Full wwPDB X-ray Structure Validation Report ⓘ

Jan 7, 2024 – 04:43 am GMT

PDB ID	:	5M7J
Title	:	Blastochloris viridis photosynthetic reaction center structure using best crystal approach
Authors	:	Sharma, A.S.; Johansson, L.; Dunevall, E.; Wahlgren, W.Y.; Neutze, R.; Katona, G.
Deposited on	:	2016-10-28
Resolution	:	3.50 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:

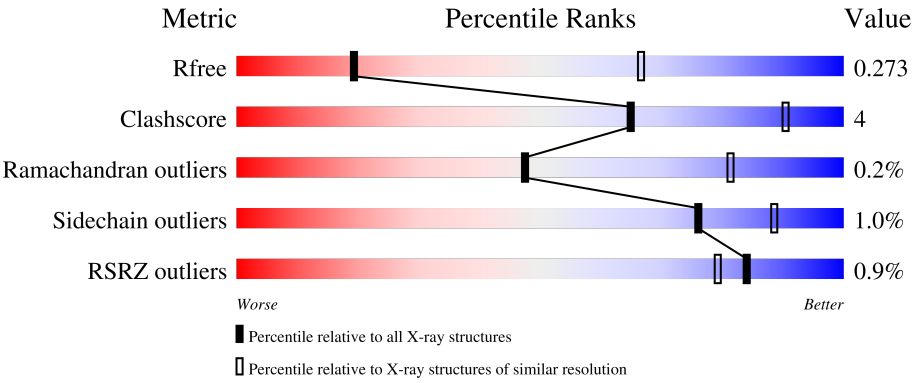
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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.

Mol	Chain	Length	Quality of chain
1	A	356	84% 9% 7%
2	B	274	87% 13%
3	C	324	91% 8% .
4	D	258	4% 89% 5% 6%

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
9	MPG	B	306	-	-	-	X
9	MPG	C	406	-	-	-	X

2 Entry composition

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
1	A	332	Total	C	N	O	S	0	0	0
			2598	1637	465	478	18			

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

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

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

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

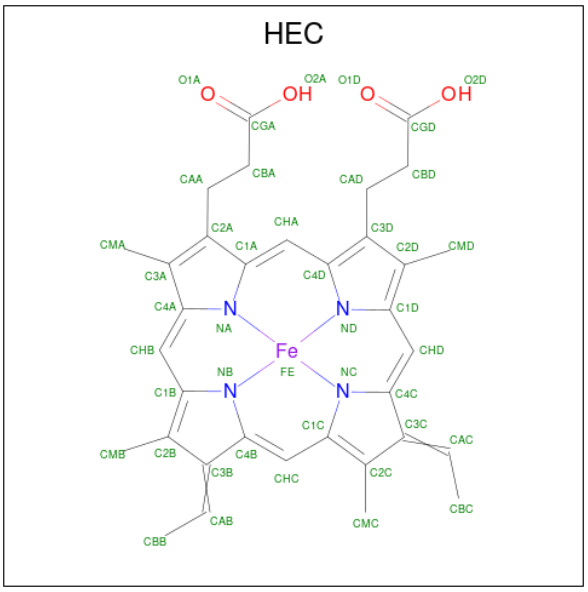
- Molecule 4 is a protein called Reaction center protein H chain.

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

There is a discrepancy between the modelled and reference sequences:

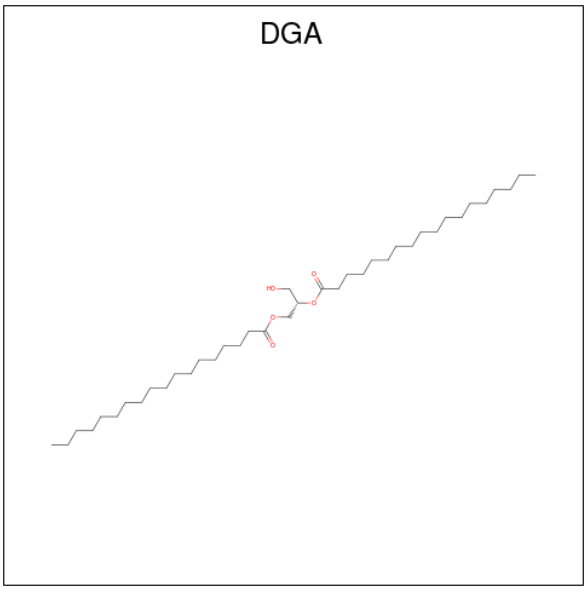
Chain	Residue	Modelled	Actual	Comment	Reference
D	1	FME	-	expression tag	UNP P06008

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



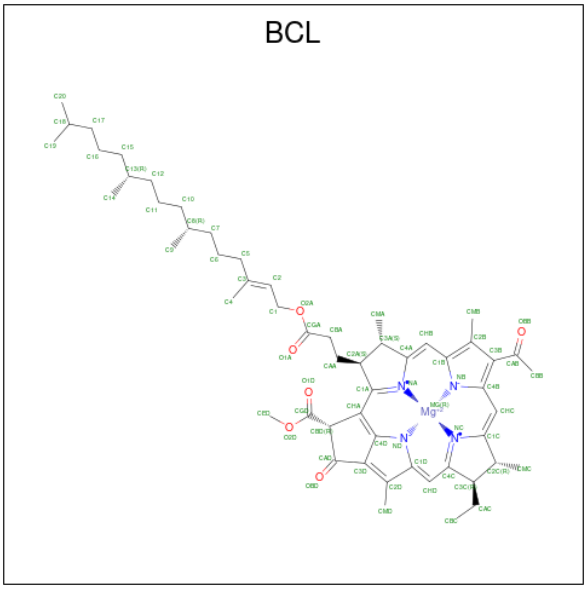
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



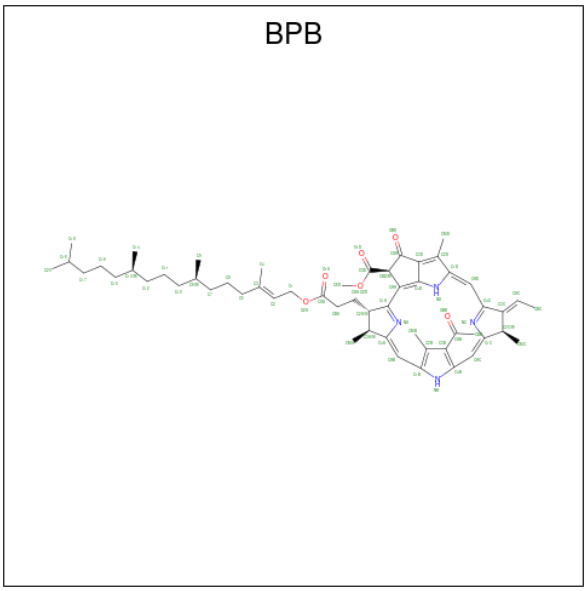
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			37	33	4		

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



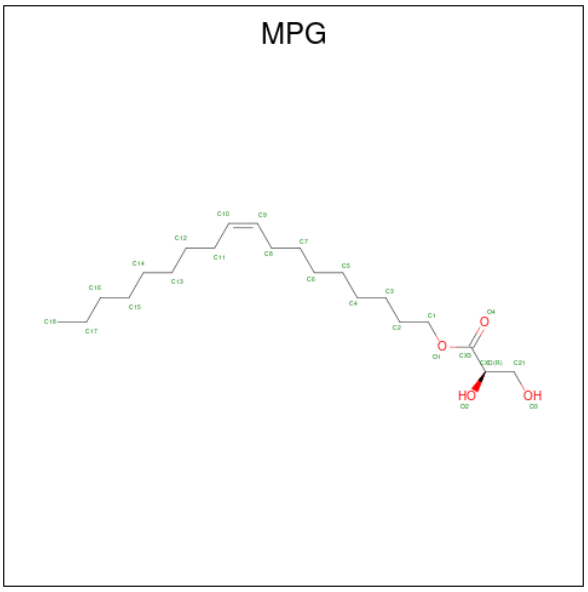
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	Mg	N	O	14	0
			65	54	1	4	6		
7	B	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	B	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	C	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- 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	6	0
			25	21	4		

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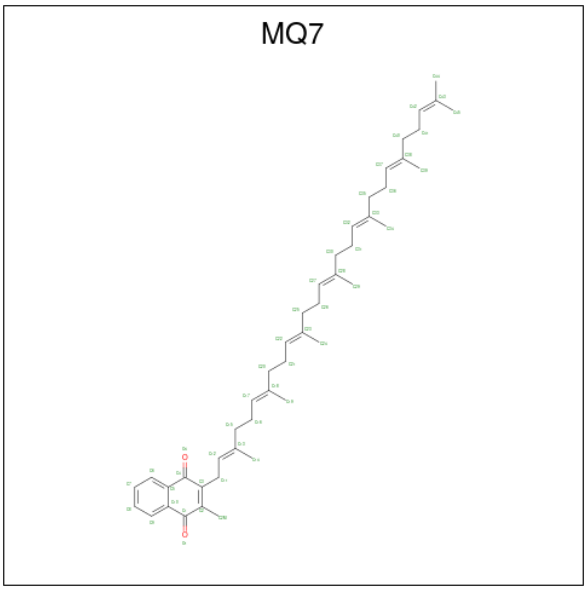
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C O 25 21 4	0	0
9	C	1	Total C 17 17	0	0

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

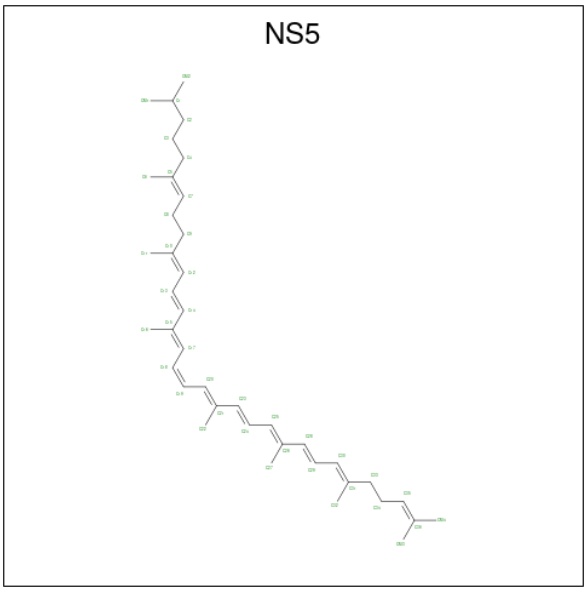
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total Fe 1 1	0	0

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



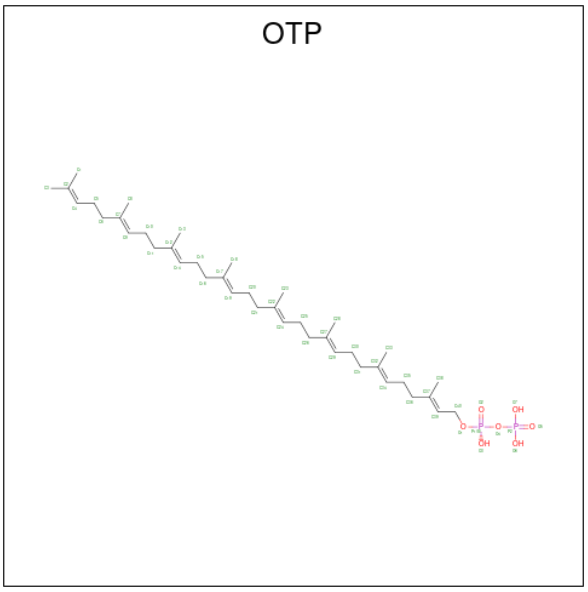
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	C	1	Total C O 48 46 2	0	0

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



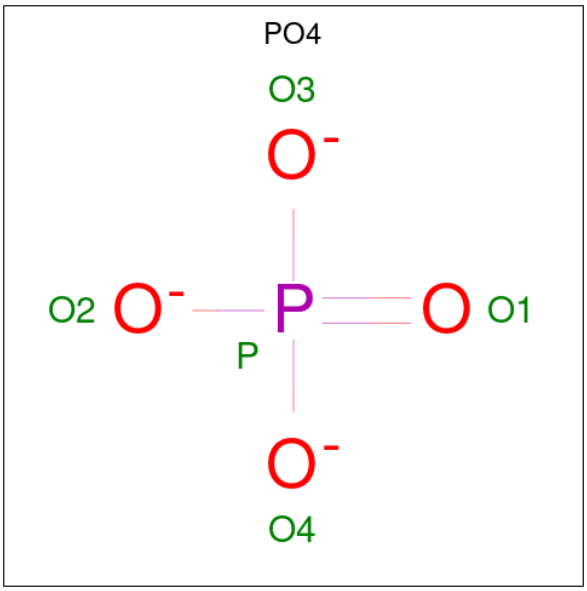
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	C	1	Total C 40 40	0	0

- 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).



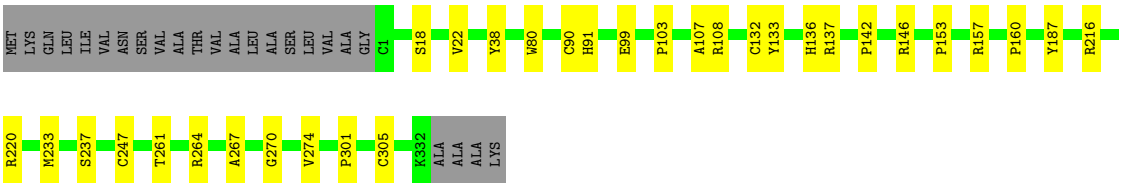
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	C	1	Total O P 5 4 1	0	0
14	C	1	Total O P 5 4 1	0	0

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.

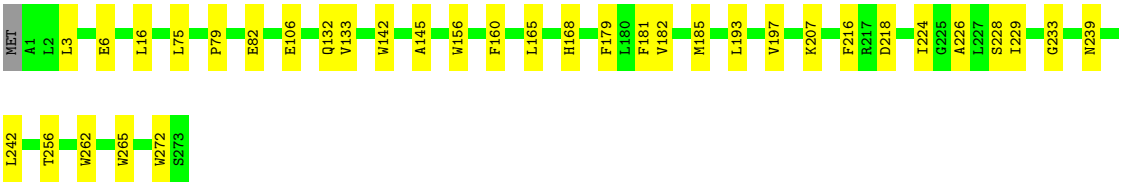
• Molecule 1: Photosynthetic reaction center cytochrome c subunit

Chain A:



• Molecule 2: Reaction center protein L chain

Chain B:

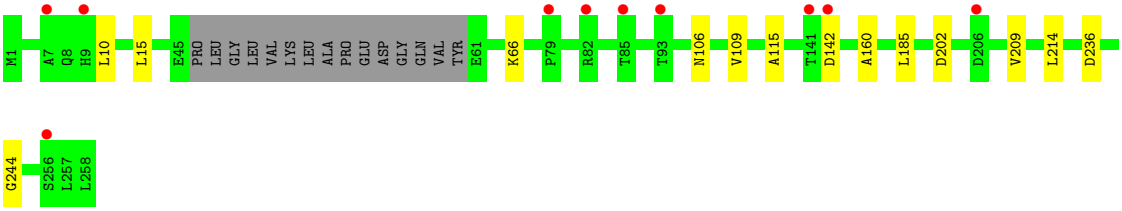


• Molecule 3: Reaction center protein M chain

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)	52.76 – 3.50 52.76 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (52.76-3.50) 99.5 (52.76-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.77 (at 3.48Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.253 , 0.273 0.253 , 0.273	Depositor DCC
R_{free} test set	1288 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å^2)	68.7	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 79.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.30$, $< L^2 > = 0.13$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.81	EDS
Total number of atoms	9890	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% 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: BCL, OTP, BPB, MQ7, FME, NS5, HEC, DGA, FE2, MPG, 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	0.26	0/2665	0.45	0/3633
2	B	0.26	0/2263	0.42	0/3089
3	C	0.25	0/2650	0.39	0/3629
4	D	0.24	0/1804	0.44	0/2485
All	All	0.25	0/9382	0.43	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	2576	24	0
2	B	2170	0	2100	22	0
3	C	2546	0	2430	19	0
4	D	1771	0	1656	7	0
5	A	172	0	128	15	0
6	A	37	0	58	3	0
7	B	197	0	218	9	0
7	C	66	0	74	4	0
8	B	65	0	74	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	C	61	0	63	2	0
9	B	50	0	80	1	0
9	C	17	0	31	0	0
10	B	1	0	0	0	0
11	C	48	0	64	1	0
12	C	40	0	60	6	0
13	C	41	0	65	1	0
14	C	10	0	0	0	0
All	All	9890	0	9677	80	0

