wwPDB X-ray Structure Validation Summary Report (i)

Dec 16, 2023 – 12:35 pm GMT

PDB ID	:	4CAS
Title	:	Serial femtosecond crystallography structure of a photosynthetic reaction center
Authors	:	Johansson, L.C.; Arnlund, D.; Katona, G.; White, T.A.; Barty, A.; DePonte, D.P.; Shoeman, R.L.; Wickstrand, C.; Sharma, A.; Williams, G.J.; Aquila, A.; Bogan, M.J.; Caleman, C.; Davidsson, J.; Doak, R.B.; Frank, M.; Fromme, R.; Galli, L.; Grotjohann, I.; Hunter, M.S.; Kassemeyer, S.; Kirian, R.A.; Kupitz, C.; Liang, M.; Lomb, L.; Malmerberg, E.; Martin, A.V.; Messerschmidt, M.; Nass, K.; Redecke, L.; Seibert, M.M.; Sjohamn, J.; Steinbrener, J.; Stellato, F.; Wang, D.; Wahlgren, W.Y.; Weierstall, U.; Westenhoff, S.; Zatsepin, N.A.; Boutet, S.; Spence, J.C.H.; Schlichting, I.; Chapman, H.N.; Fromme, P.; Neutze, R.
Deposited on	:	2013-10-09
Resolution	:	3.50 Å(reported)

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

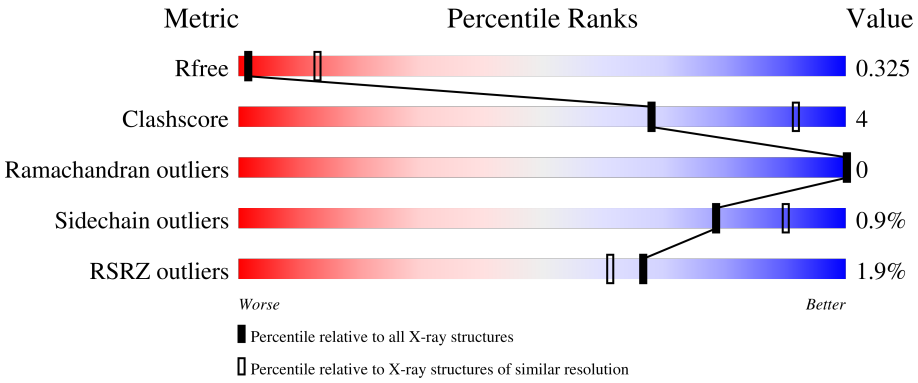
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13

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 3.50 Å.

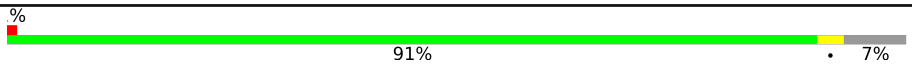
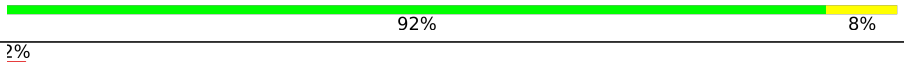
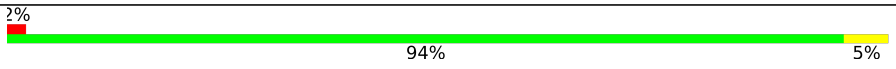
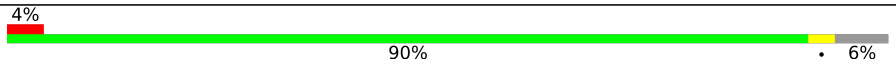
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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 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.

EDS	:	2.36
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)	:	2.36

Mol	Chain	Length	Quality of chain
1	A	356	
2	B	274	
3	C	324	
4	D	258	

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
12	NS5	C	404	-	-	-	X
6	DGA	A	405	-	-	-	X
9	MPG	B	305	-	-	-	X
9	MPG	B	306	-	-	-	X
9	MPG	C	406	-	-	-	X

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 9890 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	A	332	2598	1637	465	478	18	0	0	0

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

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

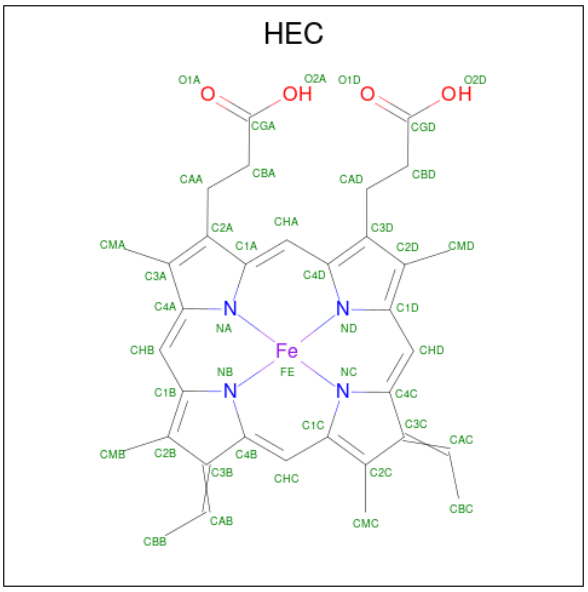
- Molecule 3 is a protein called REACTION CENTER PROTEIN M CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	323	2546	1696	417	422	11	0	0	0

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

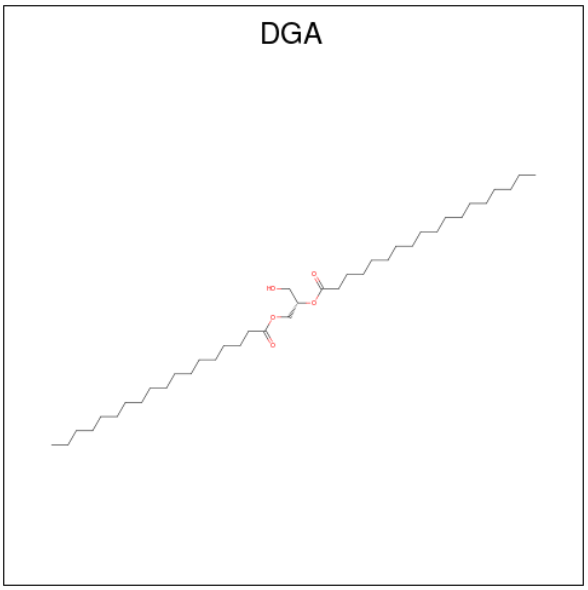
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	243	1771	1140	297	332	2	0	0	0

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



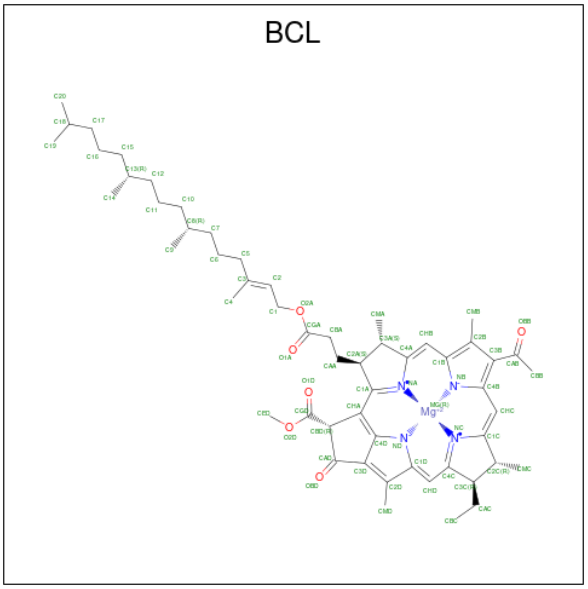
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



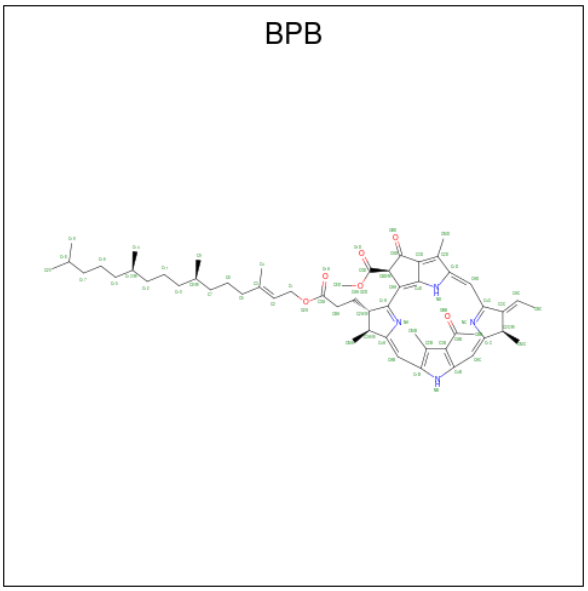
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			37	33	4		

- Molecule 7 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



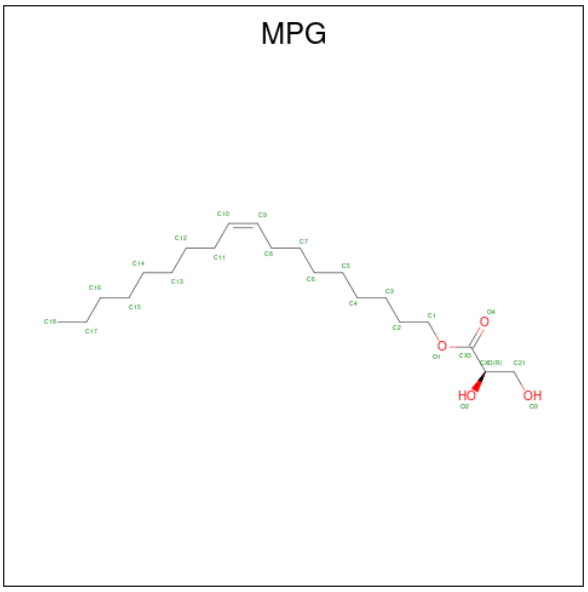
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	Mg	N	O	0	0
			65	54	1	4	6		
7	B	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	B	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	C	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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



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

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



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

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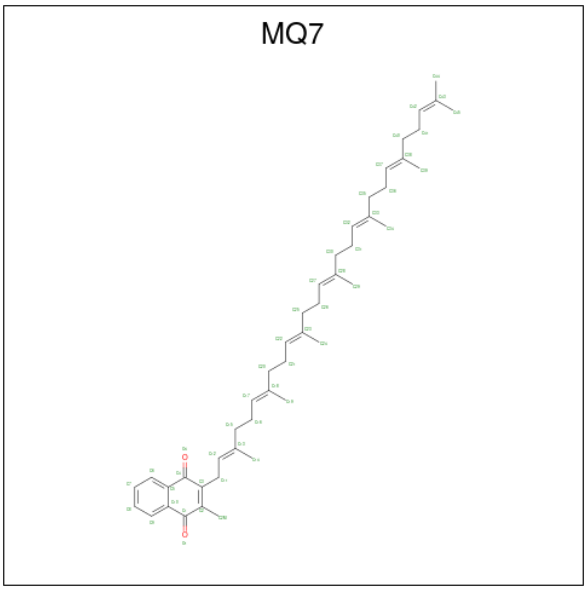
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C O 25 21 4	0	0
9	C	1	Total C 17 17	0	0

- Molecule 10 is FE (II) ION (three-letter code: FE2) (formula: Fe).

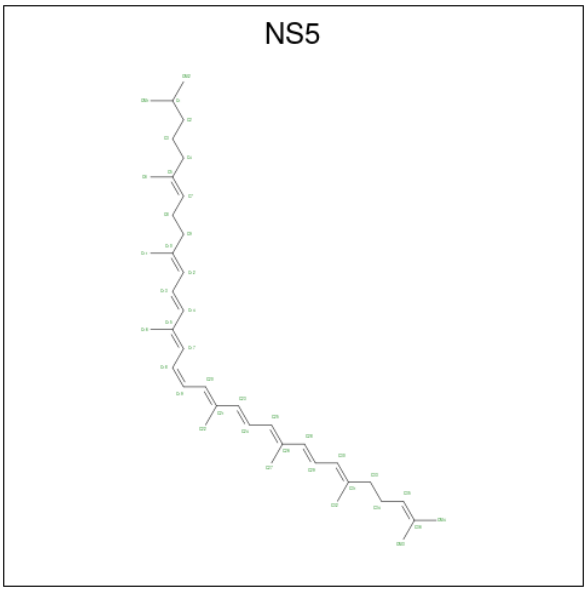
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total Fe 1 1	0	0

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



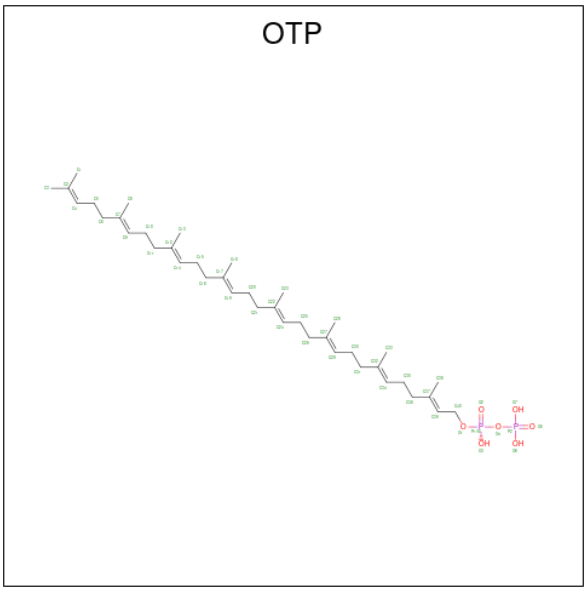
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	C	1	Total C O 48 46 2	0	0

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



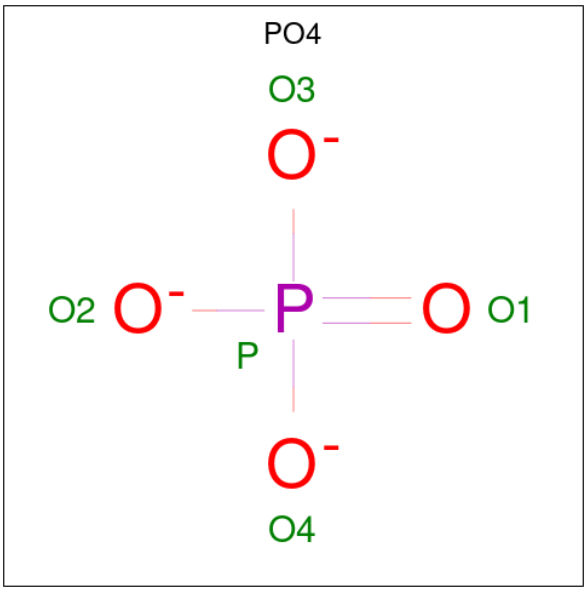
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	C	1	Total C 40 40	0	0

- Molecule 13 is (2E,6E,10E,14E,18E,22E,26E)-3,7,11,15,19,23,27,31-OCTAMETHYLD OTRIACONTA-2,6,10,14,18,22,26,30-OCTAENYL TRIHYDROGEN DIPHOSPHATE (three-letter code: OTP) (formula: $C_{40}H_{68}O_7P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	C	1	Total C O 41 40 1	0	0

- Molecule 14 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



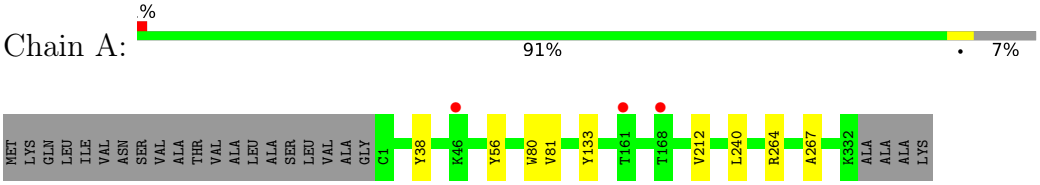
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	C	1	Total O P 5 4 1	0	0
14	C	1	Total O P 5 4 1	0	0

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.

