	ALA	N-CA-C	-8.03	103.61	113.41
4	P	303	LEU	O-C-N	7.88	130.45	122.10
3	C	163	ASP	N-CA-C	-7.73	94.34	110.80
2	B	361	LEU	N-CA-C	-7.60	102.93	111.14
4	P	304	ASP	CA-CB-CG	7.56	120.16	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	220	HIS	CA-CB-CG	7.56	121.36	113.80
1	M	380	PHE	CA-CB-CG	7.40	121.20	113.80
1	M	59	ASP	CA-CB-CG	7.35	119.95	112.60
1	M	383	ILE	CA-C-N	7.17	131.62	122.16
1	M	383	ILE	C-N-CA	7.17	131.62	122.16
2	B	264	HIS	CA-C-O	-7.11	113.35	120.82
2	N	264	HIS	CA-C-O	-7.10	113.30	120.90
2	B	264	HIS	O-C-N	-7.08	114.78	122.07
5	E	238	ASP	CB-CA-C	7.03	123.30	109.66
10	K	17	ALA	N-CA-C	-7.03	103.69	112.90
2	N	361	LEU	N-CA-C	-7.00	103.58	111.14
1	M	312	ASN	CB-CA-C	6.91	120.96	109.56
5	Q	238	ASP	CB-CA-C	6.91	123.22	110.24
2	N	400	ASP	CA-CB-CG	6.90	119.50	112.60
2	B	400	ASP	CA-CB-CG	6.88	119.48	112.60
5	Q	238	ASP	N-CA-C	-6.72	99.52	109.81
2	N	386	GLU	CB-CG-CD	6.61	123.83	112.60
5	E	238	ASP	N-CA-C	-6.58	99.45	109.85
3	C	138	PRO	N-CA-C	6.57	118.71	110.70
9	V	22	ARG	CB-CA-C	-6.56	99.47	110.56
4	D	304	ASP	N-CA-CB	6.53	121.52	110.49
3	O	138	PRO	N-CA-C	6.51	118.65	110.70
7	G	62	SER	N-CA-C	-6.50	105.27	113.72
10	K	36	TRP	CA-C-N	-6.50	111.96	120.22
10	K	36	TRP	C-N-CA	-6.50	111.96	120.22
10	K	16	LYS	N-CA-C	-6.47	105.36	113.20
7	S	62	SER	N-CA-C	-6.46	105.32	113.72
2	B	361	LEU	CB-CA-C	6.46	121.11	110.90
1	M	355	PRO	N-CA-CB	-6.40	97.78	103.35
8	H	36	GLU	N-CA-C	-6.34	105.67	113.41
2	N	361	LEU	CB-CA-C	6.33	120.91	110.90
3	O	159	PRO	N-CA-C	6.33	125.51	112.47
9	V	25	SER	O-C-N	6.30	129.55	122.11
9	V	21	MET	N-CA-C	6.14	118.36	109.71
3	C	161	VAL	N-CA-C	-6.07	95.80	106.61
3	C	164	THR	N-CA-C	-6.07	106.03	113.50
1	A	219	ILE	N-CA-C	-6.04	106.61	112.29
3	O	1	MET	CB-CG-SD	5.94	130.52	112.70
1	M	219	ILE	N-CA-C	-5.93	106.63	111.91
3	C	1	MET	CB-CG-SD	5.93	130.49	112.70
10	W	21	TRP	N-CA-CB	5.91	119.66	110.44
9	J	22	ARG	CB-CA-C	-5.84	100.85	110.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	207	VAL	CA-C-O	-5.83	115.19	121.19
1	M	387	THR	CB-CA-C	-5.76	99.74	110.56
3	C	159	PRO	CA-N-CD	-5.74	103.96	112.00
2	B	263	ASP	O-C-N	5.73	129.13	122.20
7	S	63	ALA	N-CA-C	-5.72	106.85	113.88
5	Q	207	VAL	CA-C-O	-5.69	115.25	121.28
10	K	21	TRP	N-CA-C	-5.68	105.46	112.90
7	G	63	ALA	N-CA-C	-5.67	106.91	113.88
1	M	310	ILE	CA-C-N	-5.67	114.13	121.79
1	M	310	ILE	C-N-CA	-5.67	114.13	121.79
4	P	303	LEU	CA-C-N	-5.63	116.48	126.45
4	P	303	LEU	C-N-CA	-5.63	116.48	126.45
9	V	27	TYR	CB-CA-C	5.61	121.53	111.03
1	A	309	HIS	N-CA-C	5.59	119.96	113.20
10	K	33	ILE	CA-C-O	-5.57	115.23	121.36
1	M	381	ASN	CA-CB-CG	5.57	118.17	112.60
1	A	312	ASN	N-CA-C	-5.53	106.48	113.23
10	K	35	PRO	N-CA-C	-5.53	101.08	112.47
9	V	30	PHE	CA-CB-CG	5.53	119.33	113.80
2	N	361	LEU	CA-C-O	-5.50	115.04	120.70
8	H	80	CYS	CA-CB-SG	5.49	127.03	114.40
8	T	80	CYS	CA-CB-SG	5.49	127.02	114.40
10	W	36	TRP	CA-C-N	-5.48	113.29	120.14
10	W	36	TRP	C-N-CA	-5.48	113.29	120.14
9	V	30	PHE	N-CA-C	-5.46	104.97	111.03
5	E	208	ILE	CA-C-O	-5.43	113.99	120.78
2	B	361	LEU	CA-C-O	-5.43	115.11	120.70
1	A	381	ASN	CA-CB-CG	5.42	118.02	112.60
2	N	365	ASN	N-CA-CB	5.36	120.87	111.55
1	M	357	LYS	N-CA-C	5.33	122.14	110.80
2	N	225	GLU	O-C-N	5.32	127.33	121.85
5	E	238	ASP	CA-C-O	-5.26	115.30	121.46
5	Q	179	LYS	CA-C-O	-5.24	115.07	121.78
3	C	159	PRO	CA-C-N	-5.24	112.53	121.97
3	C	159	PRO	C-N-CA	-5.24	112.53	121.97
2	B	365	ASN	N-CA-CB	5.24	120.81	111.69
9	J	52	HIS	N-CA-C	-5.23	107.56	114.31
9	V	22	ARG	N-CA-C	-5.23	106.49	112.92
9	V	52	HIS	N-CA-C	-5.23	107.57	114.31
3	O	158	ILE	CA-C-N	5.18	126.31	119.84
3	O	158	ILE	C-N-CA	5.18	126.31	119.84
1	M	357	LYS	CB-CA-C	-5.13	100.21	110.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	529	ARG	N-CA-C	-5.11	99.92	110.80
10	W	24	ALA	O-C-N	5.01	129.15	122.43
5	E	206	ILE	O-C-N	-5.01	118.17	123.03

There are no chirality outliers.

All (29) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	158	ARG	Sidechain
1	A	184	ARG	Sidechain
1	A	288	ARG	Sidechain
1	A	315	ARG	Sidechain
1	A	355	PRO	Peptide
2	B	175	ARG	Sidechain
2	B	360	MET	Mainchain
2	B	497	ARG	Sidechain
3	C	313	LYS	Peptide
3	C	5	ARG	Sidechain
5	E	164	ARG	Sidechain
5	E	242	ARG	Sidechain
9	J	22	ARG	Sidechain
9	J	23	ARG	Sidechain
1	M	158	ARG	Sidechain
1	M	184	ARG	Sidechain
1	M	288	ARG	Sidechain
1	M	315	ARG	Sidechain
1	M	453	ARG	Sidechain
2	N	175	ARG	Sidechain
2	N	360	MET	Mainchain
2	N	497	ARG	Sidechain
2	N	529	ARG	Sidechain
3	O	313	LYS	Peptide
5	Q	164	ARG	Sidechain
5	Q	178	ILE	Mainchain
5	Q	198	ARG	Sidechain
5	Q	242	ARG	Sidechain
9	V	22	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3502	0	3495	38	0
1	M	3502	0	3495	29	0
2	B	3855	0	3817	20	0
2	N	3855	0	3817	24	0
3	C	3076	0	3058	8	0
3	O	3068	0	3054	14	0
4	D	1893	0	1827	5	0
4	P	1893	0	1827	6	0
5	E	1536	0	1541	24	0
5	Q	1536	0	1540	27	0
6	F	986	0	997	5	0
6	R	986	0	997	5	0
7	G	573	0	585	1	0
7	S	573	0	585	3	0
8	H	519	0	519	3	0
8	T	519	0	521	3	0
9	J	486	0	481	8	0
9	V	486	0	481	6	0
10	K	218	0	212	16	0
10	W	218	0	212	15	0
11	B	1	0	0	0	0
11	N	1	0	0	0	0
12	B	64	0	72	3	0
12	C	64	0	72	3	0
12	N	151	0	199	6	0
12	O	121	0	130	6	0
13	C	27	0	0	0	0
13	O	27	0	0	0	0
14	C	86	0	60	1	0
14	O	86	0	60	0	0
15	C	251	0	326	12	0
15	K	30	0	34	1	0
15	O	72	0	92	0	0
15	R	86	0	123	5	0
16	D	43	0	32	2	0
16	P	43	0	32	2	0
17	E	4	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	Q	4	0	0	0	0
18	Q	25	0	31	3	0
All	All	34466	0	34324	254	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 4.

All (254) 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)
9:V:20:LEU:HG	9:V:26:VAL:HB	1.42	0.97
5:Q:207:VAL:HG12	5:Q:255:PRO:HD2	1.54	0.90
5:E:207:VAL:HG12	5:E:255:PRO:HD2	1.55	0.89
9:J:36:PHE:HZ	10:K:36:TRP:HA	1.39	0.87
2:N:205:PHE:HB2	2:N:262:LYS:HG3	1.64	0.79
1:A:309:HIS:HB3	1:A:314:GLN:HE21	1.49	0.76
12:O:407:CDL:H742	7:S:55:LYS:HE2	1.68	0.75
1:M:59:ASP:OD1	1:M:60:PHE:CD1	2.40	0.74
2:B:528:ASN:HA	9:J:24:ASN:OD1	1.92	0.69
5:Q:164:ARG:HG3	5:Q:165:GLY:H	1.57	0.69
9:J:32:ILE:HG22	10:K:30:LEU:HD12	1.73	0.69
10:W:32:LEU:HG	10:W:33:ILE:H	1.58	0.68
5:E:164:ARG:HG3	5:E:165:GLY:H	1.58	0.67
1:A:208:SER:HA	1:A:214:LEU:HD11	1.77	0.67
9:V:20:LEU:HG	9:V:26:VAL:CB	2.22	0.67
10:K:21:TRP:HA	10:K:21:TRP:CE3	2.29	0.67
2:N:150:THR:HG22	2:N:153:ARG:H	1.59	0.66
5:E:198:ARG:HH21	5:E:251:ASN:HB2	1.61	0.65
9:V:26:VAL:HA	9:V:29:THR:HG22	1.79	0.65
1:M:208:SER:HA	1:M:214:LEU:HD11	1.77	0.65
2:N:262:LYS:O	2:N:263:ASP:C	2.40	0.64
5:Q:198:ARG:HH11	5:Q:242:ARG:HB3	1.63	0.64
9:V:32:ILE:HG21	10:W:28:GLY:HA2	1.81	0.63
1:A:404:ALA:HA	1:A:407:ILE:HD12	1.80	0.63
18:Q:302:PC1:H142	7:S:41:MET:H	1.62	0.63
5:E:155:PRO:HA	5:E:172:ARG:HG3	1.81	0.62
5:Q:155:PRO:HA	5:Q:172:ARG:HG3	1.81	0.62
2:N:253:PRO:HD2	2:N:256:ASN:HD22	1.66	0.61
9:J:36:PHE:CZ	10:K:36:TRP:HA	2.30	0.61
1:A:314:GLN:HG3	1:A:497:GLY:HA2	1.83	0.61
2:N:523:ARG:HH22	2:N:528:ASN:HB2	1.65	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:523:ARG:HH22	2:B:528:ASN:HB2	1.65	0.60
2:B:253:PRO:HD2	2:B:256:ASN:HD22	1.66	0.60
5:E:207:VAL:HG23	5:E:252:LEU:HD22	1.82	0.60
9:V:20:LEU:CG	9:V:26:VAL:HB	2.26	0.59
3:O:154:LEU:HD21	3:O:286:LEU:HD11	1.85	0.59
1:M:160:GLN:HE22	1:M:456:LEU:HD12	1.69	0.58
3:O:157:ALA:HB2	3:O:292:LYS:HZ2	1.69	0.58
3:C:154:LEU:HD21	3:C:286:LEU:HD11	1.85	0.57
15:C:411:3PE:H12	3:O:12:PRO:HB3	1.86	0.57
2:N:214:ARG:HD3	2:N:258:LYS:HA	1.85	0.57
1:A:112:ILE:HB	1:A:227:ALA:HB1	1.86	0.57
1:A:315:ARG:HD2	1:A:397:GLY:HA2	1.87	0.57
1:A:160:GLN:HE22	1:A:456:LEU:HD12	1.70	0.57
2:B:214:ARG:HD3	2:B:258:LYS:HA	1.85	0.57
5:Q:207:VAL:HG23	5:Q:252:LEU:HD22	1.87	0.57
1:M:157:SER:HB2	1:M:160:GLN:H	1.70	0.56
1:M:355:PRO:HA	1:M:359:MET:HE1	1.87	0.56
10:K:21:TRP:HA	10:K:21:TRP:HE3	1.70	0.56
1:M:112:ILE:HB	1:M:227:ALA:HB1	1.86	0.56
5:Q:212:THR:HG21	5:Q:250:TYR:HB2	1.89	0.55
1:A:417:THR:HG22	1:A:419:GLY:H	1.72	0.55
5:E:212:THR:HG21	5:E:250:TYR:HB2	1.89	0.55
5:E:243:ILE:HD12	5:E:248:ALA:HB3	1.90	0.54
5:Q:243:ILE:HD12	5:Q:248:ALA:HB3	1.90	0.54
10:W:33:ILE:O	10:W:35:PRO:HD3	2.07	0.54
4:P:103:CYS:HB2	16:P:401:HEC:HAB	1.90	0.54
1:A:314:GLN:O	1:A:315:ARG:HB2	2.07	0.53
15:C:404:3PE:H231	10:W:36:TRP:CD1	2.43	0.53
10:W:33:ILE:C	10:W:35:PRO:HD3	2.32	0.53
4:D:103:CYS:HB2	16:D:501:HEC:HAB	1.89	0.53
5:Q:179:LYS:HG3	5:Q:180:LEU:N	2.24	0.53
12:O:407:CDL:H321	4:P:289:ARG:HD2	1.89	0.53
5:Q:218:PRO:HB2	5:Q:228:TRP:HB3	1.92	0.52
5:Q:190:ARG:HE	5:Q:249:PRO:HA	1.74	0.52
1:A:307:SER:HB3	1:M:236:GLU:H	1.75	0.52
12:N:603:CDL:H751	12:N:603:CDL:H341	1.92	0.51
18:Q:302:PC1:H122	7:S:41:MET:HB2	1.93	0.51
2:N:313:VAL:HG21	2:N:399:LYS:HD3	1.93	0.51
4:D:234:ALA:HB3	4:D:248:MET:HE1	1.92	0.51
10:K:32:LEU:HD11	15:K:101:3PE:H331	1.92	0.51
5:E:190:ARG:HE	5:E:249:PRO:HA	1.74	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:218:PRO:HB2	5:E:228:TRP:HB3	1.92	0.51
2:N:336:GLN:HG2	2:N:409:VAL:HG22	1.93	0.51
2:B:313:VAL:HG21	2:B:399:LYS:HD3	1.93	0.51
5:Q:207:VAL:HG12	5:Q:255:PRO:CD	2.35	0.51
3:O:157:ALA:HB2	3:O:292:LYS:NZ	2.26	0.50
4:P:234:ALA:HB3	4:P:248:MET:HE1	1.92	0.50
6:R:17:PHE:HB3	15:R:202:3PE:H341	1.94	0.50
2:N:109:THR:HG22	2:N:282:ALA:HB3	1.94	0.50
1:A:236:GLU:H	1:M:307:SER:HB3	1.75	0.50
2:N:433:VAL:N	10:W:10:ILE:HG23	2.27	0.50
5:Q:124:ARG:HG3	10:W:32:LEU:HB3	1.93	0.50
3:C:292:LYS:HD3	5:Q:213:HIS:CD2	2.47	0.49
1:A:407:ILE:HA	1:A:410:ASN:HD21	1.76	0.49
3:C:32:TYR:HB2	12:C:410:CDL:HB21	1.94	0.49
2:N:527:TRP:HB3	2:N:529:ARG:HG2	1.94	0.49
5:Q:179:LYS:HG3	5:Q:180:LEU:HG	1.95	0.49
2:B:336:GLN:HG2	2:B:409:VAL:HG22	1.93	0.49
2:N:136:ASN:HD22	2:N:253:PRO:HD3	1.77	0.49
2:B:136:ASN:HD22	2:B:253:PRO:HD3	1.77	0.49
12:O:407:CDL:H711	12:O:407:CDL:H1	1.94	0.49
1:A:310:ILE:HA	1:A:314:GLN:H	1.78	0.49
1:A:305:THR:HG21	1:A:314:GLN:HG2	1.94	0.48
8:H:39:LYS:N	8:H:40:PRO:HD2	2.28	0.48
2:N:262:LYS:HB3	2:N:262:LYS:HE3	1.53	0.48
2:B:109:THR:HG22	2:B:282:ALA:HB3	1.94	0.48
1:M:430:LYS:NZ	1:M:474:VAL:O	2.38	0.48
12:N:602:CDL:H312	12:N:602:CDL:H771	1.96	0.48
9:J:25:SER:HB3	10:K:20:MET:HB3	1.96	0.48
10:K:32:LEU:O	10:K:34:GLN:HG3	2.14	0.48
1:M:314:GLN:HB2	1:M:498:ASP:OD2	2.13	0.48
10:K:16:LYS:HA	10:K:16:LYS:HD3	1.51	0.48
5:Q:179:LYS:C	5:Q:181:ALA:H	2.20	0.48
1:M:360:TYR:HE1	2:N:159:GLU:HB3	1.78	0.48
1:A:473:GLU:O	1:A:474:VAL:C	2.54	0.47
2:B:205:PHE:HB2	2:B:262:LYS:HG3	1.95	0.47
2:B:528:ASN:CA	9:J:24:ASN:OD1	2.62	0.47
10:K:28:GLY:C	10:K:30:LEU:H	2.22	0.47
1:A:410:ASN:HA	1:A:413:LEU:HD12	1.96	0.47
1:A:157:SER:HB3	1:A:160:GLN:H	1.78	0.47
12:B:602:CDL:HA21	12:B:602:CDL:HB31	1.95	0.47
15:C:404:3PE:H231	10:W:36:TRP:HD1	1.78	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:42:CYS:SG	8:H:76:CYS:HB3	2.55	0.47
6:R:116:PRO:HG2	6:R:119:GLN:HE21	1.80	0.47
2:B:244:THR:HG21	2:B:319:ILE:H	1.79	0.47
2:B:255:GLN:HA	2:B:258:LYS:HE2	1.96	0.47
2:N:530:TYR:O	10:W:21:TRP:NE1	2.48	0.47
15:R:202:3PE:H3F1	15:R:202:3PE:H2B2	1.97	0.47
6:F:116:PRO:HG2	6:F:119:GLN:HE21	1.80	0.47
1:A:475:THR:OG1	1:A:476:LEU:N	2.47	0.46
6:R:89:THR:O	6:R:89:THR:OG1	2.33	0.46
1:M:101:ALA:HB3	1:M:175:MET:HE1	1.98	0.46
2:B:275:ALA:HB2	2:B:302:LEU:HD11	1.97	0.46
1:A:410:ASN:O	1:A:414:ALA:N	2.47	0.46
1:A:101:ALA:HB3	1:A:175:MET:HE1	1.98	0.46
2:B:262:LYS:HB3	2:B:262:LYS:HE3	1.48	0.46
2:N:244:THR:HG21	2:N:319:ILE:H	1.79	0.46
2:N:255:GLN:HA	2:N:258:LYS:HE2	1.97	0.46
5:Q:208:ILE:H	5:Q:208:ILE:HG12	1.26	0.46
9:J:36:PHE:HZ	10:K:36:TRP:CA	2.19	0.46
5:Q:219:LEU:N	5:Q:229:PHE:O	2.38	0.46
8:T:39:LYS:O	8:T:40:PRO:C	2.58	0.46
1:A:309:HIS:HB3	1:A:314:GLN:HG2	1.97	0.46
12:C:410:CDL:H222	12:C:410:CDL:H191	1.67	0.46
12:N:602:CDL:HB31	12:N:602:CDL:OA7	2.16	0.46
1:M:220:HIS:CE1	1:M:384:TYR:OH	2.69	0.46
2:N:263:ASP:O	2:N:264:HIS:C	2.57	0.46
12:N:603:CDL:HA32	3:O:9:LEU:HG	1.98	0.46
10:W:32:LEU:HG	10:W:33:ILE:N	2.27	0.46
1:A:160:GLN:HE21	1:A:160:GLN:HB3	1.35	0.45
8:H:56:ILE:HG22	8:H:64:LYS:HE2	1.98	0.45
9:J:26:VAL:O	9:J:29:THR:N	2.41	0.45
10:K:23:VAL:O	10:K:27:THR:HB	2.16	0.45
2:N:150:THR:HG22	2:N:152:LYS:H	1.81	0.45
2:N:275:ALA:HB2	2:N:302:LEU:HD11	1.97	0.45
1:M:359:MET:HE2	1:M:359:MET:HB2	1.88	0.45
9:V:29:THR:HB	10:W:24:ALA:HB1	1.98	0.45
1:A:321:ALA:HB3	1:A:492:THR:HB	1.97	0.45
15:C:411:3PE:H222	15:C:411:3PE:H252	1.78	0.45
15:C:407:3PE:H262	12:C:410:CDL:H622	1.98	0.45
10:K:20:MET:HA	10:K:23:VAL:HB	1.99	0.45
15:R:202:3PE:H361	15:R:202:3PE:H391	1.80	0.45
2:B:45:PRO:HB3	6:R:89:THR:HG22	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:213:HIS:HB2	5:E:248:ALA:HB2	1.99	0.45
1:M:321:ALA:HB3	1:M:492:THR:HB	1.97	0.45
5:E:207:VAL:CG2	5:E:252:LEU:HD22	2.47	0.44
5:Q:207:VAL:CG2	5:Q:252:LEU:HD22	2.47	0.44
8:T:56:ILE:HG22	8:T:64:LYS:HE2	1.98	0.44
15:C:406:3PE:H3D2	15:C:406:3PE:H371	2.00	0.44
3:C:115:GLU:HG3	3:C:310:PRO:HB2	2.00	0.44
5:E:169:PHE:HZ	5:E:218:PRO:HD2	1.82	0.44
1:A:268:GLU:H	1:A:268:GLU:HG3	1.27	0.44
5:Q:179:LYS:C	5:Q:181:ALA:N	2.75	0.44
15:R:202:3PE:H221	15:R:202:3PE:H252	1.75	0.44
1:A:160:GLN:NE2	1:A:456:LEU:HD12	2.33	0.44
6:F:68:LYS:HD2	7:G:26:MET:HE2	2.00	0.44
10:K:23:VAL:O	10:K:27:THR:N	2.51	0.44
3:O:137:VAL:HA	3:O:144:SER:HB3	1.99	0.44
4:P:213:LEU:HD23	4:P:223:ALA:HB1	2.00	0.44
6:F:89:THR:O	6:F:89:THR:OG1	2.33	0.44
10:W:36:TRP:CD1	10:W:36:TRP:H	2.35	0.44
15:C:411:3PE:H3A1	15:C:411:3PE:H371	1.78	0.44
1:M:159:GLU:C	1:M:160:GLN:HG2	2.43	0.43
3:O:32:TYR:CB	12:O:407:CDL:H512	2.48	0.43
4:D:213:LEU:HD23	4:D:223:ALA:HB1	2.00	0.43
1:A:403:LYS:HA	1:A:406:ASP:CG	2.42	0.43
3:O:115:GLU:HG3	3:O:310:PRO:HB2	2.00	0.43
1:A:159:GLU:C	1:A:160:GLN:HG2	2.43	0.43
5:E:146:LEU:HD23	5:E:147:GLU:H	1.83	0.43
12:N:602:CDL:H612	3:O:46:ILE:HD11	2.01	0.43
3:O:161:VAL:HG23	3:O:162:GLY:H	1.84	0.43
5:Q:213:HIS:HB2	5:Q:248:ALA:HB2	1.99	0.43
8:T:39:LYS:N	8:T:40:PRO:HD2	2.34	0.43
15:C:406:3PE:H3E2	15:C:406:3PE:H3B1	1.91	0.43
5:E:233:HIS:CD2	3:O:287:ARG:HG2	2.54	0.43
12:N:602:CDL:H331	12:N:603:CDL:H582	2.01	0.43
15:R:202:3PE:H282	15:R:202:3PE:H2B1	1.69	0.43
1:A:324:LEU:HA	1:A:325:PRO:HD3	1.91	0.43
3:C:137:VAL:HA	3:C:144:SER:HB3	1.99	0.43
12:O:407:CDL:H152	12:O:407:CDL:H181	1.55	0.43
15:C:406:3PE:H2I3	15:C:406:3PE:H2F1	1.88	0.42
4:D:106:CYS:SG	16:D:501:HEC:HAC	2.60	0.42
1:A:360:TYR:HE1	2:B:159:GLU:HB3	1.84	0.42
5:Q:146:LEU:HD23	5:Q:147:GLU:H	1.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:160:GLN:NE2	1:M:456:LEU:HD12	2.33	0.42
1:M:410:ASN:O	1:M:413:LEU:N	2.53	0.42
3:O:385:THR:HA	6:R:91:PHE:HB3	2.01	0.42
4:P:227:PRO:HG2	4:P:229:MET:HE3	2.02	0.42
5:E:207:VAL:HG12	5:E:255:PRO:CD	2.38	0.42
1:M:410:ASN:O	1:M:414:ALA:N	2.52	0.42
5:Q:169:PHE:HD1	5:Q:169:PHE:HA	1.69	0.42
3:C:20:HIS:CD2	15:C:411:3PE:H362	2.55	0.42
4:D:227:PRO:HG2	4:D:229:MET:HE3	2.02	0.42
6:F:75:MET:HE2	6:F:75:MET:HB3	1.99	0.42
1:A:307:SER:HB3	1:M:235:SER:HB2	2.02	0.42
1:A:315:ARG:CD	1:A:397:GLY:HA2	2.49	0.42
18:Q:302:PC1:H232	18:Q:302:PC1:H261	1.90	0.42
1:M:315:ARG:H	1:M:315:ARG:HG2	1.47	0.42
5:E:198:ARG:NH1	5:E:240:SER:O	2.53	0.42
5:E:213:HIS:CD2	3:O:292:LYS:HD3	2.55	0.42
2:B:392:MET:HE2	2:B:392:MET:HB3	1.96	0.41
1:M:85:LEU:HB2	1:M:89:ILE:HG22	2.02	0.41
4:P:106:CYS:SG	16:P:401:HEC:HAC	2.59	0.41
1:A:235:SER:HB2	1:M:307:SER:HB3	2.01	0.41
3:C:103:ARG:NH2	14:C:403:HEM:HBD1	2.35	0.41
5:E:169:PHE:CZ	5:E:218:PRO:HD2	2.55	0.41
1:A:410:ASN:O	1:A:413:LEU:N	2.53	0.41
10:W:30:LEU:H	10:W:30:LEU:HG	1.67	0.41
1:M:216:LEU:O	1:M:220:HIS:HD2	2.03	0.41
5:E:208:ILE:HG13	5:E:253:GLU:OE1	2.20	0.41
6:F:89:THR:HG22	2:N:45:PRO:HB3	2.03	0.41
1:M:166:ASP:OD1	1:M:166:ASP:N	2.54	0.41
2:N:392:MET:HE2	2:N:392:MET:HB3	1.96	0.41
5:Q:179:LYS:C	5:Q:180:LEU:HG	2.45	0.41
1:A:215:LEU:O	1:A:219:ILE:HG13	2.21	0.41
1:A:328:TRP:CD1	1:A:384:TYR:O	2.73	0.41
2:B:241:PHE:O	2:B:244:THR:OG1	2.38	0.41
1:A:166:ASP:OD1	1:A:166:ASP:N	2.54	0.41
12:B:602:CDL:H132	12:B:602:CDL:H161	1.89	0.41
3:C:162:GLY:O	3:C:163:ASP:HB2	2.21	0.41
5:E:257:TYR:HD2	5:E:265:LEU:HB3	1.86	0.41
10:K:29:GLY:O	10:K:30:LEU:HD23	2.21	0.41
1:M:55:ALA:HA	1:M:56:PRO:HD3	1.92	0.41
15:C:404:3PE:H242	10:W:35:PRO:HA	2.03	0.41
15:C:411:3PE:H382	15:C:411:3PE:H351	1.75	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:360:TYR:CE1	2:N:159:GLU:HB3	2.56	0.41
3:O:32:TYR:CE2	12:O:407:CDL:H121	2.56	0.41
1:M:180:VAL:O	1:M:184:ARG:HB2	2.20	0.40
1:M:357:LYS:H	1:M:357:LYS:HG3	1.54	0.40
1:A:85:LEU:HB2	1:A:89:ILE:HG22	2.02	0.40
5:E:128:LEU:HD23	5:E:128:LEU:HA	1.95	0.40
5:E:159:VAL:H	5:E:170:ILE:HG21	1.86	0.40
10:K:30:LEU:HD22	10:K:30:LEU:HA	1.85	0.40
5:E:208:ILE:H	5:E:208:ILE:HG12	1.25	0.40
2:N:433:VAL:H	10:W:10:ILE:HG23	1.86	0.40
5:Q:155:PRO:HG3	5:Q:172:ARG:HH21	1.85	0.40
5:Q:257:TYR:HD2	5:Q:265:LEU:HB3	1.85	0.40
1:A:135:ASN:HB3	2:B:75:LEU:HD21	2.03	0.40
2:B:303:SER:OG	2:B:304:THR:N	2.54	0.40
12:B:602:CDL:H592	12:B:602:CDL:H562	1.80	0.40
5:E:155:PRO:HG3	5:E:172:ARG:HH21	1.85	0.40
5:Q:159:VAL:H	5:Q:170:ILE:HG21	1.87	0.40
5:Q:197:GLU:O	5:Q:200:LYS:NZ	2.48	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	458/460 (100%)	420 (92%)	36 (8%)	2 (0%)	30	47
1	M	458/460 (100%)	422 (92%)	36 (8%)	0	100	100
2	B	485/487 (100%)	463 (96%)	21 (4%)	1 (0%)	43	62
2	N	485/487 (100%)	463 (96%)	21 (4%)	1 (0%)	43	62
3	C	384/386 (100%)	368 (96%)	13 (3%)	3 (1%)	16	29
3	O	383/386 (99%)	369 (96%)	12 (3%)	2 (0%)	24	40

