



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 01:34 pm BST

PDB ID : 5M7K
Title : Blastochloris viridis photosynthetic reaction center - RC_vir_xfel
Authors : Sharma, A.S.; Johansson, L.; Dunevall, E.; Wahlgren, W.Y.; Neutze, R.; Kato, 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

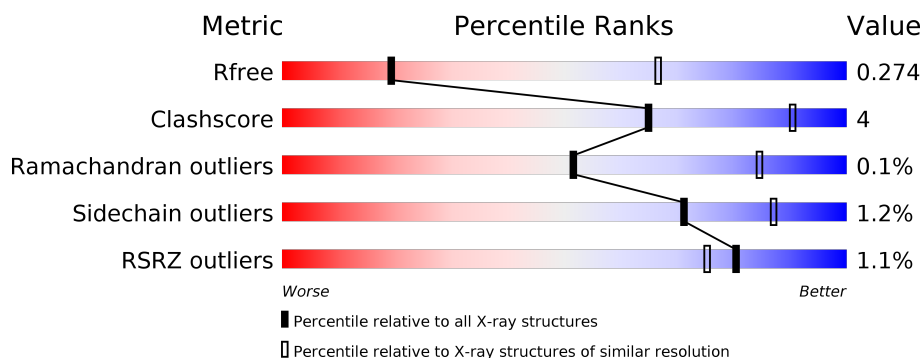
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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 on 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	MPG	B	306	-	-	-	X
9	MPG	C	407	-	-	-	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			

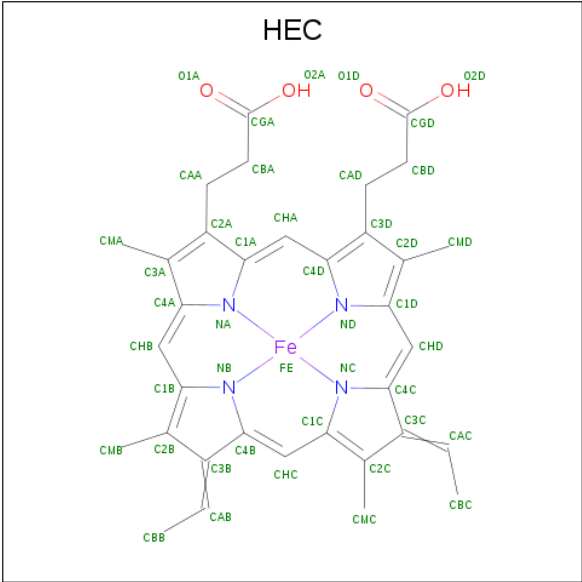
- Molecule 3 is a protein called Reaction center protein M chain.

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.

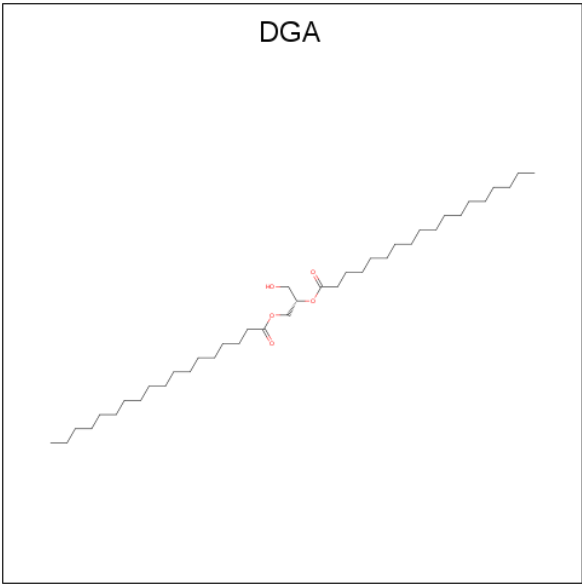
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	243	Total	C	N	O	S	0	0	0
			1771	1140	297	332	2			

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



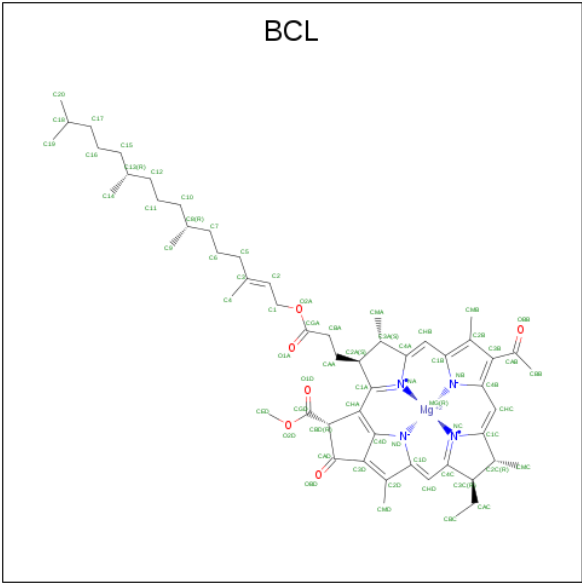
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 6 is DIACYL GLYCEROL (three-letter code: DGA) (formula: C₃₉H₇₆O₅).



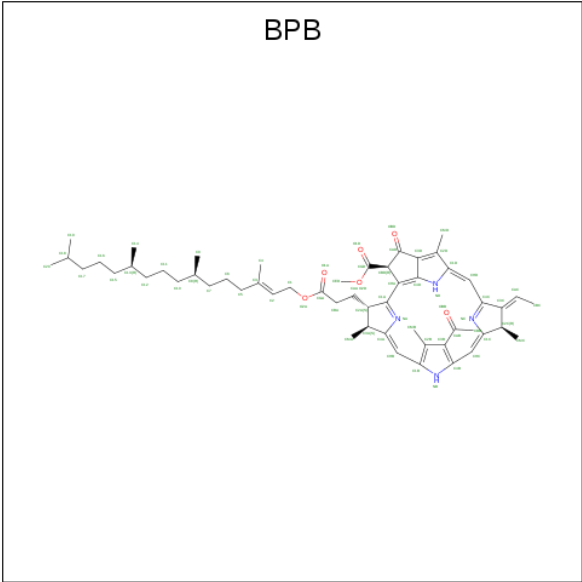
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	5	0
			37	33	4		

- Molecule 7 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C₅₅H₇₄MgN₄O₆).



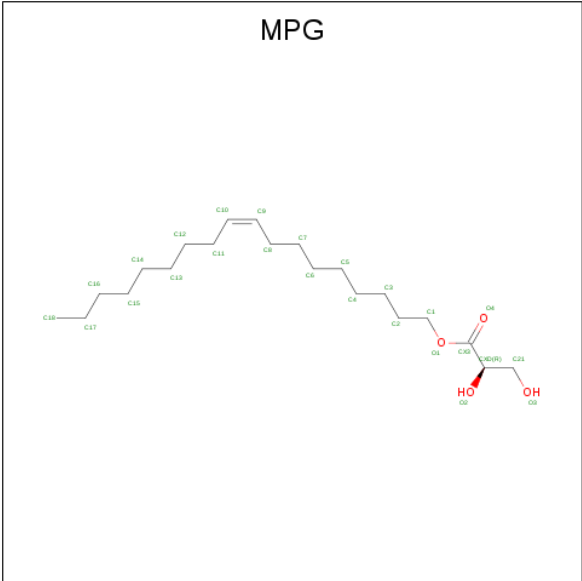
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	Mg	N	O	15	0
			65	54	1	4	6		
7	B	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	B	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	C	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 8 is BACTERIOPHEOPHYTIN B (three-letter code: BPB) (formula: C₅₅H₇₄N₄O₆).



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: C₂₁H₄₀O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	22	0
			25	21	4		

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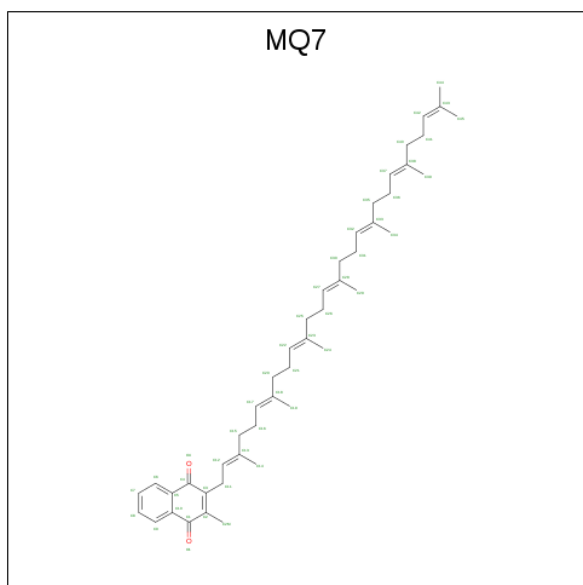
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	3	0
			25	21	4		
9	C	1	Total	C		8	0
			17	17			

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

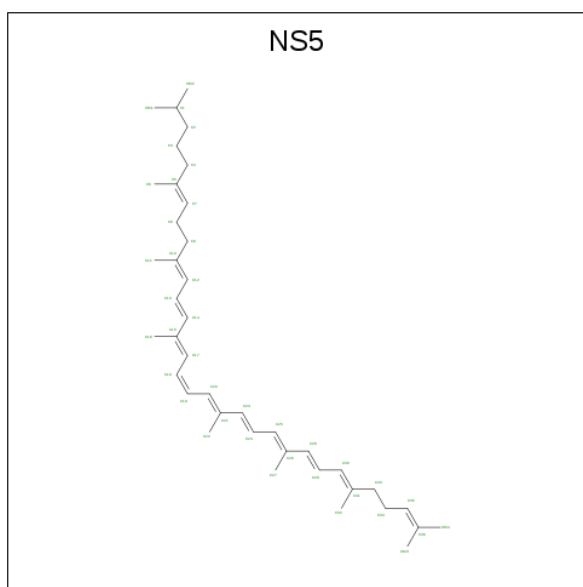
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	C	1	Total	Fe	0	0
			1	1		

- Molecule 11 is MENAQUINONE-7 (three-letter code: MQ7) (formula: C₄₆H₆₄O₂).



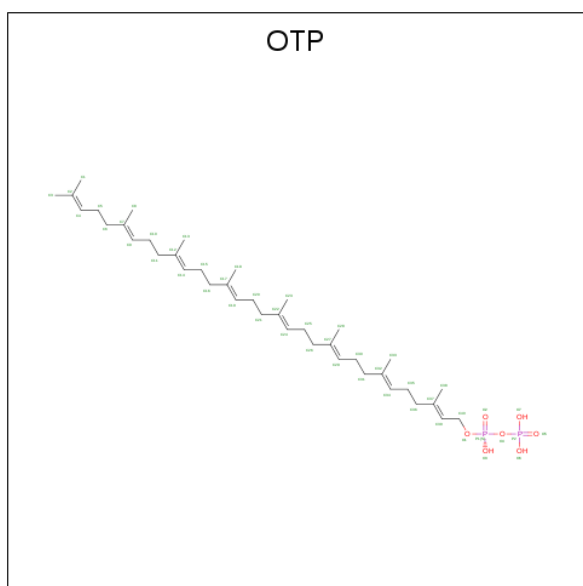
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	C	1	Total	C	O	0	0
			48	46	2		

- Molecule 12 is 15-cis-1,2-dihydroneurosporene (three-letter code: NS5) (formula: C₄₀H₆₀).



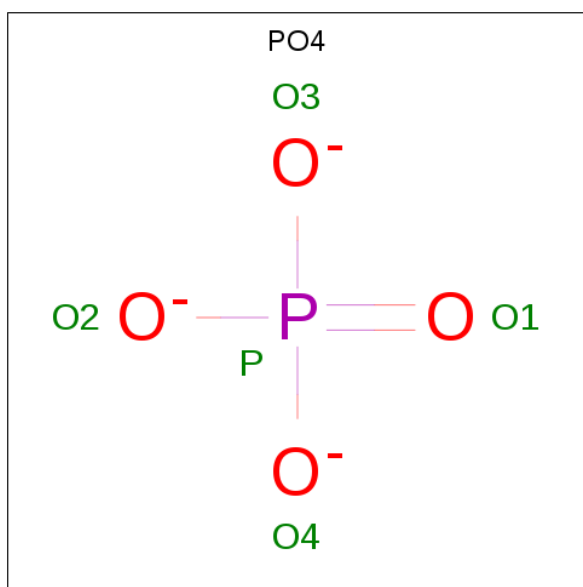
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	C	1	Total	C	9	0
			40	40		

- 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	0	0
			41	40	1		

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

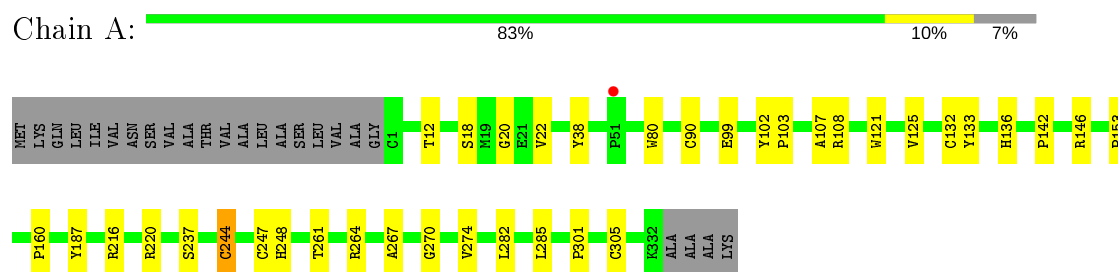


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	C	1	Total	O	P	5	0
			5	4	1		
14	C	1	Total	O	P	0	0
			5	4	1		

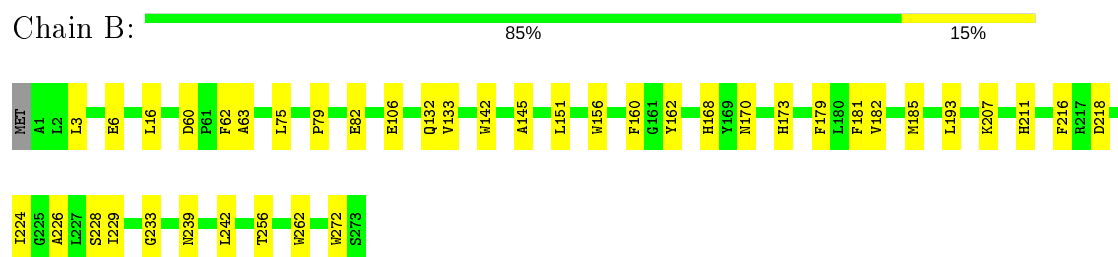
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

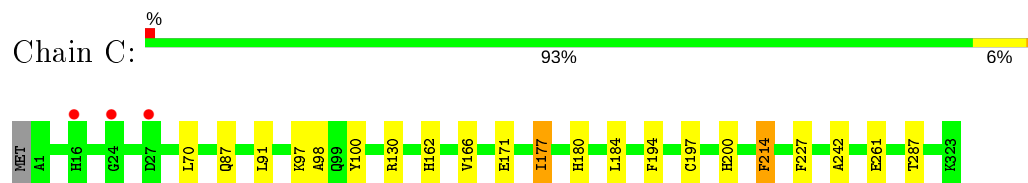
- Molecule 1: Photosynthetic reaction center cytochrome c subunit