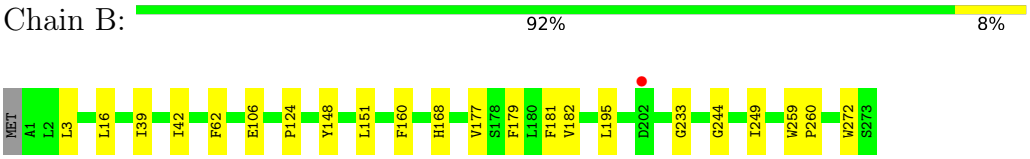
• Molecule 1: PHOTOSYNTHETIC REACTION CENTER CYTOCHROME C SUBUNIT

Chain A:



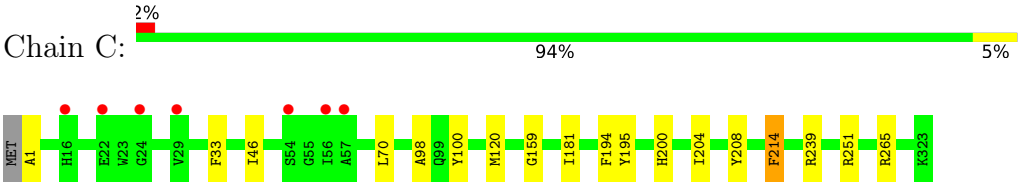
• Molecule 2: REACTION CENTER PROTEIN L CHAIN

Chain B:



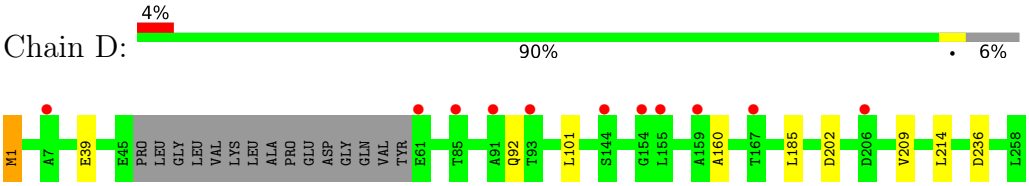
• Molecule 3: REACTION CENTER PROTEIN M CHAIN

Chain C:



• Molecule 4: REACTION CENTER PROTEIN H CHAIN

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	57.90Å 84.80Å 384.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.64 – 3.50 49.59 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.64-3.50) 99.2 (49.59-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.00 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.295 , 0.329 0.296 , 0.325	Depositor DCC
R_{free} test set	1262 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	73.5	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 77.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.32$, $< L^2 > = 0.15$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.73	EDS
Total number of atoms	9890	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% 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: MQ7, HEC, MPG, FE2, BCL, BPB, FME, NS5, DGA, OTP, PO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.56	0/2665	0.67	0/3633
2	B	0.50	0/2263	0.58	0/3089
3	C	0.52	0/2650	0.58	0/3629
4	D	0.43	0/1804	0.55	0/2485
All	All	0.51	0/9382	0.60	0/12836

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2598	0	2567	7	0
2	B	2170	0	2100	22	0
3	C	2546	0	2430	19	0
4	D	1771	0	1656	5	0
5	A	172	0	120	11	0
6	A	37	0	58	0	0
7	B	197	0	217	14	0
7	C	66	0	74	8	0
8	B	65	0	74	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	C	61	0	63	5	0
9	B	50	0	80	2	0
9	C	17	0	31	1	0
10	B	1	0	0	0	0
11	C	48	0	64	2	0
12	C	40	0	60	5	0
13	C	41	0	65	7	0
14	C	10	0	0	0	0
All	All	9890	0	9659	74	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 74 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:C:402:BPB:HHC	8:C:402:BPB:HBBB	1.62	0.81
8:B:304:BPB:HHC	8:B:304:BPB:HBBB	1.61	0.81
7:B:301:BCL:HHC	7:B:301:BCL:HBB2	1.75	0.68
2:B:181:PHE:HB3	8:C:402:BPB:HBBA	1.80	0.63
7:B:303:BCL:HMD2	7:C:401:BCL:HBB3	1.81	0.62

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	A	330/356 (93%)	323 (98%)	7 (2%)	0	100	100
2	B	273/274 (100%)	266 (97%)	7 (3%)	0	100	100
3	C	321/324 (99%)	312 (97%)	9 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	239/258 (93%)	233 (98%)	6 (2%)	0	100	100
All	All	1163/1212 (96%)	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	A	280/297 (94%)	279 (100%)	1 (0%)	91	96
2	B	218/219 (100%)	215 (99%)	3 (1%)	67	85
3	C	247/250 (99%)	245 (99%)	2 (1%)	81	91
4	D	167/212 (79%)	165 (99%)	2 (1%)	71	87
All	All	912/978 (93%)	904 (99%)	8 (1%)	78	90

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	236	ASP
4	D	185	LEU
3	C	194	PHE
2	B	272	TRP
3	C	214	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	239	ASN
3	C	200	HIS
4	D	8	GLN
1	A	302	GLN
1	A	37	GLN

5.3.3 RNA (i)

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	$\#\|Z\| > 2$
4	FME	D	1	4	8,9,10	0.81	0	7,9,11	3.34	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
4	FME	D	1	4	-	4/7/9/11	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	1	FME	CA-N-CN	-6.92	112.18	122.82
4	D	1	FME	CE-SD-CG	4.39	115.49	100.40
4	D	1	FME	O-C-CA	-2.12	119.22	124.78

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1	FME	O1-CN-N-CA
4	D	1	FME	C-CA-CB-CG
4	D	1	FME	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
4	D	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
4	D	1	FME	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 1 is monoatomic - leaving 19 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	$\#\|Z\| > 2$
7	BCL	B	302	-	64,74,74	1.78	15 (23%)	78,115,115	2.80	28 (35%)
12	NS5	C	404	-	39,39,39	2.25	7 (17%)	44,46,46	2.17	12 (27%)
13	OTP	C	405	-	40,40,48	1.57	2 (5%)	47,47,61	2.60	14 (29%)
5	HEC	A	401	1	32,50,50	1.58	5 (15%)	24,82,82	1.62	5 (20%)
5	HEC	A	402	1	32,50,50	1.39	3 (9%)	24,82,82	1.77	8 (33%)
8	BPB	C	402	-	45,66,70	2.22	9 (20%)	42,96,101	2.11	9 (21%)
9	MPG	C	406	-	16,16,24	0.42	0	15,15,25	0.65	0
9	MPG	B	306	-	24,24,24	1.58	1 (4%)	24,25,25	1.31	3 (12%)
7	BCL	C	401	-	64,74,74	1.84	14 (21%)	78,115,115	2.65	27 (34%)
11	MQ7	C	403	-	49,49,49	1.62	3 (6%)	60,63,63	1.29	8 (13%)
8	BPB	B	304	-	49,70,70	2.17	9 (18%)	47,101,101	2.00	12 (25%)
9	MPG	B	305	-	24,24,24	1.32	1 (4%)	24,25,25	1.66	3 (12%)
7	BCL	B	303	-	64,74,74	1.84	15 (23%)	78,115,115	2.71	21 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	PO4	C	408	-	4,4,4	0.70	0	6,6,6	0.66	0
7	BCL	B	301	-	63,73,74	1.80	15 (23%)	76,113,115	2.83	25 (32%)
6	DGA	A	405	1	36,36,43	1.23	2 (5%)	38,38,45	1.23	3 (7%)
5	HEC	A	404	1	32,50,50	1.48	4 (12%)	24,82,82	1.36	2 (8%)
14	PO4	C	407	-	4,4,4	0.85	0	6,6,6	0.61	0
5	HEC	A	403	1	32,50,50	1.37	5 (15%)	24,82,82	1.55	6 (25%)

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
7	BCL	B	303	-	-	7/37/137/137	-
7	BCL	B	302	-	-	4/37/137/137	-
8	BPB	C	402	-	-	16/33/101/105	0/5/6/6
12	NS5	C	404	-	-	14/43/43/43	-
7	BCL	B	301	-	-	8/36/136/137	-
11	MQ7	C	403	-	-	4/41/61/61	0/2/2/2
6	DGA	A	405	1	-	17/37/37/45	-
8	BPB	B	304	-	-	14/37/105/105	0/5/6/6
9	MPG	C	406	-	-	4/14/14/25	-
13	OTP	C	405	-	-	17/45/45/55	-
5	HEC	A	401	1	-	2/10/54/54	-
5	HEC	A	404	1	-	1/10/54/54	-
5	HEC	A	403	1	-	0/10/54/54	-
5	HEC	A	402	1	-	5/10/54/54	-
9	MPG	B	306	-	-	8/25/25/25	-
9	MPG	B	305	-	-	15/25/25/25	-
7	BCL	C	401	-	-	10/37/137/137	-

The worst 5 of 110 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	405	OTP	C39-C37	8.78	1.54	1.33
11	C	403	MQ7	C3-C2	8.07	1.50	1.35
8	B	304	BPB	CAC-C3C	7.76	1.53	1.33
12	C	404	NS5	C35-C36	7.70	1.54	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	402	BPB	CAC-C3C	7.55	1.52	1.33

The worst 5 of 186 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	302	BCL	C1C-NC-C4C	-14.26	100.29	106.71
7	B	301	BCL	C1C-NC-C4C	-14.12	100.36	106.71
7	B	303	BCL	C1C-NC-C4C	-13.80	100.50	106.71
7	C	401	BCL	C1C-NC-C4C	-12.89	100.91	106.71
13	C	405	OTP	C40-C39-C37	-9.31	112.70	127.21

There are no chirality outliers.

5 of 146 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	405	DGA	CA2-CA1-OG1-CG1
6	A	405	DGA	OA1-CA1-OG1-CG1
6	A	405	DGA	OG1-CG1-CG2-OG2
6	A	405	DGA	OG1-CG1-CG2-CG3
7	B	302	BCL	C4-C3-C5-C6

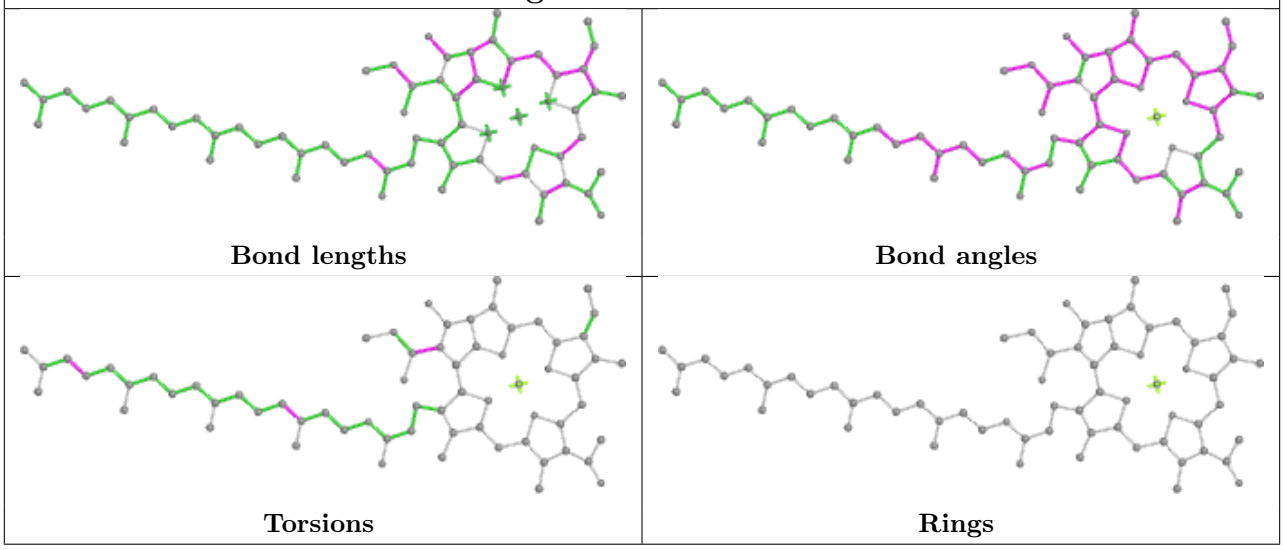
There are no ring outliers.