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	240/242 (99%)	230 (96%)	9 (4%)	1 (0%)	30	47
4	P	240/242 (99%)	230 (96%)	10 (4%)	0	100	100
5	E	194/196 (99%)	173 (89%)	20 (10%)	1 (0%)	24	40
5	Q	194/196 (99%)	172 (89%)	20 (10%)	2 (1%)	12	22
6	F	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
6	R	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
7	G	68/70 (97%)	61 (90%)	7 (10%)	0	100	100
7	S	68/70 (97%)	61 (90%)	7 (10%)	0	100	100
8	H	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
8	T	62/64 (97%)	61 (98%)	1 (2%)	0	100	100
9	J	58/60 (97%)	52 (90%)	6 (10%)	0	100	100
9	V	58/60 (97%)	47 (81%)	10 (17%)	1 (2%)	7	12
10	K	27/29 (93%)	22 (82%)	5 (18%)	0	100	100
10	W	27/29 (93%)	23 (85%)	4 (15%)	0	100	100
All	All	4181/4222 (99%)	3919 (94%)	248 (6%)	14 (0%)	37	54

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	159	PRO
3	C	163	ASP
3	O	159	PRO
3	O	162	GLY
5	Q	169	PHE
4	D	304	ASP
5	E	208	ILE
2	N	150	THR
5	Q	208	ILE
1	A	315	ARG
9	V	28	VAL
2	B	150	THR
3	C	162	GLY
1	A	310	ILE

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	384/384 (100%)	364 (95%)	20 (5%)	21	38
1	M	384/384 (100%)	363 (94%)	21 (6%)	19	35
2	B	409/409 (100%)	402 (98%)	7 (2%)	53	71
2	N	409/409 (100%)	398 (97%)	11 (3%)	39	61
3	C	331/331 (100%)	327 (99%)	4 (1%)	63	77
3	O	330/331 (100%)	327 (99%)	3 (1%)	70	82
4	D	197/197 (100%)	194 (98%)	3 (2%)	57	73
4	P	197/197 (100%)	194 (98%)	3 (2%)	57	73
5	E	169/169 (100%)	153 (90%)	16 (10%)	8	15
5	Q	169/169 (100%)	151 (89%)	18 (11%)	6	12
6	F	104/104 (100%)	103 (99%)	1 (1%)	68	80
6	R	104/104 (100%)	103 (99%)	1 (1%)	68	80
7	G	63/63 (100%)	61 (97%)	2 (3%)	34	56
7	S	63/63 (100%)	61 (97%)	2 (3%)	34	56
8	H	58/58 (100%)	50 (86%)	8 (14%)	3	5
8	T	58/58 (100%)	50 (86%)	8 (14%)	3	5
9	J	49/49 (100%)	39 (80%)	10 (20%)	1	1
9	V	49/49 (100%)	41 (84%)	8 (16%)	2	3
10	K	19/19 (100%)	9 (47%)	10 (53%)	0	0
10	W	19/19 (100%)	11 (58%)	8 (42%)	0	0
All	All	3565/3566 (100%)	3401 (95%)	164 (5%)	25	43

All (164) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	140	ARG
1	A	152	VAL
1	A	160	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	184	ARG
1	A	268	GLU
1	A	310	ILE
1	A	311	LEU
1	A	314	GLN
1	A	316	THR
1	A	330	LYS
1	A	368	LEU
1	A	381	ASN
1	A	387	THR
1	A	396	THR
1	A	418	SER
1	A	420	GLN
1	A	469	LYS
1	A	475	THR
1	A	477	LYS
1	A	488	SER
2	B	68	GLU
2	B	151	GLU
2	B	203	SER
2	B	262	LYS
2	B	263	ASP
2	B	283	SER
2	B	497	ARG
3	C	1	MET
3	C	150	VAL
3	C	161	VAL
3	C	313	LYS
4	D	108	SER
4	D	135	GLU
4	D	244	THR
5	E	146	LEU
5	E	154	GLU
5	E	157	THR
5	E	160	THR
5	E	166	LYS
5	E	170	ILE
5	E	179	LYS
5	E	183	SER
5	E	206	ILE
5	E	208	ILE
5	E	238	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	242	ARG
5	E	257	TYR
5	E	260	LEU
5	E	262	GLU
5	E	266	LEU
6	F	83	ASP
7	G	61	ILE
7	G	86	LEU
8	H	32	LYS
8	H	38	CYS
8	H	39	LYS
8	H	47	LEU
8	H	54	LYS
8	H	60	GLU
8	H	75	SER
8	H	80	CYS
9	J	21	MET
9	J	22	ARG
9	J	23	ARG
9	J	24	ASN
9	J	25	SER
9	J	28	VAL
9	J	48	LYS
9	J	51	GLU
9	J	63	SER
9	J	67	GLN
10	K	11	GLN
10	K	13	THR
10	K	14	ASP
10	K	16	LYS
10	K	20	MET
10	K	21	TRP
10	K	23	VAL
10	K	27	THR
10	K	30	LEU
10	K	33	ILE
1	M	58	LEU
1	M	152	VAL
1	M	160	GLN
1	M	184	ARG
1	M	310	ILE
1	M	311	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	314	GLN
1	M	315	ARG
1	M	330	LYS
1	M	355	PRO
1	M	357	LYS
1	M	359	MET
1	M	381	ASN
1	M	387	THR
1	M	396	THR
1	M	407	ILE
1	M	418	SER
1	M	420	GLN
1	M	469	LYS
1	M	477	LYS
1	M	488	SER
2	N	68	GLU
2	N	151	GLU
2	N	199	ILE
2	N	200	LEU
2	N	225	GLU
2	N	262	LYS
2	N	283	SER
2	N	363	SER
2	N	386	GLU
2	N	497	ARG
2	N	530	TYR
3	O	1	MET
3	O	150	VAL
3	O	313	LYS
4	P	108	SER
4	P	135	GLU
4	P	244	THR
5	Q	146	LEU
5	Q	154	GLU
5	Q	157	THR
5	Q	160	THR
5	Q	166	LYS
5	Q	167	PRO
5	Q	169	PHE
5	Q	170	ILE
5	Q	180	LEU
5	Q	183	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	Q	206	ILE
5	Q	208	ILE
5	Q	238	ASP
5	Q	242	ARG
5	Q	257	TYR
5	Q	260	LEU
5	Q	262	GLU
5	Q	266	LEU
6	R	83	ASP
7	S	61	ILE
7	S	86	LEU
8	T	32	LYS
8	T	39	LYS
8	T	41	LYS
8	T	43	VAL
8	T	47	LEU
8	T	54	LYS
8	T	60	GLU
8	T	75	SER
9	V	21	MET
9	V	22	ARG
9	V	23	ARG
9	V	26	VAL
9	V	48	LYS
9	V	51	GLU
9	V	63	SER
9	V	67	GLN
10	W	11	GLN
10	W	13	THR
10	W	14	ASP
10	W	16	LYS
10	W	20	MET
10	W	27	THR
10	W	30	LEU
10	W	34	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	GLN
1	A	160	GLN
1	A	196	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	212	GLN
1	A	314	GLN
1	A	369	ASN
1	A	420	GLN
2	B	69	ASN
2	B	87	HIS
2	B	136	ASN
2	B	144	HIS
2	B	256	ASN
2	B	294	GLN
2	B	336	GLN
2	B	365	ASN
2	B	397	ASN
3	C	4	GLN
3	C	98	HIS
3	C	177	ASN
3	C	188	HIS
3	C	201	HIS
3	C	346	GLN
4	D	171	ASN
5	E	263	ASN
7	G	78	GLN
1	M	153	GLN
1	M	160	GLN
1	M	196	GLN
1	M	212	GLN
1	M	220	HIS
1	M	314	GLN
1	M	317	HIS
1	M	369	ASN
1	M	386	ASN
2	N	87	HIS
2	N	136	ASN
2	N	144	HIS
2	N	256	ASN
2	N	294	GLN
2	N	365	ASN
2	N	397	ASN
3	O	4	GLN
3	O	98	HIS
3	O	177	ASN
3	O	187	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	O	188	HIS
3	O	217	HIS
7	S	38	GLN
7	S	78	GLN
9	V	24	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 31 ligands modelled in this entry, 2 are monoatomic - leaving 29 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
13	A1D6K	O	401	-	29,29,29	0.90	2 (6%)	33,39,39	1.98	5 (15%)
15	3PE	C	407	-	36,36,50	1.02	4 (11%)	39,41,55	1.26	3 (7%)
15	3PE	C	404	-	27,27,50	1.14	4 (14%)	30,32,55	1.25	2 (6%)
18	PC1	Q	302	-	24,24,53	1.10	1 (4%)	29,30,61	0.93	1 (3%)
15	3PE	C	409	-	33,33,50	1.05	4 (12%)	36,38,55	1.12	2 (5%)
14	HEM	O	402	3	50,50,50	1.35	7 (14%)	67,82,82	1.24	6 (8%)
13	A1D6K	C	401	-	29,29,29	0.91	2 (6%)	33,39,39	1.98	5 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CDL	N	602	-	80,80,99	0.32	0	86,92,111	0.50	1 (1%)
15	3PE	K	101	-	29,29,50	1.14	3 (10%)	32,34,55	1.18	2 (6%)
14	HEM	C	403	3	50,50,50	1.45	6 (12%)	67,82,82	1.37	11 (16%)
12	CDL	B	602	-	63,63,99	1.11	8 (12%)	69,75,111	1.13	4 (5%)
12	CDL	N	603	-	69,69,99	1.06	8 (11%)	75,81,111	1.15	4 (5%)
15	3PE	O	405	-	38,38,50	0.98	4 (10%)	41,43,55	1.17	2 (4%)
15	3PE	R	201	-	37,37,50	1.01	4 (10%)	40,42,55	1.15	2 (5%)
15	3PE	O	406	-	32,32,50	1.07	4 (12%)	35,37,55	1.21	2 (5%)
12	CDL	O	407	-	62,62,99	0.40	0	68,74,111	0.62	1 (1%)
14	HEM	C	402	3	50,50,50	1.35	7 (14%)	67,82,82	1.23	6 (8%)
15	3PE	C	408	-	32,32,50	1.08	4 (12%)	35,37,55	1.19	2 (5%)
12	CDL	O	404	-	57,57,99	1.15	8 (14%)	63,69,111	1.27	5 (7%)
15	3PE	C	405	-	31,31,50	1.07	3 (9%)	34,36,55	1.24	3 (8%)
17	FES	E	301	-	0,4,4	-	-	-	-	-
14	HEM	O	403	3	50,50,50	1.49	5 (10%)	67,82,82	1.67	12 (17%)
15	3PE	C	406	-	50,50,50	0.87	3 (6%)	53,55,55	0.96	2 (3%)
12	CDL	C	410	-	63,63,99	1.10	6 (9%)	69,75,111	1.28	5 (7%)
15	3PE	C	411	-	35,35,50	1.06	4 (11%)	38,40,55	1.23	2 (5%)
17	FES	Q	301	-	0,4,4	-	-	-	-	-
16	HEC	D	501	4	46,50,50	1.78	5 (10%)	58,82,82	1.83	7 (12%)
15	3PE	R	202	-	47,47,50	0.89	4 (8%)	50,52,55	1.12	2 (4%)
16	HEC	P	401	4	46,50,50	1.78	5 (10%)	58,82,82	1.81	7 (12%)

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
13	A1D6K	O	401	-	-	2/21/21/21	0/3/3/3
15	3PE	C	407	-	-	20/40/40/54	-
15	3PE	C	404	-	-	21/31/31/54	-
18	PC1	Q	302	-	-	13/25/25/57	-
15	3PE	C	409	-	-	27/37/37/54	-
14	HEM	O	402	3	-	5/14/54/54	-
13	A1D6K	C	401	-	-	2/21/21/21	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CDL	N	602	-	-	61/91/91/110	-
15	3PE	K	101	-	-	10/33/33/54	-
14	HEM	C	403	3	-	2/14/54/54	-
12	CDL	B	602	-	-	32/74/74/110	-
12	CDL	N	603	-	-	49/80/80/110	-
15	3PE	O	405	-	-	29/42/42/54	-
15	3PE	R	201	-	-	23/41/41/54	-
15	3PE	O	406	-	-	19/36/36/54	-
12	CDL	O	407	-	-	31/73/73/110	-
14	HEM	C	402	3	-	5/14/54/54	-
15	3PE	C	408	-	-	21/36/36/54	-
12	CDL	O	404	-	-	34/68/68/110	-
15	3PE	C	405	-	-	21/35/35/54	-
17	FES	E	301	-	-	-	0/1/1/1
14	HEM	O	403	3	-	5/14/54/54	-
15	3PE	C	406	-	-	30/54/54/54	-
12	CDL	C	410	-	-	32/74/74/110	-
15	3PE	C	411	-	-	21/39/39/54	-
17	FES	Q	301	-	-	-	0/1/1/1
16	HEC	D	501	4	-	4/14/54/54	-
15	3PE	R	202	-	-	26/51/51/54	-
16	HEC	P	401	4	-	4/14/54/54	-

All (115) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	D	501	HEC	CAB-C3B	6.21	1.55	1.35
16	P	401	HEC	CAB-C3B	6.19	1.55	1.35
16	D	501	HEC	CAC-C3C	6.02	1.54	1.35
16	P	401	HEC	CAC-C3C	6.00	1.54	1.35
16	D	501	HEC	C3D-C2D	5.15	1.52	1.38
16	P	401	HEC	C3D-C2D	5.15	1.52	1.38
14	O	403	HEM	FE-ND	4.55	2.08	1.94
14	C	403	HEM	FE-NA	4.27	2.09	1.95
14	C	403	HEM	FE-ND	3.60	2.06	1.94
14	O	403	HEM	FE-NA	3.57	2.06	1.95
13	C	401	A1D6K	C12-C10	-3.47	1.36	1.44
13	O	401	A1D6K	C12-C10	-3.44	1.36	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	O	403	HEM	FE-NB	3.40	2.05	1.94
14	C	403	HEM	CAB-C3B	3.18	1.55	1.47
14	O	403	HEM	CAB-C3B	3.17	1.55	1.47
14	C	403	HEM	CAC-C3C	3.16	1.55	1.47
14	O	403	HEM	CAC-C3C	3.16	1.55	1.47
14	C	402	HEM	CAB-C3B	3.08	1.55	1.47
14	O	402	HEM	CAB-C3B	3.07	1.55	1.47
14	C	402	HEM	CAC-C3C	2.94	1.55	1.47
15	K	101	3PE	O21-C2	-2.92	1.39	1.46
14	O	402	HEM	CAC-C3C	2.91	1.55	1.47
15	C	406	3PE	O21-C2	-2.89	1.39	1.46
14	O	402	HEM	FE-NA	2.86	2.04	1.95
14	C	402	HEM	FE-NA	2.84	2.04	1.95
15	C	411	3PE	O21-C2	-2.83	1.40	1.46
12	C	410	CDL	OA6-CA4	-2.80	1.40	1.46
15	R	202	3PE	O21-C2	-2.75	1.40	1.46
14	C	403	HEM	FE-NB	2.72	2.03	1.94
15	O	406	3PE	O31-C3	-2.72	1.39	1.45
15	C	405	3PE	O21-C2	-2.70	1.40	1.46
12	B	602	CDL	OA6-CA4	-2.69	1.40	1.46
12	B	602	CDL	OB6-CB4	-2.68	1.40	1.46
15	C	408	3PE	O21-C2	-2.66	1.40	1.46
12	N	603	CDL	OB6-CB4	-2.65	1.40	1.46
12	C	410	CDL	OA8-CA7	2.65	1.41	1.33
12	N	603	CDL	OA6-CA4	-2.65	1.40	1.46
12	C	410	CDL	OB8-CB6	-2.64	1.39	1.45
15	C	407	3PE	O21-C2	-2.61	1.40	1.46
15	C	409	3PE	O31-C3	-2.60	1.39	1.45
12	N	603	CDL	OB8-CB6	-2.59	1.39	1.45
15	R	201	3PE	O21-C2	-2.56	1.40	1.46
12	C	410	CDL	OB6-CB5	2.56	1.41	1.34
15	C	411	3PE	O31-C31	2.54	1.40	1.33
12	O	404	CDL	OB6-CB5	2.54	1.41	1.34
14	O	402	HEM	FE-NB	2.54	2.02	1.94
15	O	405	3PE	O31-C31	2.53	1.40	1.33
15	C	406	3PE	O31-C31	2.52	1.40	1.33
14	C	402	HEM	FE-NC	2.51	2.03	1.95
12	B	602	CDL	OB8-CB7	2.51	1.40	1.33
12	O	404	CDL	OA8-CA7	2.51	1.40	1.33
14	C	402	HEM	FE-NB	2.48	2.02	1.94
15	C	409	3PE	O21-C2	-2.48	1.40	1.46
12	O	404	CDL	OB6-CB4	-2.48	1.40	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	O	402	HEM	FE-NC	2.47	2.03	1.95
14	C	402	HEM	FE-ND	2.47	2.02	1.94
15	K	101	3PE	O31-C31	2.47	1.40	1.33
12	B	602	CDL	OA8-CA6	-2.45	1.39	1.45
13	C	401	A1D6K	O4-N1	2.45	1.42	1.39
15	C	407	3PE	O31-C31	2.44	1.40	1.33
15	C	408	3PE	O31-C3	-2.44	1.39	1.45
14	O	402	HEM	FE-ND	2.42	2.02	1.94
12	O	404	CDL	OB8-CB7	2.41	1.40	1.33
12	N	603	CDL	OA8-CA7	2.41	1.40	1.33
15	R	201	3PE	O31-C31	2.40	1.40	1.33
13	O	401	A1D6K	O4-N1	2.39	1.42	1.39
18	Q	302	PC1	O21-C21	2.37	1.40	1.33
15	O	406	3PE	O21-C2	-2.36	1.41	1.46
15	C	404	3PE	O21-C21	2.33	1.40	1.34
15	C	404	3PE	O31-C3	-2.32	1.40	1.45
12	O	404	CDL	OA6-CA5	2.31	1.40	1.34
15	R	202	3PE	O31-C31	2.31	1.40	1.33
15	C	405	3PE	O31-C31	2.30	1.40	1.33
12	N	603	CDL	OA6-CA5	2.29	1.40	1.34
15	C	408	3PE	O21-C21	2.28	1.40	1.34
15	R	201	3PE	O21-C21	2.28	1.40	1.34
14	O	402	HEM	C2A-C3A	-2.27	1.33	1.38
16	D	501	HEC	C3B-C2B	-2.27	1.33	1.41
15	C	405	3PE	O31-C3	-2.27	1.40	1.45
12	N	603	CDL	OA8-CA6	-2.25	1.40	1.45
15	C	404	3PE	O21-C2	-2.24	1.41	1.46
15	O	405	3PE	O21-C21	2.24	1.40	1.34
14	C	402	HEM	C2A-C3A	-2.24	1.33	1.38
15	C	409	3PE	O21-C21	2.23	1.40	1.34
12	O	404	CDL	OB8-CB6	-2.23	1.40	1.45
15	O	405	3PE	O21-C2	-2.22	1.41	1.46
12	N	603	CDL	OB6-CB5	2.22	1.40	1.34
16	P	401	HEC	C3B-C2B	-2.22	1.33	1.41
15	R	201	3PE	O31-C3	-2.22	1.40	1.45
12	O	404	CDL	OA6-CA4	-2.21	1.41	1.46
15	R	202	3PE	O31-C3	-2.21	1.40	1.45
12	N	603	CDL	OB8-CB7	2.21	1.39	1.33
15	O	406	3PE	O21-C21	2.20	1.40	1.34
15	C	407	3PE	O31-C3	-2.20	1.40	1.45
15	C	408	3PE	O31-C31	2.18	1.39	1.33
12	B	602	CDL	OB8-CB6	-2.18	1.40	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	C	404	3PE	O31-C31	2.18	1.39	1.33
12	B	602	CDL	OB6-CB5	2.18	1.40	1.34
15	C	407	3PE	O21-C21	2.18	1.40	1.34
16	D	501	HEC	C3C-C2C	-2.18	1.33	1.41
16	P	401	HEC	C3C-C2C	-2.18	1.33	1.41
15	C	411	3PE	O31-C3	-2.17	1.40	1.45
15	C	409	3PE	O31-C31	2.16	1.39	1.33
12	C	410	CDL	OA6-CA5	2.15	1.40	1.34
15	K	101	3PE	O31-C3	-2.14	1.40	1.45
12	B	602	CDL	OA8-CA7	2.13	1.39	1.33
14	C	403	HEM	C2A-C3A	-2.12	1.33	1.38
12	B	602	CDL	OA6-CA5	2.12	1.40	1.34
12	C	410	CDL	OB8-CB7	2.12	1.39	1.33
12	O	404	CDL	OA8-CA6	-2.07	1.40	1.45
15	C	411	3PE	O21-C21	2.04	1.40	1.34
15	C	406	3PE	O31-C3	-2.04	1.40	1.45
15	O	405	3PE	O31-C3	-2.03	1.40	1.45
15	O	406	3PE	O31-C31	2.02	1.39	1.33
15	R	202	3PE	O21-C21	2.01	1.39	1.34

