



# Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 07:24 am BST

PDB ID : 5NJ4  
Title : From macrocrystals to microcrystals: a strategy for membrane protein serial crystallography  
Authors : Dods, R.; Baath, P.; Branden, G.; Neutze, R.  
Deposited on : 2017-03-28  
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

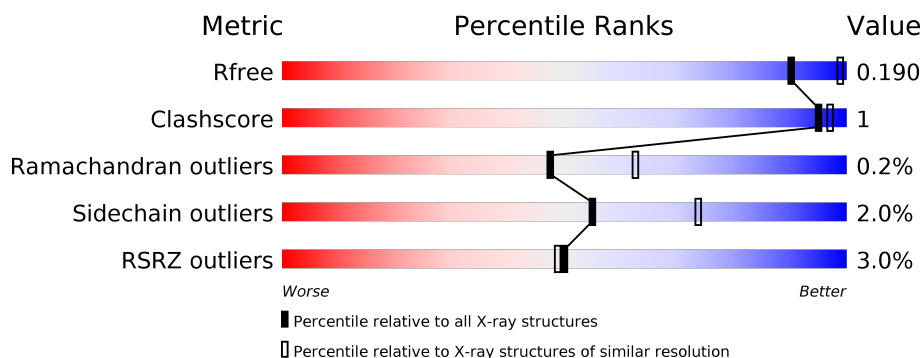
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C	336	<div> <div>2%</div> <div>96%</div> <div>••</div> </div>
2	H	258	<div> <div>5%</div> <div>97%</div> <div>••</div> </div>
3	L	273	<div> <div>3%</div> <div>98%</div> <div>•</div> </div>
4	M	323	<div> <div>2%</div> <div>96%</div> <div>•</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	DGA	C	405	-	-	-	X
8	LDA	M	415	-	-	-	X
8	LDA	M	416	-	-	-	X

## 2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 10402 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Photosynthetic reaction center cytochrome c subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	332	Total	C	N	O	S	0	0	0
			2602	1640	466	478	18			

- Molecule 2 is a protein called Reaction center protein H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	258	Total	C	N	O	S	0	0	0
			2018	1292	344	380	2			

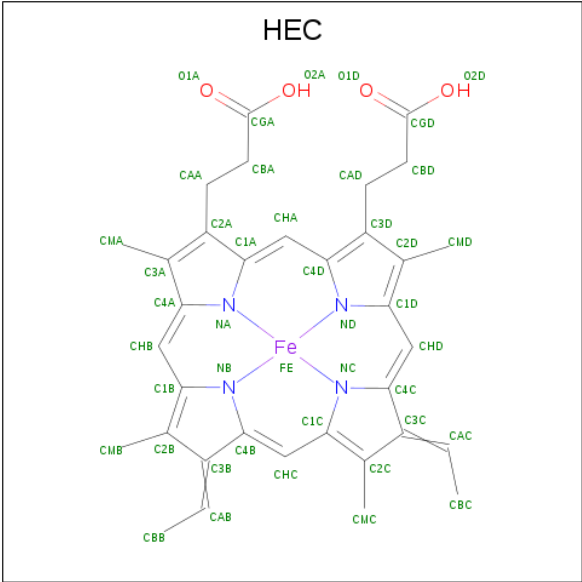
- Molecule 3 is a protein called Reaction center protein L chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	273	Total	C	N	O	S	0	1	0
			2172	1460	350	355	7			

- Molecule 4 is a protein called Reaction center protein M chain.

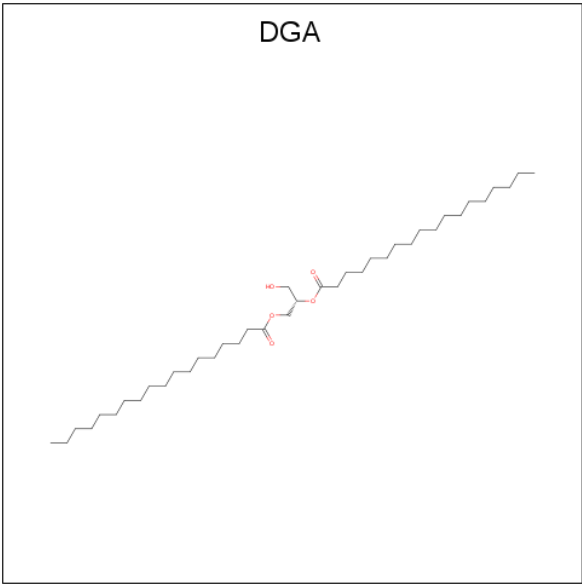
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	323	Total	C	N	O	S	0	0	0
			2555	1702	419	423	11			

- Molecule 5 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



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

- Molecule 6 is DIACYL GLYCEROL (three-letter code: DGA) (formula: C<sub>39</sub>H<sub>76</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			37	33	4		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



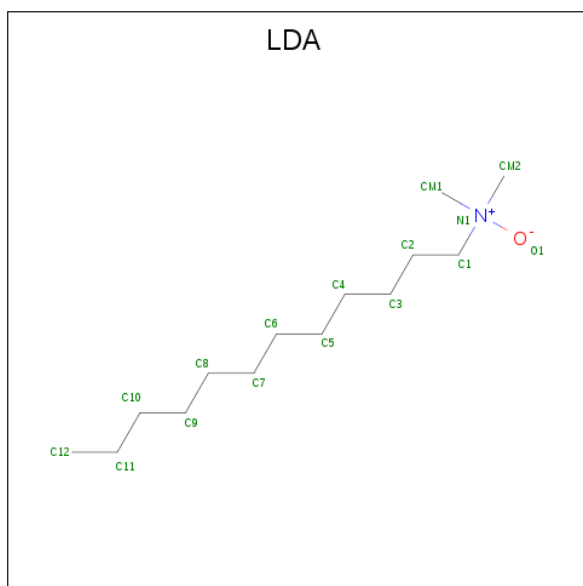
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	H	1	Total	O	S	0	0
			5	4	1		
7	H	1	Total	O	S	0	0
			5	4	1		
7	H	1	Total	O	S	0	0
			5	4	1		
7	H	1	Total	O	S	0	0
			5	4	1		
7	M	1	Total	O	S	0	0
			5	4	1		
7	M	1	Total	O	S	0	0
			5	4	1		
7	M	1	Total	O	S	0	0
			5	4	1		
7	M	1	Total	O	S	0	0
			5	4	1		

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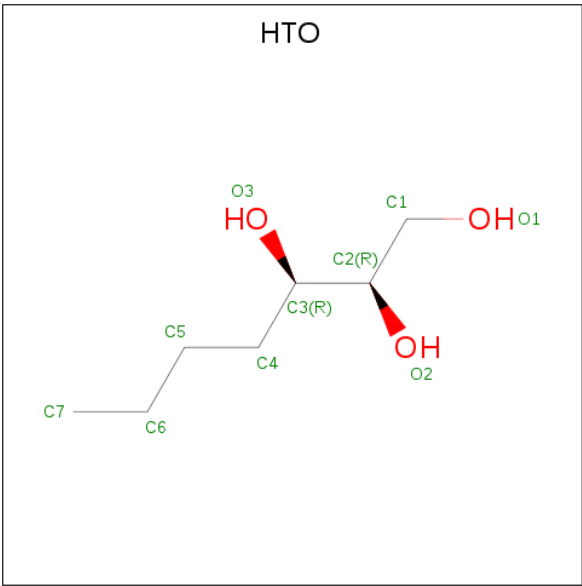
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	M	1	Total	O	S	0	0
			5	4	1		
7	M	1	Total	O	S	0	0
			5	4	1		
7	M	1	Total	O	S	0	0
			5	4	1		
7	M	1	Total	O	S	0	0
			5	4	1		

- Molecule 8 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula:  $C_{14}H_{31}NO$ ).



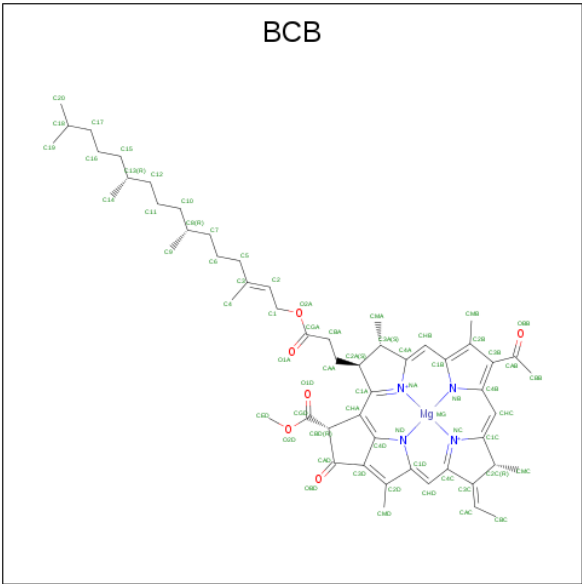
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	H	1	Total	C	N	O	0	0
			16	14	1	1		
8	H	1	Total	C	N	O	0	0
			16	14	1	1		
8	H	1	Total	C	N	O	0	0
			16	14	1	1		
8	L	1	Total	C	N	O	0	0
			16	14	1	1		
8	M	1	Total	C	N	O	0	0
			16	14	1	1		
8	M	1	Total	C	N	O	0	0
			16	14	1	1		
8	M	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 9 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: C<sub>7</sub>H<sub>16</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	H	1	Total	C	O	0	0
			10	7	3		
9	H	1	Total	C	O	0	0
			10	7	3		
9	L	1	Total	C	O	0	0
			10	7	3		

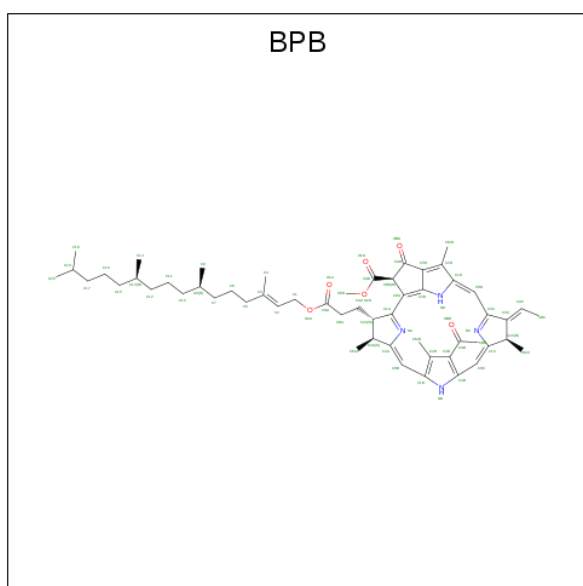
- Molecule 10 is BACTERIOCHLOROPHYLL B (three-letter code: BCB) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>6</sub>).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	L	1	Total	C	Mg	N	O	
			66	55	1	4	6	0
10	L	1	Total	C	Mg	N	O	
			66	55	1	4	6	0
10	M	1	Total	C	Mg	N	O	
			66	55	1	4	6	0
10	M	1	Total	C	Mg	N	O	
			66	55	1	4	6	0

- Molecule 11 is BACTERIOPHEOPHYTIN B (three-letter code: BPB) (formula:  $C_{55}H_{74}N_4O_6$ ).

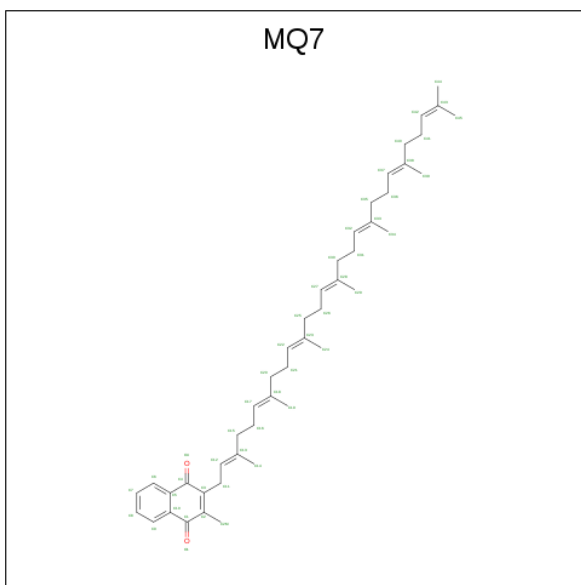


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	L	1	Total	C	N	O		
			65	55	4	6	0	0
11	M	1	Total	C	N	O		
			65	55	4	6	0	0

- Molecule 12 is FE (II) ION (three-letter code: FE2) (formula: Fe).