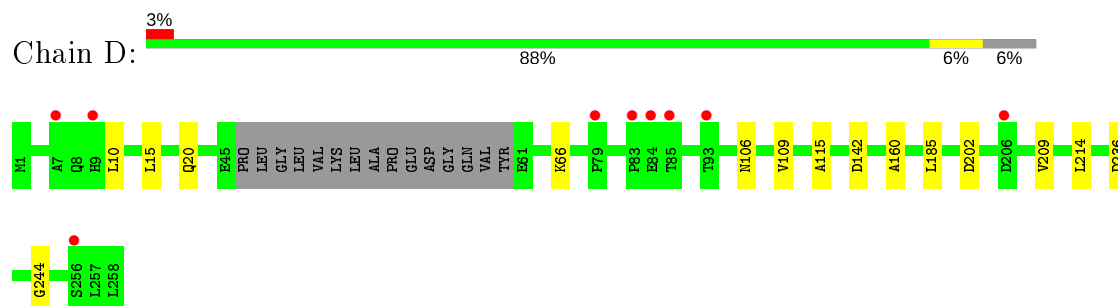
- Molecule 2: Reaction center protein L chain



- Molecule 3: Reaction center protein M chain



- Molecule 4: Reaction center protein H chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.90 Å 84.80 Å 384.30 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.44 – 3.50 55.44 – 3.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (55.44-3.50) 100.0 (55.44-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 3.49 Å)	Xtriage
Refinement program	PHENIX (1.10 _2155: ???)	Depositor
R, R_{free}	0.253 , 0.274 0.253 , 0.274	Depositor DCC
R_{free} test set	1294 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å ²)	77.1	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 75.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.34$, $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	9890	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.27	0/2665	0.46	0/3633
2	B	0.26	0/2263	0.42	0/3089
3	C	0.26	0/2650	0.40	0/3629
4	D	0.25	0/1804	0.45	0/2485
All	All	0.26	0/9382	0.43	0/12836

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	248	HIS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2598	0	2576	31	0
2	B	2170	0	2100	24	0
3	C	2546	0	2430	14	0
4	D	1771	0	1656	7	0
5	A	172	0	128	14	0
6	A	37	0	58	2	0
7	B	197	0	218	8	0
7	C	66	0	74	3	0
8	B	65	0	74	2	0
8	C	61	0	63	1	0
9	B	50	0	80	0	0
9	C	17	0	31	0	0
10	C	1	0	0	0	0
11	C	48	0	64	1	0
12	C	40	0	60	2	0
13	C	41	0	65	2	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)
1:A:244:CYS:HB3	5:A:403:HEC:C3B	2.28	0.63
1:A:153:PRO:HD3	1:A:160:PRO:HB3	1.81	0.61
1:A:80:TRP:CD1	1:A:133:TYR:HB2	2.36	0.61
1:A:244:CYS:SG	2:B:162:TYR:HB3	2.41	0.60
1:A:99:GLU:OE2	1:A:108:ARG:NH2	2.35	0.59
7:B:303:BCL:HMD2	7:C:401:BCL:HBB3	1.85	0.58
1:A:305:CYS:HA	5:A:404:HEC:HHC	1.86	0.57
4:D:160:ALA:HB3	4:D:214:LEU:HD23	1.88	0.56
2:B:168:HIS:CE1	7:B:302:BCL:HMC2	2.41	0.55
1:A:136:HIS:NE2	5:A:402:HEC:NB	2.54	0.55
4:D:202:ASP:HB3	4:D:209:VAL:HB	1.87	0.55
1:A:274:VAL:HG22	5:A:404:HEC:HMC2	1.92	0.52
1:A:220:ARG:NH2	3:C:171:GLU:OE2	2.42	0.51
1:A:247:CYS:HA	1:A:261:THR:OG1	2.09	0.51
1:A:282:LEU:HA	1:A:285:LEU:HD12	1.94	0.49
2:B:133:VAL:HA	2:B:142:TRP:HZ3	1.77	0.49
2:B:193:LEU:HD22	2:B:216:PHE:HE2	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:224:ILE:HG12	2:B:228:SER:HB2	1.94	0.49
2:B:75:LEU:HA	2:B:142:TRP:CD1	2.46	0.49
3:C:70:LEU:HD21	12:C:405:NS5:H29	1.94	0.49
7:B:302:BCL:H193	11:C:404:MQ7:H292	1.94	0.49
1:A:244:CYS:HB3	5:A:403:HEC:C4B	2.43	0.48
7:B:301:BCL:HBB3	7:C:401:BCL:H62	1.96	0.48
1:A:142:PRO:HD2	5:A:402:HEC:HBD2	1.96	0.48
2:B:16:LEU:HD13	2:B:106:GLU:HG2	1.96	0.48
2:B:233:GLY:HA3	3:C:214:PHE:CE1	2.49	0.48
7:B:303:BCL:HMD2	7:C:401:BCL:CBB	2.44	0.48
2:B:132:GLN:OE1	2:B:145:ALA:HB1	2.14	0.48
3:C:98:ALA:HB3	3:C:100:TYR:CZ	2.48	0.48
7:B:301:BCL:H3C	3:C:184:LEU:HD21	1.97	0.47
4:D:10:LEU:HD21	4:D:15:LEU:HD21	1.97	0.47
2:B:218:ASP:O	3:C:130:ARG:NH2	2.47	0.47
2:B:226:ALA:O	2:B:229:ILE:HG22	2.15	0.47
3:C:162:HIS:O	3:C:166:VAL:HG22	2.15	0.46
1:A:107:ALA:CB	5:A:401:HEC:HAC	2.46	0.46
4:D:106:ASN:HB3	4:D:109:VAL:HG22	1.98	0.46
1:A:264:ARG:HG2	5:A:403:HEC:HMD3	1.98	0.45
1:A:22:VAL:HG12	2:B:256:THR:HB	1.99	0.45
5:A:404:HEC:HMC1	5:A:404:HEC:CBC	2.47	0.45
1:A:270:GLY:O	1:A:274:VAL:HG23	2.17	0.45
7:B:303:BCL:HED3	13:C:406:OTP:H282	1.98	0.45
4:D:142:ASP:OD1	4:D:142:ASP:N	2.43	0.45
3:C:227:PHE:HB2	3:C:242:ALA:HB2	1.99	0.45
6:A:405:DGA:HA22	6:A:405:DGA:HG11	1.76	0.44
3:C:261:GLU:OE2	4:D:66:LYS:NZ	2.51	0.44
12:C:405:NS5:H18	12:C:405:NS5:H161	1.81	0.44
1:A:18:SER:HB2	2:B:156:TRP:CD1	2.52	0.44
2:B:181:PHE:HB3	8:C:402:BPB:HBBA	1.99	0.44
1:A:80:TRP:HB3	1:A:132:CYS:HB2	1.99	0.44
1:A:80:TRP:HE3	1:A:132:CYS:HG	1.64	0.44
2:B:60:ASP:HB3	2:B:63:ALA:HB3	2.00	0.43
4:D:115:ALA:HB2	4:D:244:GLY:HA3	2.00	0.43
1:A:187:TYR:CE2	3:C:97:LYS:HD3	2.54	0.43
1:A:244:CYS:HB3	5:A:403:HEC:CAB	2.48	0.43
13:C:406:OTP:H81	13:C:406:OTP:H51	1.69	0.43
3:C:87:GLN:O	3:C:91:LEU:HG	2.18	0.43
1:A:267:ALA:CB	5:A:403:HEC:HAC	2.48	0.43
1:A:301:PRO:HG2	5:A:402:HEC:HBD1	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:401:HEC:HMB1	5:A:401:HEC:CBB	2.48	0.43
2:B:179:PHE:HA	2:B:182:VAL:HG12	1.99	0.43
3:C:177:ILE:O	3:C:180:HIS:ND1	2.52	0.43
2:B:170:ASN:HB3	2:B:173:HIS:HB2	2.01	0.42
1:A:102:TYR:CG	1:A:103:PRO:HD3	2.54	0.42
1:A:12:THR:HG23	1:A:20:GLY:HA2	2.02	0.42
8:B:304:BPB:HBBB	8:B:304:BPB:HHC	2.01	0.42
1:A:237:SER:OG	5:A:403:HEC:HAB	2.19	0.42
2:B:239:ASN:HA	2:B:242:LEU:HB2	2.02	0.42
8:B:304:BPB:H14	8:B:304:BPB:H16A	1.83	0.41
1:A:121:TRP:O	1:A:125:VAL:HG22	2.20	0.41
1:A:216:ARG:NH2	3:C:287:THR:O	2.52	0.41
6:A:405:DGA:HB22	2:B:262:TRP:HH2	1.85	0.41
3:C:197:CYS:O	3:C:200:HIS:HB3	2.21	0.41
7:B:302:BCL:H41	7:B:302:BCL:H61	1.85	0.41
2:B:207:LYS:HB3	2:B:211:HIS:CG	2.55	0.41
1:A:247:CYS:HA	1:A:261:THR:HG1	1.86	0.41
1:A:90:CYS:SG	1:A:103:PRO:HB2	2.61	0.40
2:B:3:LEU:HB2	2:B:6:GLU:HB2	2.04	0.40
2:B:62:PHE:HB3	2:B:151:LEU:HD12	2.02	0.40
2:B:193:LEU:HD22	2:B:216:PHE:CE2	2.55	0.40
2:B:79:PRO:HB2	2:B:82[B]:GLU:HB2	2.02	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%)	313 (95%)	17 (5%)	0	100	100
2	B	273/274 (100%)	262 (96%)	11 (4%)	0	100	100
3	C	321/324 (99%)	313 (98%)	7 (2%)	1 (0%)	41	75

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	239/258 (93%)	234 (98%)	5 (2%)	0	100	100
All	All	1163/1212 (96%)	1122 (96%)	40 (3%)	1 (0%)	51	84

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	177	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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%)	277 (99%)	3 (1%)	73	88
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%)	164 (98%)	3 (2%)	59	81
All	All	912/978 (93%)	901 (99%)	11 (1%)	71	87

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

Mol	Chain	Res	Type
1	A	38	TYR
1	A	146	ARG
1	A	244	CYS
2	B	160	PHE
2	B	185	MET
2	B	272	TRP
3	C	194	PHE
3	C	214	PHE
4	D	20	GLN
4	D	185	LEU
4	D	236	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no

such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	FME	D	1	4	8,9,10	0.92	0	7,9,11	0.80	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	CA-CB-CG-SD
4	D	1	FME	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 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	C	401	-	58,74,74	1.24	5 (8%)	69,115,115	1.45	11 (15%)
6	DGA	A	405	-	36,36,43	1.17	3 (8%)	38,38,45	3.13	6 (15%)
7	BCL	B	302	-	58,74,74	1.28	5 (8%)	69,115,115	1.51	12 (17%)
14	PO4	C	408	-	4,4,4	0.92	0	6,6,6	0.43	0
7	BCL	B	301	-	57,73,74	1.29	5 (8%)	67,113,115	1.25	8 (11%)
12	NS5	C	405	-	39,39,39	2.33	18 (46%)	44,46,46	2.07	13 (29%)
5	HEC	A	401	1	26,50,50	2.19	4 (15%)	18,82,82	2.01	7 (38%)
9	MPG	B	305	-	24,24,24	1.24	1 (4%)	24,25,25	1.53	3 (12%)
14	PO4	C	409	-	4,4,4	0.88	0	6,6,6	0.50	0
8	BPB	B	304	-	64,70,70	1.11	5 (7%)	64,101,101	1.19	6 (9%)
7	BCL	B	303	-	58,74,74	1.31	5 (8%)	69,115,115	1.38	11 (15%)
9	MPG	B	306	-	24,24,24	1.26	1 (4%)	24,25,25	1.30	2 (8%)
11	MQ7	C	404	-	49,49,49	1.81	10 (20%)	60,63,63	1.60	15 (25%)
9	MPG	C	407	-	16,16,24	0.79	0	15,15,25	0.75	0
5	HEC	A	402	1	26,50,50	2.14	5 (19%)	18,82,82	2.22	8 (44%)
5	HEC	A	403	1	26,50,50	2.16	4 (15%)	18,82,82	2.03	6 (33%)
8	BPB	C	402	-	60,66,70	1.15	5 (8%)	59,96,101	1.24	6 (10%)
5	HEC	A	404	1	26,50,50	2.21	4 (15%)	18,82,82	1.82	5 (27%)
13	OTP	C	406	-	40,40,48	0.66	0	47,47,61	1.97	16 (34%)

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	C	401	-	-	6/37/137/137	-
6	DGA	A	405	-	-	14/37/37/45	-
7	BCL	B	302	-	-	4/37/137/137	-
7	BCL	B	301	-	-	6/36/136/137	-
12	NS5	C	405	-	-	13/43/43/43	-
5	HEC	A	401	1	-	0/6/54/54	-
9	MPG	B	305	-	-	14/25/25/25	-
9	MPG	B	306	-	-	11/25/25/25	-
5	HEC	A	402	1	-	1/6/54/54	-
8	BPB	B	304	-	-	7/47/105/105	0/5/6/6
11	MQ7	C	404	-	-	3/41/61/61	0/2/2/2
9	MPG	C	407	-	-	6/14/14/25	-
7	BCL	B	303	-	-	5/37/137/137	-
5	HEC	A	403	1	-	0/6/54/54	-
8	BPB	C	402	-	-	11/43/101/105	0/5/6/6
5	HEC	A	404	1	-	0/6/54/54	-
13	OTP	C	406	-	-	13/45/45/55	-