16 monomers are involved in 56 short contacts:

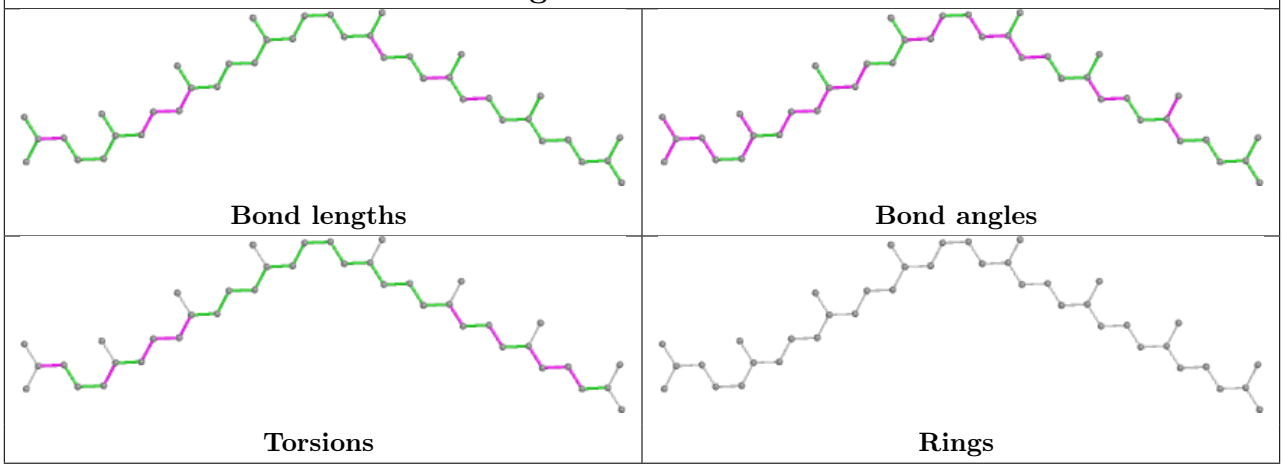
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	302	BCL	5	0
12	C	404	NS5	5	0
13	C	405	OTP	7	0
5	A	401	HEC	4	0
5	A	402	HEC	2	0
8	C	402	BPB	5	0
9	C	406	MPG	1	0
9	B	306	MPG	1	0
7	C	401	BCL	8	0
11	C	403	MQ7	2	0
8	B	304	BPB	8	0
9	B	305	MPG	1	0
7	B	303	BCL	6	0
7	B	301	BCL	3	0
5	A	404	HEC	4	0
5	A	403	HEC	1	0

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 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.