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	O	401	A1D6K	C19-O4-N1	9.43	119.98	109.98
13	C	401	A1D6K	C19-O4-N1	9.40	119.95	109.98
16	D	501	HEC	CBC-CAC-C3C	-7.61	112.22	127.43
16	P	401	HEC	CBC-CAC-C3C	-7.56	112.33	127.43
16	D	501	HEC	CBB-CAB-C3B	-7.38	112.69	127.43
16	P	401	HEC	CBB-CAB-C3B	-7.28	112.89	127.43
14	O	403	HEM	CAD-C3D-C4D	5.71	134.65	124.70
14	O	403	HEM	CAD-C3D-C2D	-5.23	118.07	127.87
12	C	410	CDL	OB6-CB5-C51	4.88	122.04	111.48
15	O	406	3PE	O21-C21-C22	4.39	120.97	111.48
12	O	404	CDL	OB6-CB5-C51	4.37	120.92	111.48
15	C	405	3PE	O21-C21-C22	4.33	120.86	111.48
12	C	410	CDL	OA6-CA5-C11	4.30	120.79	111.48
12	O	404	CDL	OA6-CA5-C11	4.29	120.76	111.48
15	R	201	3PE	O21-C21-C22	4.12	120.39	111.48
15	C	411	3PE	O21-C21-C22	4.08	120.31	111.48
15	R	202	3PE	O21-C21-C22	4.07	120.28	111.48
15	C	407	3PE	O21-C21-C22	4.06	120.26	111.48
15	K	101	3PE	O21-C21-C22	4.02	120.17	111.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	O	405	3PE	O21-C21-C22	3.90	119.92	111.48
12	N	603	CDL	OB6-CB5-C51	3.84	119.78	111.48
15	C	404	3PE	O21-C21-C22	3.82	119.74	111.48
15	C	408	3PE	O21-C21-C22	3.82	119.74	111.48
12	N	603	CDL	OA6-CA5-C11	3.79	119.68	111.48
12	B	602	CDL	OB6-CB5-C51	3.65	119.38	111.48
12	B	602	CDL	OA6-CA5-C11	3.64	119.36	111.48
15	C	407	3PE	O31-C31-C32	3.58	122.75	111.83
14	C	403	HEM	CAA-C2A-C1A	3.46	131.69	124.94
14	O	403	HEM	CHA-C4D-C3D	3.41	131.52	125.23
12	C	410	CDL	OA8-CA7-C31	3.37	121.37	111.15
15	C	409	3PE	O21-C21-C22	3.27	118.56	111.48
15	C	406	3PE	O21-C21-C22	3.22	118.45	111.48
14	C	402	HEM	CMB-C2B-C1B	-3.21	120.02	125.03
14	O	402	HEM	CMB-C2B-C1B	-3.16	120.09	125.03
16	P	401	HEC	C4D-ND-C1D	3.10	110.88	105.82
16	D	501	HEC	C4D-ND-C1D	3.08	110.84	105.82
13	C	401	A1D6K	C11-C12-C10	3.08	106.01	104.22
14	O	403	HEM	C3D-C4D-ND	-3.06	106.81	110.17
15	C	411	3PE	O31-C31-C32	3.05	121.14	111.83
13	O	401	A1D6K	C11-C12-C10	3.01	105.98	104.22
15	O	405	3PE	O31-C31-C32	2.96	120.87	111.83
14	O	403	HEM	C4D-ND-C1D	2.95	108.70	105.21
12	B	602	CDL	OB8-CB7-C71	2.91	120.72	111.83
15	R	201	3PE	O31-C31-C32	2.89	120.64	111.83
15	C	408	3PE	O31-C31-C32	2.86	120.56	111.83
14	C	403	HEM	CAA-C2A-C3A	-2.84	120.70	127.07
12	O	404	CDL	OB8-CB7-C71	2.77	120.28	111.83
12	O	404	CDL	OA8-CA7-C31	2.71	120.10	111.83
14	C	403	HEM	C2A-C1A-NA	-2.70	107.15	110.15
15	C	409	3PE	O31-C31-C32	2.69	120.04	111.83
18	Q	302	PC1	O21-C21-C22	2.69	120.02	111.83
14	O	402	HEM	C3D-C4D-ND	-2.68	107.23	110.17
14	C	402	HEM	C3D-C4D-ND	-2.68	107.24	110.17
13	C	401	A1D6K	C12-C10-N2	-2.67	111.60	113.57
14	C	403	HEM	CMB-C2B-C1B	-2.67	120.86	125.03
12	O	407	CDL	OB6-CB5-C51	2.66	117.24	111.48
13	O	401	A1D6K	C12-C10-N2	-2.65	111.62	113.57
15	K	101	3PE	O31-C31-C32	2.64	119.89	111.83
15	C	404	3PE	O31-C31-C32	2.62	119.82	111.83
14	C	402	HEM	C3B-C2B-C1B	2.62	108.38	106.41
15	C	405	3PE	O31-C31-C32	2.60	119.78	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	O	403	HEM	CMB-C2B-C1B	-2.60	120.98	125.03
15	C	406	3PE	O31-C31-C32	2.58	119.71	111.83
14	O	402	HEM	C3B-C2B-C1B	2.57	108.34	106.41
12	N	603	CDL	OB8-CB7-C71	2.55	119.61	111.83
14	O	403	HEM	CBD-CAD-C3D	2.54	119.56	112.53
12	N	603	CDL	OA8-CA7-C31	2.52	119.50	111.83
15	R	202	3PE	O31-C31-C32	2.49	119.42	111.83
14	C	403	HEM	C1B-NB-C4B	2.48	108.14	105.21
14	O	403	HEM	C2A-C1A-NA	-2.46	107.42	110.15
12	C	410	CDL	OB6-CB5-OB7	-2.44	118.00	123.70
16	P	401	HEC	CMD-C2D-C1D	2.44	129.13	125.42
16	D	501	HEC	CMD-C2D-C1D	2.43	129.12	125.42
14	C	402	HEM	C4D-ND-C1D	2.42	108.07	105.21
14	C	403	HEM	CBA-CAA-C2A	2.41	119.18	112.53
14	O	402	HEM	C4D-ND-C1D	2.40	108.06	105.21
13	C	401	A1D6K	C13-N3-N2	-2.39	117.03	119.93
12	O	404	CDL	OA8-CA6-CA4	2.38	115.25	108.40
14	O	403	HEM	C1D-C2D-C3D	2.37	109.47	106.98
13	O	401	A1D6K	C13-N3-N2	-2.36	117.07	119.93
12	N	602	CDL	OB6-CB4-CB6	2.35	116.77	108.34
14	O	403	HEM	C1B-NB-C4B	2.33	107.96	105.21
16	D	501	HEC	CAA-CBA-CGA	-2.27	107.65	113.67
16	P	401	HEC	CAA-CBA-CGA	-2.25	107.70	113.67
16	D	501	HEC	CHD-C4C-NC	2.24	126.89	124.45
14	C	403	HEM	C3D-C4D-ND	-2.19	107.77	110.17
16	P	401	HEC	CHD-C4C-NC	2.19	126.84	124.45
14	C	403	HEM	C4D-ND-C1D	2.19	107.80	105.21
14	O	403	HEM	CHA-C4D-ND	-2.18	121.67	124.37
12	B	602	CDL	OA8-CA7-C31	2.17	117.72	111.15
14	O	402	HEM	CMC-C2C-C1C	-2.15	120.93	124.73
12	C	410	CDL	OB8-CB7-C71	2.15	118.38	111.83
13	C	401	A1D6K	C10-N2-N3	2.14	104.98	103.11
14	C	402	HEM	CMC-C2C-C1C	-2.14	120.97	124.73
13	O	401	A1D6K	C10-N2-N3	2.12	104.96	103.11
14	C	403	HEM	CAC-C3C-C4C	-2.12	119.77	124.82
16	P	401	HEC	C2A-C1A-NA	-2.09	108.30	110.32
15	C	407	3PE	O31-C31-O32	-2.08	118.43	123.63
16	D	501	HEC	C2A-C1A-NA	-2.07	108.33	110.32
14	C	403	HEM	C4A-C3A-C2A	2.06	109.18	106.82
14	O	403	HEM	CAC-C3C-C4C	-2.06	119.89	124.82
15	C	405	3PE	C2-O21-C21	-2.05	112.89	117.80
14	C	403	HEM	C3B-C2B-C1B	2.04	107.94	106.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	C	402	HEM	CAC-C3C-C4C	-2.03	119.98	124.82
14	O	402	HEM	CAC-C3C-C4C	-2.03	119.98	124.82
15	O	406	3PE	O31-C31-C32	2.00	117.95	111.83

There are no chirality outliers.

All (549) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	B	602	CDL	O1-C1-CB2-OB2
12	B	602	CDL	CA3-OA5-PA1-OA2
12	B	602	CDL	CA3-OA5-PA1-OA4
12	C	410	CDL	C11-CA5-OA6-CA4
12	C	410	CDL	CB2-OB2-PB2-OB4
12	C	410	CDL	CB2-OB2-PB2-OB5
12	C	410	CDL	C51-CB5-OB6-CB4
12	N	602	CDL	CB2-C1-CA2-OA2
12	N	602	CDL	CA2-OA2-PA1-OA4
12	N	602	CDL	CA2-OA2-PA1-OA5
12	N	602	CDL	CA3-OA5-PA1-OA3
12	N	602	CDL	OA7-CA5-OA6-CA4
12	N	602	CDL	C11-CA5-OA6-CA4
12	N	602	CDL	CB2-OB2-PB2-OB3
12	N	602	CDL	CB2-OB2-PB2-OB4
12	N	602	CDL	CB2-OB2-PB2-OB5
12	N	602	CDL	CB3-OB5-PB2-OB2
12	N	602	CDL	CB3-OB5-PB2-OB3
12	N	602	CDL	CB3-OB5-PB2-OB4
12	N	603	CDL	O1-C1-CA2-OA2
12	N	603	CDL	CA3-OA5-PA1-OA2
12	N	603	CDL	CA3-OA5-PA1-OA3
12	N	603	CDL	CA3-OA5-PA1-OA4
12	N	603	CDL	C11-CA5-OA6-CA4
12	N	603	CDL	CB2-OB2-PB2-OB3
12	N	603	CDL	CB2-OB2-PB2-OB4
12	N	603	CDL	CB2-OB2-PB2-OB5
12	N	603	CDL	CB3-OB5-PB2-OB2
12	N	603	CDL	CB3-OB5-PB2-OB3
12	N	603	CDL	CB3-OB5-PB2-OB4
12	O	404	CDL	CA2-OA2-PA1-OA4
12	O	404	CDL	CA2-OA2-PA1-OA5
12	O	404	CDL	CA3-OA5-PA1-OA3
12	O	404	CDL	CA3-OA5-PA1-OA4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
12	O	404	CDL	C11-CA5-OA6-CA4
12	O	404	CDL	CB2-OB2-PB2-OB3
12	O	404	CDL	OB7-CB5-OB6-CB4
12	O	407	CDL	CB2-C1-CA2-OA2
12	O	407	CDL	CA2-C1-CB2-OB2
12	O	407	CDL	C11-CA5-OA6-CA4
14	C	403	HEM	C1A-C2A-CAA-CBA
14	O	403	HEM	C2D-C3D-CAD-CBD
14	O	403	HEM	C4D-C3D-CAD-CBD
15	C	404	3PE	C1-O11-P-O12
15	C	404	3PE	C1-O11-P-O13
15	C	404	3PE	C1-O11-P-O14
15	C	404	3PE	C11-O13-P-O11
15	C	404	3PE	C11-O13-P-O12
15	C	404	3PE	O13-C11-C12-N
15	C	404	3PE	C22-C21-O21-C2
15	C	405	3PE	C11-O13-P-O11
15	C	405	3PE	C11-O13-P-O12
15	C	405	3PE	C11-O13-P-O14
15	C	405	3PE	O13-C11-C12-N
15	C	406	3PE	O13-C11-C12-N
15	C	407	3PE	C11-O13-P-O11
15	C	407	3PE	C11-O13-P-O14
15	C	407	3PE	O13-C11-C12-N
15	C	407	3PE	C22-C21-O21-C2
15	C	408	3PE	C11-O13-P-O11
15	C	408	3PE	C11-O13-P-O12
15	C	408	3PE	C11-O13-P-O14
15	C	408	3PE	O13-C11-C12-N
15	C	409	3PE	C1-O11-P-O12
15	C	409	3PE	C1-O11-P-O13
15	C	409	3PE	C11-O13-P-O11
15	C	409	3PE	C11-O13-P-O12
15	C	411	3PE	C1-O11-P-O12
15	C	411	3PE	C1-O11-P-O13
15	C	411	3PE	C1-O11-P-O14
15	C	411	3PE	C11-O13-P-O11
15	C	411	3PE	C11-O13-P-O12
15	C	411	3PE	C11-O13-P-O14
15	C	411	3PE	O22-C21-O21-C2
15	K	101	3PE	C11-O13-P-O11
15	K	101	3PE	C11-O13-P-O12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	K	101	3PE	C11-O13-P-O14
15	O	405	3PE	C1-O11-P-O13
15	O	405	3PE	C1-O11-P-O14
15	O	405	3PE	O13-C11-C12-N
15	O	406	3PE	C11-O13-P-O11
15	O	406	3PE	C11-O13-P-O12
15	O	406	3PE	C11-O13-P-O14
15	O	406	3PE	O13-C11-C12-N
15	O	406	3PE	O21-C2-C3-O31
15	O	406	3PE	C22-C21-O21-C2
15	R	201	3PE	C11-O13-P-O11
15	R	201	3PE	C11-O13-P-O12
15	R	201	3PE	O13-C11-C12-N
15	R	201	3PE	O22-C21-O21-C2
15	R	201	3PE	C22-C21-O21-C2
15	R	202	3PE	C1-O11-P-O13
15	R	202	3PE	C1-O11-P-O14
15	R	202	3PE	C11-O13-P-O11
15	R	202	3PE	C11-O13-P-O12
15	R	202	3PE	O13-C11-C12-N
15	R	202	3PE	C22-C21-O21-C2
16	D	501	HEC	C2C-C3C-CAC-CBC
16	P	401	HEC	C2C-C3C-CAC-CBC
18	Q	302	PC1	C11-O13-P-O14
18	Q	302	PC1	C11-O13-P-O11
18	Q	302	PC1	C1-O11-P-O14
18	Q	302	PC1	O11-C1-C2-O21
12	B	602	CDL	OB9-CB7-OB8-CB6
15	C	407	3PE	O32-C31-O31-C3
15	C	411	3PE	O32-C31-O31-C3
15	O	405	3PE	O32-C31-O31-C3
18	Q	302	PC1	O22-C21-O21-C2
12	B	602	CDL	C71-CB7-OB8-CB6
12	O	404	CDL	C31-CA7-OA8-CA6
15	C	407	3PE	C32-C31-O31-C3
15	C	411	3PE	C32-C31-O31-C3
15	O	405	3PE	C32-C31-O31-C3
18	Q	302	PC1	C22-C21-O21-C2
12	C	410	CDL	OA9-CA7-OA8-CA6
12	N	602	CDL	OB9-CB7-OB8-CB6
12	O	404	CDL	OA9-CA7-OA8-CA6
12	O	404	CDL	OB9-CB7-OB8-CB6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
12	C	410	CDL	OA7-CA5-OA6-CA4
12	C	410	CDL	OB7-CB5-OB6-CB4
12	N	602	CDL	OB7-CB5-OB6-CB4
12	N	603	CDL	OA7-CA5-OA6-CA4
12	O	404	CDL	OA7-CA5-OA6-CA4
12	O	407	CDL	OA7-CA5-OA6-CA4
15	C	404	3PE	O22-C21-O21-C2
15	C	407	3PE	O22-C21-O21-C2
15	C	409	3PE	O22-C21-O21-C2
15	O	406	3PE	O22-C21-O21-C2
15	R	202	3PE	O22-C21-O21-C2
12	N	602	CDL	C71-CB7-OB8-CB6
12	O	404	CDL	C71-CB7-OB8-CB6
12	O	404	CDL	C51-CB5-OB6-CB4
15	C	411	3PE	C22-C21-O21-C2
15	C	408	3PE	O32-C31-O31-C3
12	C	410	CDL	C31-CA7-OA8-CA6
15	C	404	3PE	C32-C31-O31-C3
12	N	602	CDL	O1-C1-CA2-OA2
12	O	407	CDL	O1-C1-CA2-OA2
12	O	407	CDL	O1-C1-CB2-OB2
12	N	602	CDL	C51-CB5-OB6-CB4
15	C	409	3PE	C22-C21-O21-C2
15	O	405	3PE	C22-C21-O21-C2
15	C	408	3PE	C32-C31-O31-C3
15	C	404	3PE	O32-C31-O31-C3
12	O	407	CDL	CB5-C51-C52-C53
15	O	405	3PE	O22-C21-O21-C2
12	B	602	CDL	CB2-C1-CA2-OA2
12	C	410	CDL	C71-CB7-OB8-CB6
12	O	407	CDL	C31-CA7-OA8-CA6
15	O	406	3PE	C32-C33-C34-C35
12	O	407	CDL	C15-C16-C17-C18
12	O	407	CDL	C17-C18-C19-C20
12	B	602	CDL	O1-C1-CA2-OA2
12	O	407	CDL	OA9-CA7-OA8-CA6
15	C	405	3PE	C31-C32-C33-C34
14	C	403	HEM	C3A-C2A-CAA-CBA
15	C	405	3PE	C22-C21-O21-C2
12	B	602	CDL	OA6-CA4-CA6-OA8
12	N	602	CDL	C31-CA7-OA8-CA6
12	N	603	CDL	C71-CB7-OB8-CB6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
12	N	603	CDL	CA7-C31-C32-C33
15	R	202	3PE	C21-C22-C23-C24
12	O	407	CDL	C71-CB7-OB8-CB6
12	N	603	CDL	CB5-C51-C52-C53
12	C	410	CDL	C13-C14-C15-C16
12	B	602	CDL	CB5-C51-C52-C53
12	N	603	CDL	CA5-C11-C12-C13
15	C	408	3PE	C21-C22-C23-C24
15	C	411	3PE	C31-C32-C33-C34
15	K	101	3PE	C21-C22-C23-C24
15	O	406	3PE	C31-C32-C33-C34
12	C	410	CDL	OB9-CB7-OB8-CB6
15	C	407	3PE	C31-C32-C33-C34
12	N	602	CDL	OA9-CA7-OA8-CA6
12	N	603	CDL	OB9-CB7-OB8-CB6
12	O	407	CDL	OB9-CB7-OB8-CB6
15	C	405	3PE	O22-C21-O21-C2
12	B	602	CDL	CA2-C1-CB2-OB2
12	N	603	CDL	CB2-C1-CA2-OA2
15	R	201	3PE	C32-C31-O31-C3
15	O	406	3PE	C21-C22-C23-C24
12	C	410	CDL	CB6-CB4-OB6-CB5
15	C	404	3PE	C3-C2-O21-C21
15	O	406	3PE	C1-C2-O21-C21
12	B	602	CDL	C17-C18-C19-C20
12	N	603	CDL	C19-C20-C21-C22
12	O	404	CDL	C15-C16-C17-C18
15	C	406	3PE	C34-C35-C36-C37
15	C	406	3PE	C2A-C2B-C2C-C2D
15	R	202	3PE	C37-C38-C39-C3A
12	B	602	CDL	C54-C55-C56-C57
12	C	410	CDL	C11-C12-C13-C14
12	N	602	CDL	C18-C19-C20-C21
12	N	602	CDL	C54-C55-C56-C57
15	O	405	3PE	C28-C29-C2A-C2B
12	C	410	CDL	C15-C16-C17-C18
12	C	410	CDL	C54-C55-C56-C57
12	C	410	CDL	C57-C58-C59-C60
12	N	602	CDL	C72-C73-C74-C75
15	C	405	3PE	C23-C24-C25-C26
15	C	406	3PE	C31-C32-C33-C34
12	N	602	CDL	C23-C24-C25-C26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
12	N	602	CDL	CA5-C11-C12-C13
12	N	602	CDL	C13-C14-C15-C16
12	O	407	CDL	C16-C17-C18-C19
12	O	407	CDL	C72-C73-C74-C75
15	C	407	3PE	C36-C37-C38-C39
15	C	409	3PE	C35-C36-C37-C38
12	C	410	CDL	C12-C13-C14-C15
12	N	603	CDL	C12-C13-C14-C15
15	C	411	3PE	C26-C27-C28-C29
15	O	405	3PE	C23-C24-C25-C26
12	O	404	CDL	CA7-C31-C32-C33
15	C	408	3PE	C36-C37-C38-C39
12	N	602	CDL	C74-C75-C76-C77
12	N	603	CDL	C23-C24-C25-C26
15	R	202	3PE	C3C-C3D-C3E-C3F
15	C	409	3PE	C36-C37-C38-C39
15	C	411	3PE	C32-C33-C34-C35
12	C	410	CDL	C56-C57-C58-C59
12	N	602	CDL	C55-C56-C57-C58
15	C	406	3PE	C38-C39-C3A-C3B
15	R	201	3PE	C36-C37-C38-C39
12	O	404	CDL	CA5-C11-C12-C13
12	O	407	CDL	CA7-C31-C32-C33
12	B	602	CDL	C57-C58-C59-C60
12	N	602	CDL	C31-C32-C33-C34
12	N	602	CDL	C63-C64-C65-C66
12	O	404	CDL	C71-C72-C73-C74
15	C	406	3PE	C3A-C3B-C3C-C3D
15	C	408	3PE	C32-C33-C34-C35
15	C	409	3PE	C33-C34-C35-C36
15	R	201	3PE	O32-C31-O31-C3
15	O	405	3PE	C35-C36-C37-C38
15	C	408	3PE	C22-C23-C24-C25
15	C	409	3PE	C32-C33-C34-C35
12	O	404	CDL	C51-C52-C53-C54
12	N	603	CDL	C51-CB5-OB6-CB4
15	K	101	3PE	C22-C21-O21-C2
12	N	602	CDL	C15-C16-C17-C18
12	O	404	CDL	C12-C13-C14-C15
15	C	409	3PE	C22-C23-C24-C25
12	C	410	CDL	C51-C52-C53-C54
12	N	602	CDL	C56-C57-C58-C59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
12	N	602	CDL	CB7-C71-C72-C73
12	C	410	CDL	C16-C17-C18-C19
15	R	202	3PE	C2B-C2C-C2D-C2E
15	C	408	3PE	C34-C35-C36-C37
15	C	408	3PE	C35-C36-C37-C38
15	O	405	3PE	C22-C23-C24-C25
15	R	202	3PE	C31-C32-C33-C34
12	N	603	CDL	C71-C72-C73-C74
12	C	410	CDL	C53-C54-C55-C56
15	K	101	3PE	C32-C33-C34-C35
15	O	406	3PE	C35-C36-C37-C38
15	C	409	3PE	C38-C39-C3A-C3B
15	O	406	3PE	C25-C26-C27-C28
15	C	411	3PE	C25-C26-C27-C28
12	N	602	CDL	C73-C74-C75-C76
15	R	201	3PE	C33-C34-C35-C36
18	Q	302	PC1	C11-C12-N-C13
18	Q	302	PC1	C11-C12-N-C14
15	C	409	3PE	C34-C35-C36-C37
15	R	202	3PE	C22-C23-C24-C25
15	R	201	3PE	C38-C39-C3A-C3B
15	K	101	3PE	O22-C21-O21-C2
15	R	201	3PE	C3A-C3B-C3C-C3D
12	B	602	CDL	C18-C19-C20-C21
15	C	406	3PE	C23-C24-C25-C26
15	R	201	3PE	C31-C32-C33-C34
12	B	602	CDL	C53-C54-C55-C56
15	C	408	3PE	O21-C2-C3-O31
15	K	101	3PE	O21-C2-C3-O31
15	K	101	3PE	C23-C24-C25-C26
15	R	202	3PE	C3A-C3B-C3C-C3D
12	N	602	CDL	C59-C60-C61-C62
12	N	602	CDL	C62-C63-C64-C65
12	N	603	CDL	C16-C17-C18-C19
12	N	603	CDL	C22-C23-C24-C25
15	R	201	3PE	C22-C23-C24-C25
14	O	403	HEM	C3D-CAD-CBD-CGD
12	N	603	CDL	OB7-CB5-OB6-CB4
15	R	202	3PE	C27-C28-C29-C2A
15	C	405	3PE	C22-C23-C24-C25
15	R	202	3PE	C3D-C3E-C3F-C3G
12	N	603	CDL	CB7-C71-C72-C73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	O	405	3PE	C31-C32-C33-C34
12	N	603	CDL	C55-C56-C57-C58
12	O	407	CDL	C51-C52-C53-C54
12	B	602	CDL	C59-C60-C61-C62
12	N	603	CDL	C20-C21-C22-C23
12	N	603	CDL	C72-C73-C74-C75
15	C	406	3PE	C39-C3A-C3B-C3C
12	N	603	CDL	C15-C16-C17-C18
15	O	405	3PE	O11-C1-C2-C3
15	C	404	3PE	C24-C25-C26-C27
12	O	407	CDL	C12-C13-C14-C15
15	C	409	3PE	C31-C32-C33-C34
15	C	409	3PE	C21-C22-C23-C24
18	Q	302	PC1	C21-C22-C23-C24
18	Q	302	PC1	C25-C26-C27-C28
15	C	406	3PE	C22-C21-O21-C2
12	C	410	CDL	C19-C20-C21-C22
15	C	405	3PE	C24-C25-C26-C27
15	C	406	3PE	C29-C2A-C2B-C2C
12	B	602	CDL	CA3-CA4-CA6-OA8
15	C	404	3PE	C1-C2-C3-O31
15	C	405	3PE	C1-C2-C3-O31
15	C	408	3PE	C1-C2-C3-O31
18	Q	302	PC1	C11-C12-N-C15
12	B	602	CDL	C15-C16-C17-C18
12	N	603	CDL	C13-C14-C15-C16
15	R	201	3PE	C39-C3A-C3B-C3C
12	N	602	CDL	C1-CA2-OA2-PA1
12	O	404	CDL	C1-CB2-OB2-PB2
12	N	603	CDL	C17-C18-C19-C20
12	B	602	CDL	C51-C52-C53-C54
12	N	602	CDL	CB6-CB4-OB6-CB5
15	C	409	3PE	C1-C2-O21-C21
12	B	602	CDL	C19-C20-C21-C22
12	N	602	CDL	C60-C61-C62-C63
12	N	603	CDL	C33-C34-C35-C36
15	C	404	3PE	C25-C26-C27-C28
15	C	411	3PE	C33-C34-C35-C36
15	C	404	3PE	O11-C1-C2-O21
15	C	408	3PE	O11-C1-C2-O21
15	R	201	3PE	O11-C1-C2-O21
12	N	602	CDL	C33-C34-C35-C36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
12	B	602	CDL	C60-C61-C62-C63
15	R	202	3PE	C33-C34-C35-C36
15	C	411	3PE	O21-C2-C3-O31
15	R	202	3PE	C2C-C2D-C2E-C2F
12	N	603	CDL	C14-C15-C16-C17
15	O	405	3PE	C2B-C2C-C2D-C2E
12	C	410	CDL	C20-C21-C22-C23
15	R	202	3PE	C3B-C3C-C3D-C3E
12	O	407	CDL	C14-C15-C16-C17
15	C	411	3PE	C23-C24-C25-C26
12	B	602	CDL	C61-C62-C63-C64
12	O	407	CDL	C32-C33-C34-C35
15	C	408	3PE	C38-C39-C3A-C3B
12	B	602	CDL	C1-CB2-OB2-PB2
12	N	602	CDL	C61-C62-C63-C64
12	O	407	CDL	C31-C32-C33-C34
14	C	402	HEM	C2A-CAA-CBA-CGA
14	O	402	HEM	C2A-CAA-CBA-CGA
12	N	602	CDL	C19-C20-C21-C22
15	C	411	3PE	C27-C28-C29-C2A
12	N	602	CDL	OB5-CB3-CB4-CB6
15	C	407	3PE	O11-C1-C2-C3
12	N	603	CDL	C52-C53-C54-C55
12	N	602	CDL	C64-C65-C66-C67
15	C	407	3PE	C33-C34-C35-C36
15	C	406	3PE	C2C-C2D-C2E-C2F
12	O	407	CDL	C19-C20-C21-C22
12	O	404	CDL	C53-C54-C55-C56
12	O	404	CDL	C54-C55-C56-C57
12	B	602	CDL	CB3-CB4-CB6-OB8
12	N	603	CDL	CB3-CB4-CB6-OB8
15	C	409	3PE	C1-C2-C3-O31
15	K	101	3PE	C1-C2-C3-O31
15	O	406	3PE	C1-C2-C3-O31
12	N	602	CDL	C71-C72-C73-C74
12	N	603	CDL	C32-C33-C34-C35
15	O	405	3PE	C34-C35-C36-C37
12	O	407	CDL	C54-C55-C56-C57
12	N	602	CDL	OA5-CA3-CA4-OA6
12	N	602	CDL	OB5-CB3-CB4-OB6
12	C	410	CDL	C1-CB2-OB2-PB2
15	C	406	3PE	C24-C25-C26-C27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
12	O	404	CDL	OA6-CA4-CA6-OA8
15	O	405	3PE	O21-C2-C3-O31
12	N	603	CDL	C31-C32-C33-C34
15	C	406	3PE	C21-C22-C23-C24
12	N	602	CDL	C24-C25-C26-C27
15	C	406	3PE	C33-C34-C35-C36
12	O	407	CDL	C55-C56-C57-C58
12	O	404	CDL	C13-C14-C15-C16
15	C	406	3PE	O11-C1-C2-C3
15	R	201	3PE	O11-C1-C2-C3
15	R	201	3PE	C37-C38-C39-C3A
15	C	406	3PE	O22-C21-O21-C2
12	B	602	CDL	CB7-C71-C72-C73
12	C	410	CDL	CB7-C71-C72-C73
15	O	405	3PE	C1-C2-O21-C21
15	C	409	3PE	C32-C31-O31-C3
12	O	407	CDL	OB5-CB3-CB4-OB6
15	C	405	3PE	O11-C1-C2-O21
15	C	406	3PE	O11-C1-C2-O21
15	O	405	3PE	C1-C2-C3-O31
15	C	404	3PE	C12-C11-O13-P
15	C	409	3PE	O21-C2-C3-O31
12	N	602	CDL	C11-C12-C13-C14
15	C	409	3PE	O32-C31-O31-C3
15	C	407	3PE	C26-C27-C28-C29
15	C	406	3PE	C36-C37-C38-C39
12	B	602	CDL	OA5-CA3-CA4-CA6
12	N	602	CDL	OA5-CA3-CA4-CA6
12	O	407	CDL	OB5-CB3-CB4-CB6
15	C	405	3PE	O11-C1-C2-C3
12	N	603	CDL	C1-CB2-OB2-PB2
16	D	501	HEC	C4B-C3B-CAB-CBB
16	D	501	HEC	C4C-C3C-CAC-CBC
16	P	401	HEC	C4B-C3B-CAB-CBB
16	P	401	HEC	C4C-C3C-CAC-CBC
15	C	407	3PE	O11-C1-C2-O21
15	O	405	3PE	O11-C1-C2-O21
12	O	404	CDL	C72-C73-C74-C75
12	N	602	CDL	C20-C21-C22-C23
15	O	406	3PE	C26-C27-C28-C29
12	B	602	CDL	OB6-CB4-CB6-OB8
12	N	603	CDL	OB6-CB4-CB6-OB8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	C	404	3PE	O21-C2-C3-O31
15	C	405	3PE	O21-C2-C3-O31
12	O	404	CDL	CA3-CA4-CA6-OA8
15	C	409	3PE	O21-C21-C22-C23
12	C	410	CDL	C61-C62-C63-C64
15	C	411	3PE	C24-C25-C26-C27
15	C	405	3PE	C36-C37-C38-C39
15	C	405	3PE	C33-C34-C35-C36
12	B	602	CDL	C16-C17-C18-C19
12	N	602	CDL	CA3-OA5-PA1-OA2
12	N	602	CDL	CA3-OA5-PA1-OA4
12	O	404	CDL	CA2-OA2-PA1-OA3
12	O	404	CDL	CA3-OA5-PA1-OA2
12	O	407	CDL	CB3-OB5-PB2-OB3
15	C	405	3PE	C1-O11-P-O12
15	C	405	3PE	C1-O11-P-O13
15	C	405	3PE	C1-O11-P-O14
15	C	406	3PE	C1-O11-P-O14
15	C	407	3PE	C11-O13-P-O12
15	C	408	3PE	C1-O11-P-O12
15	C	408	3PE	C1-O11-P-O13
15	C	409	3PE	C11-O13-P-O14
15	O	405	3PE	C1-O11-P-O12
15	O	405	3PE	C11-O13-P-O11
15	O	405	3PE	C11-O13-P-O12
15	O	405	3PE	C11-O13-P-O14
15	R	201	3PE	C1-O11-P-O12
15	R	201	3PE	C1-O11-P-O13
15	R	201	3PE	C1-O11-P-O14
15	R	202	3PE	C1-O11-P-O12
15	R	202	3PE	C11-O13-P-O14
16	D	501	HEC	C2B-C3B-CAB-CBB
16	P	401	HEC	C2B-C3B-CAB-CBB
18	Q	302	PC1	C1-O11-P-O12
18	Q	302	PC1	C1-O11-P-O13
12	C	410	CDL	C32-C31-CA7-OA8
12	B	602	CDL	CA4-CA3-OA5-PA1
12	N	602	CDL	CA4-CA3-OA5-PA1
15	C	409	3PE	C2-C1-O11-P
15	R	202	3PE	C32-C33-C34-C35
12	O	404	CDL	C73-C74-C75-C76
12	O	404	CDL	CA3-CA4-OA6-CA5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	C	408	3PE	C33-C34-C35-C36
15	C	404	3PE	O11-C1-C2-C3
15	C	408	3PE	O11-C1-C2-C3
12	B	602	CDL	OA5-CA3-CA4-OA6
15	C	406	3PE	C3F-C3G-C3H-C3I
15	O	405	3PE	C2C-C2D-C2E-C2F
12	O	404	CDL	CB5-C51-C52-C53
12	B	602	CDL	C14-C15-C16-C17
12	B	602	CDL	C12-C11-CA5-OA6
15	C	408	3PE	C23-C24-C25-C26
15	C	411	3PE	C1-C2-C3-O31
15	O	406	3PE	C23-C24-C25-C26
15	C	411	3PE	C36-C37-C38-C39
12	C	410	CDL	C32-C31-CA7-OA9
15	C	407	3PE	C35-C36-C37-C38
15	O	405	3PE	C29-C2A-C2B-C2C
15	C	407	3PE	C21-C22-C23-C24
12	N	603	CDL	CB4-CB3-OB5-PB2
15	C	407	3PE	C28-C29-C2A-C2B
15	R	201	3PE	C34-C35-C36-C37
15	O	405	3PE	C36-C37-C38-C39
12	N	602	CDL	C16-C17-C18-C19
12	N	602	CDL	C14-C15-C16-C17
12	N	602	CDL	C58-C59-C60-C61
15	O	406	3PE	C2-C1-O11-P
13	C	401	A1D6K	C3-N1-O4-C19
13	O	401	A1D6K	C3-N1-O4-C19
12	O	407	CDL	C18-C19-C20-C21
12	C	410	CDL	C18-C19-C20-C21
15	C	407	3PE	C25-C26-C27-C28
15	R	202	3PE	O31-C31-C32-C33
15	C	406	3PE	C2D-C2E-C2F-C2G
12	N	603	CDL	C32-C31-CA7-OA8
14	O	402	HEM	CAA-CBA-CGA-O1A
15	C	406	3PE	C37-C38-C39-C3A
15	C	406	3PE	C32-C33-C34-C35
15	C	406	3PE	C2E-C2F-C2G-C2H
12	C	410	CDL	OB6-CB4-CB6-OB8
15	C	406	3PE	C28-C29-C2A-C2B
12	O	407	CDL	CB4-CB6-OB8-CB7
15	C	407	3PE	C32-C33-C34-C35
14	O	402	HEM	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
12	N	603	CDL	OA9-CA7-OA8-CA6
12	N	602	CDL	C52-C53-C54-C55
15	C	406	3PE	C1-C2-C3-O31
15	C	409	3PE	O11-C1-C2-O21
15	C	409	3PE	O11-C1-C2-C3
15	R	201	3PE	O21-C2-C3-O31
12	N	603	CDL	C31-CA7-OA8-CA6
15	O	406	3PE	C22-C23-C24-C25
14	C	402	HEM	CAA-CBA-CGA-O2A
12	O	407	CDL	C13-C14-C15-C16
12	C	410	CDL	C60-C61-C62-C63
12	N	603	CDL	CA3-CA4-CA6-OA8
15	R	201	3PE	C1-C2-C3-O31
15	R	202	3PE	C2A-C2B-C2C-C2D
12	N	603	CDL	OA6-CA4-CA6-OA8
15	O	405	3PE	O31-C31-C32-C33
12	N	602	CDL	C53-C54-C55-C56
14	C	402	HEM	CAA-CBA-CGA-O1A
15	O	406	3PE	C36-C37-C38-C39
15	O	405	3PE	C32-C33-C34-C35
12	O	404	CDL	C52-C53-C54-C55
12	N	602	CDL	C51-C52-C53-C54
15	C	406	3PE	C22-C23-C24-C25
15	C	404	3PE	O31-C31-C32-C33
12	N	602	CDL	C52-C51-CB5-OB6
14	O	402	HEM	CAD-CBD-CGD-O2D
12	N	602	CDL	C75-C76-C77-C78
15	C	409	3PE	C37-C38-C39-C3A
14	C	402	HEM	CAD-CBD-CGD-O2D
15	R	202	3PE	C28-C29-C2A-C2B
12	O	404	CDL	C11-C12-C13-C14
15	C	405	3PE	O31-C31-C32-C33
13	C	401	A1D6K	C4-C3-N1-C2
13	O	401	A1D6K	C4-C3-N1-C2
15	C	406	3PE	O21-C21-C22-C23
14	O	402	HEM	CAD-CBD-CGD-O1D
15	C	409	3PE	O22-C21-C22-C23
14	O	403	HEM	CAA-CBA-CGA-O2A
15	C	404	3PE	C2-C1-O11-P
14	C	402	HEM	CAD-CBD-CGD-O1D
15	C	404	3PE	O32-C31-C32-C33
15	C	406	3PE	C3D-C3E-C3F-C3G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	O	405	3PE	O32-C31-C32-C33
15	C	407	3PE	C22-C23-C24-C25
15	R	202	3PE	C36-C37-C38-C39
12	O	407	CDL	C53-C54-C55-C56
15	C	406	3PE	O22-C21-C22-C23
15	C	405	3PE	C32-C33-C34-C35
14	O	403	HEM	CAA-CBA-CGA-O1A
12	N	603	CDL	C12-C11-CA5-OA6
12	C	410	CDL	C72-C71-CB7-OB8
12	N	603	CDL	C52-C51-CB5-OB6
12	O	404	CDL	C12-C11-CA5-OA6