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	404	MQ7	C3-C2	7.19	1.48	1.35
5	A	404	HEC	C3B-C2B	-5.62	1.34	1.40
5	A	401	HEC	C3B-C2B	-5.57	1.34	1.40
5	A	404	HEC	C3C-C2C	-5.51	1.35	1.40
5	A	403	HEC	C3C-C2C	-5.29	1.35	1.40
5	A	401	HEC	C3C-C2C	-5.26	1.35	1.40
5	A	402	HEC	C3C-C2C	-5.25	1.35	1.40
7	B	301	BCL	C1B-NB	5.17	1.39	1.35
5	A	403	HEC	C3B-C2B	-5.12	1.35	1.40
7	B	303	BCL	C1B-NB	5.01	1.39	1.35
7	B	302	BCL	MG-NA	4.96	2.18	2.06
7	B	302	BCL	C1B-NB	4.96	1.39	1.35
5	A	402	HEC	C3B-C2B	-4.96	1.35	1.40
7	C	401	BCL	C1B-NB	4.95	1.39	1.35
12	C	405	NS5	C30-C31	4.90	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	305	MPG	O1-CX3	4.81	1.43	1.33
9	B	306	MPG	O1-CX3	4.81	1.43	1.33
7	B	301	BCL	MG-NA	4.77	2.17	2.06
7	C	401	BCL	MG-NA	4.67	2.17	2.06
7	B	303	BCL	MG-NA	4.61	2.17	2.06
12	C	405	NS5	C14-C15	4.25	1.55	1.45
8	B	304	BPB	C3B-C4B	4.19	1.46	1.41
5	A	403	HEC	CBC-CAC	-4.13	1.34	1.49
5	A	402	HEC	CBB-CAB	-4.12	1.34	1.49
11	C	404	MQ7	C5-C4	4.09	1.56	1.48
8	C	402	BPB	C3B-C4B	4.09	1.46	1.41
5	A	401	HEC	CBC-CAC	-4.07	1.34	1.49
5	A	403	HEC	CBB-CAB	-4.07	1.34	1.49
5	A	402	HEC	CBC-CAC	-4.06	1.34	1.49
5	A	404	HEC	CBB-CAB	-4.04	1.34	1.49
5	A	401	HEC	CBB-CAB	-3.96	1.34	1.49
5	A	404	HEC	CBC-CAC	-3.94	1.34	1.49
11	C	404	MQ7	C10-C1	3.79	1.55	1.48
12	C	405	NS5	C19-C20	3.79	1.55	1.43
12	C	405	NS5	C12-C10	3.72	1.38	1.34
7	B	303	BCL	MG-NC	3.65	2.14	2.06
12	C	405	NS5	C28-C26	3.52	1.53	1.45
12	C	405	NS5	C18-C17	3.48	1.54	1.43
6	A	405	DGA	OG1-CA1	3.44	1.43	1.33
7	B	301	BCL	MG-NC	3.43	2.14	2.06
6	A	405	DGA	CG1-CG2	3.41	1.58	1.50
7	B	302	BCL	MG-NC	3.37	2.14	2.06
12	C	405	NS5	C23-C21	3.35	1.53	1.45
12	C	405	NS5	C29-C30	3.29	1.53	1.43
12	C	405	NS5	C24-C25	3.23	1.53	1.43
8	C	402	BPB	CAC-C3C	3.18	1.42	1.33
6	A	405	DGA	OG2-CB1	3.18	1.43	1.34
8	B	304	BPB	CAC-C3C	3.18	1.42	1.33
12	C	405	NS5	C4-C5	2.99	1.57	1.51
7	C	401	BCL	MG-NC	2.99	2.13	2.06
12	C	405	NS5	C13-C12	2.95	1.52	1.43
12	C	405	NS5	C20-C21	2.87	1.39	1.35
7	B	303	BCL	C4B-NB	2.80	1.37	1.35
7	B	303	BCL	OBD-CAD	2.68	1.26	1.22
11	C	404	MQ7	C20-C18	2.64	1.56	1.51
12	C	405	NS5	C7-C5	2.63	1.39	1.33
8	C	402	BPB	CHD-C1D	2.61	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	304	BPB	C4C-C3C	2.58	1.51	1.45
8	C	402	BPB	C4C-C3C	2.53	1.51	1.45
11	C	404	MQ7	C12-C13	2.52	1.39	1.33
12	C	405	NS5	C33-C31	2.52	1.56	1.51
11	C	404	MQ7	C17-C18	2.49	1.39	1.33
7	C	401	BCL	OBD-CAD	2.43	1.25	1.22
8	B	304	BPB	CHD-C1D	2.42	1.43	1.38
12	C	405	NS5	C13-C14	2.42	1.40	1.34
7	B	301	BCL	C4B-NB	2.40	1.37	1.35
7	B	302	BCL	C4B-NB	2.38	1.37	1.35
11	C	404	MQ7	C27-C28	2.36	1.38	1.33
7	C	401	BCL	C4B-NB	2.34	1.37	1.35
8	C	402	BPB	C2C-C3C	2.30	1.54	1.51
11	C	404	MQ7	C32-C33	2.29	1.38	1.33
11	C	404	MQ7	C11-C3	2.29	1.55	1.51
12	C	405	NS5	C17-C15	2.26	1.38	1.35
7	B	302	BCL	OBD-CAD	2.25	1.25	1.22
12	C	405	NS5	C29-C28	2.18	1.40	1.34
12	C	405	NS5	C35-C36	2.07	1.38	1.32
11	C	404	MQ7	C22-C23	2.06	1.37	1.33
7	B	301	BCL	OBD-CAD	2.06	1.25	1.22
8	B	304	BPB	OBD-CAD	2.04	1.26	1.22
5	A	402	HEC	CAD-C3D	2.04	1.55	1.52

All (135) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	405	DGA	OG2-CG2-CG3	-12.84	78.58	107.93
6	A	405	DGA	OG2-CG2-CG1	-10.09	82.77	106.13
6	A	405	DGA	CG3-CG2-CG1	7.00	132.75	112.63
12	C	405	NS5	C18-C17-C15	-6.46	118.10	127.31
12	C	405	NS5	C19-C20-C21	-5.98	118.78	127.31
9	B	305	MPG	O1-CX3-CXD	5.44	122.52	111.68
13	C	406	OTP	C33-C32-C31	4.81	123.36	115.27
7	B	303	BCL	CMB-C2B-C1B	-4.63	121.35	128.46
9	B	306	MPG	O1-CX3-CXD	4.44	120.53	111.68
13	C	406	OTP	C40-C39-C37	-4.33	120.46	127.21
7	B	302	BCL	CMB-C2B-C1B	-4.31	121.83	128.46
7	C	401	BCL	CMB-C2B-C1B	-4.28	121.89	128.46
8	B	304	BPB	CBD-CHA-C4D	-4.25	103.75	108.54
8	C	402	BPB	CBD-CHA-C4D	-4.15	103.87	108.54
5	A	402	HEC	CMB-C2B-C1B	-4.06	122.22	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	402	HEC	CMB-C2B-C3B	3.89	130.39	125.82
5	A	403	HEC	CMB-C2B-C1B	-3.83	122.58	128.46
7	C	401	BCL	C4D-C3D-CAD	-3.70	106.40	108.47
7	C	401	BCL	C2A-C1A-CHA	3.64	130.23	123.86
6	A	405	DGA	OG2-CB1-CB2	3.58	119.22	111.50
7	B	302	BCL	C4D-C3D-CAD	-3.58	106.47	108.47
11	C	404	MQ7	C21-C22-C23	-3.56	119.08	127.66
7	B	302	BCL	OBD-CAD-CBD	-3.53	120.85	125.89
7	B	301	BCL	CMB-C2B-C1B	-3.51	123.06	128.46
5	A	401	HEC	CMC-C2C-C1C	-3.51	123.06	128.46
5	A	401	HEC	CMB-C2B-C1B	-3.48	123.11	128.46
7	C	401	BCL	CHA-C1A-NA	-3.47	118.46	126.40
12	C	405	NS5	C11-C10-C9	3.43	121.04	115.27
5	A	402	HEC	CBA-CAA-C2A	-3.41	106.20	112.48
5	A	404	HEC	CMB-C2B-C1B	-3.38	123.26	128.46
11	C	404	MQ7	C11-C12-C13	-3.34	121.23	126.79
7	B	303	BCL	CMB-C2B-C3B	3.29	130.84	124.68
7	B	302	BCL	C2A-C1A-CHA	3.29	129.61	123.86
7	B	302	BCL	C4A-NA-C1A	3.28	108.18	106.71
7	B	301	BCL	CHA-C1A-NA	-3.25	118.96	126.40
7	B	302	BCL	C1-C2-C3	-3.20	120.52	126.04
5	A	403	HEC	CMC-C2C-C1C	-3.18	123.57	128.46
5	A	403	HEC	CMB-C2B-C3B	3.17	129.55	125.82
7	B	302	BCL	CHA-C1A-NA	-3.17	119.14	126.40
13	C	406	OTP	C38-C37-C36	3.16	120.58	115.27
5	A	404	HEC	CMC-C2C-C1C	-3.15	123.62	128.46
13	C	406	OTP	C8-C7-C6	3.13	120.53	115.27
12	C	405	NS5	C6-C5-C4	3.12	120.51	115.27
7	C	401	BCL	CMB-C2B-C3B	3.08	130.44	124.68
7	B	301	BCL	OBD-CAD-CBD	-3.06	121.52	125.89
5	A	402	HEC	CMC-C2C-C1C	-3.06	123.75	128.46
5	A	401	HEC	CBD-CAD-C3D	-3.06	106.84	112.49
7	B	302	BCL	CMB-C2B-C3B	3.06	130.41	124.68
13	C	406	OTP	C35-C34-C32	-3.03	120.36	127.66
11	C	404	MQ7	C26-C27-C28	-3.03	120.36	127.66
13	C	406	OTP	C28-C27-C26	3.03	120.37	115.27
13	C	406	OTP	C23-C22-C21	3.00	120.33	115.27
7	B	303	BCL	OBD-CAD-CBD	-3.00	121.61	125.89
13	C	406	OTP	C15-C14-C12	-2.95	120.56	127.66
12	C	405	NS5	C24-C25-C26	-2.94	123.12	127.31
7	C	401	BCL	OBD-CAD-CBD	-2.94	121.70	125.89
11	C	404	MQ7	C31-C32-C33	-2.94	120.59	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	C	406	OTP	C13-C12-C11	2.93	120.20	115.27
7	B	303	BCL	C2A-C1A-CHA	2.93	128.98	123.86
7	C	401	BCL	C4A-NA-C1A	2.91	108.02	106.71
11	C	404	MQ7	C39-C38-C40	2.90	120.16	115.27
7	B	303	BCL	CHA-C1A-NA	-2.88	119.80	126.40
5	A	402	HEC	CBD-CAD-C3D	-2.85	107.23	112.49
13	C	406	OTP	C10-C9-C7	-2.83	120.84	127.66
13	C	406	OTP	C18-C17-C16	2.80	119.98	115.27
12	C	405	NS5	C25-C24-C23	-2.78	114.55	123.22
11	C	404	MQ7	C24-C23-C25	2.75	119.90	115.27
5	A	403	HEC	CAA-CBA-CGA	-2.75	108.06	112.67
5	A	401	HEC	CMB-C2B-C3B	2.73	129.03	125.82
8	C	402	BPB	C11-C10-C8	2.73	124.76	115.92
7	C	401	BCL	C11-C10-C8	-2.73	107.08	115.92
13	C	406	OTP	C30-C29-C27	-2.73	121.09	127.66
11	C	404	MQ7	C29-C28-C30	2.73	119.86	115.27
9	B	305	MPG	O1-CX3-O4	-2.72	118.98	124.13
11	C	404	MQ7	C34-C33-C35	2.72	119.84	115.27
8	B	304	BPB	C3D-C4D-CHA	2.71	116.81	109.49
5	A	401	HEC	CMC-C2C-C3C	2.71	129.01	125.82
8	C	402	BPB	C3D-C4D-CHA	2.71	116.79	109.49
7	C	401	BCL	C1C-NC-C4C	2.70	107.92	106.71
11	C	404	MQ7	C19-C18-C20	2.68	119.78	115.27
6	A	405	DGA	OG1-CA1-CA2	2.67	120.30	111.91
11	C	404	MQ7	C16-C17-C18	-2.66	121.26	127.66
7	B	301	BCL	C4A-NA-C1A	2.62	107.89	106.71
5	A	403	HEC	CMC-C2C-C3C	2.61	128.89	125.82
8	B	304	BPB	CMB-C2B-C3B	2.59	129.53	124.68
7	B	301	BCL	C2A-C1A-CHA	2.59	128.38	123.86
12	C	405	NS5	C34-C35-C36	-2.58	118.93	127.75
7	B	302	BCL	C1C-NC-C4C	2.58	107.86	106.71
7	B	302	BCL	CMD-C2D-C3D	2.55	129.44	124.68
7	B	303	BCL	C1C-NC-C4C	2.54	107.85	106.71
12	C	405	NS5	CM4-C36-CM3	2.51	120.15	114.60
7	B	301	BCL	C4D-C3D-CAD	-2.49	107.08	108.47
12	C	405	NS5	C16-C15-C17	-2.47	119.47	122.92
8	C	402	BPB	CMB-C2B-C3B	2.45	129.26	124.68
5	A	404	HEC	CMC-C2C-C3C	2.43	128.68	125.82
5	A	404	HEC	CMB-C2B-C3B	2.42	128.66	125.82
7	C	401	BCL	CMD-C2D-C3D	2.41	129.18	124.68
13	C	406	OTP	C1-C2-C3	2.40	119.91	114.60
11	C	404	MQ7	C14-C13-C15	2.40	119.31	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	304	BPB	CHD-C1D-ND	-2.38	119.62	124.58
7	B	303	BCL	C4A-NA-C1A	2.38	107.78	106.71
7	B	303	BCL	C1-C2-C3	-2.37	121.94	126.04
6	A	405	DGA	CG2-OG2-CB1	-2.37	114.83	117.88
11	C	404	MQ7	C2M-C2-C3	-2.36	120.56	124.40
8	C	402	BPB	CHD-C1D-ND	-2.35	119.68	124.58
12	C	405	NS5	C13-C14-C15	-2.34	119.84	126.42
7	B	301	BCL	CMB-C2B-C3B	2.34	129.05	124.68
7	B	303	BCL	C4B-C3B-CAB	-2.33	122.62	127.13
5	A	403	HEC	CBD-CAD-C3D	-2.33	108.19	112.49
5	A	402	HEC	CAD-CBD-CGD	-2.31	108.79	112.67
7	B	301	BCL	CMD-C2D-C3D	2.30	128.99	124.68
12	C	405	NS5	C32-C31-C33	2.30	119.14	115.27
5	A	404	HEC	CBD-CAD-C3D	-2.30	108.25	112.49
7	B	303	BCL	OBB-CAB-CBB	-2.27	115.05	120.17
13	C	406	OTP	C18-C17-C19	-2.26	117.89	123.68
11	C	404	MQ7	C45-C43-C44	2.25	119.58	114.60
7	B	302	BCL	OBB-CAB-CBB	-2.25	115.11	120.17
9	B	305	MPG	O4-CX3-CXD	-2.24	118.49	123.68
5	A	402	HEC	CMC-C2C-C3C	2.24	128.45	125.82
5	A	402	HEC	CMD-C2D-C1D	-2.24	125.03	128.46
7	C	401	BCL	OBB-CAB-CBB	-2.23	115.16	120.17
8	B	304	BPB	C17-C16-C15	2.21	123.38	113.24
9	B	306	MPG	O4-CX3-CXD	-2.19	118.62	123.68
11	C	404	MQ7	C36-C37-C38	-2.18	122.40	127.66
7	B	302	BCL	C4B-C3B-CAB	-2.17	122.94	127.13
13	C	406	OTP	C33-C32-C34	-2.15	118.16	123.68
7	B	303	BCL	C4D-C3D-CAD	-2.09	107.31	108.47
5	A	401	HEC	CMD-C2D-C1D	-2.08	125.26	128.46
8	C	402	BPB	C4B-CHC-C1C	2.06	131.22	128.57
12	C	405	NS5	C34-C33-C31	-2.05	106.23	112.98
5	A	401	HEC	CAA-CBA-CGA	-2.04	109.24	112.67
8	B	304	BPB	OBB-CAB-CBB	-2.03	115.59	120.17
11	C	404	MQ7	C2M-C2-C1	2.03	119.63	116.27
12	C	405	NS5	C9-C8-C7	-2.02	105.25	111.88
13	C	406	OTP	C5-C4-C2	-2.00	120.90	127.75

There are no chirality outliers.