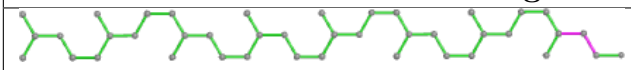
Ligand BCL B 302



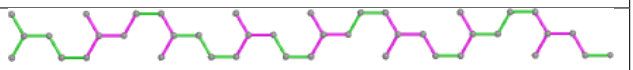
Ligand NS5 C 404



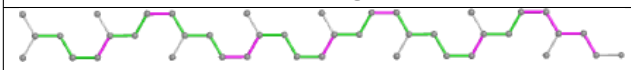
Ligand OTP C 405



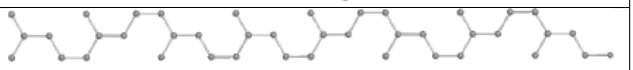
Bond lengths



Bond angles

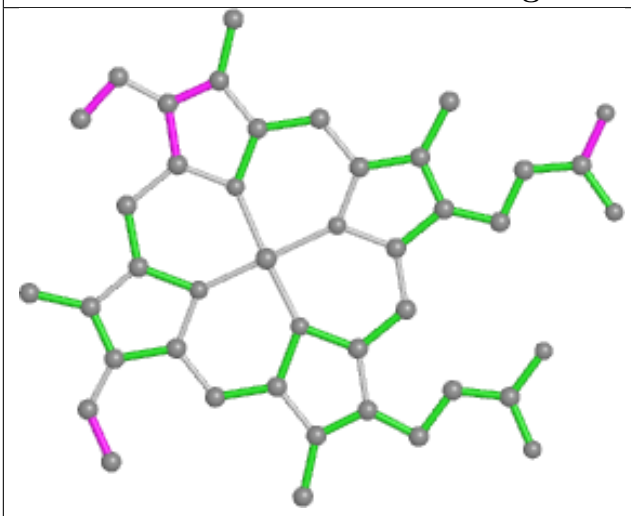


Torsions

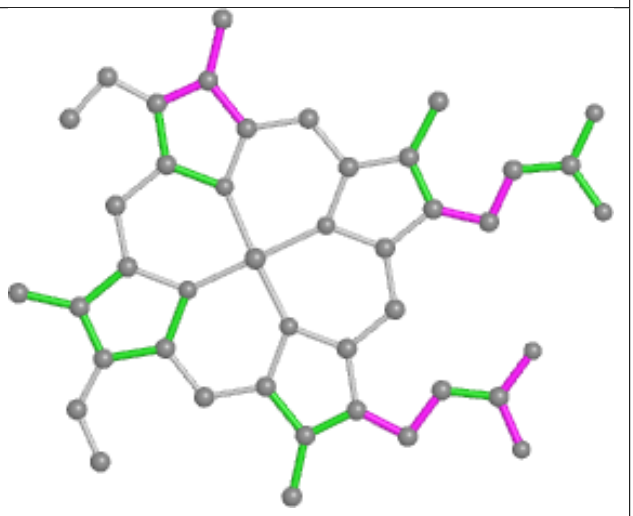


Rings

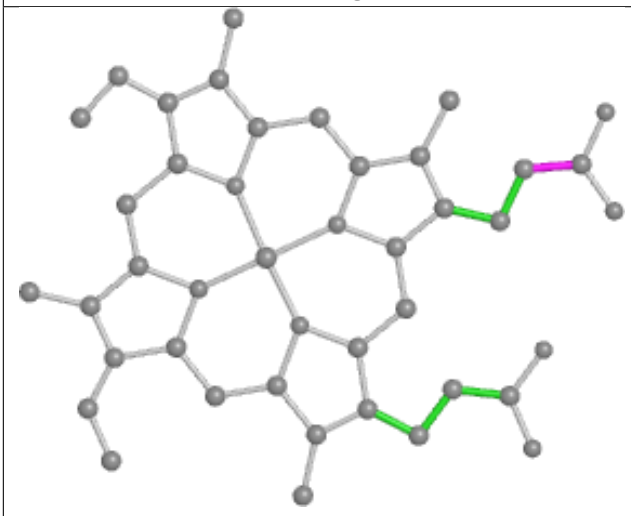
Ligand HEC A 401



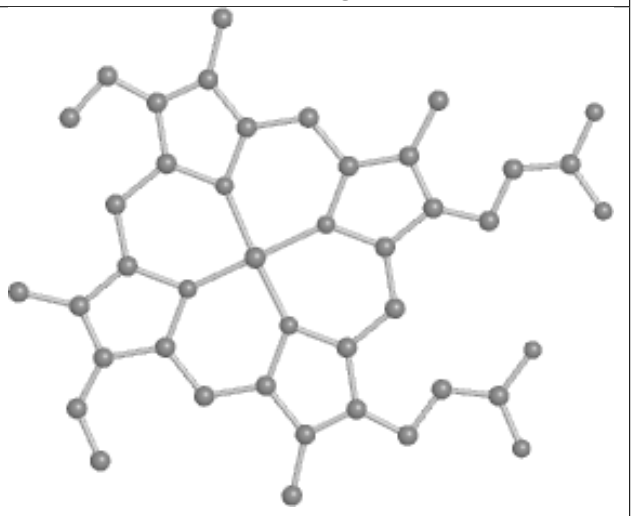
Bond lengths



Bond angles

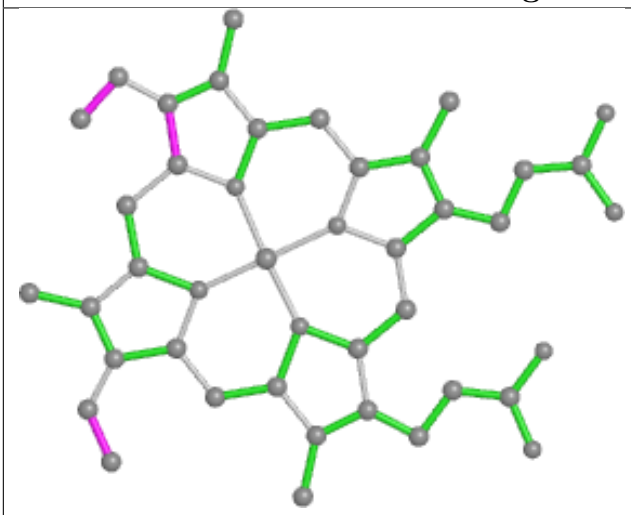


Torsions

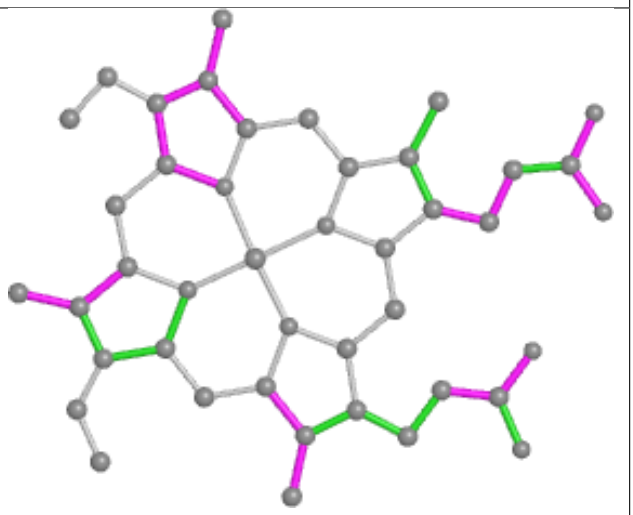


Rings

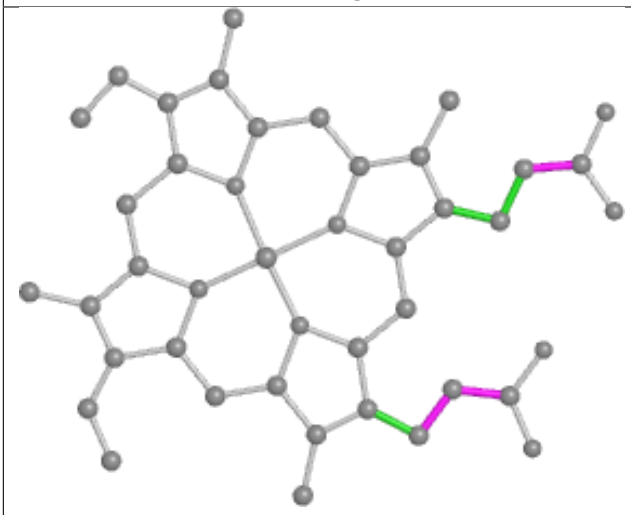
Ligand HEC A 402



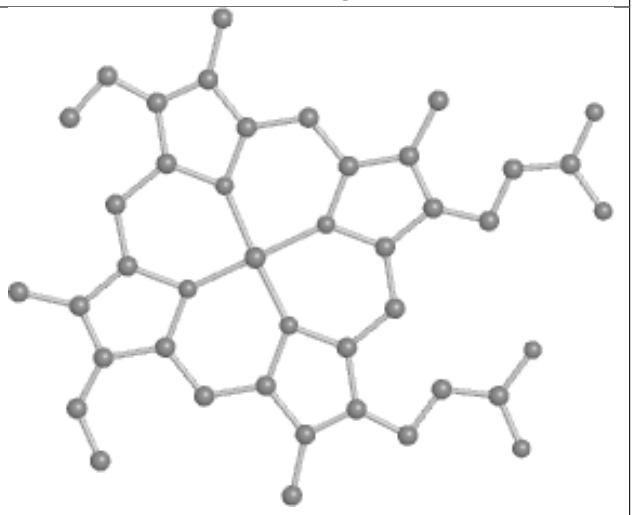
Bond lengths



Bond angles

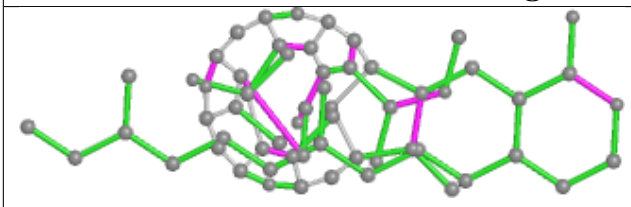


Torsions

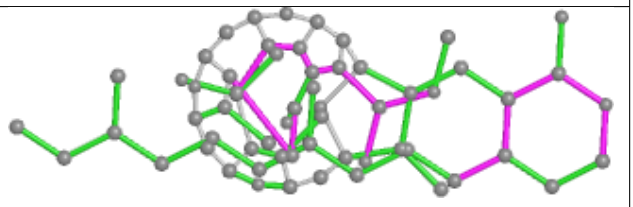


Rings

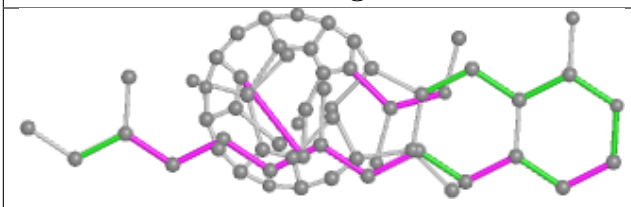
Ligand BPB C 402



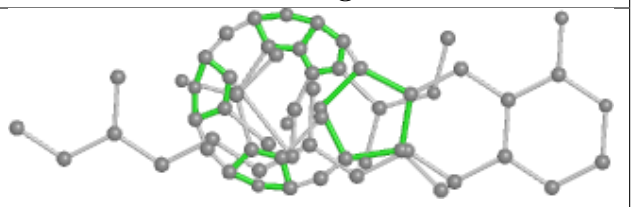
Bond lengths



Bond angles

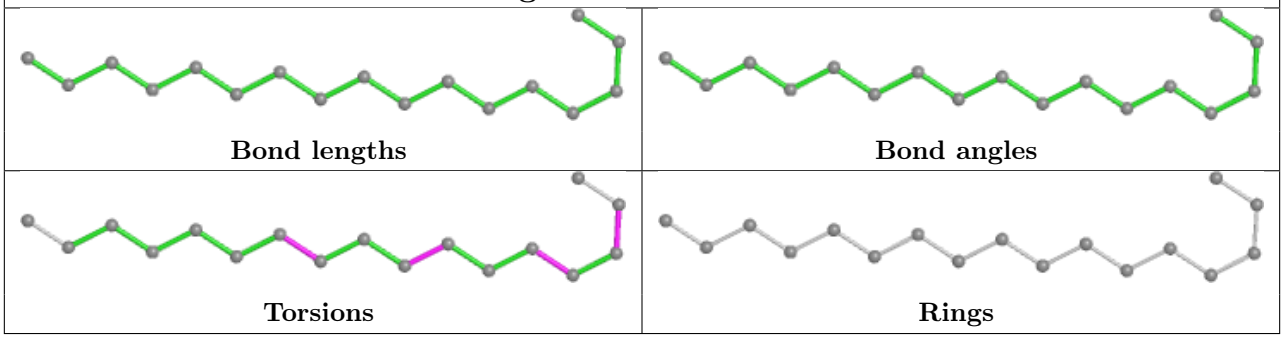


Torsions

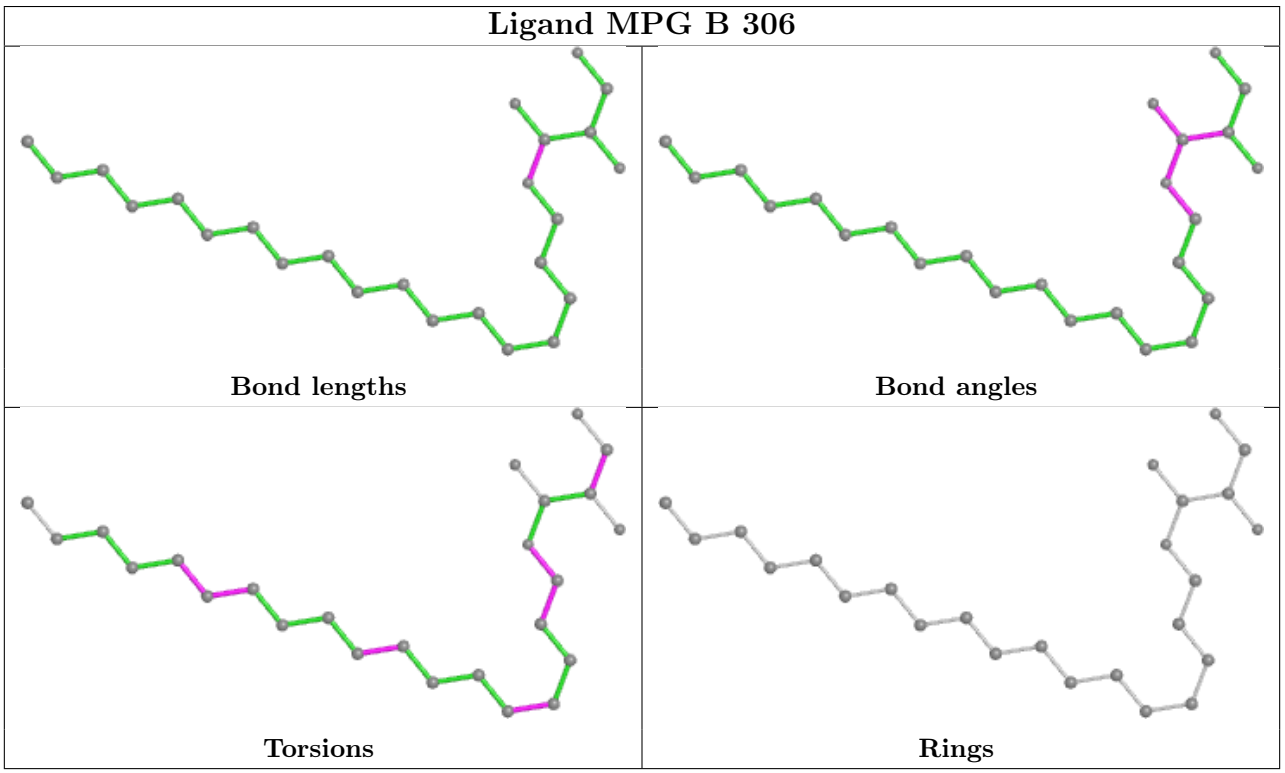


Rings

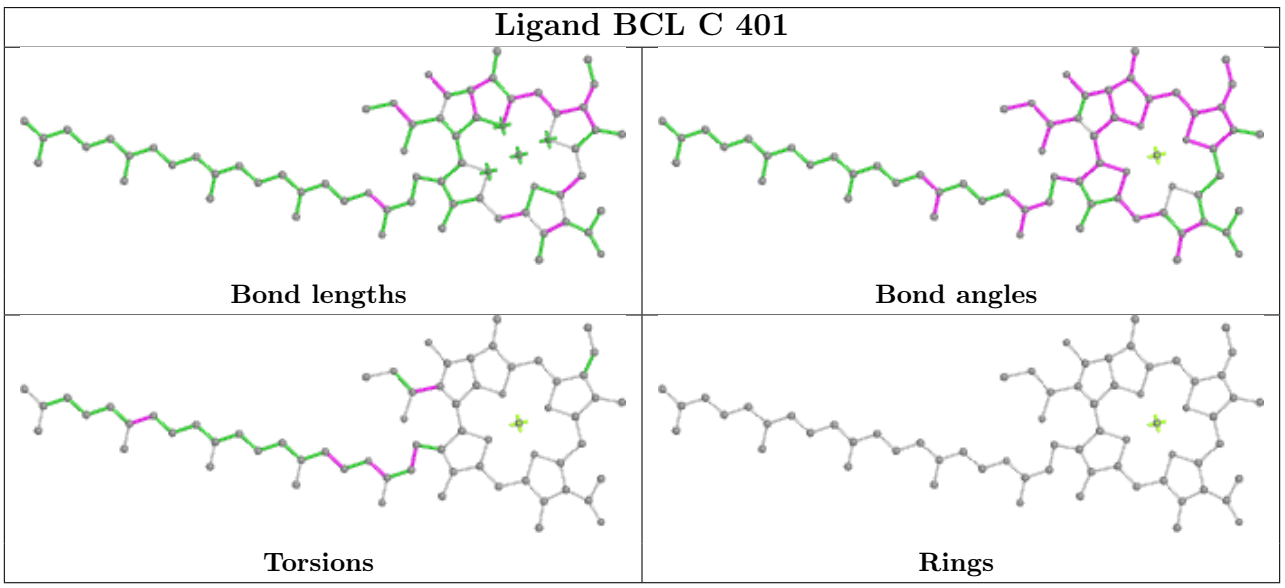
Ligand MPG C 406



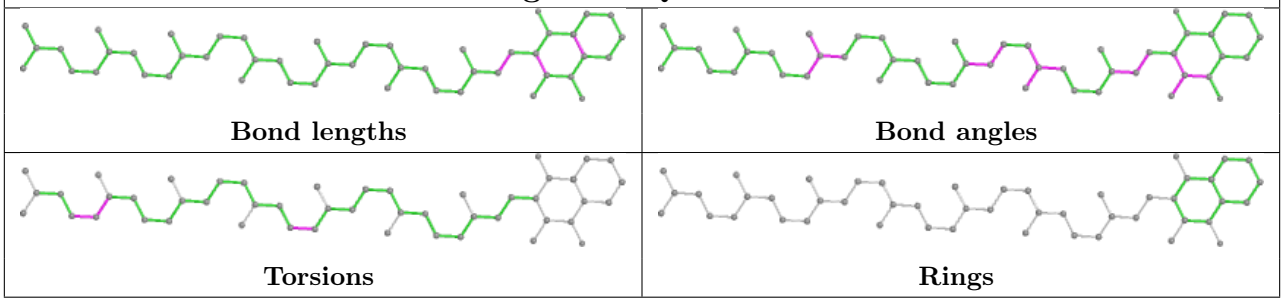
Ligand MPG B 306



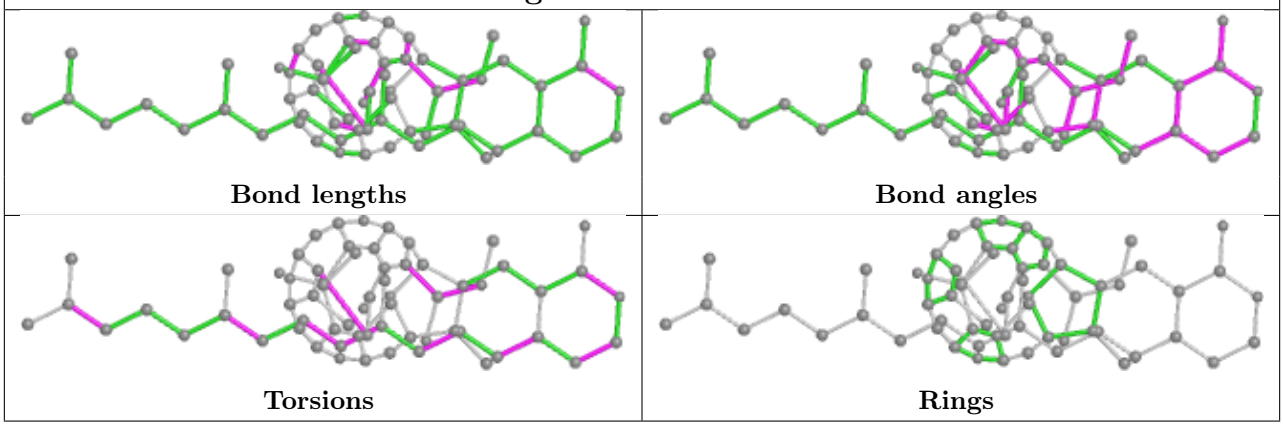
Ligand BCL C 401



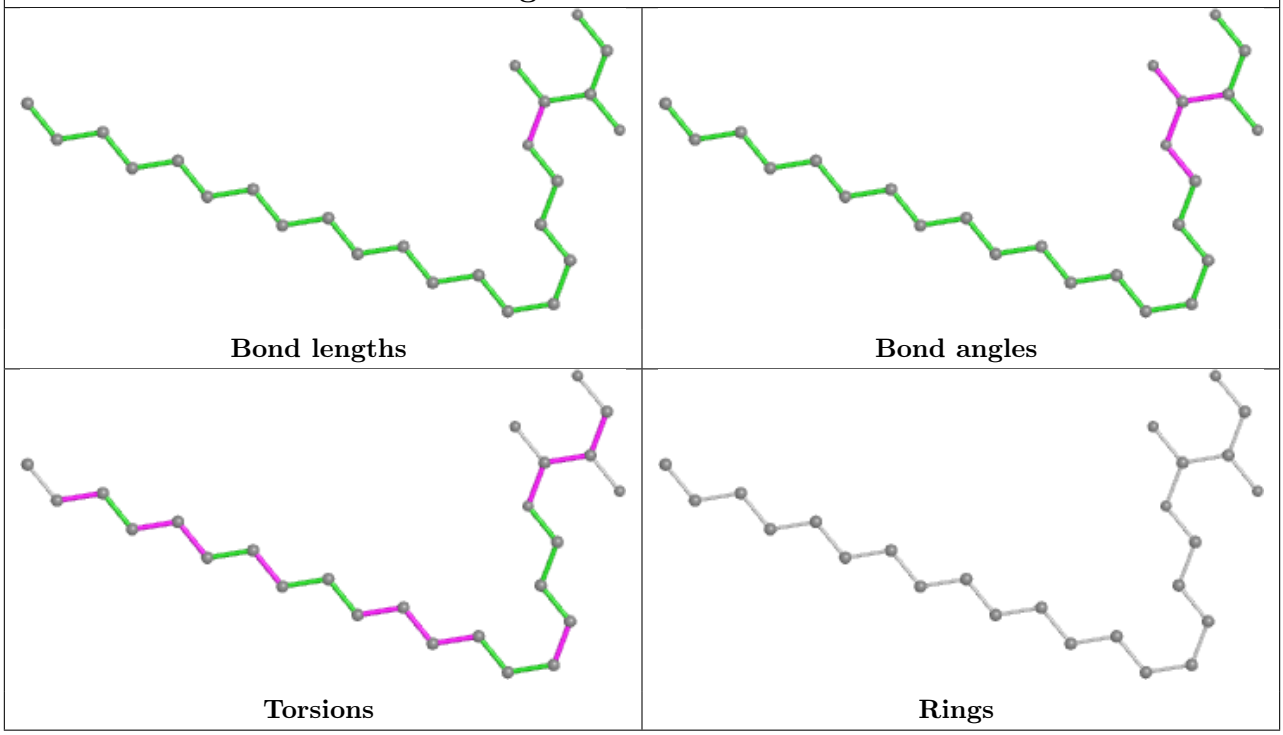
Ligand MQ7 C 403



Ligand BPB B 304



Ligand MPG B 305



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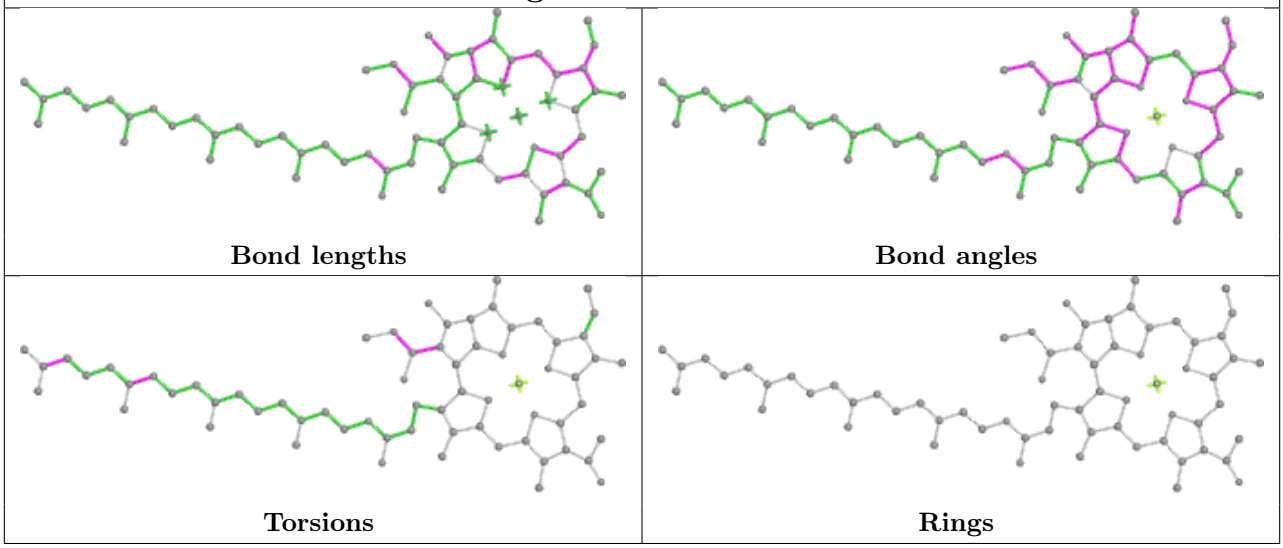
