Full wwPDB X-ray Structure Validation Report ⓘ

Aug 23, 2026 – 05:35 pm BST

PDB ID	:	2WJM / pdb_00002wjm
Title	:	Lipidic sponge phase crystal structure of the photosynthetic reaction centre from Blastochloris viridis (low dose)
Authors	:	Woehri, A.B.; Wahlgren, W.Y.; Malmerberg, E.; Johansson, L.C.; Neutze, R.; Katona, G.
Deposited on	:	2009-05-27
Resolution	:	1.95 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
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:

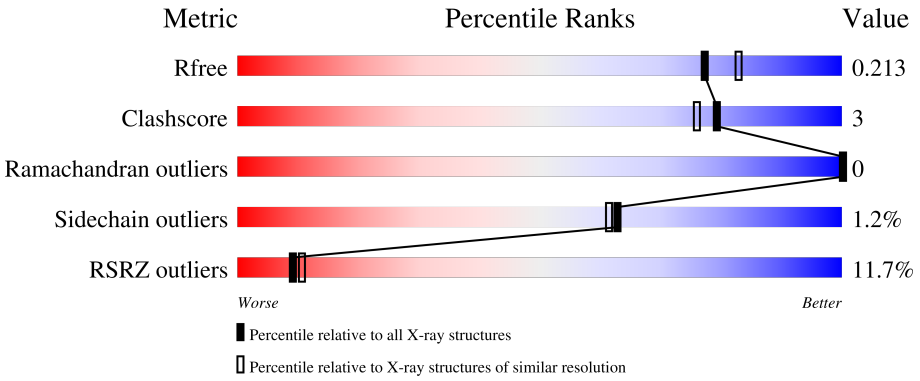
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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 of the lower 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 <=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	4% 94% 5%
2	H	258	24% 90% 6%
3	L	274	19% 93% 7%
4	M	324	3% 94% 5%

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	HEC	C	401	X	-	-	-
5	HEC	C	402	X	-	-	-
5	HEC	C	403	X	-	-	-
5	HEC	C	404	X	-	-	-
7	BCB	L	301	X	-	-	-
7	BCB	L	302	X	-	-	-
7	BCB	M	401	X	-	-	-
7	BCB	M	402	X	-	-	-

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 10671 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
			Total	C	N	O	S			
1	C	332	2598	1637	465	478	18	0	0	0

- Molecule 2 is a protein called REACTION CENTER PROTEIN H CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	243	1880	1205	326	347	2	0	0	0

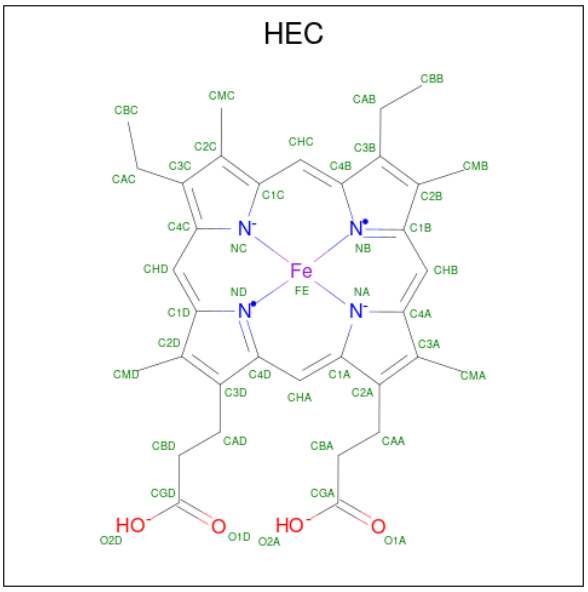
- Molecule 3 is a protein called REACTION CENTER PROTEIN L CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	273	2170	1458	350	355	7	0	2	0

- Molecule 4 is a protein called REACTION CENTER PROTEIN M CHAIN.

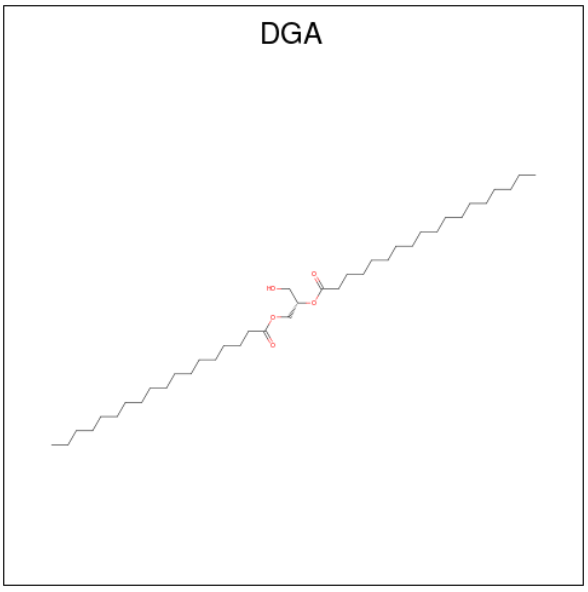
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	M	323	2548	1697	417	423	11	0	0	0

- Molecule 5 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



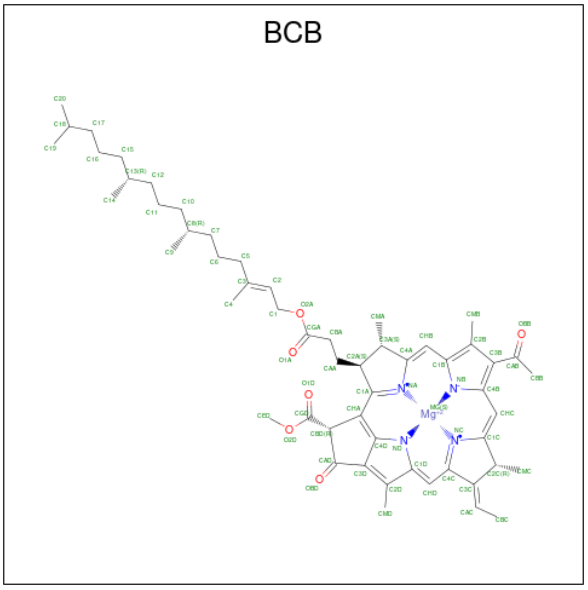
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 6 is DIACYL GLYCEROL (CCD ID: DGA) (formula: $C_{39}H_{76}O_5$).



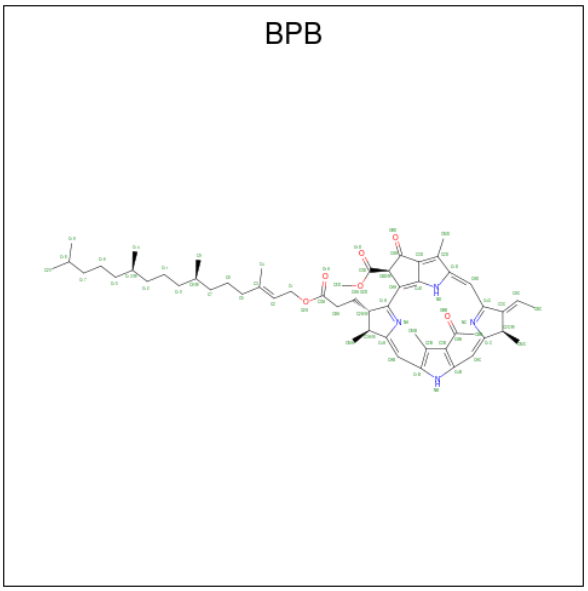
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			37	33	4		

- Molecule 7 is BACTERIOCHLOROPHYLL B (CCD ID: BCB) (formula: $C_{55}H_{72}MgN_4O_6$).



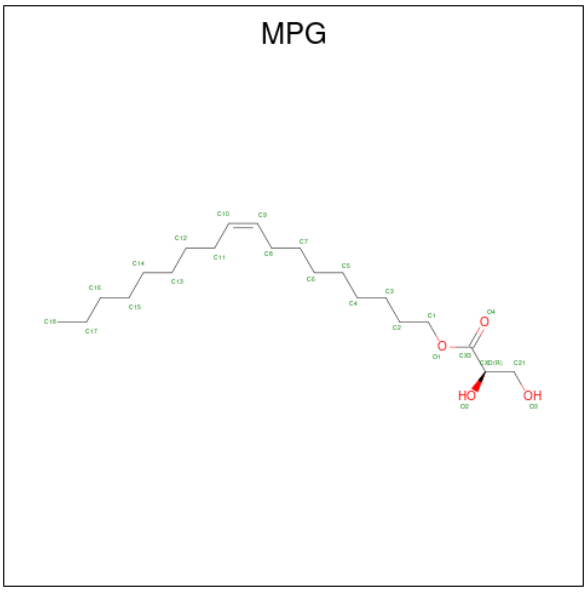
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	M	1	Total	C	Mg	N	O	0	0
			65	54	1	4	6		
7	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 8 is BACTERIOPHEOPHYTIN B (CCD ID: BPB) (formula: $C_{55}H_{74}N_4O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	L	1	Total	C	N	O	0	0
			65	55	4	6		
8	M	1	Total	C	N	O	0	0
			61	51	4	6		

- Molecule 9 is [(Z)-octadec-9-enyl] (2R)-2,3-bis(oxidanyl)propanoate (CCD ID: MPG) (formula: $C_{21}H_{40}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	L	1	Total	C	O	0	0
			25	21	4		

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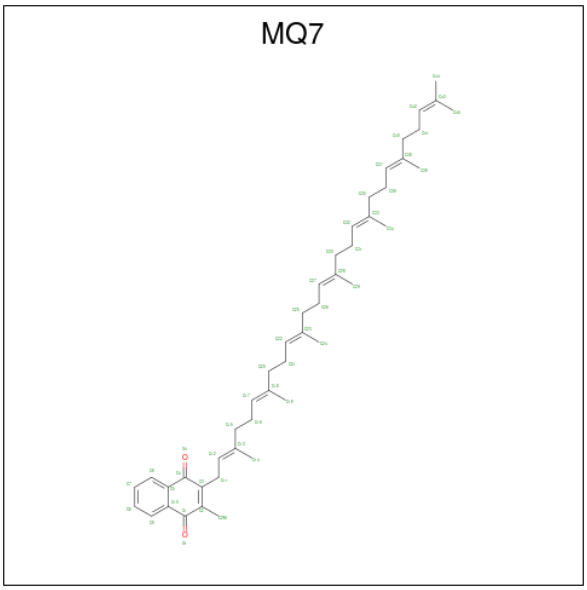
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	L	1	Total C O 25 21 4	0	0
9	M	1	Total C 17 17	0	0

- Molecule 10 is FE (II) ION (CCD ID: FE2) (formula: Fe).

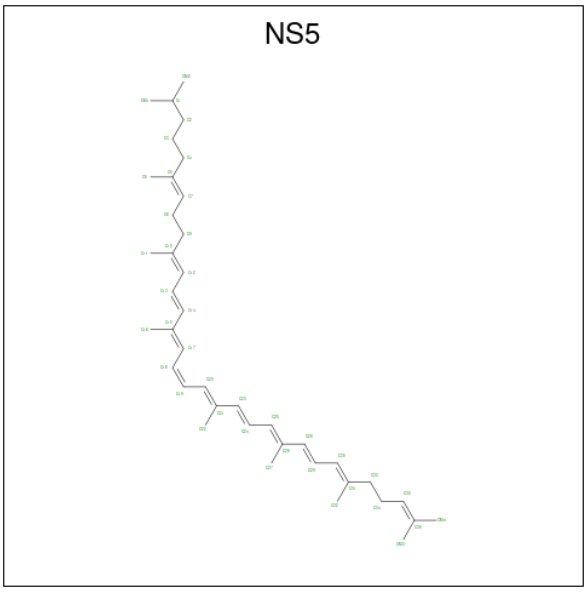
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	L	1	Total Fe 1 1	0	0

- Molecule 11 is MENAQUINONE-7 (CCD ID: MQ7) (formula: $C_{46}H_{64}O_2$).



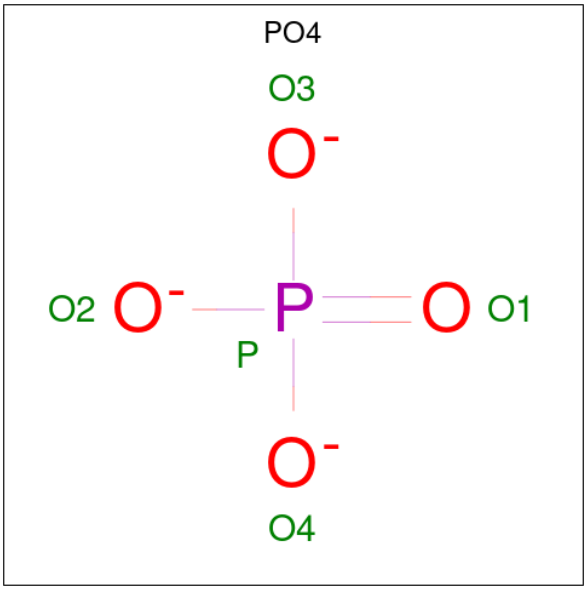
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	M	1	Total C O 48 46 2	0	0

- Molecule 12 is 15-cis-1,2-dihydroneurosporene (CCD ID: NS5) (formula: $C_{40}H_{60}$).



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

- Molecule 13 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	M	1	Total O P 5 4 1	0	0
13	M	1	Total O P 5 4 1	0	0

- Molecule 14 is water.

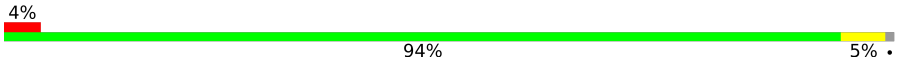
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	C	311	Total O 311 311	0	0
14	H	146	Total O 146 146	0	0
14	L	92	Total O 92 92	0	0
14	M	162	Total O 162 162	0	0

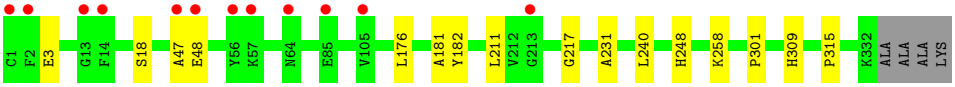
3 Residue-property plots (i)

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

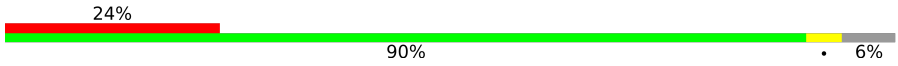
Chain C:

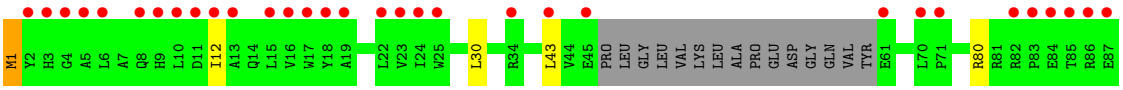


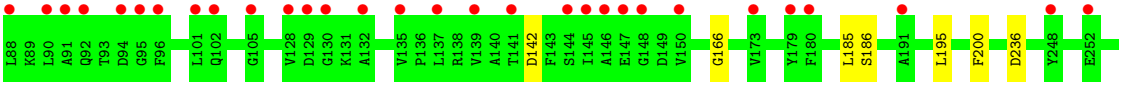


• Molecule 2: REACTION CENTER PROTEIN H CHAIN

Chain H:



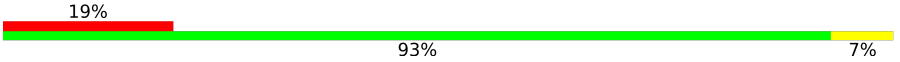


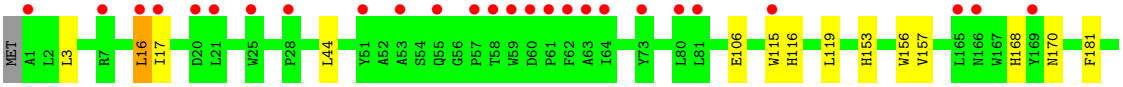


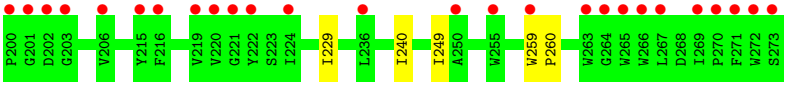


• Molecule 3: REACTION CENTER PROTEIN L CHAIN

Chain L:

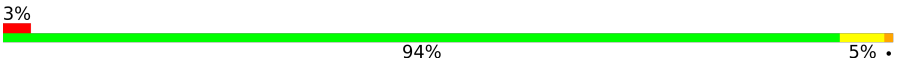


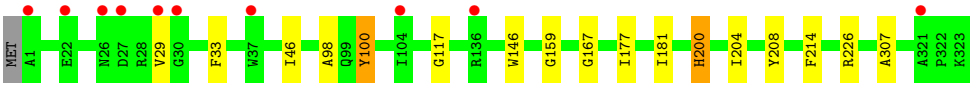




• Molecule 4: REACTION CENTER PROTEIN M CHAIN

Chain M:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	84.45Å 138.50Å 177.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	176.78 – 1.95 176.78 – 1.95	Depositor EDS
% Data completeness (in resolution range)	95.8 (176.78-1.95) 95.9 (176.78-1.95)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.20 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.173 , 0.201 0.186 , 0.213	Depositor DCC
R_{free} test set	7313 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	25.5	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 50.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10671	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEC, BCB, PO4, FME, FE2, BPB, MPG, NS5, MQ7, DGA

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	0.87	1/2665 (0.0%)	0.92	3/3633 (0.1%)
2	H	0.75	0/1913	0.81	1/2613 (0.0%)
3	L	0.79	0/2263	0.87	1/3089 (0.0%)
4	M	0.82	0/2652	0.87	2/3630 (0.1%)
All	All	0.81	1/9493 (0.0%)	0.87	7/12965 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	231	ALA	CA-CB	5.38	1.61	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	48	GLU	N-CA-C	-8.50	94.15	108.26
1	C	3	GLU	CA-C-N	-6.18	115.21	119.66
1	C	3	GLU	C-N-CA	-6.18	115.21	119.66
2	H	12	ILE	N-CA-C	5.93	116.11	110.42
4	M	100	TYR	N-CA-C	-5.82	105.38	112.88
3	L	240	ILE	N-CA-C	-5.57	105.08	110.42
4	M	200	HIS	N-CA-C	-5.38	105.50	111.36