All (114) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	401	BCL	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
7	C	401	BCL	CAD-CBD-CGD-O2D
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
12	C	405	NS5	C3-C4-C5-C6
12	C	405	NS5	C3-C4-C5-C7
13	C	406	OTP	C30-C31-C32-C34
13	C	406	OTP	C30-C31-C32-C33
13	C	406	OTP	C14-C15-C16-C17
13	C	406	OTP	C9-C10-C11-C12
13	C	406	OTP	C5-C6-C7-C8
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
9	B	305	MPG	O4-CX3-CXD-C21
9	B	306	MPG	O3-C21-CXD-O2
8	B	304	BPB	NB-C4B-CHC-C1C
8	B	304	BPB	C3B-C4B-CHC-C1C
8	C	402	BPB	C4-C3-C5-C6
8	C	402	BPB	C11-C10-C8-C9
8	C	402	BPB	NB-C4B-CHC-C1C
8	C	402	BPB	C3B-C4B-CHC-C1C
12	C	405	NS5	C2-C3-C4-C5
13	C	406	OTP	C5-C6-C7-C9
8	C	402	BPB	C2-C3-C5-C6
12	C	405	NS5	C11-C10-C9-C8
12	C	405	NS5	C12-C10-C9-C8
7	C	401	BCL	C2A-CAA-CBA-CGA
12	C	405	NS5	C28-C29-C30-C31
7	B	301	BCL	C14-C13-C15-C16
12	C	405	NS5	C27-C26-C28-C29
12	C	405	NS5	C25-C26-C28-C29
7	B	302	BCL	C15-C16-C17-C18
7	B	303	BCL	C11-C12-C13-C15
13	C	406	OTP	C24-C25-C26-C27
9	B	305	MPG	C2-C3-C4-C5
9	B	305	MPG	C5-C6-C7-C8
9	B	306	MPG	C11-C12-C13-C14
6	A	405	DGA	CBB-CAB-CB9-CB8

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Mol	Chain	Res	Type	Atoms
6	A	405	DGA	CCB-CDB-CEB-CFB
7	B	303	BCL	C16-C17-C18-C19
8	B	304	BPB	C4-C3-C5-C6
9	B	305	MPG	C10-C11-C12-C13
9	C	407	MPG	C10-C11-C12-C13
13	C	406	OTP	C34-C35-C36-C37
9	B	306	MPG	C3-C4-C5-C6
6	A	405	DGA	CA7-CA8-CA9-CAA
6	A	405	DGA	CA5-CA6-CA7-CA8
8	B	304	BPB	O2A-C1-C2-C3
8	B	304	BPB	C2-C3-C5-C6
6	A	405	DGA	CB9-CAB-CBB-CCB
7	B	301	BCL	C2-C3-C5-C6
6	A	405	DGA	CB4-CB5-CB6-CB7
7	B	303	BCL	C16-C17-C18-C20
6	A	405	DGA	CB6-CB7-CB8-CB9
9	B	306	MPG	C12-C13-C14-C15
9	B	305	MPG	C6-C7-C8-C9
7	B	303	BCL	C11-C12-C13-C14
9	C	407	MPG	C4-C5-C6-C7
7	B	301	BCL	C4-C3-C5-C6
12	C	405	NS5	C1-C2-C3-C4
6	A	405	DGA	CEB-CFB-CGB-CHB
9	B	305	MPG	O4-CX3-CXD-O2
8	C	402	BPB	C6-C7-C8-C10
8	C	402	BPB	C11-C10-C8-C7
9	B	306	MPG	O3-C21-CXD-CX3
8	C	402	BPB	C6-C7-C8-C9
12	C	405	NS5	CM2-C1-C2-C3
5	A	402	HEC	C3D-CAD-CBD-CGD
9	B	305	MPG	C12-C13-C14-C15
13	C	406	OTP	C15-C16-C17-C18
12	C	405	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	C13-C14-C15-C16
9	B	306	MPG	O4-CX3-CXD-C21
9	C	407	MPG	C13-C14-C15-C16
9	C	407	MPG	C2-C3-C4-C5
12	C	405	NS5	C26-C28-C29-C30
6	A	405	DGA	CBB-CCB-CDB-CEB
13	C	406	OTP	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
7	C	401	BCL	O2A-C1-C2-C3
9	C	407	MPG	C7-C8-C9-C10
12	C	405	NS5	C15-C17-C18-C19
11	C	404	MQ7	C39-C38-C40-C41
9	B	306	MPG	C6-C7-C8-C9
7	B	303	BCL	C15-C16-C17-C18
11	C	404	MQ7	C38-C40-C41-C42
13	C	406	OTP	C15-C16-C17-C19
11	C	404	MQ7	C37-C38-C40-C41
9	B	306	MPG	O1-CX3-CXD-C21
7	B	302	BCL	CAD-CBD-CGD-O2D
7	B	301	BCL	CAD-CBD-CGD-O2D
9	B	305	MPG	C7-C8-C9-C10
9	C	407	MPG	C9-C10-C11-C12
7	C	401	BCL	CHA-CBD-CGD-O1D
7	C	401	BCL	CHA-CBD-CGD-O2D
7	B	301	BCL	CHA-CBD-CGD-O2D
8	B	304	BPB	CHA-CBD-CGD-O2D
9	B	306	MPG	C1-C2-C3-C4
9	B	306	MPG	C7-C8-C9-C10
9	B	306	MPG	C2-C3-C4-C5
13	C	406	OTP	C20-C21-C22-C24
8	C	402	BPB	C11-C12-C13-C15
8	C	402	BPB	C11-C12-C13-C14
6	A	405	DGA	OG2-CB1-CB2-CB3
7	B	301	BCL	C12-C13-C15-C16
13	C	406	OTP	C19-C20-C21-C22
8	B	304	BPB	C8-C10-C11-C12
6	A	405	DGA	OB1-CB1-CB2-CB3

There are no ring outliers.

14 monomers are involved in 30 short contacts:

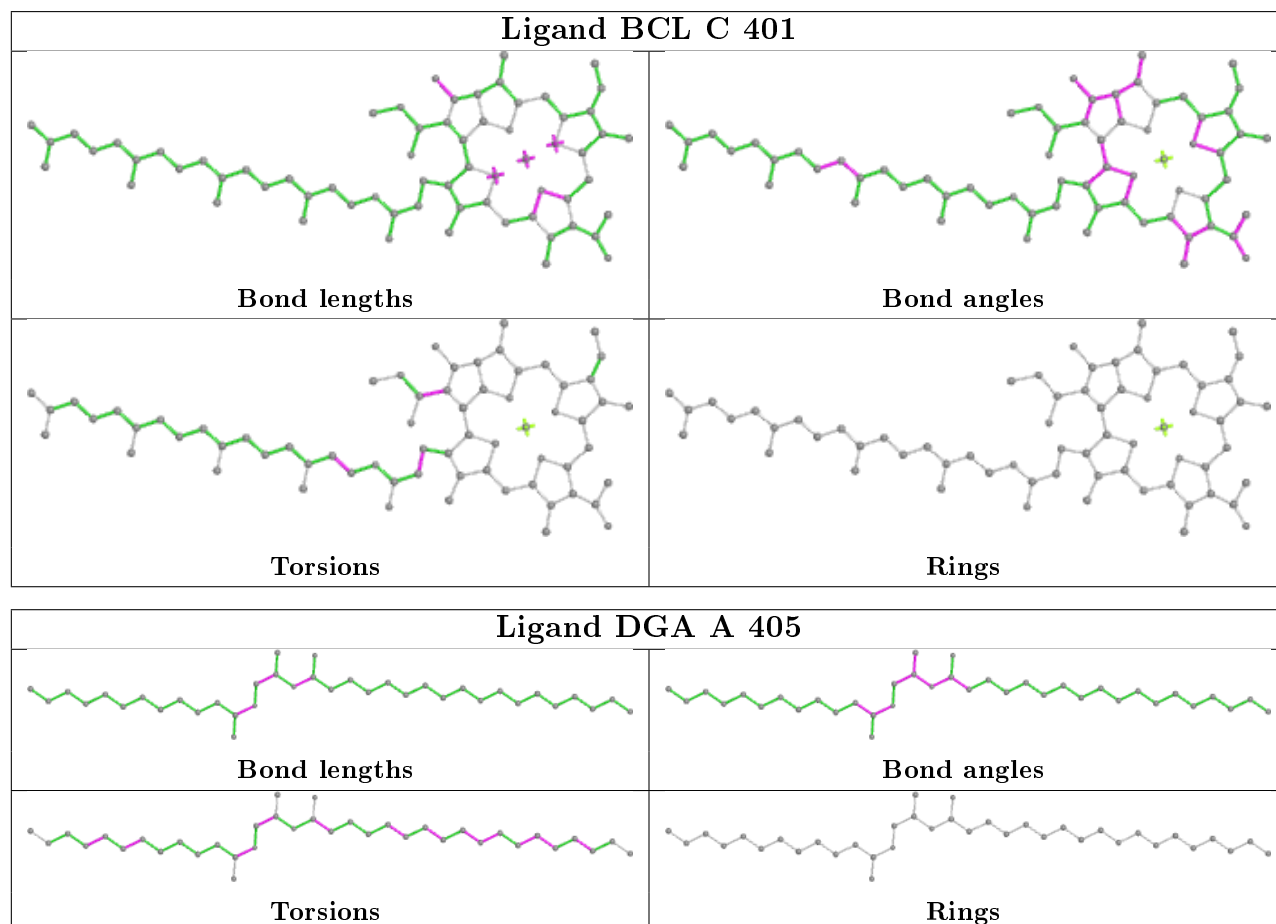
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	401	BCL	3	0
6	A	405	DGA	2	0
7	B	302	BCL	3	0
7	B	301	BCL	2	0
12	C	405	NS5	2	0
5	A	401	HEC	2	0
8	B	304	BPB	2	0
7	B	303	BCL	3	0