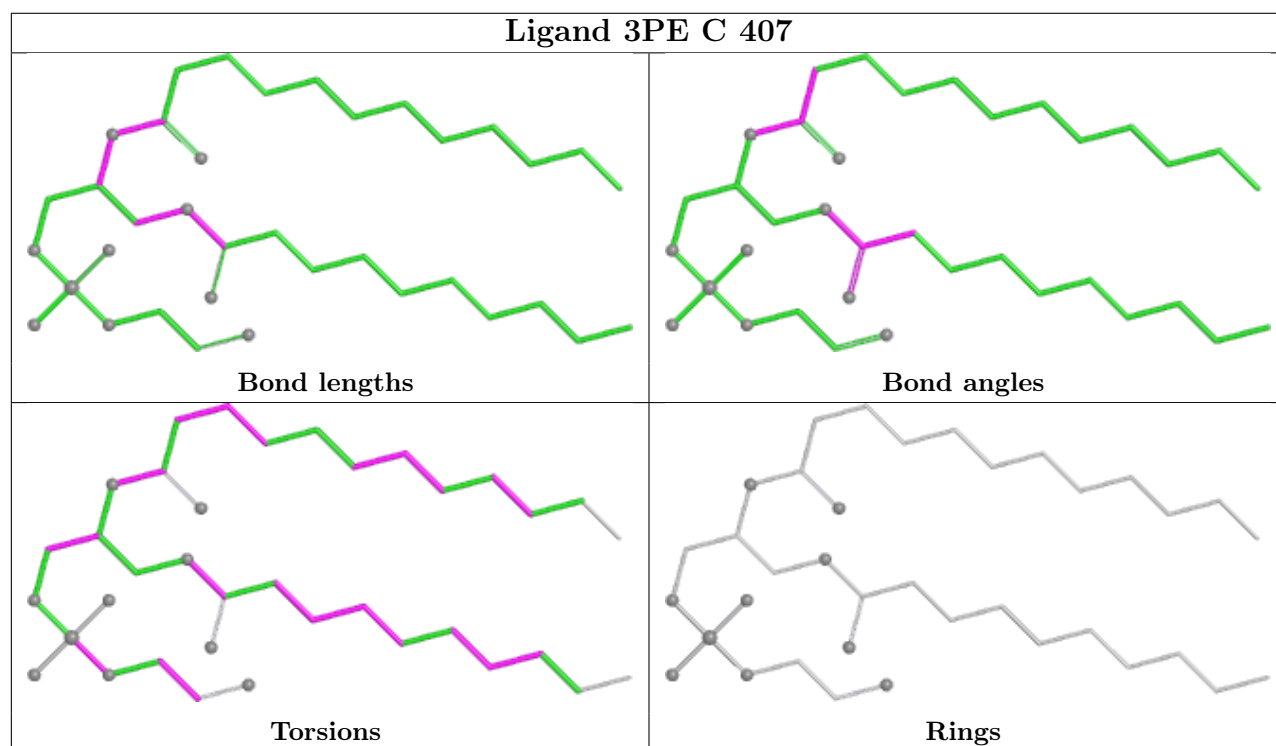
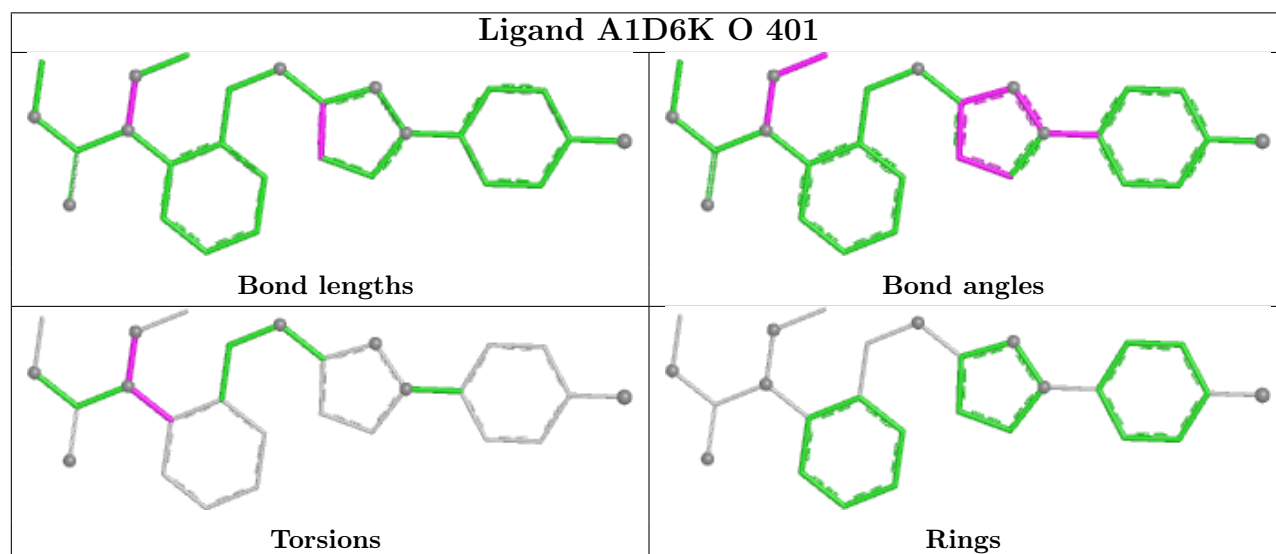
There are no ring outliers.

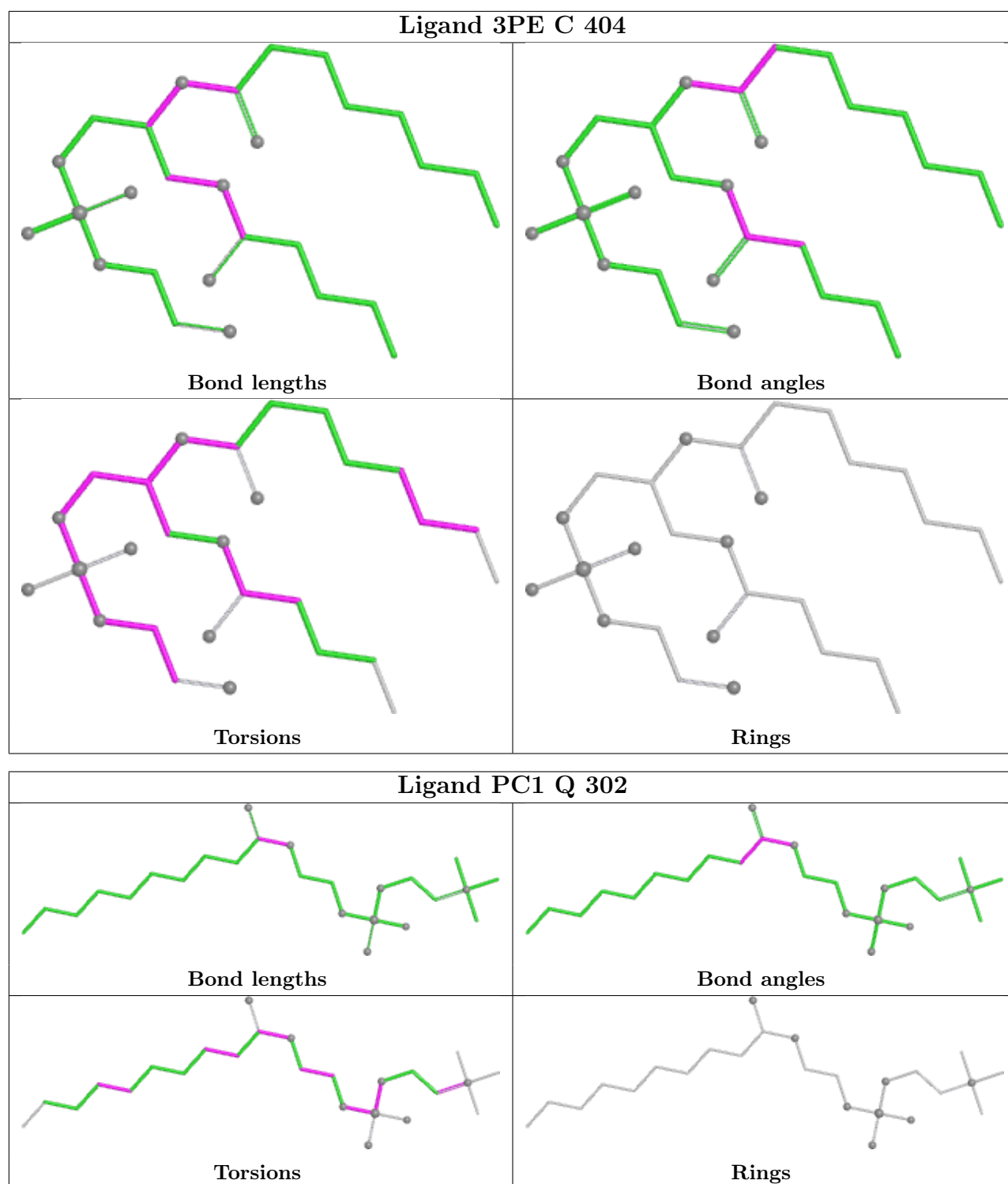
15 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	C	407	3PE	1	0
15	C	404	3PE	3	0
18	Q	302	PC1	3	0
12	N	602	CDL	4	0
15	K	101	3PE	1	0
14	C	403	HEM	1	0
12	B	602	CDL	3	0
12	N	603	CDL	3	0
12	O	407	CDL	6	0
15	C	406	3PE	3	0
12	C	410	CDL	3	0
15	C	411	3PE	5	0
16	D	501	HEC	2	0
15	R	202	3PE	5	0
16	P	401	HEC	2	0

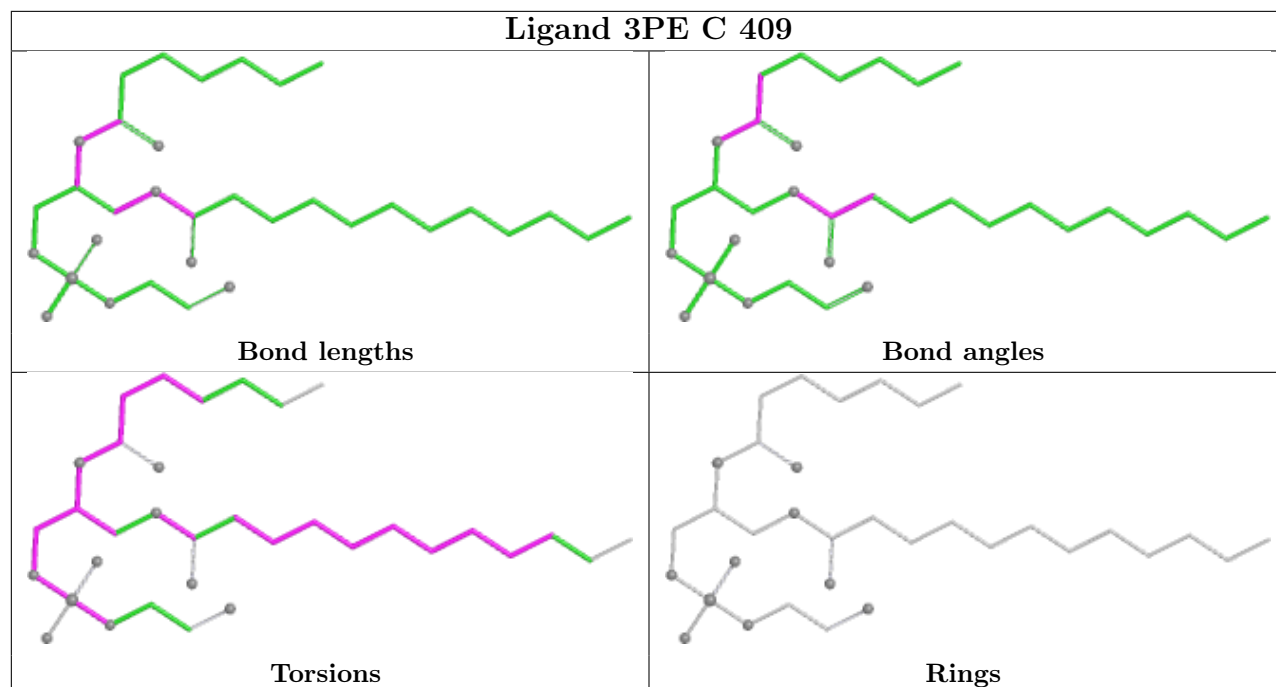
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