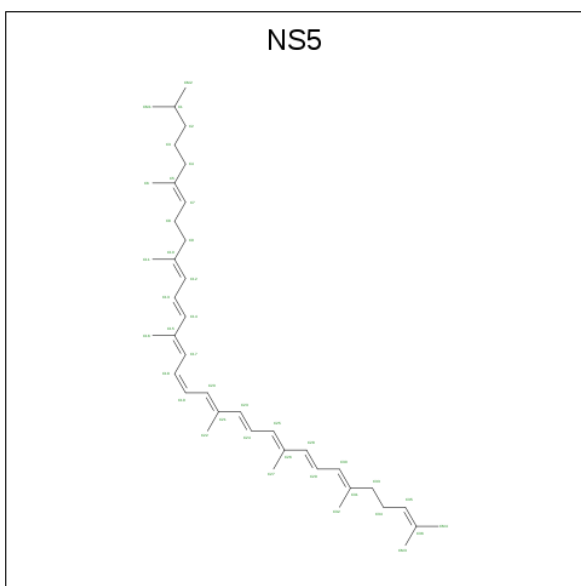
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	L	1	Total	Fe		
			1	1	0	0

- Molecule 13 is MENAQUINONE-7 (three-letter code: MQ7) (formula:  $C_{46}H_{64}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	M	1	Total	C	O	0	0
			48	46	2		

- Molecule 14 is 15-cis-1,2-dihydroneurosporene (three-letter code: NS5) (formula: C<sub>40</sub>H<sub>60</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	M	1	Total	C	0	0
			40	40		

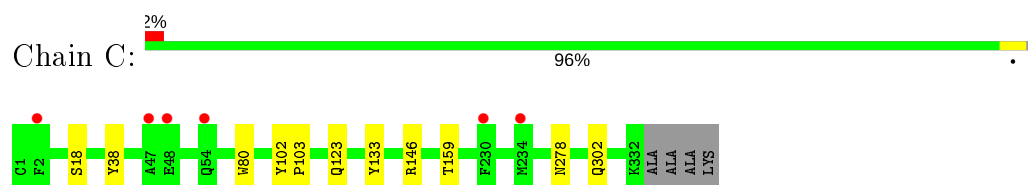
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	C	58	Total 58	O 58	0	0
15	H	23	Total 23	O 23	0	0
15	L	24	Total 24	O 24	0	0
15	M	41	Total 41	O 41	0	0

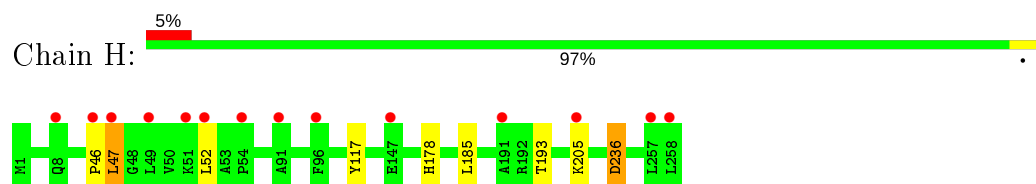
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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 electron 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 dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

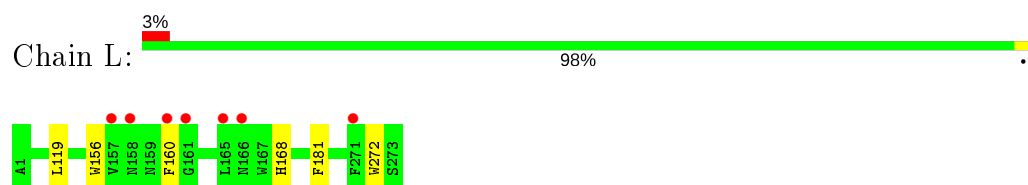
- Molecule 1: Photosynthetic reaction center cytochrome c subunit



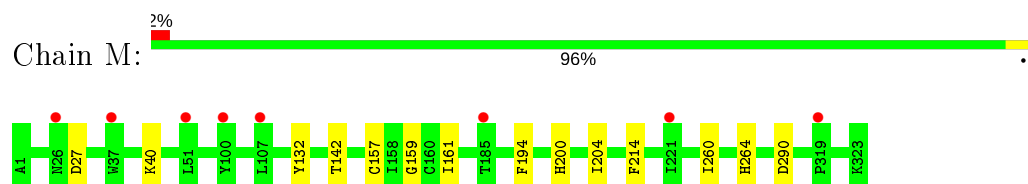
- Molecule 2: Reaction center protein H chain



- Molecule 3: Reaction center protein L chain



- Molecule 4: Reaction center protein M chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	226.50 Å   226.50 Å   113.90 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	35.70 – 2.40 35.55 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (35.70-2.40) 100.0 (35.55-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.55 (at 2.39 Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.161   ,   0.186 0.168   ,   0.190	Depositor DCC
$R_{free}$ test set	5711 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	73.2	Xtriage
Anisotropy	0.005	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 62.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	10402	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.81% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LDA, DGA, HTO, BCB, BPB, FE2, SO4, MQ7, HEC, FME, NS5

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	C	0.40	0/2669	0.66	0/3637
2	H	0.43	0/2055	0.66	0/2807
3	L	0.43	0/2267	0.60	0/3095
4	M	0.43	0/2659	0.59	0/3637
All	All	0.42	0/9650	0.62	0/13176

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2602	0	2578	6	0
2	H	2018	0	2020	1	0
3	L	2172	0	2097	4	0
4	M	2555	0	2452	5	0
5	C	172	0	120	3	0
6	C	37	0	58	0	0
7	C	15	0	0	0	0
7	H	20	0	0	0	0
7	M	40	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	48	0	93	0	0
8	L	16	0	31	0	0
8	M	48	0	93	0	0
9	H	20	0	32	0	0
9	L	10	0	16	0	0
10	L	132	0	144	4	0
10	M	132	0	144	1	0
11	L	65	0	74	1	0
11	M	65	0	74	3	0
12	L	1	0	0	0	0
13	M	48	0	64	0	0
14	M	40	0	60	1	0
15	C	58	0	0	1	0
15	H	23	0	0	0	0
15	L	24	0	0	0	0
15	M	41	0	0	0	0
All	All	10402	0	10150	24	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 1.

All (24) 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)
4:M:159:GLY:HA3	14:M:405:NS5:H272	1.73	0.70
11:L:303:BPB:HBBB	11:L:303:BPB:HMB	1.75	0.69
11:M:404:BPB:HBBB	11:M:404:BPB:HHC	1.78	0.66
10:M:402:BCB:HBB2	10:M:402:BCB:HHC	1.82	0.62
5:C:401:HEC:HBC3	5:C:401:HEC:HMC1	1.85	0.58
3:L:181:PHE:CD2	11:M:404:BPB:HBB	2.40	0.57
3:L:168:HIS:CE1	10:L:301:BCB:HMC2	2.42	0.53
3:L:181:PHE:HB3	11:M:404:BPB:CBB	2.40	0.51
5:C:403:HEC:HBC1	5:C:404:HEC:HMA1	1.93	0.51
5:C:402:HEC:HMC1	5:C:402:HEC:HBC3	1.93	0.51
1:C:278:ASN:HB3	1:C:302:GLN:HE21	1.76	0.50
10:L:302:BCB:HMB1	10:L:302:BCB:HBB2	1.96	0.48
1:C:80:TRP:CD1	1:C:133:TYR:HB2	2.52	0.45
4:M:200:HIS:CE1	4:M:204:ILE:HD11	2.53	0.44
1:C:102:TYR:CG	1:C:103:PRO:HD3	2.53	0.44
10:L:301:BCB:HBB3	10:L:301:BCB:HMB1	2.00	0.43
10:L:302:BCB:CBB	10:L:302:BCB:HMB1	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:260:ILE:O	4:M:264:HIS:ND1	2.52	0.43
4:M:132:TYR:CE1	4:M:142:THR:HG21	2.54	0.42
1:C:102:TYR:CD2	1:C:103:PRO:HD3	2.55	0.42
4:M:157:CYS:HA	4:M:161:ILE:HB	2.01	0.42
1:C:302:GLN:NE2	15:C:502:HOH:O	2.47	0.41
1:C:18:SER:HB2	3:L:156:TRP:CD1	2.56	0.41
2:H:117:TYR:HB2	2:H:236:ASP:HB3	2.04	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 X-ray entries followed by that with respect to entries of similar resolution.

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	C	330/336 (98%)	324 (98%)	6 (2%)	0	100	100
2	H	256/258 (99%)	249 (97%)	5 (2%)	2 (1%)	19	29
3	L	272/273 (100%)	265 (97%)	7 (3%)	0	100	100
4	M	321/323 (99%)	311 (97%)	10 (3%)	0	100	100
All	All	1179/1190 (99%)	1149 (98%)	28 (2%)	2 (0%)	47	62

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	46	PRO
2	H	47	LEU

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.



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	C	281/282 (100%)	277 (99%)	4 (1%)	67	82
2	H	212/212 (100%)	205 (97%)	7 (3%)	38	57
3	L	219/218 (100%)	216 (99%)	3 (1%)	67	82
4	M	249/249 (100%)	244 (98%)	5 (2%)	55	74
All	All	961/961 (100%)	942 (98%)	19 (2%)	55	74

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	38	TYR
1	C	123	GLN
1	C	146	ARG
1	C	159	THR
2	H	47	LEU
2	H	52	LEU
2	H	178	HIS
2	H	185	LEU
2	H	193	THR
2	H	205	LYS
2	H	236	ASP
3	L	119	LEU
3	L	160	PHE
3	L	272	TRP
4	M	27	ASP
4	M	40	LYS
4	M	194	PHE
4	M	214	PHE
4	M	290	ASP

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

Mol	Chain	Res	Type
1	C	123	GLN
1	C	302	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	FME	H	1	2	8,9,10	0.79	0	7,9,11	3.41	3 (42%)

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
2	FME	H	1	2	-	3/7/9/11	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1	FME	CA-N-CN	-7.77	110.88	122.82
2	H	1	FME	CE-SD-CG	3.06	110.90	100.40
2	H	1	FME	O1-CN-N	-2.22	119.42	125.27

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	1	FME	O1-CN-N-CA
2	H	1	FME	C-CA-CB-CG
2	H	1	FME	CB-CA-N-CN

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 39 ligands modelled in this entry, 1 is monoatomic - leaving 38 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	$\# Z  > 2$
9	HTO	H	709	-	9,9,9	0.41	0	10,10,10	0.58	0
7	SO4	M	412	-	4,4,4	0.35	0	6,6,6	0.19	0
8	LDA	M	416	-	12,15,15	2.01	1 (8%)	14,17,17	0.38	0
6	DGA	C	405	1	36,36,43	1.22	2 (5%)	38,38,45	1.17	4 (10%)
5	HEC	C	403	1	26,50,50	1.66	3 (11%)	18,82,82	1.68	4 (22%)
7	SO4	M	410	-	4,4,4	0.32	0	6,6,6	0.18	0
8	LDA	H	706	-	12,15,15	2.04	1 (8%)	14,17,17	0.76	1 (7%)
5	HEC	C	402	1	26,50,50	1.56	2 (7%)	18,82,82	2.00	6 (33%)
7	SO4	M	407	-	4,4,4	0.28	0	6,6,6	0.06	0
9	HTO	L	305	-	9,9,9	0.51	0	10,10,10	0.76	0
7	SO4	M	409	-	4,4,4	0.39	0	6,6,6	0.18	0
7	SO4	C	408	-	4,4,4	0.33	0	6,6,6	0.14	0
13	MQ7	M	401	-	49,49,49	1.59	2 (4%)	60,63,63	1.13	6 (10%)
5	HEC	C	401	1	26,50,50	1.74	2 (7%)	18,82,82	2.25	4 (22%)
8	LDA	H	707	-	12,15,15	2.06	1 (8%)	14,17,17	0.82	0
7	SO4	M	408	-	4,4,4	0.22	0	6,6,6	0.49	0
7	SO4	M	413	-	4,4,4	0.34	0	6,6,6	0.07	0
8	LDA	M	414	-	12,15,15	2.11	1 (8%)	14,17,17	0.48	0
8	LDA	M	415	-	12,15,15	2.08	1 (8%)	14,17,17	0.34	0
7	SO4	C	407	-	4,4,4	0.34	0	6,6,6	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	NS5	M	405	-	39,39,39	1.44	1 (2%)	44,46,46	1.89	11 (25%)
10	BCB	L	301	-	60,74,74	2.94	20 (33%)	48,115,115	2.25	16 (33%)
7	SO4	C	406	-	4,4,4	0.37	0	6,6,6	0.31	0
7	SO4	M	411	-	4,4,4	0.36	0	6,6,6	0.17	0
10	BCB	M	402	-	60,74,74	2.93	23 (38%)	48,115,115	1.94	11 (22%)
9	HTO	H	708	-	9,9,9	0.53	0	10,10,10	0.55	0
8	LDA	H	701	-	12,15,15	1.90	1 (8%)	14,17,17	0.54	0
8	LDA	L	304	-	12,15,15	2.09	1 (8%)	14,17,17	0.50	0
10	BCB	M	403	-	60,74,74	2.89	21 (35%)	48,115,115	2.20	13 (27%)
7	SO4	H	703	-	4,4,4	0.34	0	6,6,6	0.08	0
7	SO4	H	704	-	4,4,4	0.28	0	6,6,6	0.17	0
7	SO4	H	702	-	4,4,4	0.32	0	6,6,6	0.27	0
7	SO4	H	705	-	4,4,4	0.34	0	6,6,6	0.17	0
10	BCB	L	302	-	60,74,74	2.88	24 (40%)	48,115,115	2.10	14 (29%)
11	BPB	M	404	-	64,70,70	2.16	17 (26%)	64,101,101	1.72	13 (20%)
5	HEC	C	404	1	26,50,50	1.52	3 (11%)	18,82,82	1.88	6 (33%)
11	BPB	L	303	-	64,70,70	2.03	13 (20%)	64,101,101	1.75	12 (18%)
7	SO4	M	406	-	4,4,4	0.22	0	6,6,6	0.26	0

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
9	HTO	H	709	-	-	0/10/10/10	-
8	LDA	M	416	-	-	6/13/13/13	-
6	DGA	C	405	1	-	15/37/37/45	-
5	HEC	C	403	1	-	0/6/54/54	-
8	LDA	H	706	-	-	6/13/13/13	-
5	HEC	C	402	1	-	1/6/54/54	-
9	HTO	L	305	-	-	4/10/10/10	-
8	LDA	M	414	-	-	4/13/13/13	-
13	MQ7	M	401	-	-	0/41/61/61	0/2/2/2
5	HEC	C	401	1	-	0/6/54/54	-
8	LDA	H	707	-	-	7/13/13/13	-
8	LDA	M	415	-	-	3/13/13/13	-
14	NS5	M	405	-	-	8/43/43/43	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	BCB	L	301	-	-	9/41/177/177	-
10	BCB	M	402	-	-	10/41/177/177	-
9	HTO	H	708	-	-	4/10/10/10	-
8	LDA	H	701	-	-	2/13/13/13	-
8	LDA	L	304	-	-	7/13/13/13	-
10	BCB	M	403	-	-	13/41/177/177	-
10	BCB	L	302	-	-	9/41/177/177	-
11	BPB	M	404	-	-	6/47/105/105	0/5/6/6
5	HEC	C	404	1	-	0/6/54/54	-
11	BPB	L	303	-	-	6/47/105/105	0/5/6/6