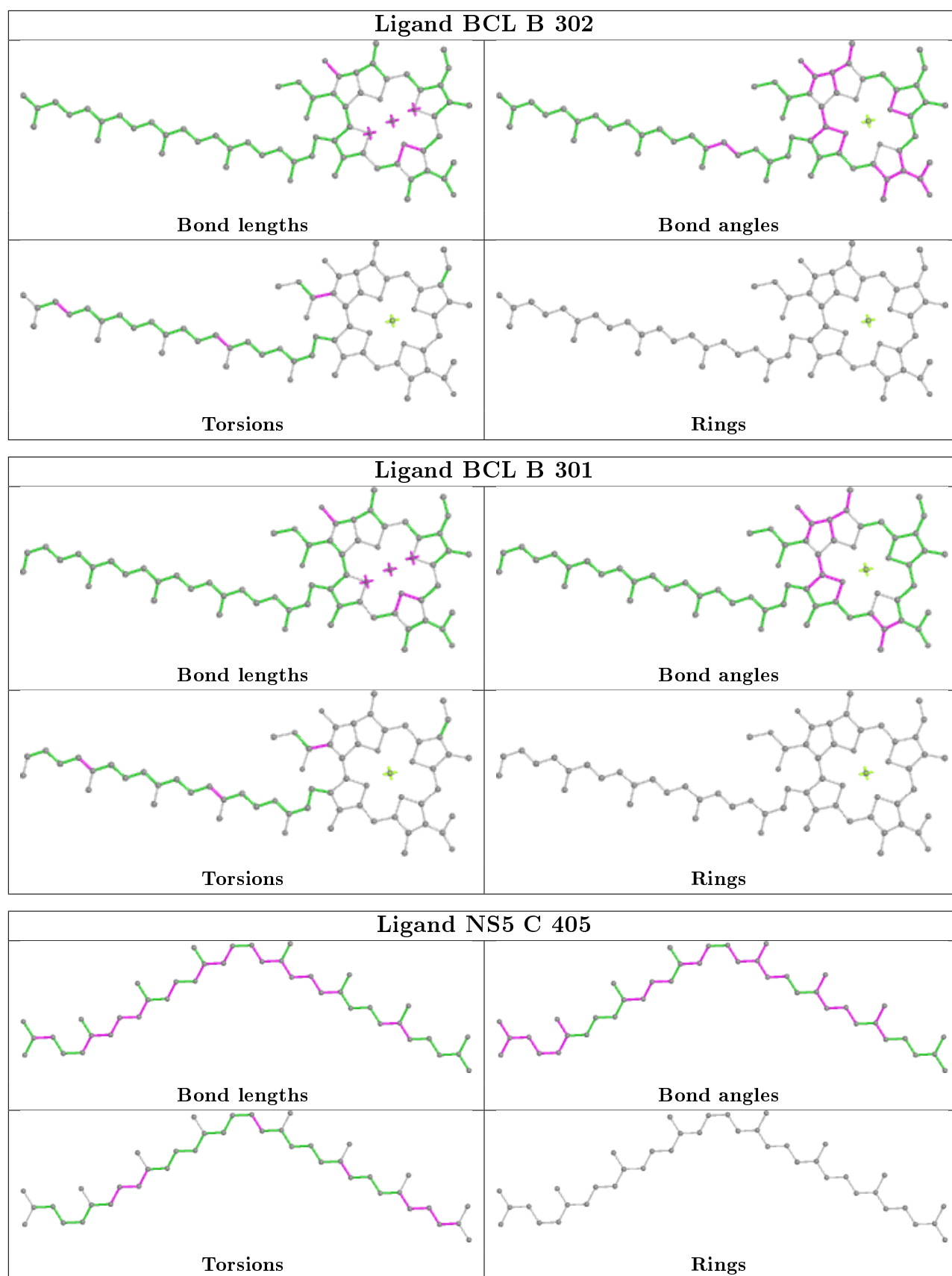
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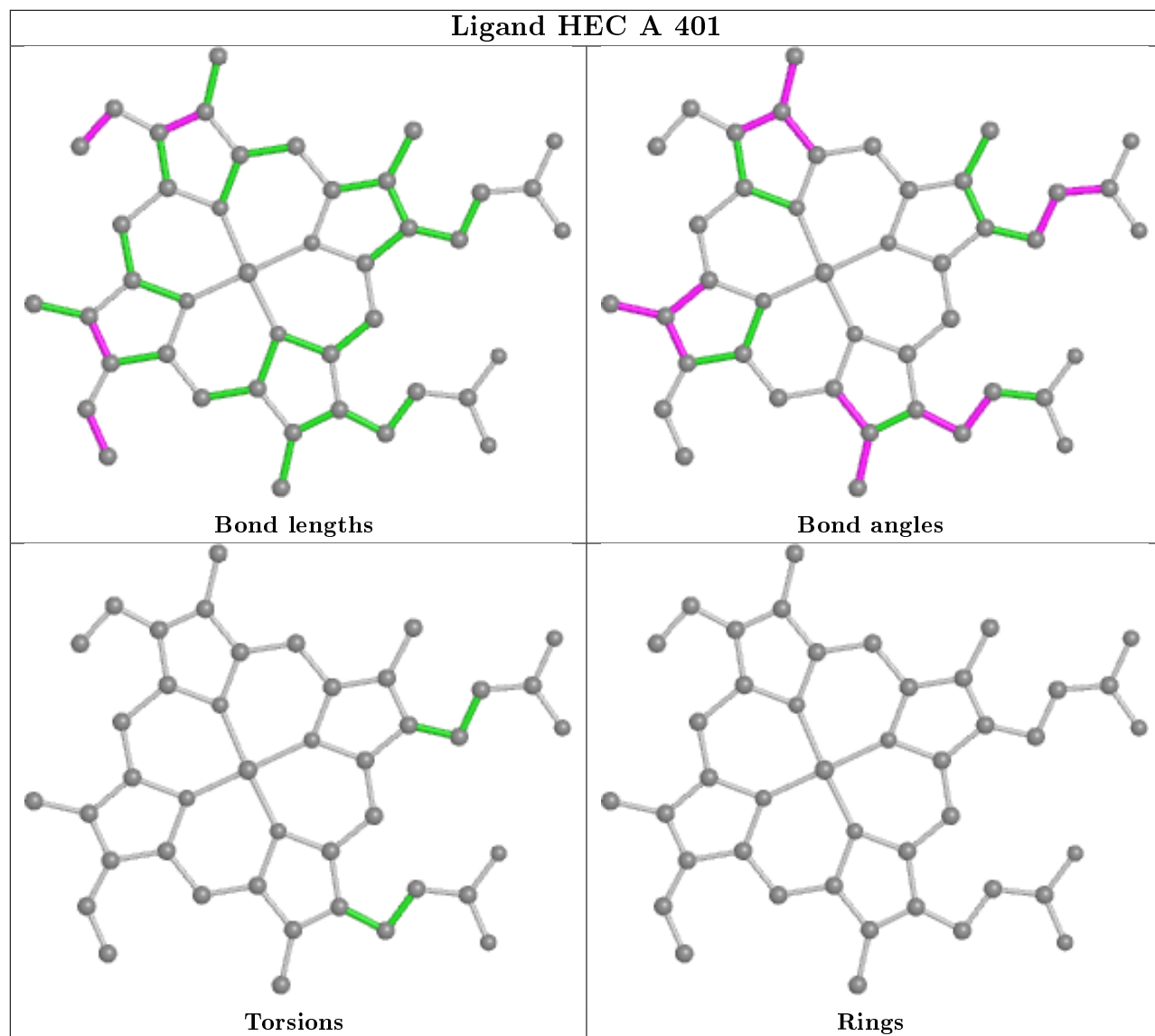
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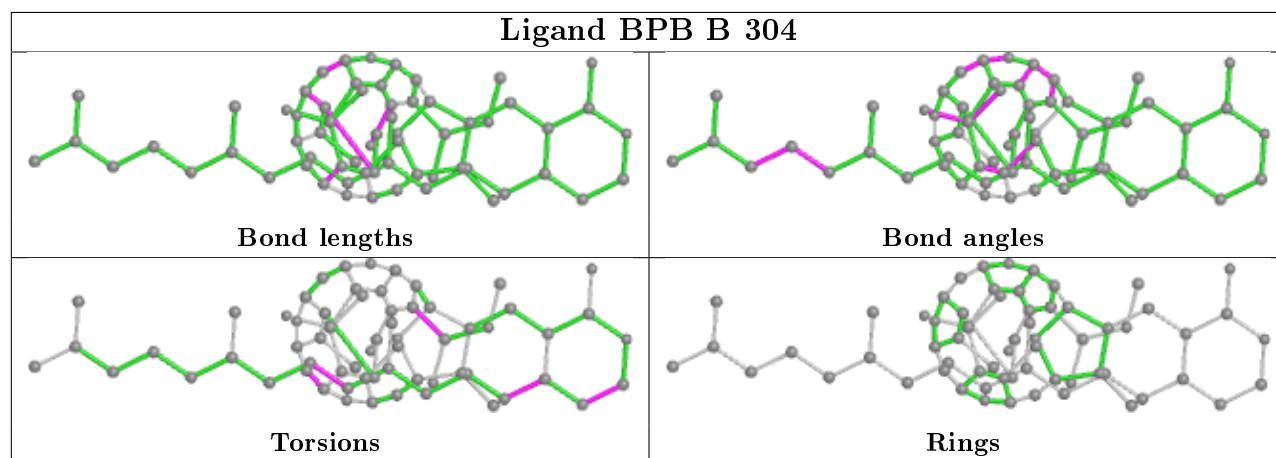
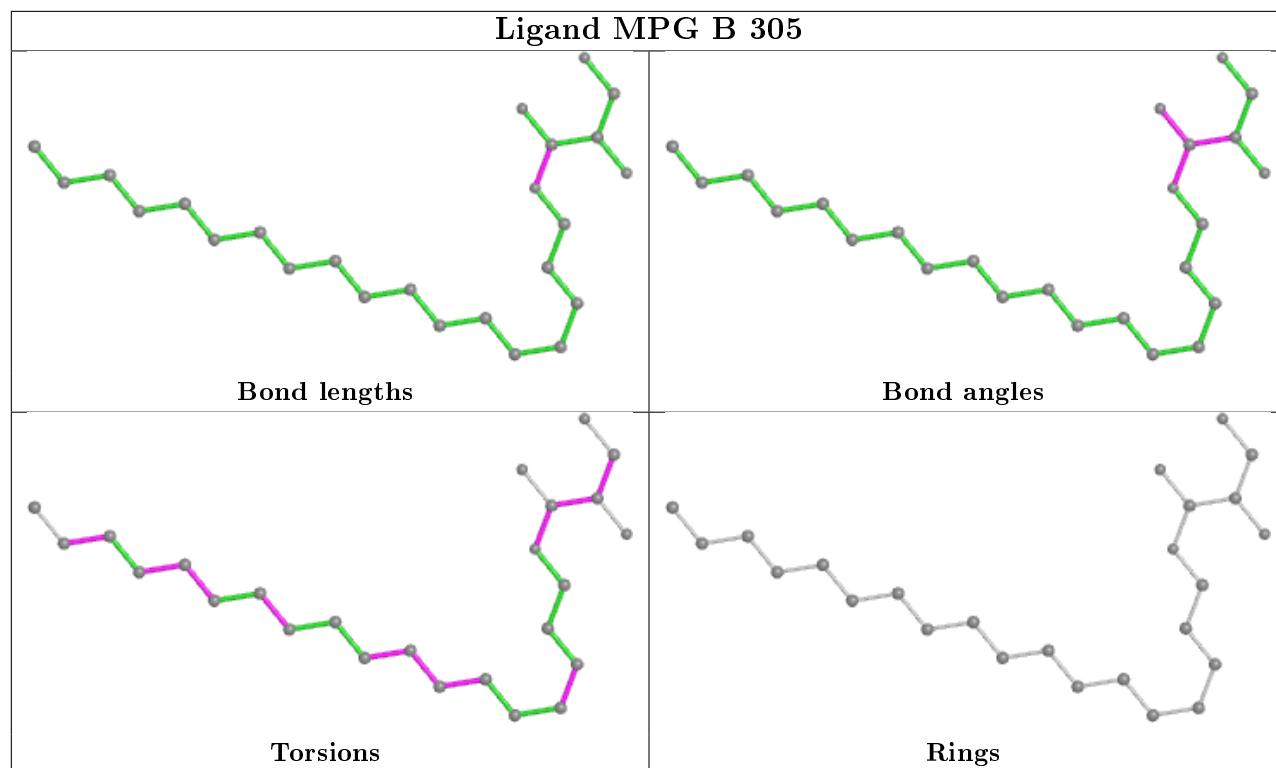
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	C	404	MQ7	1	0
5	A	402	HEC	3	0
5	A	403	HEC	6	0
8	C	402	BPB	1	0
5	A	404	HEC	3	0
13	C	406	OTP	2	0

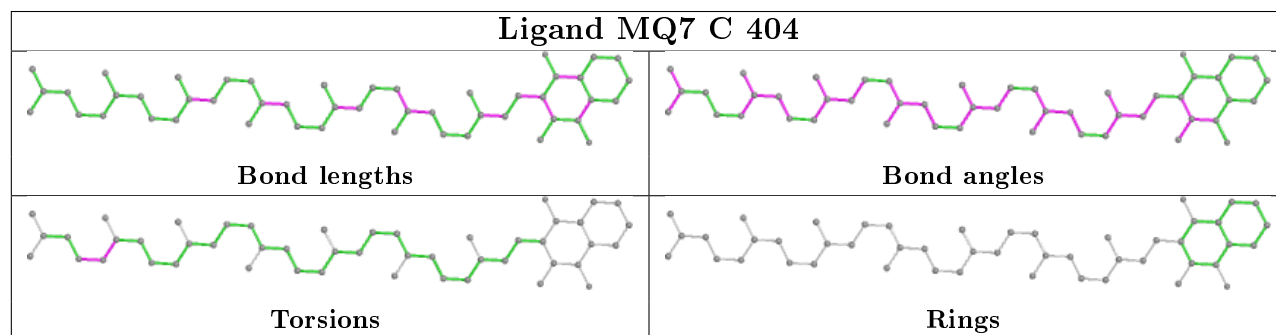
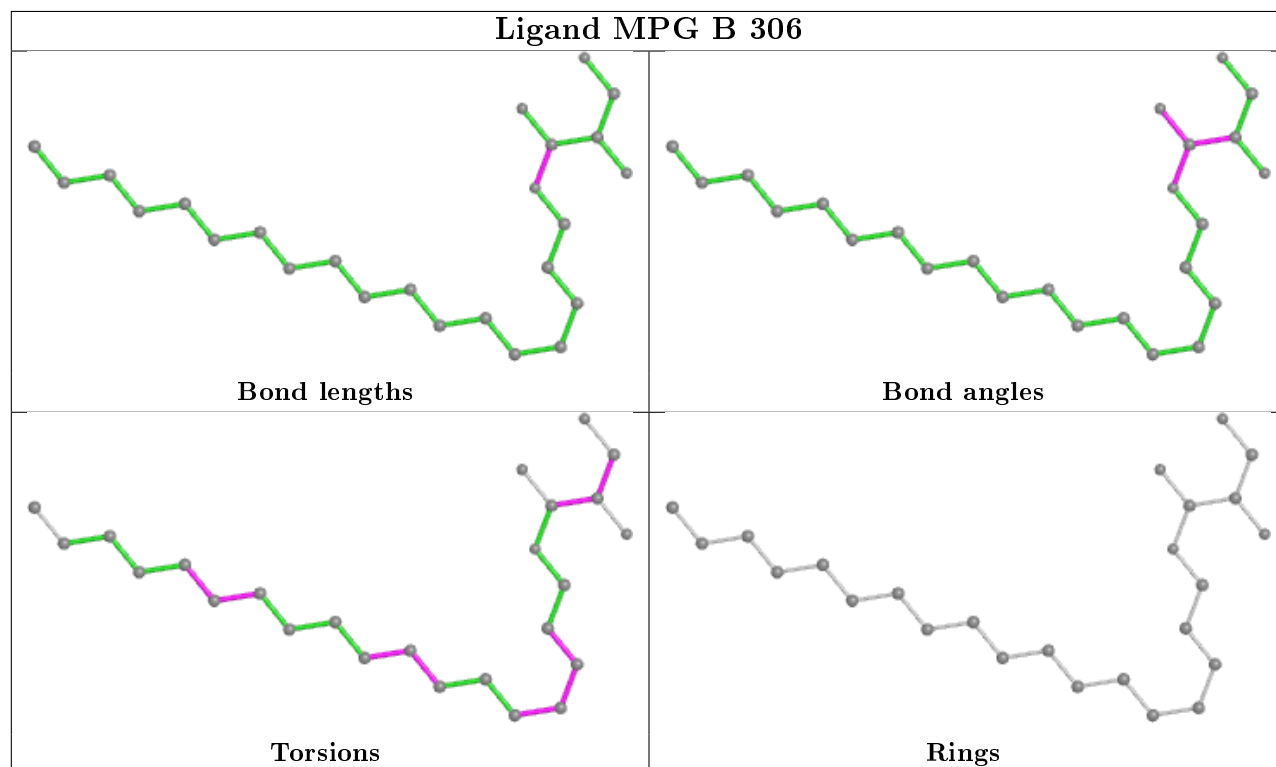
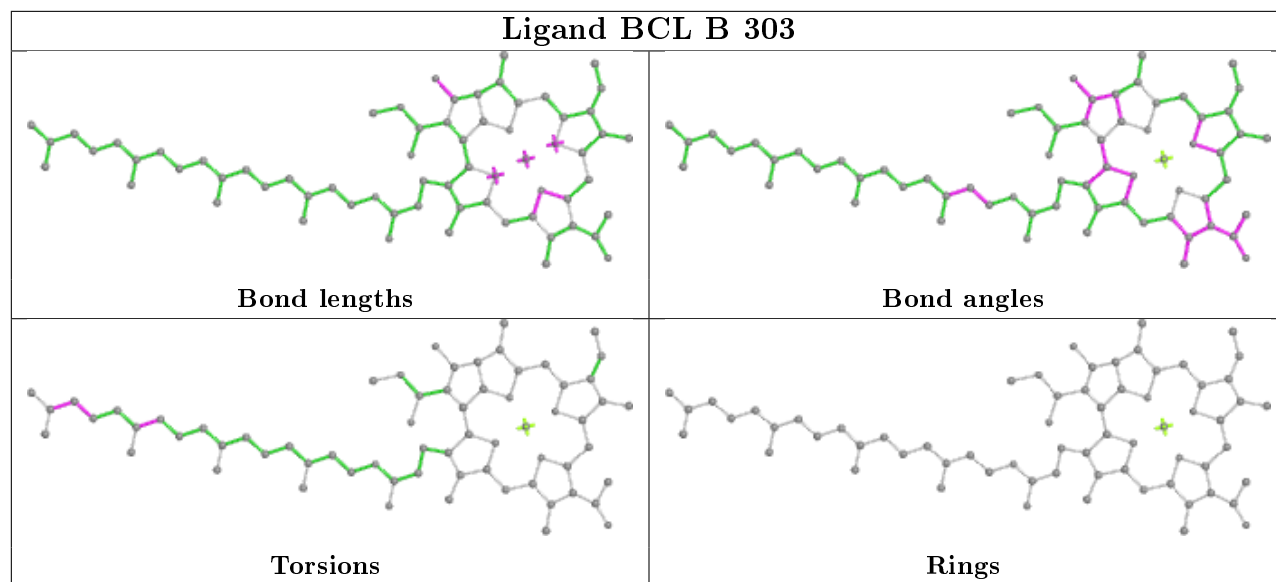
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