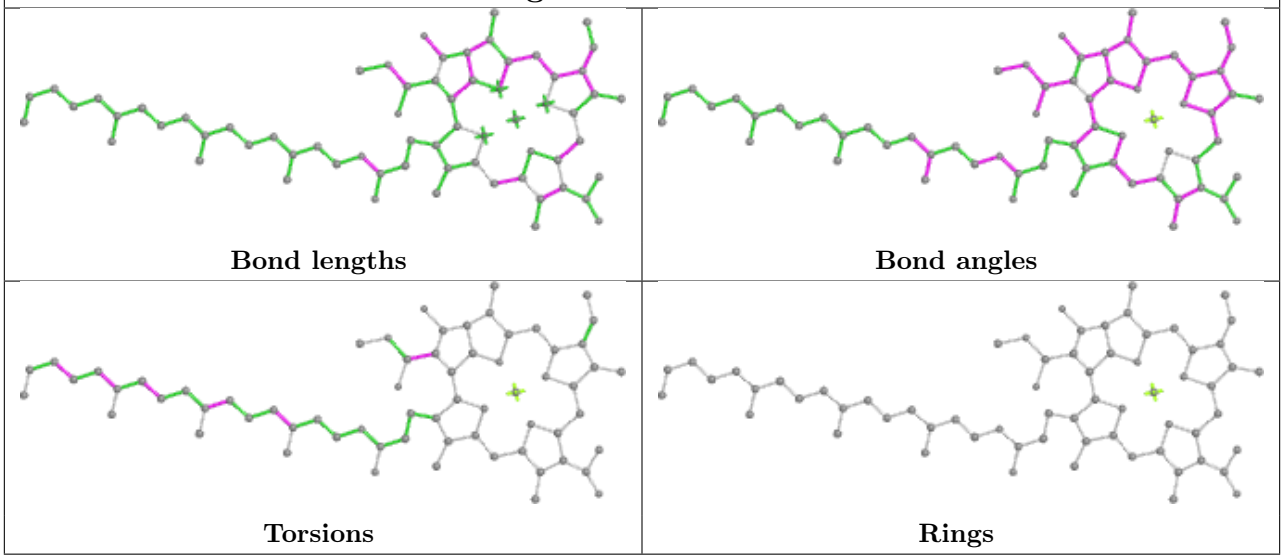
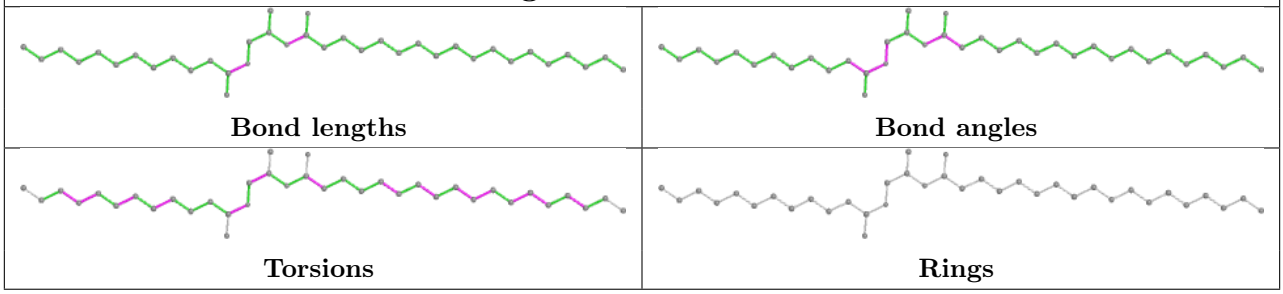


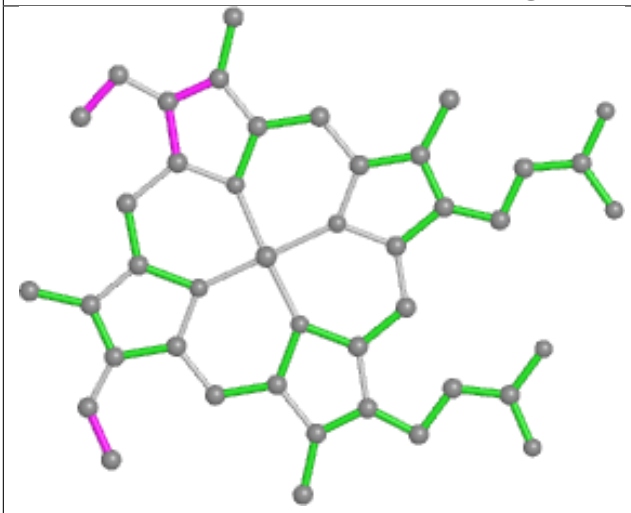
Ligand BCL B 301



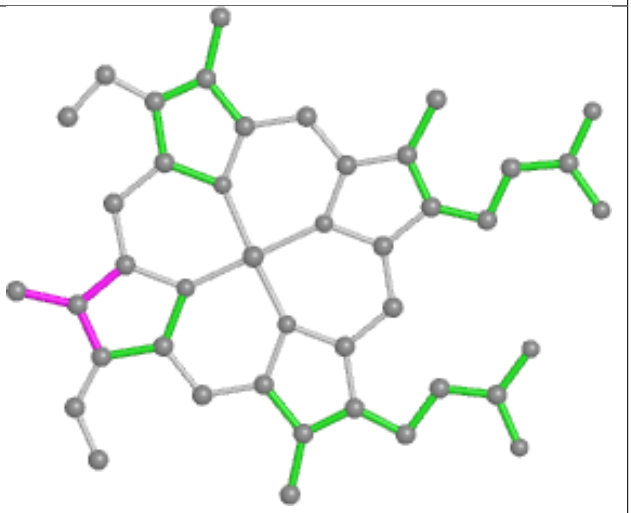
Ligand DGA A 405



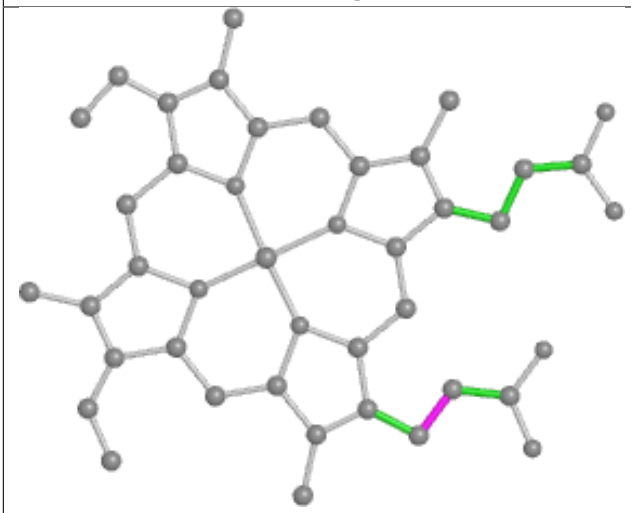
Ligand HEC A 404



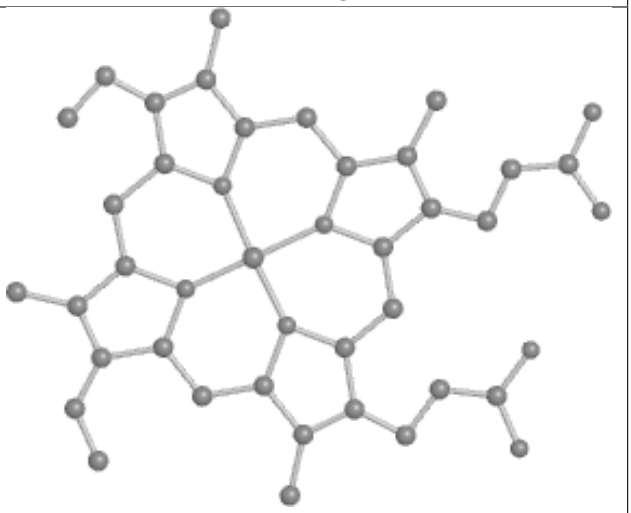
Bond lengths



Bond angles

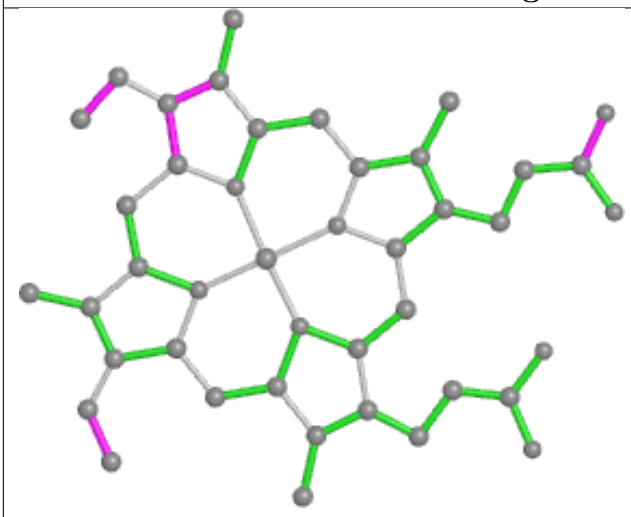


Torsions

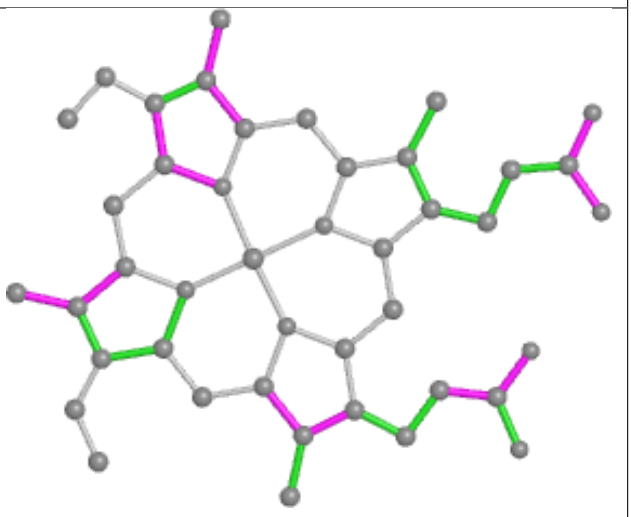


Rings

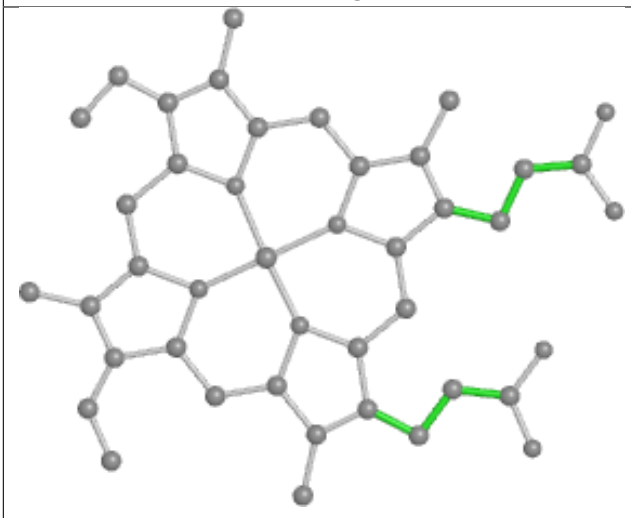
Ligand HEC A 403



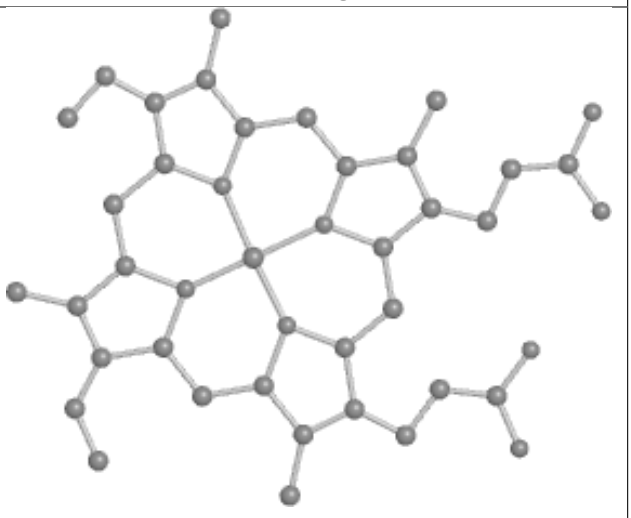
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 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^{th} 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	A	332/356 (93%)	-0.11	3 (0%)	84	79	21, 38, 56, 78	0
2	B	273/274 (99%)	-0.09	1 (0%)	92	90	27, 55, 89, 113	0
3	C	323/324 (99%)	0.01	7 (2%)	62	56	28, 56, 88, 109	0
4	D	242/258 (93%)	0.48	11 (4%)	33	29	63, 92, 115, 136	0
All	All	1170/1212 (96%)	0.05	22 (1%)	66	61	21, 54, 101, 136	0

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	85	THR	4.5
2	B	202	ASP	3.4
3	C	54	SER	3.3
4	D	159	ALA	2.9
4	D	144	SER	2.8

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^{th} 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
4	FME	D	1	10/11	0.86	0.38	64,69,72,73	0

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

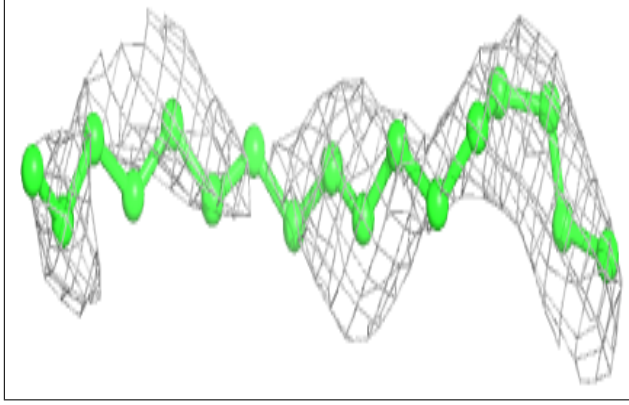
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