All (140) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	402	BCB	CHB-C4A	-8.57	1.33	1.52
13	M	401	MQ7	C3-C2	8.41	1.50	1.35
10	L	301	BCB	C1D-ND	-8.34	1.32	1.50
10	L	302	BCB	CHB-C4A	-8.28	1.34	1.52
10	M	403	BCB	C1D-ND	-8.19	1.33	1.50
10	M	402	BCB	C1D-ND	-8.17	1.33	1.50
10	L	301	BCB	CHB-C4A	-8.15	1.34	1.52
10	M	403	BCB	CHB-C4A	-8.15	1.34	1.52
10	L	302	BCB	C1D-ND	-7.99	1.33	1.50
10	L	301	BCB	C1B-NB	-7.39	1.34	1.50
14	M	405	NS5	C35-C36	7.36	1.53	1.32
8	M	414	LDA	O1-N1	-7.21	1.25	1.42
10	L	302	BCB	C1B-NB	-7.19	1.35	1.50
10	M	402	BCB	C1B-NB	-7.17	1.35	1.50
8	L	304	LDA	O1-N1	-7.14	1.25	1.42
8	H	707	LDA	O1-N1	-7.11	1.25	1.42
8	M	415	LDA	O1-N1	-7.08	1.25	1.42
8	H	706	LDA	O1-N1	-7.01	1.25	1.42
10	M	403	BCB	C1B-NB	-7.01	1.35	1.50
10	M	403	BCB	C4B-NB	-7.01	1.35	1.50
11	M	404	BPB	CAC-C3C	6.94	1.52	1.33
8	M	416	LDA	O1-N1	-6.82	1.26	1.42
10	M	402	BCB	C4B-NB	-6.82	1.35	1.50
11	L	303	BPB	CAC-C3C	6.55	1.51	1.33
10	L	301	BCB	C4D-ND	-6.53	1.36	1.50
10	L	302	BCB	C4B-NB	-6.51	1.36	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	701	LDA	O1-N1	-6.50	1.26	1.42
10	L	302	BCB	C4D-ND	-6.41	1.36	1.50
10	L	301	BCB	C4B-NB	-6.24	1.37	1.50
10	M	402	BCB	C4D-ND	-6.22	1.37	1.50
10	M	403	BCB	C4D-ND	-6.15	1.37	1.50
13	M	401	MQ7	C10-C5	5.75	1.50	1.40
5	C	401	HEC	C3B-C2B	-5.67	1.34	1.40
11	M	404	BPB	C3B-C4B	5.55	1.48	1.41
10	L	301	BCB	CHD-C1D	-5.49	1.45	1.53
11	L	303	BPB	C3B-C4B	5.40	1.48	1.41
5	C	404	HEC	C3B-C2B	-5.38	1.35	1.40
5	C	403	HEC	C3B-C2B	-5.30	1.35	1.40
10	L	302	BCB	CHD-C1D	-5.29	1.45	1.53
10	M	403	BCB	CHD-C1D	-5.25	1.45	1.53
10	M	402	BCB	CHD-C1D	-5.20	1.45	1.53
10	M	403	BCB	CHD-C4C	-5.17	1.44	1.53
11	M	404	BPB	C1A-NA	-5.04	1.27	1.36
11	L	303	BPB	C1A-NA	-5.02	1.27	1.36
10	M	402	BCB	CHD-C4C	-4.98	1.44	1.53
10	L	301	BCB	OBD-CAD	4.95	1.29	1.21
10	L	301	BCB	O2D-CGD	4.95	1.45	1.33
10	L	301	BCB	CHD-C4C	-4.93	1.44	1.53
5	C	402	HEC	C3B-C2B	-4.91	1.35	1.40
11	M	404	BPB	CHD-C1D	4.87	1.48	1.38
6	C	405	DGA	OG2-CB1	4.72	1.47	1.34
5	C	401	HEC	C3C-C2C	-4.66	1.35	1.40
11	L	303	BPB	O2D-CGD	4.65	1.44	1.33
11	M	404	BPB	O2A-CGA	4.61	1.46	1.33
6	C	405	DGA	OG1-CA1	4.60	1.46	1.33
10	L	301	BCB	CHB-C1B	-4.56	1.46	1.53
11	L	303	BPB	C3B-C2B	4.53	1.47	1.39
10	M	402	BCB	O2D-CGD	4.48	1.44	1.33
10	L	302	BCB	CHD-C4C	-4.48	1.45	1.53
10	M	403	BCB	CHB-C1B	-4.46	1.46	1.53
10	M	402	BCB	CHB-C1B	-4.46	1.46	1.53
11	M	404	BPB	C4C-NC	-4.43	1.26	1.36
11	M	404	BPB	O2D-CGD	4.42	1.44	1.33
10	M	403	BCB	O2D-CGD	4.39	1.43	1.33
10	L	302	BCB	C2D-C1D	-4.39	1.45	1.53
10	L	302	BCB	O2D-CGD	4.30	1.43	1.33
10	L	301	BCB	C2D-C1D	-4.20	1.45	1.53
5	C	403	HEC	C3C-C2C	-4.15	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	402	BCB	O2A-CGA	4.13	1.45	1.33
11	M	404	BPB	C3B-C2B	4.13	1.46	1.39
10	M	403	BCB	OBD-CAD	4.12	1.28	1.21
10	L	302	BCB	O2A-CGA	4.00	1.45	1.33
10	M	402	BCB	OBD-CAD	3.95	1.28	1.21
11	L	303	BPB	C4C-NC	-3.93	1.27	1.36
10	M	403	BCB	O2A-CGA	3.91	1.44	1.33
10	L	302	BCB	CHB-C1B	-3.84	1.47	1.53
10	L	302	BCB	OBD-CAD	3.80	1.27	1.21
10	M	403	BCB	C2D-C1D	-3.74	1.46	1.53
11	L	303	BPB	O2A-CGA	3.73	1.44	1.33
10	L	301	BCB	O2A-CGA	3.72	1.44	1.33
11	L	303	BPB	CHD-C1D	3.68	1.45	1.38
11	M	404	BPB	C3D-C2D	3.52	1.48	1.39
10	M	403	BCB	C1A-CHA	-3.50	1.48	1.54
5	C	402	HEC	C3C-C2C	-3.49	1.37	1.40
10	L	302	BCB	C1A-CHA	-3.47	1.48	1.54
10	M	403	BCB	CBD-CAD	-3.40	1.48	1.53
10	M	402	BCB	C2D-C1D	-3.39	1.47	1.53
10	L	302	BCB	CHC-C4B	-3.39	1.48	1.53
11	L	303	BPB	OBD-CAD	3.34	1.28	1.22
10	M	402	BCB	C1A-CHA	-3.32	1.48	1.54
10	L	301	BCB	C4A-C3A	-3.22	1.49	1.53
10	M	402	BCB	C3B-C2B	-3.21	1.46	1.55
10	L	301	BCB	C3D-C2D	-3.20	1.46	1.55
11	M	404	BPB	OBD-CAD	3.20	1.28	1.22
11	L	303	BPB	C3D-C2D	3.19	1.47	1.39
11	M	404	BPB	C1C-NC	-3.10	1.32	1.38
10	M	402	BCB	C2B-C1B	-3.05	1.47	1.53
10	M	403	BCB	C2B-C1B	-3.00	1.47	1.53
5	C	404	HEC	C3C-C2C	-2.99	1.37	1.40
10	L	302	BCB	C3D-C2D	-2.98	1.47	1.55
10	M	402	BCB	C3D-C2D	-2.97	1.47	1.55
10	L	302	BCB	C3B-C2B	-2.89	1.47	1.55
10	M	403	BCB	C3D-C2D	-2.84	1.47	1.55
10	L	301	BCB	C1A-CHA	-2.83	1.49	1.54
10	L	301	BCB	C2B-C1B	-2.81	1.48	1.53
11	M	404	BPB	CHD-C4C	2.80	1.47	1.40
11	L	303	BPB	C1C-NC	-2.77	1.33	1.38
10	L	301	BCB	C3B-C2B	-2.72	1.48	1.55
10	M	403	BCB	CHC-C4B	-2.68	1.49	1.53
10	L	302	BCB	CBD-CAD	-2.64	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	402	BCB	CBD-CAD	-2.63	1.49	1.53
10	M	402	BCB	CHC-C1C	-2.61	1.46	1.52
10	M	402	BCB	CHC-C4B	-2.61	1.49	1.53
10	L	301	BCB	CBD-CAD	-2.61	1.49	1.53
10	M	403	BCB	CHC-C1C	-2.58	1.46	1.52
10	L	301	BCB	CHC-C4B	-2.51	1.49	1.53
10	M	402	BCB	C4A-C3A	-2.49	1.50	1.53
10	M	402	BCB	C3B-CAB	-2.48	1.49	1.52
10	L	302	BCB	C2B-C1B	-2.46	1.48	1.53
10	M	403	BCB	C4A-C3A	-2.45	1.50	1.53
11	L	303	BPB	C1D-ND	-2.44	1.33	1.38
10	M	403	BCB	C3B-C2B	-2.43	1.48	1.55
5	C	403	HEC	C3C-C4C	2.41	1.47	1.43
10	L	302	BCB	C4A-C3A	-2.40	1.50	1.53
11	L	303	BPB	CHD-C4C	2.39	1.46	1.40
10	L	302	BCB	C3D-CAD	-2.39	1.46	1.51
11	M	404	BPB	C1D-ND	-2.35	1.33	1.38
10	L	302	BCB	CHC-C1C	-2.33	1.47	1.52
11	M	404	BPB	C4B-CHC	2.23	1.49	1.41
11	M	404	BPB	C1B-CHB	2.22	1.49	1.41
11	M	404	BPB	C4C-C3C	2.21	1.50	1.45
10	M	402	BCB	CBD-CGD	-2.20	1.48	1.52
11	M	404	BPB	C4A-NA	-2.19	1.32	1.37
10	M	403	BCB	CHA-CBD	-2.17	1.46	1.53
10	L	302	BCB	CBD-CGD	-2.14	1.48	1.52
10	M	402	BCB	C3D-CAD	-2.10	1.47	1.51
10	L	302	BCB	C3B-CAB	-2.09	1.49	1.52
10	L	301	BCB	CHC-C1C	-2.05	1.48	1.52
5	C	404	HEC	C3C-C4C	2.04	1.46	1.43
10	L	302	BCB	CHA-CBD	-2.03	1.47	1.53