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

All (80) 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)
7:B:303:BCL:HMD2	7:C:401:BCL:HBB3	1.76	0.67
1:A:99:GLU:OE2	1:A:108:ARG:NH2	2.33	0.61
1:A:80:TRP:CD1	1:A:133:TYR:HB2	2.38	0.59
9:B:305:MPG:H21C	3:C:1:ALA:HA	1.85	0.59
1:A:220:ARG:NH2	3:C:171:GLU:OE2	2.35	0.58
4:D:160:ALA:HB3	4:D:214:LEU:HD23	1.87	0.57
1:A:136:HIS:NE2	5:A:402:HEC:NB	2.53	0.56
1:A:305:CYS:HA	5:A:404:HEC:HHC	1.88	0.55
1:A:247:CYS:HA	1:A:261:THR:OG1	2.07	0.54
2:B:168:HIS:CE1	7:B:302:BCL:HMC2	2.43	0.52
7:B:302:BCL:H193	11:C:403:MQ7:H292	1.91	0.52
3:C:117:GLY:HA3	12:C:404:NS5:H92	1.92	0.52
2:B:239:ASN:HA	2:B:242:LEU:HB2	1.93	0.50
6:A:405:DGA:HB22	2:B:262:TRP:HH2	1.76	0.50
1:A:274:VAL:HG22	5:A:404:HEC:HMC2	1.94	0.50
2:B:132:GLN:OE1	2:B:145:ALA:HB1	2.13	0.49
2:B:193:LEU:HD22	2:B:216:PHE:HE2	1.77	0.49
1:A:301:PRO:HG2	5:A:402:HEC:HBD1	1.94	0.49
2:B:75:LEU:HA	2:B:142:TRP:CD1	2.47	0.48
1:A:153:PRO:HD3	1:A:160:PRO:HB3	1.95	0.48
1:A:233:MET:HB3	5:A:403:HEC:C3B	2.42	0.48
1:A:264:ARG:HG2	5:A:403:HEC:HMD3	1.96	0.48
6:A:405:DGA:HA22	6:A:405:DGA:HG11	1.70	0.48
2:B:133:VAL:HA	2:B:142:TRP:HZ3	1.79	0.48
8:B:304:BPB:HHC	8:B:304:BPB:HBBB	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:16:LEU:HD13	2:B:106:GLU:HG2	1.95	0.48
1:A:137:ARG:HB2	1:A:157:ARG:HH22	1.78	0.48
1:A:237:SER:OG	5:A:403:HEC:HAB	2.14	0.48
4:D:202:ASP:HB3	4:D:209:VAL:HB	1.95	0.48
1:A:107:ALA:CB	5:A:401:HEC:HAC	2.45	0.47
5:A:403:HEC:HBB1	2:B:165:LEU:HD22	1.96	0.47
7:B:301:BCL:H3C	3:C:184:LEU:HD21	1.96	0.47
2:B:181:PHE:HB3	8:C:402:BPB:HBBA	1.95	0.47
3:C:160:CYS:HB3	12:C:404:NS5:H82	1.97	0.47
4:D:106:ASN:HB3	4:D:109:VAL:HG22	1.97	0.47
3:C:70:LEU:HD21	12:C:404:NS5:H29	1.97	0.46
3:C:162:HIS:O	3:C:166:VAL:HG22	2.14	0.46
2:B:79:PRO:HB2	2:B:82[B]:GLU:HB2	1.97	0.46
2:B:218:ASP:O	3:C:130:ARG:NH2	2.48	0.46
3:C:261:GLU:OE2	4:D:66:LYS:NZ	2.49	0.46
1:A:270:GLY:O	1:A:274:VAL:HG23	2.16	0.46
1:A:18:SER:HB2	2:B:156:TRP:CD1	2.51	0.46
2:B:179:PHE:HA	2:B:182:VAL:HG12	1.96	0.45
12:C:404:NS5:H18	12:C:404:NS5:H161	1.79	0.45
2:B:233:GLY:HA3	3:C:214:PHE:CE1	2.52	0.45
1:A:267:ALA:CB	5:A:403:HEC:HAC	2.47	0.45
5:A:404:HEC:CBC	5:A:404:HEC:HMC1	2.47	0.45
1:A:216:ARG:NH2	3:C:287:THR:O	2.50	0.44
1:A:80:TRP:HB3	1:A:132:CYS:HB2	1.98	0.44
2:B:224:ILE:HG12	2:B:228:SER:HB2	1.99	0.44
7:B:303:BCL:HMD2	7:C:401:BCL:CBB	2.44	0.44
7:B:301:BCL:HBB3	7:C:401:BCL:H62	2.00	0.44
4:D:142:ASP:OD1	4:D:142:ASP:N	2.45	0.44
12:C:404:NS5:H63	12:C:404:NS5:H32	1.93	0.43
3:C:281:GLY:O	3:C:285:THR:OG1	2.31	0.43
1:A:90:CYS:SG	1:A:103:PRO:HB2	2.58	0.43
7:B:301:BCL:HHC	7:B:301:BCL:HBB2	1.99	0.43
3:C:98:ALA:HB3	3:C:100:TYR:CZ	2.53	0.43
5:A:404:HEC:CBB	5:A:404:HEC:HMB1	2.49	0.43
4:D:115:ALA:HB2	4:D:244:GLY:HA3	2.00	0.43
3:C:177:ILE:O	3:C:180:HIS:ND1	2.51	0.43
3:C:227:PHE:HB2	3:C:242:ALA:HB2	2.00	0.42
13:C:405:OTP:H51	13:C:405:OTP:H81	1.71	0.42
5:A:401:HEC:CBB	5:A:401:HEC:HMB1	2.49	0.42
2:B:168:HIS:NE2	7:B:302:BCL:HMC2	2.35	0.42
7:B:302:BCL:H61	7:B:302:BCL:H41	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:405:DGA:HB21	2:B:265:TRP:CZ2	2.55	0.42
1:A:22:VAL:HG12	2:B:256:THR:HB	2.02	0.42
3:C:87:GLN:O	3:C:91:LEU:HG	2.20	0.41
4:D:10:LEU:HD21	4:D:15:LEU:HD21	2.03	0.41
3:C:106:PRO:O	3:C:111:GLY:N	2.49	0.41
1:A:142:PRO:HD2	5:A:402:HEC:HBD2	2.03	0.41
8:C:402:BPB:HHC	8:C:402:BPB:HBBB	2.02	0.41
2:B:226:ALA:O	2:B:229:ILE:HG22	2.20	0.41
2:B:3:LEU:HB2	2:B:6:GLU:HB2	2.02	0.41
3:C:195:TYR:CE2	7:C:401:BCL:HMC2	2.56	0.41
12:C:404:NS5:H341	12:C:404:NS5:H321	1.83	0.40
1:A:91:HIS:NE2	5:A:401:HEC:NA	2.69	0.40
1:A:187:TYR:CE2	3:C:97:LYS:HD3	2.57	0.40
2:B:197:VAL:HG13	2:B:207:LYS:HB2	2.03	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	A	330/356 (93%)	315 (96%)	15 (4%)	0	100	100
2	B	273/274 (100%)	263 (96%)	10 (4%)	0	100	100
3	C	321/324 (99%)	312 (97%)	7 (2%)	2 (1%)	25	64
4	D	239/258 (93%)	231 (97%)	8 (3%)	0	100	100
All	All	1163/1212 (96%)	1121 (96%)	40 (3%)	2 (0%)	47	81

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	193	ASN

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Mol	Chain	Res	Type
3	C	177	ILE

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%)	278 (99%)	2 (1%)	84 93
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%)	903 (99%)	9 (1%)	76 88

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	TYR
1	A	146	ARG
2	B	160	PHE
2	B	185	MET
2	B	272	TRP
3	C	194	PHE
3	C	214	PHE
4	D	185	LEU
4	D	236	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	0.93	0	7,9,11	0.81	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FME	D	1	4	-	4/7/9/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

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	$\#\|Z\| > 2$
14	PO4	C	407	-	4,4,4	0.90	0	6,6,6	0.44	0
7	BCL	B	302	-	64,74,74	1.30	6 (9%)	78,115,115	1.62	12 (15%)
13	OTP	C	405	-	40,40,48	0.63	0	47,47,61	1.96	15 (31%)
14	PO4	C	408	-	4,4,4	0.90	0	6,6,6	0.47	0
5	HEC	A	401	1	32,50,50	2.02	4 (12%)	24,82,82	1.77	5 (20%)
7	BCL	C	401	-	64,74,74	1.30	6 (9%)	78,115,115	1.57	11 (14%)
5	HEC	A	404	1	32,50,50	2.05	4 (12%)	24,82,82	1.58	5 (20%)
8	BPB	C	402	-	45,66,70	0.98	3 (6%)	42,96,101	1.22	5 (11%)
5	HEC	A	403	1	32,50,50	1.98	4 (12%)	24,82,82	1.86	5 (20%)
9	MPG	B	305	-	24,24,24	1.24	1 (4%)	24,25,25	1.54	3 (12%)
11	MQ7	C	403	-	49,49,49	1.79	10 (20%)	60,63,63	1.62	15 (25%)
9	MPG	B	306	-	24,24,24	1.23	1 (4%)	24,25,25	1.28	2 (8%)
8	BPB	B	304	-	49,70,70	0.99	3 (6%)	47,101,101	1.16	5 (10%)
7	BCL	B	301	-	63,73,74	1.28	6 (9%)	76,113,115	1.47	8 (10%)
6	DGA	A	405	-	36,36,43	1.18	3 (8%)	38,38,45	3.08	6 (15%)
12	NS5	C	404	-	39,39,39	2.34	18 (46%)	44,46,46	2.03	11 (25%)
5	HEC	A	402	1	32,50,50	1.97	4 (12%)	24,82,82	1.94	6 (25%)
9	MPG	C	406	-	16,16,24	0.78	0	15,15,25	0.78	0
7	BCL	B	303	-	64,74,74	1.31	7 (10%)	78,115,115	1.51	12 (15%)

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
5	HEC	A	401	1	-	2/10/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BPB	B	304	-	-	4/37/105/105	0/5/6/6
7	BCL	B	303	-	-	5/37/137/137	-
11	MQ7	C	403	-	-	3/41/61/61	0/2/2/2
9	MPG	B	306	-	-	11/25/25/25	-
7	BCL	B	302	-	-	4/37/137/137	-
7	BCL	C	401	-	-	6/37/137/137	-
6	DGA	A	405	-	-	16/37/37/45	-
13	OTP	C	405	-	-	13/45/45/55	-
5	HEC	A	404	1	-	0/10/54/54	-
12	NS5	C	404	-	-	14/43/43/43	-
5	HEC	A	402	1	-	5/10/54/54	-
8	BPB	C	402	-	-	9/33/101/105	0/5/6/6
5	HEC	A	403	1	-	0/10/54/54	-
9	MPG	C	406	-	-	6/14/14/25	-
9	MPG	B	305	-	-	15/25/25/25	-
7	BCL	B	301	-	-	5/36/136/137	-

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	403	MQ7	C3-C2	7.13	1.48	1.35
5	A	404	HEC	C2B-C3B	-5.71	1.34	1.40
5	A	401	HEC	C2B-C3B	-5.50	1.35	1.40
5	A	404	HEC	C3C-C2C	-5.45	1.35	1.40
5	A	401	HEC	C3C-C2C	-5.40	1.35	1.40
5	A	402	HEC	C2B-C3B	-5.34	1.35	1.40
5	A	403	HEC	C3C-C2C	-5.31	1.35	1.40
7	C	401	BCL	C1B-NB	5.07	1.39	1.35
7	B	303	BCL	C1B-NB	5.06	1.39	1.35
7	B	301	BCL	C1B-NB	5.04	1.39	1.35
7	B	302	BCL	C1B-NB	4.96	1.39	1.35
12	C	404	NS5	C30-C31	4.96	1.39	1.34
5	A	403	HEC	C2B-C3B	-4.95	1.35	1.40
5	A	402	HEC	C3C-C2C	-4.92	1.35	1.40
7	B	302	BCL	MG-NA	4.83	2.17	2.06
9	B	305	MPG	O1-CX3	4.80	1.43	1.33
7	C	401	BCL	MG-NA	4.78	2.17	2.06
9	B	306	MPG	O1-CX3	4.74	1.43	1.33
7	B	301	BCL	MG-NA	4.70	2.17	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	303	BCL	MG-NA	4.66	2.17	2.06
12	C	404	NS5	C14-C15	4.30	1.55	1.45
5	A	403	HEC	CBC-CAC	-4.06	1.34	1.49
11	C	403	MQ7	C5-C4	4.04	1.55	1.48
5	A	403	HEC	CBB-CAB	-4.04	1.34	1.49
5	A	402	HEC	CBC-CAC	-4.04	1.34	1.49
5	A	402	HEC	CBB-CAB	-4.04	1.34	1.49
5	A	404	HEC	CBB-CAB	-4.02	1.34	1.49
5	A	401	HEC	CBC-CAC	-4.00	1.34	1.49
5	A	401	HEC	CBB-CAB	-4.00	1.34	1.49
5	A	404	HEC	CBC-CAC	-3.98	1.34	1.49
12	C	404	NS5	C12-C10	3.84	1.38	1.34
11	C	403	MQ7	C10-C1	3.78	1.55	1.48
12	C	404	NS5	C19-C20	3.75	1.55	1.43
8	B	304	BPB	CBD-CGD	-3.71	1.47	1.52
6	A	405	DGA	OG1-CA1	3.53	1.43	1.33
12	C	404	NS5	C23-C21	3.50	1.53	1.45
12	C	404	NS5	C18-C17	3.49	1.54	1.43
8	C	402	BPB	CBD-CGD	-3.48	1.47	1.52
6	A	405	DGA	CG1-CG2	3.45	1.58	1.50
7	B	303	BCL	MG-NC	3.44	2.14	2.06
12	C	404	NS5	C28-C26	3.40	1.53	1.45
7	B	301	BCL	MG-NC	3.37	2.14	2.06
7	B	302	BCL	MG-NC	3.28	2.14	2.06
8	C	402	BPB	CAC-C3C	3.27	1.41	1.33
12	C	404	NS5	C29-C30	3.27	1.53	1.43
12	C	404	NS5	C24-C25	3.24	1.53	1.43
6	A	405	DGA	OG2-CB1	3.24	1.43	1.34
8	B	304	BPB	CAC-C3C	3.22	1.41	1.33
7	C	401	BCL	MG-NC	3.13	2.13	2.06
12	C	404	NS5	C13-C12	3.02	1.52	1.43
12	C	404	NS5	C4-C5	2.95	1.57	1.51
12	C	404	NS5	C20-C21	2.84	1.39	1.35
7	B	303	BCL	CHD-C1D	2.70	1.43	1.38
11	C	403	MQ7	C20-C18	2.67	1.56	1.51
12	C	404	NS5	C7-C5	2.67	1.39	1.33
11	C	403	MQ7	C12-C13	2.54	1.39	1.33
12	C	404	NS5	C33-C31	2.53	1.56	1.51
7	B	302	BCL	CHD-C1D	2.52	1.43	1.38
11	C	403	MQ7	C17-C18	2.49	1.39	1.33
7	B	301	BCL	CHD-C1D	2.46	1.43	1.38
8	B	304	BPB	OBD-CAD	2.45	1.25	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	401	BCL	CHD-C1D	2.43	1.43	1.38
12	C	404	NS5	C13-C14	2.40	1.40	1.34
7	B	303	BCL	C4B-NB	2.38	1.37	1.35
11	C	403	MQ7	C27-C28	2.35	1.38	1.33
11	C	403	MQ7	C32-C33	2.30	1.38	1.33
7	C	401	BCL	C4B-NB	2.22	1.37	1.35
11	C	403	MQ7	C11-C3	2.18	1.55	1.51
12	C	404	NS5	C17-C15	2.18	1.38	1.35
7	B	301	BCL	C4B-NB	2.16	1.37	1.35
7	C	401	BCL	C1D-ND	2.16	1.40	1.37
7	B	302	BCL	C4B-NB	2.13	1.37	1.35
12	C	404	NS5	C29-C28	2.10	1.40	1.34
7	B	303	BCL	OBD-CAD	2.08	1.26	1.22
12	C	404	NS5	C35-C36	2.07	1.38	1.32
7	B	302	BCL	C1D-C2D	-2.04	1.41	1.45
8	C	402	BPB	OBD-CAD	2.04	1.25	1.22
7	B	301	BCL	C3D-C4D	-2.02	1.39	1.44
7	B	303	BCL	C3D-C4D	-2.01	1.39	1.44
11	C	403	MQ7	C22-C23	2.00	1.37	1.33