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	248	HIS	Peptide
1	C	47	ALA	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2598	0	2567	9	0
2	H	1880	0	1869	6	0
3	L	2170	0	2100	13	0
4	M	2548	0	2432	14	0
5	C	172	0	120	1	0
6	C	37	0	58	0	0
7	L	132	0	144	6	0
7	M	131	0	140	4	0
8	L	65	0	74	7	0
8	M	61	0	63	6	0
9	L	50	0	80	3	0
9	M	17	0	31	0	0
10	L	1	0	0	0	0
11	M	48	0	64	0	0
12	M	40	0	60	7	0
13	M	10	0	0	0	0
14	C	311	0	0	1	0
14	H	146	0	0	2	0
14	L	92	0	0	0	0
14	M	162	0	0	0	0
All	All	10671	0	9802	53	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (53) 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)
8:M:403:BPB:HHC	8:M:403:BPB:HBBB	1.44	0.98
7:M:401:BCB:HBB2	7:M:401:BCB:HHC	1.53	0.89
8:L:303:BPB:HHC	8:L:303:BPB:HBBB	1.55	0.88
2:H:142:ASP:OD1	14:H:301:HOH:O	2.04	0.73
7:M:401:BCB:HHC	7:M:401:BCB:CBB	2.19	0.73
3:L:181:PHE:HB3	8:M:403:BPB:HBBA	1.75	0.68
8:M:403:BPB:HHC	8:M:403:BPB:CBB	2.21	0.67
3:L:181:PHE:CD2	8:M:403:BPB:HBB	2.33	0.63
8:L:303:BPB:HBB	4:M:208:TYR:CD2	2.34	0.63
3:L:116:HIS:CE1	9:L:304:MPG:H32C	2.33	0.63
4:M:117:GLY:HA3	12:M:405:NS5:H92	1.83	0.60
8:L:303:BPB:HHC	8:L:303:BPB:CBB	2.30	0.59
4:M:159:GLY:HA3	12:M:405:NS5:C11	2.32	0.59
3:L:16:LEU:HD13	3:L:106:GLU:HG2	1.88	0.56
1:C:176:LEU:HD12	14:C:733:HOH:O	2.07	0.55
8:L:303:BPB:HBBA	4:M:208:TYR:HB3	1.88	0.55
8:M:403:BPB:C9	12:M:405:NS5:HM33	2.39	0.53
7:L:301:BCB:HMB1	7:L:301:BCB:HBB3	1.89	0.53
3:L:168:HIS:CE1	7:L:301:BCB:HMC2	2.46	0.50
4:M:177:ILE:HD11	12:M:405:NS5:H273	1.94	0.50
7:M:401:BCB:CBB	7:M:401:BCB:CHC	2.90	0.50
4:M:159:GLY:HA3	12:M:405:NS5:H113	1.96	0.48
3:L:259:TRP:N	3:L:260:PRO:CD	2.78	0.47
4:M:98:ALA:HB3	4:M:100:TYR:CZ	2.50	0.47
4:M:146:TRP:HA	4:M:146:TRP:CE3	2.49	0.47
2:H:43:LEU:CD2	3:L:3:LEU:HD23	2.46	0.46
1:C:309:HIS:CE1	1:C:315:PRO:HD3	2.51	0.46
1:C:240:LEU:HD22	1:C:309:HIS:CG	2.50	0.45
1:C:211:LEU:HD12	2:H:1:FME:O	2.17	0.45
8:M:403:BPB:CBB	8:M:403:BPB:CHC	2.91	0.45
7:L:302:BCB:HMA1	7:L:302:BCB:H142	1.99	0.44
4:M:33:PHE:CE2	4:M:46:ILE:HD12	2.53	0.44
1:C:258:LYS:HG2	4:M:307:ALA:HB2	2.00	0.44
12:M:405:NS5:H161	12:M:405:NS5:H18	1.78	0.44
1:C:217:GLY:HA2	4:M:167:GLY:O	2.18	0.43
7:M:401:BCB:HBB3	7:M:402:BCB:H41	2.01	0.43
3:L:170:ASN:C	3:L:170:ASN:OD1	2.62	0.43
7:L:302:BCB:C1B	8:L:303:BPB:H19A	2.49	0.43
7:L:302:BCB:C2B	8:L:303:BPB:H19A	2.49	0.42
4:M:200:HIS:CE1	4:M:204:ILE:HD11	2.53	0.42
7:L:301:BCB:H203	7:L:301:BCB:H161	1.88	0.42
2:H:80:ARG:HD2	14:H:435:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:119:LEU:HD23	9:L:304:MPG:H72C	2.02	0.42
8:L:303:BPB:CBB	4:M:208:TYR:CD2	3.03	0.42
12:M:405:NS5:H24	12:M:405:NS5:H221	1.82	0.42
1:C:181:ALA:O	1:C:182:TYR:HB2	2.20	0.41
3:L:153:HIS:O	3:L:157:VAL:HG23	2.20	0.41
1:C:18:SER:HB2	3:L:156:TRP:CD1	2.57	0.40
2:H:166:GLY:HA3	2:H:186:SER:O	2.21	0.40
1:C:301:PRO:HG2	5:C:402:HEC:HBD1	2.03	0.40
3:L:229:ILE:HD12	3:L:229:ILE:O	2.20	0.40
2:H:200:PHE:CZ	4:M:226:ARG:HD3	2.57	0.40
3:L:115:TRP:CE3	9:L:304:MPG:H212	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)	321 (97%)	9 (3%)	0	100	100
2	H	239/258 (93%)	235 (98%)	4 (2%)	0	100	100
3	L	273/274 (100%)	266 (97%)	7 (3%)	0	100	100
4	M	321/324 (99%)	312 (97%)	9 (3%)	0	100	100
All	All	1163/1192 (98%)	1134 (98%)	29 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	280/282 (99%)	280 (100%)	0	100	100
2	H	192/212 (91%)	188 (98%)	4 (2%)	47	41
3	L	218/219 (100%)	214 (98%)	4 (2%)	51	47
4	M	247/250 (99%)	244 (99%)	3 (1%)	63	61
All	All	937/963 (97%)	926 (99%)	11 (1%)	63	61

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	30	LEU
2	H	185	LEU
2	H	195	LEU
2	H	236	ASP
3	L	16	LEU
3	L	17	ILE
3	L	44	LEU
3	L	249	ILE
4	M	29	VAL
4	M	181	ILE
4	M	214	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	120	ASN
1	C	302	GLN
2	H	102	GLN
3	L	183	ASN
3	L	213	ASN
4	M	16	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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	0.83	1 (12%)	7,9,11	3.07	2 (28%)

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	-	4/7/9/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1	FME	CN-N	2.05	1.40	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	1	FME	CA-N-CN	-7.35	111.52	122.82
2	H	1	FME	CE-SD-CG	2.25	108.13	100.40

There are no chirality outliers.

All (4) 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	N-CA-CB-CG
2	H	1	FME	CB-CG-SD-CE

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	1	FME	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 19 ligands modelled in this entry, 1 is monoatomic - leaving 18 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	$\#\|Z\| > 2$
11	MQ7	M	404	-	49,49,49	1.44	2 (4%)	60,63,63	1.18	6 (10%)
7	BCB	L	301	3	68,74,74	1.94	17 (25%)	79,115,115	3.13	28 (35%)
5	HEC	C	401	1	50,50,50	1.94	10 (20%)	68,82,82	1.62	9 (13%)
7	BCB	L	302	3	68,74,74	1.86	15 (22%)	79,115,115	2.98	24 (30%)
8	BPB	L	303	-	57,70,70	2.48	15 (26%)	56,101,101	2.30	15 (26%)
5	HEC	C	402	1	50,50,50	1.90	7 (14%)	68,82,82	1.58	12 (17%)
8	BPB	M	403	-	53,66,70	2.54	14 (26%)	51,96,101	2.57	17 (33%)
7	BCB	M	402	4	68,74,74	1.91	15 (22%)	79,115,115	2.99	25 (31%)
9	MPG	L	305	-	24,24,24	1.50	2 (8%)	24,25,25	1.64	3 (12%)
12	NS5	M	405	-	39,39,39	2.17	5 (12%)	44,46,46	2.16	15 (34%)
9	MPG	L	304	-	24,24,24	1.40	2 (8%)	24,25,25	1.51	2 (8%)
9	MPG	M	406	-	16,16,24	0.27	0	15,15,25	0.62	0
5	HEC	C	404	1	50,50,50	1.83	7 (14%)	68,82,82	1.32	7 (10%)
13	PO4	M	408	-	4,4,4	0.61	0	6,6,6	1.85	2 (33%)
6	DGA	C	405	1	36,36,43	1.28	2 (5%)	38,38,45	1.20	2 (5%)
7	BCB	M	401	4	67,73,74	1.98	16 (23%)	77,113,115	3.12	17 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	HEC	C	403	1	50,50,50	1.95	9 (18%)	68,82,82	1.62	11 (16%)
13	PO4	M	407	-	4,4,4	0.64	0	6,6,6	1.50	2 (33%)

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
11	MQ7	M	404	-	-	3/41/61/61	0/2/2/2
7	BCB	L	301	3	3/3/21/26	5/41/137/137	-
5	HEC	C	401	1	1/1/3/7	6/14/54/54	-
7	BCB	L	302	3	3/3/21/26	8/41/137/137	-
8	BPB	L	303	-	-	7/37/105/105	0/5/6/6
5	HEC	C	402	1	1/1/3/7	7/14/54/54	-
8	BPB	M	403	-	-	17/33/101/105	0/5/6/6
7	BCB	M	402	4	3/3/21/26	7/41/137/137	-
9	MPG	L	305	-	-	13/25/25/25	-
12	NS5	M	405	-	-	13/43/43/43	-
9	MPG	L	304	-	-	16/25/25/25	-
9	MPG	M	406	-	-	3/14/14/25	-
5	HEC	C	404	1	1/1/3/7	3/14/54/54	-
6	DGA	C	405	1	-	15/37/37/45	-
7	BCB	M	401	4	3/3/20/26	6/40/136/137	-
5	HEC	C	403	1	1/1/3/7	4/14/54/54	-

All (138) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	403	BPB	C1B-C2B	8.74	1.49	1.39
12	M	405	NS5	C35-C36	7.73	1.54	1.32
8	L	303	BPB	CAC-C3C	7.62	1.52	1.33
5	C	404	HEC	C3D-C2D	7.50	1.52	1.36
11	M	404	MQ7	C3-C2	7.45	1.48	1.35
8	L	303	BPB	C1B-C2B	7.42	1.47	1.39
5	C	403	HEC	C3D-C2D	7.31	1.52	1.36
8	M	403	BPB	CAC-C3C	7.23	1.51	1.33
5	C	402	HEC	C3D-C2D	7.22	1.52	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	M	405	NS5	C29-C28	7.14	1.53	1.34
5	C	401	HEC	C3D-C2D	6.92	1.51	1.36
8	M	403	BPB	C1D-C2D	6.87	1.47	1.39
9	L	305	MPG	O1-CX3	6.41	1.46	1.33
9	L	304	MPG	O1-CX3	6.21	1.46	1.33
7	M	401	BCB	C2C-C3C	-6.05	1.43	1.51
8	L	303	BPB	C1D-C2D	5.85	1.46	1.39
7	L	301	BCB	CAC-C3C	5.81	1.49	1.33
5	C	403	HEC	FE-ND	5.68	2.12	1.94
7	L	302	BCB	CAC-C3C	5.65	1.49	1.33
12	M	405	NS5	C9-C8	-5.51	1.35	1.53
8	L	303	BPB	C3D-C2D	5.50	1.49	1.39
5	C	402	HEC	FE-NB	5.48	2.11	1.94
7	M	402	BCB	C2C-C3C	-5.44	1.44	1.51
7	L	302	BCB	CHC-C1C	5.38	1.49	1.37
7	M	401	BCB	CAC-C3C	5.35	1.48	1.33
7	M	402	BCB	CAC-C3C	5.31	1.48	1.33
6	C	405	DGA	OG2-CB1	5.14	1.48	1.34
7	L	301	BCB	O2D-CGD	4.95	1.45	1.33
8	L	303	BPB	C4D-CHA	4.94	1.47	1.39
7	L	301	BCB	CHC-C1C	4.88	1.48	1.37
7	M	402	BCB	OBD-CAD	4.85	1.30	1.22
11	M	404	MQ7	C10-C5	4.85	1.48	1.40
8	M	403	BPB	OBD-CAD	4.85	1.29	1.22
5	C	402	HEC	FE-ND	4.84	2.09	1.94
8	L	303	BPB	C3B-C2B	4.84	1.48	1.39
5	C	401	HEC	FE-ND	4.82	2.09	1.94
7	M	401	BCB	C1D-ND	-4.79	1.31	1.37
6	C	405	DGA	OG1-CA1	4.78	1.47	1.33
7	M	402	BCB	O2D-CGD	4.77	1.44	1.33
5	C	404	HEC	FE-NB	4.70	2.09	1.94
8	L	303	BPB	OBD-CAD	4.58	1.28	1.22
7	L	301	BCB	CHC-C4B	4.57	1.49	1.39
7	L	302	BCB	CHC-C4B	4.50	1.49	1.39
7	L	302	BCB	C2C-C3C	-4.41	1.46	1.51
8	L	303	BPB	C3B-C4B	4.40	1.49	1.41
7	M	402	BCB	CHC-C4B	4.40	1.49	1.39
7	L	301	BCB	OBD-CAD	4.39	1.30	1.22
8	M	403	BPB	C3B-C2B	4.37	1.47	1.39
8	M	403	BPB	C4D-CHA	4.35	1.46	1.39
7	M	401	BCB	CHC-C4B	4.33	1.49	1.39
8	M	403	BPB	C3D-C2D	4.33	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	303	BPB	O2D-CGD	4.29	1.43	1.33
7	M	401	BCB	CHC-C1C	4.29	1.47	1.37
7	L	301	BCB	C3B-C4B	4.11	1.48	1.41
7	M	402	BCB	CHC-C1C	4.09	1.46	1.37
5	C	401	HEC	FE-NA	4.07	2.08	1.95
5	C	403	HEC	CBB-CAB	-4.06	1.33	1.51
7	M	402	BCB	C3B-C4B	4.06	1.48	1.41
7	L	301	BCB	C2C-C3C	-3.99	1.46	1.51
5	C	404	HEC	FE-ND	3.80	2.06	1.94
8	M	403	BPB	C3B-C4B	3.79	1.48	1.41
5	C	401	HEC	CBB-CAB	-3.77	1.34	1.51
8	M	403	BPB	O2D-CGD	3.75	1.42	1.33
5	C	404	HEC	CBB-CAB	-3.74	1.34	1.51
5	C	403	HEC	FE-NA	3.71	2.07	1.95
7	M	401	BCB	O2A-CGA	3.71	1.44	1.33
7	L	302	BCB	O2D-CGD	3.68	1.42	1.33
5	C	402	HEC	CBC-CAC	-3.67	1.35	1.51
7	L	302	BCB	C3B-C4B	3.64	1.47	1.41
7	M	401	BCB	OBD-CAD	3.63	1.28	1.22
7	M	401	BCB	O2D-CGD	3.60	1.42	1.33
7	M	401	BCB	C3D-C2D	3.59	1.48	1.39
5	C	401	HEC	CBC-CAC	-3.56	1.35	1.51
7	M	401	BCB	CHB-C1B	3.55	1.47	1.39
5	C	404	HEC	CBC-CAC	-3.54	1.35	1.51
7	L	302	BCB	O2A-CGA	3.50	1.43	1.33
8	L	303	BPB	C3A-C2A	-3.45	1.51	1.54
5	C	403	HEC	FE-NB	3.43	2.05	1.94
7	L	301	BCB	C1D-ND	-3.37	1.33	1.37
5	C	402	HEC	CBB-CAB	-3.35	1.36	1.51
5	C	401	HEC	FE-NB	3.31	2.05	1.94
5	C	403	HEC	CBC-CAC	-3.30	1.36	1.51
8	M	403	BPB	O2A-CGA	3.26	1.42	1.33
8	M	403	BPB	C4C-NC	-3.24	1.27	1.37
8	L	303	BPB	O2A-CGA	3.22	1.42	1.33
7	L	302	BCB	CHD-C1D	3.17	1.44	1.38
7	L	301	BCB	O2A-CGA	3.17	1.42	1.33
7	M	402	BCB	O2A-CGA	3.11	1.42	1.33
7	L	301	BCB	CHB-C1B	3.06	1.46	1.39
7	L	302	BCB	CHB-C1B	3.02	1.46	1.39
7	M	402	BCB	CHB-C1B	3.02	1.46	1.39
5	C	403	HEC	CMC-C2C	3.02	1.57	1.50
5	C	401	HEC	FE-NC	3.01	2.05	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	301	BCB	C1B-C2B	2.98	1.50	1.43
7	L	302	BCB	C3D-C2D	2.98	1.47	1.39
7	M	402	BCB	C3D-C2D	2.93	1.47	1.39
7	M	402	BCB	C1D-ND	-2.88	1.34	1.37
7	M	401	BCB	CHD-C1D	2.85	1.43	1.38
12	M	405	NS5	C29-C30	2.85	1.52	1.43
7	M	402	BCB	CHD-C4C	2.83	1.45	1.39
7	M	401	BCB	C3B-C4B	2.81	1.46	1.41
12	M	405	NS5	C30-C31	2.79	1.37	1.34
7	L	302	BCB	OBD-CAD	2.75	1.27	1.22
7	L	302	BCB	CHD-C4C	2.74	1.45	1.39
8	L	303	BPB	C1D-ND	-2.74	1.33	1.38
5	C	401	HEC	CMA-C3A	2.72	1.56	1.50
5	C	402	HEC	CMB-C2B	2.63	1.56	1.50
8	L	303	BPB	C4C-NC	-2.62	1.29	1.37
8	L	303	BPB	CHA-CBD	-2.58	1.48	1.51
8	M	403	BPB	C3A-C2A	-2.53	1.52	1.54
7	M	401	BCB	C1B-NB	-2.52	1.34	1.37
7	L	301	BCB	CHD-C1D	2.51	1.43	1.38
7	M	402	BCB	C1B-C2B	2.47	1.49	1.43
7	L	301	BCB	C3D-C2D	2.47	1.45	1.39
5	C	401	HEC	CMB-C2B	2.45	1.56	1.50
8	M	403	BPB	C1D-ND	-2.43	1.34	1.38
7	L	301	BCB	CHD-C4C	2.38	1.44	1.39
7	M	401	BCB	C4D-CHA	2.38	1.46	1.38
7	L	301	BCB	C1B-NB	-2.37	1.34	1.37
7	L	301	BCB	C3D-C4D	-2.37	1.38	1.44
7	M	401	BCB	C3D-C4D	-2.35	1.38	1.44
7	M	401	BCB	C1B-C2B	2.28	1.48	1.43
5	C	403	HEC	C4C-C3C	2.26	1.49	1.44
7	M	402	BCB	CHD-C1D	2.26	1.42	1.38
9	L	305	MPG	C21-CXD	2.22	1.55	1.51
5	C	401	HEC	O2D-CGD	-2.19	1.23	1.30
7	L	302	BCB	C1D-ND	-2.16	1.35	1.37
7	L	302	BCB	C1B-NB	-2.14	1.35	1.37
7	L	301	BCB	C4D-CHA	2.13	1.46	1.38
5	C	404	HEC	O1D-CGD	2.12	1.29	1.22
9	L	304	MPG	C21-CXD	2.12	1.55	1.51
8	L	303	BPB	CBD-CGD	-2.11	1.49	1.52
8	M	403	BPB	C4B-NB	-2.10	1.34	1.38
7	M	402	BCB	C4D-CHA	2.08	1.45	1.38
7	L	302	BCB	C1B-C2B	2.06	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	403	HEC	FE-NC	2.06	2.02	1.95
5	C	402	HEC	FE-NC	2.05	2.02	1.95
5	C	404	HEC	CHD-C4C	-2.01	1.34	1.39