All (121) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	L	301	BCB	CMB-C2B-C3B	7.59	133.15	114.29
10	M	403	BCB	CMB-C2B-C3B	7.51	132.95	114.29
10	L	302	BCB	CMB-C2B-C3B	7.03	131.76	114.29
5	C	401	HEC	CBA-CAA-C2A	-6.46	100.58	112.48
10	M	402	BCB	CMB-C2B-C3B	6.44	130.28	114.29
11	M	404	BPB	CMD-C2D-C1D	6.02	134.33	125.06
11	L	303	BPB	CMD-C2D-C1D	5.57	133.64	125.06
10	L	302	BCB	OBD-CAD-C3D	-5.48	117.08	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	L	303	BPB	CBC-CAC-C3C	-5.43	110.85	126.72
10	L	302	BCB	C3B-C4B-NB	5.07	113.00	103.75
10	M	403	BCB	CHA-CBD-CGD	-5.01	103.68	115.02
5	C	402	HEC	CBA-CAA-C2A	-5.01	103.24	112.48
11	M	404	BPB	O2D-CGD-CBD	4.91	119.99	111.27
10	M	402	BCB	C1D-CHD-C4C	4.88	122.78	112.37
10	M	402	BCB	OBD-CAD-C3D	-4.79	118.30	126.73
10	M	403	BCB	C3B-C4B-NB	4.79	112.48	103.75
10	L	301	BCB	C3B-C4B-NB	4.77	112.45	103.75
6	C	405	DGA	OG2-CB1-CB2	4.57	121.35	111.50
11	M	404	BPB	CBC-CAC-C3C	-4.53	113.47	126.72
14	M	405	NS5	C34-C35-C36	-4.52	112.31	127.75
10	L	301	BCB	CHA-CBD-CGD	-4.47	104.90	115.02
10	M	402	BCB	C3B-C4B-NB	4.44	111.84	103.75
10	L	302	BCB	C1D-CHD-C4C	4.41	121.77	112.37
5	C	401	HEC	CBD-CAD-C3D	-4.32	104.52	112.49
11	L	303	BPB	O2D-CGD-CBD	4.28	118.88	111.27
10	L	301	BCB	C1D-CHD-C4C	4.24	121.41	112.37
10	L	301	BCB	OBD-CAD-C3D	-4.22	119.31	126.73
10	M	403	BCB	C1D-CHD-C4C	4.21	121.35	112.37
14	M	405	NS5	CM4-C36-C35	-4.08	110.85	122.65
14	M	405	NS5	CM3-C36-C35	-4.06	110.92	122.65
11	M	404	BPB	CMD-C2D-C3D	-3.92	118.61	127.61
5	C	404	HEC	CMC-C2C-C1C	-3.90	122.48	128.46
14	M	405	NS5	C19-C20-C21	-3.83	121.85	127.31
10	L	301	BCB	CBB-CAB-C3B	3.68	120.55	116.80
10	M	403	BCB	O2D-CGD-CBD	3.66	119.70	111.11
10	M	403	BCB	O2D-CGD-O1D	-3.61	116.78	123.84
10	L	301	BCB	C4-C3-C5	3.55	121.25	115.27
10	M	403	BCB	CBB-CAB-C3B	3.51	120.38	116.80
5	C	403	HEC	CBA-CAA-C2A	-3.49	106.04	112.48
11	L	303	BPB	CMD-C2D-C3D	-3.46	119.67	127.61
10	L	302	BCB	O2D-CGD-CBD	3.42	119.15	111.11
11	L	303	BPB	CHD-C4C-C3C	-3.41	119.67	125.11
5	C	402	HEC	CMC-C2C-C1C	-3.37	123.29	128.46
14	M	405	NS5	C18-C19-C20	3.29	130.22	123.47
5	C	404	HEC	CAD-CBD-CGD	-3.26	107.20	112.67
14	M	405	NS5	C14-C15-C17	-3.26	113.94	118.94
11	L	303	BPB	OBD-CAD-C3D	-3.19	120.85	128.52
11	M	404	BPB	OBD-CAD-C3D	-3.16	120.92	128.52
10	M	402	BCB	O2D-CGD-CBD	3.13	118.47	111.11
14	M	405	NS5	C18-C17-C15	-3.13	122.84	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	L	302	BCB	CED-O2D-CGD	3.11	122.96	115.94
11	L	303	BPB	C3C-C4C-NC	3.08	114.50	109.58
10	M	403	BCB	OBD-CAD-C3D	-3.05	121.36	126.73
5	C	402	HEC	CMB-C2B-C1B	-3.01	123.83	128.46
10	M	403	BCB	CED-O2D-CGD	2.96	122.62	115.94
11	L	303	BPB	CAD-C3D-C2D	2.95	155.06	140.80
10	M	402	BCB	C4A-C3A-C2A	-2.92	99.40	103.86
10	L	301	BCB	CED-O2D-CGD	2.92	122.53	115.94
10	M	403	BCB	CMD-C2D-C3D	2.91	121.52	114.29
10	L	302	BCB	O1D-CGD-CBD	-2.85	118.90	124.54
6	C	405	DGA	OG1-CA1-CA2	2.84	120.82	111.91
11	M	404	BPB	CAD-C3D-C2D	2.84	154.50	140.80
11	M	404	BPB	CED-O2D-CGD	2.82	122.31	115.94
10	L	302	BCB	CMD-C2D-C3D	2.82	121.28	114.29
10	L	301	BCB	O2D-CGD-CBD	2.70	117.46	111.11
10	L	301	BCB	C5-C3-C2	-2.70	115.66	121.12
11	L	303	BPB	CMB-C2B-C3B	2.68	129.70	124.68
10	L	301	BCB	O2A-CGA-CBA	2.68	120.32	111.91
5	C	404	HEC	CMC-C2C-C3C	2.67	128.96	125.82
14	M	405	NS5	C16-C15-C14	2.66	122.26	118.08
5	C	403	HEC	CMC-C2C-C1C	-2.64	124.41	128.46
5	C	404	HEC	CMB-C2B-C1B	-2.61	124.45	128.46
14	M	405	NS5	C6-C5-C7	-2.61	116.99	123.68
10	L	302	BCB	CBA-CAA-C2A	-2.60	112.19	115.72
5	C	403	HEC	C1D-C2D-C3D	2.58	108.79	107.00
11	M	404	BPB	OBB-CAB-C3B	2.56	124.53	119.99
13	M	401	MQ7	C12-C11-C3	-2.51	105.27	112.05
10	L	301	BCB	O2D-CGD-O1D	-2.50	118.95	123.84
10	L	301	BCB	O2A-CGA-O1A	-2.48	117.32	123.59
6	C	405	DGA	OG2-CG2-CG1	2.47	111.85	106.13
10	M	402	BCB	CMD-C2D-C3D	2.47	120.42	114.29
5	C	402	HEC	CMD-C2D-C1D	-2.45	124.70	128.46
14	M	405	NS5	C11-C10-C9	2.44	119.37	115.27
10	L	301	BCB	CHC-C4B-C3B	2.42	124.11	118.17
13	M	401	MQ7	C39-C38-C40	2.42	119.34	115.27
10	L	301	BCB	CMD-C2D-C3D	2.41	120.28	114.29
11	L	303	BPB	CHB-C4A-NA	2.41	128.07	125.20
13	M	401	MQ7	C26-C27-C28	-2.40	121.89	127.66
11	M	404	BPB	O1D-CGD-CBD	-2.39	119.60	124.48
10	M	403	BCB	CHC-C4B-C3B	2.33	123.89	118.17
10	M	402	BCB	C4-C3-C5	2.32	119.17	115.27
14	M	405	NS5	C8-C9-C10	-2.32	105.36	112.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	L	303	BPB	O1D-CGD-CBD	-2.31	119.75	124.48
10	L	302	BCB	C4A-C3A-C2A	-2.30	100.35	103.86
10	L	302	BCB	C6-C5-C3	-2.29	107.44	113.45
11	M	404	BPB	C1-O2A-CGA	2.28	122.41	116.44
6	C	405	DGA	OG1-CA1-OA1	-2.25	117.90	123.59
5	C	402	HEC	CMC-C2C-C3C	2.25	128.46	125.82
13	M	401	MQ7	C2M-C2-C3	-2.25	120.74	124.40
10	M	402	BCB	CHC-C4B-C3B	2.23	123.64	118.17
5	C	404	HEC	CBA-CAA-C2A	-2.21	108.42	112.48
11	L	303	BPB	CED-O2D-CGD	2.20	120.92	115.94
11	M	404	BPB	C4B-CHC-C1C	2.20	131.41	128.57
10	L	301	BCB	C4A-C3A-C2A	-2.18	100.52	103.86
10	L	302	BCB	CBB-CAB-C3B	2.18	119.02	116.80
5	C	401	HEC	C4B-C3B-C2B	2.17	108.70	106.35
5	C	404	HEC	CMB-C2B-C3B	2.14	128.34	125.82
11	M	404	BPB	CBB-CAB-C3B	-2.14	113.98	120.34
5	C	401	HEC	CAD-CBD-CGD	2.13	116.25	112.67
11	M	404	BPB	O2A-C1-C2	2.12	114.21	108.64
5	C	403	HEC	CMB-C2B-C1B	-2.12	125.21	128.46
10	M	403	BCB	C4A-C3A-C2A	-2.08	100.69	103.86
13	M	401	MQ7	C2M-C2-C1	2.07	119.71	116.27
10	M	403	BCB	C1-C2-C3	-2.07	122.45	126.04
13	M	401	MQ7	C29-C28-C30	2.07	118.75	115.27
10	L	302	BCB	C4D-C3D-CAD	-2.06	100.06	104.73
5	C	402	HEC	CMB-C2B-C3B	2.05	128.23	125.82
10	L	302	BCB	CHC-C4B-C3B	2.04	123.17	118.17
10	M	402	BCB	O1D-CGD-CBD	-2.03	120.51	124.54
8	H	706	LDA	CM2-N1-C1	2.03	114.50	110.23
10	M	402	BCB	O2A-CGA-CBA	2.03	118.28	111.91

There are no chirality outliers.

All (120) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	405	DGA	OG1-CG1-CG2-OG2
6	C	405	DGA	OG1-CG1-CG2-CG3
8	H	706	LDA	C2-C1-N1-O1
8	H	706	LDA	C2-C1-N1-CM1
8	H	706	LDA	C2-C1-N1-CM2
9	H	708	HTO	C1-C2-C3-O3
9	H	708	HTO	O2-C2-C3-O3
9	H	708	HTO	O2-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
8	H	707	LDA	N1-C1-C2-C3
9	L	305	HTO	O2-C2-C3-C4
10	L	301	BCB	C2B-C3B-CAB-OBB
10	L	301	BCB	C2B-C3B-CAB-CBB
10	L	301	BCB	C2C-C3C-CAC-CBC
10	L	301	BCB	C4-C3-C5-C6
10	M	402	BCB	C2C-C3C-CAC-CBC
10	M	402	BCB	C4C-C3C-CAC-CBC
10	M	403	BCB	C2B-C3B-CAB-OBB
10	M	403	BCB	C2B-C3B-CAB-CBB
10	M	403	BCB	C2C-C3C-CAC-CBC
10	M	403	BCB	CAD-CBD-CGD-O1D
10	M	403	BCB	CAD-CBD-CGD-O2D
10	L	302	BCB	C2B-C3B-CAB-OBB
10	L	302	BCB	C2B-C3B-CAB-CBB
10	L	302	BCB	C2C-C3C-CAC-CBC
11	M	404	BPB	C2C-C3C-CAC-CBC
11	L	303	BPB	C2C-C3C-CAC-CBC
14	M	405	NS5	C34-C35-C36-CM3
10	M	403	BCB	C2A-CAA-CBA-CGA
10	M	402	BCB	CBD-CGD-O2D-CED
14	M	405	NS5	C34-C35-C36-CM4
10	L	301	BCB	C2-C3-C5-C6
11	M	404	BPB	C13-C15-C16-C17
10	L	301	BCB	C13-C15-C16-C17
10	M	403	BCB	C15-C16-C17-C18
8	H	707	LDA	C3-C4-C5-C6
8	M	416	LDA	C2-C3-C4-C5
8	M	414	LDA	C5-C6-C7-C8
10	M	402	BCB	O1D-CGD-O2D-CED
8	H	701	LDA	C4-C5-C6-C7
8	M	415	LDA	C6-C7-C8-C9
8	H	701	LDA	C6-C7-C8-C9
8	M	416	LDA	C5-C6-C7-C8
8	L	304	LDA	C7-C8-C9-C10
6	C	405	DGA	CBB-CAB-CB9-CB8
8	M	416	LDA	C3-C4-C5-C6
11	L	303	BPB	O2A-C1-C2-C3
8	H	707	LDA	C5-C6-C7-C8
6	C	405	DGA	CA2-CA1-OG1-CG1
10	M	403	BCB	C12-C13-C15-C16
6	C	405	DGA	OA1-CA1-OG1-CG1

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Mol	Chain	Res	Type	Atoms
6	C	405	DGA	CCB-CDB-CEB-CFB
10	M	403	BCB	C14-C13-C15-C16
8	H	706	LDA	C1-C2-C3-C4
8	H	706	LDA	C6-C7-C8-C9
8	L	304	LDA	C3-C4-C5-C6
8	L	304	LDA	C9-C10-C11-C12
8	M	416	LDA	C1-C2-C3-C4
9	H	708	HTO	C4-C5-C6-C7
8	H	707	LDA	C2-C3-C4-C5
10	L	302	BCB	C12-C13-C15-C16
10	L	302	BCB	C14-C13-C15-C16
11	M	404	BPB	CBA-CGA-O2A-C1
5	C	402	HEC	C3D-CAD-CBD-CGD
10	M	402	BCB	C5-C6-C7-C8
11	M	404	BPB	O1A-CGA-O2A-C1
6	C	405	DGA	CB9-CAB-CBB-CCB
6	C	405	DGA	CA3-CA4-CA5-CA6
10	M	403	BCB	C13-C15-C16-C17
14	M	405	NS5	C31-C33-C34-C35
14	M	405	NS5	C22-C21-C23-C24
11	L	303	BPB	C4-C3-C5-C6
8	M	416	LDA	C4-C5-C6-C7
11	M	404	BPB	CAD-CBD-CGD-O2D
11	L	303	BPB	C8-C10-C11-C12
10	M	403	BCB	C8-C10-C11-C12
8	H	707	LDA	C9-C10-C11-C12
8	M	415	LDA	C2-C1-N1-CM1
8	H	706	LDA	C3-C4-C5-C6
9	L	305	HTO	C4-C5-C6-C7
8	H	707	LDA	C7-C8-C9-C10
11	L	303	BPB	C2-C3-C5-C6
8	M	414	LDA	C11-C10-C9-C8
9	L	305	HTO	O3-C3-C4-C5
10	L	302	BCB	C13-C15-C16-C17
14	M	405	NS5	C3-C4-C5-C6
10	M	402	BCB	C8-C10-C11-C12
9	L	305	HTO	C2-C3-C4-C5
8	M	414	LDA	C4-C5-C6-C7
8	M	416	LDA	N1-C1-C2-C3
6	C	405	DGA	CAB-CBB-CCB-CDB
6	C	405	DGA	CB6-CB7-CB8-CB9
8	L	304	LDA	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
10	L	301	BCB	C1A-C2A-CAA-CBA
10	M	403	BCB	C1A-C2A-CAA-CBA
10	L	302	BCB	C1A-C2A-CAA-CBA
14	M	405	NS5	C20-C21-C23-C24
10	L	301	BCB	C16-C17-C18-C20
10	M	402	BCB	CHA-CBD-CGD-O2D
10	L	302	BCB	CHA-CBD-CGD-O1D
8	H	707	LDA	C4-C5-C6-C7
8	L	304	LDA	C1-C2-C3-C4
6	C	405	DGA	CBB-CCB-CDB-CEB
10	M	402	BCB	C10-C11-C12-C13
10	L	301	BCB	C16-C17-C18-C19
6	C	405	DGA	CA9-CAA-CBA-CCA
11	L	303	BPB	CAD-CBD-CGD-O2D
6	C	405	DGA	CEB-CFB-CGB-CHB
10	M	403	BCB	O2A-C1-C2-C3
10	M	402	BCB	CHA-CBD-CGD-O1D
10	L	302	BCB	CHA-CBD-CGD-O2D
8	M	415	LDA	C2-C1-N1-CM2
11	M	404	BPB	CHA-CBD-CGD-O2D
8	L	304	LDA	C6-C7-C8-C9
8	M	414	LDA	C6-C7-C8-C9
6	C	405	DGA	CB2-CB3-CB4-CB5
10	M	402	BCB	C4B-C3B-CAB-CBB
14	M	405	NS5	C3-C4-C5-C7
14	M	405	NS5	C7-C8-C9-C10
8	L	304	LDA	C2-C1-N1-O1
6	C	405	DGA	OG2-CB1-CB2-CB3

There are no ring outliers.