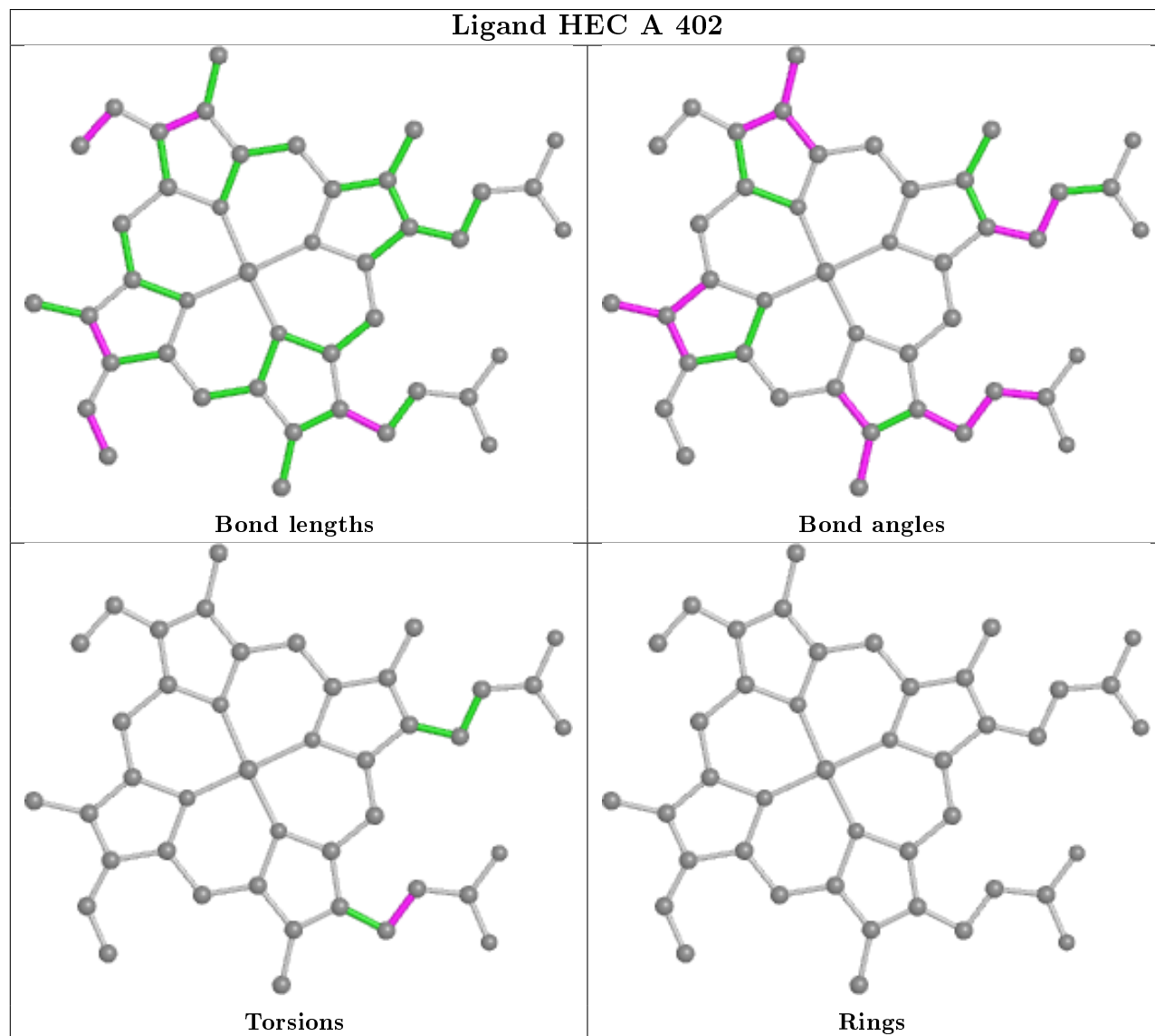
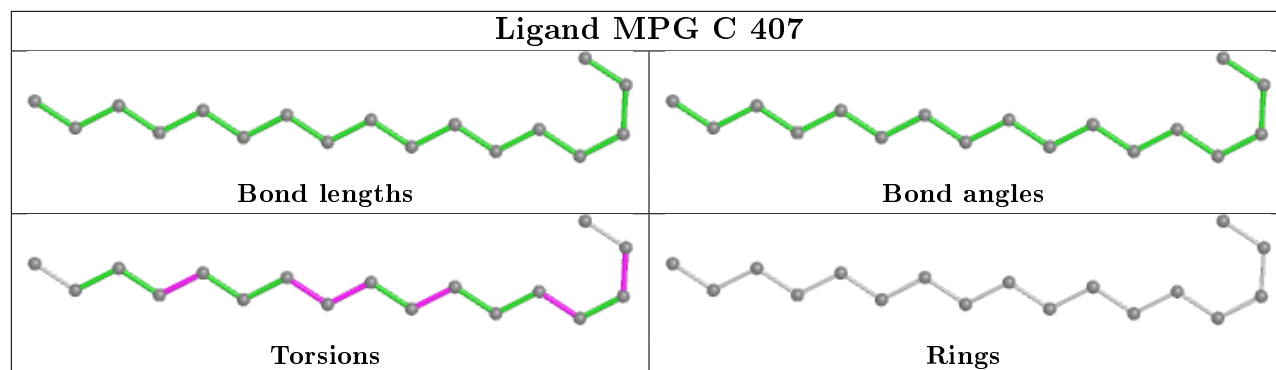




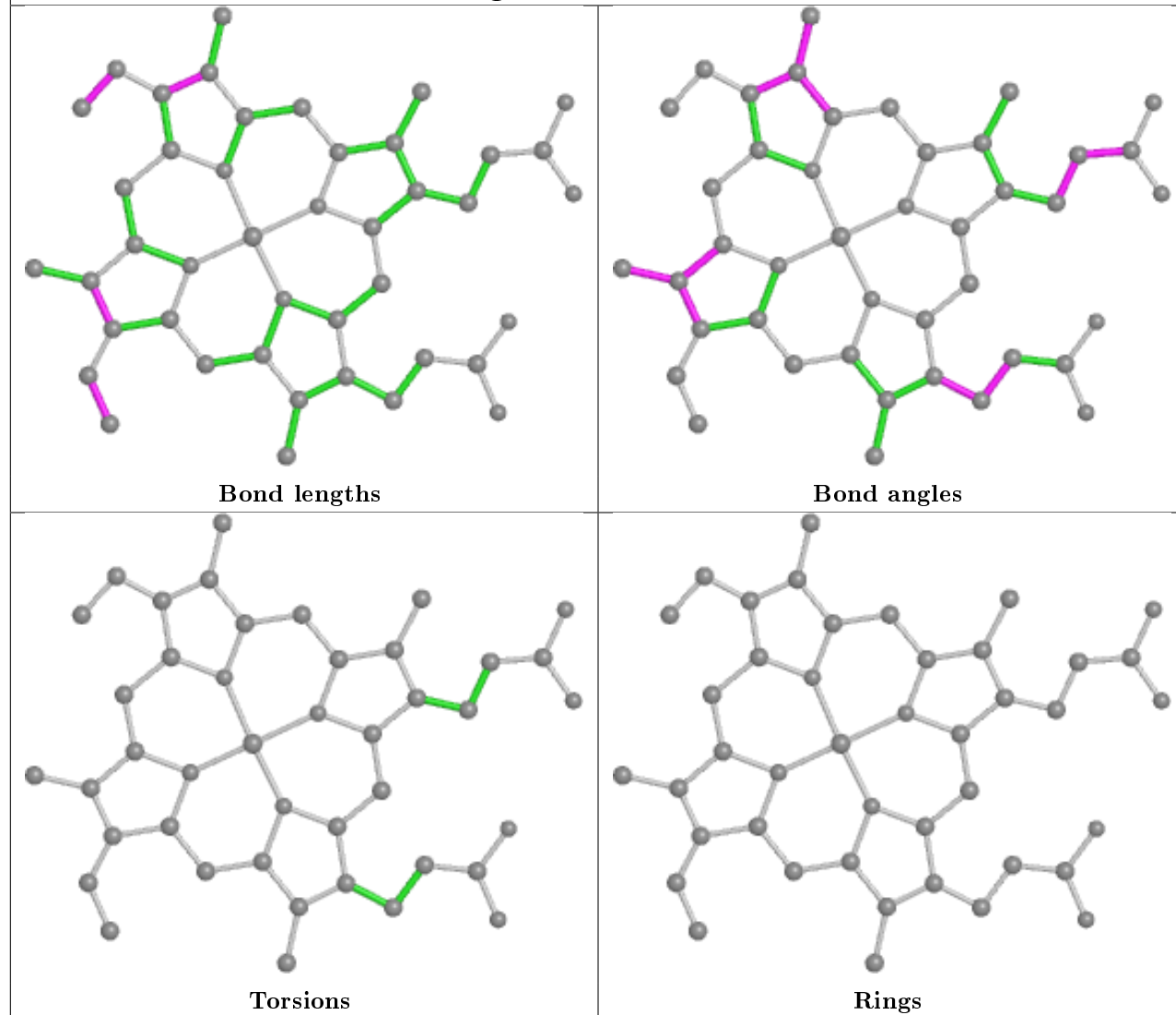




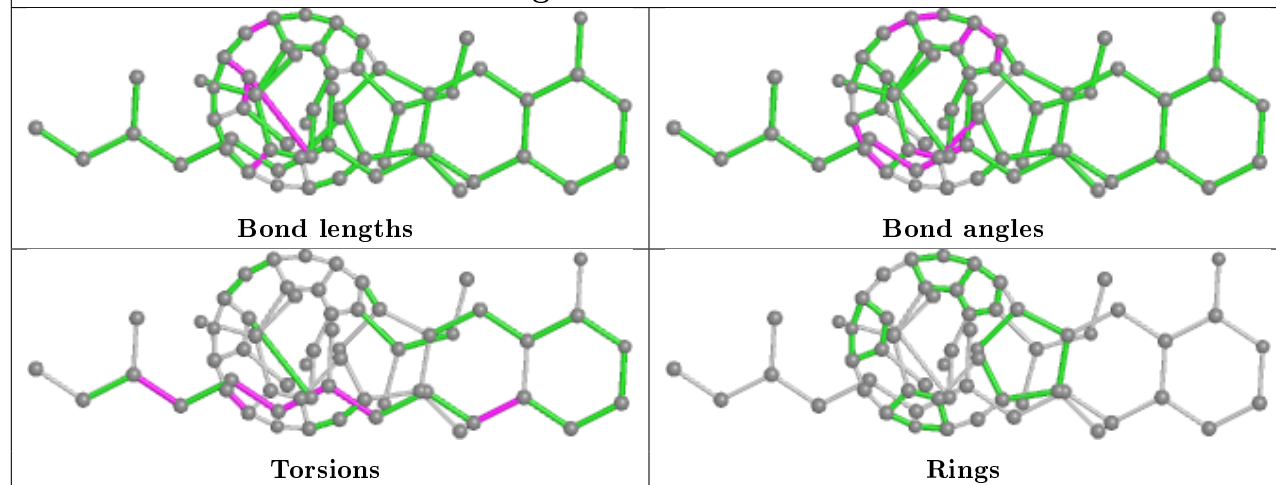


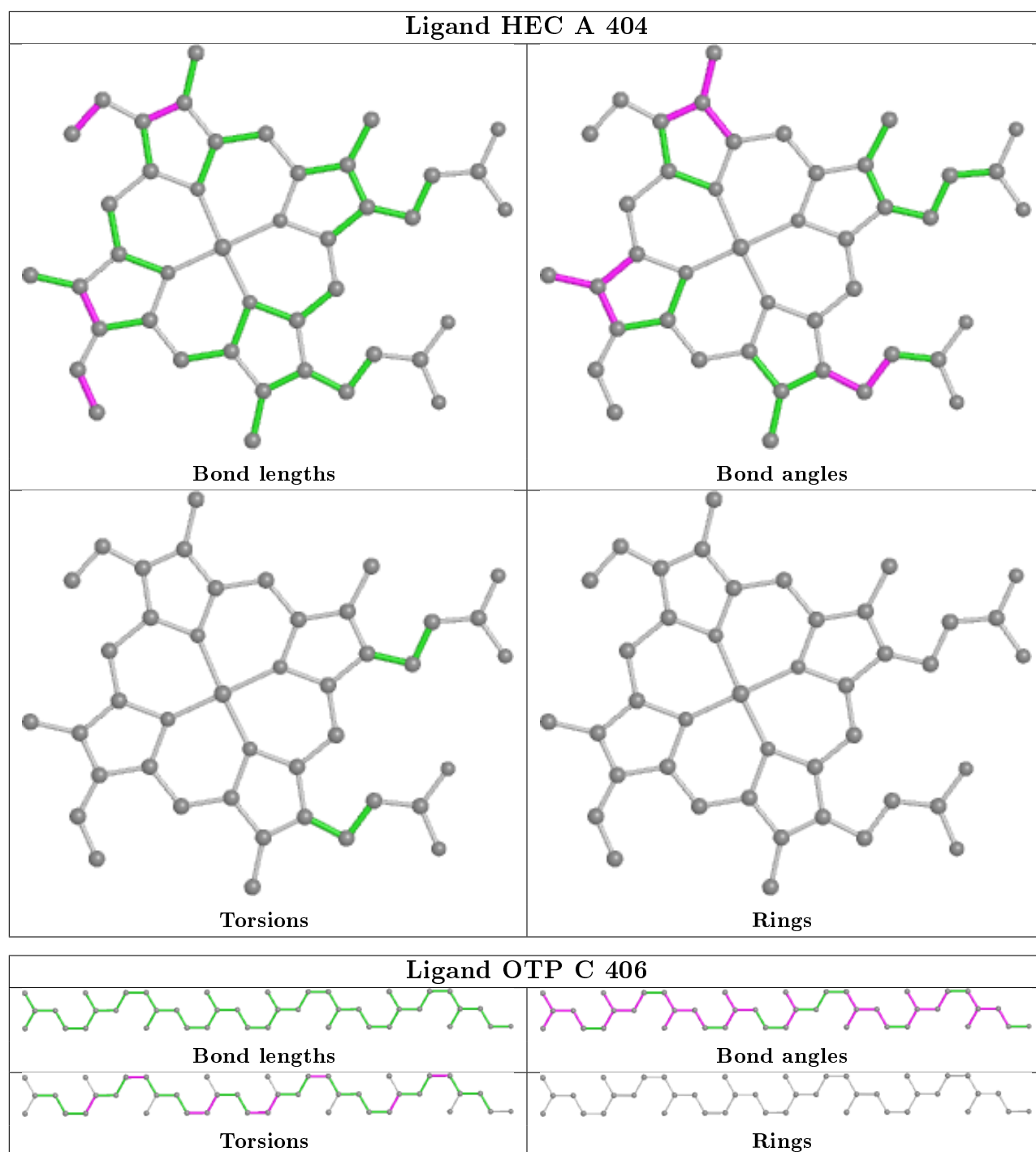


Ligand HEC A 403



Ligand BPB C 402





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	332/356 (93%)	-0.35	1 (0%) 94 91	30, 44, 65, 82	0
2	B	273/274 (99%)	-0.32	0 100 100	34, 56, 91, 111	0
3	C	323/324 (99%)	-0.20	3 (0%) 84 79	33, 61, 90, 110	0
4	D	242/258 (93%)	0.23	9 (3%) 41 37	53, 96, 116, 147	0
All	All	1170/1212 (96%)	-0.18	13 (1%) 80 75	30, 58, 104, 147	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	85	THR	3.6
4	D	84	GLU	3.1
3	C	24	GLY	3.1
4	D	7	ALA	2.4
4	D	256	SER	2.4
4	D	206	ASP	2.3
1	A	51	PRO	2.3
4	D	93	THR	2.2
3	C	16	HIS	2.1
4	D	9	HIS	2.1
4	D	83	PRO	2.1
4	D	79	PRO	2.1
3	C	27	ASP	2.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	FME	D	1	10/11	0.87	0.46	57,67,76,92	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