All (197) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	M	401	BCB	C1C-NC-C4C	-20.68	97.41	106.71
7	L	302	BCB	C1C-NC-C4C	-17.91	98.66	106.71
7	L	301	BCB	C1C-NC-C4C	-17.81	98.70	106.71
7	M	402	BCB	C1C-NC-C4C	-17.02	99.05	106.71
7	L	301	BCB	C2B-C1B-NB	7.59	115.32	110.23
8	L	303	BPB	C2B-C1B-NB	7.22	114.51	109.53
7	M	402	BCB	C2B-C1B-NB	7.11	115.00	110.23
7	M	401	BCB	C2B-C1B-NB	7.07	114.97	110.23
7	M	402	BCB	C4D-C3D-CAD	-6.92	99.93	108.10
5	C	402	HEC	C1D-ND-C4D	6.90	112.20	105.07
8	M	403	BPB	O2D-CGD-CBD	6.79	119.59	111.00
8	L	303	BPB	C3D-C4D-ND	6.74	116.90	107.72
7	L	302	BCB	C4D-C3D-CAD	-6.69	100.22	108.10
7	L	301	BCB	CMD-C2D-C1D	6.56	136.28	124.71
5	C	403	HEC	C1D-ND-C4D	6.55	111.84	105.07
7	M	401	BCB	C4D-C3D-CAD	-6.48	100.46	108.10
5	C	401	HEC	C1D-ND-C4D	6.39	111.67	105.07
8	M	403	BPB	C3D-C4D-ND	6.39	116.42	107.72
7	L	302	BCB	CMD-C2D-C1D	6.37	135.94	124.71
8	M	403	BPB	C2B-C1B-NB	6.33	113.90	109.53
7	L	302	BCB	C2B-C1B-NB	6.23	114.41	110.23
8	M	403	BPB	CBC-CAC-C3C	-5.80	111.30	126.70
12	M	405	NS5	C29-C28-C26	-5.74	110.28	126.42
8	L	303	BPB	OBD-CAD-C3D	-5.72	118.48	127.98
9	L	305	MPG	O1-CX3-CXD	5.63	122.90	111.68
9	L	304	MPG	O1-CX3-CXD	5.41	122.46	111.68
5	C	404	HEC	C1D-ND-C4D	5.29	110.54	105.07
7	L	302	BCB	C2D-C1D-ND	5.17	113.92	110.10
7	L	301	BCB	C4D-C3D-CAD	-5.16	102.01	108.10
7	M	402	BCB	O2D-CGD-CBD	5.15	120.41	111.27
7	M	402	BCB	O2D-CGD-O1D	-5.13	113.81	123.84
7	L	301	BCB	C4-C3-C5	5.07	123.80	115.27
7	L	301	BCB	C1D-ND-C4D	-4.87	102.87	106.33
7	L	301	BCB	C1-C2-C3	-4.87	117.62	126.04
8	M	403	BPB	C4D-CHA-CBD	-4.81	106.34	108.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	M	401	BCB	CMD-C2D-C1D	4.76	133.10	124.71
8	M	403	BPB	C4D-ND-C1D	-4.66	104.09	108.83
6	C	405	DGA	OG2-CB1-CB2	4.63	121.47	111.50
8	L	303	BPB	C4D-CHA-CBD	-4.61	106.43	108.52
7	M	401	BCB	OBD-CAD-C3D	-4.52	117.64	128.52
12	M	405	NS5	C18-C17-C15	-4.51	120.87	127.31
7	M	402	BCB	C2D-C1D-ND	4.51	113.43	110.10
8	L	303	BPB	CBC-CAC-C3C	-4.50	114.77	126.70
7	L	301	BCB	OBD-CAD-C3D	-4.47	117.76	128.52
7	L	302	BCB	C1D-ND-C4D	-4.40	103.21	106.33
5	C	403	HEC	C4B-NB-C1B	4.28	109.50	105.07
7	L	301	BCB	C2D-C1D-ND	4.26	113.24	110.10
8	L	303	BPB	C4D-ND-C1D	-4.26	104.50	108.83
7	M	402	BCB	C4D-CHA-C1A	4.22	126.39	121.25
7	M	401	BCB	C2D-C1D-ND	4.21	113.20	110.10
7	L	301	BCB	C3D-C4D-ND	4.14	116.94	110.24
12	M	405	NS5	C19-C18-C17	4.12	131.91	123.47
7	M	402	BCB	CMD-C2D-C1D	4.10	131.94	124.71
8	L	303	BPB	O2D-CGD-CBD	4.09	116.18	111.00
7	L	302	BCB	C3D-C4D-ND	4.09	116.86	110.24
9	L	304	MPG	O1-CX3-O4	-4.07	116.43	124.13
12	M	405	NS5	CM3-C36-C35	-4.04	110.96	122.65
7	M	401	BCB	C2C-C1C-CHC	-4.04	114.14	123.64
7	L	302	BCB	OBD-CAD-C3D	-4.01	118.86	128.52
7	M	402	BCB	C3D-C4D-ND	3.99	116.69	110.24
8	M	403	BPB	OBD-CAD-C3D	-3.91	121.49	127.98
7	M	402	BCB	OBD-CAD-C3D	-3.91	119.12	128.52
5	C	402	HEC	C4B-NB-C1B	3.89	109.09	105.07
5	C	403	HEC	CBC-CAC-C3C	3.82	122.97	112.43
8	M	403	BPB	C2D-C1D-ND	3.76	112.12	109.53
7	L	301	BCB	O2D-CGD-CBD	3.73	117.90	111.27
12	M	405	NS5	C34-C35-C36	-3.72	115.04	127.75
8	M	403	BPB	O2D-CGD-O1D	-3.71	116.59	123.84
7	M	401	BCB	C3D-C4D-ND	3.68	116.19	110.24
7	L	301	BCB	CMD-C2D-C3D	-3.66	119.19	127.61
12	M	405	NS5	C24-C25-C26	-3.64	122.12	127.31
5	C	401	HEC	CMD-C2D-C1D	3.61	130.54	125.04
8	L	303	BPB	C2D-C1D-ND	3.59	112.01	109.53
7	M	401	BCB	CHC-C1C-NC	-3.59	119.55	124.51
5	C	403	HEC	C3B-C4B-NB	-3.57	106.19	110.17
7	M	402	BCB	CAD-C3D-C2D	3.54	157.88	140.80
7	L	302	BCB	CHD-C4C-C3C	-3.53	121.47	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	401	HEC	C4A-NA-C1A	3.51	108.79	105.35
7	L	301	BCB	CHC-C1C-NC	-3.51	119.66	124.51
8	M	403	BPB	C4-C3-C5	3.51	121.17	115.27
7	M	402	BCB	C4A-NA-C1A	3.49	108.28	106.71
7	L	301	BCB	C4A-NA-C1A	3.48	108.27	106.71
9	L	305	MPG	O1-CX3-O4	-3.46	117.57	124.13
7	M	401	BCB	CAD-C3D-C2D	3.45	157.46	140.80
7	L	301	BCB	CHD-C4C-C3C	-3.41	121.62	125.89
7	L	302	BCB	O2D-CGD-CBD	3.38	117.27	111.27
7	M	402	BCB	C2C-C1C-CHC	-3.37	115.70	123.64
7	L	302	BCB	CHC-C1C-NC	-3.35	119.89	124.51
7	L	301	BCB	O2D-CGD-O1D	-3.31	117.36	123.84
7	L	302	BCB	C2C-C1C-CHC	-3.29	115.89	123.64
7	M	401	BCB	O2D-CGD-CBD	3.28	117.11	111.27
7	M	402	BCB	CAA-C2A-C1A	3.28	122.74	111.97
13	M	408	PO4	O3-P-O1	-3.27	98.92	110.89
8	L	303	BPB	CMB-C2B-C3B	3.24	130.74	124.68
7	L	302	BCB	CAD-C3D-C2D	3.24	156.42	140.80
7	M	402	BCB	C1D-ND-C4D	-3.23	104.04	106.33
7	L	301	BCB	C2C-C1C-CHC	-3.19	116.12	123.64
7	L	301	BCB	CAA-C2A-C1A	3.17	122.35	111.97
12	M	405	NS5	C22-C21-C20	3.12	127.30	122.92
5	C	401	HEC	C3D-C4D-ND	-3.11	107.34	110.36
12	M	405	NS5	CM4-C36-C35	-3.08	113.75	122.65
7	L	301	BCB	CAD-C3D-C2D	3.06	155.57	140.80
5	C	401	HEC	C2A-C1A-NA	-3.02	107.39	110.32
8	L	303	BPB	C3D-CAD-CBD	2.99	111.55	107.61
5	C	404	HEC	CAA-CBA-CGA	-2.97	107.20	113.60
7	M	402	BCB	CHC-C1C-NC	-2.95	120.43	124.51
5	C	401	HEC	CBD-CAD-C3D	-2.95	104.42	112.63
7	L	302	BCB	CMB-C2B-C3B	2.91	133.79	125.93
7	M	402	BCB	C4-C3-C5	2.91	120.16	115.27
5	C	404	HEC	CBC-CAC-C3C	2.90	120.42	112.43
5	C	402	HEC	C3B-C4B-NB	-2.88	106.96	110.17
8	M	403	BPB	C1-C2-C3	-2.85	121.11	126.04
5	C	403	HEC	CAD-C3D-C4D	2.85	129.63	124.66
7	L	301	BCB	O2A-CGA-O1A	-2.84	116.43	123.59
8	M	403	BPB	CMD-C2D-C3D	-2.82	119.41	124.68
7	M	402	BCB	C1D-CHD-C4C	-2.80	120.03	126.06
6	C	405	DGA	OG1-CA1-CA2	2.79	120.68	111.91
11	M	404	MQ7	C24-C23-C25	2.78	119.94	115.27
5	C	401	HEC	C4B-NB-C1B	2.77	107.94	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	M	403	BPB	CMC-C2C-C1C	-2.73	109.77	114.36
7	M	401	BCB	CHC-C4B-C3B	-2.72	122.69	132.35
11	M	404	MQ7	C34-C33-C35	2.70	119.81	115.27
7	L	302	BCB	CMD-C2D-C3D	-2.68	121.44	127.61
5	C	404	HEC	C4B-NB-C1B	2.68	107.84	105.07
7	M	402	BCB	CMB-C2B-C3B	2.66	133.12	125.93
7	L	302	BCB	CHB-C1B-C2B	-2.65	119.75	127.24
7	M	402	BCB	CHA-C4D-ND	-2.64	126.97	132.50
8	M	403	BPB	C3D-CAD-CBD	2.63	111.07	107.61
12	M	405	NS5	C8-C9-C10	2.62	121.61	112.98
12	M	405	NS5	CM4-C36-CM3	-2.60	108.86	114.60
12	M	405	NS5	C9-C8-C7	2.59	120.38	111.88
5	C	402	HEC	CBC-CAC-C3C	2.57	119.52	112.43
5	C	402	HEC	O1D-CGD-CBD	-2.56	114.87	123.08
7	M	401	BCB	C1D-ND-C4D	-2.54	104.53	106.33
7	M	401	BCB	O2D-CGD-O1D	-2.54	118.88	123.84
8	M	403	BPB	OBB-CAB-C3B	2.53	124.48	119.99
5	C	402	HEC	CHB-C4A-NA	2.52	127.16	124.44
7	M	402	BCB	CHD-C4C-C3C	-2.52	122.74	125.89
7	L	302	BCB	O1D-CGD-CBD	-2.50	119.38	124.48
7	L	302	BCB	CHC-C4B-C3B	-2.47	123.55	132.35
12	M	405	NS5	C30-C29-C28	-2.46	115.53	123.22
8	M	403	BPB	C3B-C4B-NB	2.46	111.72	108.04
12	M	405	NS5	C18-C19-C20	2.45	128.48	123.47
5	C	403	HEC	C4A-NA-C1A	2.43	107.72	105.35
7	M	402	BCB	C1-O2A-CGA	2.41	122.78	116.44
7	M	401	BCB	CMB-C2B-C1B	2.40	129.03	125.37
8	L	303	BPB	C4A-C3A-C2A	-2.39	100.56	102.84
12	M	405	NS5	C23-C21-C20	-2.39	115.28	118.94
5	C	403	HEC	C2A-C1A-NA	-2.39	108.00	110.32
5	C	402	HEC	O2D-CGD-CBD	2.38	121.67	114.03
8	L	303	BPB	CED-O2D-CGD	2.38	121.31	115.94
7	L	302	BCB	C3D-C2D-C1D	-2.35	102.62	105.83
7	M	401	BCB	C1-C2-C3	-2.35	121.98	126.04
5	C	401	HEC	C1D-C2D-C3D	-2.35	104.49	106.96
13	M	408	PO4	O4-P-O2	2.34	115.48	107.97
5	C	403	HEC	CHA-C1A-NA	2.33	126.96	124.44
8	L	303	BPB	C1-C2-C3	-2.33	122.02	126.04
7	L	301	BCB	CMB-C2B-C1B	2.29	128.86	125.37
7	M	402	BCB	CHB-C1B-C2B	-2.27	120.82	127.24
8	L	303	BPB	CMA-C3A-C4A	-2.27	109.40	114.38
13	M	407	PO4	O3-P-O1	-2.27	102.59	110.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	L	301	BCB	C7-C6-C5	-2.26	107.21	113.36
11	M	404	MQ7	C21-C22-C23	-2.24	122.28	127.66
7	L	302	BCB	C1D-CHD-C4C	-2.23	121.25	126.06
7	L	301	BCB	CHC-C4B-C3B	-2.21	124.48	132.35
8	L	303	BPB	CBA-CAA-C2A	-2.21	107.36	113.81
7	L	302	BCB	C5-C3-C2	-2.21	116.65	121.12
7	L	301	BCB	C5-C3-C2	-2.21	116.65	121.12
5	C	401	HEC	CBB-CAB-C3B	2.20	118.50	112.43
5	C	402	HEC	C4C-NC-C1C	2.20	107.50	105.35
13	M	407	PO4	O4-P-O3	2.19	115.01	107.97
7	L	302	BCB	CHA-C4D-ND	-2.18	127.94	132.50
7	L	301	BCB	O2A-CGA-CBA	2.17	118.73	111.91
5	C	404	HEC	C2A-C1A-NA	-2.17	108.21	110.32
5	C	403	HEC	CHB-C1B-NB	2.15	126.75	124.42
5	C	403	HEC	CBB-CAB-C3B	2.14	118.34	112.43
8	M	403	BPB	CBB-CAB-C3B	-2.14	113.99	120.34
5	C	402	HEC	C3D-C4D-ND	-2.13	108.29	110.36
7	L	301	BCB	CHD-C1D-ND	-2.11	122.52	124.45
11	M	404	MQ7	C26-C27-C28	-2.10	122.60	127.66
7	L	301	BCB	CED-O2D-CGD	2.10	120.69	115.94
12	M	405	NS5	C11-C10-C9	2.07	118.75	115.27
11	M	404	MQ7	C45-C43-C44	2.07	119.17	114.60
5	C	403	HEC	C4C-NC-C1C	2.07	107.37	105.35
7	M	401	BCB	CMD-C2D-C3D	-2.06	122.87	127.61
5	C	402	HEC	CMD-C2D-C1D	2.05	128.16	125.04
7	L	302	BCB	C2A-C1A-CHA	-2.04	120.28	123.86
7	L	301	BCB	C3C-C4C-NC	2.03	112.79	110.57
11	M	404	MQ7	C19-C18-C20	2.02	118.68	115.27
7	M	402	BCB	CMA-C3A-C4A	2.02	117.19	111.77
5	C	402	HEC	C1D-C2D-C3D	-2.02	104.84	106.96
5	C	402	HEC	CBD-CAD-C3D	-2.02	107.03	112.63
5	C	404	HEC	CAD-CBD-CGD	-2.01	109.27	113.60
5	C	404	HEC	CHB-C4A-NA	2.01	126.62	124.44
9	L	305	MPG	C1-O1-CX3	2.01	120.83	116.58
7	M	402	BCB	CHC-C4B-C3B	-2.01	125.22	132.35
7	L	302	BCB	C11-C12-C13	-2.00	109.45	115.92

All (16) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	C	401	HEC	NA
5	C	402	HEC	NA

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Mol	Chain	Res	Type	Atom
5	C	403	HEC	NA
5	C	404	HEC	NA
7	L	301	BCB	ND
7	L	301	BCB	NA
7	L	301	BCB	NC
7	L	302	BCB	ND
7	L	302	BCB	NA
7	L	302	BCB	NC
7	M	401	BCB	ND
7	M	401	BCB	NA
7	M	401	BCB	NC
7	M	402	BCB	ND
7	M	402	BCB	NA
7	M	402	BCB	NC

All (133) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	405	DGA	CA2-CA1-OG1-CG1
6	C	405	DGA	OA1-CA1-OG1-CG1
6	C	405	DGA	OG1-CG1-CG2-OG2
6	C	405	DGA	OG1-CG1-CG2-CG3
7	L	302	BCB	C2C-C3C-CAC-CBC
7	M	402	BCB	CAD-CBD-CGD-O1D
7	M	402	BCB	CAD-CBD-CGD-O2D
8	L	303	BPB	C2C-C3C-CAC-CBC
8	M	403	BPB	C2C-C3C-CAC-CBC
9	L	304	MPG	CXD-CX3-O1-C1
9	L	304	MPG	O4-CX3-O1-C1
9	L	304	MPG	O3-C21-CXD-O2
9	L	304	MPG	O1-CX3-CXD-C21
9	L	304	MPG	O4-CX3-CXD-C21
9	L	305	MPG	O3-C21-CXD-O2
9	L	305	MPG	O1-CX3-CXD-C21
12	M	405	NS5	C25-C26-C28-C29
12	M	405	NS5	C27-C26-C28-C29
12	M	405	NS5	C26-C28-C29-C30
12	M	405	NS5	C28-C29-C30-C31
12	M	405	NS5	C2-C3-C4-C5
7	M	402	BCB	C2A-CAA-CBA-CGA
5	C	403	HEC	C2B-C3B-CAB-CBB
12	M	405	NS5	C34-C35-C36-CM4