All (126) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	405	DGA	OG2-CG2-CG3	-12.63	79.06	107.93
6	A	405	DGA	OG2-CG2-CG1	-9.98	83.03	106.13
6	A	405	DGA	CG3-CG2-CG1	7.09	133.01	112.63
12	C	404	NS5	C18-C17-C15	-6.40	118.18	127.31
12	C	404	NS5	C19-C20-C21	-5.69	119.19	127.31
7	C	401	BCL	CHD-C1D-ND	-5.62	119.29	124.45
9	B	305	MPG	O1-CX3-CXD	5.44	122.54	111.68
7	B	302	BCL	CHD-C1D-ND	-5.41	119.48	124.45
7	B	301	BCL	CHD-C1D-ND	-5.33	119.56	124.45
7	B	303	BCL	CHD-C1D-ND	-5.28	119.60	124.45
7	C	401	BCL	C4D-CHA-C1A	5.23	127.61	121.25
7	B	302	BCL	C4D-CHA-C1A	5.22	127.60	121.25
7	B	301	BCL	C4D-CHA-C1A	5.10	127.46	121.25
13	C	405	OTP	C33-C32-C31	4.62	123.05	115.27
7	B	302	BCL	CMB-C2B-C1B	-4.59	121.40	128.46
7	B	303	BCL	CMB-C2B-C1B	-4.41	121.69	128.46
7	B	303	BCL	C4D-CHA-C1A	4.39	126.60	121.25
9	B	306	MPG	O1-CX3-CXD	4.38	120.41	111.68
7	C	401	BCL	CMB-C2B-C1B	-4.37	121.74	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	403	HEC	CMB-C2B-C1B	-4.13	122.11	128.46
7	B	301	BCL	C1D-ND-C4D	-4.10	103.42	106.33
7	B	303	BCL	C1D-ND-C4D	-3.86	103.59	106.33
5	A	402	HEC	CMB-C2B-C1B	-3.81	122.61	128.46
13	C	405	OTP	C40-C39-C37	-3.74	121.39	127.21
5	A	402	HEC	CBA-CAA-C2A	-3.71	106.35	112.60
11	C	403	MQ7	C21-C22-C23	-3.67	118.83	127.66
5	A	401	HEC	CMB-C2B-C1B	-3.62	122.91	128.46
5	A	403	HEC	CMB-C2B-C3B	3.61	130.06	125.82
5	A	403	HEC	CMC-C2C-C1C	-3.52	123.05	128.46
7	B	301	BCL	CMB-C2B-C1B	-3.49	123.10	128.46
7	C	401	BCL	C2A-C1A-CHA	3.42	129.84	123.86
7	C	401	BCL	C1D-ND-C4D	-3.38	103.93	106.33
7	B	302	BCL	C4A-NA-C1A	3.38	108.22	106.71
8	C	402	BPB	OBD-CAD-CBD	-3.37	120.88	125.82
5	A	401	HEC	CMC-C2C-C1C	-3.36	123.29	128.46
12	C	404	NS5	C11-C10-C9	3.36	120.92	115.27
13	C	405	OTP	C23-C22-C21	3.35	120.91	115.27
5	A	402	HEC	CMC-C2C-C1C	-3.35	123.32	128.46
5	A	402	HEC	CMB-C2B-C3B	3.34	129.75	125.82
7	B	302	BCL	C2A-C1A-CHA	3.28	129.60	123.86
5	A	401	HEC	CBD-CAD-C3D	-3.28	107.03	112.62
7	B	302	BCL	C1D-ND-C4D	-3.27	104.01	106.33
7	B	302	BCL	CMB-C2B-C3B	3.23	130.72	124.68
11	C	403	MQ7	C11-C12-C13	-3.22	121.44	126.79
7	B	302	BCL	CHA-C1A-NA	-3.20	119.06	126.40
7	C	401	BCL	CHA-C1A-NA	-3.19	119.10	126.40
5	A	404	HEC	CMC-C2C-C1C	-3.17	123.58	128.46
13	C	405	OTP	C8-C7-C6	3.17	120.61	115.27
6	A	405	DGA	OG2-CB1-CB2	3.17	118.33	111.50
13	C	405	OTP	C13-C12-C11	3.14	120.55	115.27
7	B	301	BCL	CHA-C1A-NA	-3.13	119.23	126.40
12	C	404	NS5	C24-C25-C26	-3.12	122.85	127.31
7	B	303	BCL	CMB-C2B-C3B	3.12	130.52	124.68
7	C	401	BCL	CMB-C2B-C3B	3.11	130.50	124.68
13	C	405	OTP	C35-C34-C32	-3.10	120.19	127.66
8	B	304	BPB	OBD-CAD-CBD	-3.09	121.29	125.82
5	A	404	HEC	CMB-C2B-C1B	-3.05	123.77	128.46
13	C	405	OTP	C28-C27-C26	3.03	120.36	115.27
11	C	403	MQ7	C31-C32-C33	-3.02	120.38	127.66
13	C	405	OTP	C18-C17-C16	3.00	120.33	115.27
13	C	405	OTP	C15-C14-C12	-2.99	120.47	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	C	403	MQ7	C26-C27-C28	-2.98	120.48	127.66
7	B	302	BCL	C1-C2-C3	-2.97	120.91	126.04
9	B	305	MPG	O1-CX3-O4	-2.97	118.51	124.13
13	C	405	OTP	C30-C29-C27	-2.93	120.60	127.66
11	C	403	MQ7	C24-C23-C25	2.90	120.14	115.27
7	B	303	BCL	C4A-NA-C1A	2.89	108.01	106.71
7	B	303	BCL	CHA-C1A-NA	-2.87	119.82	126.40
12	C	404	NS5	C6-C5-C4	2.87	120.10	115.27
11	C	403	MQ7	C39-C38-C40	2.86	120.08	115.27
11	C	403	MQ7	C19-C18-C20	2.81	120.00	115.27
5	A	401	HEC	CMB-C2B-C3B	2.78	129.09	125.82
13	C	405	OTP	C10-C9-C7	-2.78	120.98	127.66
11	C	403	MQ7	C16-C17-C18	-2.76	121.00	127.66
11	C	403	MQ7	C34-C33-C35	2.75	119.90	115.27
11	C	403	MQ7	C29-C28-C30	2.75	119.90	115.27
5	A	402	HEC	CBD-CAD-C3D	-2.71	107.99	112.62
8	C	402	BPB	C11-C10-C8	2.71	124.69	115.92
7	B	303	BCL	C2A-C1A-CHA	2.70	128.58	123.86
5	A	403	HEC	CMC-C2C-C3C	2.69	128.98	125.82
6	A	405	DGA	OG1-CA1-CA2	2.67	120.28	111.91
7	B	301	BCL	C4A-NA-C1A	2.64	107.89	106.71
11	C	403	MQ7	C2M-C2-C3	-2.62	120.12	124.40
7	B	301	BCL	C2A-C1A-CHA	2.59	128.39	123.86
7	C	401	BCL	C4A-NA-C1A	2.57	107.86	106.71
12	C	404	NS5	C34-C35-C36	-2.56	119.00	127.75
13	C	405	OTP	C38-C37-C36	2.54	119.55	115.27
12	C	404	NS5	C13-C14-C15	-2.52	119.33	126.42
5	A	402	HEC	CMC-C2C-C3C	2.52	128.78	125.82
8	B	304	BPB	CMB-C2B-C3B	2.49	129.34	124.68
11	C	403	MQ7	C14-C13-C15	2.47	119.42	115.27
12	C	404	NS5	CM4-C36-CM3	2.46	120.03	114.60
7	B	302	BCL	C1C-NC-C4C	2.44	107.81	106.71
13	C	405	OTP	C1-C2-C3	2.44	119.98	114.60
7	B	302	BCL	OBB-CAB-CBB	-2.43	114.71	120.17
12	C	404	NS5	C32-C31-C33	2.42	119.34	115.27
8	B	304	BPB	CMD-C2D-C3D	2.41	129.19	124.68
5	A	404	HEC	CMC-C2C-C3C	2.41	128.65	125.82
12	C	404	NS5	C25-C24-C23	-2.41	115.70	123.22
12	C	404	NS5	C16-C15-C17	-2.41	119.55	122.92
8	C	402	BPB	CMD-C2D-C3D	2.40	129.17	124.68
7	C	401	BCL	OBB-CAB-CBB	-2.35	114.88	120.17
7	C	401	BCL	C11-C10-C8	-2.33	108.38	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	304	BPB	CBC-CAC-C3C	-2.32	120.53	126.70
8	C	402	BPB	CMB-C2B-C3B	2.32	129.01	124.68
5	A	403	HEC	CBD-CAD-C3D	-2.31	108.69	112.62
13	C	405	OTP	C18-C17-C19	-2.30	117.78	123.68
11	C	403	MQ7	C45-C43-C44	2.30	119.68	114.60
7	B	303	BCL	OBB-CAB-CBB	-2.30	115.00	120.17
5	A	401	HEC	CMC-C2C-C3C	2.25	128.46	125.82
11	C	403	MQ7	C36-C37-C38	-2.25	122.25	127.66
7	B	301	BCL	CMB-C2B-C3B	2.23	128.84	124.68
7	B	303	BCL	C1-C2-C3	-2.22	122.20	126.04
13	C	405	OTP	C21-C20-C19	-2.20	104.64	111.88
11	C	403	MQ7	C2M-C2-C1	2.18	119.89	116.27
6	A	405	DGA	OG1-CG1-CG2	2.16	114.60	108.38
7	B	303	BCL	C4B-C3B-CAB	-2.13	123.01	127.13
8	C	402	BPB	O2D-CGD-CBD	2.13	113.70	111.00
7	C	401	BCL	C1C-NC-C4C	2.09	107.65	106.71
7	B	303	BCL	C1C-NC-C4C	2.06	107.63	106.71
5	A	404	HEC	CBD-CAD-C3D	-2.06	109.11	112.62
9	B	306	MPG	O4-CX3-CXD	-2.05	118.93	123.68
7	B	302	BCL	C2D-C1D-ND	2.05	111.61	110.10
9	B	305	MPG	O4-CX3-CXD	-2.04	118.95	123.68
8	B	304	BPB	OBB-CAB-CBB	-2.04	115.58	120.17
5	A	404	HEC	CMB-C2B-C3B	2.03	128.20	125.82

There are no chirality outliers.

All (118) 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
7	B	302	BCL	C2-C3-C5-C6
7	B	302	BCL	C4-C3-C5-C6
7	C	401	BCL	CAD-CBD-CGD-O1D
7	C	401	BCL	CAD-CBD-CGD-O2D
8	C	402	BPB	C2-C3-C5-C6
8	C	402	BPB	C4-C3-C5-C6
8	C	402	BPB	C11-C10-C8-C9
9	B	305	MPG	CXD-CX3-O1-C1
9	B	305	MPG	O4-CX3-O1-C1
9	B	305	MPG	O3-C21-CXD-O2
9	B	305	MPG	O1-CX3-CXD-C21

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Mol	Chain	Res	Type	Atoms
9	B	305	MPG	O4-CX3-CXD-C21
9	B	306	MPG	O3-C21-CXD-O2
9	B	306	MPG	O1-CX3-CXD-C21
12	C	404	NS5	C3-C4-C5-C6
12	C	404	NS5	C3-C4-C5-C7
13	C	405	OTP	C30-C31-C32-C34
13	C	405	OTP	C30-C31-C32-C33
13	C	405	OTP	C5-C6-C7-C8
13	C	405	OTP	C20-C21-C22-C23
13	C	405	OTP	C5-C6-C7-C9
12	C	404	NS5	C2-C3-C4-C5
12	C	404	NS5	C11-C10-C9-C8
12	C	404	NS5	C12-C10-C9-C8
7	C	401	BCL	C2A-CAA-CBA-CGA
13	C	405	OTP	C24-C25-C26-C27
12	C	404	NS5	C28-C29-C30-C31
13	C	405	OTP	C20-C21-C22-C24
7	B	301	BCL	C14-C13-C15-C16
12	C	404	NS5	C27-C26-C28-C29
12	C	404	NS5	C25-C26-C28-C29
13	C	405	OTP	C34-C35-C36-C37
13	C	405	OTP	C14-C15-C16-C17
13	C	405	OTP	C9-C10-C11-C12
7	B	302	BCL	C15-C16-C17-C18
9	B	305	MPG	C10-C11-C12-C13
9	C	406	MPG	C10-C11-C12-C13
9	B	305	MPG	C2-C3-C4-C5
6	A	405	DGA	CCB-CDB-CEB-CFB
7	B	303	BCL	C16-C17-C18-C19
9	B	305	MPG	C5-C6-C7-C8
9	B	306	MPG	C11-C12-C13-C14
6	A	405	DGA	CBB-CAB-CB9-CB8
9	B	306	MPG	C3-C4-C5-C6
8	B	304	BPB	O2A-C1-C2-C3
6	A	405	DGA	CA7-CA8-CA9-CAA
6	A	405	DGA	CB9-CAB-CBB-CCB
8	B	304	BPB	C4-C3-C5-C6
7	B	303	BCL	C11-C12-C13-C15
8	B	304	BPB	C2-C3-C5-C6
9	B	306	MPG	C12-C13-C14-C15
6	A	405	DGA	CB4-CB5-CB6-CB7
7	B	301	BCL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
7	B	303	BCL	C11-C12-C13-C14
7	B	303	BCL	C16-C17-C18-C20
6	A	405	DGA	CA5-CA6-CA7-CA8
6	A	405	DGA	CB6-CB7-CB8-CB9
7	B	301	BCL	C4-C3-C5-C6
13	C	405	OTP	C15-C16-C17-C18
12	C	404	NS5	C1-C2-C3-C4
12	C	404	NS5	CM2-C1-C2-C3
9	C	406	MPG	C4-C5-C6-C7
6	A	405	DGA	CEB-CFB-CGB-CHB
8	C	402	BPB	C6-C7-C8-C10
8	C	402	BPB	C11-C10-C8-C7
8	C	402	BPB	C6-C7-C8-C9
9	B	306	MPG	O3-C21-CXD-CX3
9	B	305	MPG	C12-C13-C14-C15
12	C	404	NS5	CM1-C1-C2-C3
9	B	305	MPG	C15-C16-C17-C18
8	C	402	BPB	C8-C10-C11-C12
9	B	305	MPG	C6-C7-C8-C9
9	B	306	MPG	O4-CX3-CXD-C21
9	C	406	MPG	C13-C14-C15-C16
7	B	301	BCL	CAD-CBD-CGD-O2D
9	B	305	MPG	O4-CX3-CXD-O2
9	C	406	MPG	C2-C3-C4-C5
5	A	402	HEC	C3D-CAD-CBD-CGD
6	A	405	DGA	CBB-CCB-CDB-CEB
9	B	305	MPG	C13-C14-C15-C16
12	C	404	NS5	C26-C28-C29-C30
13	C	405	OTP	C15-C16-C17-C19
9	B	306	MPG	C1-C2-C3-C4
9	B	306	MPG	C6-C7-C8-C9
5	A	402	HEC	CAD-CBD-CGD-O1D
7	C	401	BCL	O2A-C1-C2-C3
5	A	402	HEC	CAA-CBA-CGA-O1A
9	C	406	MPG	C7-C8-C9-C10
5	A	402	HEC	CAD-CBD-CGD-O2D
6	A	405	DGA	CAB-CBB-CCB-CDB
5	A	401	HEC	CAA-CBA-CGA-O2A
5	A	402	HEC	CAA-CBA-CGA-O2A
11	C	403	MQ7	C39-C38-C40-C41
11	C	403	MQ7	C38-C40-C41-C42
8	C	402	BPB	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
8	C	402	BPB	C11-C12-C13-C14
9	C	406	MPG	C9-C10-C11-C12
11	C	403	MQ7	C37-C38-C40-C41
5	A	401	HEC	CAA-CBA-CGA-O1A
9	B	305	MPG	C7-C8-C9-C10
7	C	401	BCL	CHA-CBD-CGD-O1D
7	C	401	BCL	CHA-CBD-CGD-O2D
9	B	306	MPG	C7-C8-C9-C10
8	B	304	BPB	CHA-CBD-CGD-O1D
9	B	305	MPG	O3-C21-CXD-CX3
6	A	405	DGA	CA8-CA9-CAA-CBA
7	B	303	BCL	C15-C16-C17-C18
9	B	306	MPG	C2-C3-C4-C5
13	C	405	OTP	C17-C19-C20-C21
7	B	302	BCL	CAD-CBD-CGD-O1D
6	A	405	DGA	OG2-CB1-CB2-CB3
7	B	301	BCL	C12-C13-C15-C16
12	C	404	NS5	C15-C17-C18-C19
6	A	405	DGA	OB1-CB1-CB2-CB3
12	C	404	NS5	C32-C31-C33-C34

There are no ring outliers.

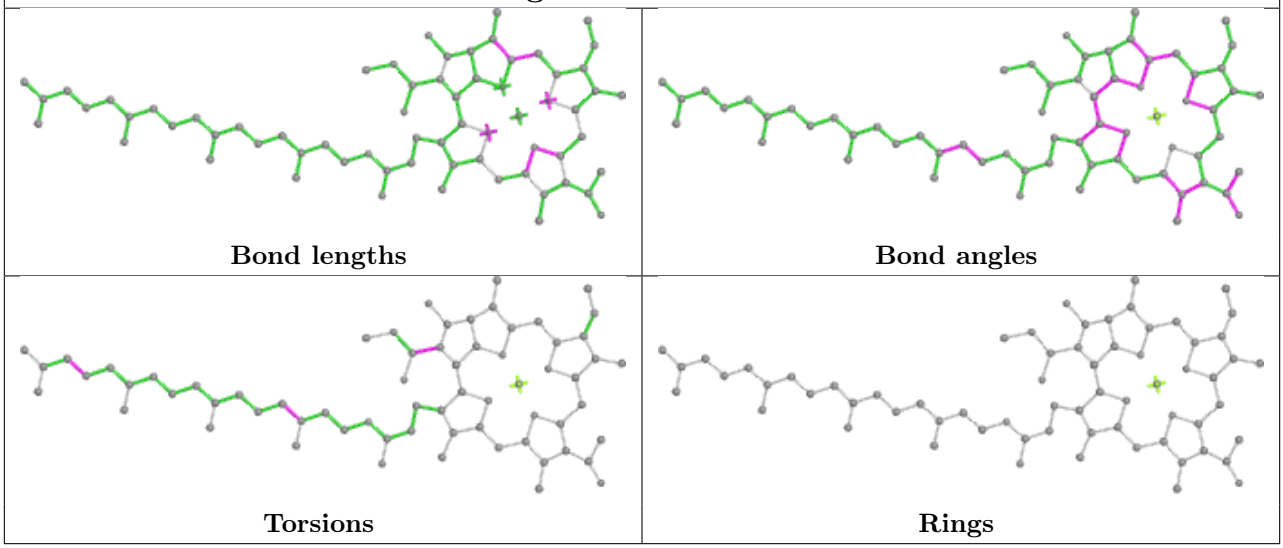
15 monomers are involved in 39 short contacts:

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

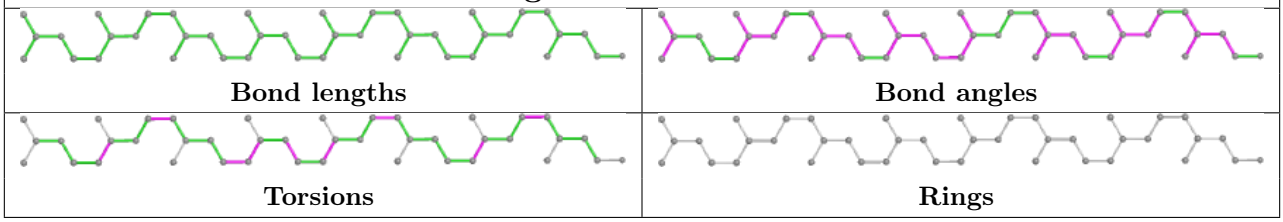
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