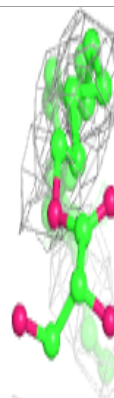
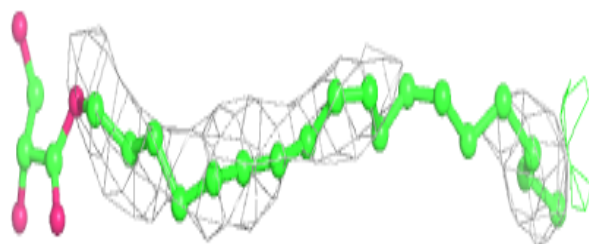
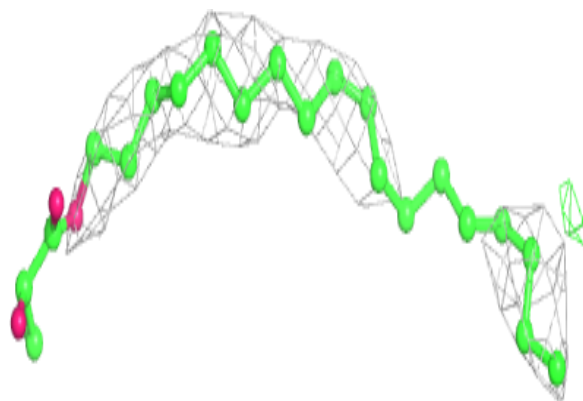
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
9	MPG	B	306	25/25	0.68	0.43	69,82,90,94	3
9	MPG	C	407	17/25	0.71	0.49	73,81,109,112	8
12	NS5	C	405	40/40	0.82	0.36	47,68,89,96	9
13	OTP	C	406	41/49	0.83	0.32	45,67,80,85	0
8	BPB	C	402	61/65	0.91	0.29	52,64,78,80	0
11	MQ7	C	404	48/48	0.91	0.30	43,63,70,72	0
14	PO4	C	409	5/5	0.91	0.25	95,95,101,106	0
9	MPG	B	305	25/25	0.92	0.30	64,91,97,99	22
5	HEC	A	401	43/43	0.94	0.30	42,49,54,57	0
8	BPB	B	304	65/65	0.94	0.22	38,47,56,57	0
10	FE2	C	403	1/1	0.95	0.10	67,67,67,67	0
7	BCL	B	301	65/66	0.95	0.20	42,50,158,164	15
7	BCL	B	303	66/66	0.96	0.20	34,40,47,52	0
5	HEC	A	403	43/43	0.96	0.23	24,35,39,45	0
5	HEC	A	404	43/43	0.96	0.20	36,43,50,53	0
5	HEC	A	402	43/43	0.96	0.27	39,44,48,62	0
14	PO4	C	408	5/5	-	-	81,82,84,85	5
6	DGA	A	405	37/44	0.75	0.39	50,71,91,92	5
7	BCL	B	302	66/66	0.94	0.23	40,45,52,58	0
7	BCL	C	401	66/66	0.94	0.24	41,45,58,60	0

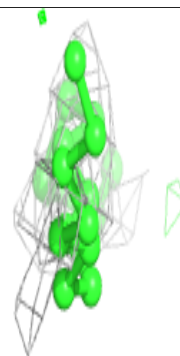
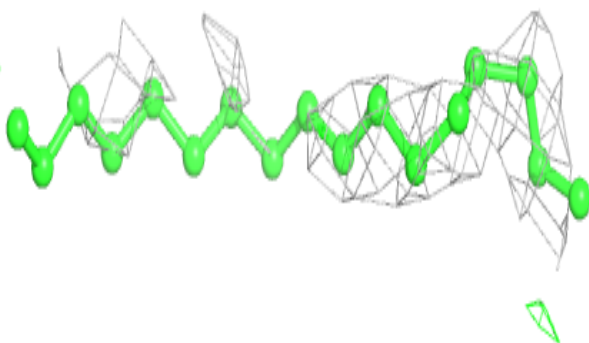
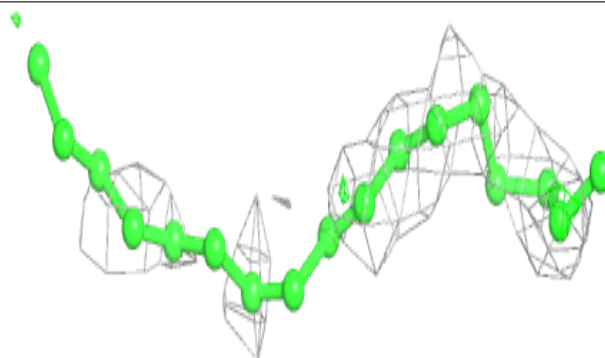
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around MPG 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)

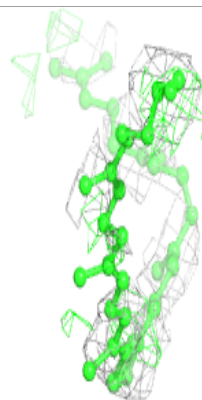
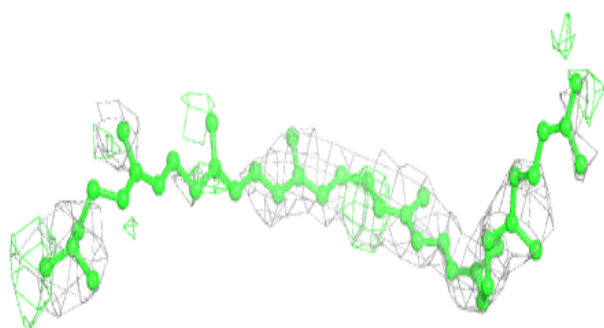
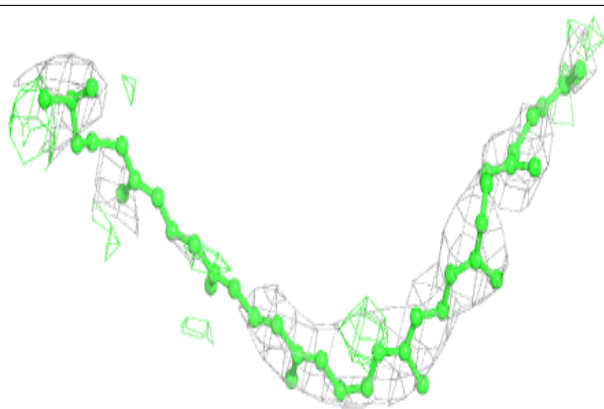
**Electron density around MPG C 407:**

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

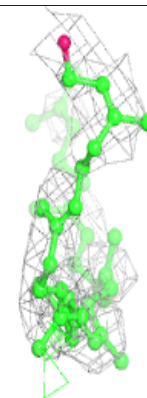
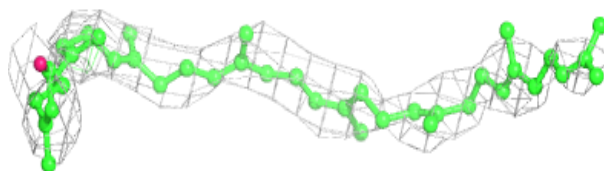
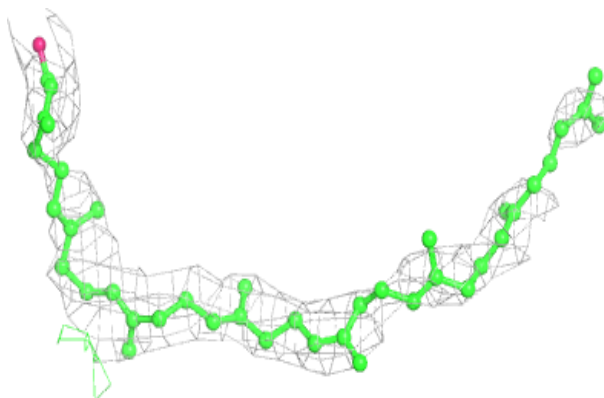


Electron density around NS5 C 405:

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

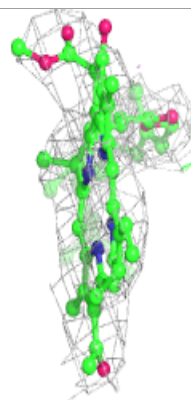
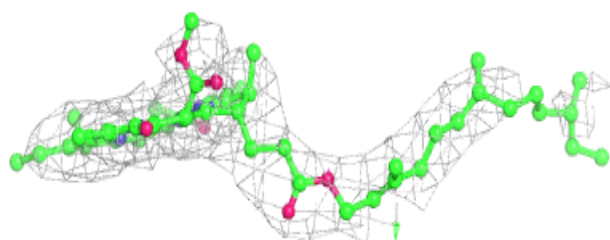
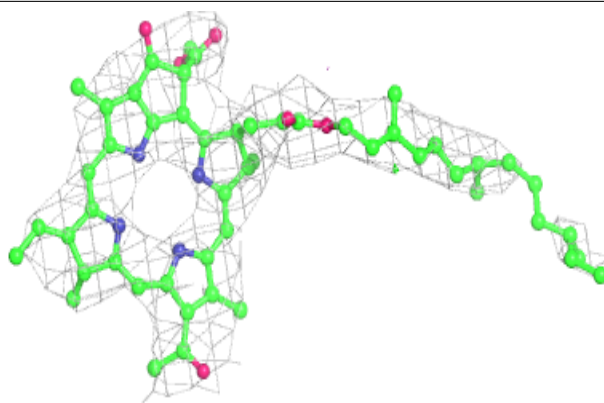
**Electron density around OTP C 406:**

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

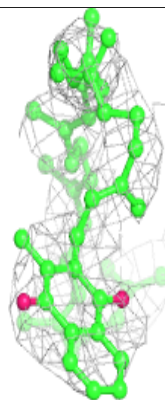
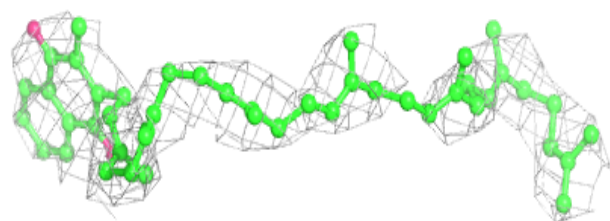
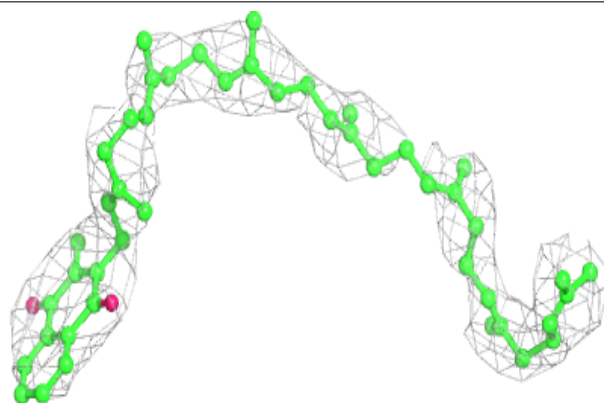


Electron density around BPB C 402:

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

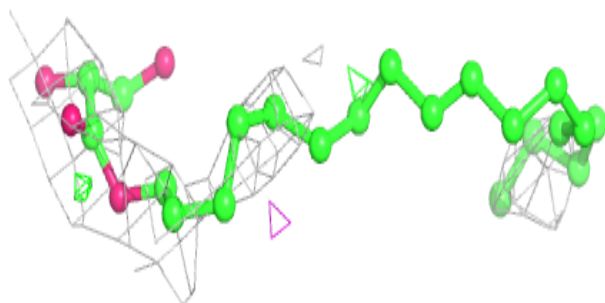
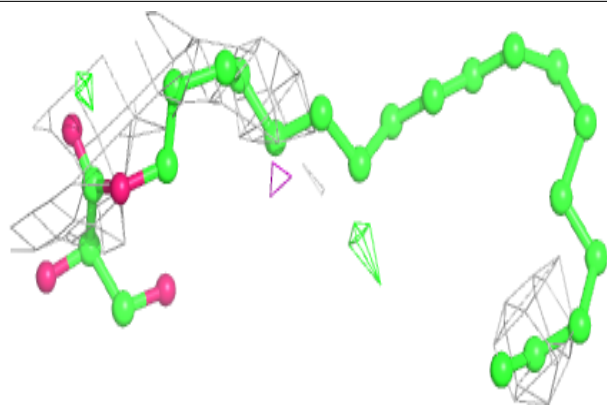
**Electron density around MQ7 C 404:**

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

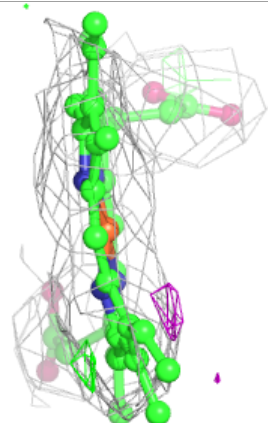
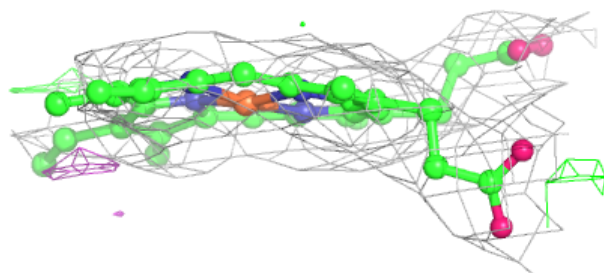
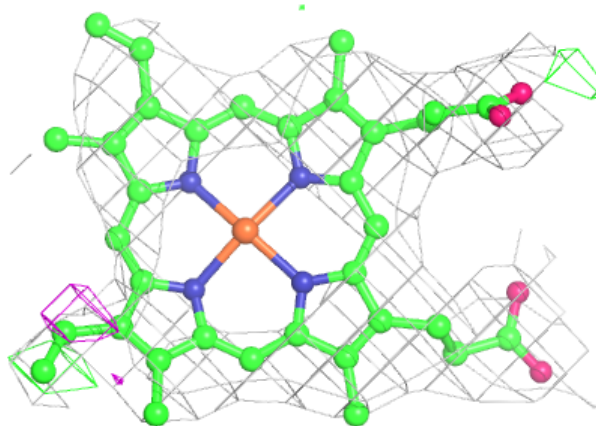


Electron density around MPG B 305:

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

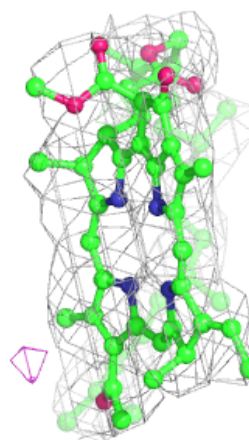
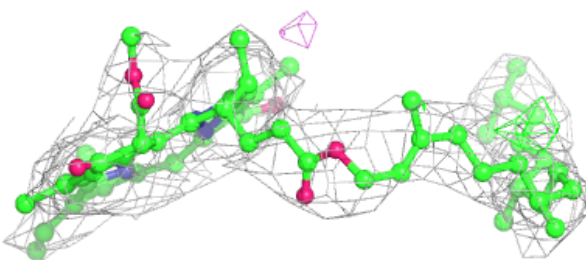
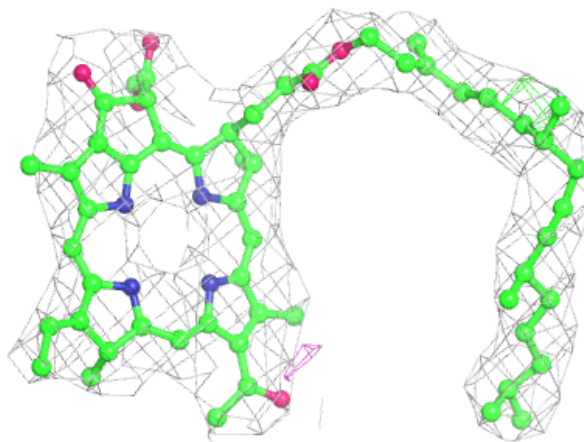
**Electron density around HEC A 401:**