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Mol	Chain	Res	Type	Atoms
7	L	301	BCB	C4-C3-C5-C6
12	M	405	NS5	C11-C10-C9-C8
7	L	301	BCB	C2-C3-C5-C6
12	M	405	NS5	C12-C10-C9-C8
5	C	401	HEC	C2B-C3B-CAB-CBB
5	C	404	HEC	C2B-C3B-CAB-CBB
7	M	401	BCB	C14-C13-C15-C16
8	M	403	BPB	C11-C10-C8-C9
5	C	403	HEC	C4B-C3B-CAB-CBB
7	L	301	BCB	C15-C16-C17-C18
12	M	405	NS5	C34-C35-C36-CM3
5	C	401	HEC	C2C-C3C-CAC-CBC
12	M	405	NS5	C32-C31-C33-C34
9	L	305	MPG	O1-C1-C2-C3
9	L	304	MPG	C5-C6-C7-C8
7	L	302	BCB	C16-C17-C18-C19
9	L	305	MPG	C11-C12-C13-C14
9	L	305	MPG	C12-C13-C14-C15
9	L	304	MPG	C2-C3-C4-C5
6	C	405	DGA	CB6-CB7-CB8-CB9
9	L	304	MPG	C12-C13-C14-C15
8	M	403	BPB	C8-C10-C11-C12
5	C	401	HEC	C4B-C3B-CAB-CBB
7	L	302	BCB	C16-C17-C18-C20
6	C	405	DGA	CCB-CDB-CEB-CFB
5	C	402	HEC	C2B-C3B-CAB-CBB
9	L	304	MPG	C10-C11-C12-C13
9	L	305	MPG	O4-CX3-O1-C1
6	C	405	DGA	CDB-CEB-CFB-CGB
7	M	401	BCB	C15-C16-C17-C18
9	M	406	MPG	C3-C4-C5-C6
8	M	403	BPB	C6-C7-C8-C10
9	L	305	MPG	CXD-CX3-O1-C1
5	C	404	HEC	C4B-C3B-CAB-CBB
5	C	401	HEC	C4C-C3C-CAC-CBC
12	M	405	NS5	C30-C31-C33-C34
8	M	403	BPB	C6-C7-C8-C9
5	C	403	HEC	C2C-C3C-CAC-CBC
6	C	405	DGA	CBB-CAB-CB9-CB8
8	L	303	BPB	C4-C3-C5-C6
6	C	405	DGA	CEB-CFB-CGB-CHB
9	M	406	MPG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
7	M	401	BCB	C4-C3-C5-C6
8	L	303	BPB	C2-C3-C5-C6
7	M	401	BCB	C2-C3-C5-C6
8	M	403	BPB	C3-C5-C6-C7
7	L	302	BCB	C11-C12-C13-C14
8	M	403	BPB	C11-C12-C13-C14
9	L	304	MPG	O3-C21-CXD-CX3
9	L	305	MPG	O3-C21-CXD-CX3
6	C	405	DGA	CB9-CAB-CBB-CCB
5	C	403	HEC	C4C-C3C-CAC-CBC
6	C	405	DGA	CA6-CA7-CA8-CA9
12	M	405	NS5	C1-C2-C3-C4
5	C	402	HEC	C3D-CAD-CBD-CGD
8	L	303	BPB	O2A-C1-C2-C3
6	C	405	DGA	CA7-CA8-CA9-CAA
9	L	304	MPG	C15-C16-C17-C18
6	C	405	DGA	CA5-CA6-CA7-CA8
7	L	302	BCB	C11-C12-C13-C15
7	M	401	BCB	C12-C13-C15-C16
8	M	403	BPB	C11-C10-C8-C7
8	M	403	BPB	C11-C12-C13-C15
8	L	303	BPB	C16-C17-C18-C19
9	L	305	MPG	O4-CX3-CXD-C21
7	M	401	BCB	CAD-CBD-CGD-O2D
8	L	303	BPB	CAD-CBD-CGD-O2D
8	M	403	BPB	CAD-CBD-CGD-O2D
8	L	303	BPB	C8-C10-C11-C12
8	M	403	BPB	C10-C11-C12-C13
9	L	305	MPG	C3-C4-C5-C6
7	L	301	BCB	C16-C17-C18-C20
9	L	304	MPG	C1-C2-C3-C4
7	L	301	BCB	CAD-CBD-CGD-O1D
7	M	402	BCB	C11-C12-C13-C14
9	L	304	MPG	C13-C14-C15-C16
5	C	402	HEC	C4B-C3B-CAB-CBB
9	L	304	MPG	O4-CX3-CXD-O2
7	M	402	BCB	C11-C12-C13-C15
5	C	402	HEC	CAA-CBA-CGA-O1A
9	L	305	MPG	C7-C8-C9-C10
9	L	305	MPG	C2-C1-O1-CX3
8	M	403	BPB	O2A-C1-C2-C3
8	M	403	BPB	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
11	M	404	MQ7	C39-C38-C40-C41
5	C	402	HEC	CAD-CBD-CGD-O1D
5	C	402	HEC	CAA-CBA-CGA-O2A
5	C	401	HEC	CAA-CBA-CGA-O1A
8	M	403	BPB	C14-C13-C15-C16
5	C	401	HEC	CAA-CBA-CGA-O2A
7	L	302	BCB	C2-C1-O2A-CGA
9	L	305	MPG	C14-C15-C16-C17
8	M	403	BPB	C4-C3-C5-C6
9	L	304	MPG	O1-C1-C2-C3
11	M	404	MQ7	C37-C38-C40-C41
8	M	403	BPB	C12-C13-C15-C16
5	C	402	HEC	CAD-CBD-CGD-O2D
7	L	302	BCB	CAD-CBD-CGD-O2D
9	L	304	MPG	C7-C8-C9-C10
9	M	406	MPG	C7-C8-C9-C10
7	M	402	BCB	CHA-CBD-CGD-O1D
7	M	402	BCB	CHA-CBD-CGD-O2D
7	L	302	BCB	C13-C15-C16-C17
11	M	404	MQ7	C38-C40-C41-C42
6	C	405	DGA	CA2-CA3-CA4-CA5
6	C	405	DGA	CA8-CA9-CAA-CBA
5	C	404	HEC	C4C-C3C-CAC-CBC
8	M	403	BPB	C2-C3-C5-C6
12	M	405	NS5	C31-C33-C34-C35

There are no ring outliers.

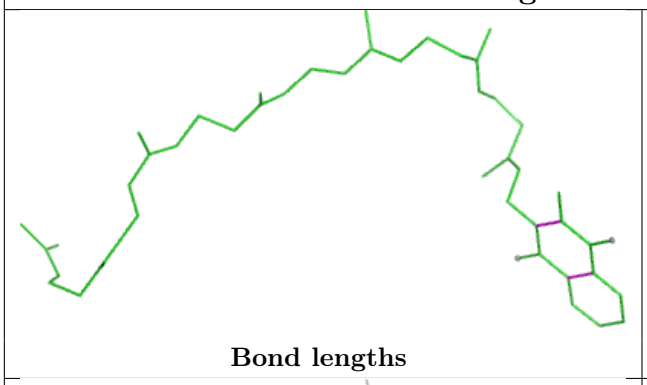
9 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	L	301	BCB	3	0
7	L	302	BCB	3	0
8	L	303	BPB	7	0
5	C	402	HEC	1	0
8	M	403	BPB	6	0
7	M	402	BCB	1	0
12	M	405	NS5	7	0
9	L	304	MPG	3	0
7	M	401	BCB	4	0

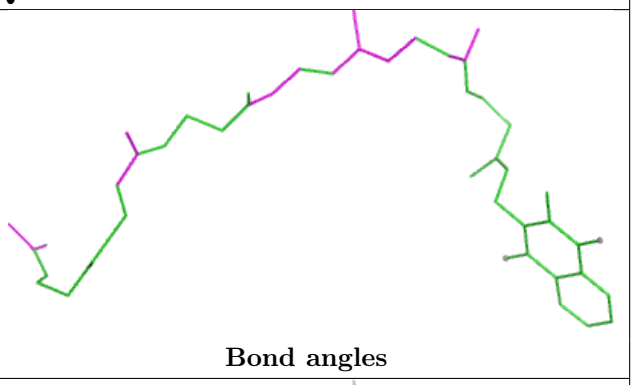
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

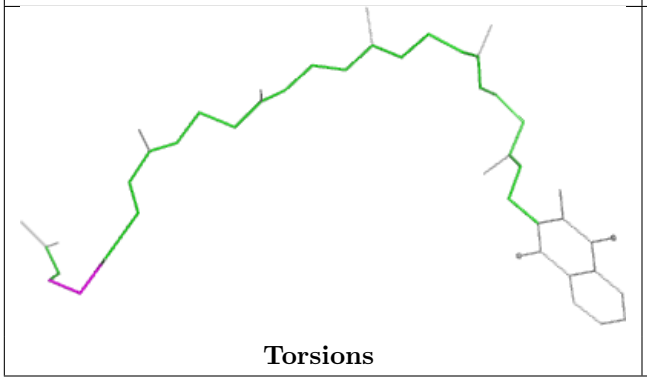
Ligand MQ7 M 404



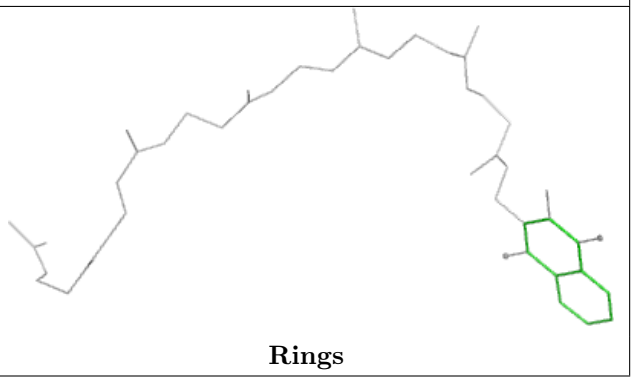
Bond lengths



Bond angles

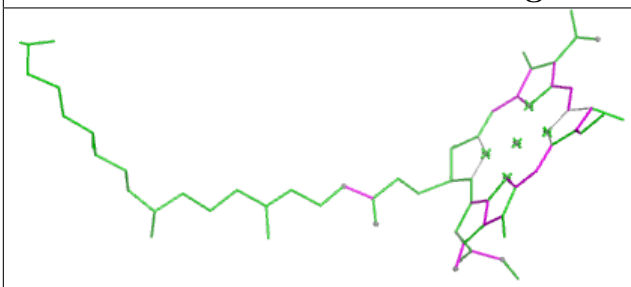


Torsions

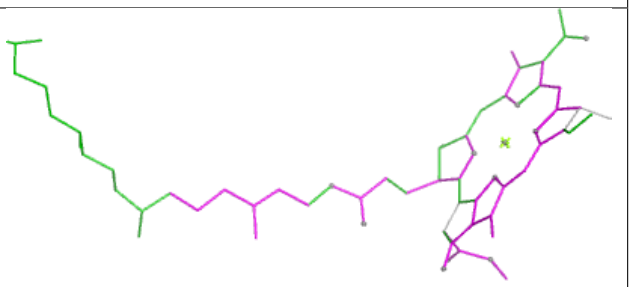


Rings

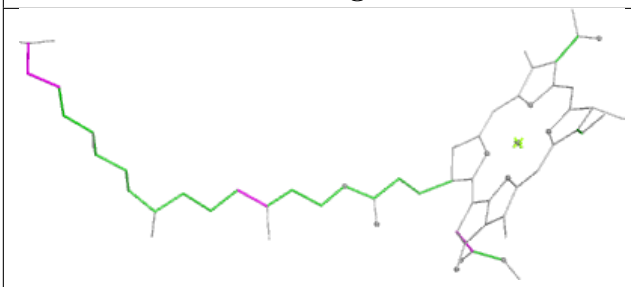
Ligand BCB L 301



Bond lengths



Bond angles



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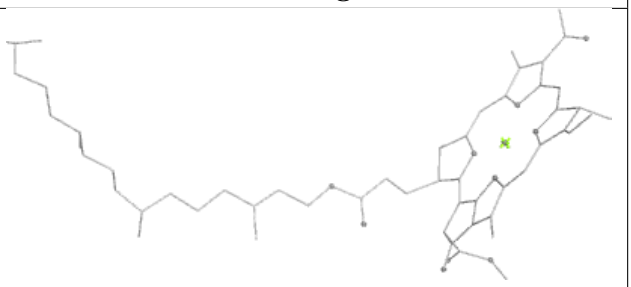
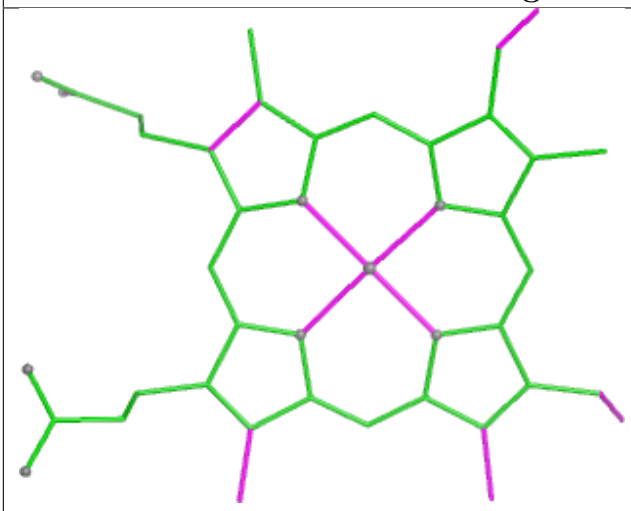
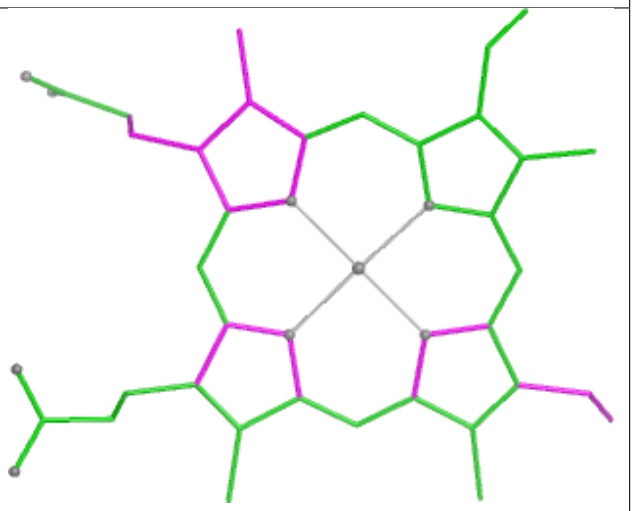


Rings

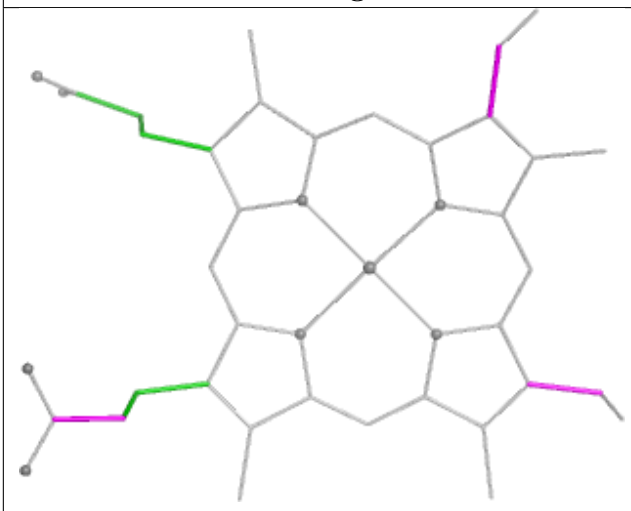
Ligand HEC C 401



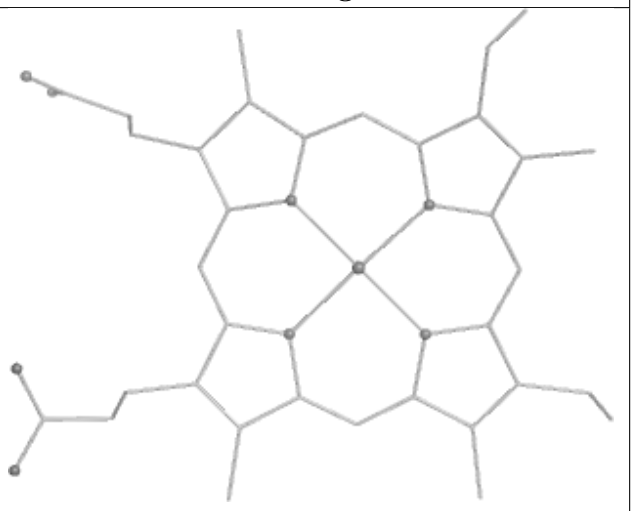
Bond lengths



Bond angles

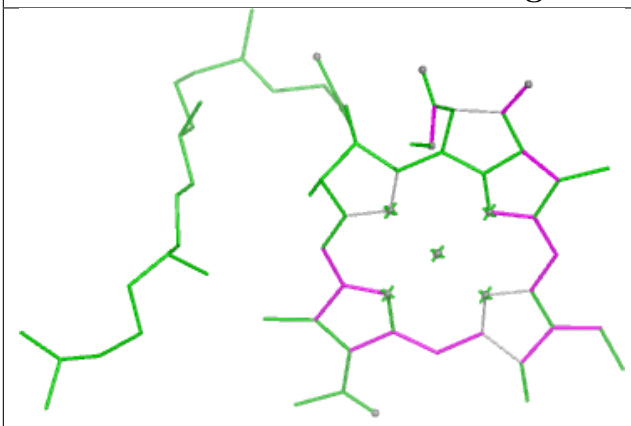


Torsions



Rings

Ligand BCB L 302



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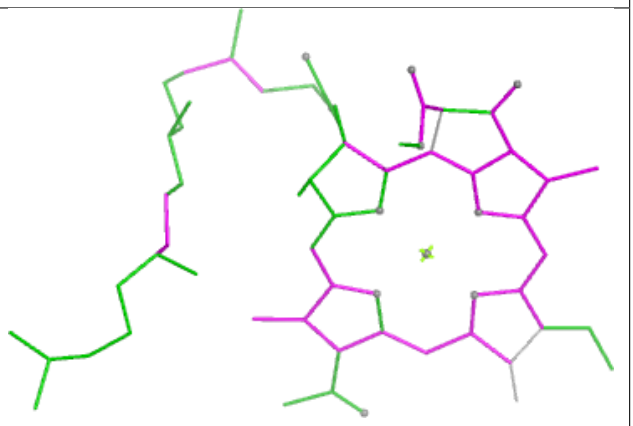

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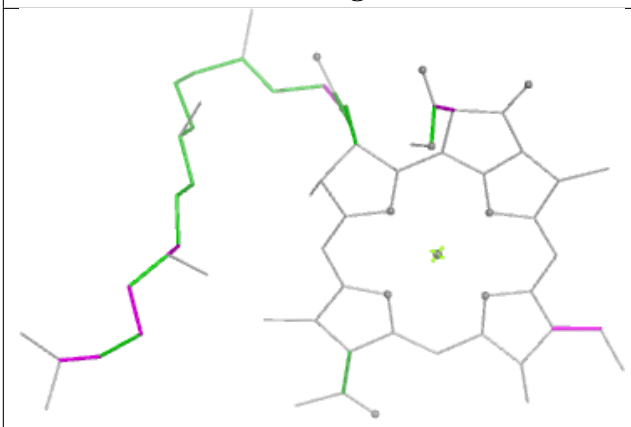
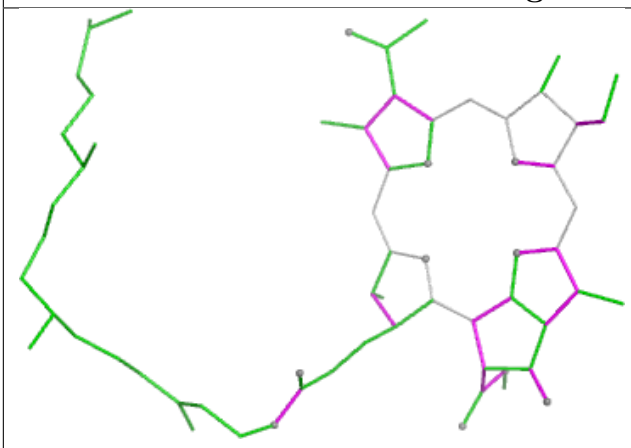


Torsions



Rings

Ligand BPB L 303



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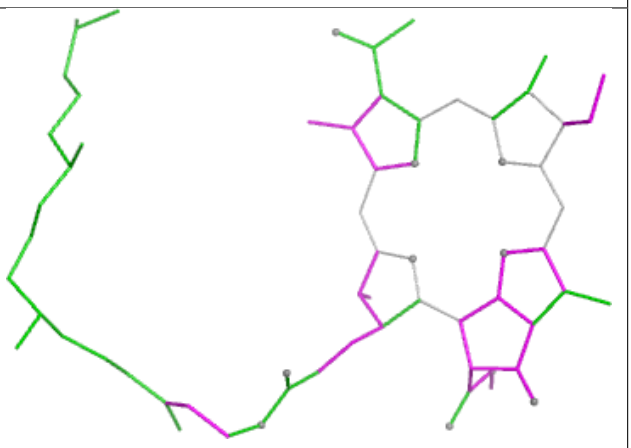
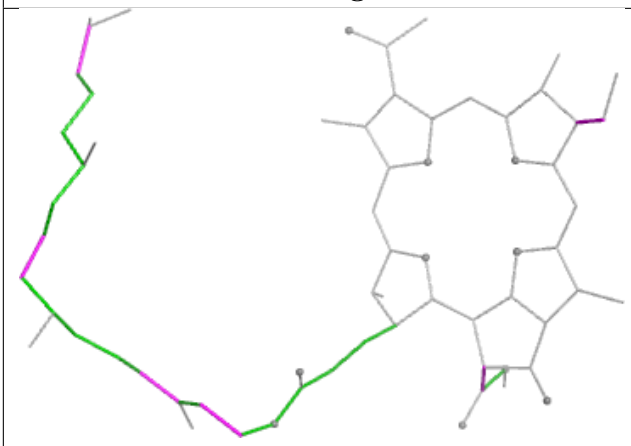