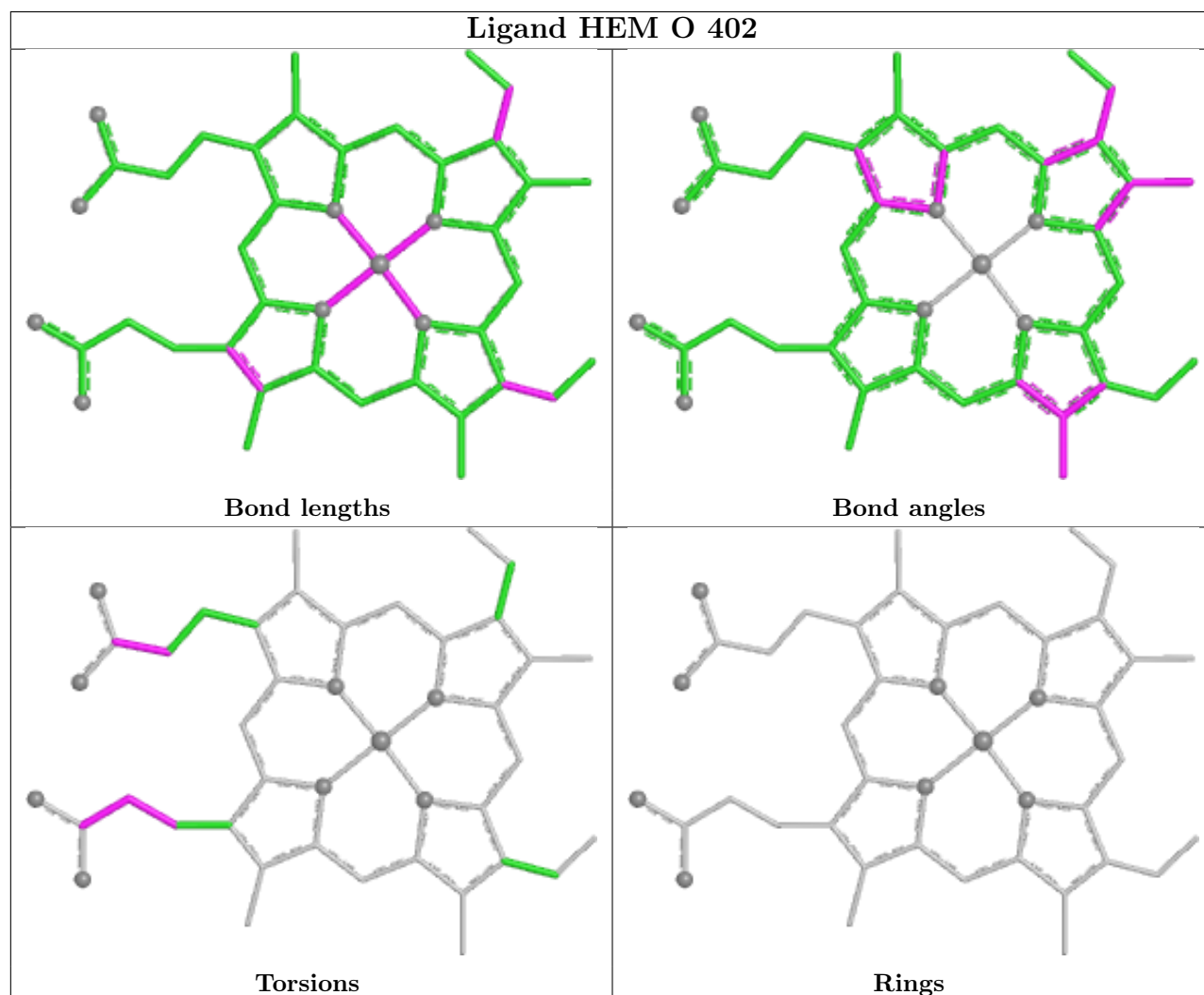


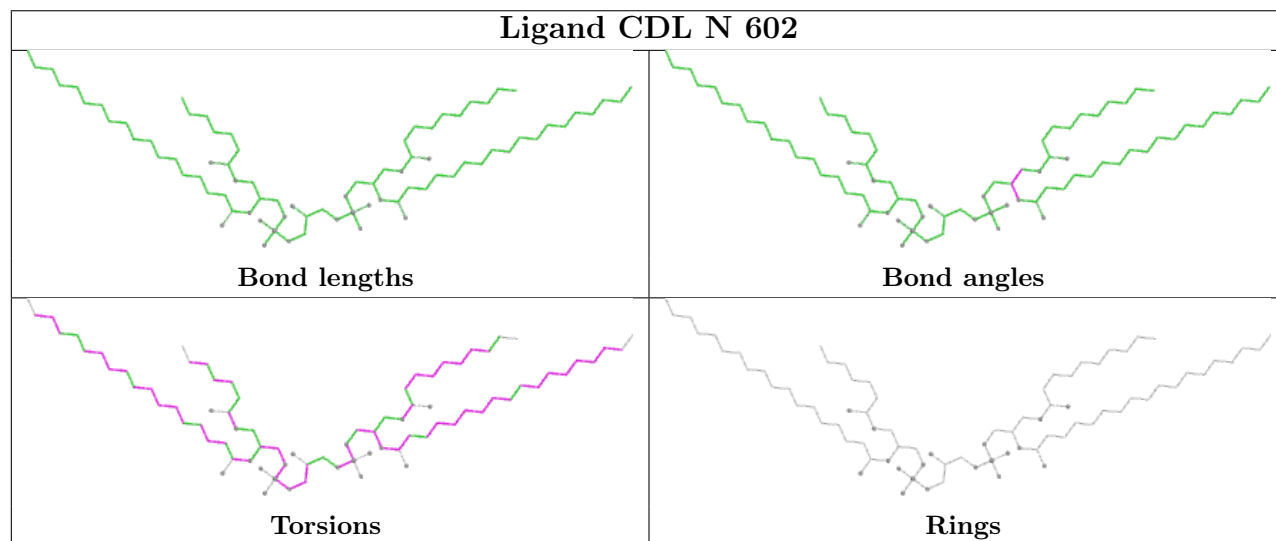
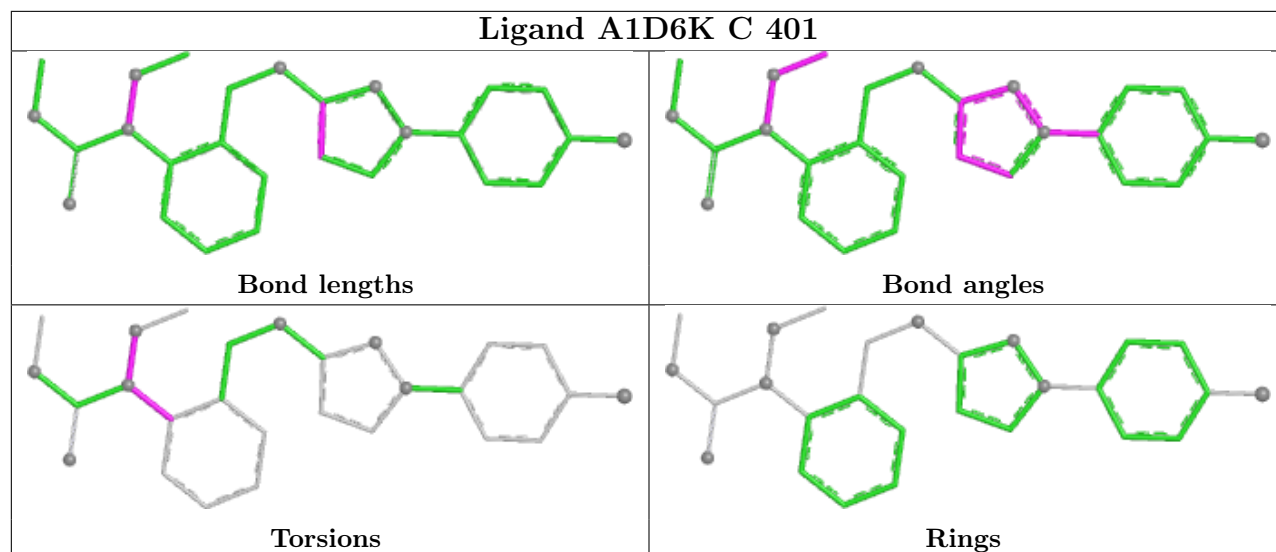


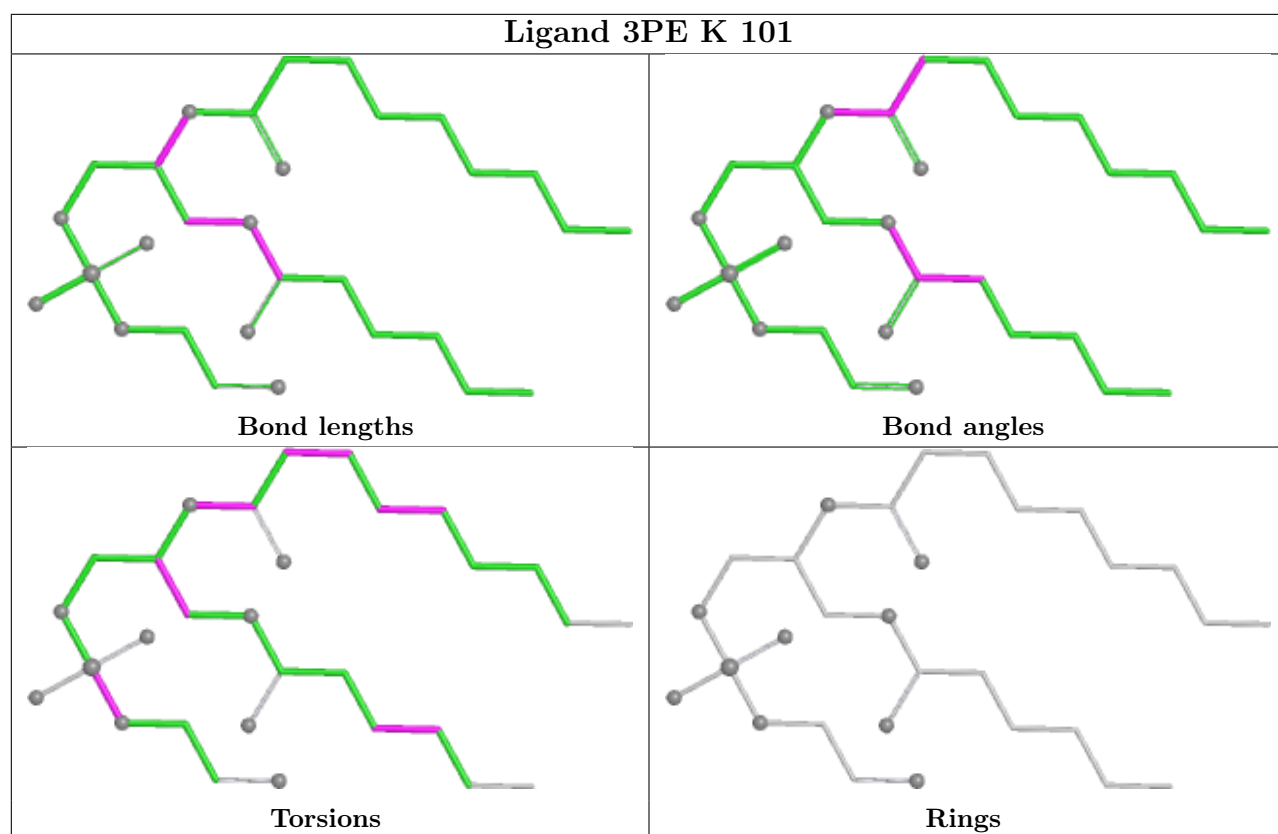
Ligand 3PE C 409

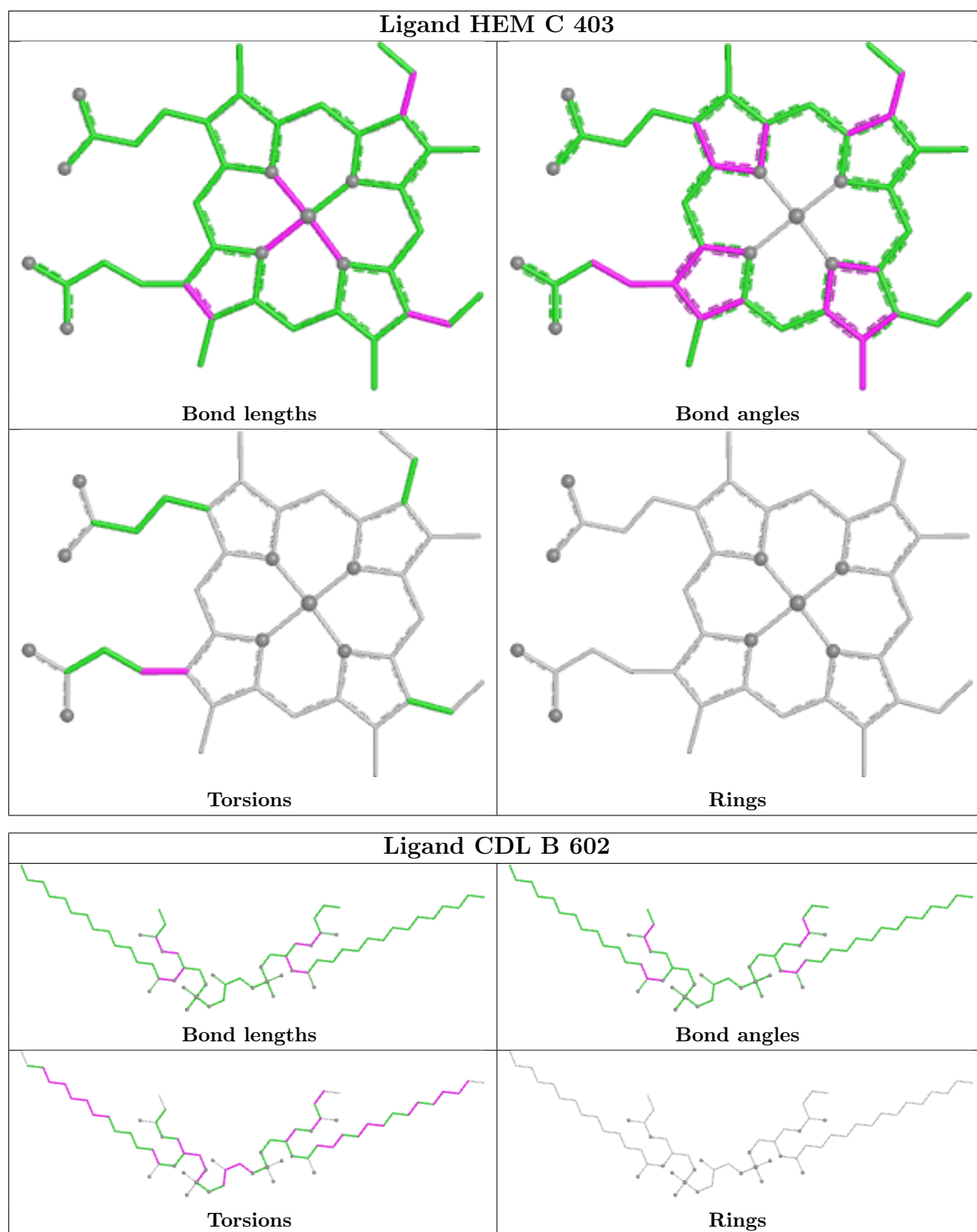


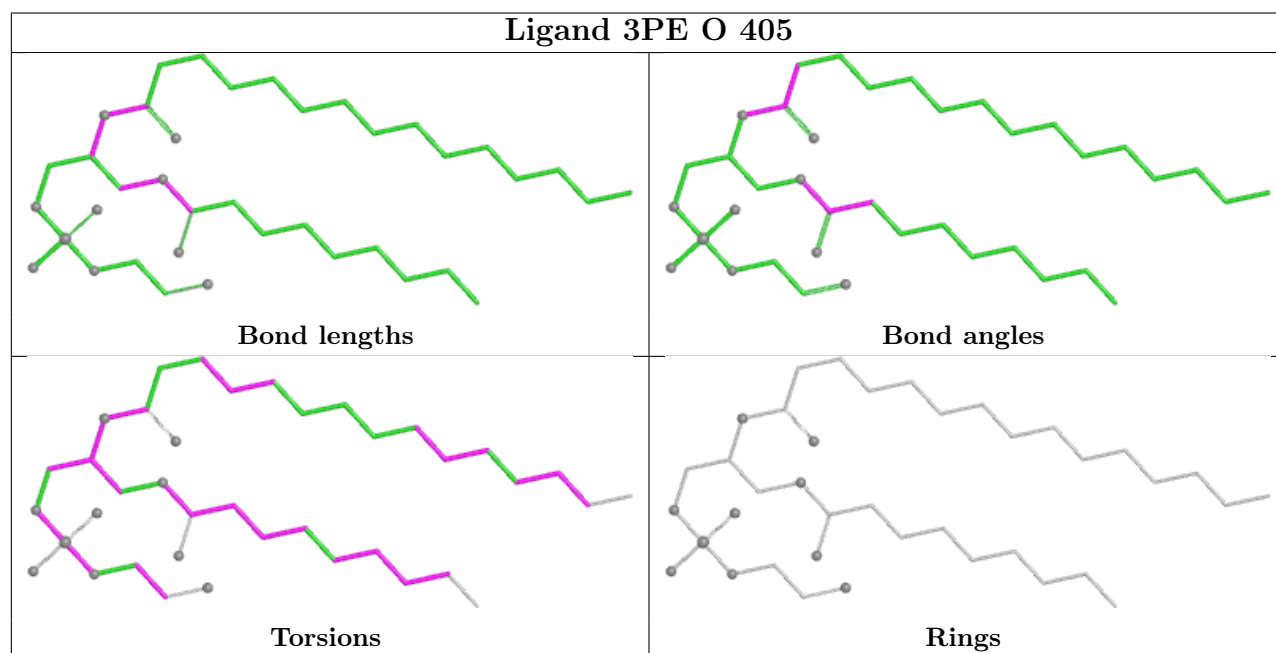
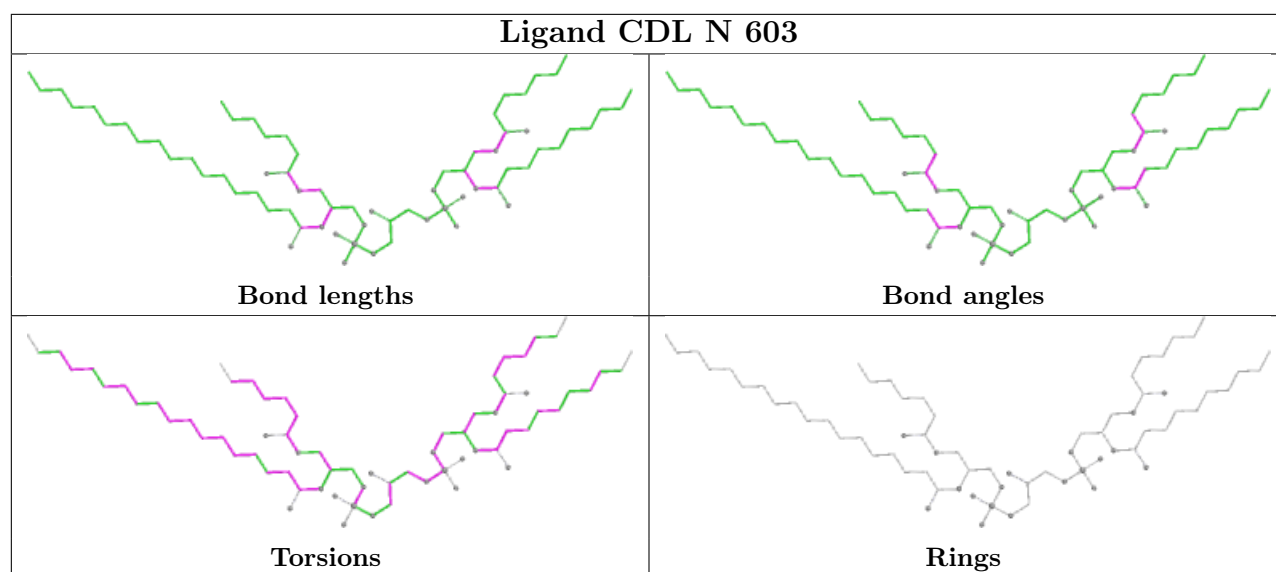
Ligand HEM O 402

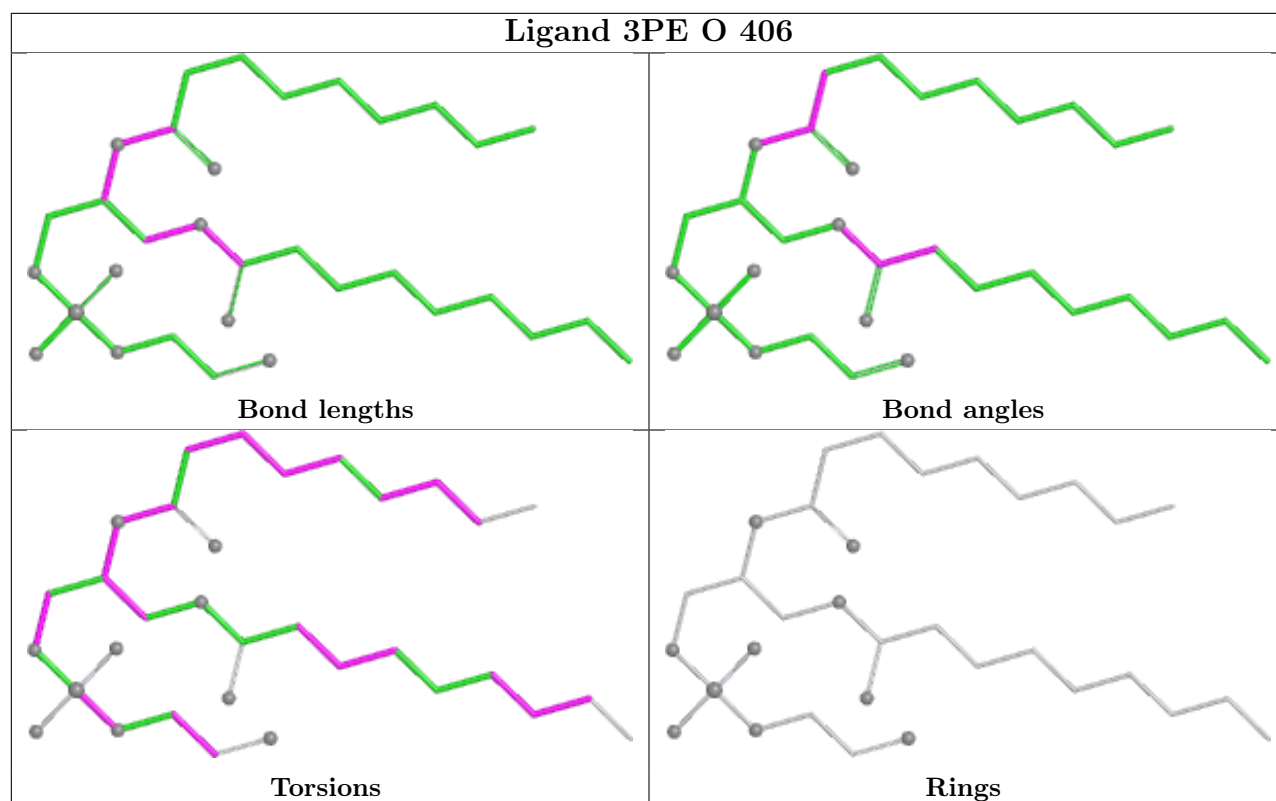
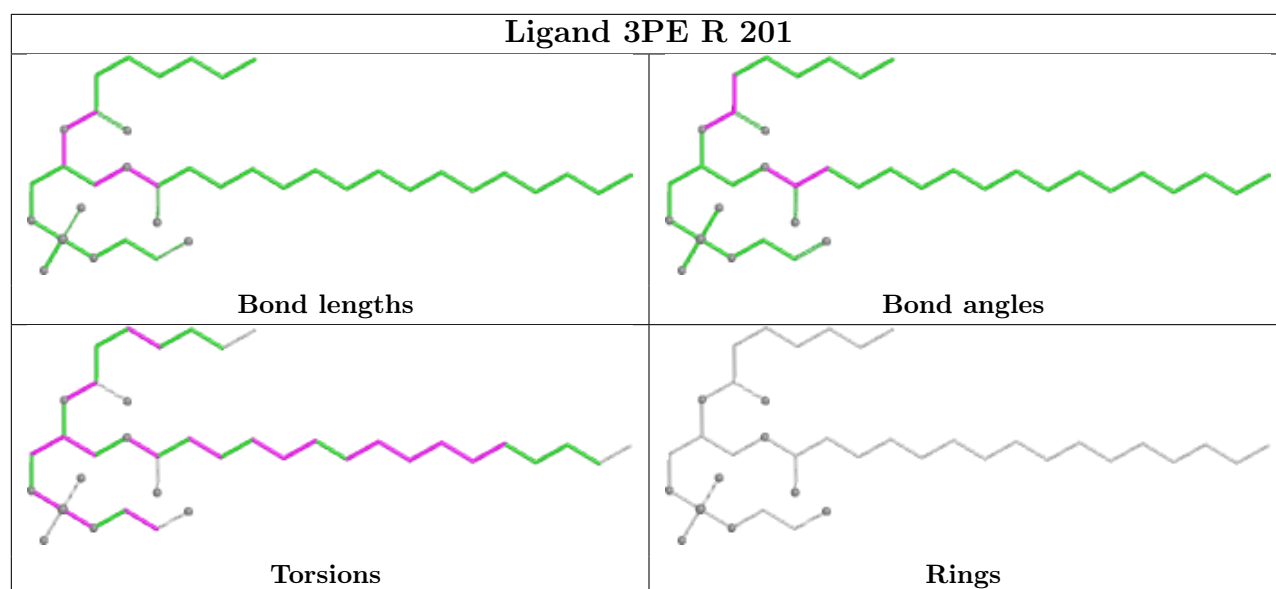