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



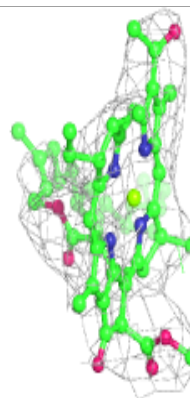
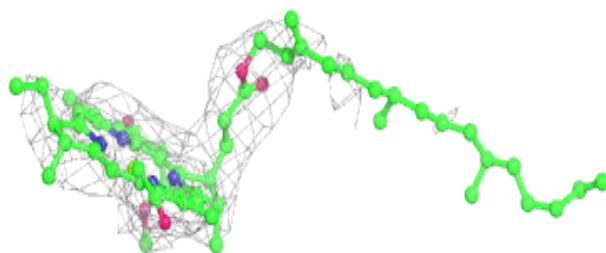
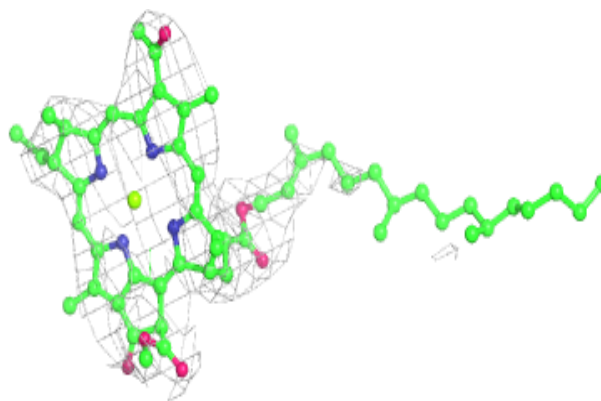
Electron density around BPB B 304:

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

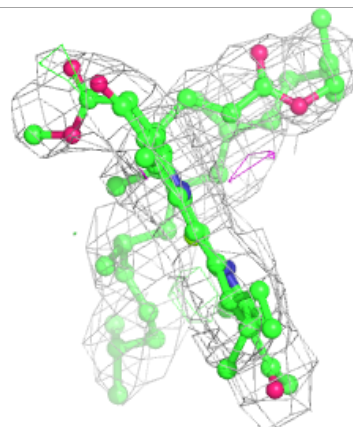
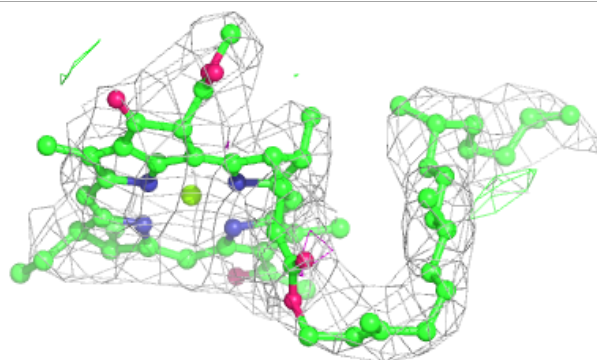
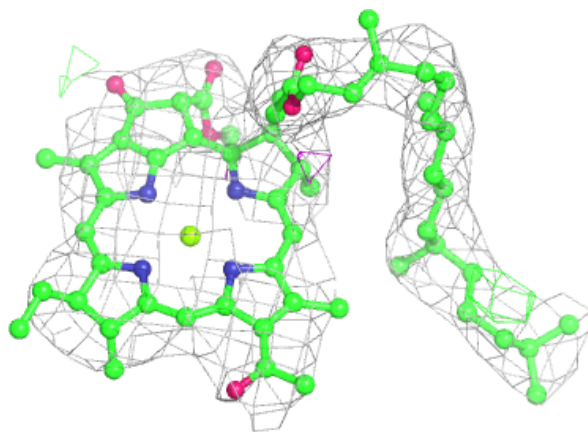


Electron density around BCL B 301:

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

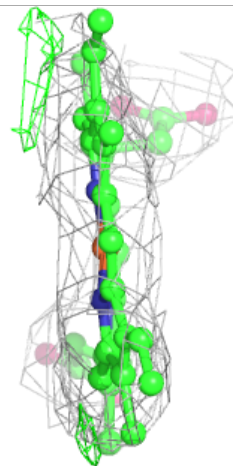
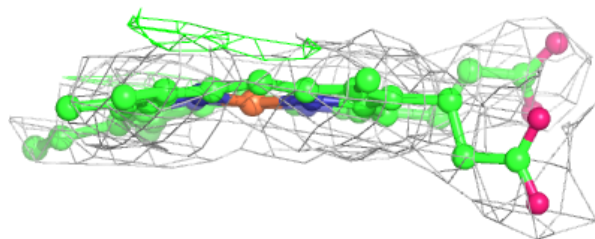
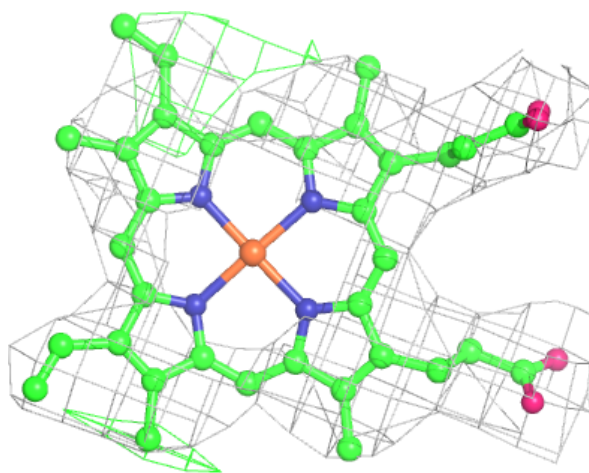
**Electron density around BCL B 303:**

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



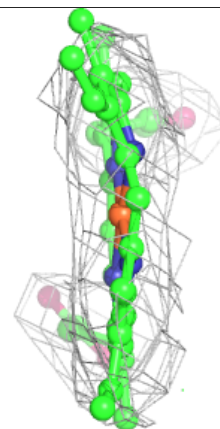
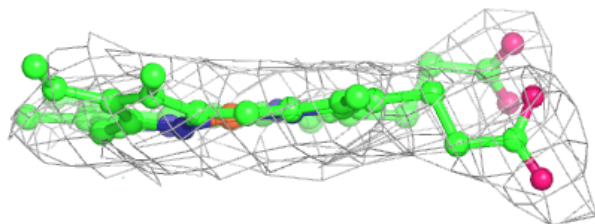
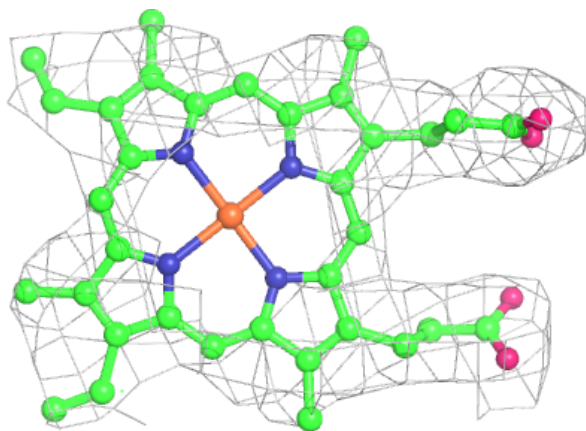
Electron density around HEC A 403:

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



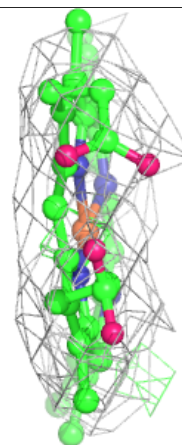
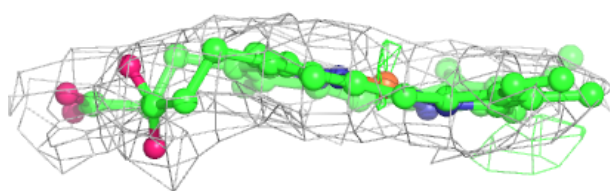
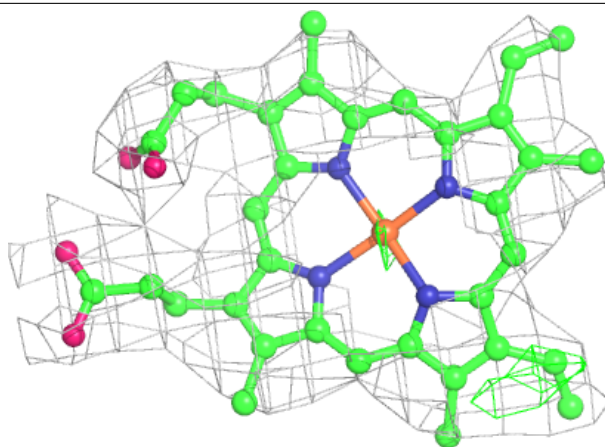
Electron density around HEC A 404:

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



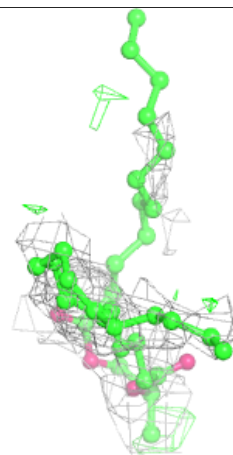
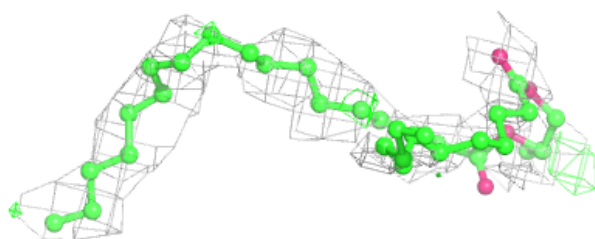
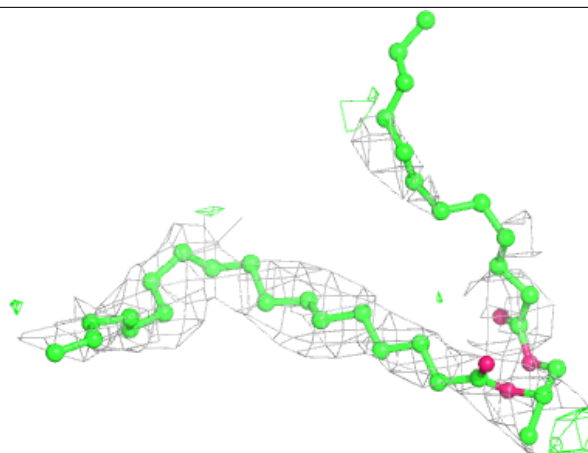
Electron density around HEC A 402:

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

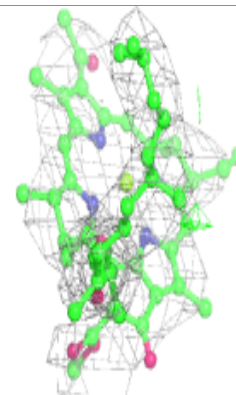
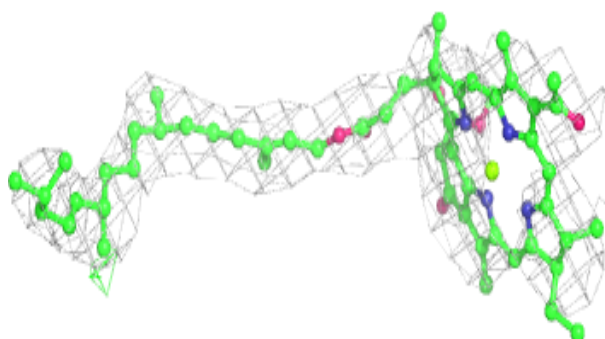
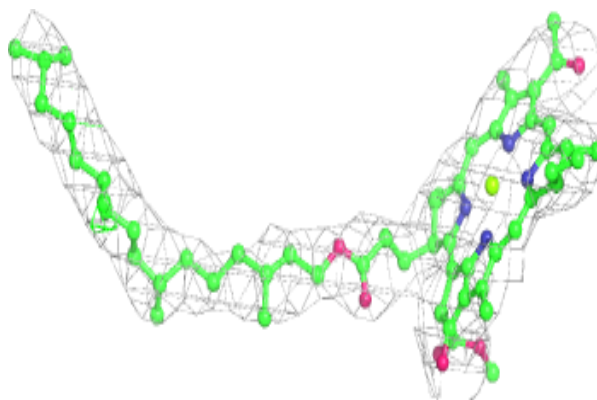


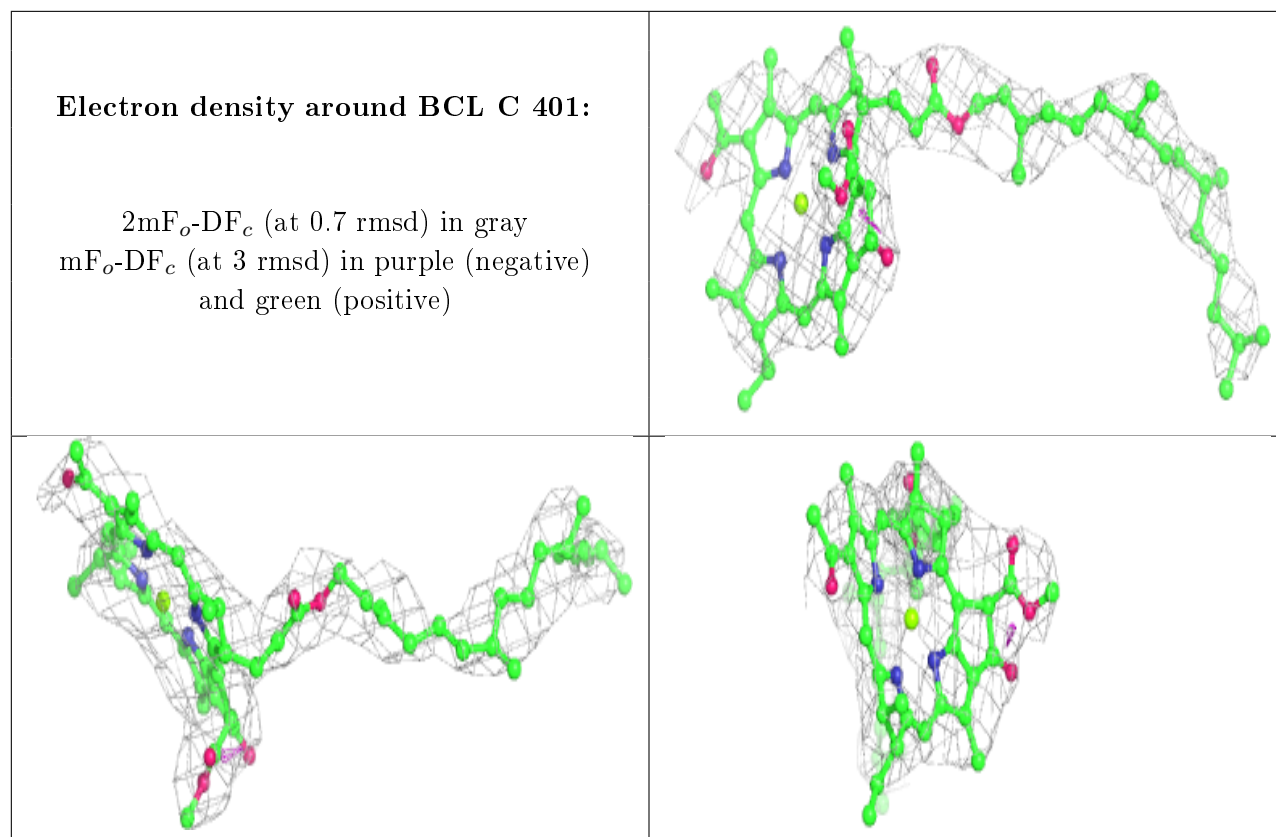
Electron density around DGA A 405:

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

**Electron density around 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.