Bond angles



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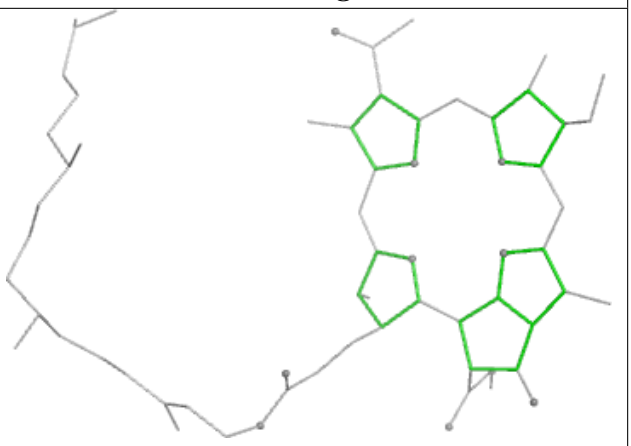
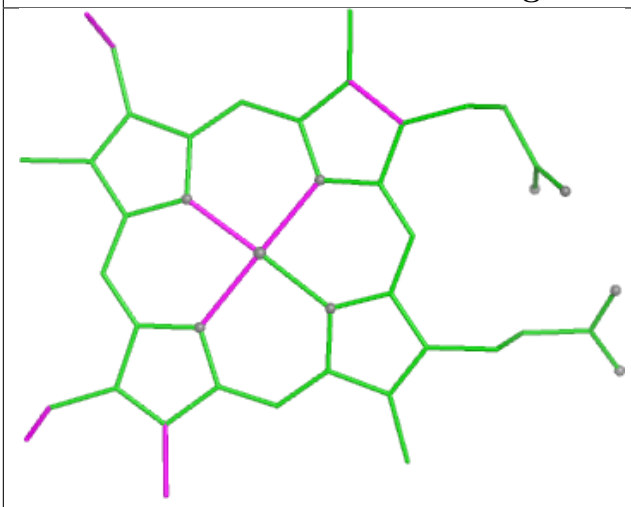


Rings

Ligand HEC C 402



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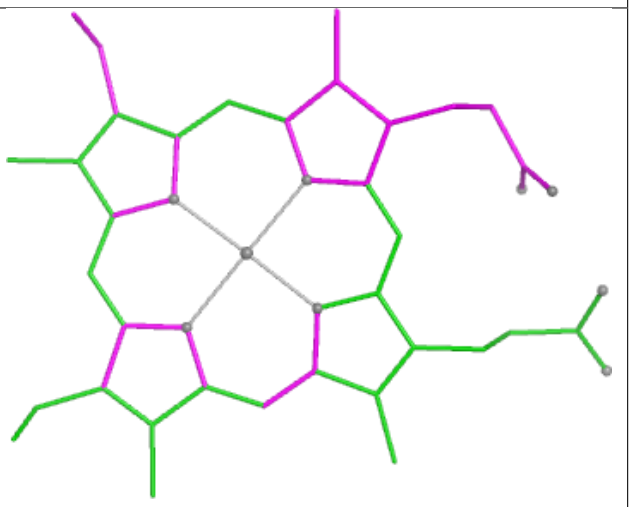

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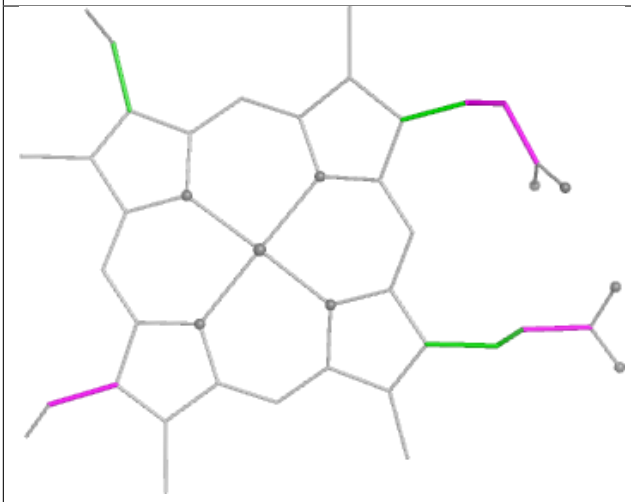

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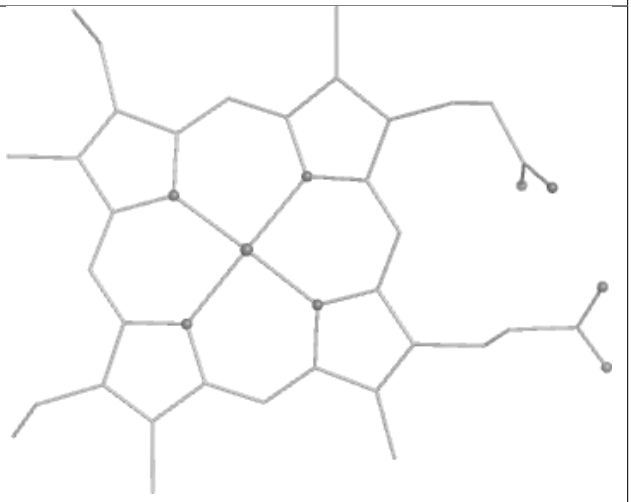
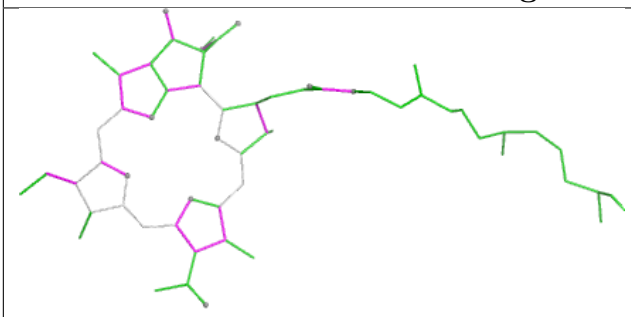


Rings

Ligand BPB M 403



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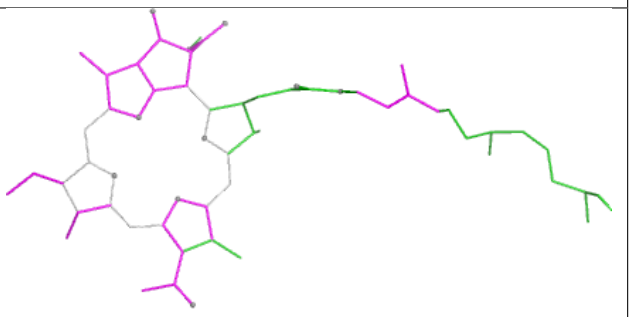
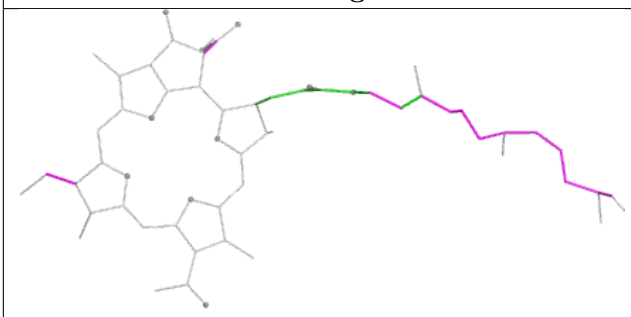


Bond angles



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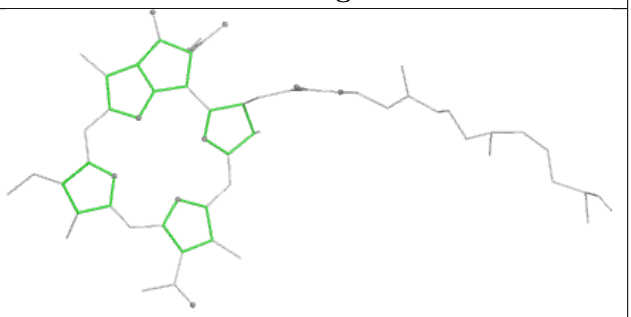

Rings

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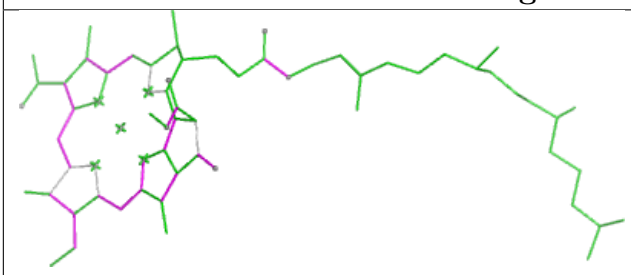

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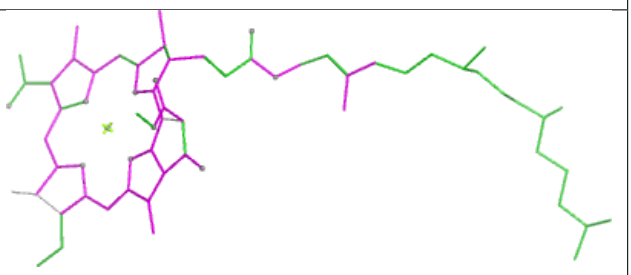

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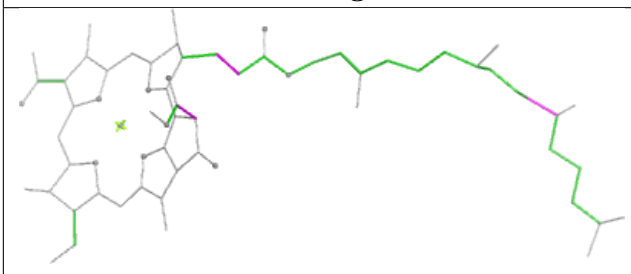

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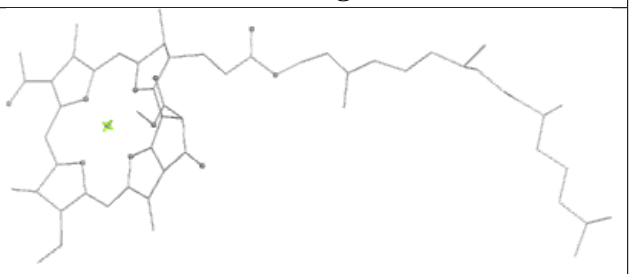
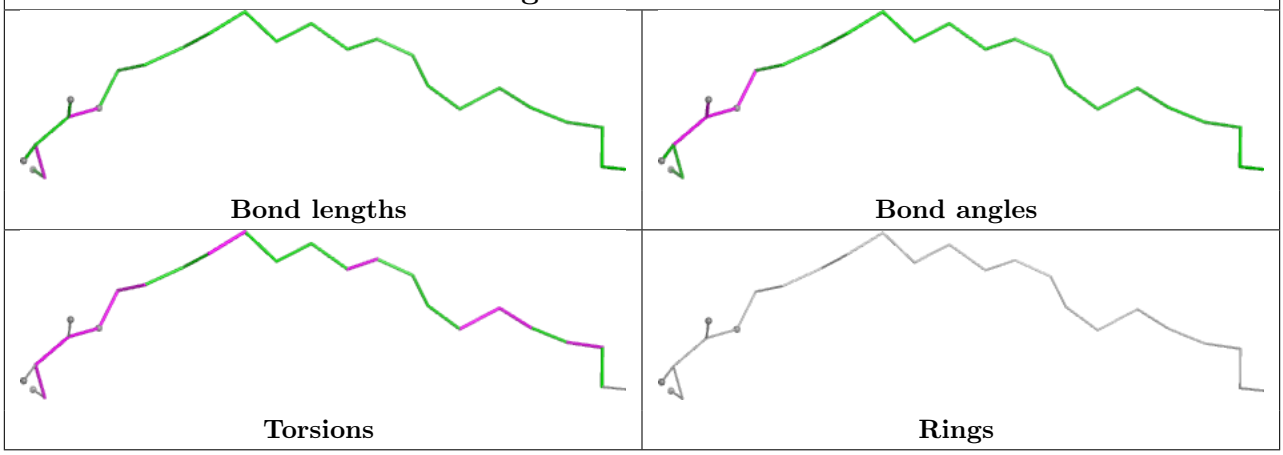
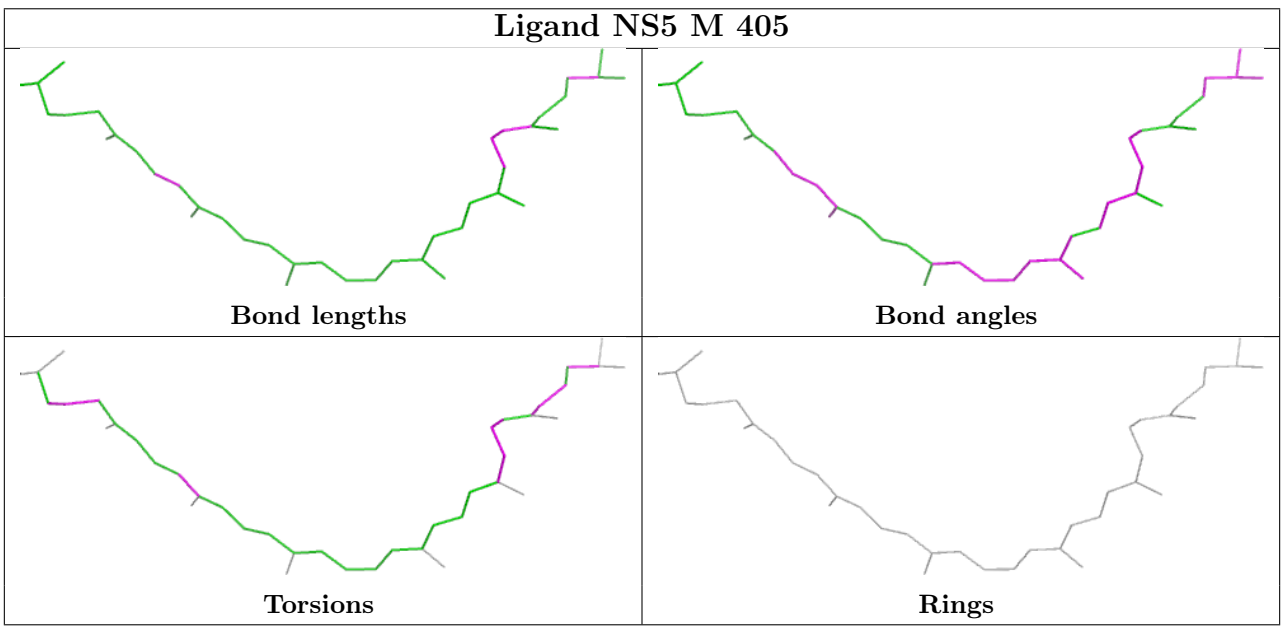