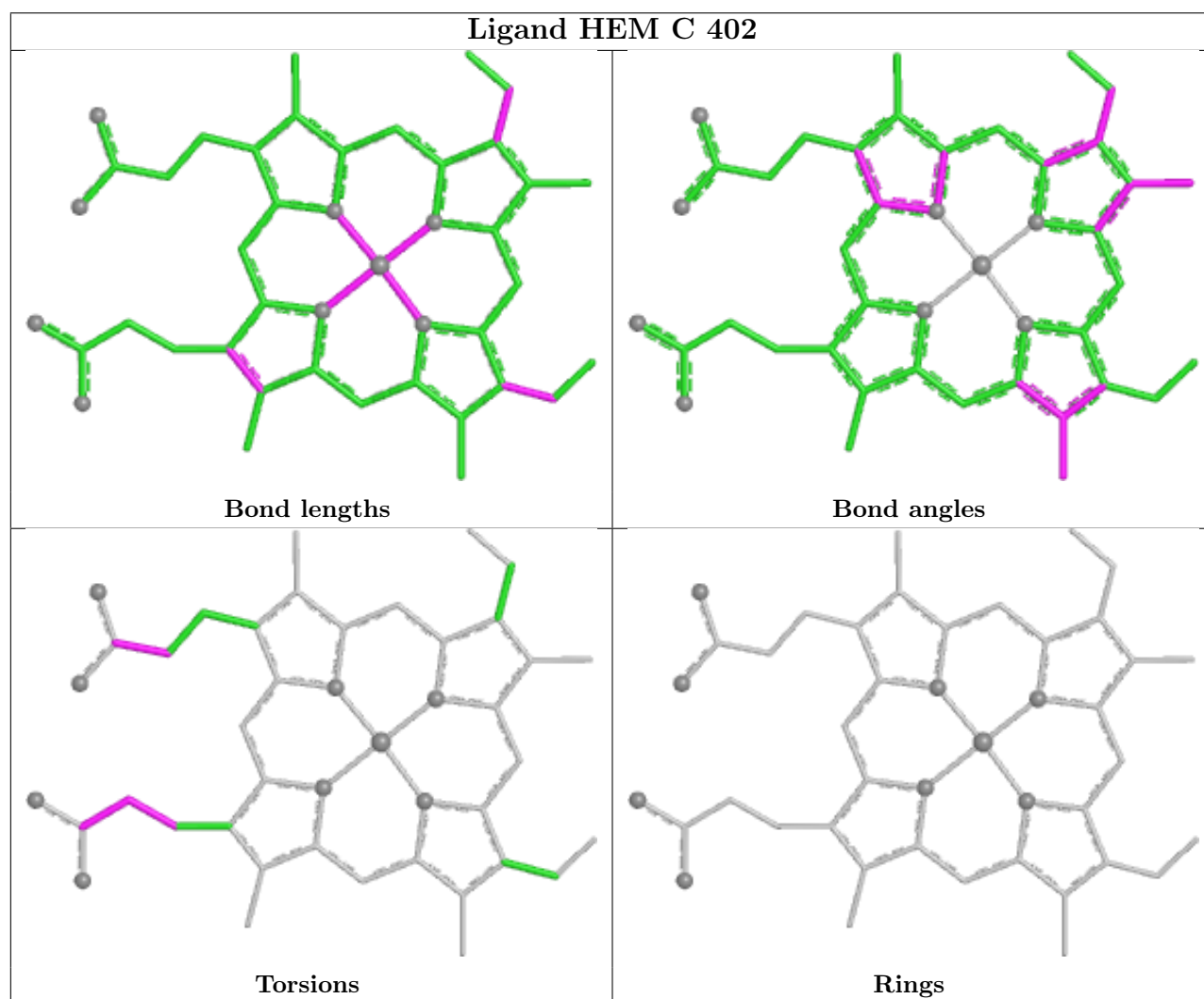
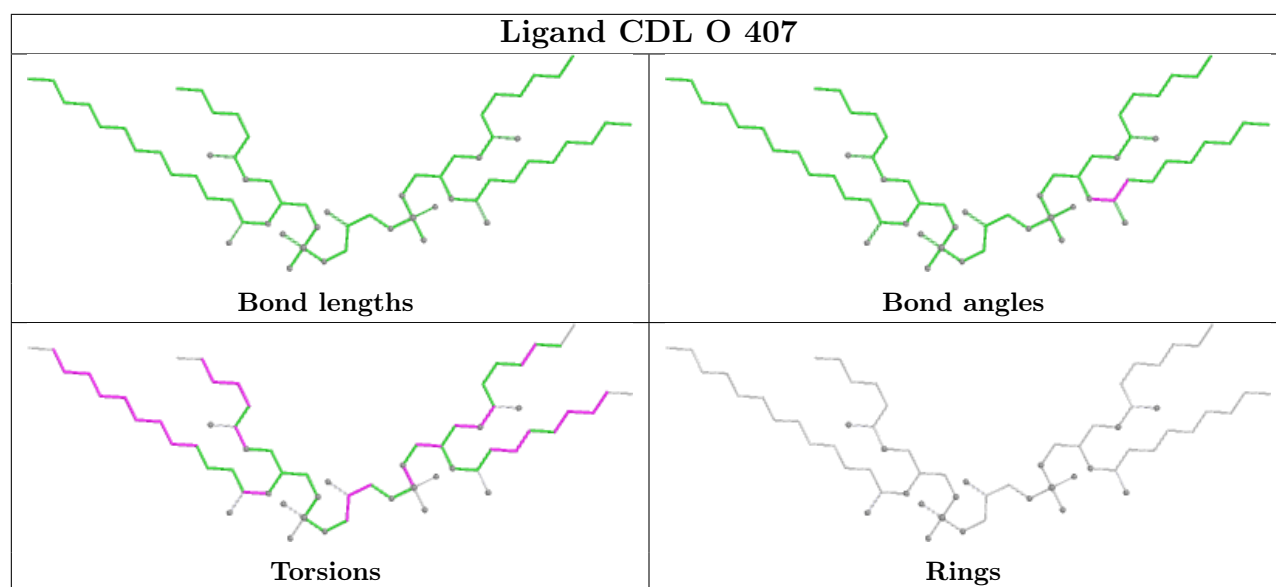


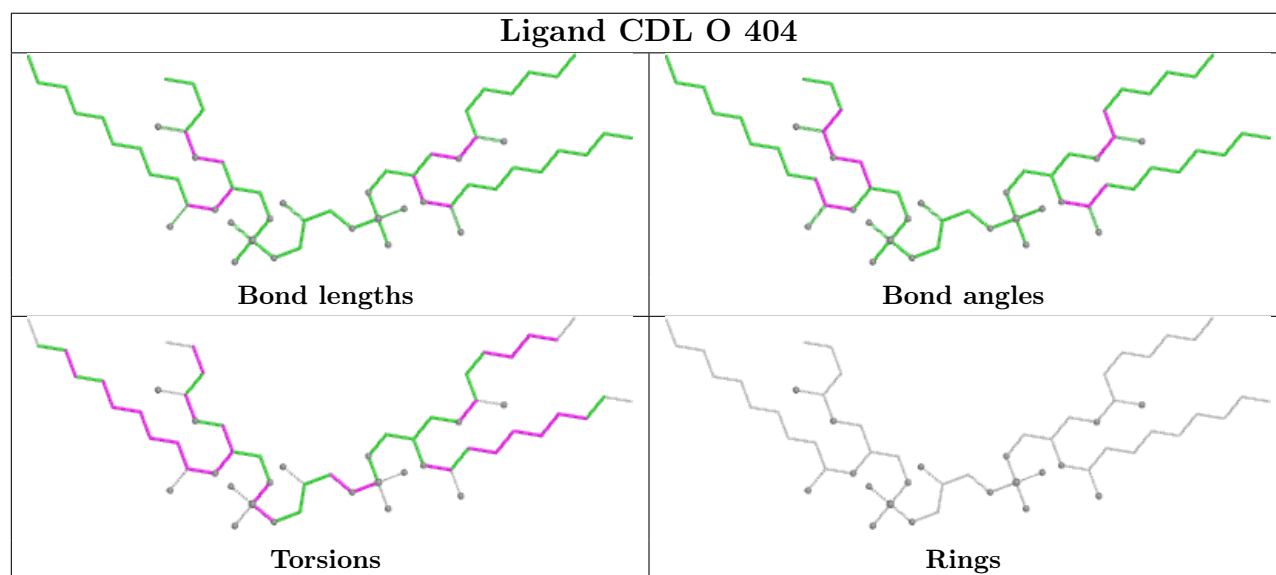
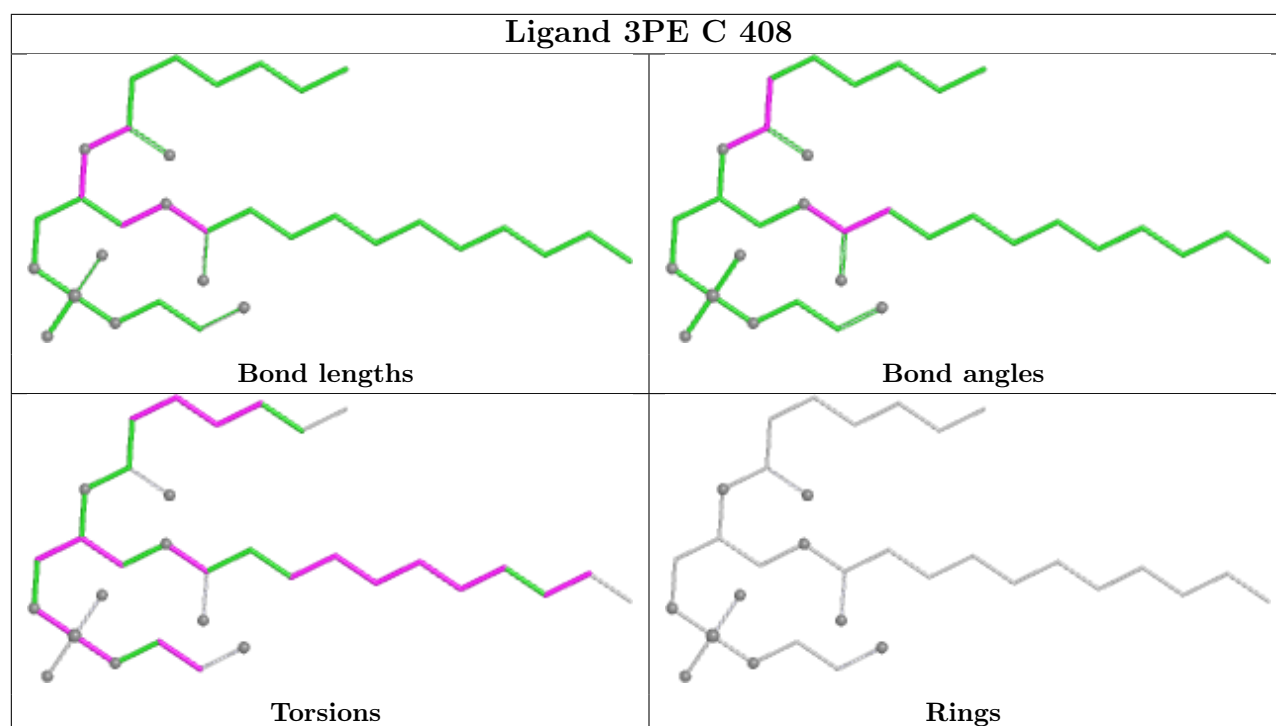


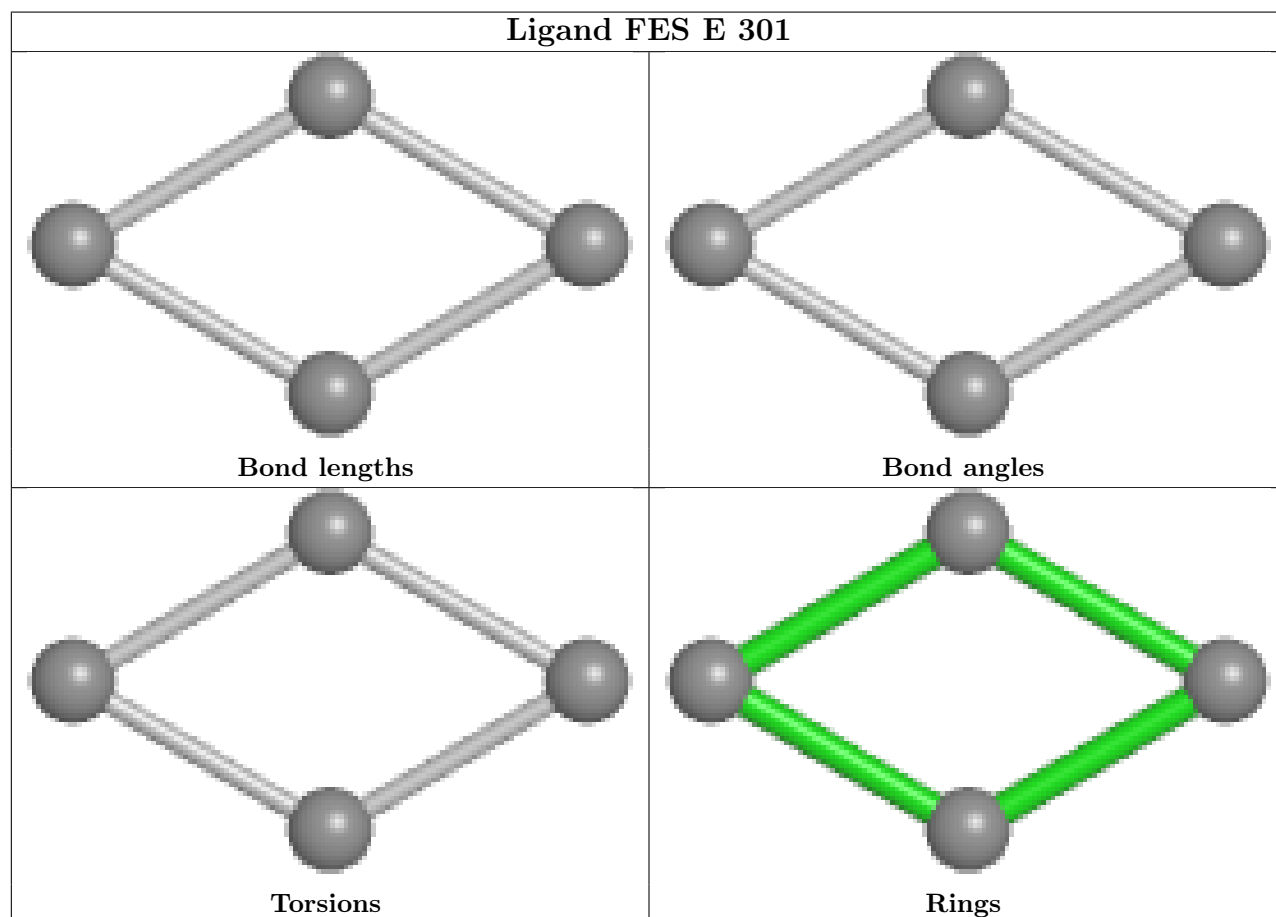
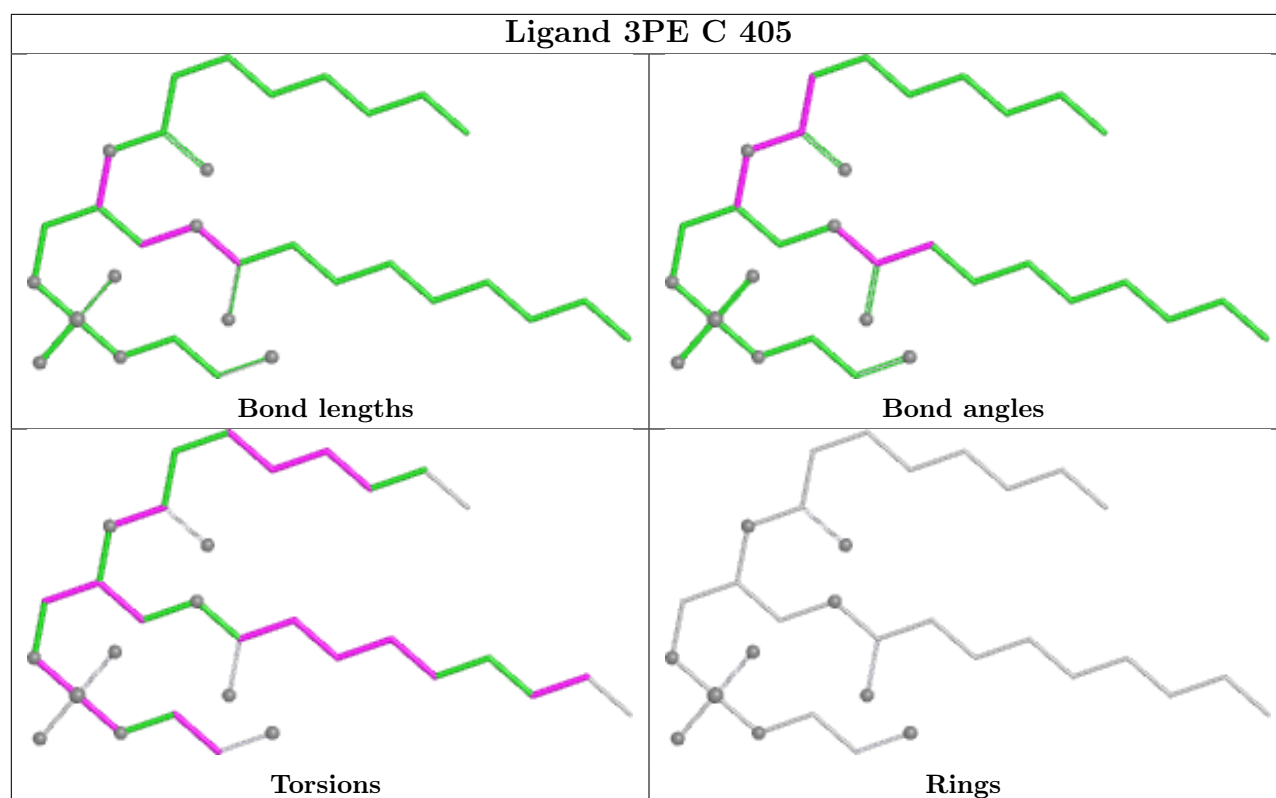


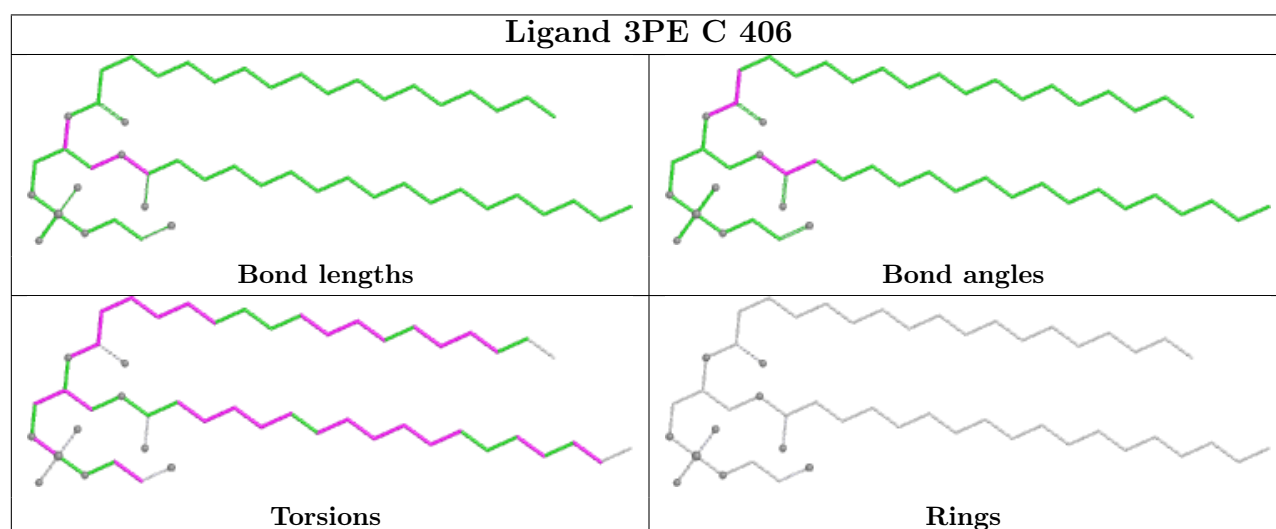
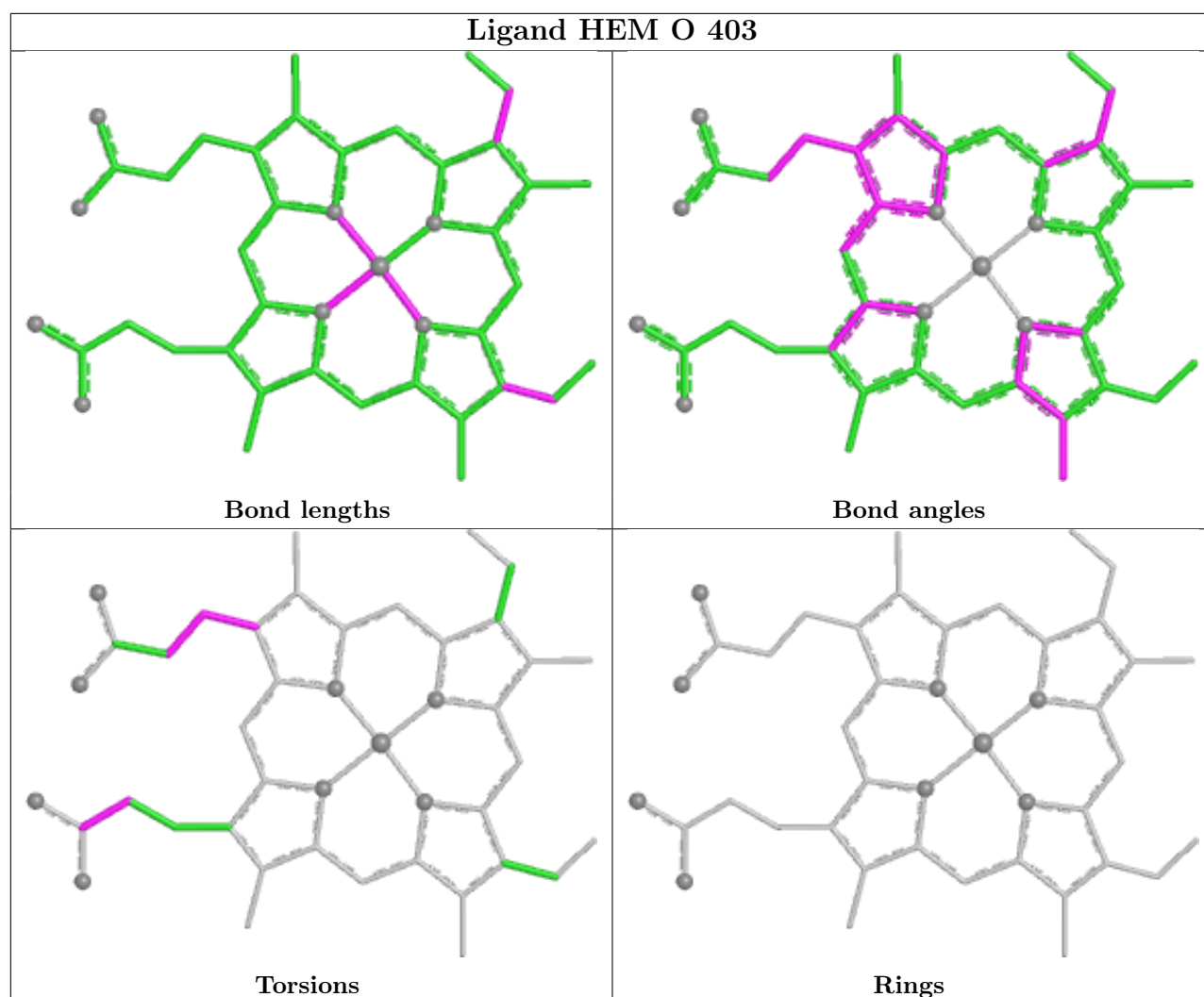


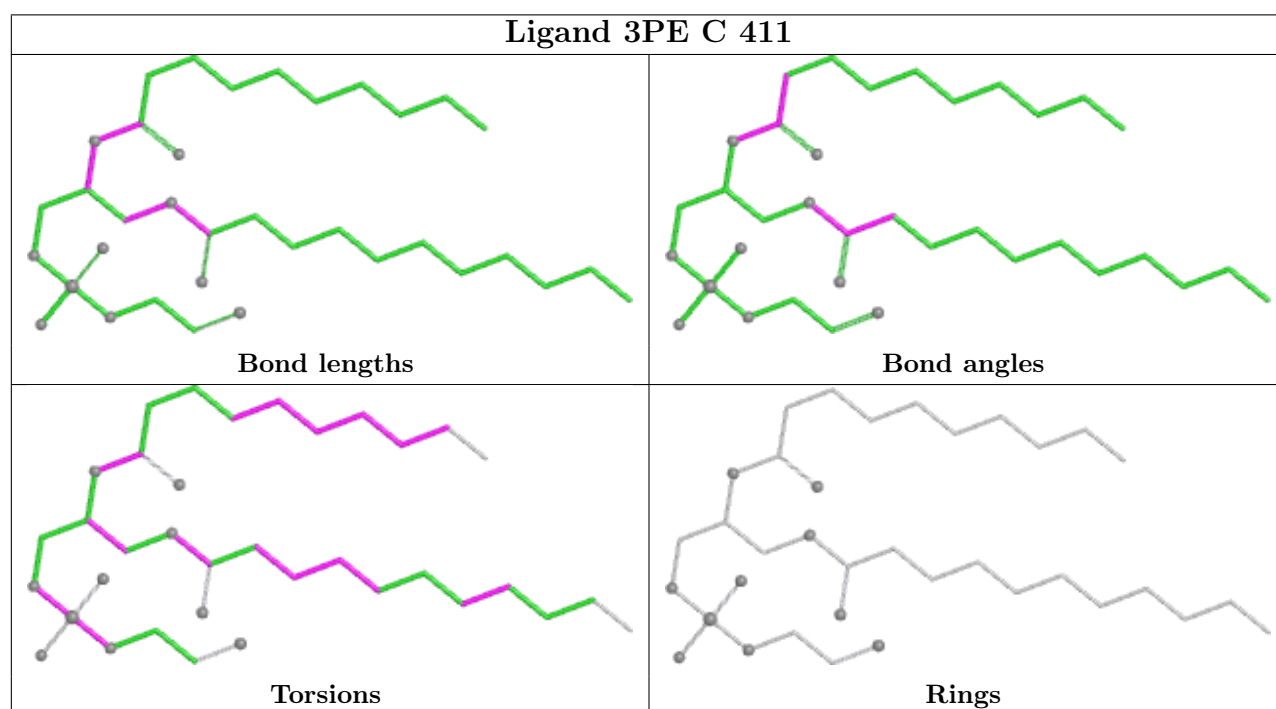
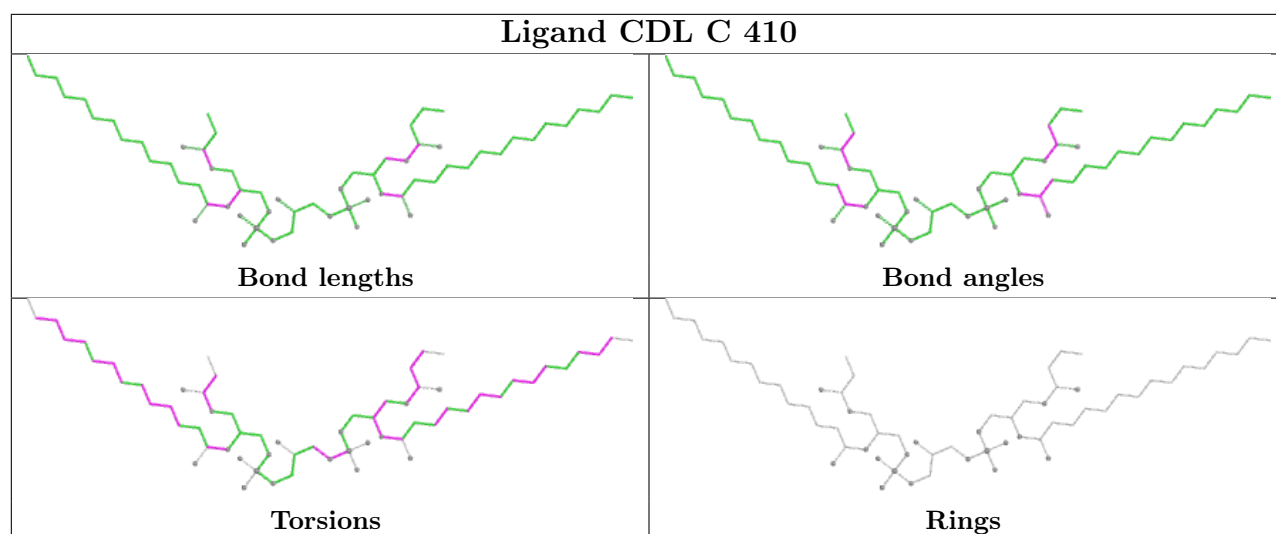