10 monomers are involved in 13 short contacts:

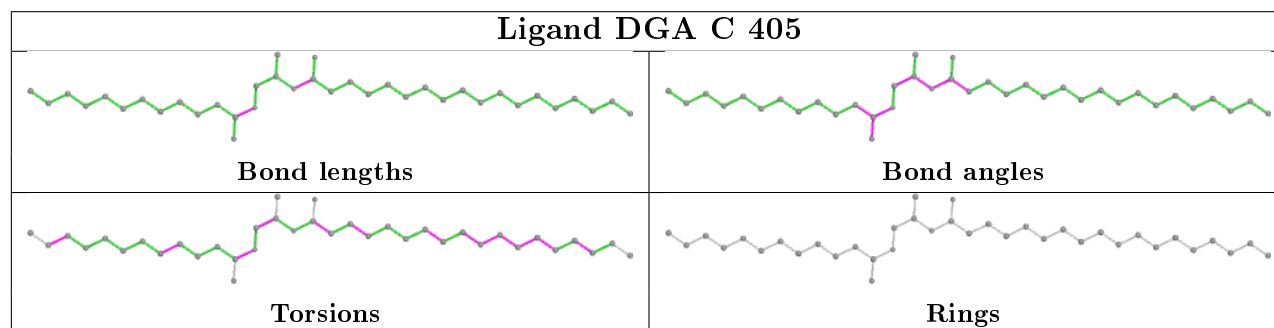
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	403	HEC	1	0
5	C	402	HEC	1	0
5	C	401	HEC	1	0
14	M	405	NS5	1	0
10	L	301	BCB	2	0
10	M	402	BCB	1	0
10	L	302	BCB	2	0
11	M	404	BPB	3	0
5	C	404	HEC	1	0

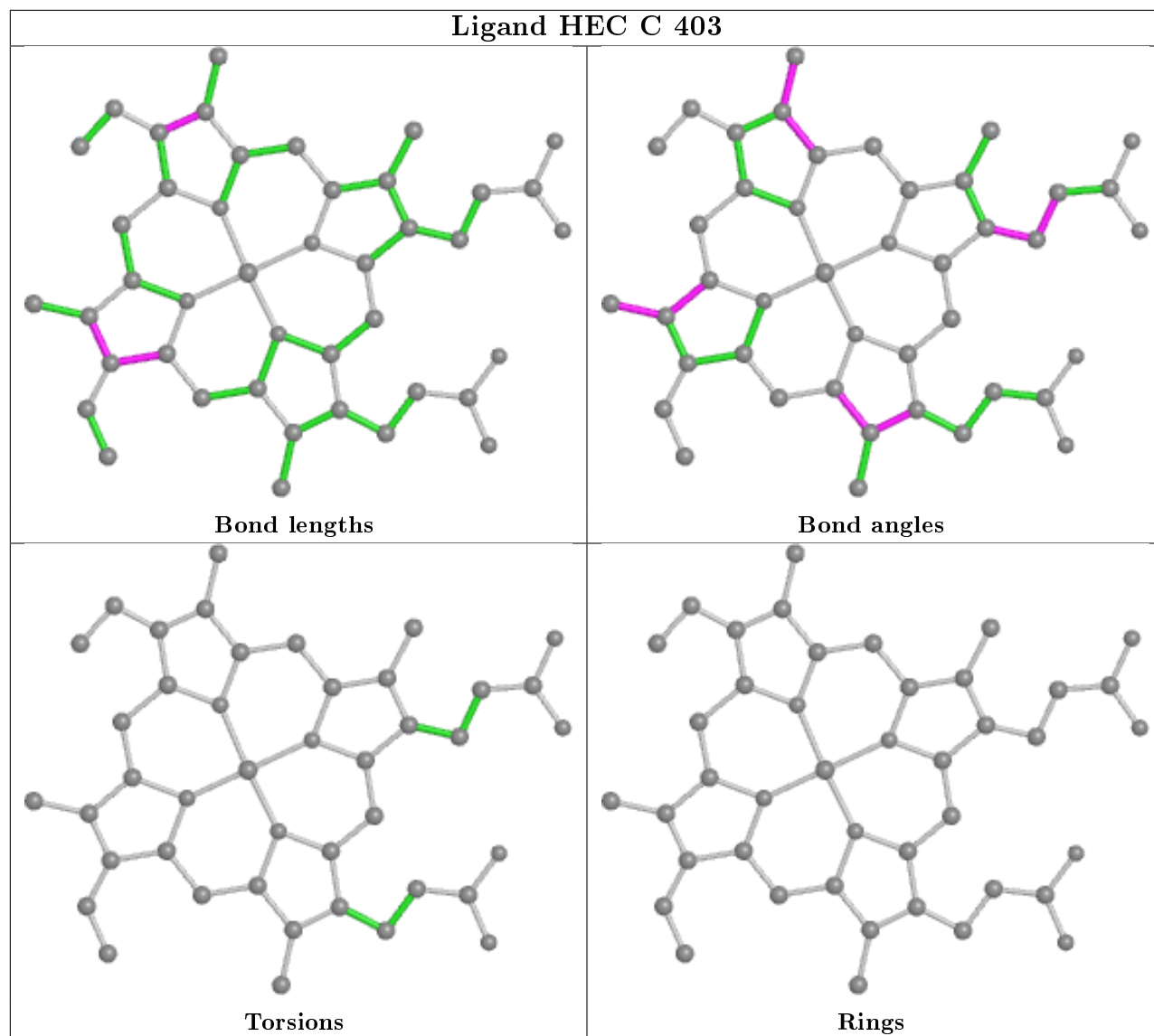
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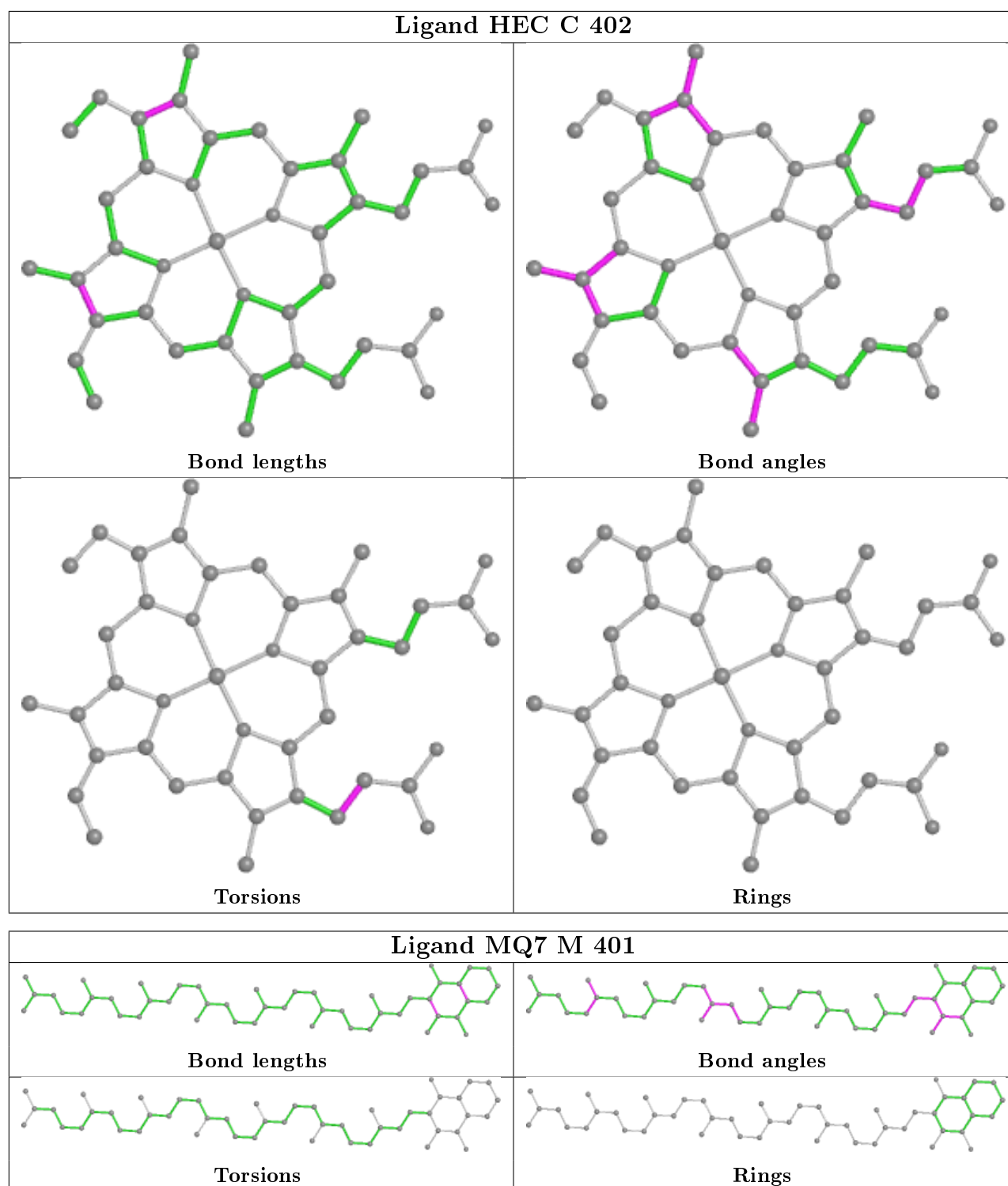
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	L	303	BPB	1	0

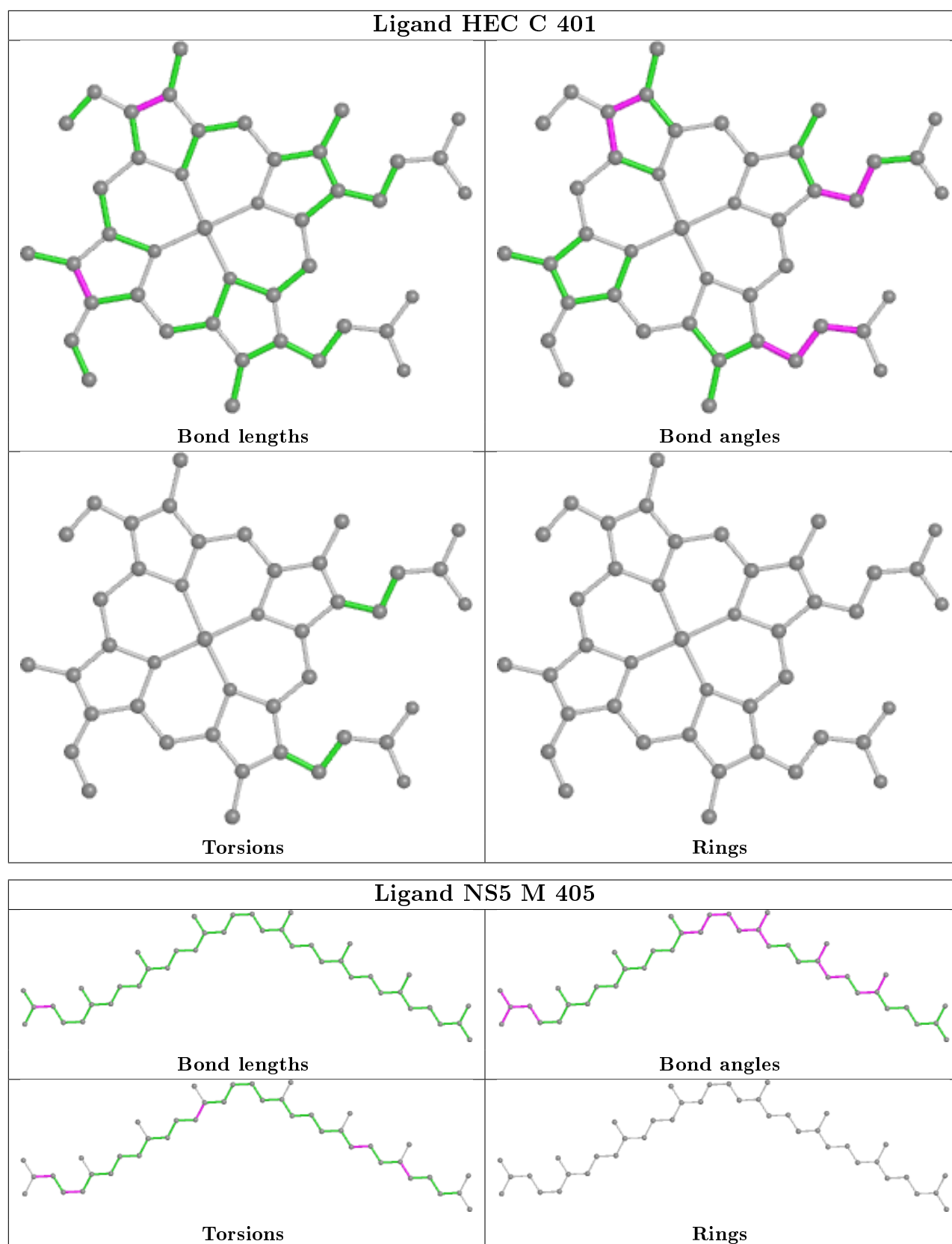
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