Rings

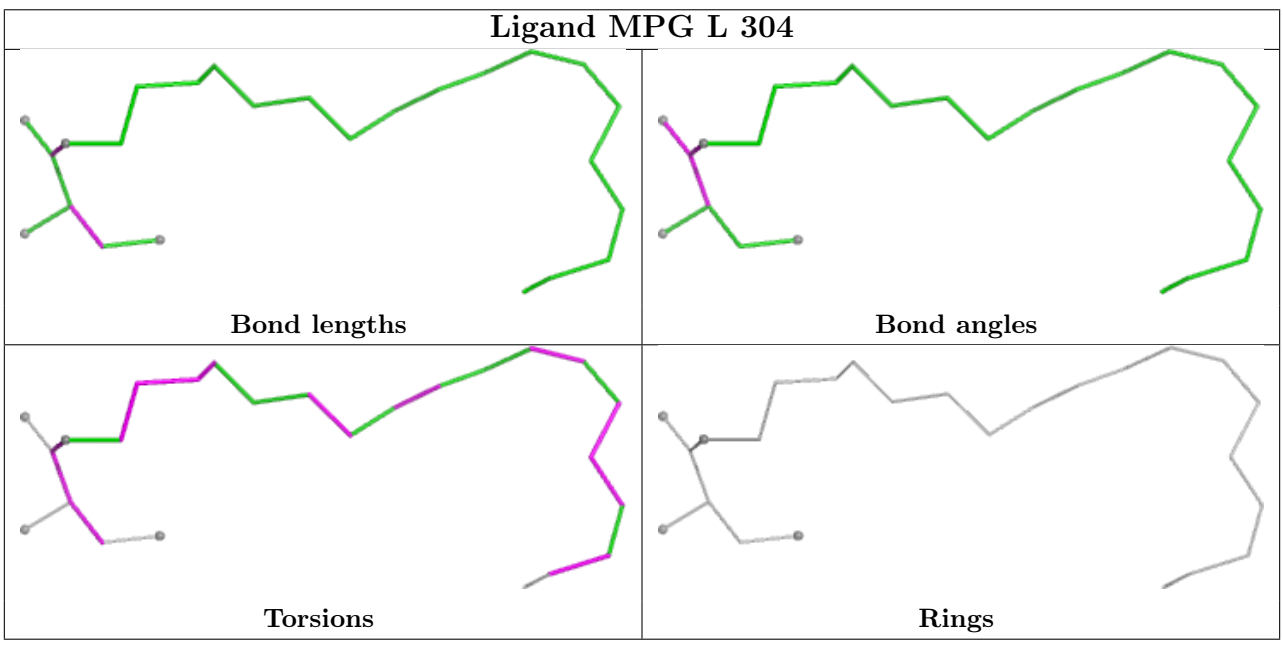
Ligand MPG L 305



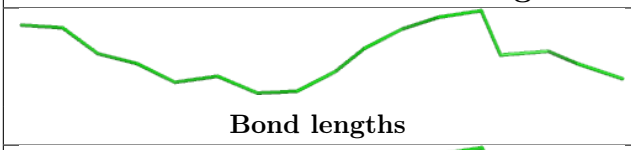
Ligand NS5 M 405



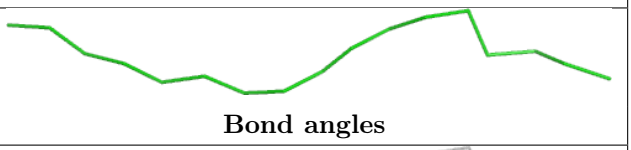
Ligand MPG L 304



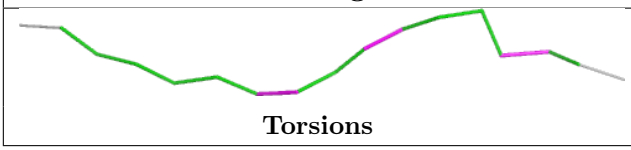
Ligand MPG M 406



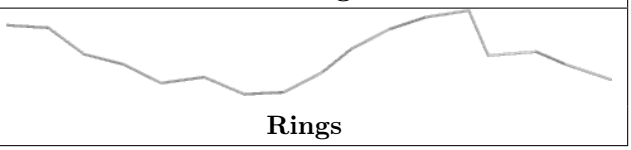
Bond lengths



Bond angles

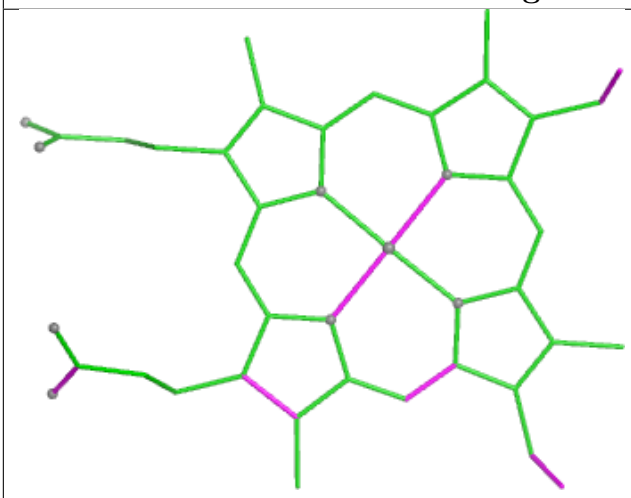


Torsions



Rings

Ligand HEC C 404



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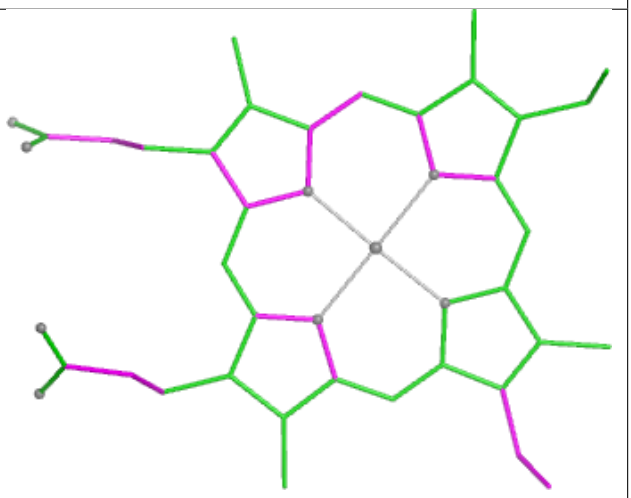
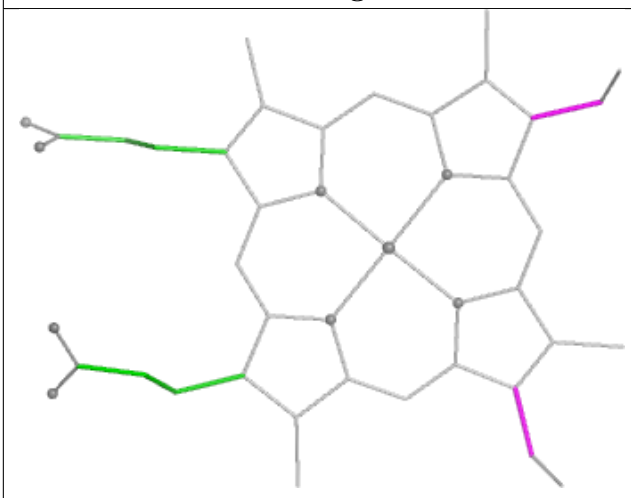


Bond angles



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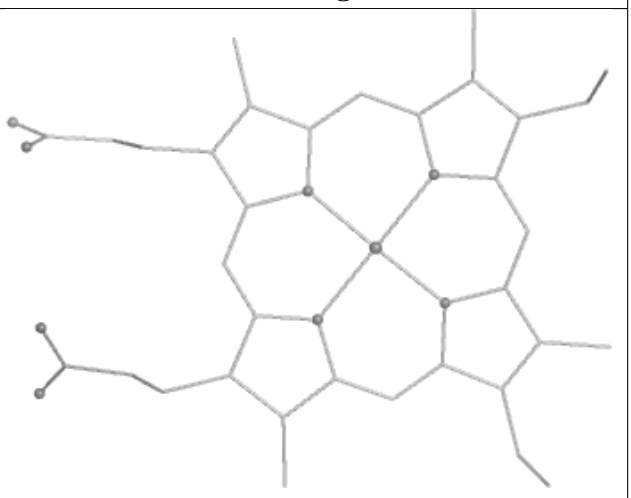
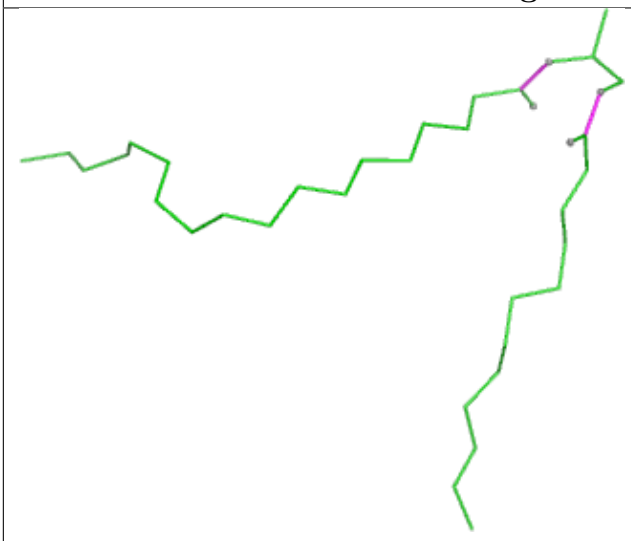
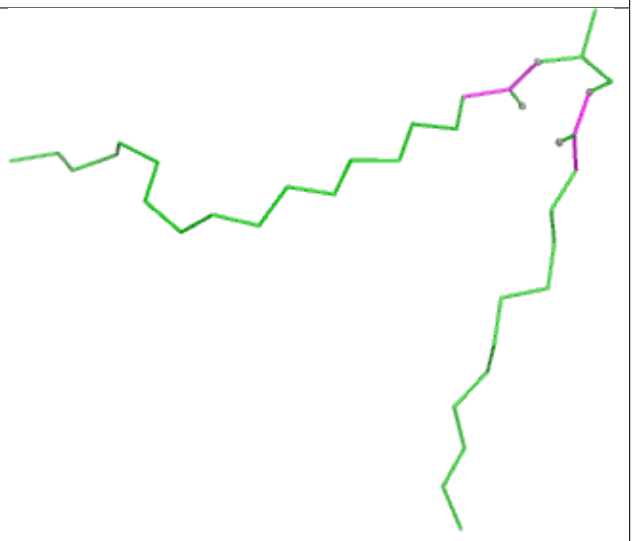


Rings

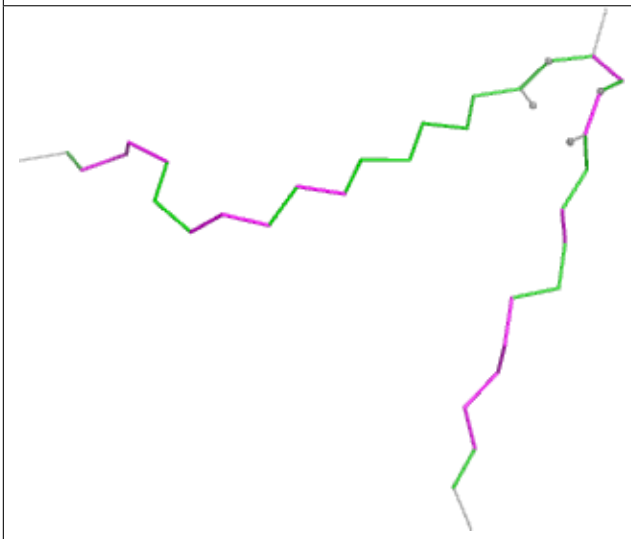
Ligand DGA C 405



Bond lengths



Bond angles

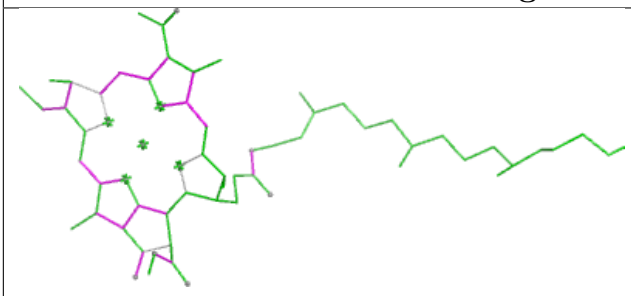


Torsions

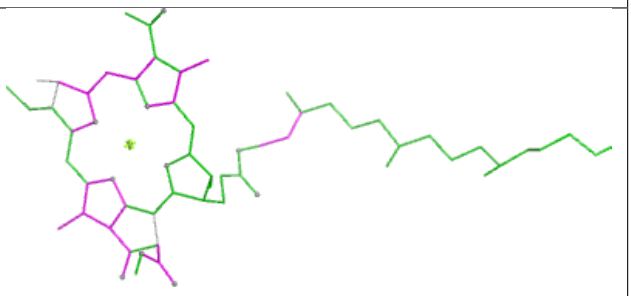


Rings

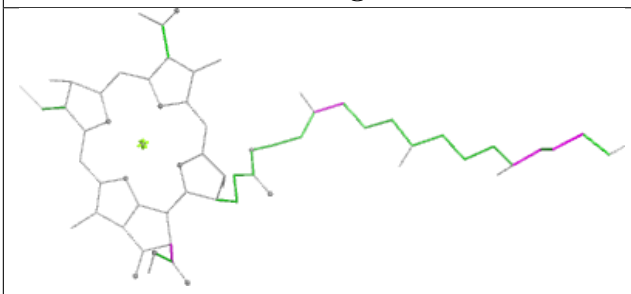
Ligand BCB M 401



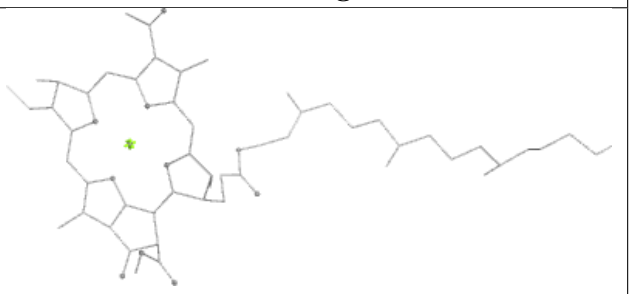
Bond lengths



Bond angles

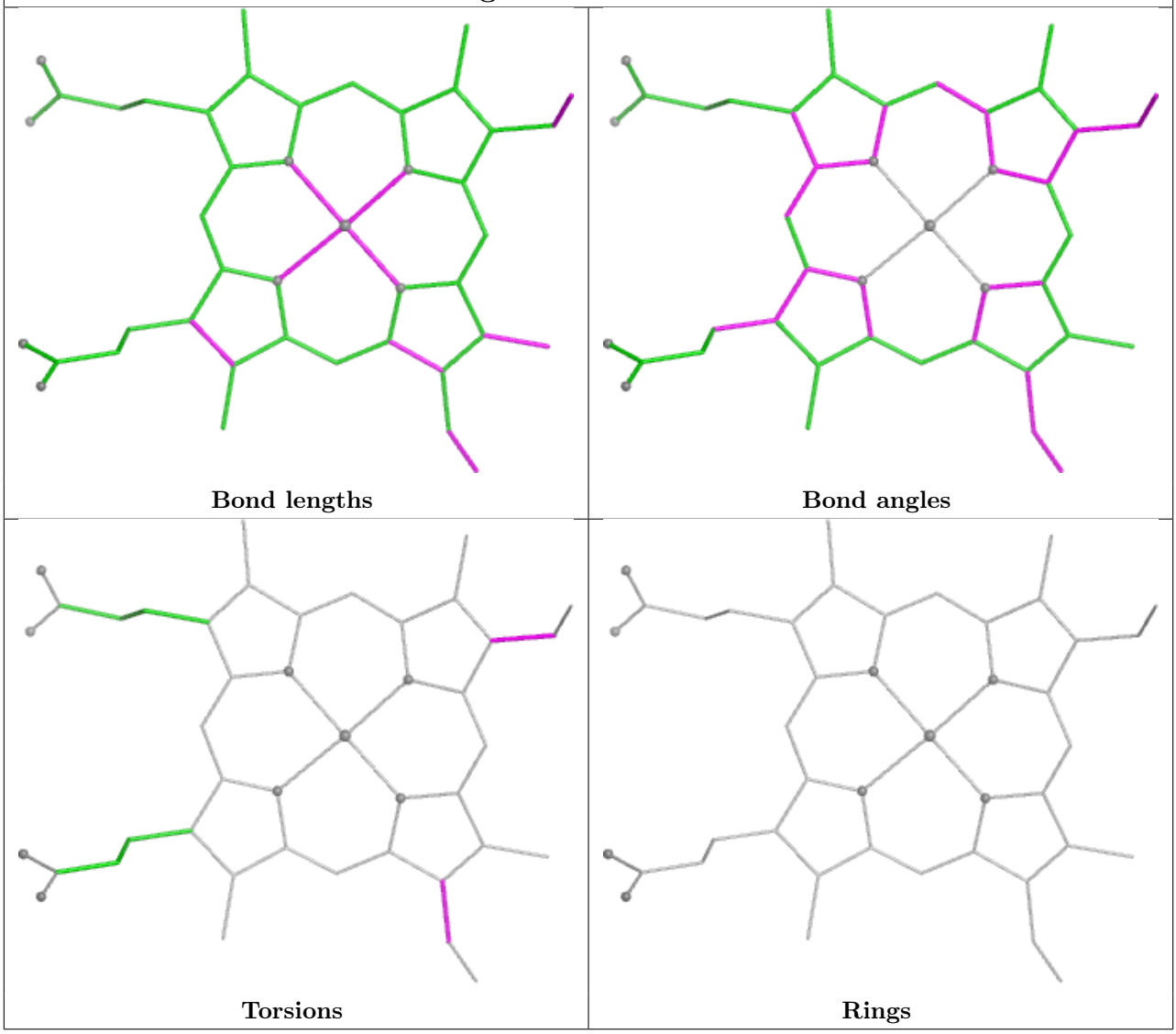


Torsions



Rings

Ligand HEC C 403



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 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, 95th 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^2)	Q<0.9
1	C	332/336 (98%)	0.65	12 (3%) 46 53	27, 32, 38, 53	0
2	H	242/258 (93%)	1.47	63 (26%) 1 1	26, 31, 43, 58	0
3	L	273/274 (99%)	1.34	52 (19%) 3 3	21, 32, 41, 54	2 (0%)
4	M	323/324 (99%)	0.49	10 (3%) 51 58	27, 31, 40, 43	0
All	All	1170/1192 (98%)	0.94	137 (11%) 9 11	21, 31, 41, 58	2 (0%)

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	63	ALA	6.7
2	H	83	PRO	6.6
2	H	84	GLU	6.2
2	H	85	THR	5.9
3	L	1	ALA	5.3
3	L	202	ASP	5.1
3	L	59	TRP	4.9
1	C	1	CYS	4.9
3	L	51	TYR	4.6
3	L	272	TRP	4.3
3	L	60	ASP	4.3
3	L	81	LEU	4.2
2	H	45	GLU	4.2
3	L	269	ILE	4.1
1	C	2	PHE	4.0
2	H	82	ARG	4.0
2	H	9	HIS	4.0
3	L	271	PHE	3.9
2	H	102	GLN	3.8
3	L	58	THR	3.8
3	L	115	TRP	3.7

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Mol	Chain	Res	Type	RSRZ
3	L	57	PRO	3.7
3	L	267	LEU	3.7
2	H	12	ILE	3.7
2	H	91	ALA	3.6
3	L	222	TYR	3.5
2	H	10	LEU	3.5
3	L	203	GLY	3.5
2	H	4	GLY	3.4
2	H	2	TYR	3.4
3	L	20	ASP	3.4
3	L	264	GLY	3.4
3	L	64	ILE	3.3
2	H	19	ALA	3.3
3	L	266	TRP	3.3
3	L	273	SER	3.3
2	H	96	PHE	3.3
1	C	48	GLU	3.3
2	H	16	VAL	3.2
2	H	88	LEU	3.2
2	H	87	GLU	3.2
2	H	8	GLN	3.2
2	H	61	GLU	3.2
2	H	25	TRP	3.1
3	L	61	PRO	3.1
2	H	147	GLU	3.1
4	M	37	TRP	3.1
3	L	62	PHE	3.1
2	H	6	LEU	3.0
2	H	148	GLY	3.0
3	L	215	TYR	2.9
3	L	25	TRP	2.9
3	L	219	VAL	2.9
2	H	132	ALA	2.9
2	H	15	LEU	2.9
2	H	258	LEU	2.9
3	L	270	PRO	2.8
3	L	200	PRO	2.8
3	L	265	TRP	2.8
1	C	64	ASN	2.7
2	H	145	ILE	2.7
2	H	92	GLN	2.7
2	H	179	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
3	L	169	TYR	2.7
2	H	5	ALA	2.7
2	H	23	VAL	2.7
4	M	1	ALA	2.6
3	L	263	TRP	2.6
3	L	236	LEU	2.6
2	H	150	VAL	2.6
2	H	144	SER	2.6
3	L	259	TRP	2.6
2	H	13	ALA	2.5
3	L	216	PHE	2.5
2	H	129	ASP	2.5
3	L	21	LEU	2.5
3	L	201	GLY	2.5
2	H	34	ARG	2.5
2	H	191	ALA	2.5
2	H	94	ASP	2.5
4	M	26	ASN	2.4
4	M	104	ILE	2.4
1	C	57	LYS	2.4
3	L	53	ALA	2.4
3	L	255	TRP	2.4
2	H	3	HIS	2.4
4	M	22	GLU	2.4
3	L	224	ILE	2.4
1	C	47	ALA	2.4
1	C	85	GLU	2.4
3	L	55	GLN	2.4
2	H	137	LEU	2.4
2	H	18	TYR	2.4
2	H	141	THR	2.4
4	M	29	VAL	2.4
2	H	146	ALA	2.3
2	H	11	ASP	2.3
2	H	43	LEU	2.3
1	C	14	PHE	2.3
2	H	71	PRO	2.3
3	L	166	ASN	2.3
3	L	80	LEU	2.3
4	M	30	GLY	2.2
4	M	27	ASP	2.2
2	H	139	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
3	L	220	VAL	2.2
2	H	105	GLY	2.2
3	L	28	PRO	2.2
2	H	173	VAL	2.2
2	H	180	PHE	2.2
2	H	95	GLY	2.2
3	L	165	LEU	2.2
2	H	86	ARG	2.2
2	H	248	TYR	2.1
3	L	17	ILE	2.1
1	C	105	VAL	2.1
2	H	130	GLY	2.1
2	H	101	LEU	2.1
1	C	56	TYR	2.1
3	L	73	TYR	2.1
3	L	206	VAL	2.1
4	M	321	ALA	2.1
3	L	7	ARG	2.1
3	L	221	GLY	2.1
2	H	17	TRP	2.1
2	H	135	VAL	2.1
2	H	70	LEU	2.1
3	L	250	ALA	2.1
4	M	136	ARG	2.1
2	H	24	ILE	2.0
2	H	252	GLU	2.0
1	C	13	GLY	2.0
2	H	22	LEU	2.0
2	H	90	LEU	2.0
3	L	16	LEU	2.0
1	C	213	GLY	2.0
2	H	128	VAL	2.0