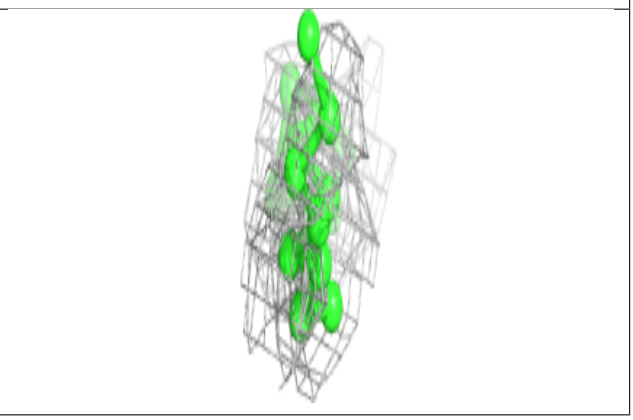
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	MPG	C	406	17/25	0.64	0.46	60,84,100,103	0
9	MPG	B	306	25/25	0.68	0.47	67,77,97,98	0
12	NS5	C	404	40/40	0.71	0.48	50,79,103,106	0
6	DGA	A	405	37/44	0.72	0.40	53,77,94,103	0
9	MPG	B	305	25/25	0.73	0.45	80,101,116,120	0
13	OTP	C	405	41/49	0.81	0.38	48,60,78,84	0
8	BPB	C	402	61/65	0.89	0.31	51,68,83,88	0
11	MQ7	C	403	48/48	0.89	0.29	32,42,66,70	0
14	PO4	C	407	5/5	0.91	0.49	93,95,102,104	0
7	BCL	B	301	65/66	0.92	0.27	32,43,164,175	0
14	PO4	C	408	5/5	0.92	0.27	66,68,71,71	0
7	BCL	B	302	66/66	0.94	0.23	27,33,42,50	0
7	BCL	C	401	66/66	0.94	0.23	29,37,54,66	0
8	BPB	B	304	65/65	0.94	0.23	27,35,47,60	0
7	BCL	B	303	66/66	0.95	0.23	18,27,47,48	0
5	HEC	A	404	43/43	0.95	0.21	32,37,53,58	0
5	HEC	A	401	43/43	0.95	0.29	23,31,34,35	0
5	HEC	A	402	43/43	0.96	0.23	23,25,29,35	0
5	HEC	A	403	43/43	0.96	0.20	22,25,27,30	0
10	FE2	B	307	1/1	0.98	0.05	48,48,48,48	0

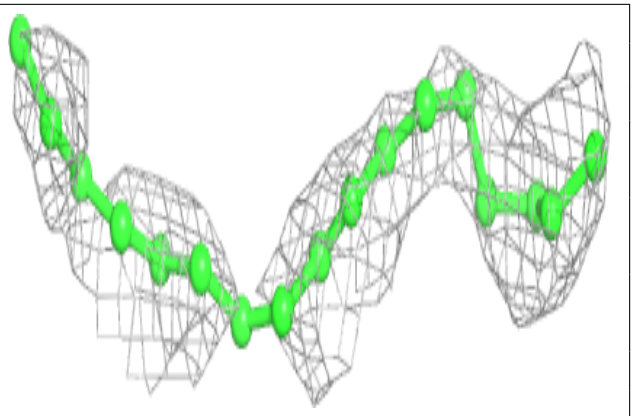
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around MPG C 406:

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

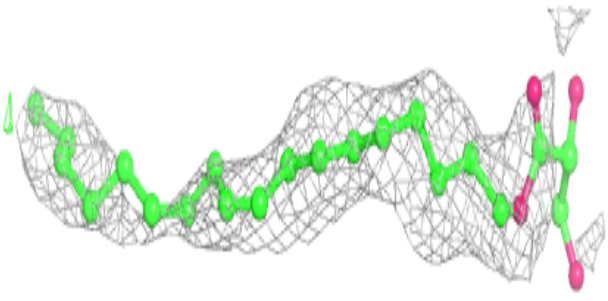


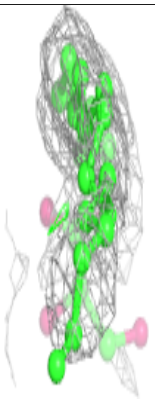


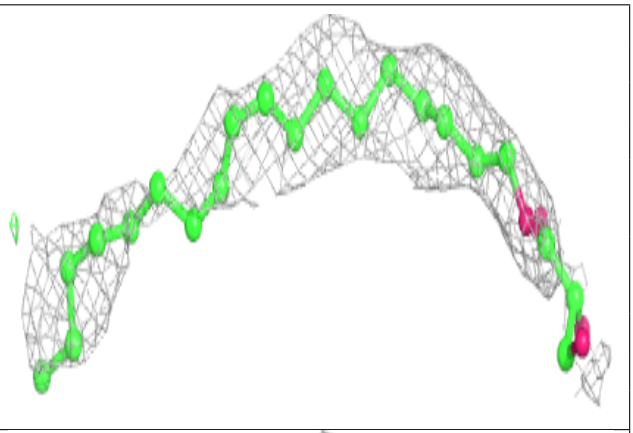


Electron density around MPG B 306:

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

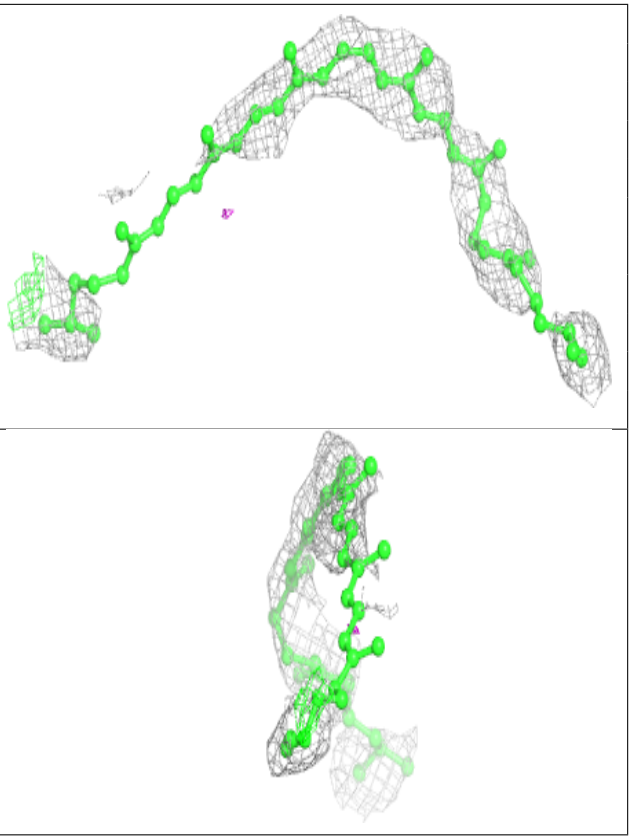


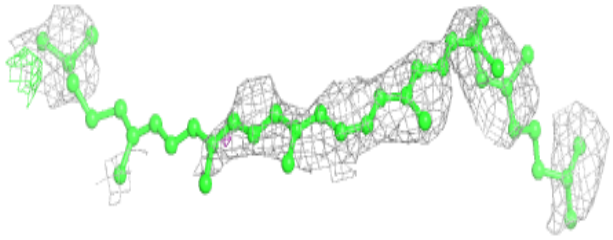




Electron density around NS5 C 404:

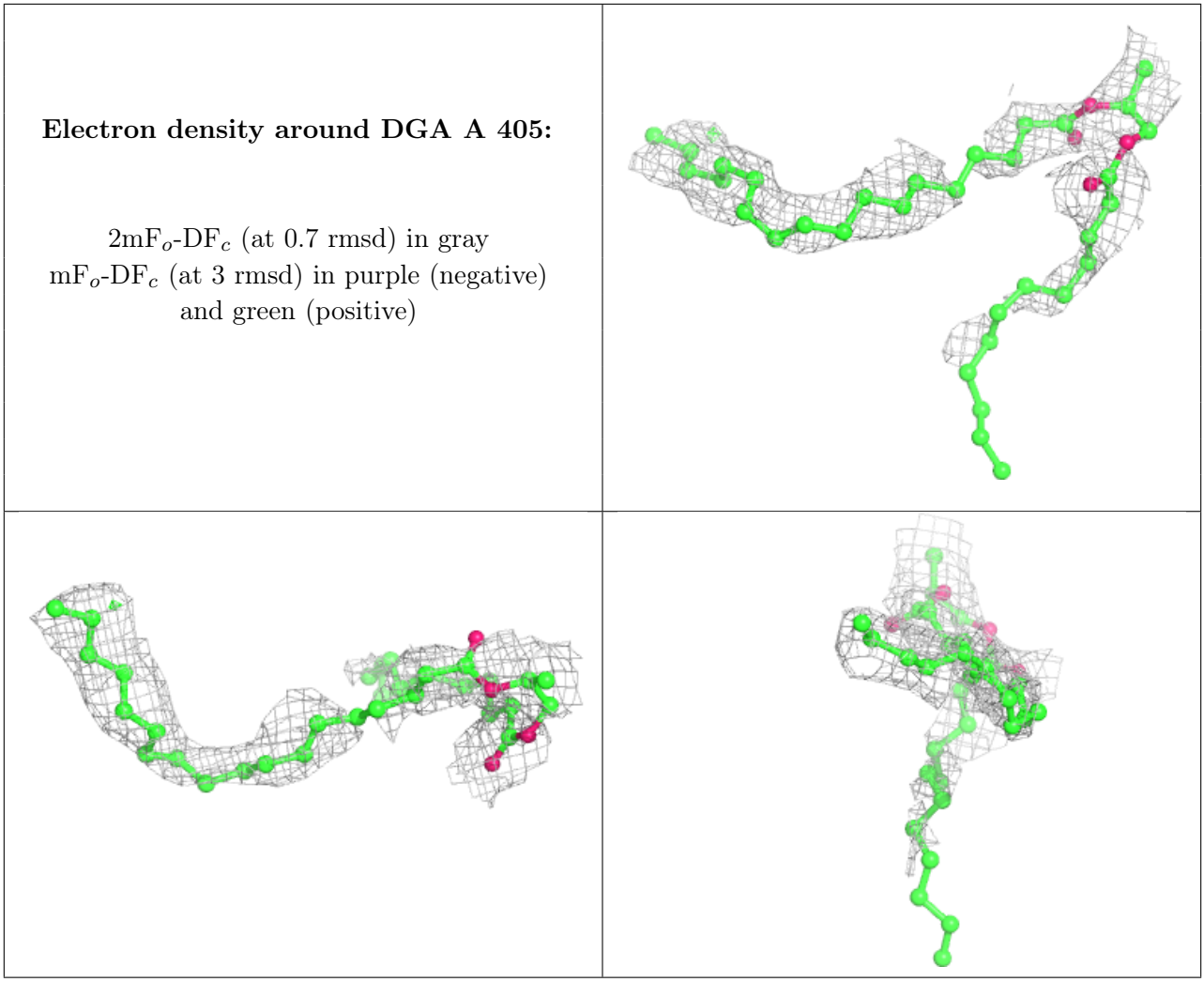
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





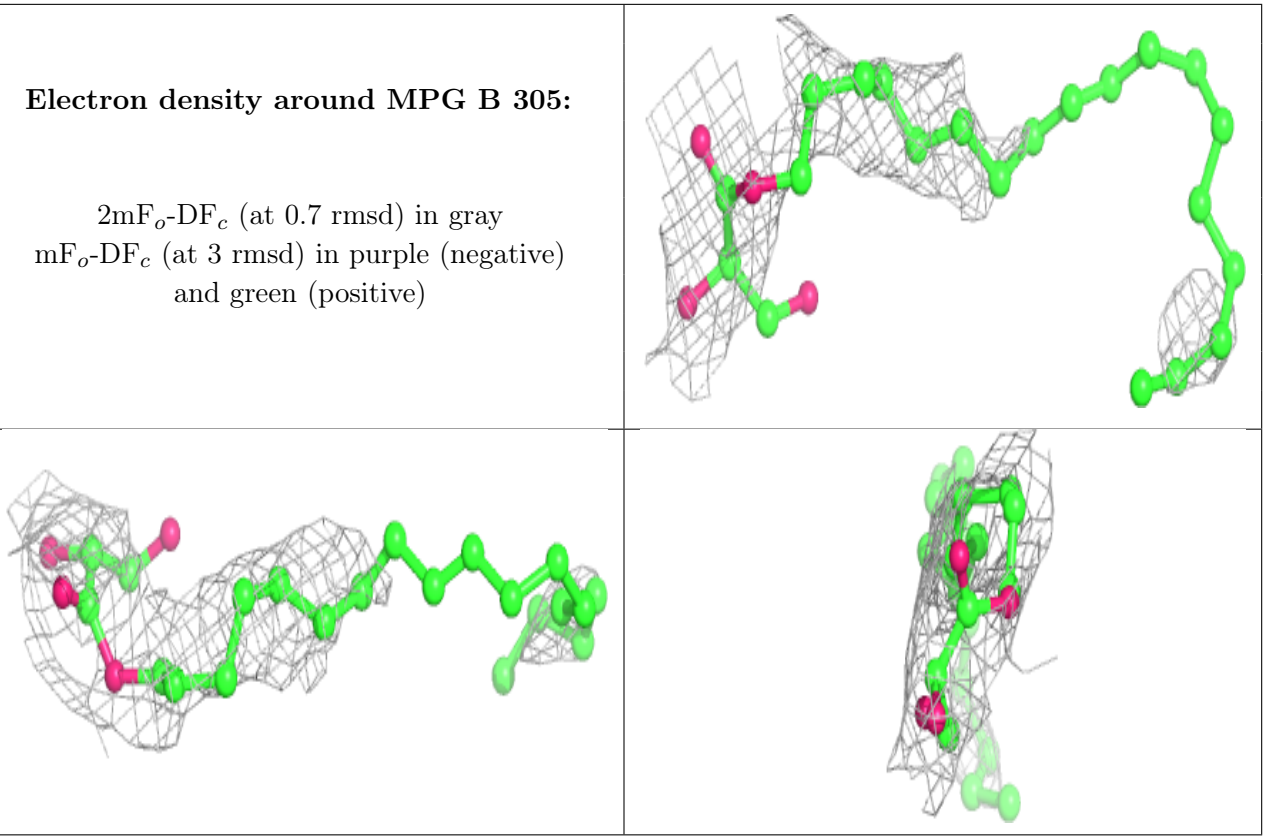
Electron density around DGA A 405:

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



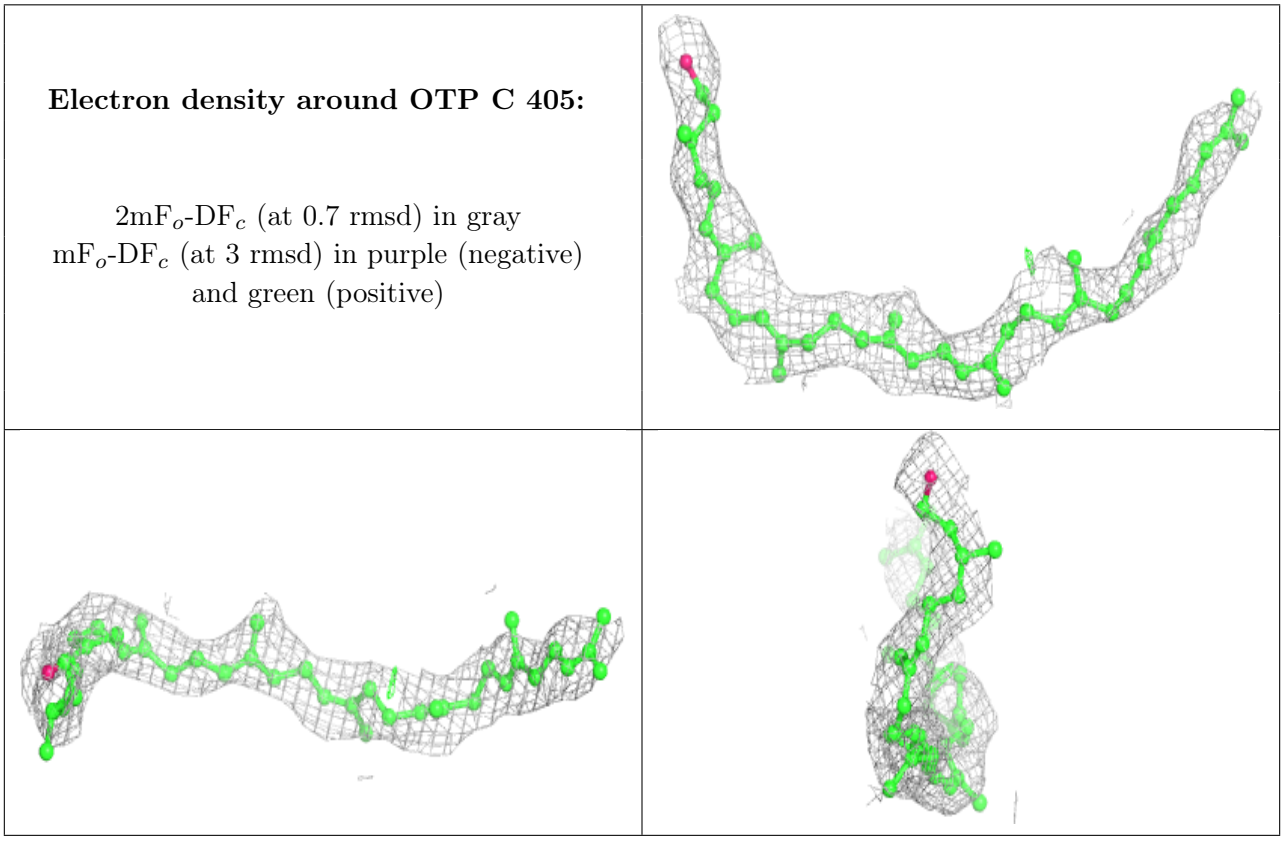
Electron density around MPG B 305:

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



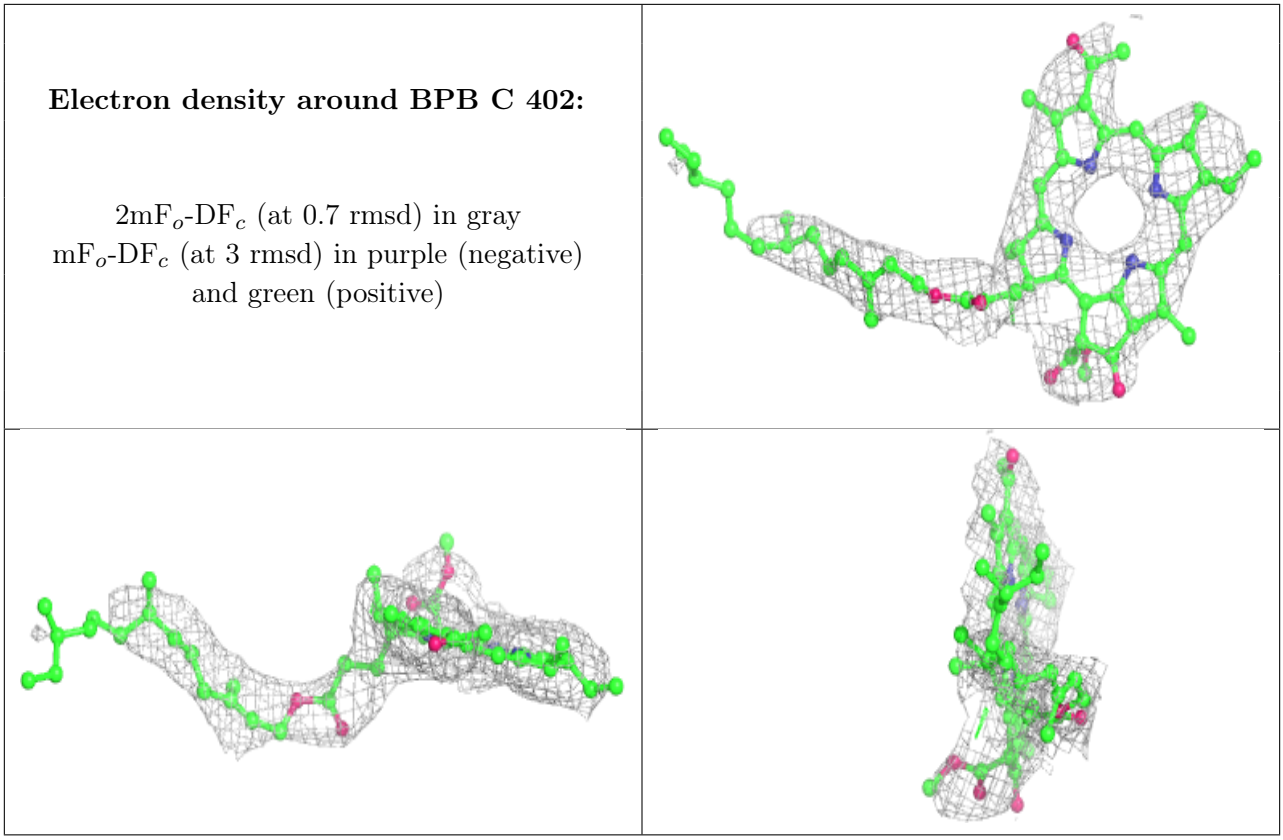
Electron density around OTP C 405:

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



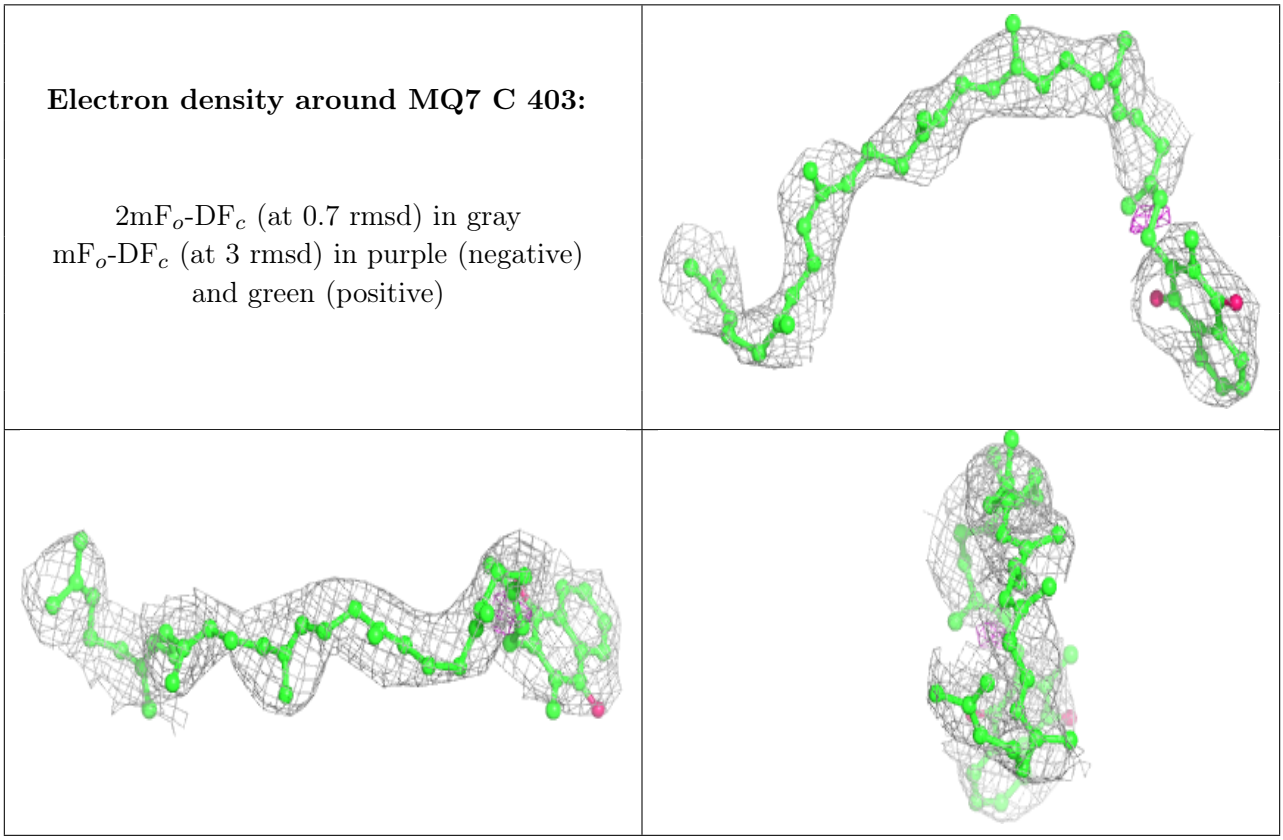
Electron density around BPB C 402:

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



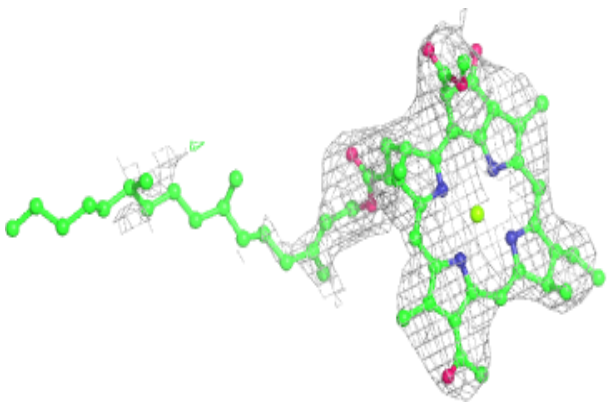
Electron density around MQ7 C 403:

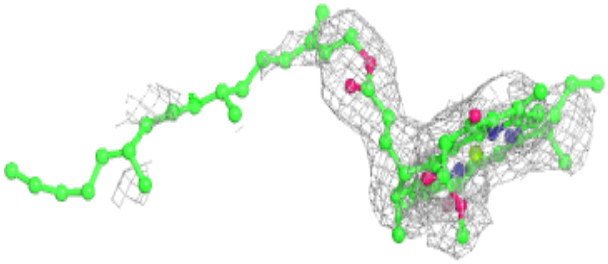
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

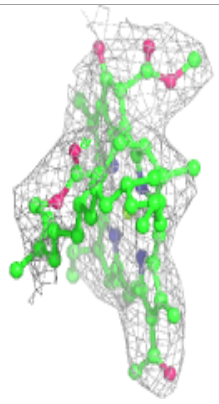


Electron density around BCL B 301:

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

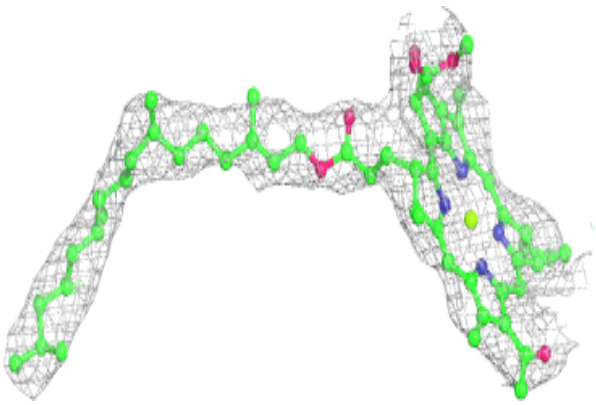


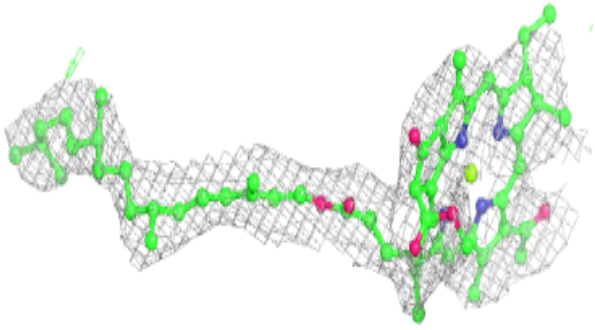


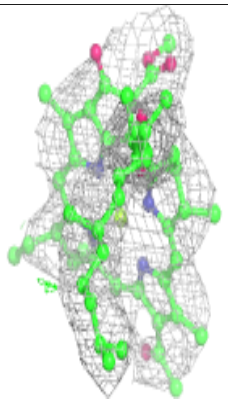


Electron density around BCL B 302:

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

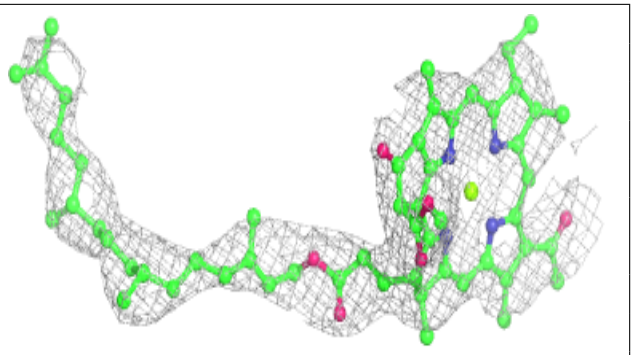


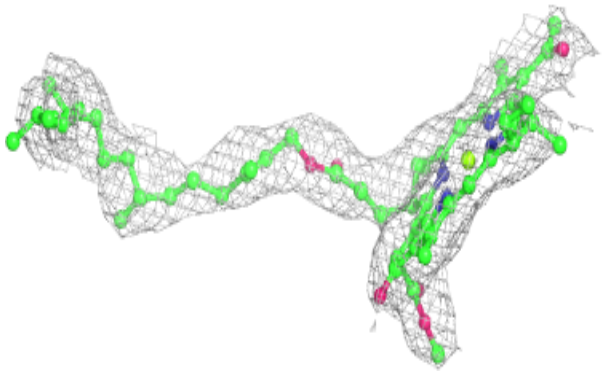


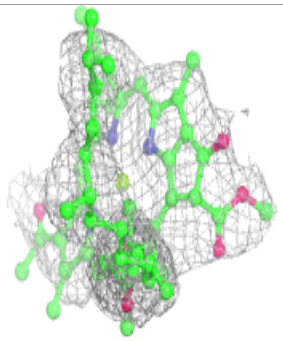


Electron density around BCL C 401:

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

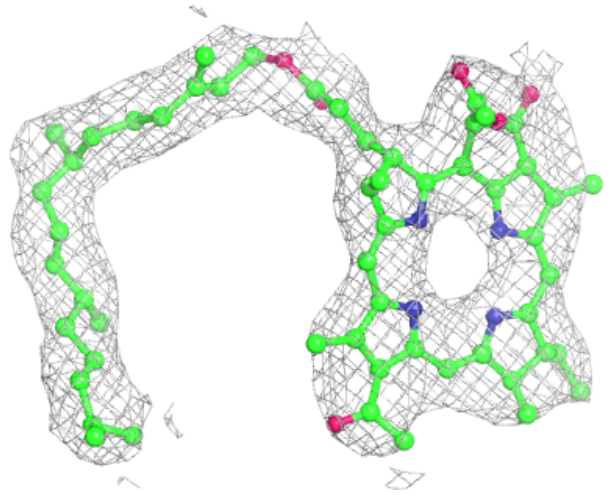


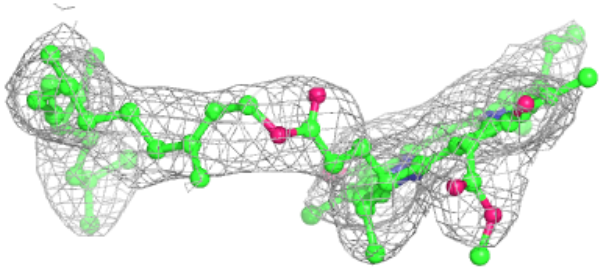


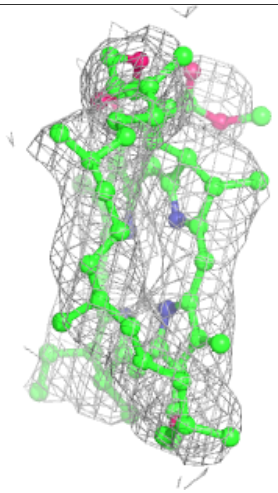


Electron density around BPB B 304:

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

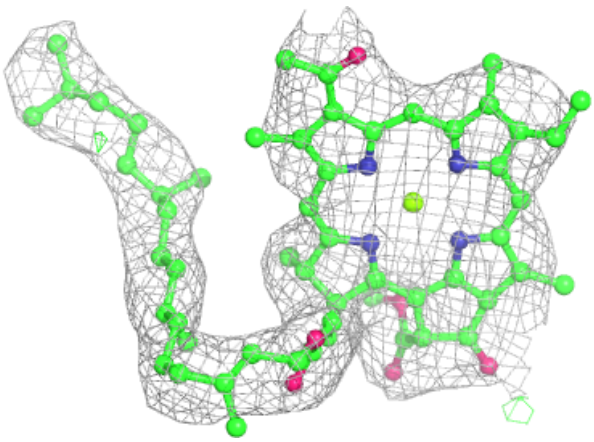


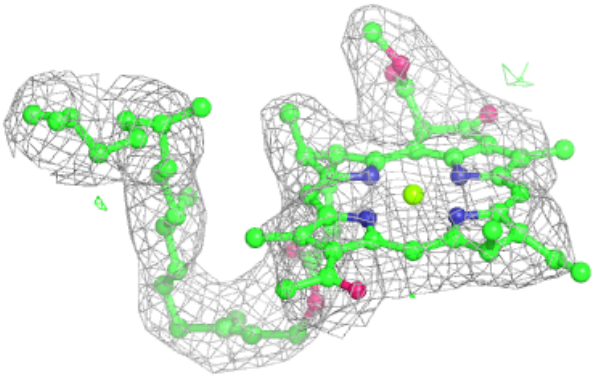


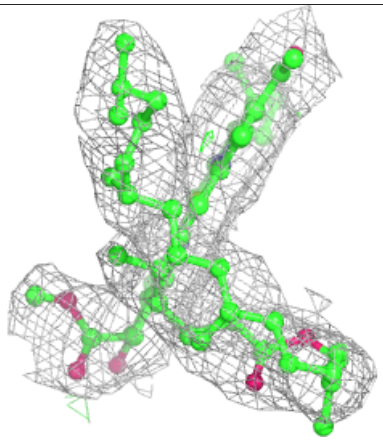


Electron density around BCL B 303:

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

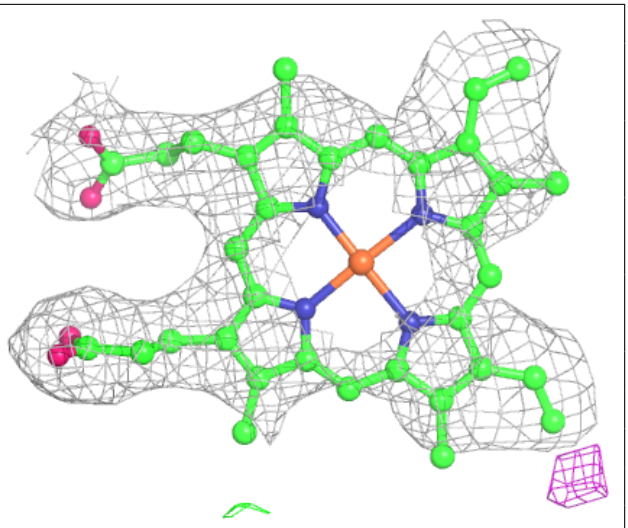


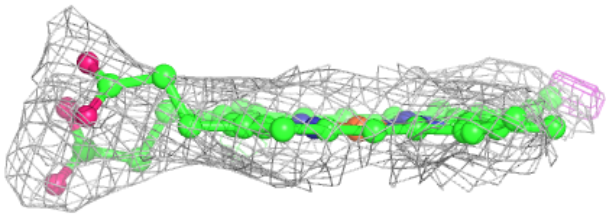


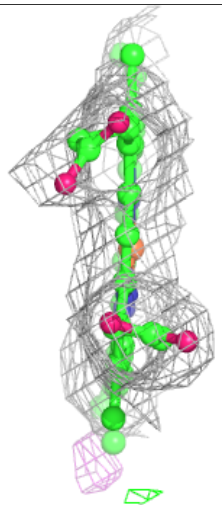


Electron density around HEC A 404:

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

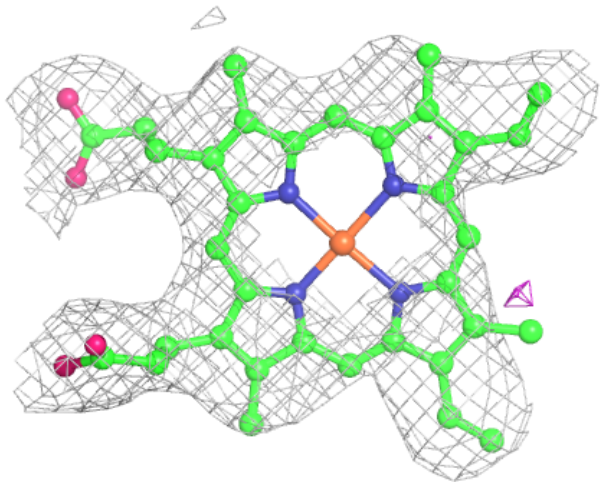


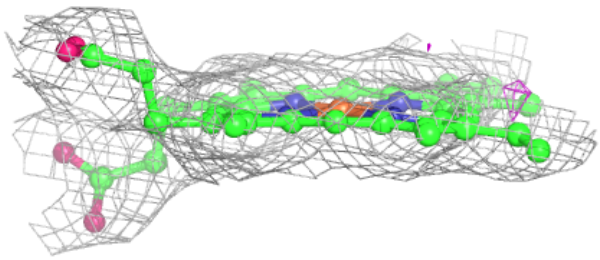


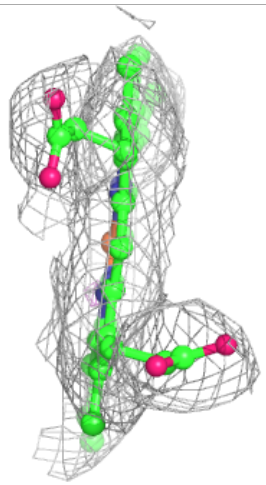


Electron density around HEC A 401:

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

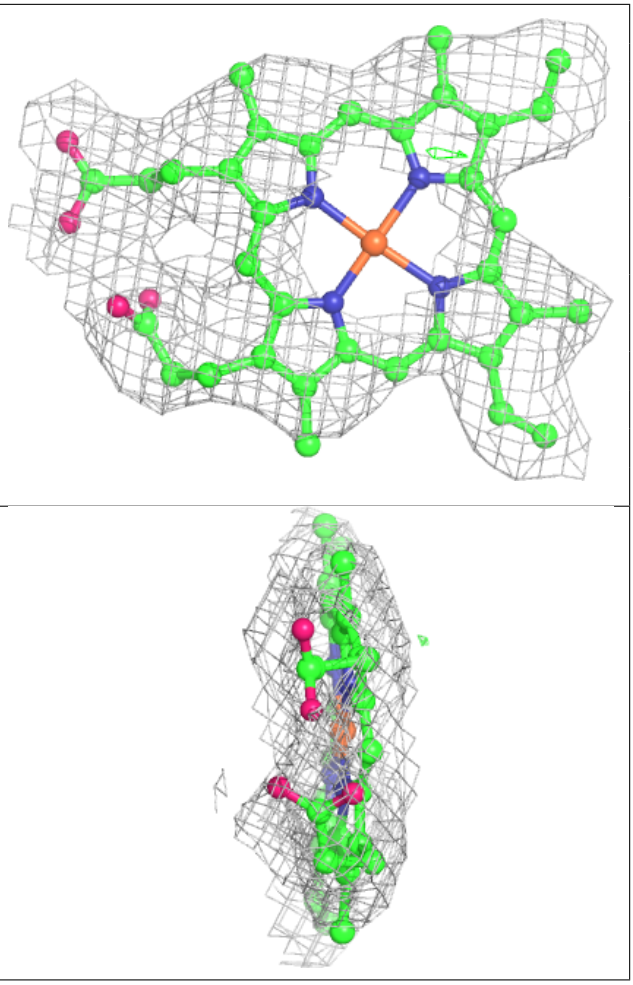






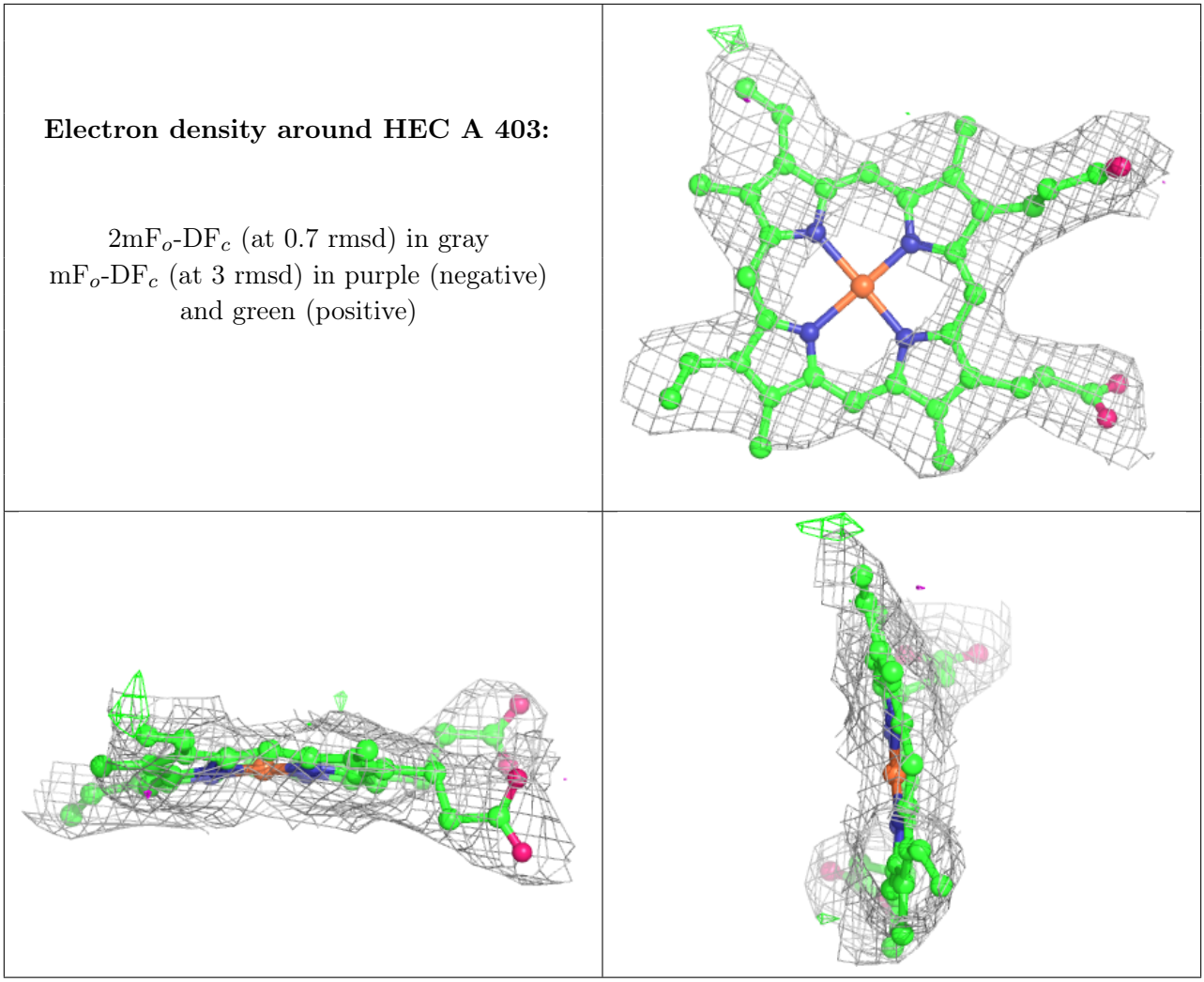
Electron density around HEC A 402:

$2mF_o$-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 A 403:

$2mF_o$-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

There are no such residues in this entry.