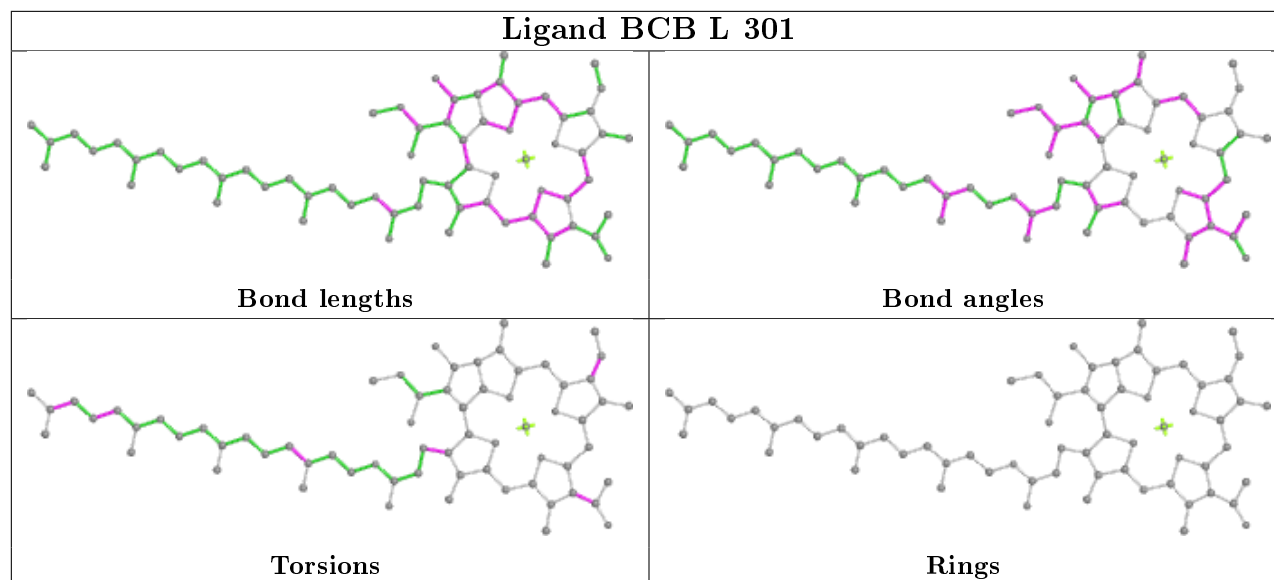
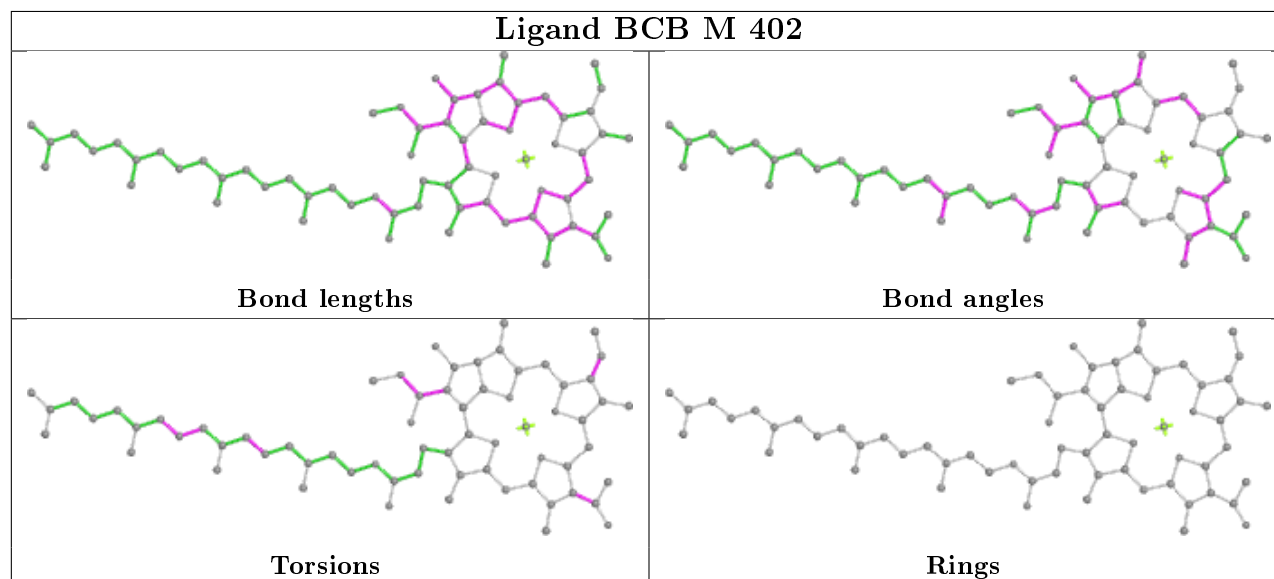
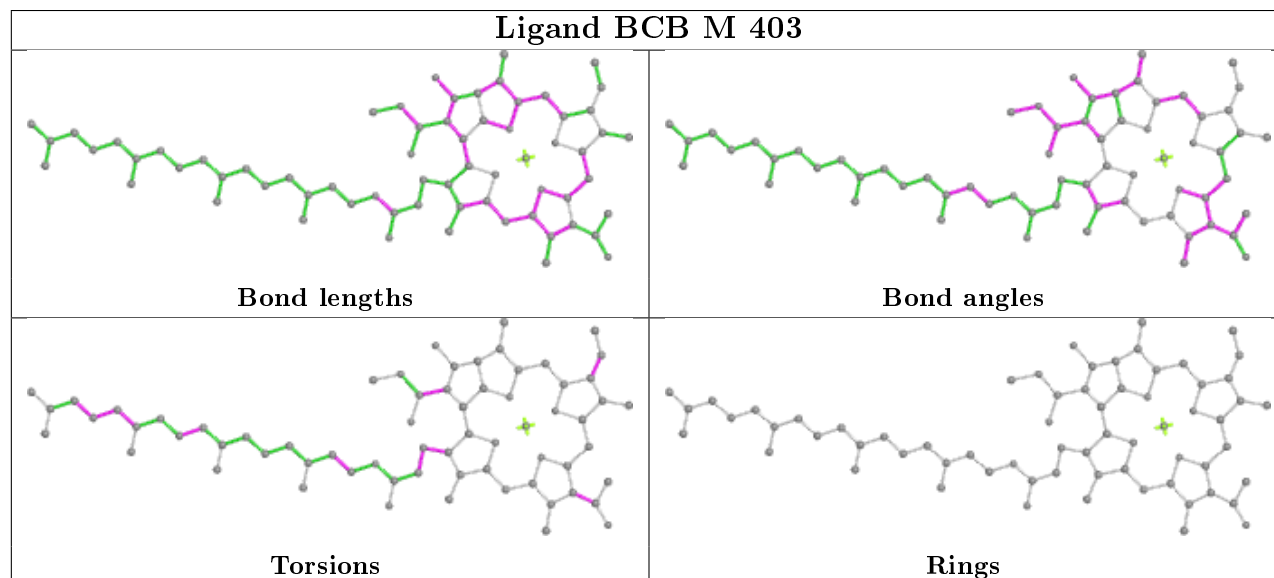


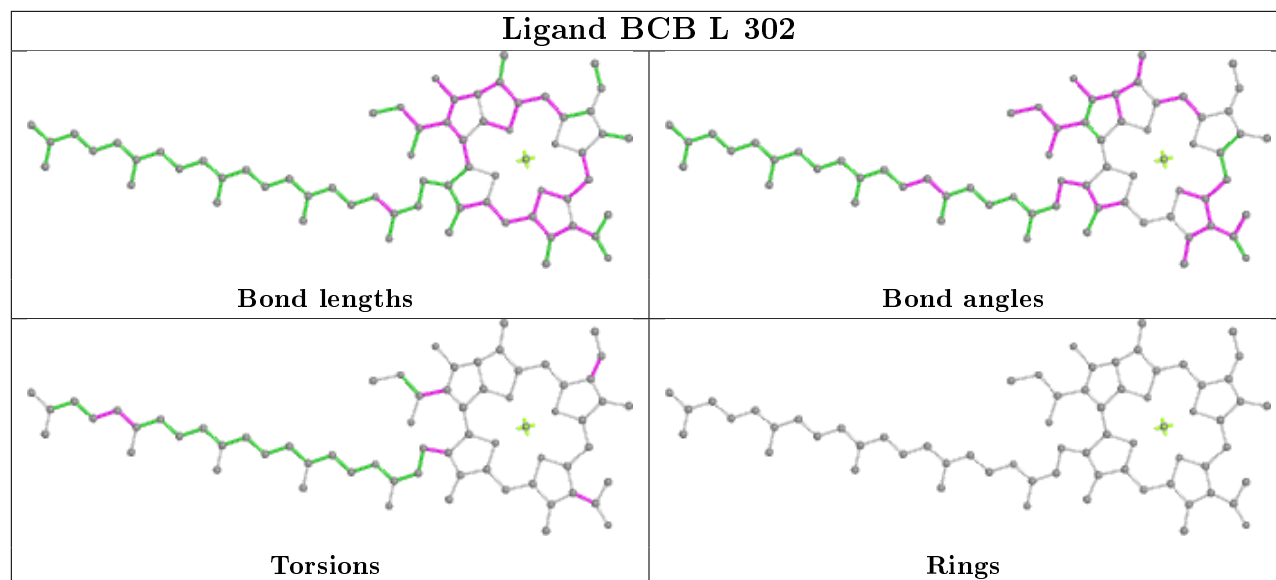
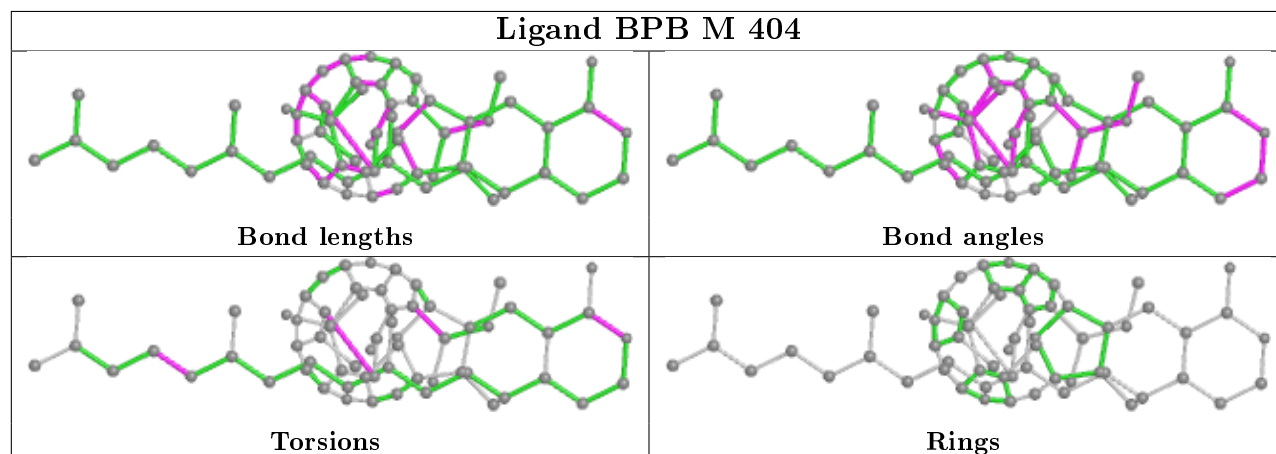


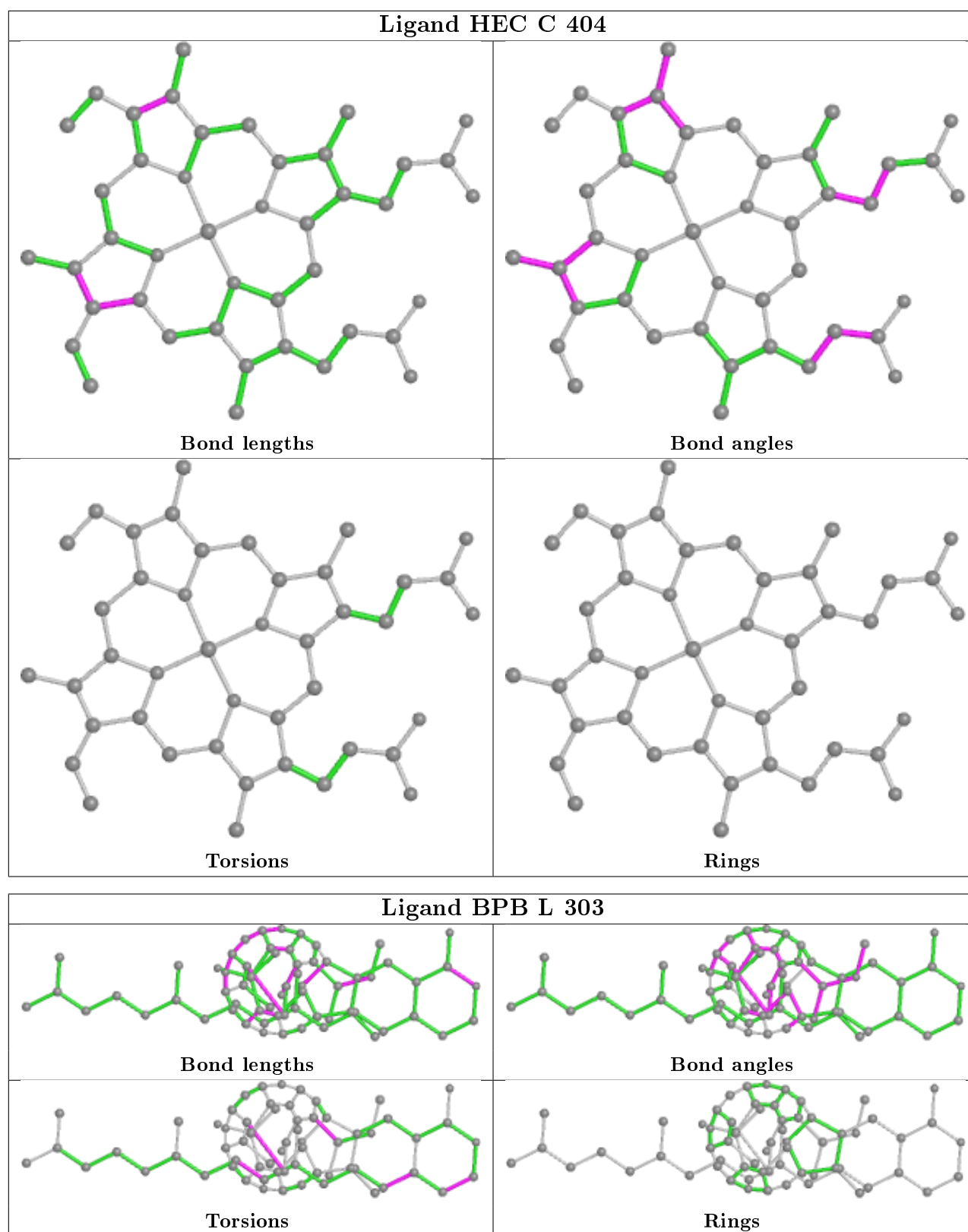






**Ligand BCB L 301****Ligand BCB M 402****Ligand BCB M 403**

**Ligand BCB L 302****Ligand BPB M 404**



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	C	332/336 (98%)	-0.35	6 (1%) 68 66	60, 76, 106, 138	0
2	H	257/258 (99%)	-0.20	14 (5%) 25 24	67, 89, 139, 200	0
3	L	273/273 (100%)	-0.43	7 (2%) 56 54	60, 74, 102, 120	0
4	M	323/323 (100%)	-0.18	8 (2%) 57 55	60, 74, 103, 128	0
All	All	1185/1190 (99%)	-0.29	35 (2%) 50 49	60, 77, 112, 200	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	52	LEU	4.9
4	M	37	TRP	4.4
2	H	47	LEU	4.2
2	H	49	LEU	3.9
2	H	46	PRO	3.5
2	H	51	LYS	3.2
3	L	271	PHE	3.1
2	H	257	LEU	3.0
2	H	96	PHE	2.8
1	C	48	GLU	2.6
4	M	107	LEU	2.6
4	M	51	LEU	2.6
2	H	8	GLN	2.6
2	H	205	LYS	2.5
3	L	158	ASN	2.5
4	M	319	PRO	2.5
2	H	191	ALA	2.4
2	H	258	LEU	2.4
4	M	26	ASN	2.3
3	L	161	GLY	2.3
3	L	166	ASN	2.3