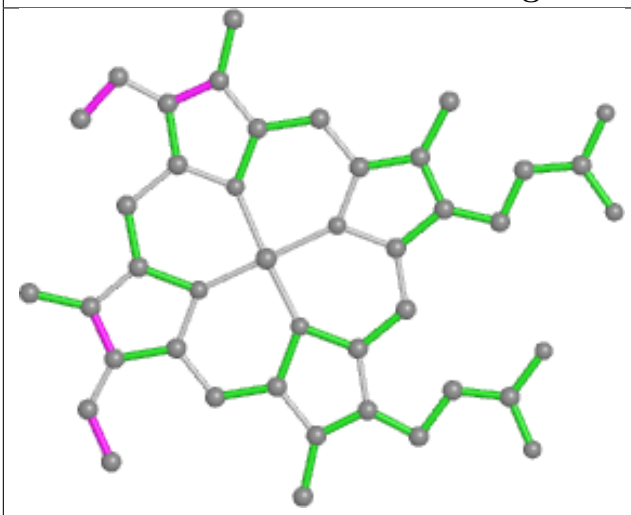
Ligand BCL B 302



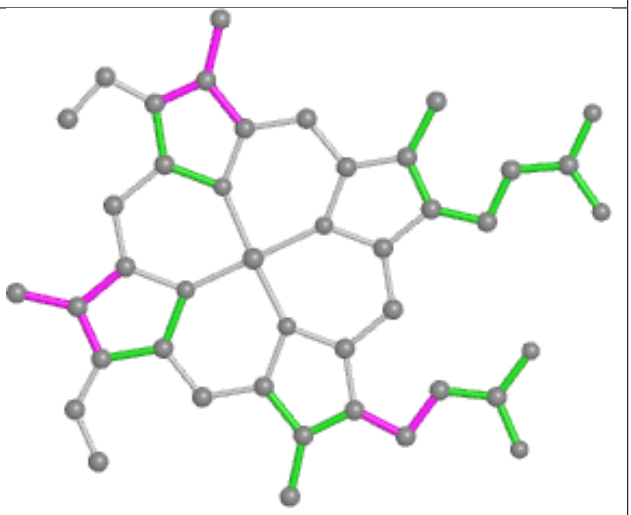
Ligand OTP C 405



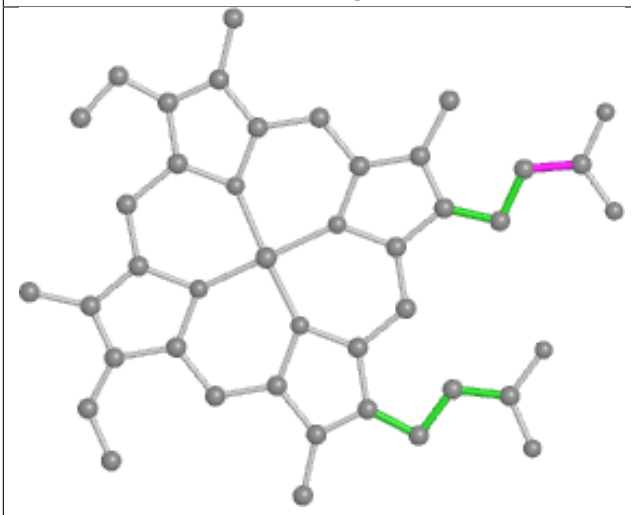
Ligand HEC A 401



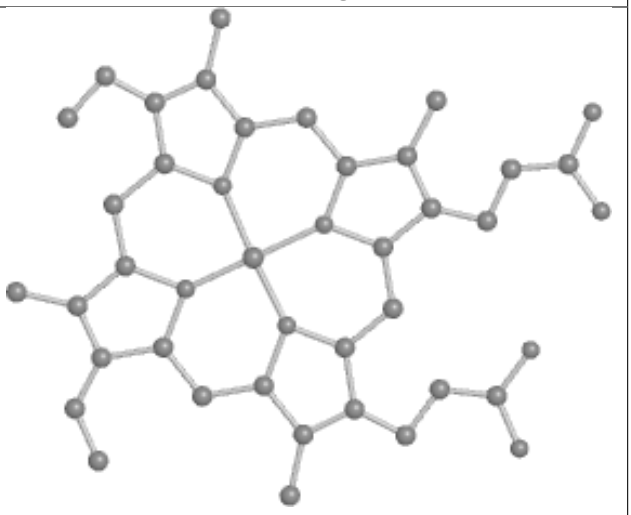
Bond lengths



Bond angles

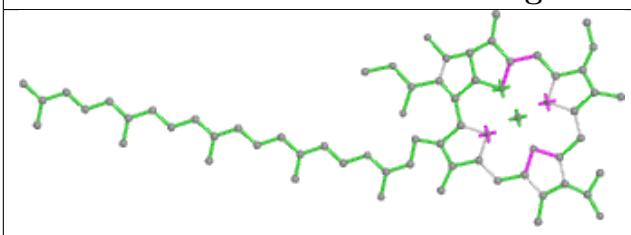


Torsions

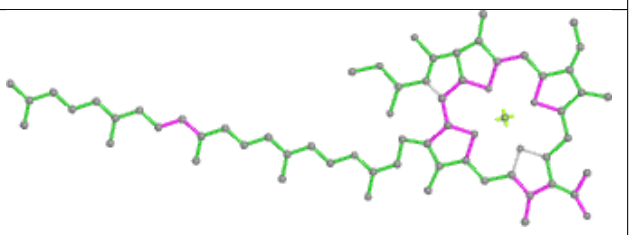


Rings

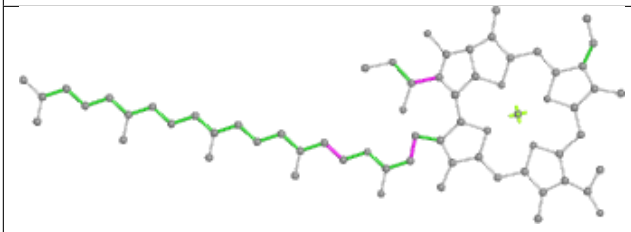
Ligand BCL C 401



Bond lengths



Bond angles



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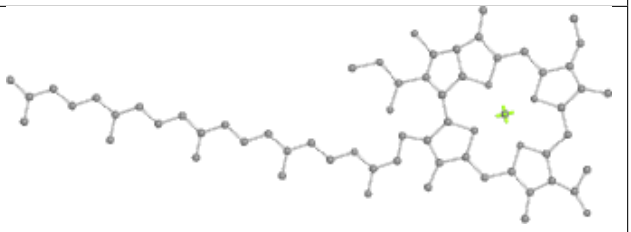
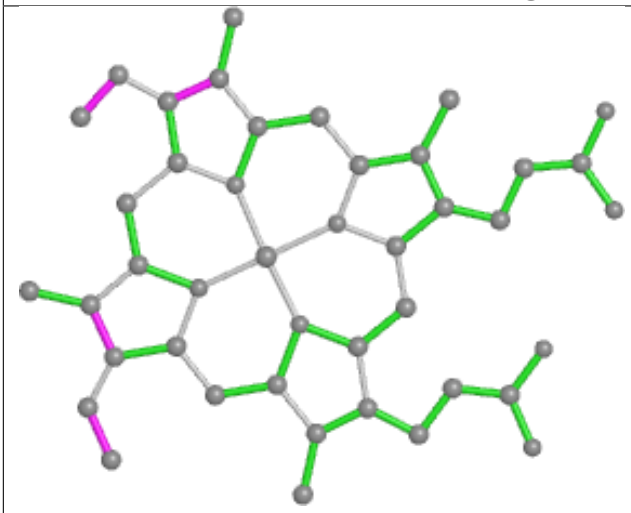
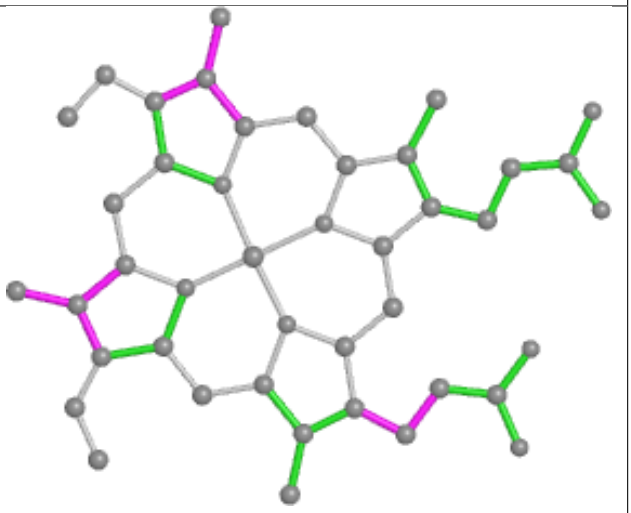


Rings

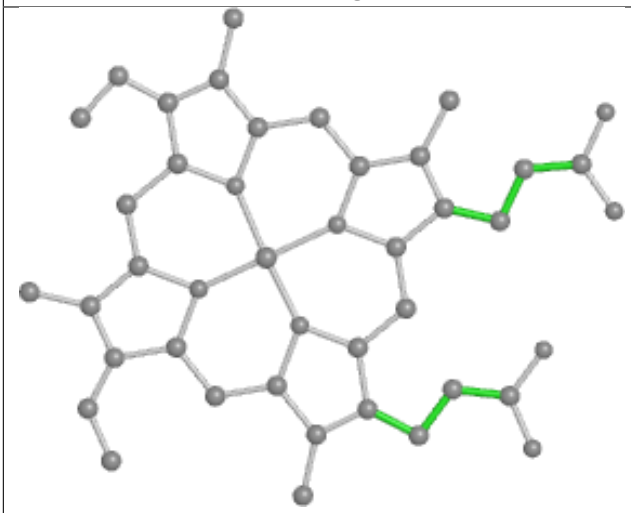
Ligand HEC A 404



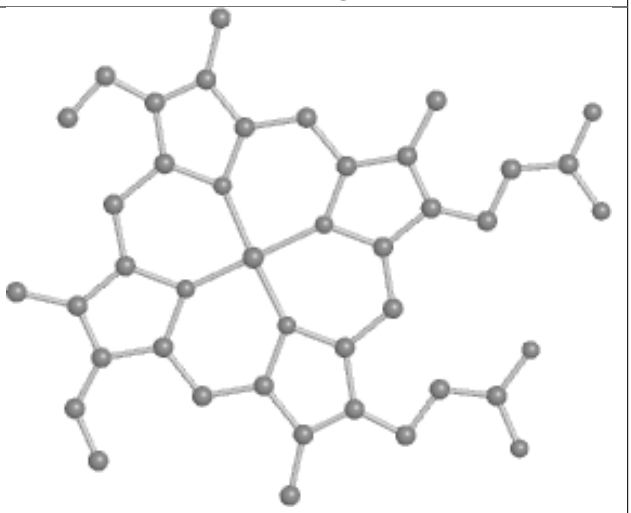
Bond lengths



Bond angles

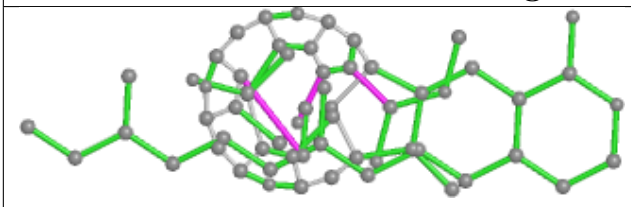


Torsions

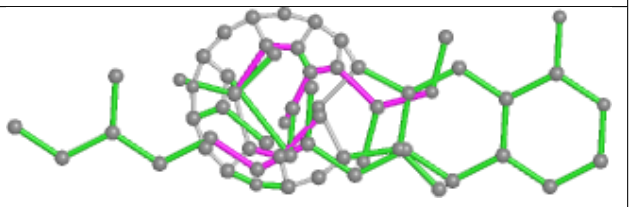


Rings

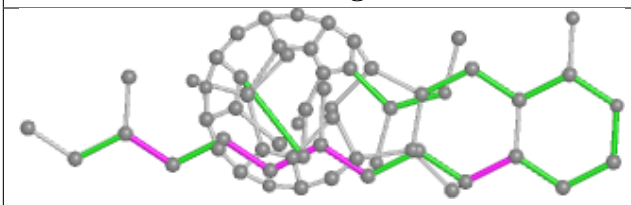
Ligand BPB C 402



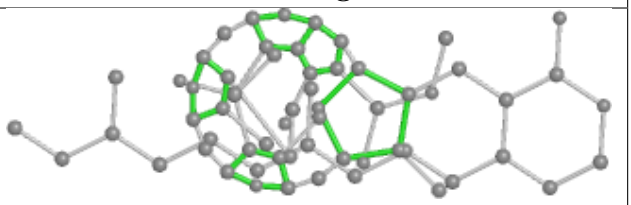
Bond lengths



Bond angles

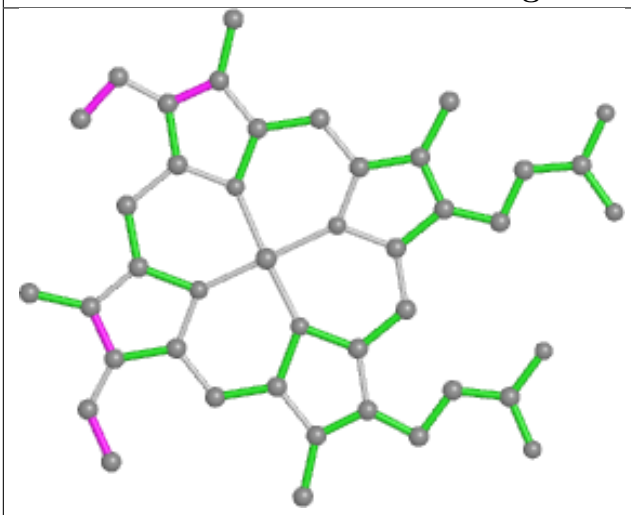


Torsions



Rings

Ligand HEC A 403



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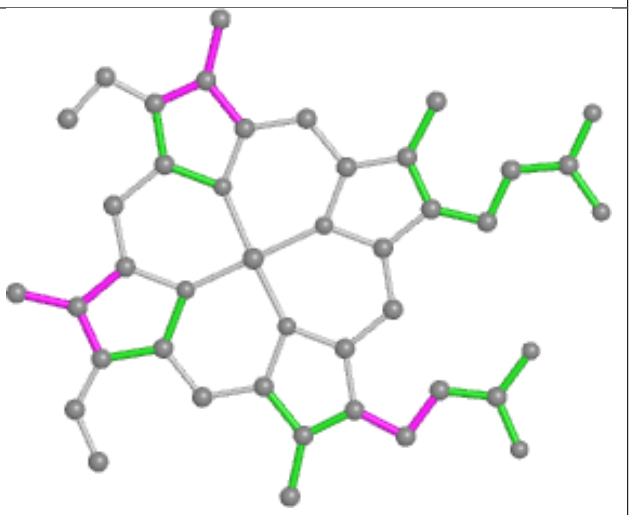
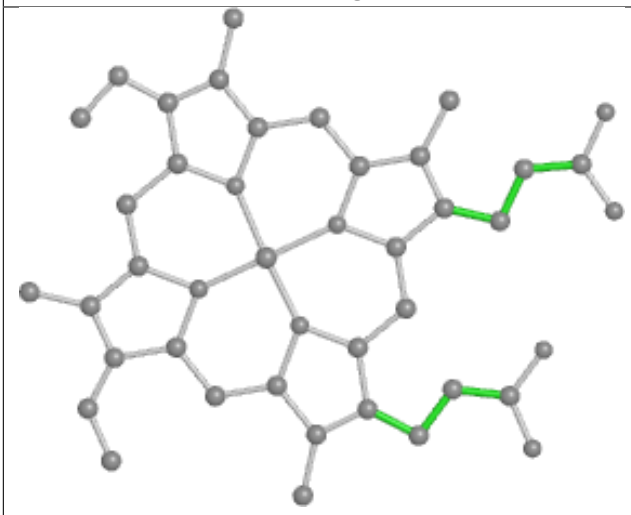
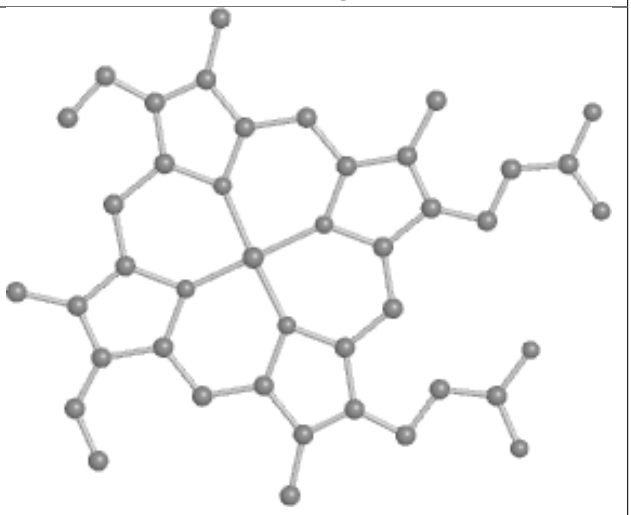