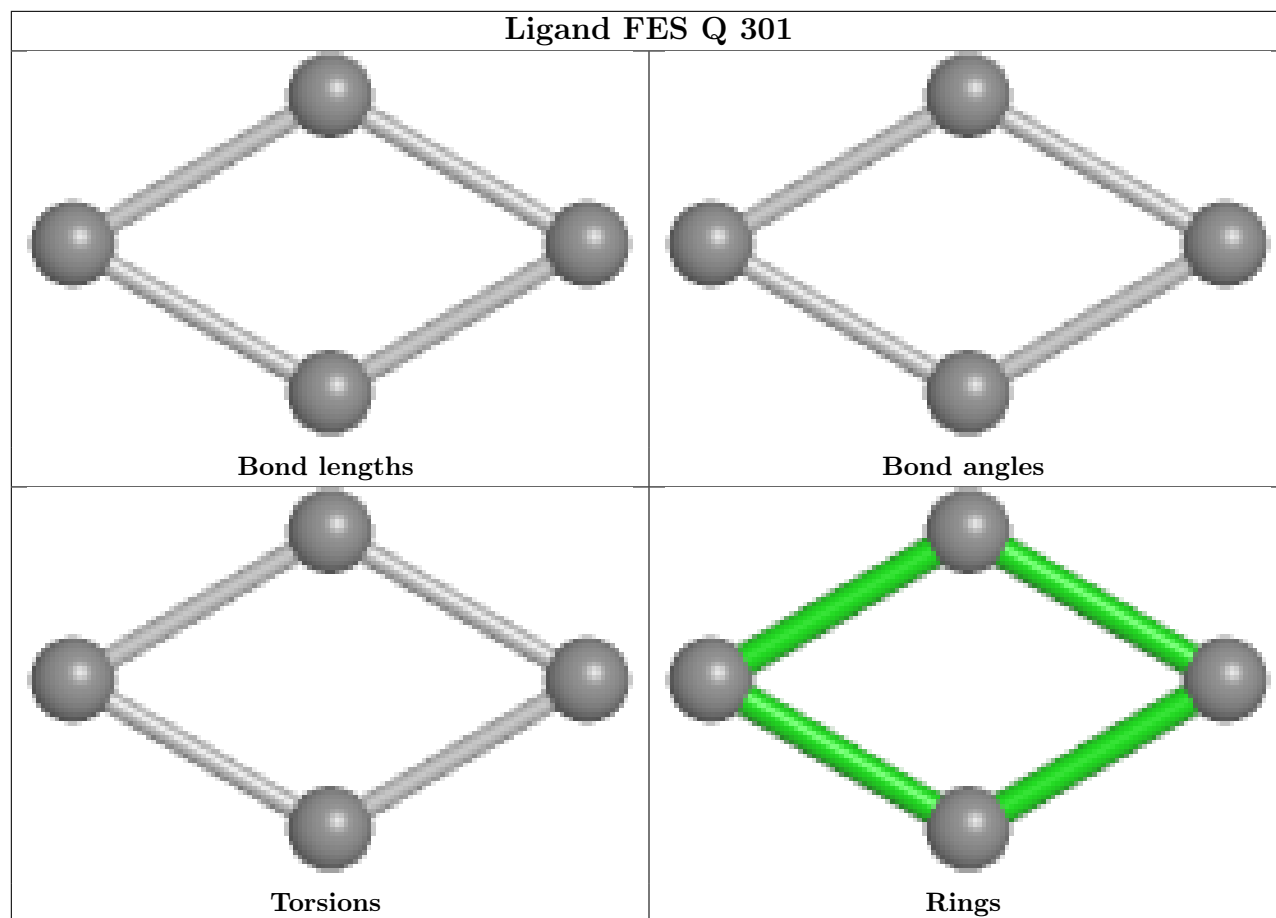


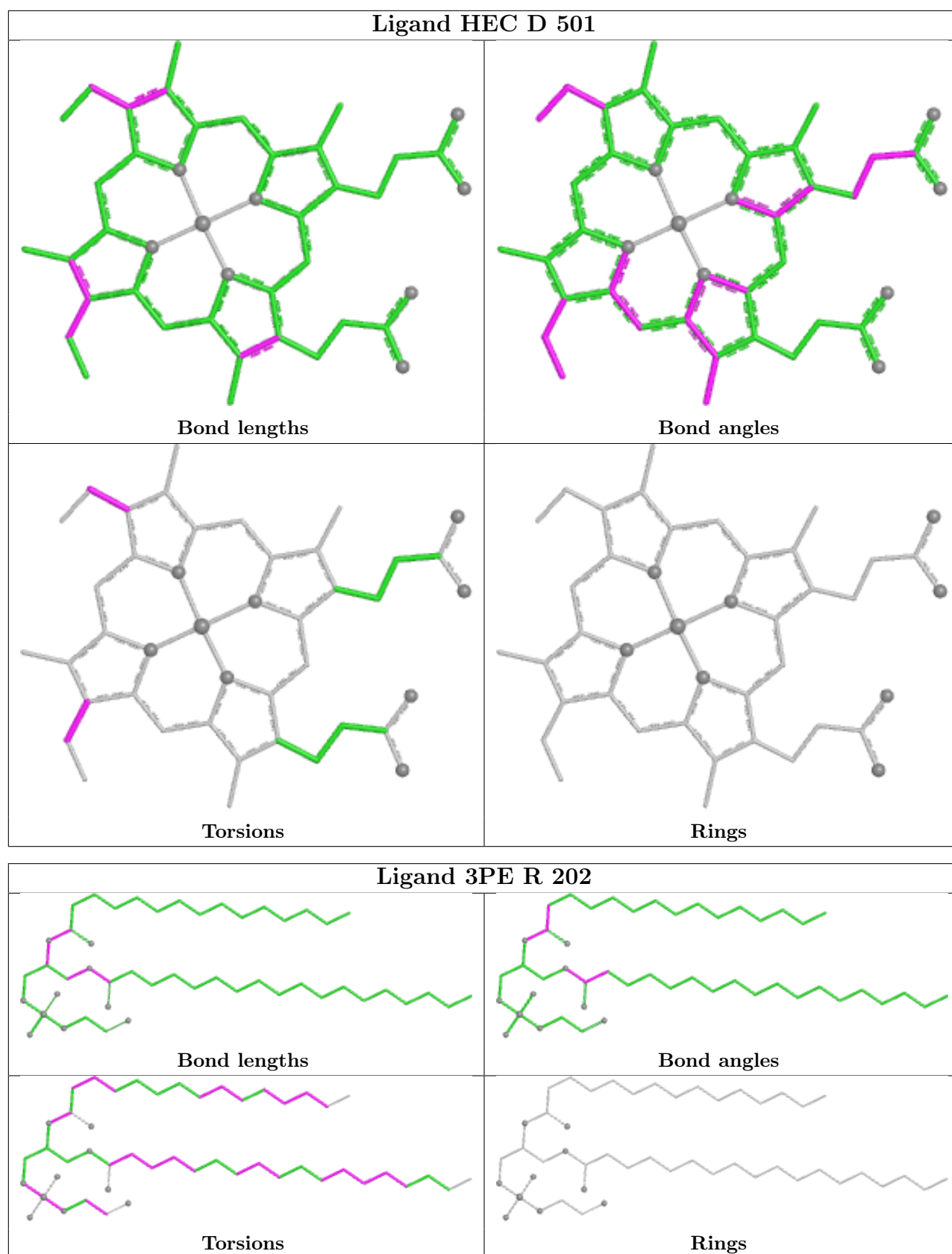


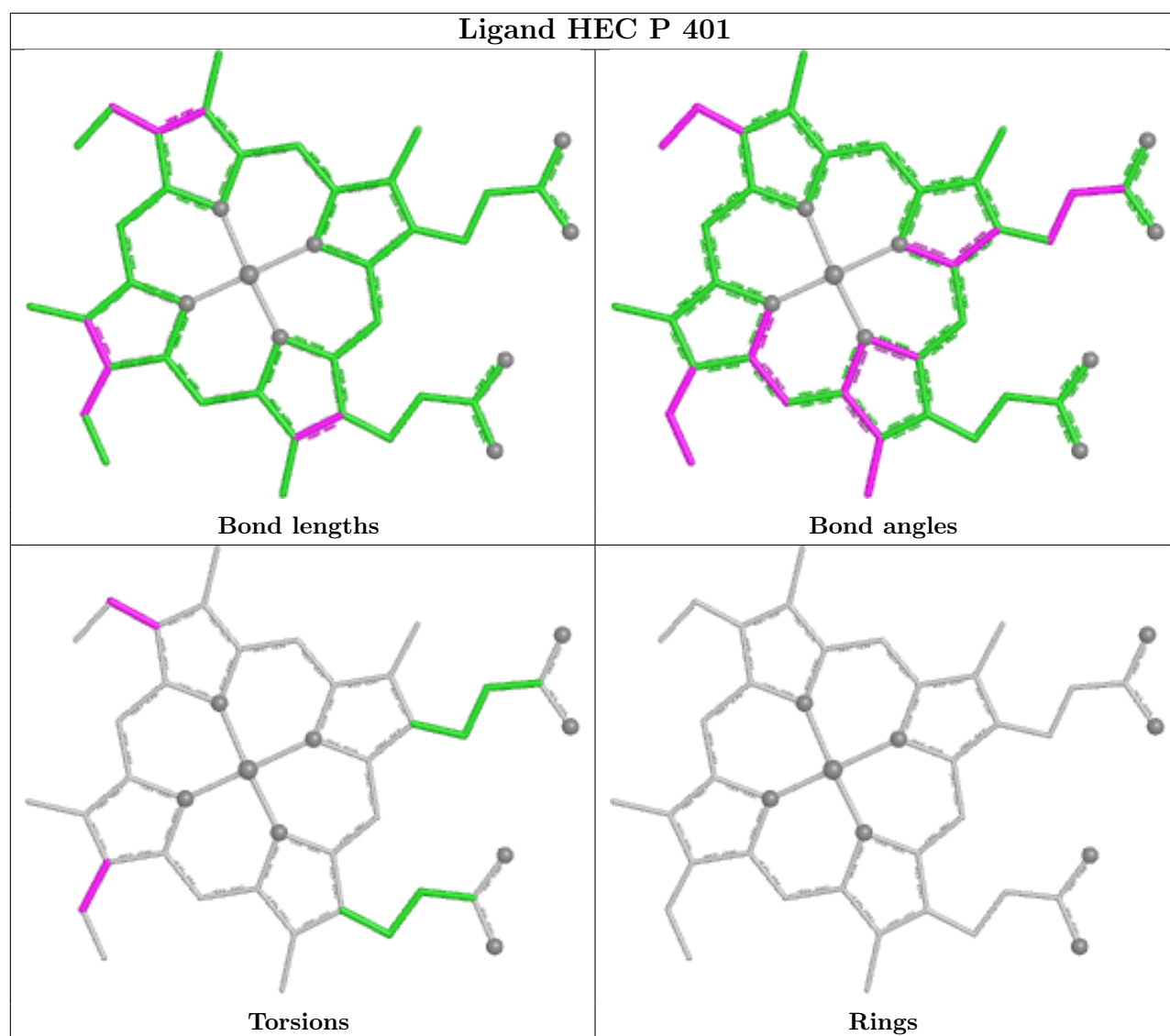












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

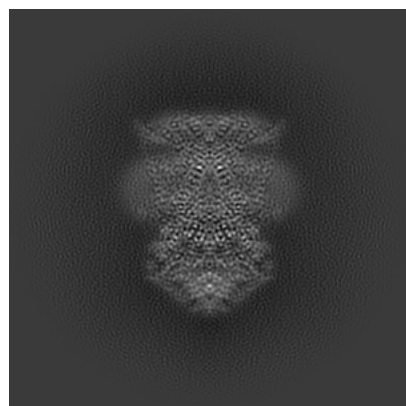
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60307. These allow visual inspection of the internal detail of the map and identification of artifacts.

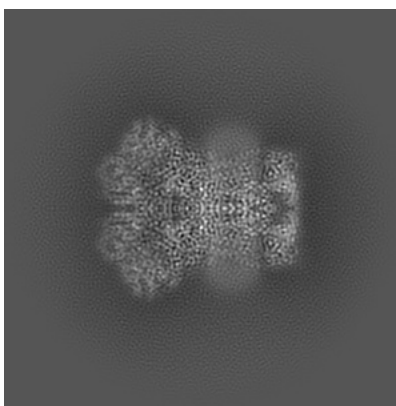
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

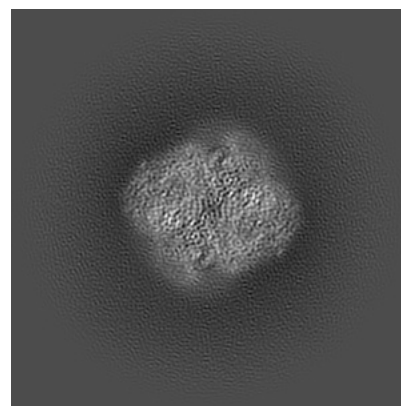
6.1.1 Primary map



X

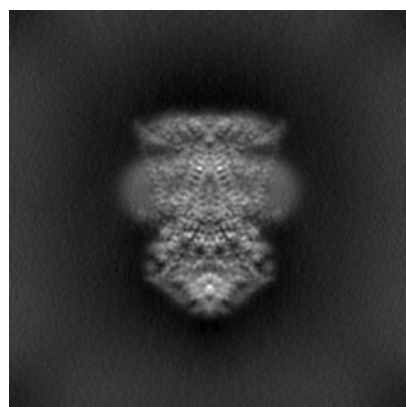


Y

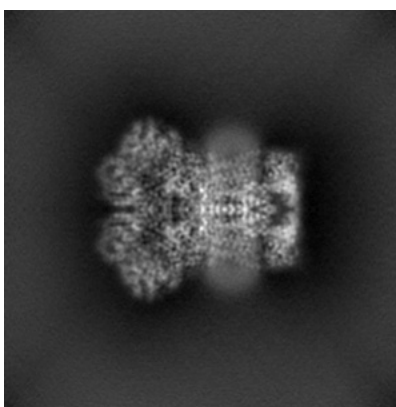


Z

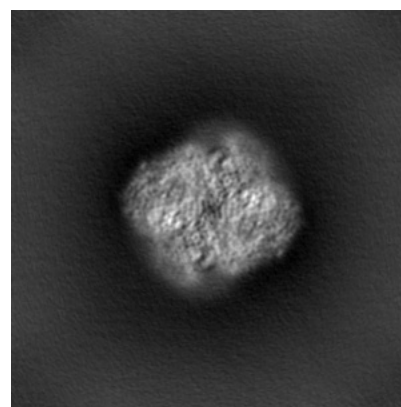
6.1.2 Raw map



X



Y

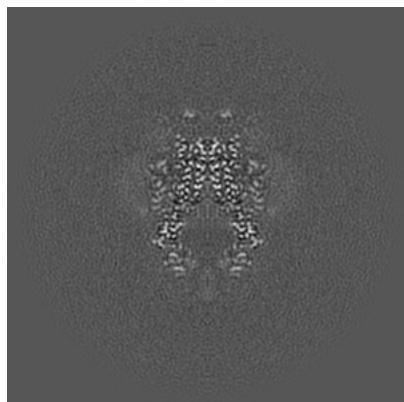


Z

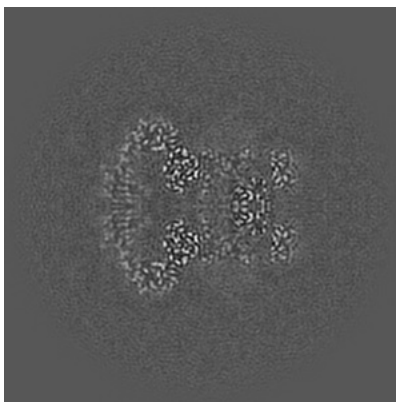
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

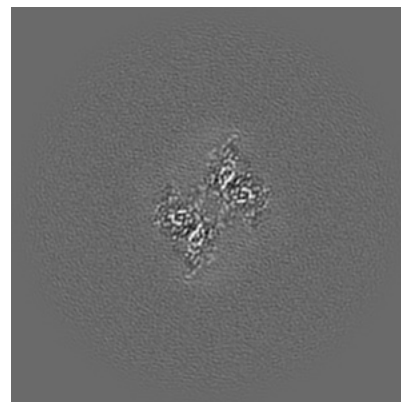
6.2.1 Primary map



X Index: 160

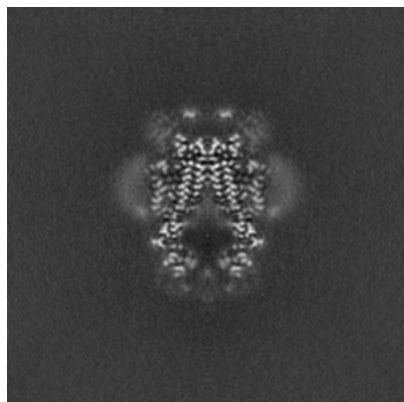


Y Index: 160

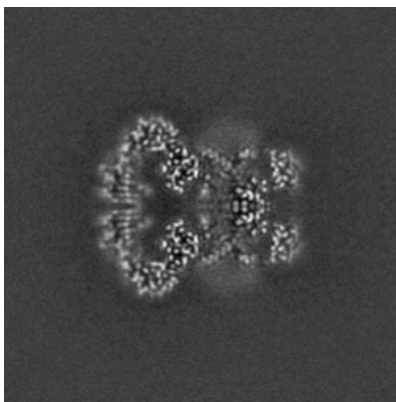


Z Index: 160

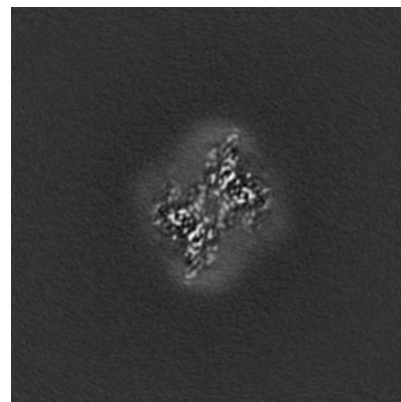
6.2.2 Raw map



X Index: 160



Y Index: 160

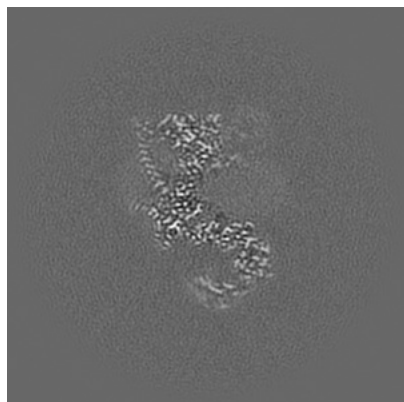


Z Index: 160

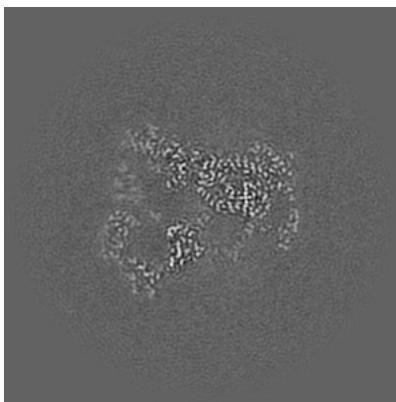
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

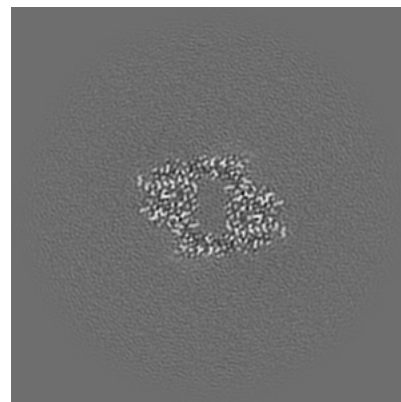
6.3.1 Primary map



X Index: 141

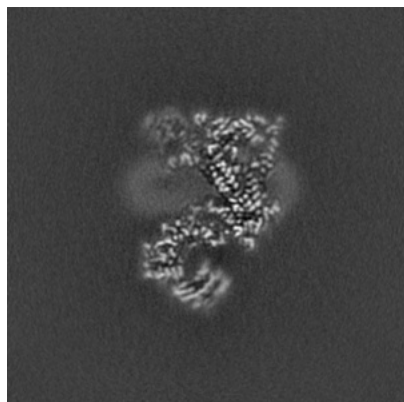


Y Index: 168

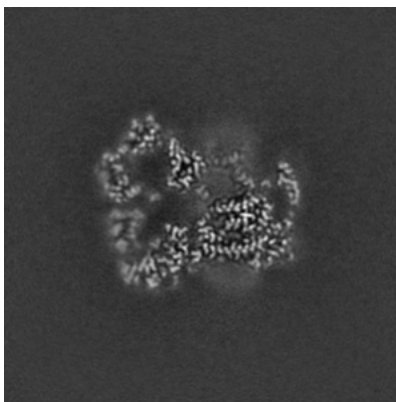


Z Index: 140

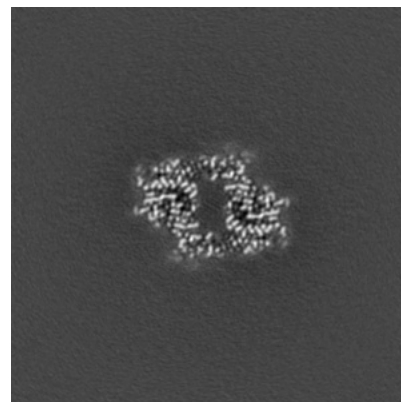
6.3.2 Raw map



X Index: 175



Y Index: 153

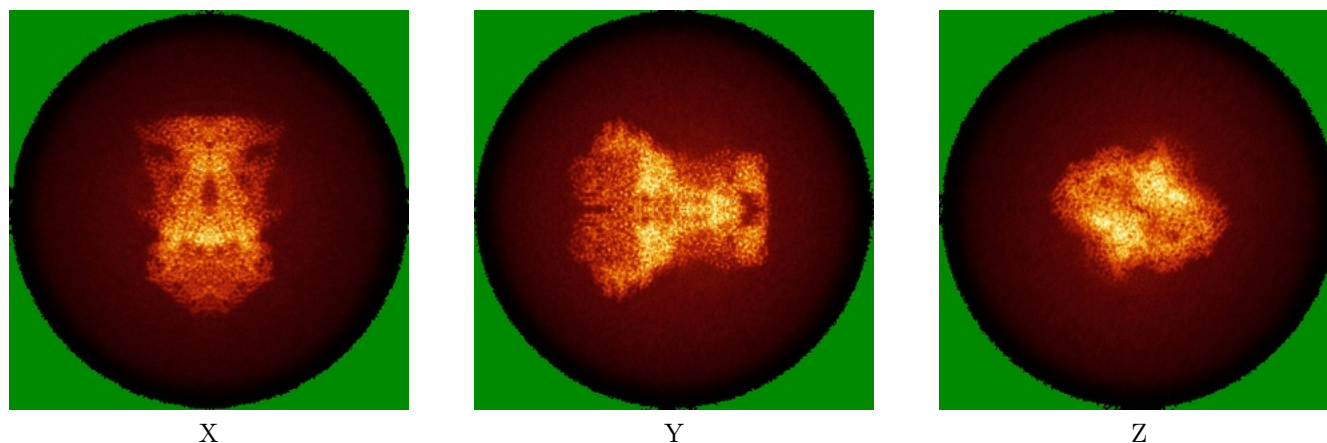


Z Index: 139

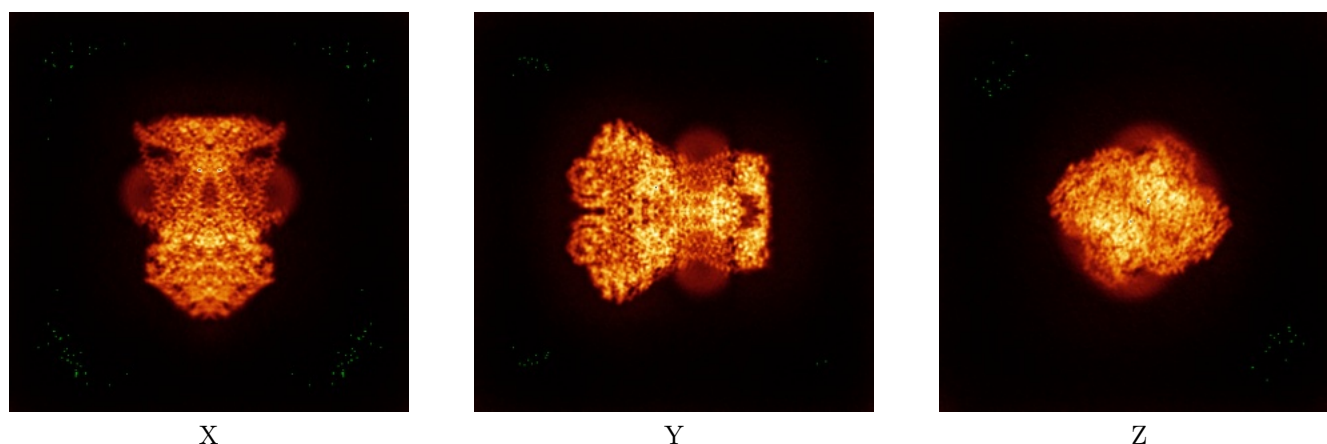
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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

6.5 Orthogonal surface views [i](#)

This section was not generated.