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*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	L	165	LEU	2.3
1	C	47	ALA	2.2
3	L	157	VAL	2.2
2	H	147	GLU	2.2
4	M	185	THR	2.2
4	M	221	ILE	2.1
1	C	54	GLN	2.1
2	H	54	PRO	2.1
2	H	91	ALA	2.1
1	C	2	PHE	2.1
1	C	234	MET	2.1
4	M	100	TYR	2.1
1	C	230	PHE	2.0
3	L	160	PHE	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	FME	H	1	10/11	0.98	0.10	74,90,102,110	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	DGA	C	405	37/44	0.54	0.43	106,133,171,173	0
8	LDA	M	415	16/16	0.61	0.46	100,129,160,162	0
8	LDA	H	706	16/16	0.67	0.34	88,103,162,165	0

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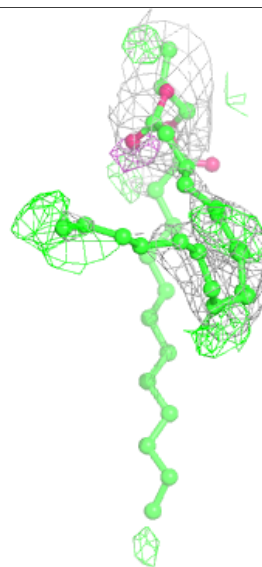
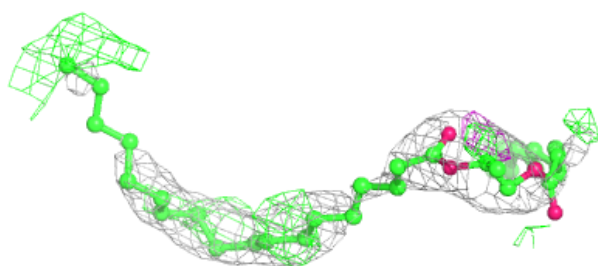
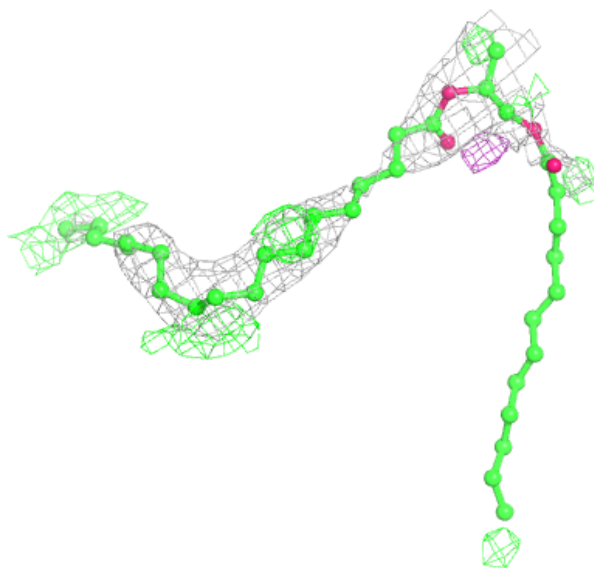
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	LDA	M	416	16/16	0.71	0.41	119,131,154,155	0
7	SO4	M	413	5/5	0.75	0.39	208,211,215,229	0
9	HTO	L	305	10/10	0.75	0.39	102,114,122,129	0
7	SO4	C	408	5/5	0.81	0.46	100,103,108,108	5
8	LDA	L	304	16/16	0.81	0.45	133,139,169,169	0
7	SO4	H	704	5/5	0.82	0.40	90,93,97,98	5
9	HTO	H	709	10/10	0.83	0.16	108,116,128,129	0
7	SO4	C	406	5/5	0.84	0.22	128,143,148,152	0
7	SO4	M	411	5/5	0.84	0.32	140,148,160,162	0
7	SO4	M	410	5/5	0.84	0.25	89,97,101,105	5
7	SO4	C	407	5/5	0.84	0.66	102,107,112,113	5
9	HTO	H	708	10/10	0.85	0.43	102,117,128,128	0
7	SO4	M	412	5/5	0.86	0.49	143,150,158,164	0
14	NS5	M	405	40/40	0.86	0.22	70,89,128,128	0
8	LDA	M	414	16/16	0.88	0.35	115,120,158,159	0
7	SO4	M	409	5/5	0.92	0.35	130,130,144,150	0
13	MQ7	M	401	48/48	0.94	0.22	64,71,114,126	0
8	LDA	H	707	16/16	0.95	0.26	95,110,135,135	0
8	LDA	H	701	16/16	0.96	0.24	72,87,99,100	0
7	SO4	M	407	5/5	0.96	0.10	102,105,117,122	0
7	SO4	H	703	5/5	0.96	0.39	163,163,172,174	0
10	BCB	M	402	66/66	0.96	0.17	60,70,151,157	0
10	BCB	L	301	66/66	0.97	0.19	55,60,78,91	0
7	SO4	H	705	5/5	0.97	0.06	95,96,112,113	5
11	BPB	M	404	65/65	0.97	0.16	64,75,157,163	0
5	HEC	C	403	43/43	0.98	0.18	51,63,70,77	0
5	HEC	C	401	43/43	0.98	0.11	69,81,90,98	0
7	SO4	H	702	5/5	0.98	0.09	95,100,107,112	0
5	HEC	C	402	43/43	0.98	0.13	69,75,86,94	0
10	BCB	L	302	66/66	0.98	0.20	59,64,105,109	0
10	BCB	M	403	66/66	0.98	0.18	54,63,95,99	0
5	HEC	C	404	43/43	0.98	0.12	60,67,86,105	0
11	BPB	L	303	65/65	0.98	0.18	60,66,76,80	0
12	FE2	L	306	1/1	0.99	0.15	68,68,68,68	0
7	SO4	M	408	5/5	0.99	0.07	77,83,86,90	0
7	SO4	M	406	5/5	0.99	0.09	88,96,107,109	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

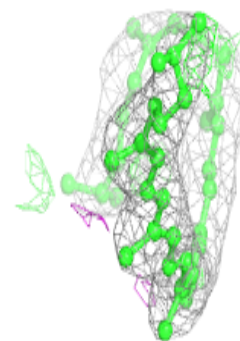
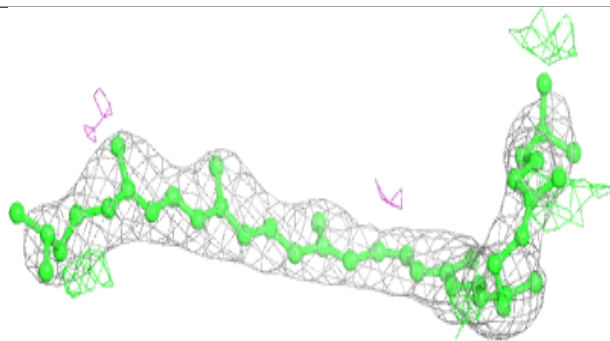
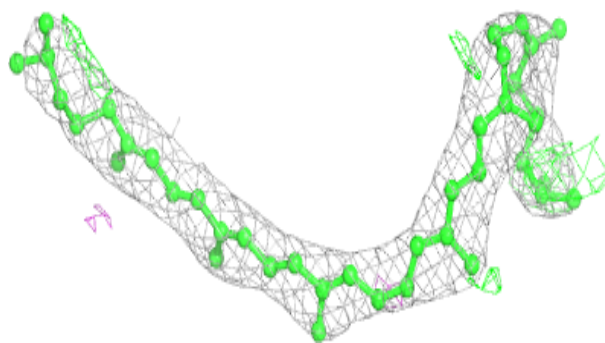
**Electron density around DGA C 405:**

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and green (positive)

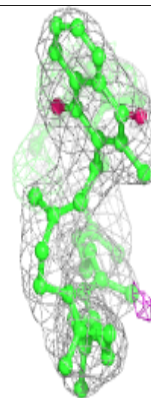
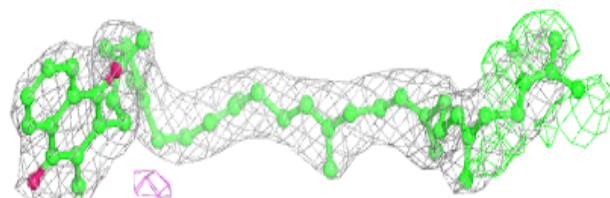
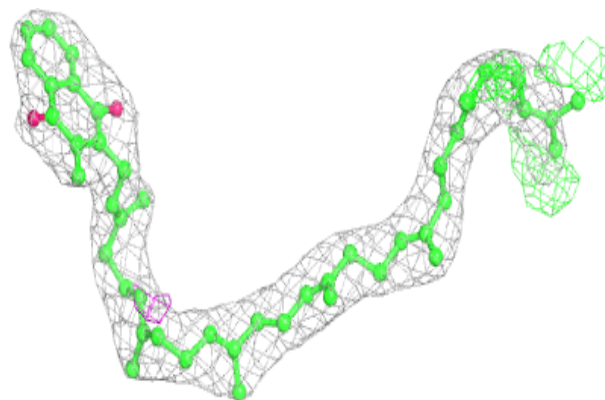


**Electron density around NS5 M 405:**

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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

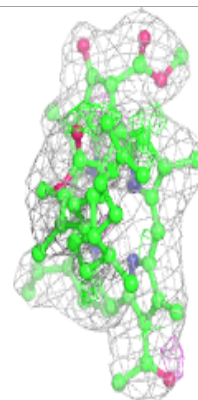
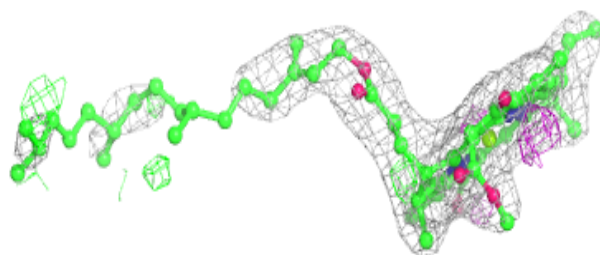
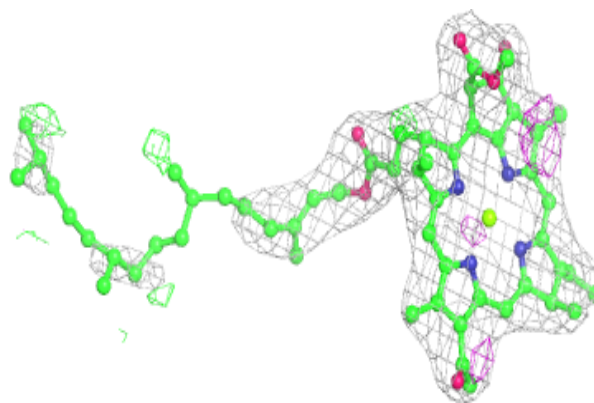
**Electron density around MQ7 M 401:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

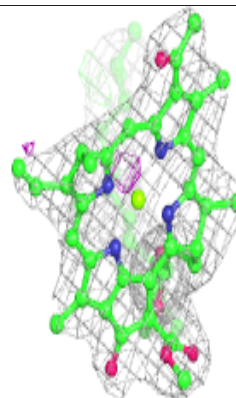
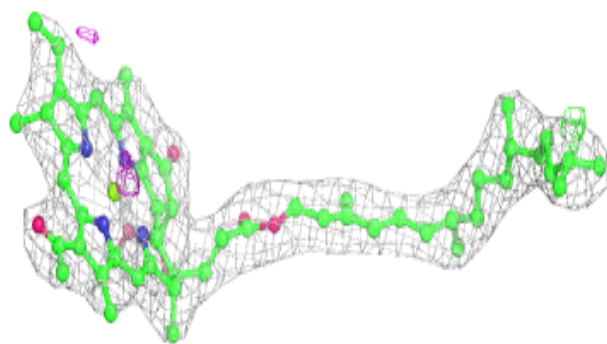
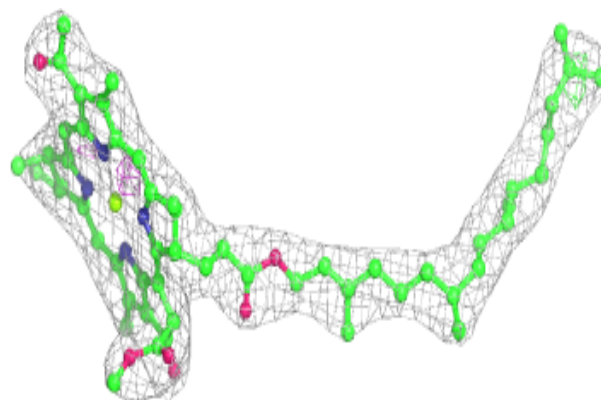