Bond angles

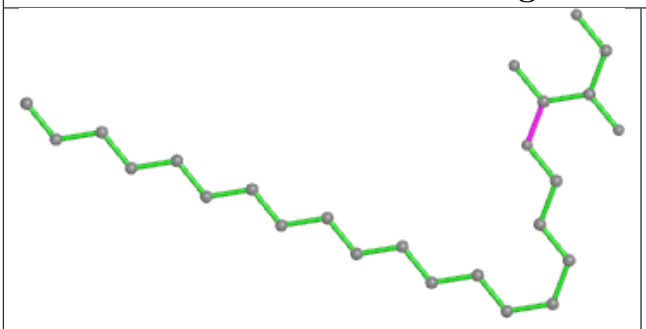


Torsions

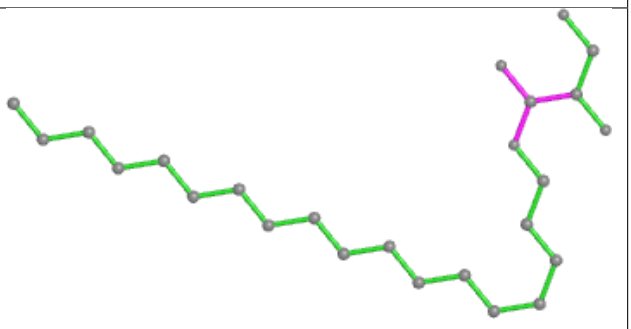


Rings

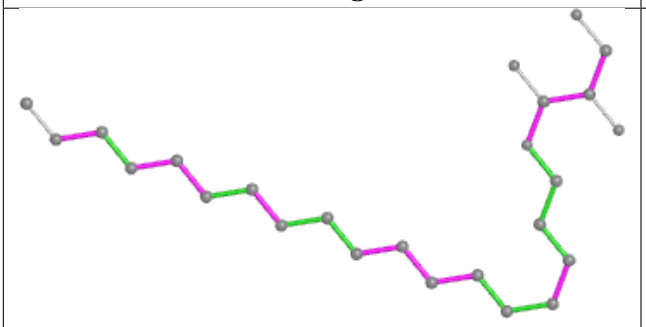
Ligand MPG B 305



Bond lengths



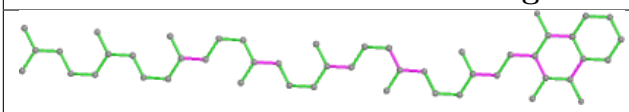
Bond angles



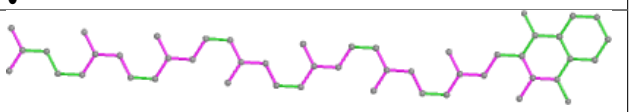
Torsions

Rings

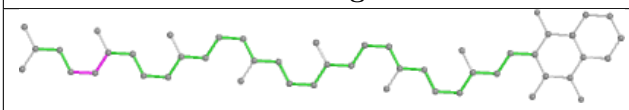
Ligand MQ7 C 403



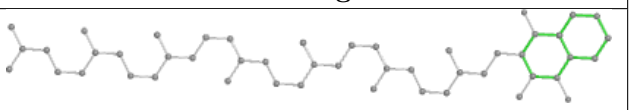
Bond lengths



Bond angles

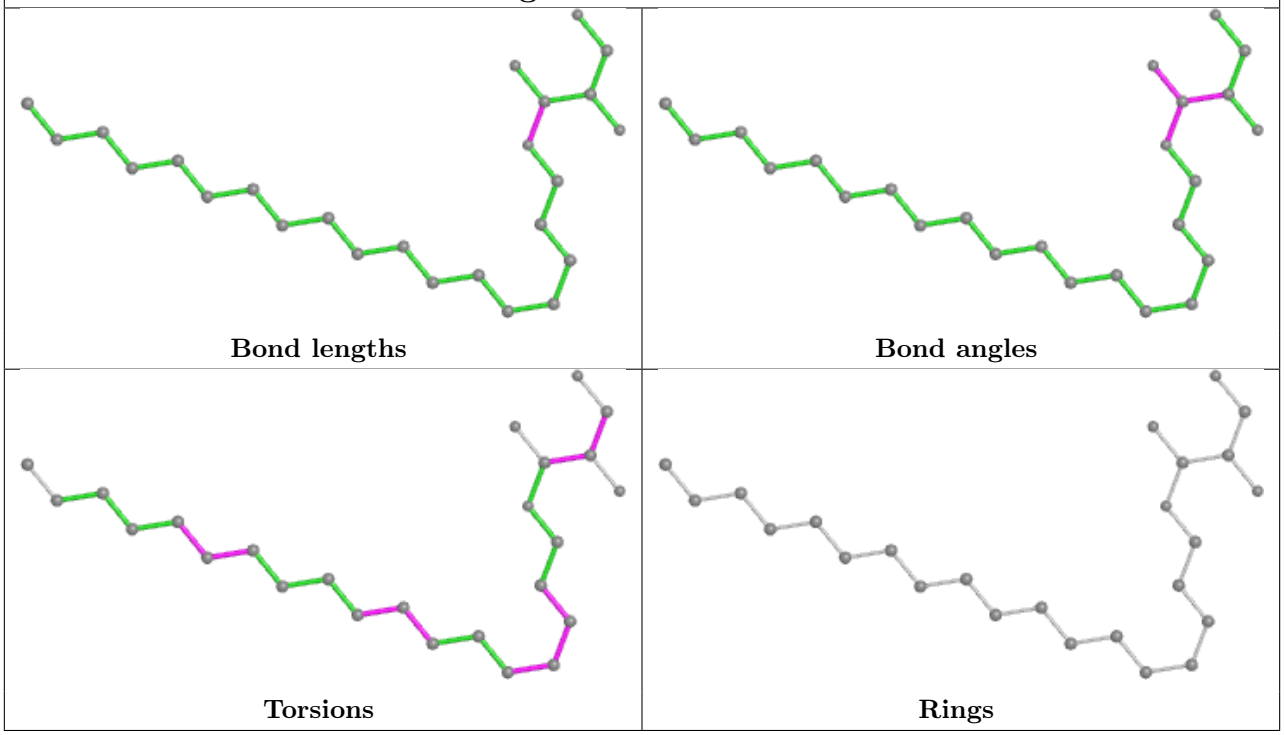


Torsions

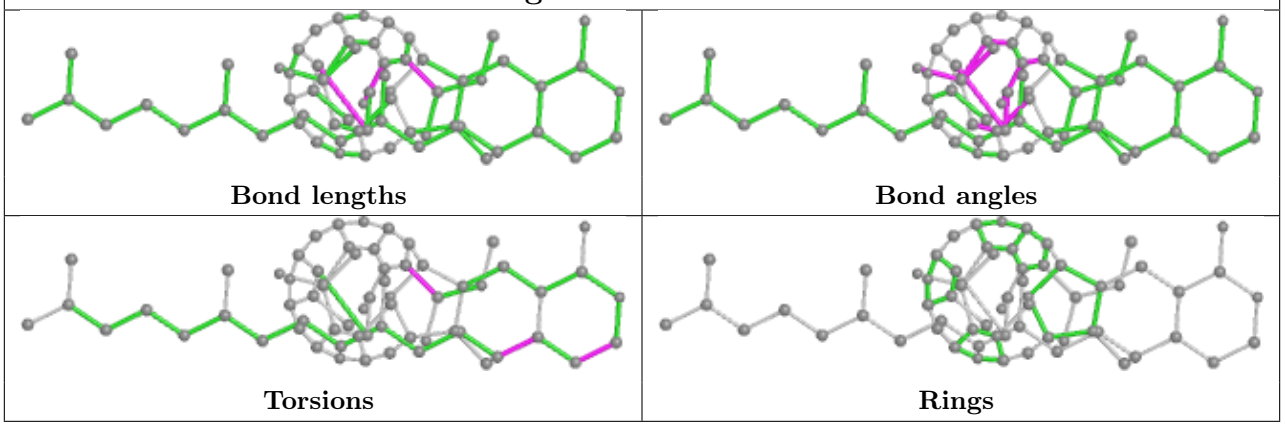


Rings

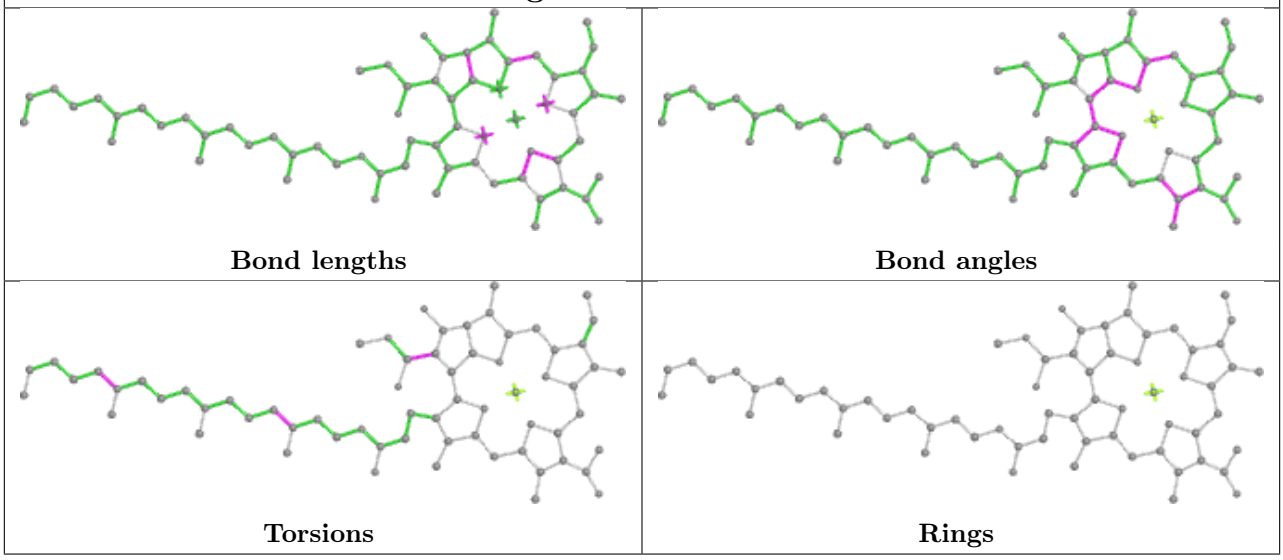
Ligand MPG B 306



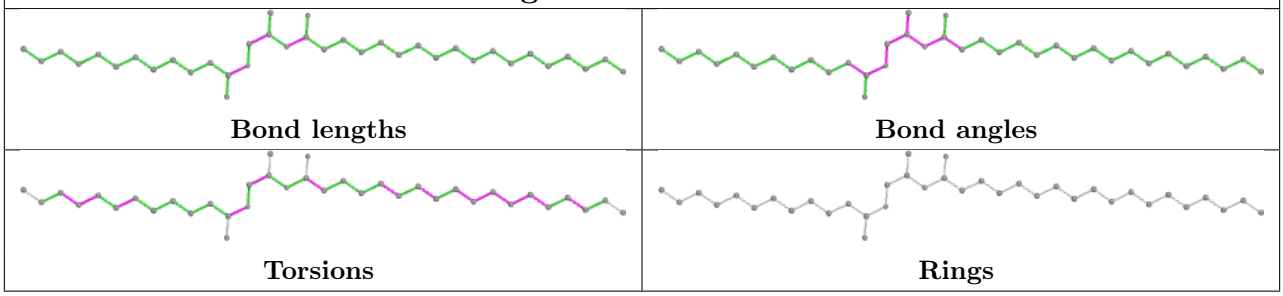
Ligand BPB B 304



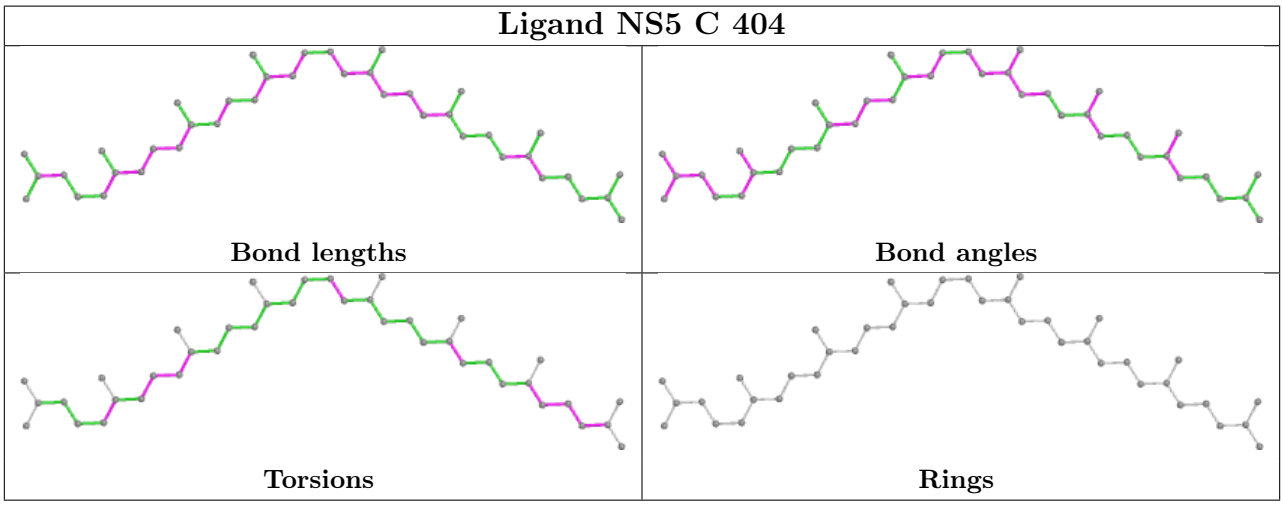
Ligand BCL B 301



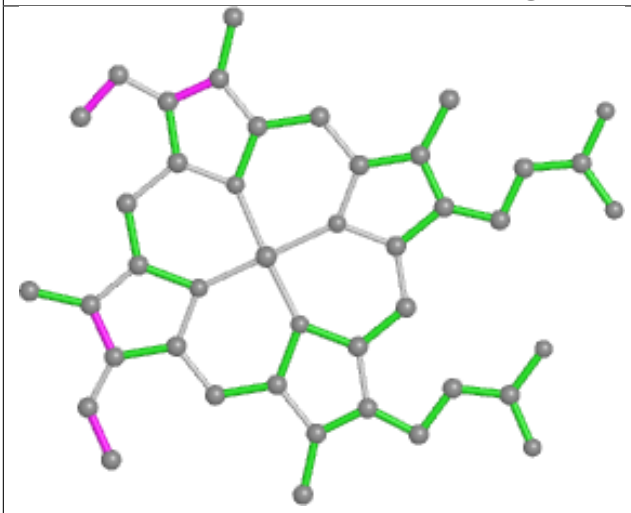
Ligand DGA A 405



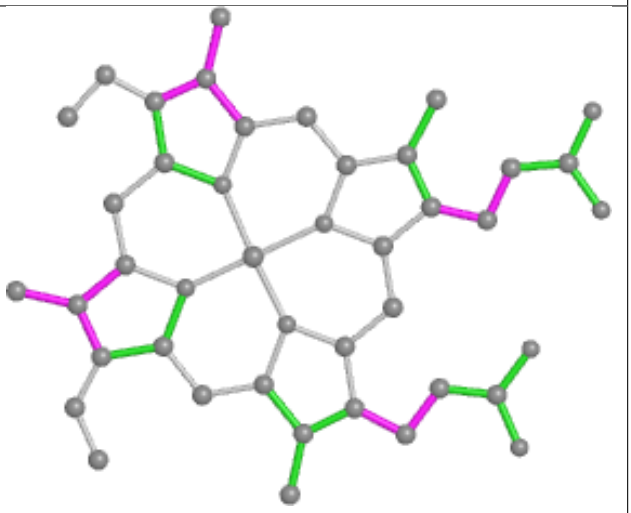
Ligand NS5 C 404



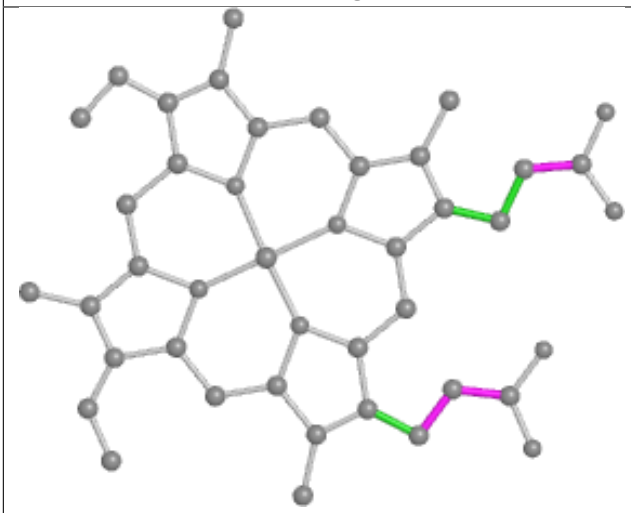
Ligand HEC A 402



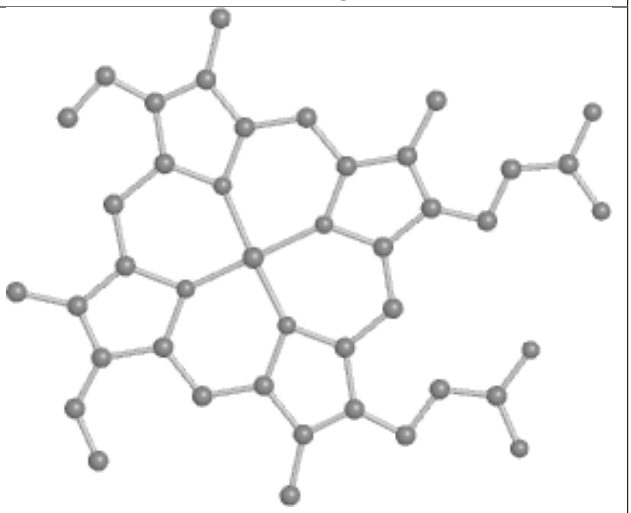
Bond lengths



Bond angles

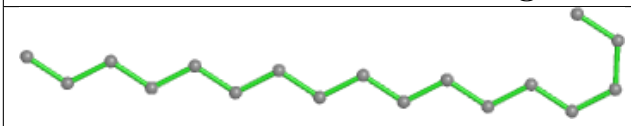


Torsions

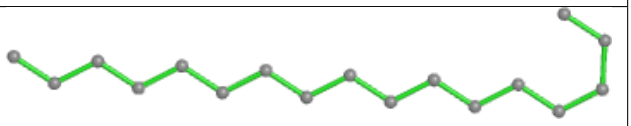


Rings

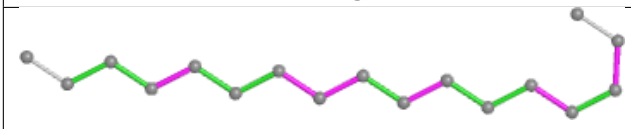
Ligand MPG C 406



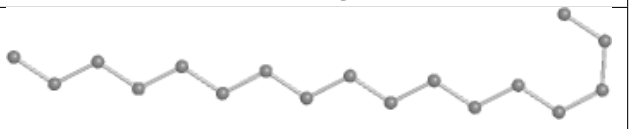
Bond lengths



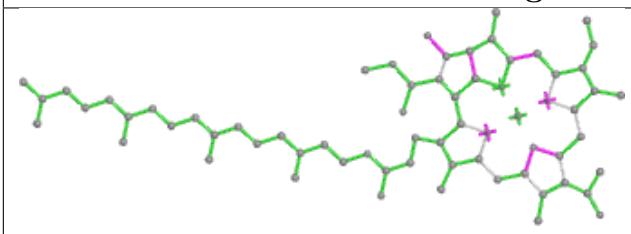
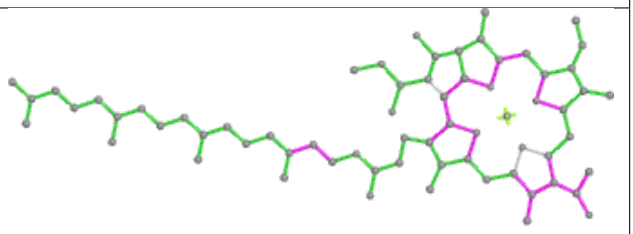
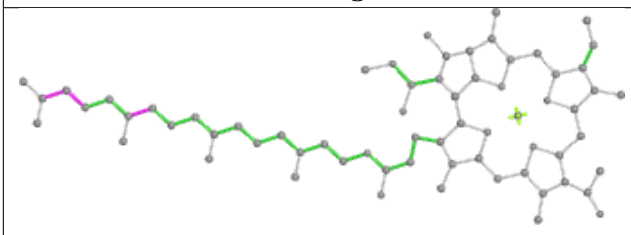
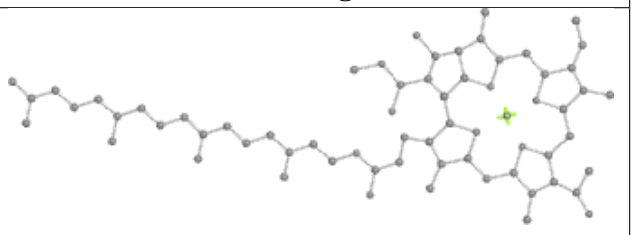
Bond angles



Torsions



Rings

Ligand BCL B 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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%)	-0.45	0 100 100	19, 37, 59, 79	0
2	B	273/274 (99%)	-0.37	0 100 100	24, 50, 84, 107	0
3	C	323/324 (99%)	-0.32	1 (0%) 94 91	23, 54, 82, 106	0
4	D	242/258 (93%)	0.17	10 (4%) 37 33	48, 90, 110, 142	0