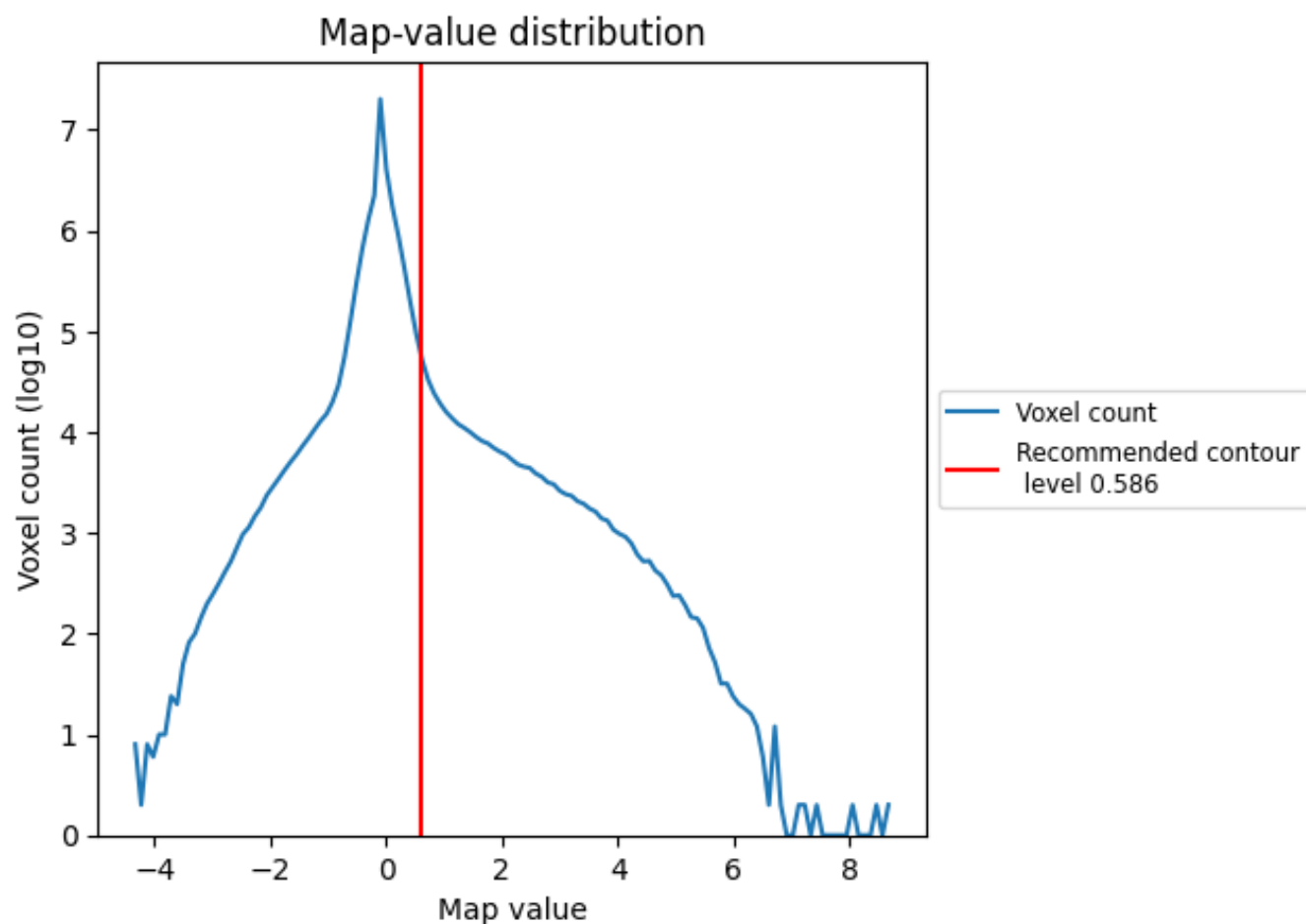
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

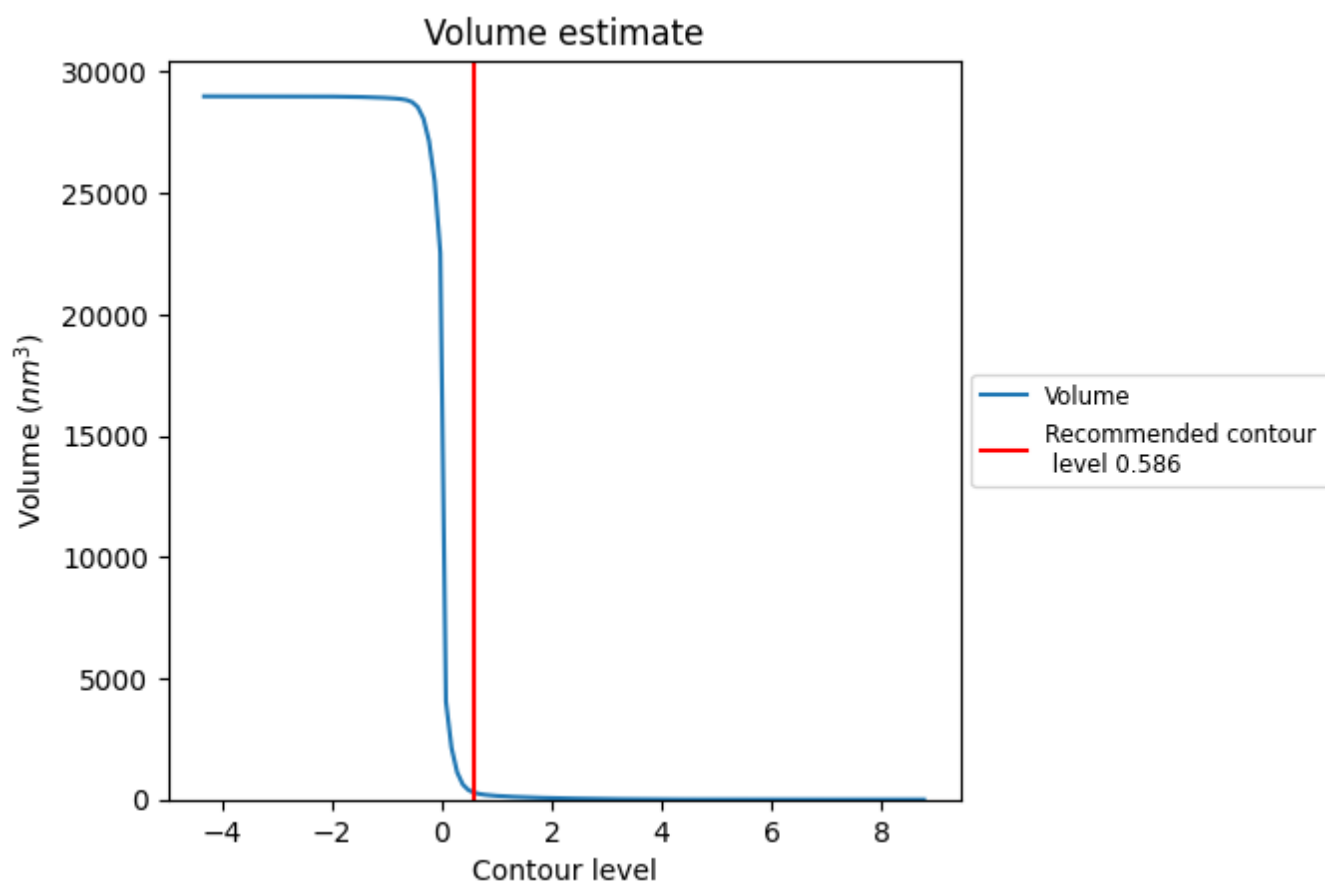
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

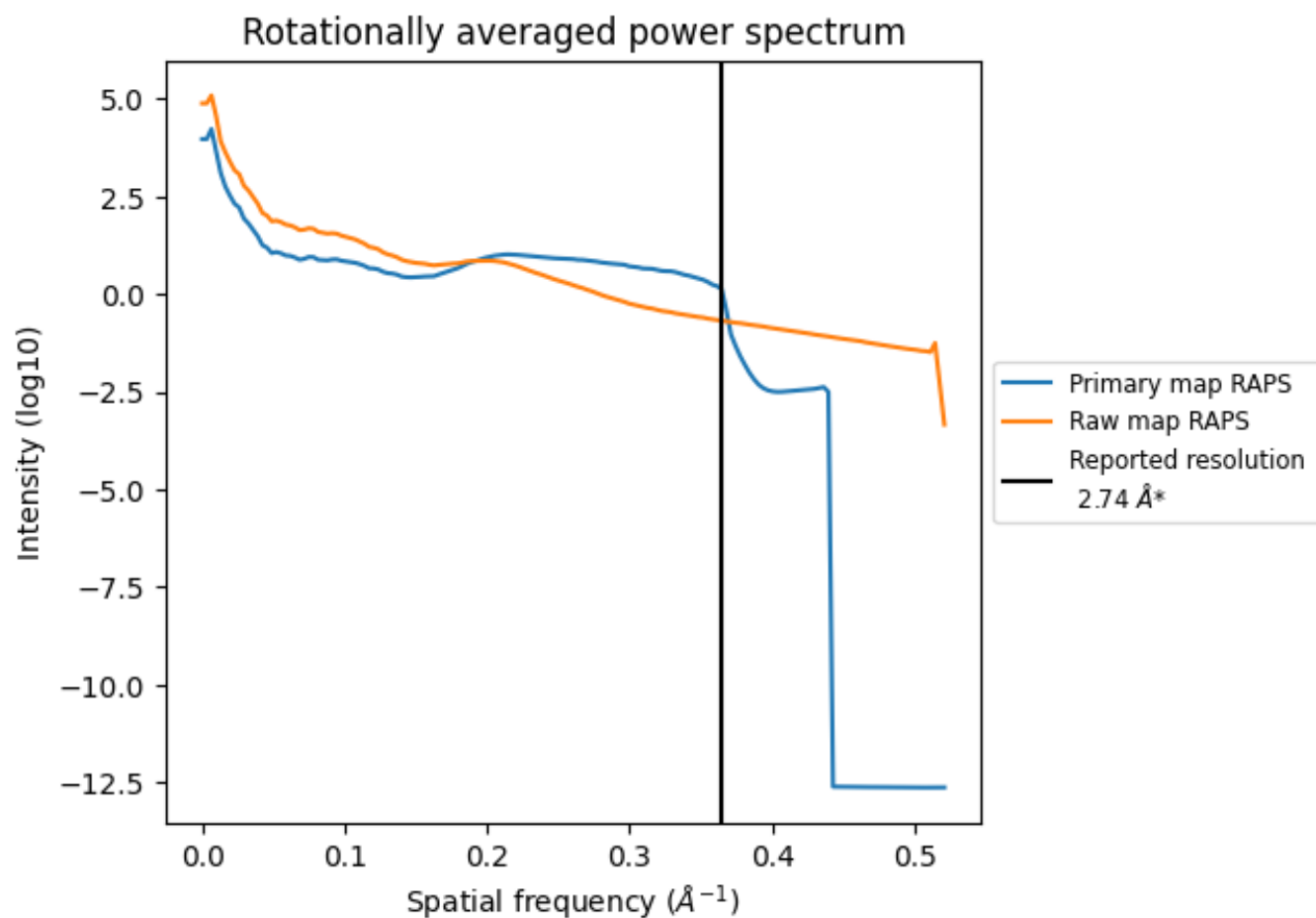
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 286 nm^3 ; this corresponds to an approximate mass of 259 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 ⓘ

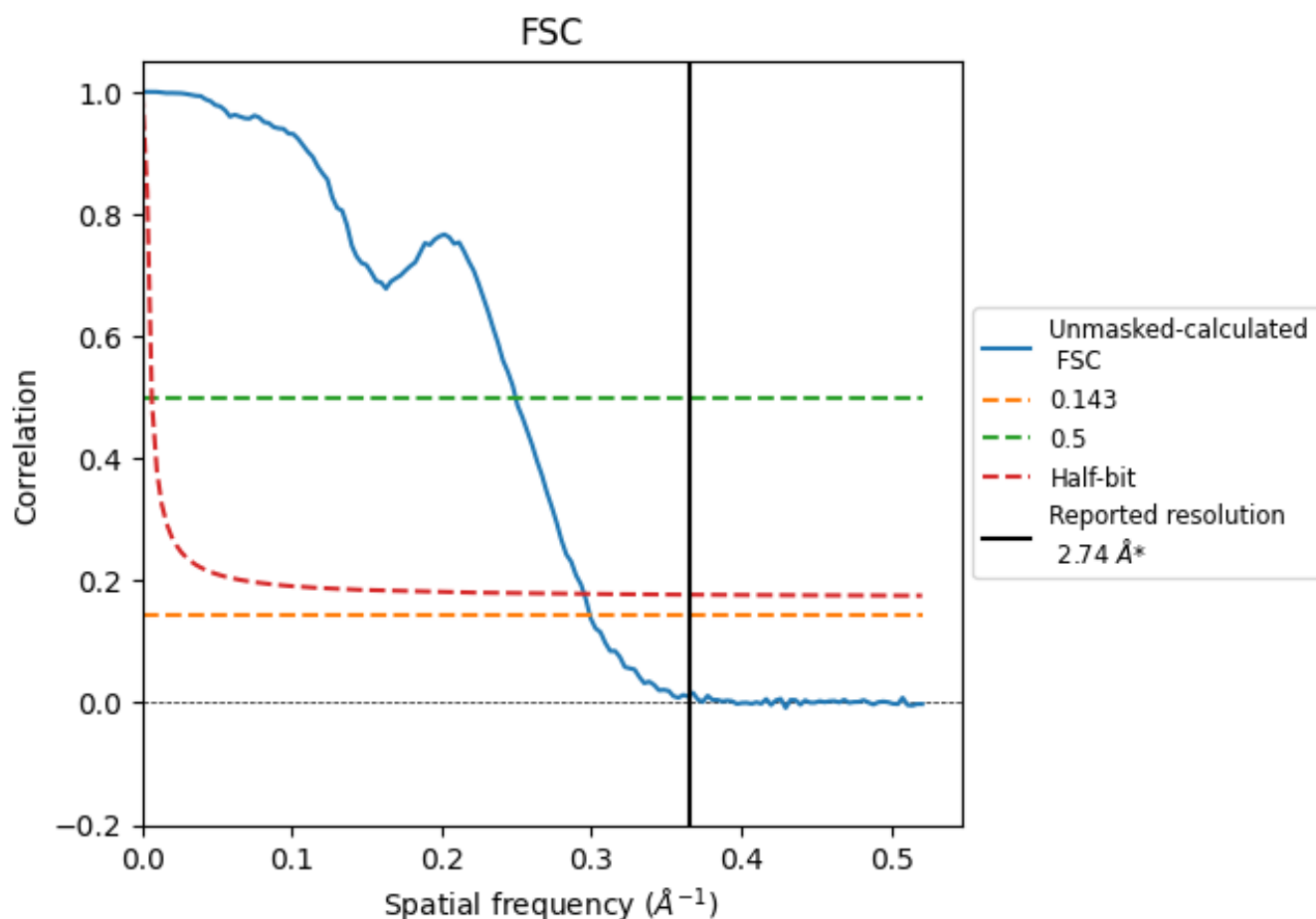


*Reported resolution corresponds to spatial frequency of $0.365 \text{ \AA}^{-1}$

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 0.365 Å⁻¹

8.2 Resolution estimates [i](#)

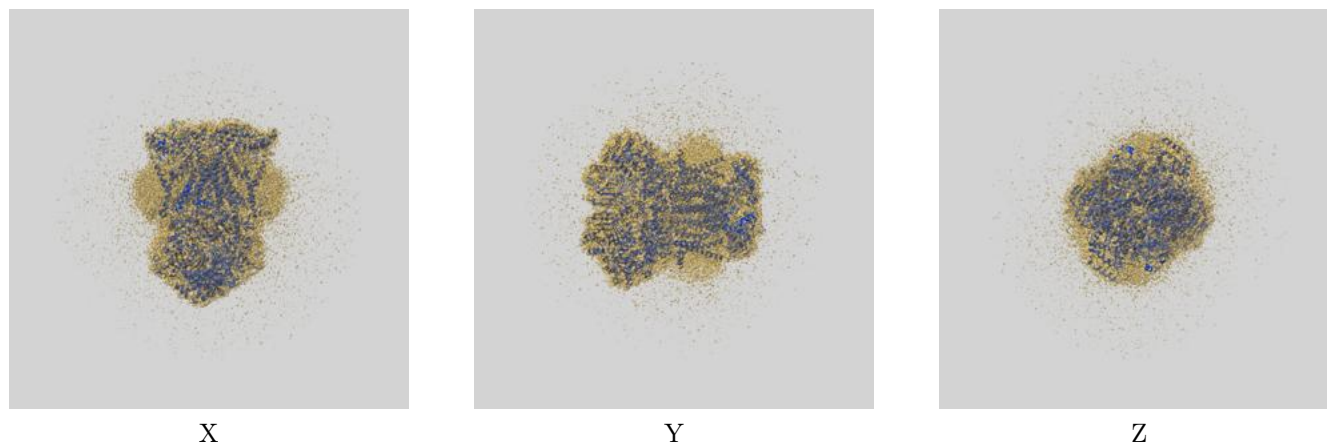
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.74	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.34	4.01	3.39

*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 3.34 differs from the reported value 2.74 by more than 10 %

9 Map-model fit [i](#)

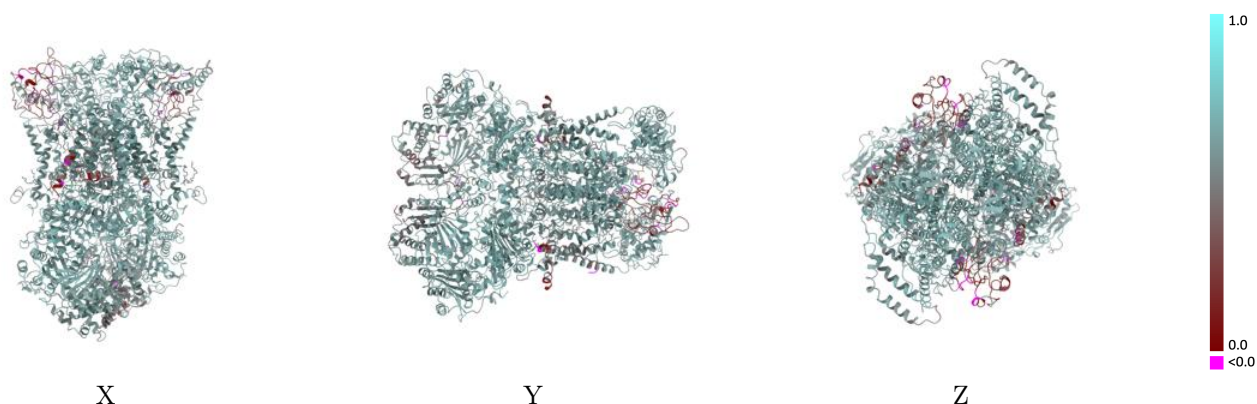
This section contains information regarding the fit between EMDB map EMD-60307 and PDB model 8ZOM. Per-residue inclusion information can be found in section [3](#) on page [12](#).

9.1 Map-model overlay [i](#)



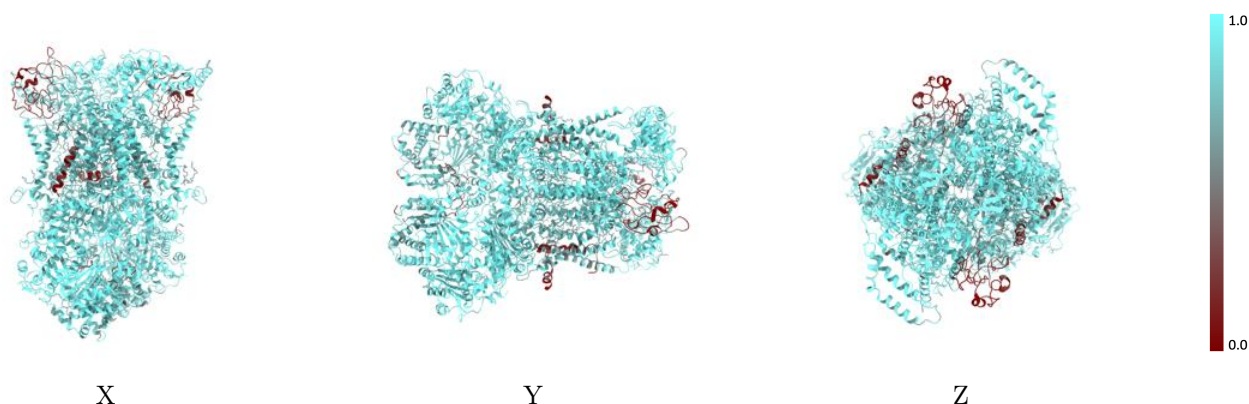
The images above show the 3D surface view of the map at the recommended contour level 0.586 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



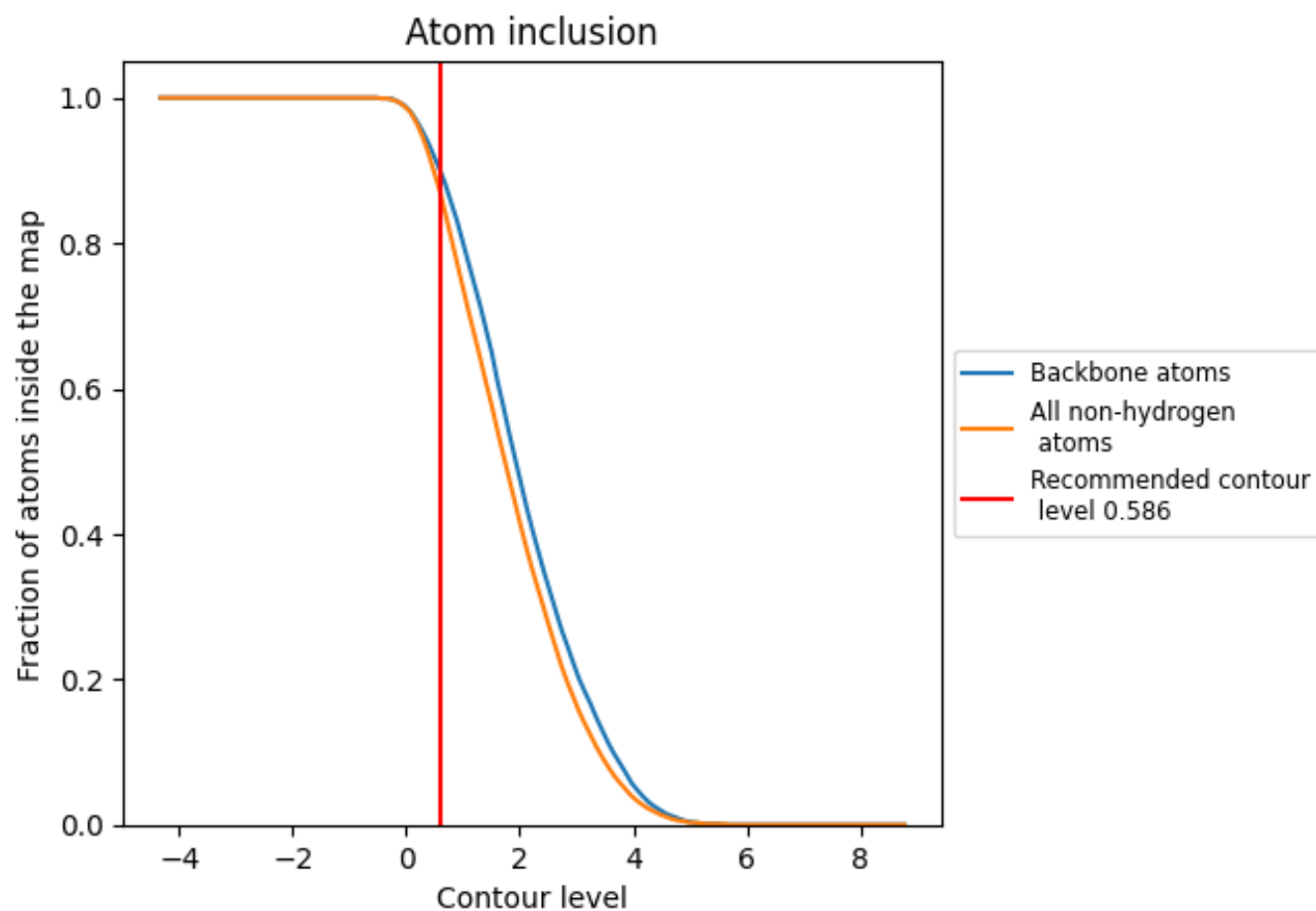
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.586).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 87% 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 (0.586) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8730	 0.5780
A	 0.8730	 0.5630
B	 0.9450	 0.6170
C	 0.9530	 0.6290
D	 0.9740	 0.6310
E	 0.4790	 0.3750
F	 0.9680	 0.6350
G	 0.8810	 0.5880
H	 0.8910	 0.5660
J	 0.7010	 0.5000
K	 0.2300	 0.2620
M	 0.8720	 0.5620
N	 0.9370	 0.6180
O	 0.9610	 0.6330
P	 0.9720	 0.6300
Q	 0.4830	 0.3740
R	 0.9380	 0.6270
S	 0.8850	 0.5890
T	 0.8830	 0.5650
V	 0.6900	 0.4890
W	 0.2150	 0.2390