**Electron density around BCB M 402:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

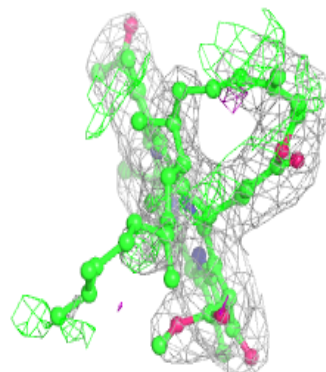
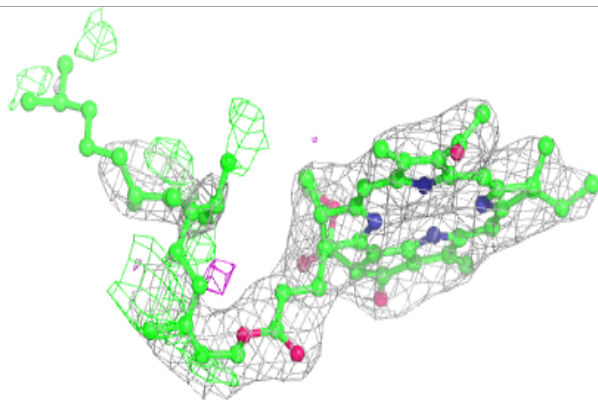
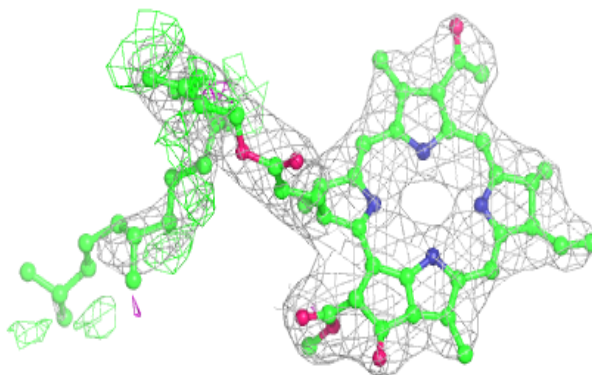
**Electron density around BCB L 301:**

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and green (positive)

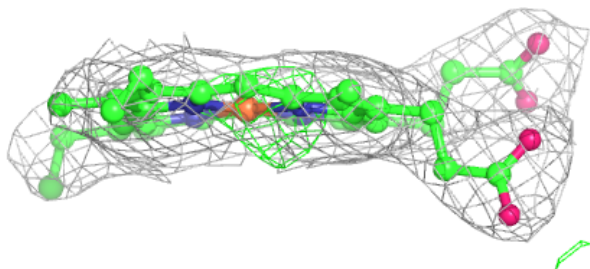
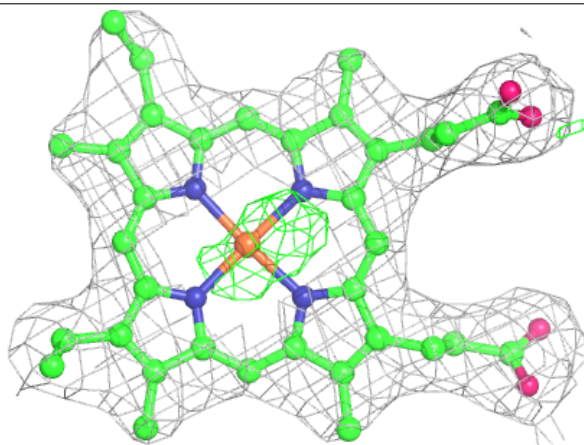


**Electron density around BPB M 404:**

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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

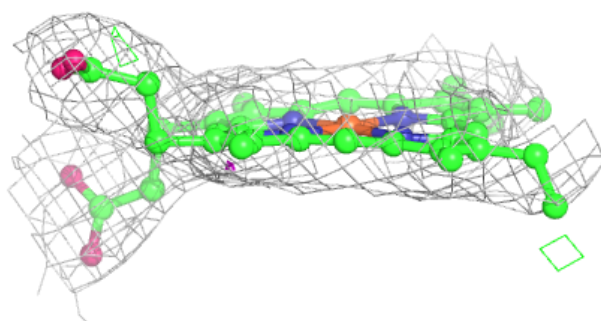
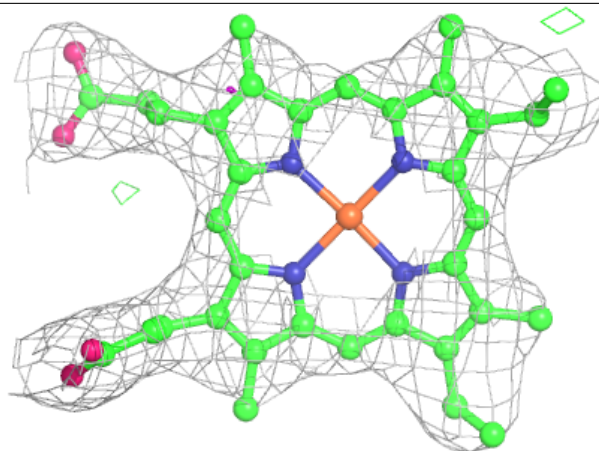
**Electron density around HEC C 403:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEC C 401:**

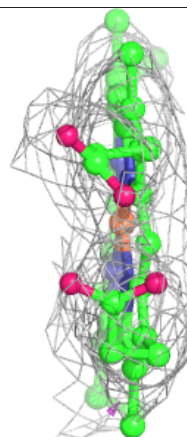
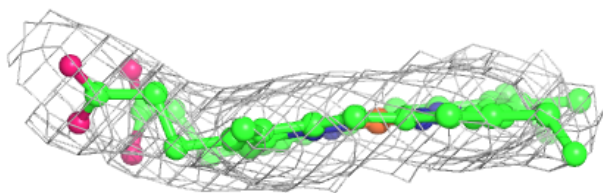
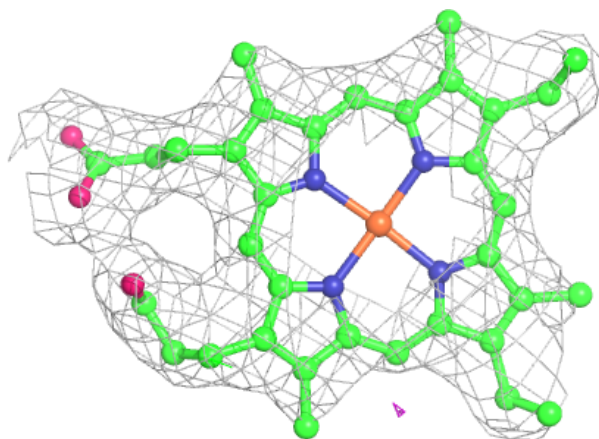
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





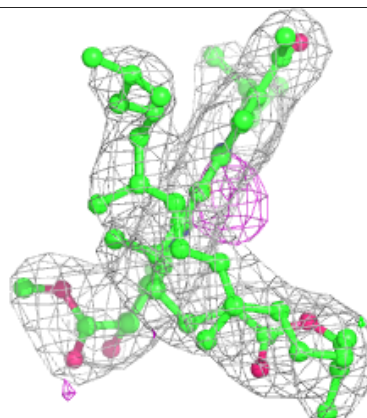
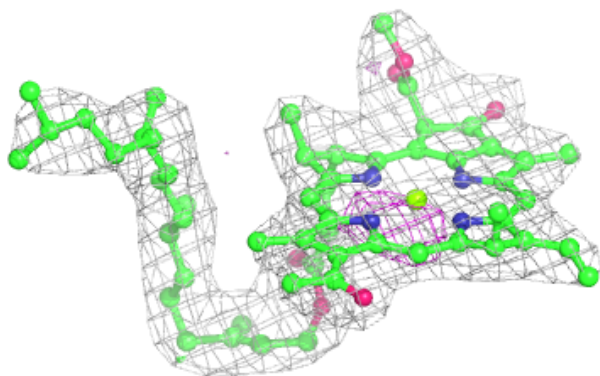
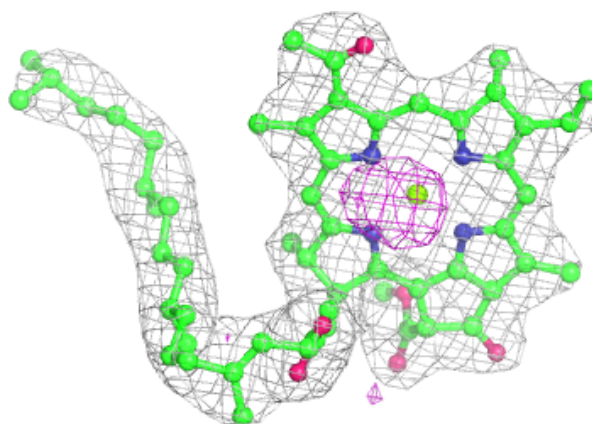
**Electron density around HEC C 402:**

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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

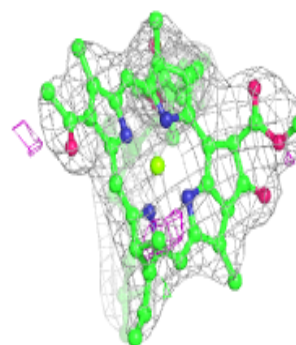
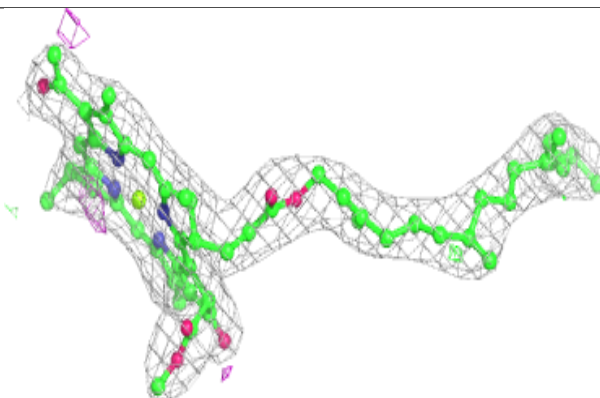
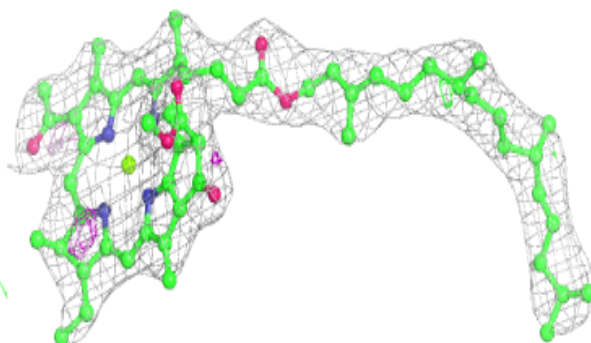


**Electron density around BCB L 302:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around BCB M 403:**

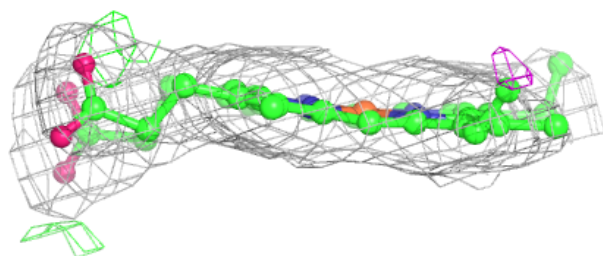
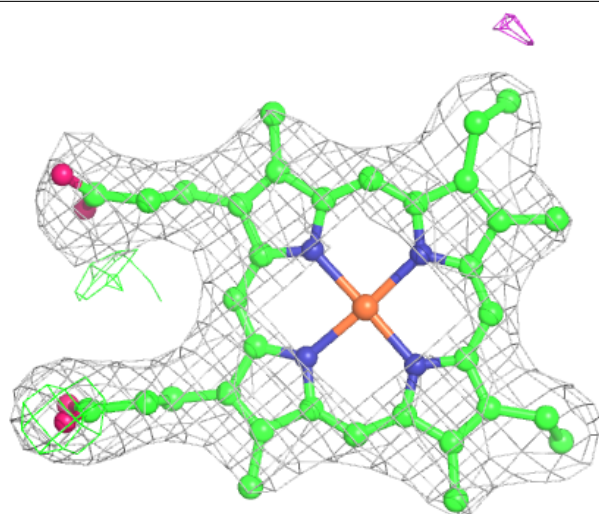
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





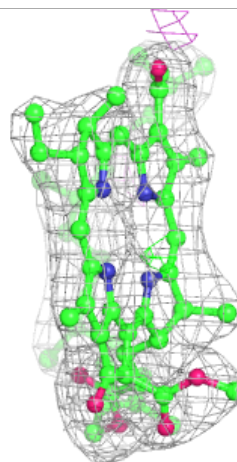
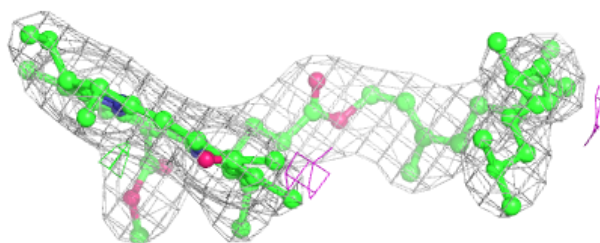
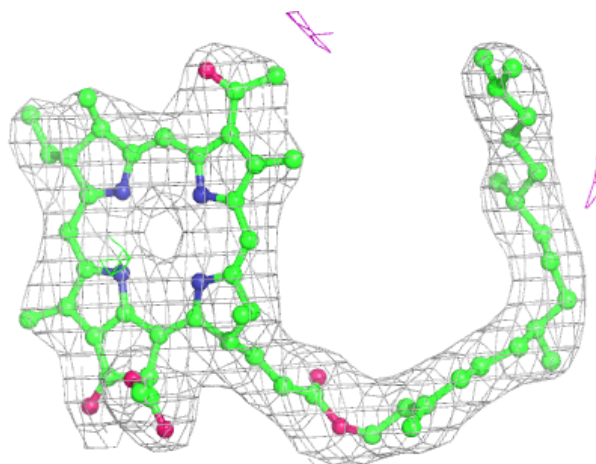
**Electron density around HEC C 404:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around BPB L 303:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.