All	All	1170/1212 (96%)	-0.27	11 (0%) 84 79	19, 52, 98, 142	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	24	GLY	3.3
4	D	206	ASP	2.8
4	D	141	THR	2.5
4	D	9	HIS	2.4
4	D	7	ALA	2.4
4	D	256	SER	2.4
4	D	85	THR	2.3
4	D	142	ASP	2.2
4	D	79	PRO	2.2
4	D	93	THR	2.2
4	D	82	ARG	2.1

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	0.92	0.44	45,61,73,80	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

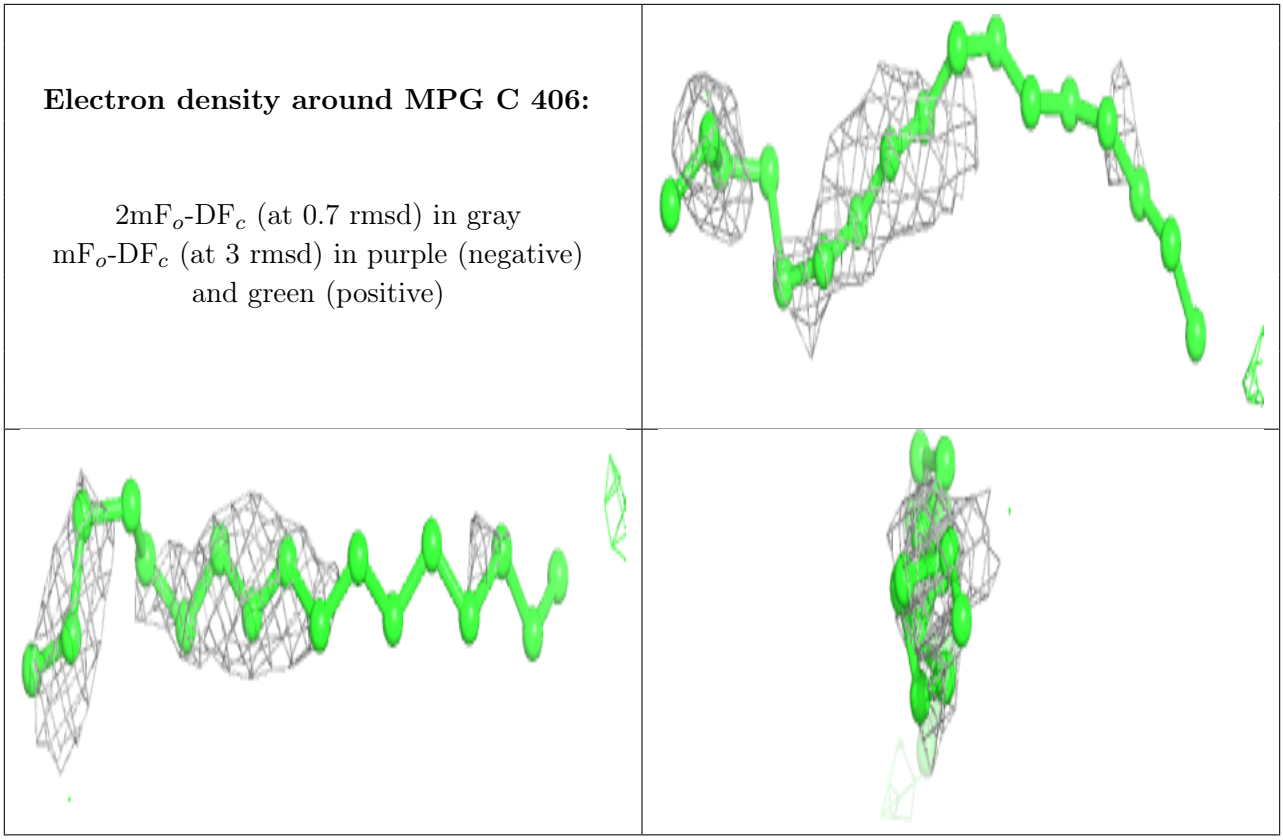
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	0.70	0.57	61,79,106,107	0
9	MPG	B	306	25/25	0.74	0.42	54,74,89,101	0
6	DGA	A	405	37/44	0.74	0.38	43,71,89,91	0
9	MPG	B	305	25/25	0.76	0.34	54,81,92,93	6
12	NS5	C	404	40/40	0.84	0.33	31,61,90,94	0
13	OTP	C	405	41/49	0.87	0.30	37,59,79,90	0
14	PO4	C	407	5/5	0.88	0.46	90,90,98,107	0
11	MQ7	C	403	48/48	0.91	0.29	27,53,66,69	0
8	BPB	C	402	61/65	0.92	0.26	43,57,71,72	0
14	PO4	C	408	5/5	0.93	0.19	79,82,84,88	0
10	FE2	B	307	1/1	0.94	0.12	54,54,54,54	0
8	BPB	B	304	65/65	0.94	0.21	28,43,51,57	0
7	BCL	B	302	66/66	0.95	0.20	25,36,45,56	0
5	HEC	A	401	43/43	0.95	0.29	35,45,55,56	0
7	BCL	C	401	66/66	0.96	0.20	30,38,49,57	0
7	BCL	B	301	65/66	0.96	0.18	30,45,152,159	14
5	HEC	A	404	43/43	0.96	0.18	24,36,46,48	0
7	BCL	B	303	66/66	0.96	0.19	25,33,44,51	0
5	HEC	A	403	43/43	0.97	0.20	17,26,32,35	0
5	HEC	A	402	43/43	0.97	0.22	14,31,37,49	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.

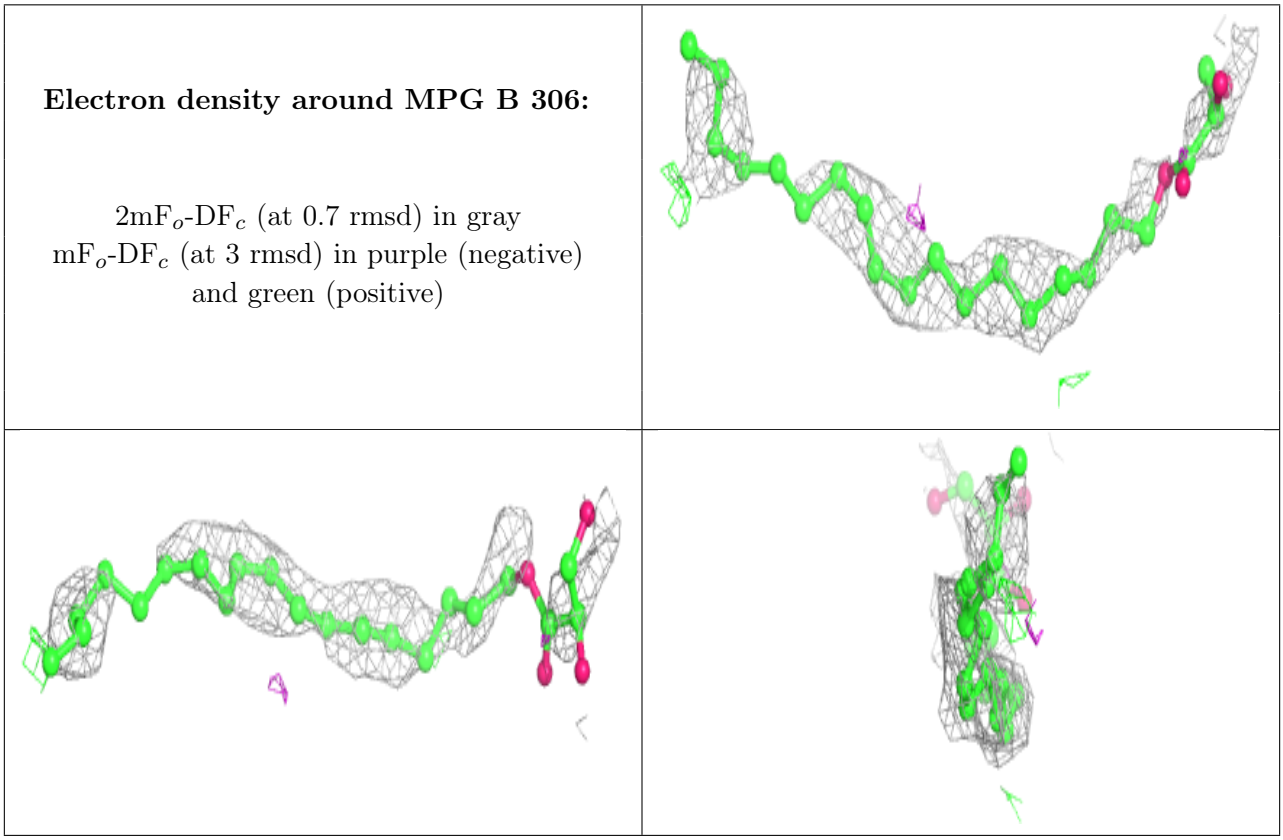
Electron density around MPG C 406:

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



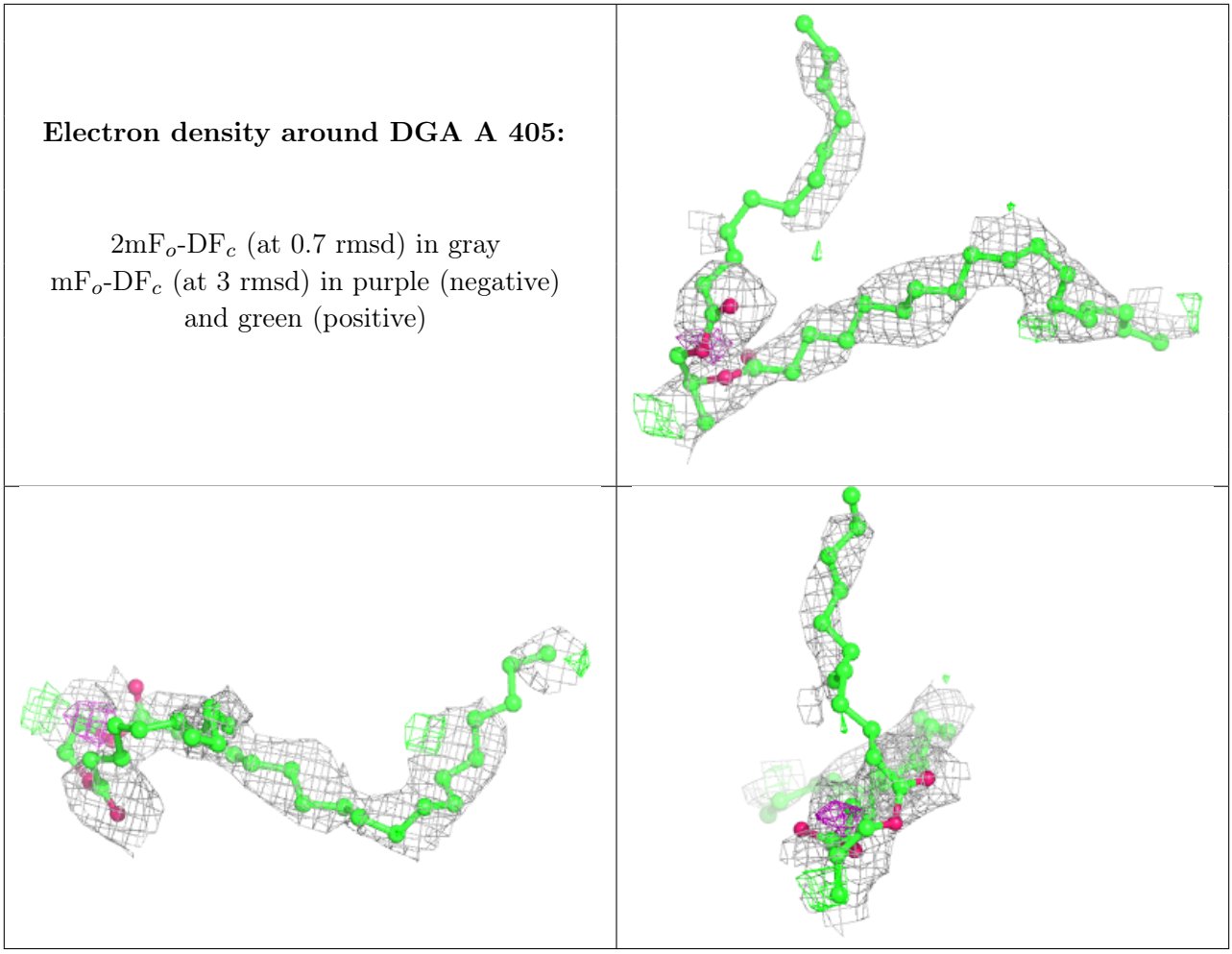
Electron density around MPG B 306:

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



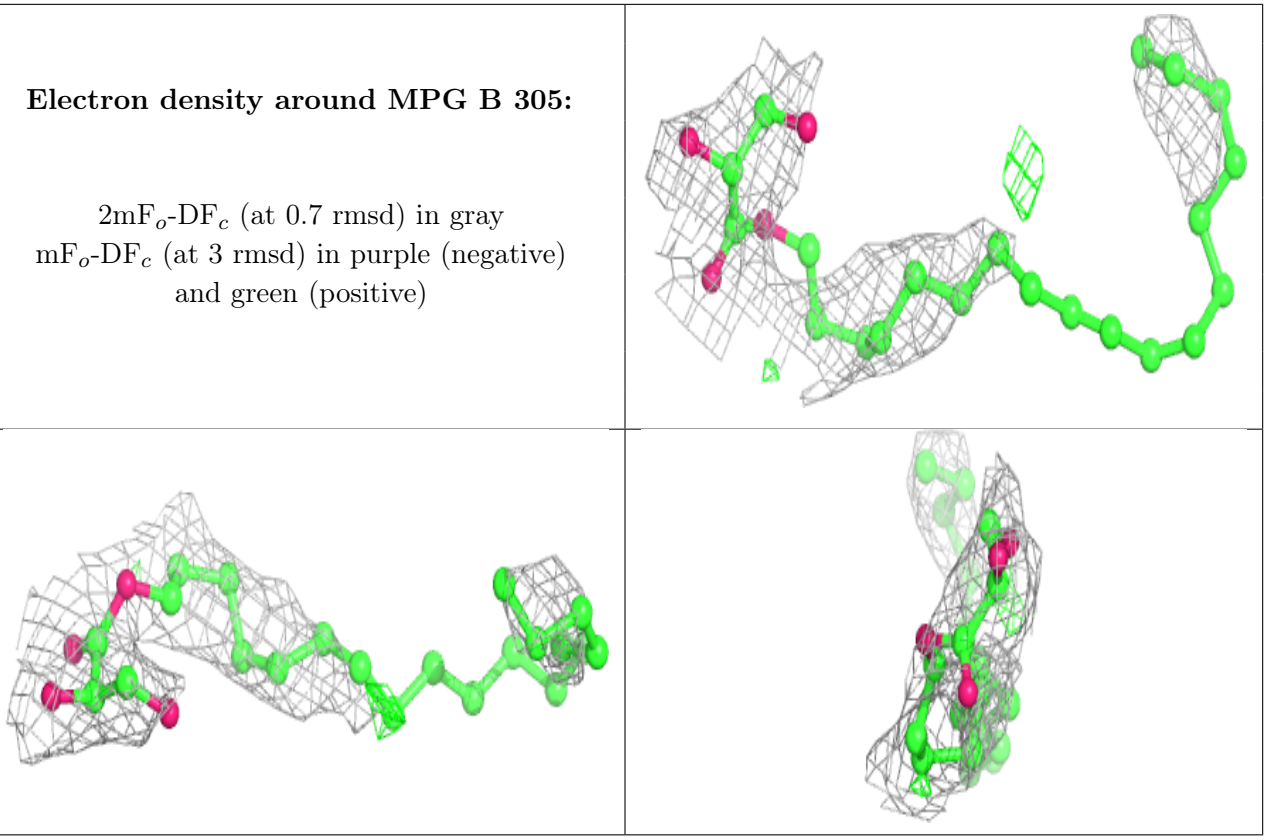
Electron density around DGA A 405:

$2mF_o$-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 NS5 C 404:

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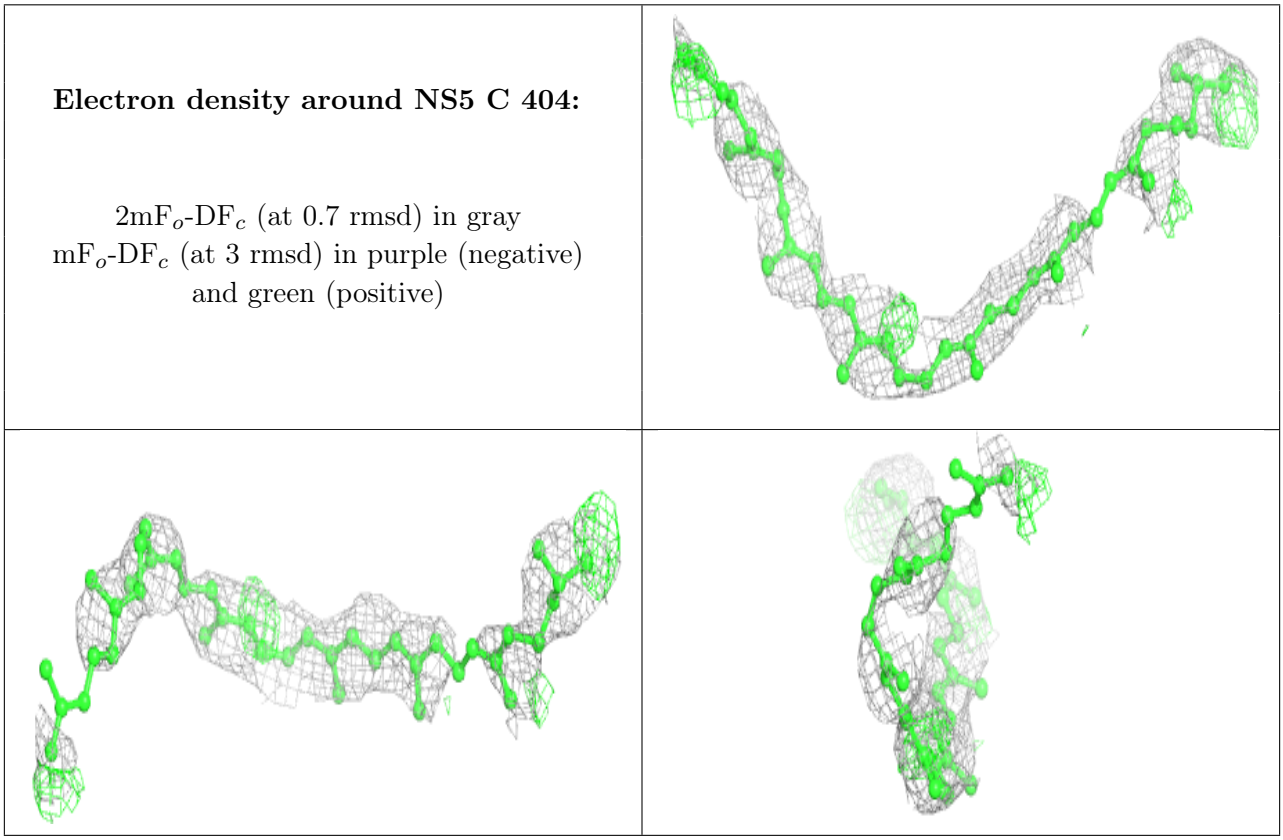
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around OTP C 405:

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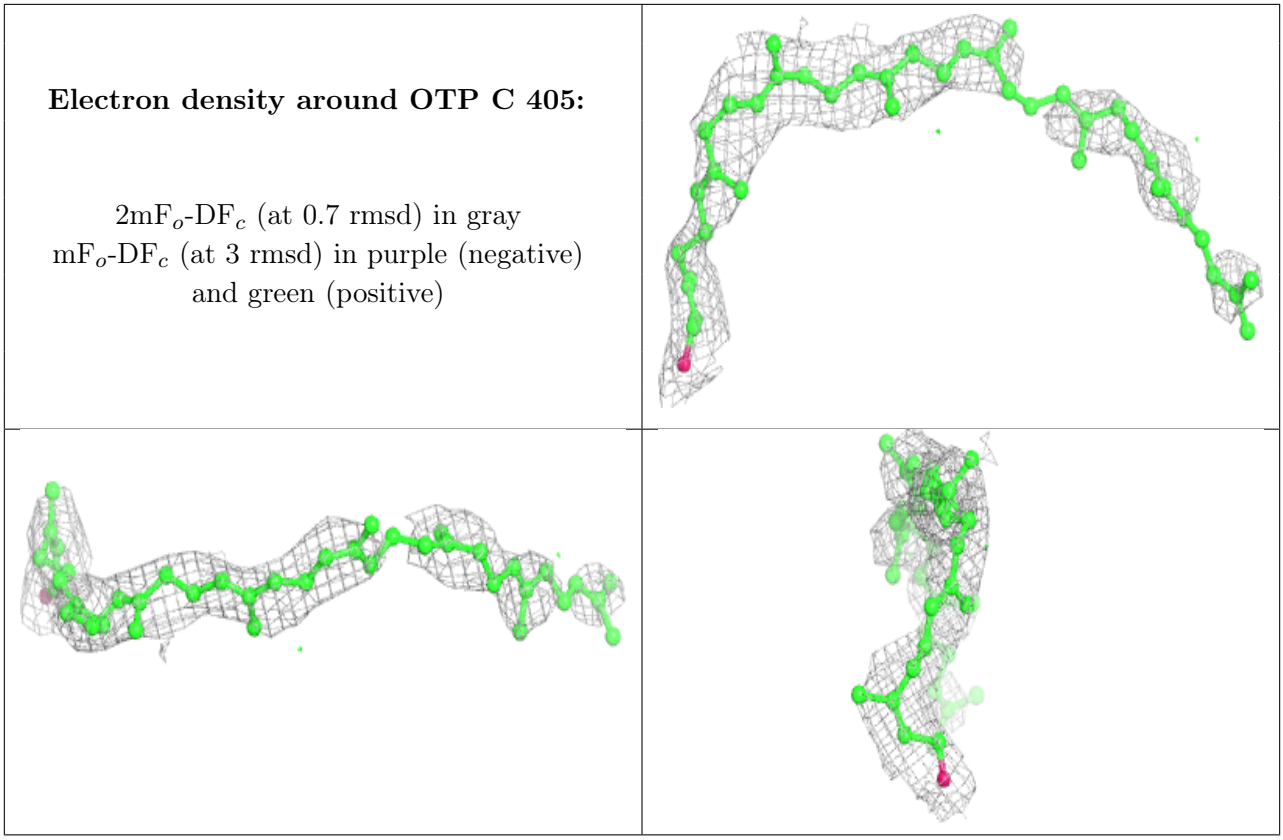
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around MQ7 C 403:

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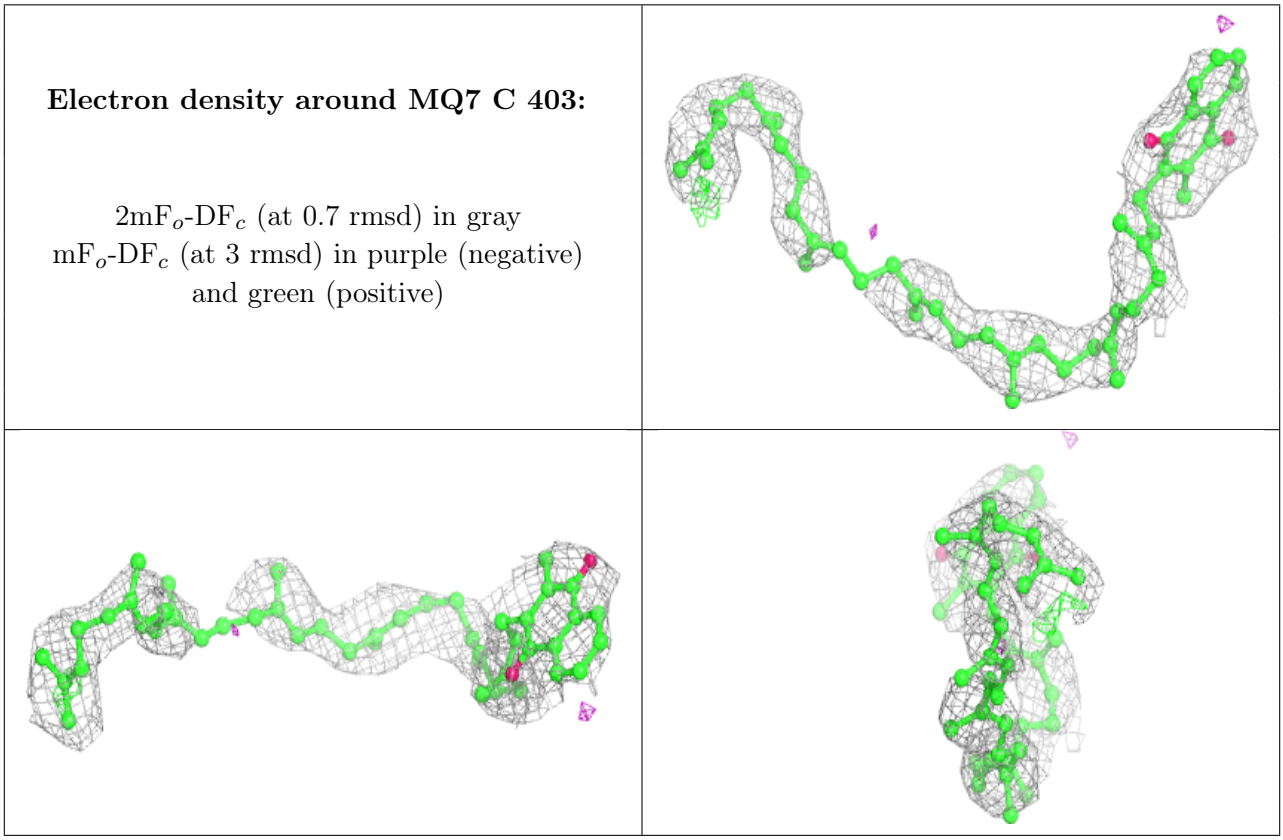
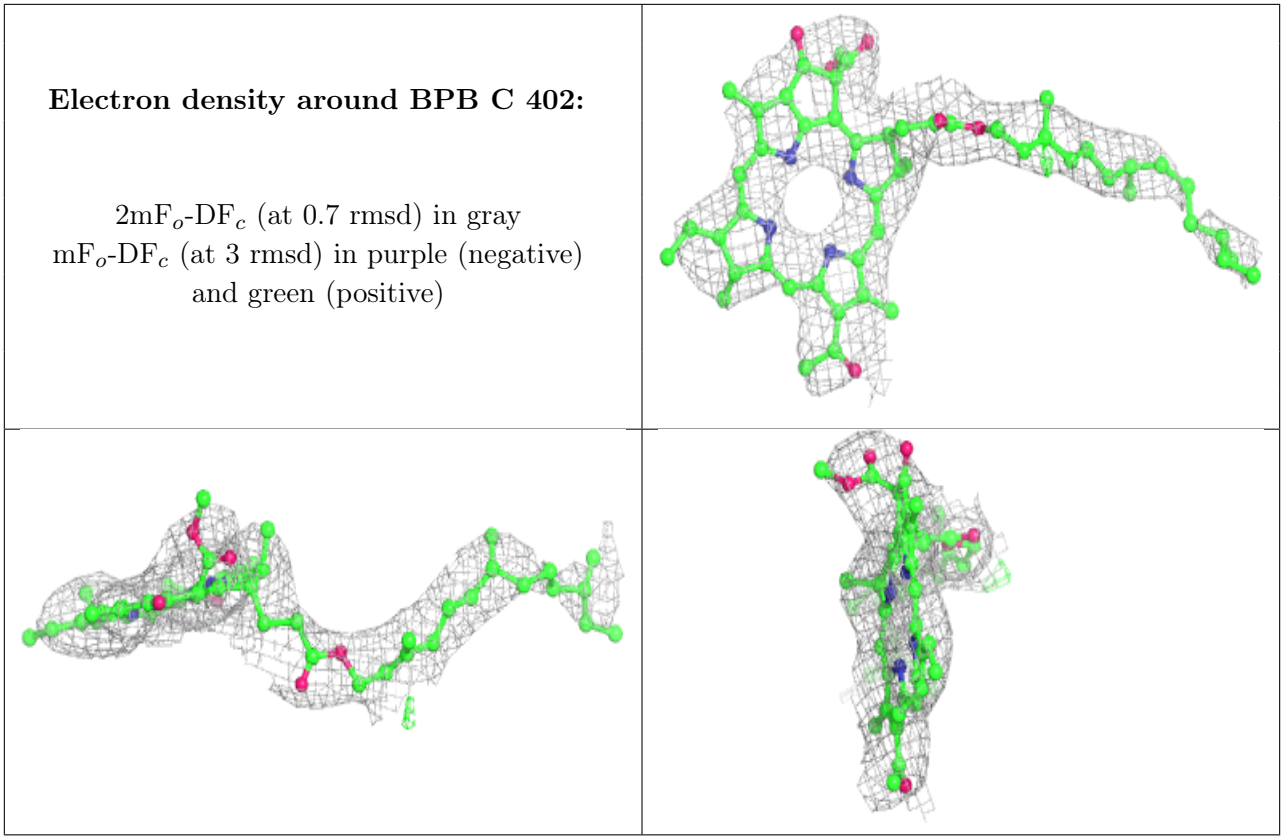
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



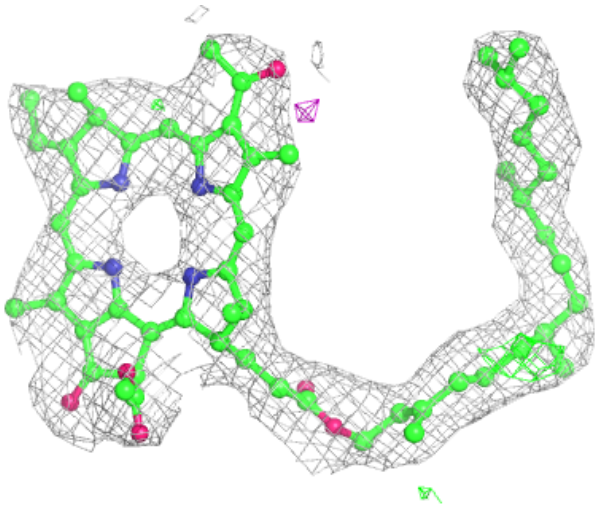
Electron density around BPB C 402:

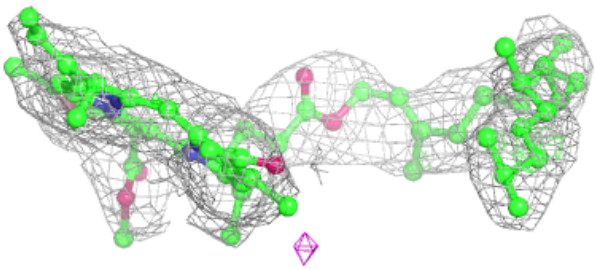
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

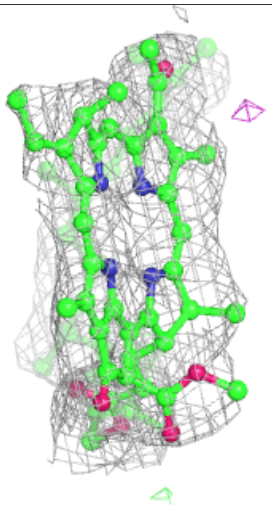


Electron density around BPB B 304:

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

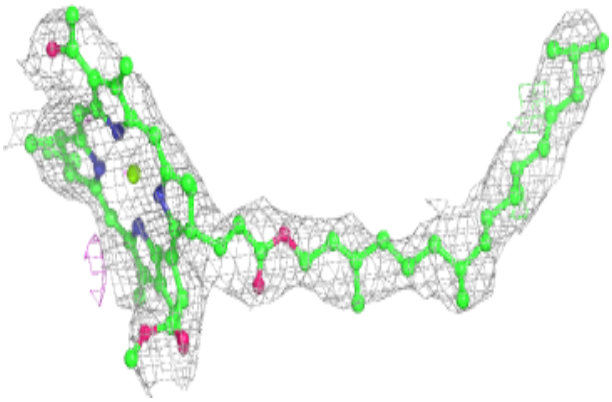


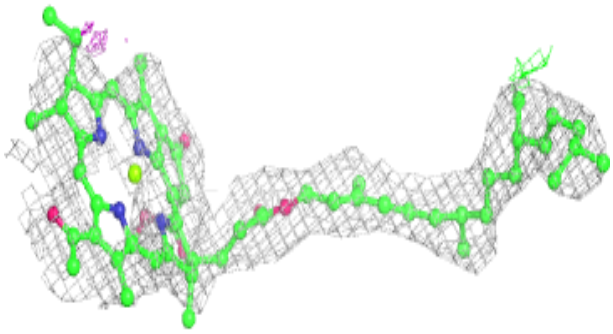


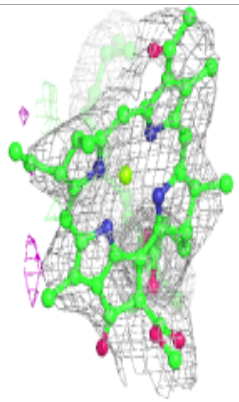


Electron density around BCL B 302:

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

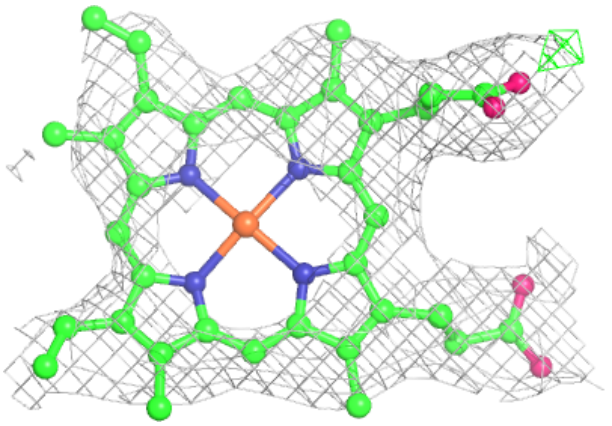


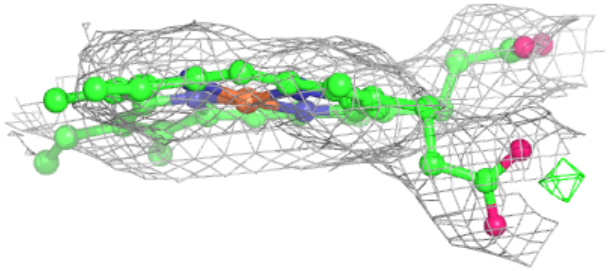


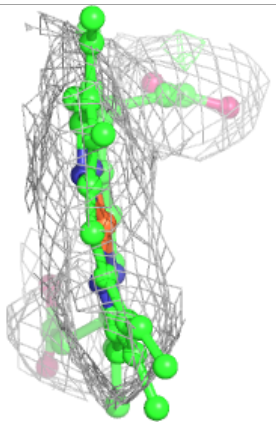


Electron density around HEC A 401:

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

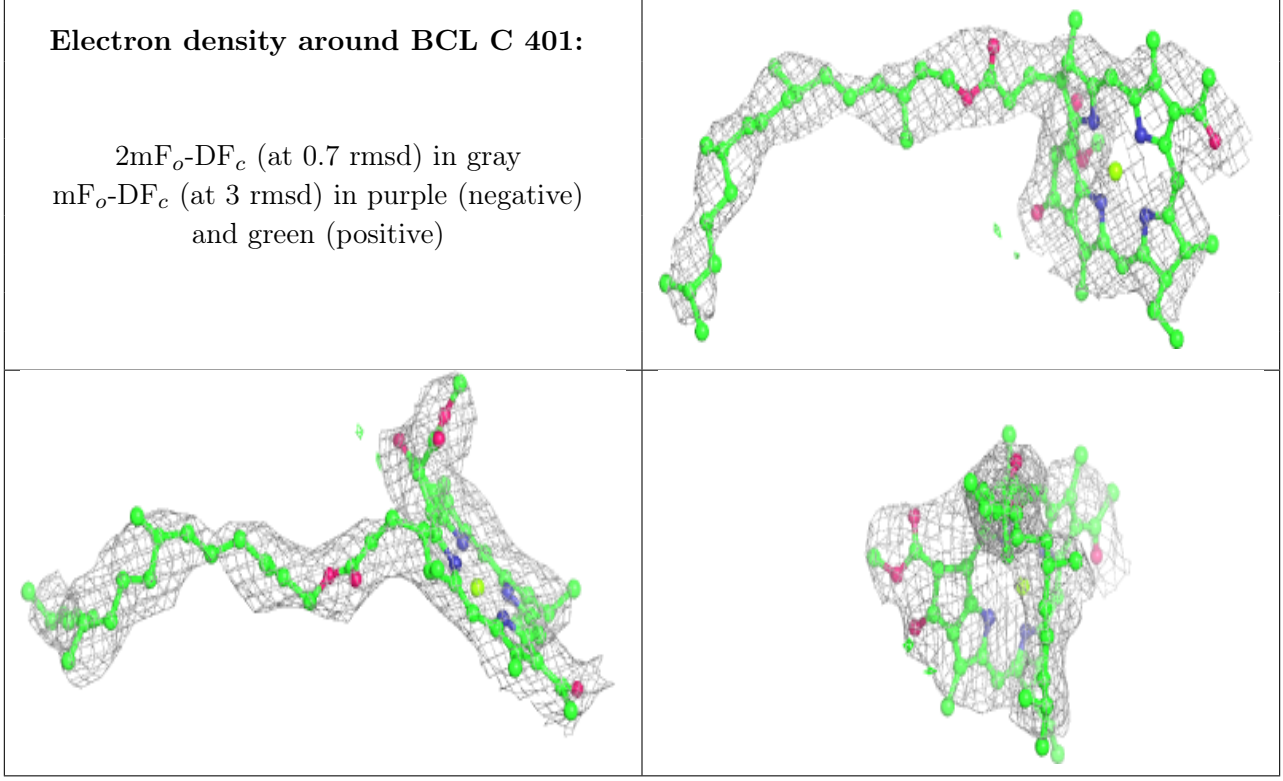






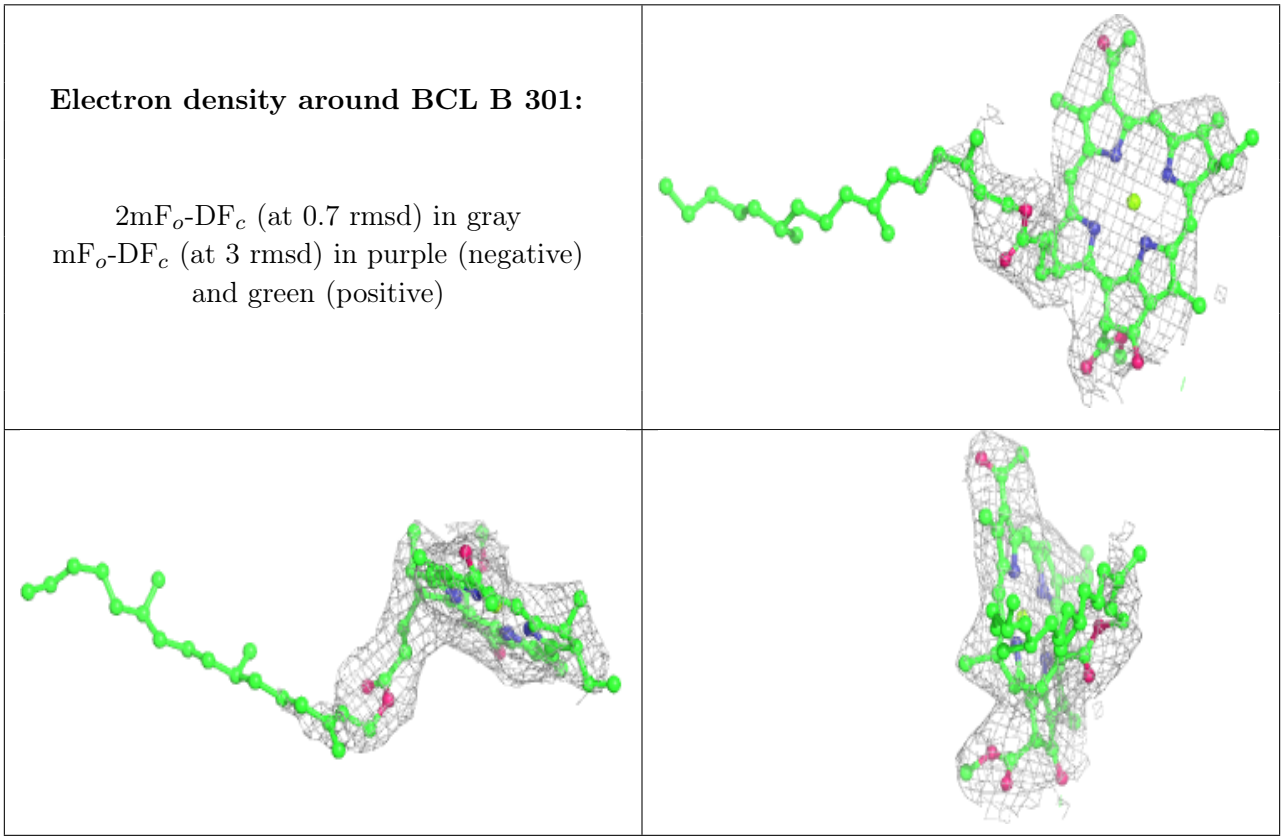
Electron density around BCL C 401:

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



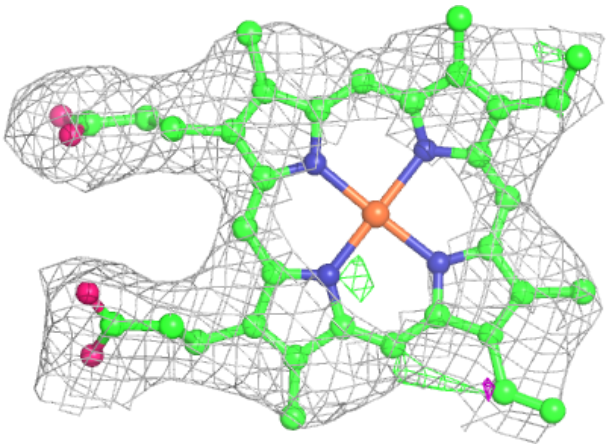
Electron density around BCL B 301:

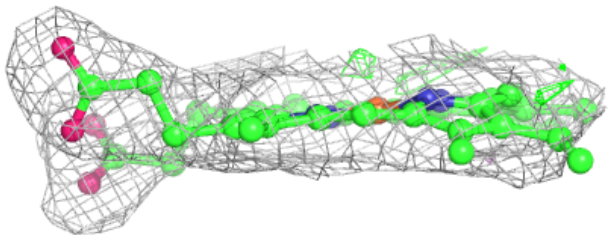
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

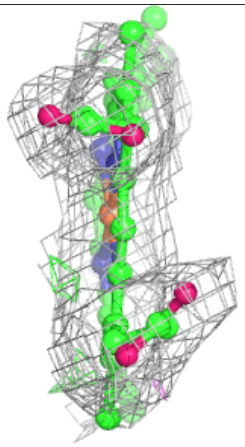


Electron density around HEC A 404:

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

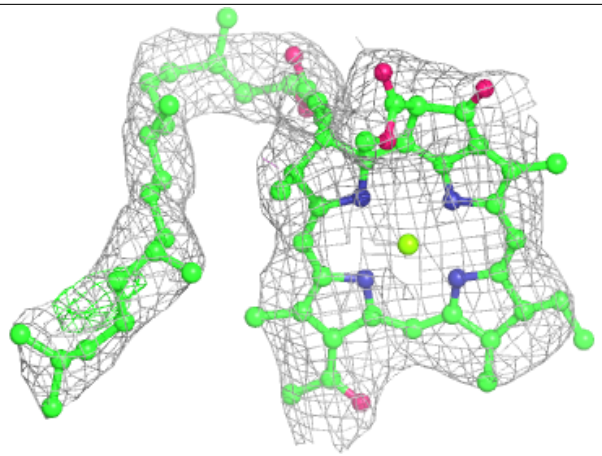


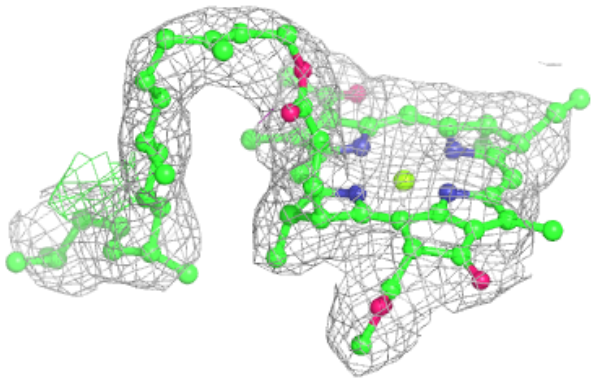


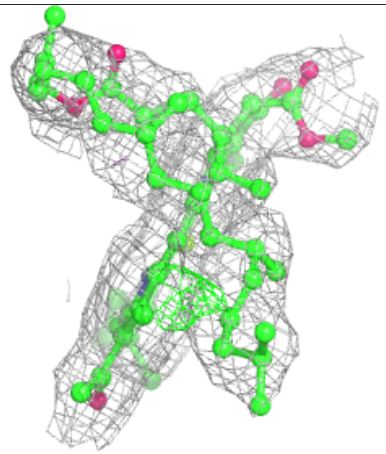


Electron density around BCL B 303:

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

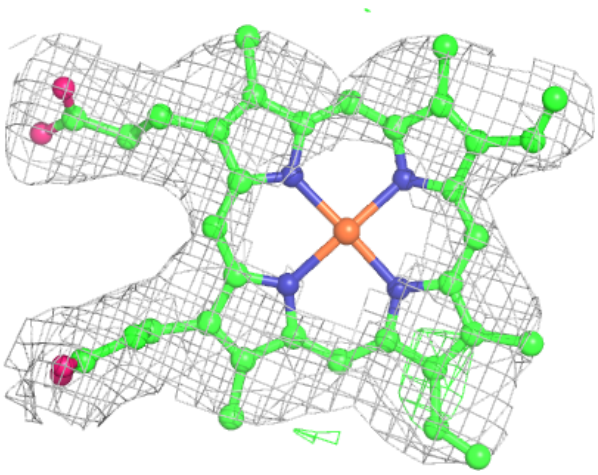


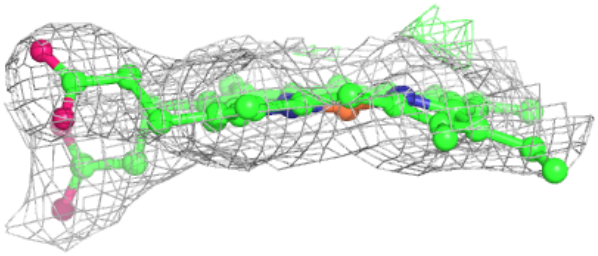


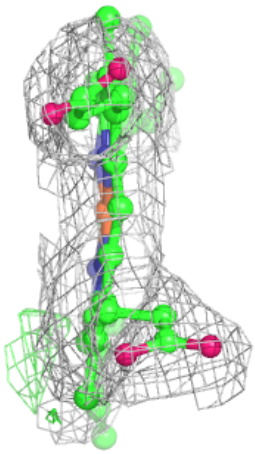


Electron density around HEC A 403:

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

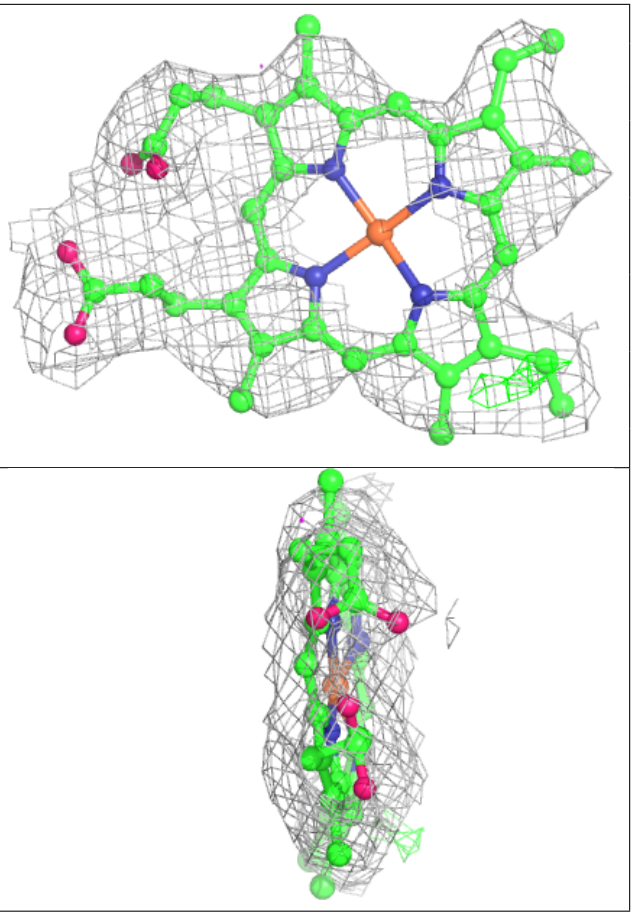






Electron density around HEC A 402:

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



6.5 Other polymers

There are no such residues in this entry.