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

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, 95th 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^2)	Q<0.9
2	FME	H	1	10/11	0.66	0.21	31,36,49,51	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

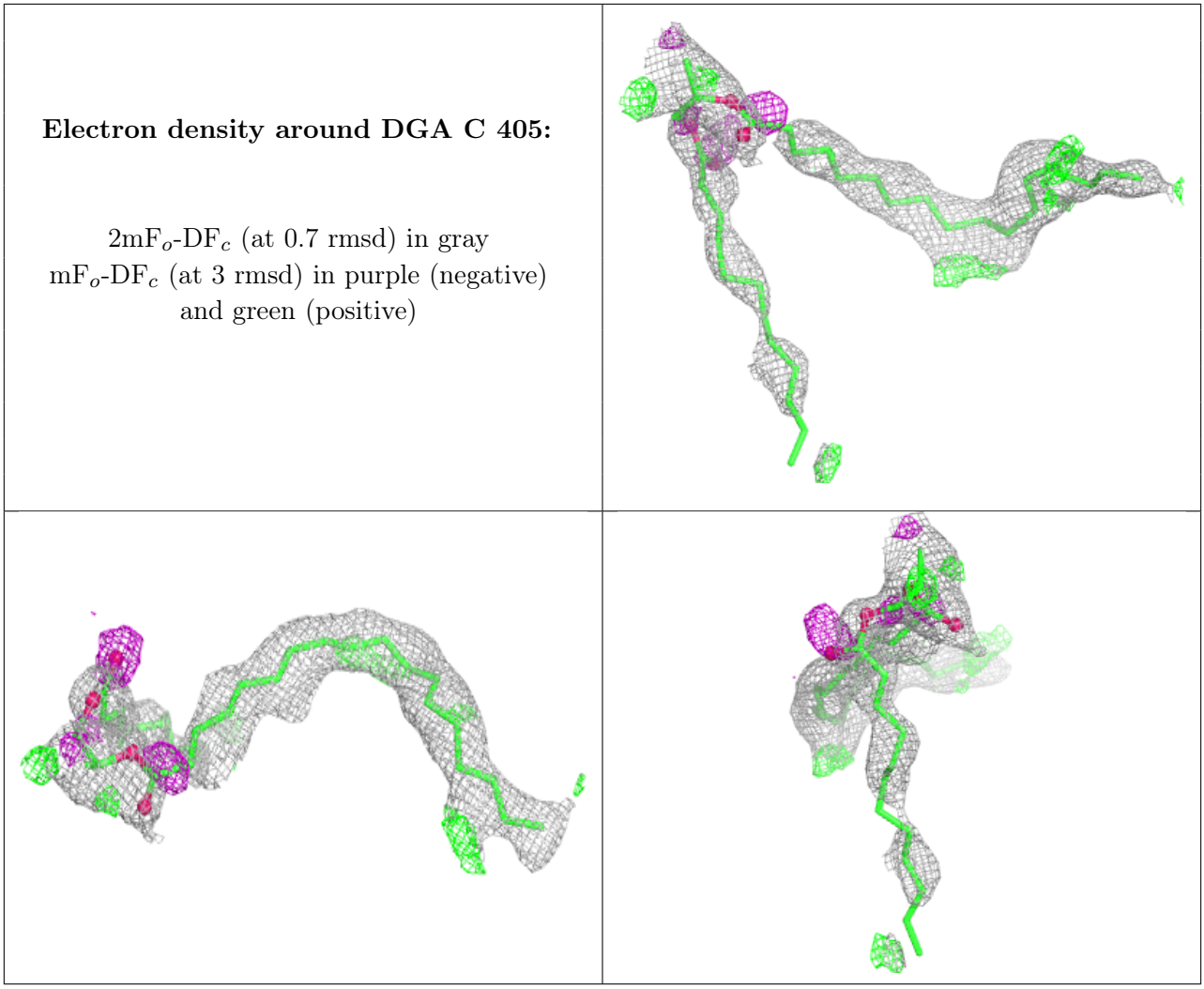
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	DGA	C	405	37/44	0.72	0.26	54,66,76,76	0
13	PO4	M	407	5/5	0.77	0.18	50,52,60,61	0
9	MPG	L	304	25/25	0.78	0.23	47,56,76,76	0
9	MPG	L	305	25/25	0.79	0.26	34,43,48,49	25
12	NS5	M	405	40/40	0.82	0.21	38,50,65,66	0
9	MPG	M	406	17/25	0.83	0.21	53,56,57,57	0
13	PO4	M	408	5/5	0.90	0.30	42,45,49,54	0
11	MQ7	M	404	48/48	0.92	0.12	26,30,44,46	0
8	BPB	L	303	65/65	0.94	0.10	22,29,34,36	0
7	BCB	L	302	66/66	0.94	0.11	22,25,49,52	0
8	BPB	M	403	61/65	0.95	0.11	19,25,56,58	0
7	BCB	L	301	66/66	0.96	0.09	19,25,35,38	0
7	BCB	M	401	65/66	0.96	0.11	20,23,65,67	0
7	BCB	M	402	66/66	0.96	0.09	19,22,35,36	0
5	HEC	C	401	43/43	0.97	0.09	26,30,32,33	0
5	HEC	C	404	43/43	0.97	0.09	20,24,35,43	0
5	HEC	C	403	43/43	0.98	0.08	19,23,25,27	0
5	HEC	C	402	43/43	0.98	0.09	23,26,32,35	0
10	FE2	L	306	1/1	0.99	0.07	26,26,26,26	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.

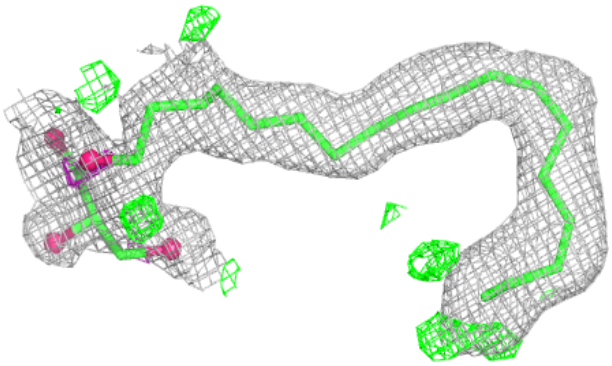
Electron density around DGA C 405:

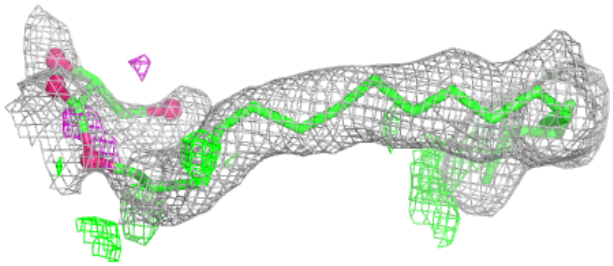
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

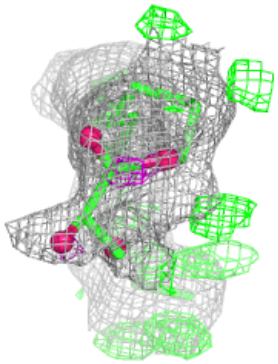


Electron density around MPG L 304:

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

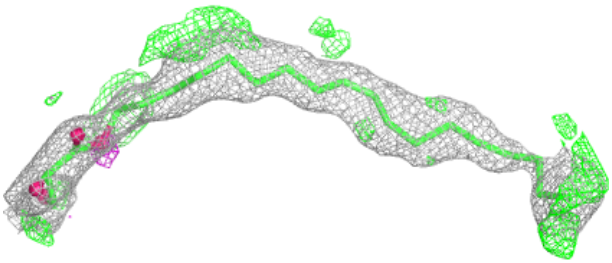


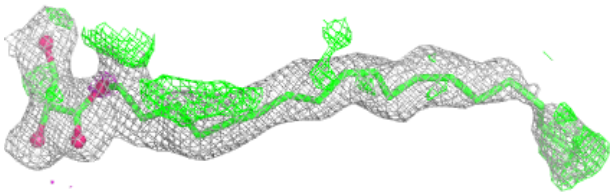


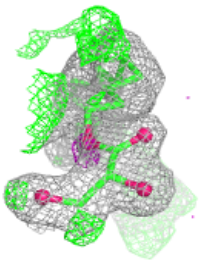


Electron density around MPG L 305:

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

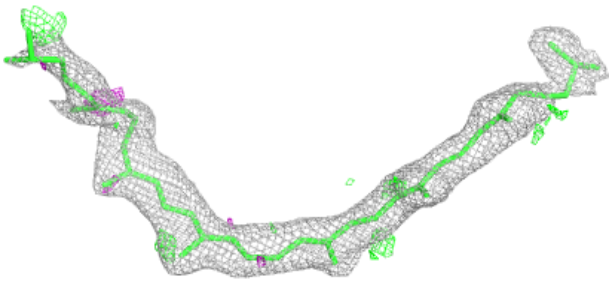


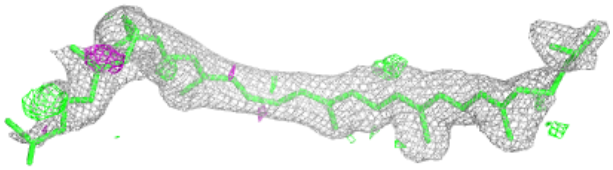


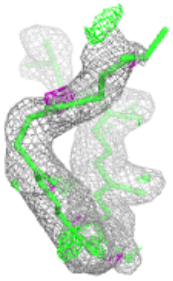


Electron density around NS5 M 405:

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

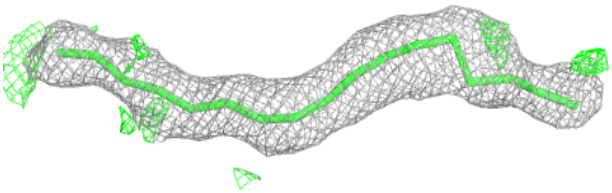


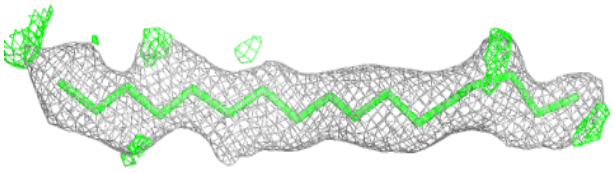


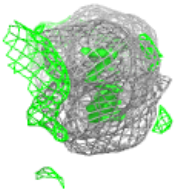


Electron density around MPG M 406:

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

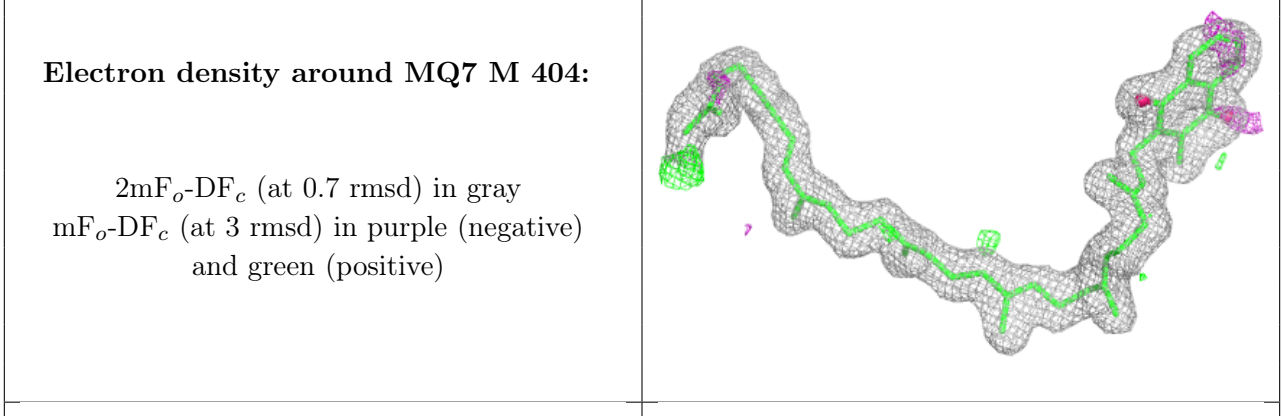






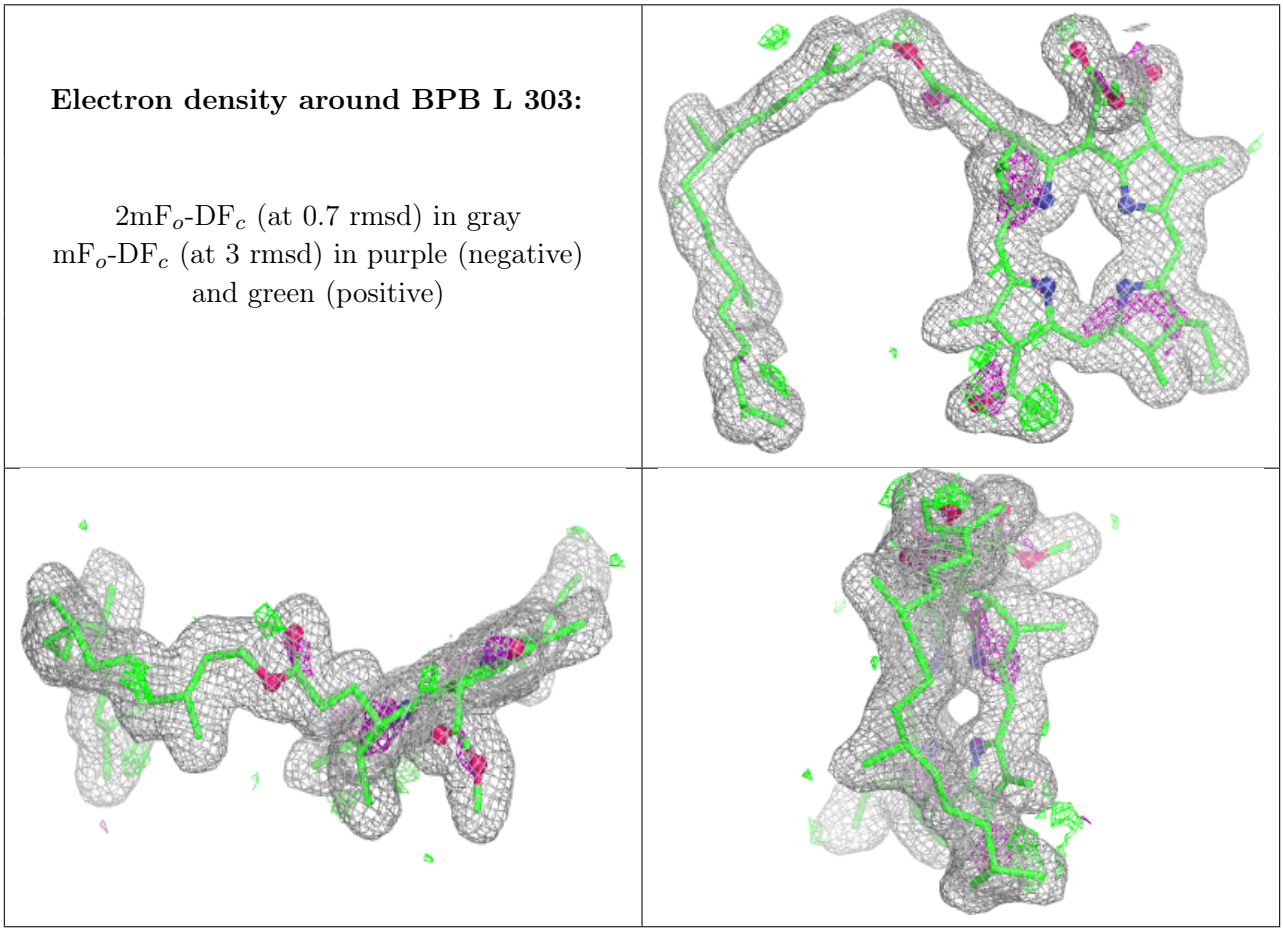
Electron density around MQ7 M 404:

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



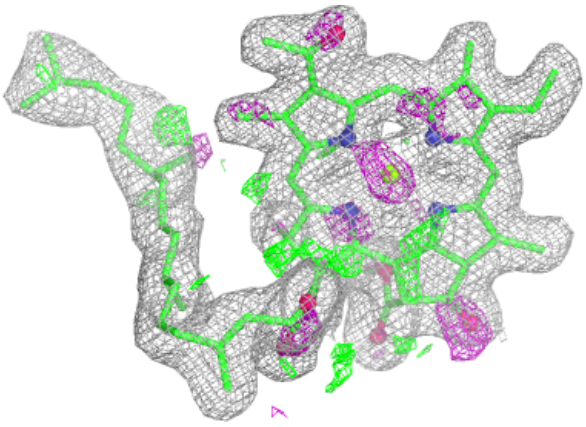
Electron density around BPB L 303:

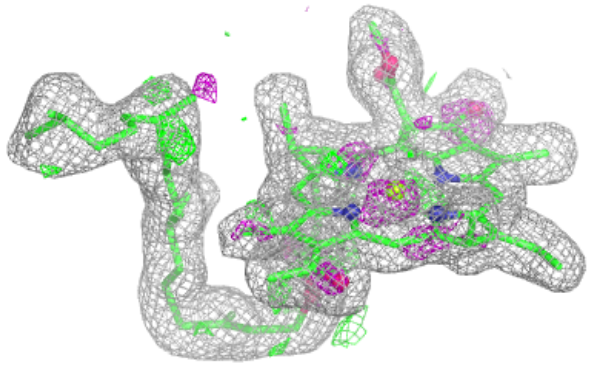
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

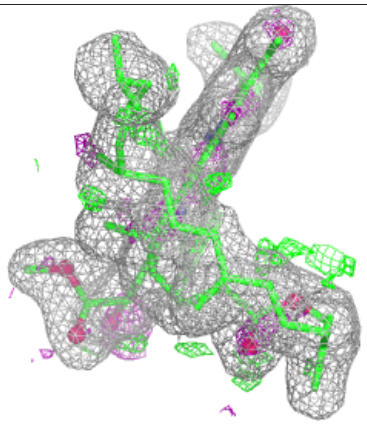


Electron density around BCB L 302:

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

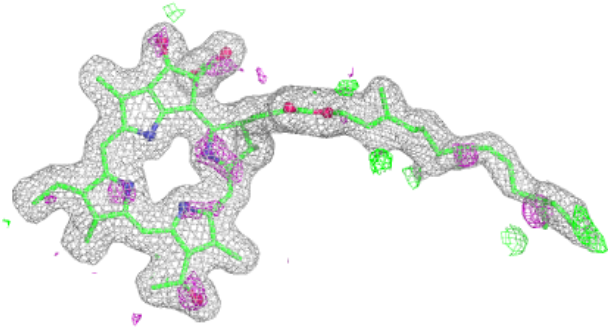


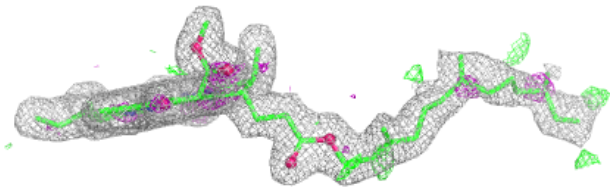


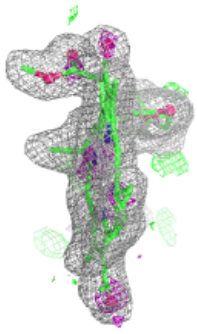


Electron density around BPB M 403:

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

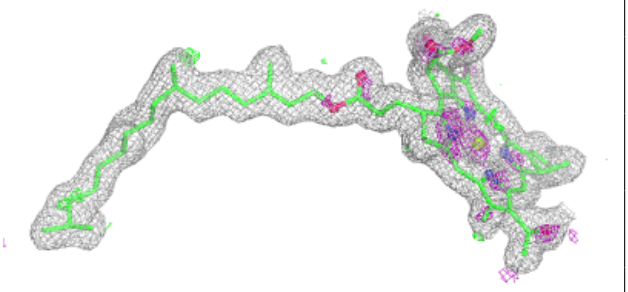


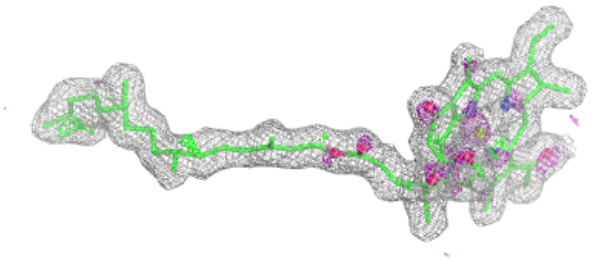


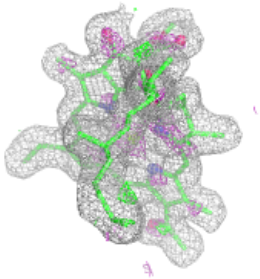


Electron density around BCB L 301:

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

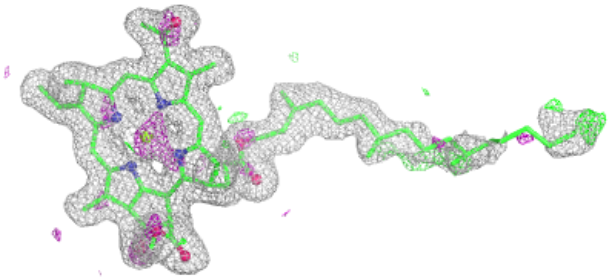


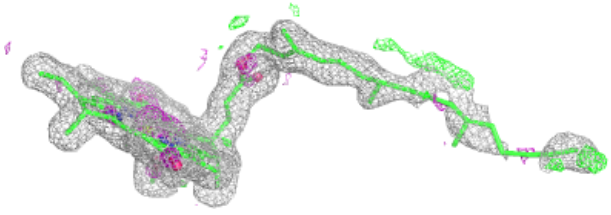


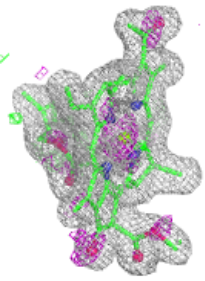


Electron density around BCB M 401:

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

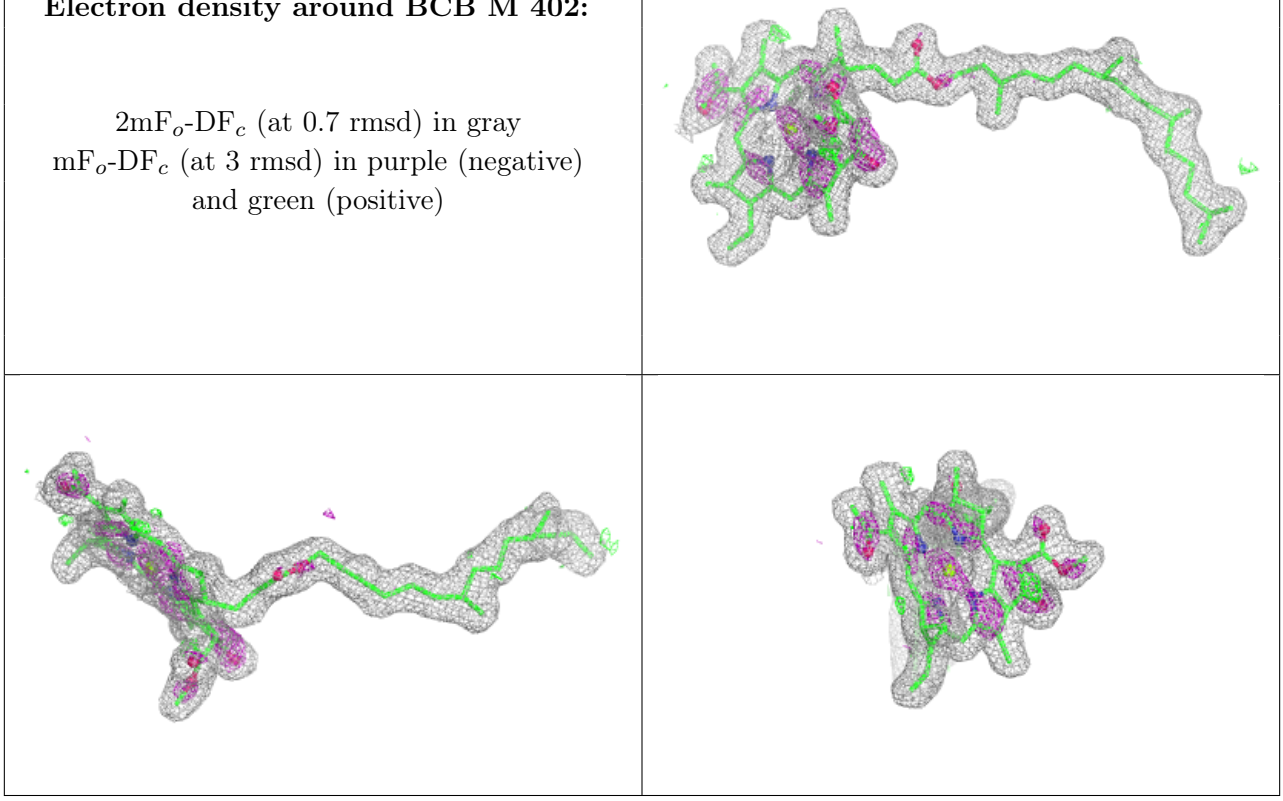






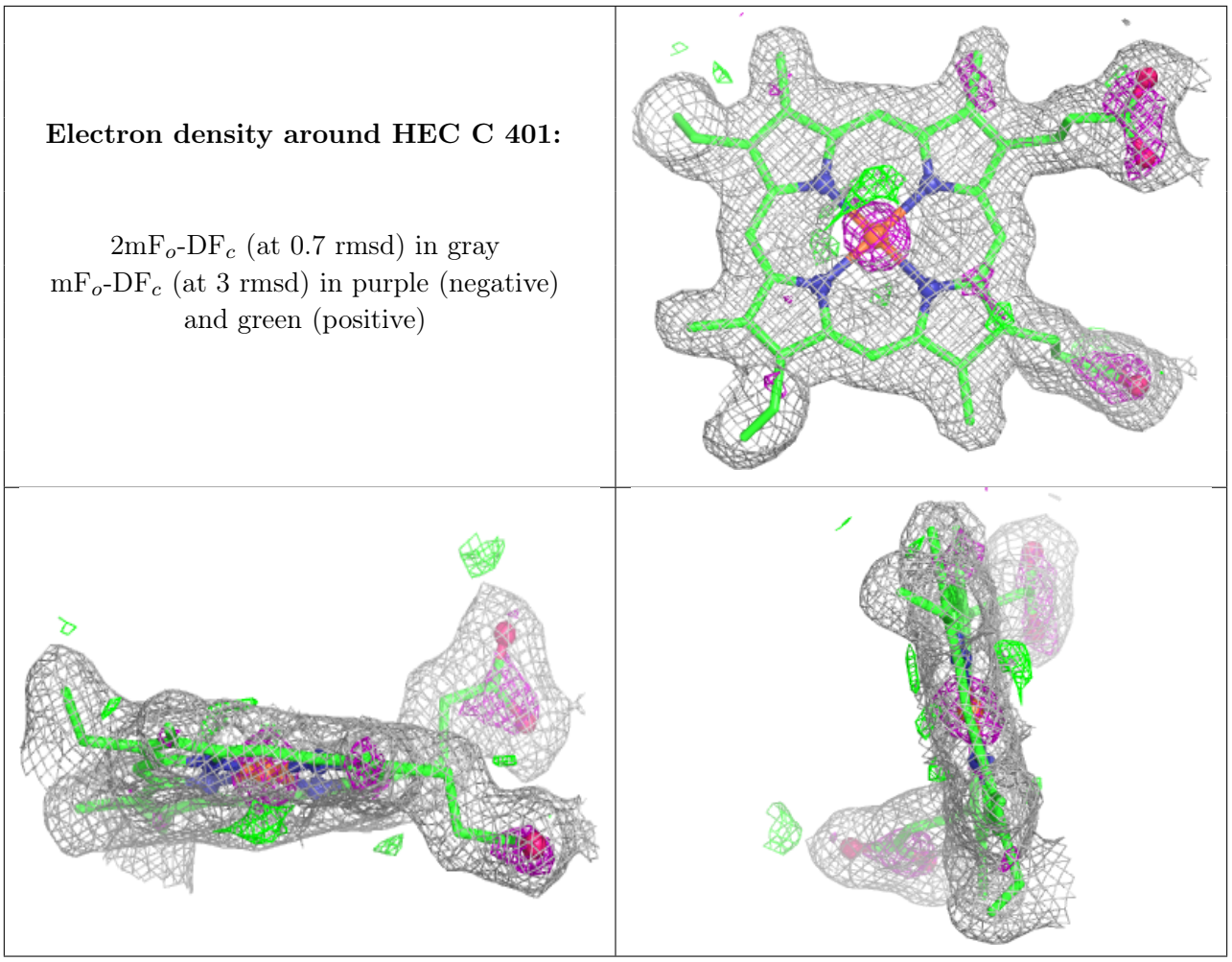
Electron density around BCB M 402:

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



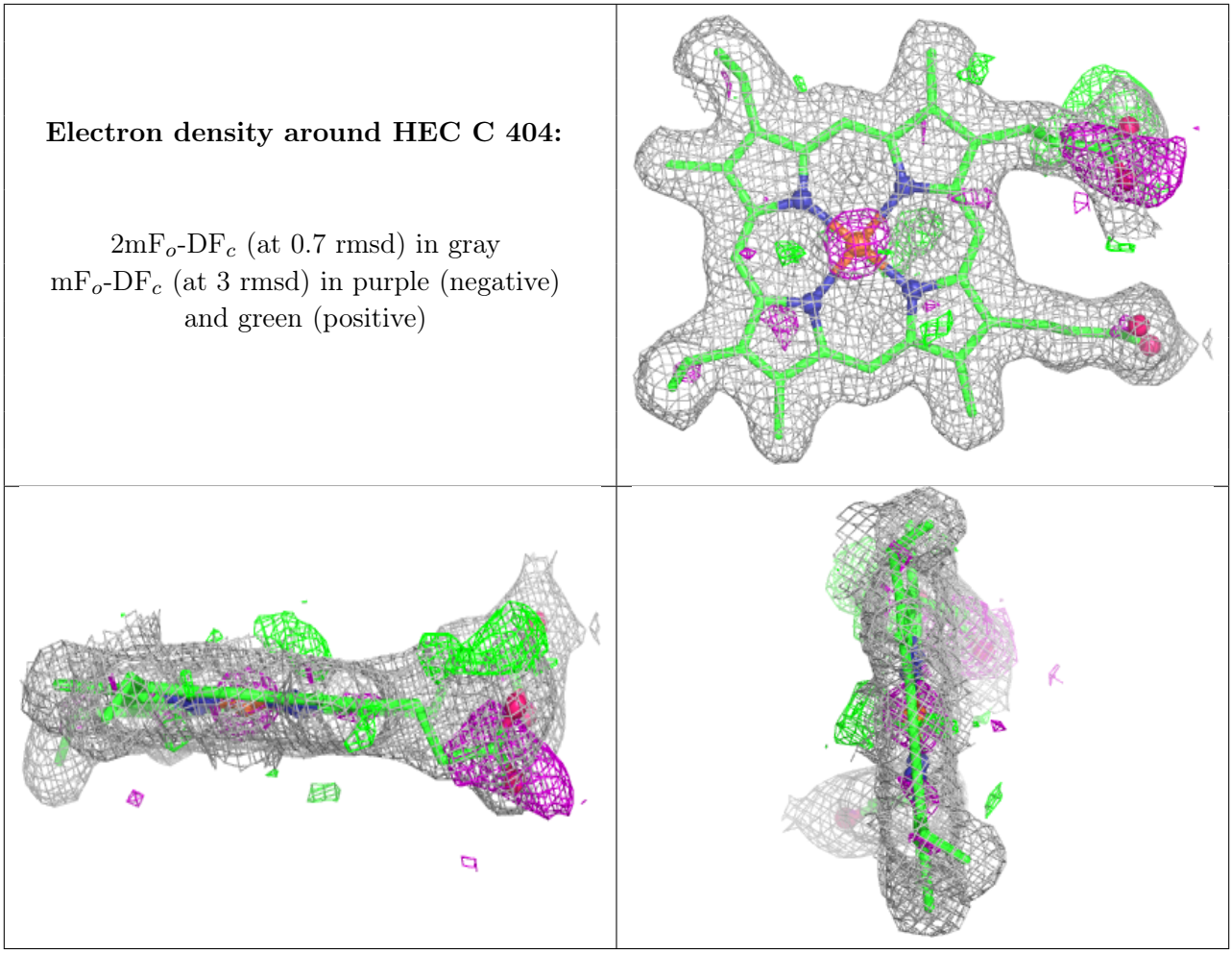
Electron density around HEC C 401:

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



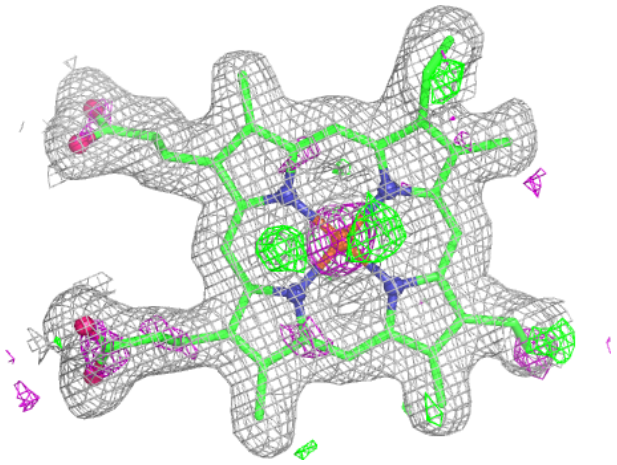
Electron density around HEC C 404:

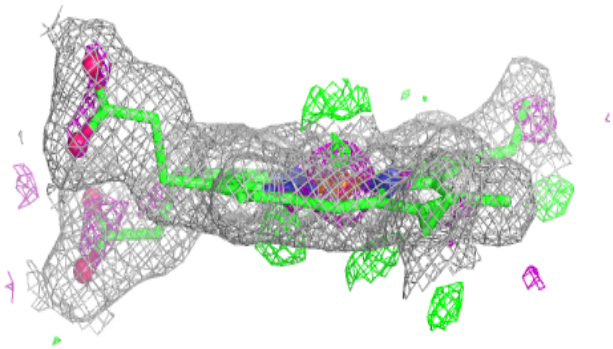
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

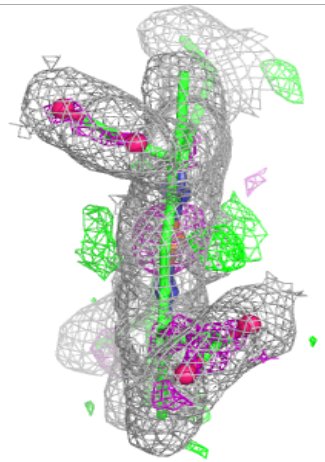


Electron density around HEC C 403:

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

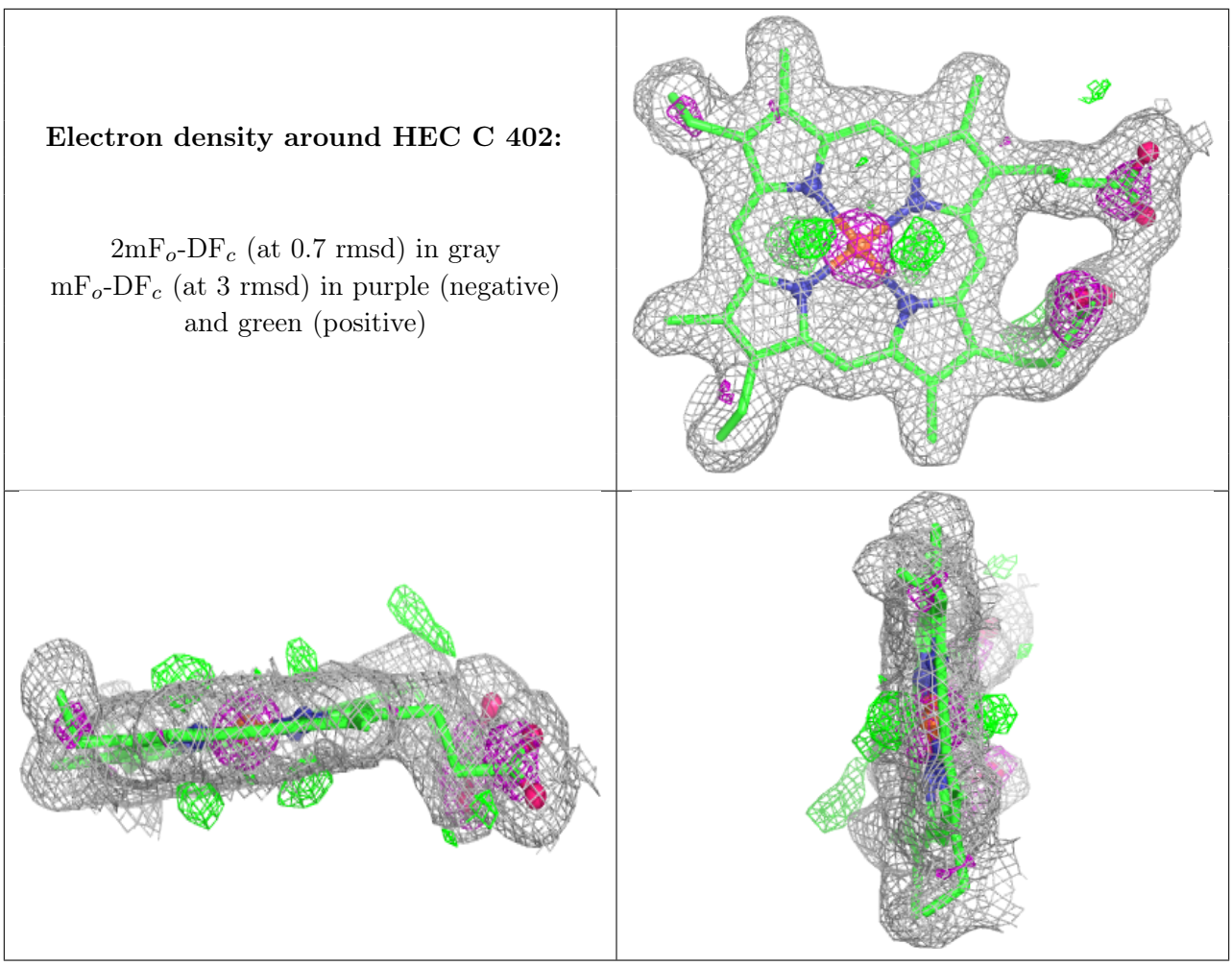






Electron density around HEC C 402:

$2mF_o$-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.