Full wwPDB X-ray Structure Validation Report (i)

Aug 18, 2026 – 11:05 am BST

PDB ID	:	5O4C / pdb_00005o4c
Title	:	From macrocrystals to microcrystals: a strategy for membrane protein serial crystallography
Authors	:	Dods, R.; Baath, P.; Branden, G.; Neutze, R.
Deposited on	:	2017-05-28
Resolution	:	2.80 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 (i) 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 (i)) were used in the production of this report:

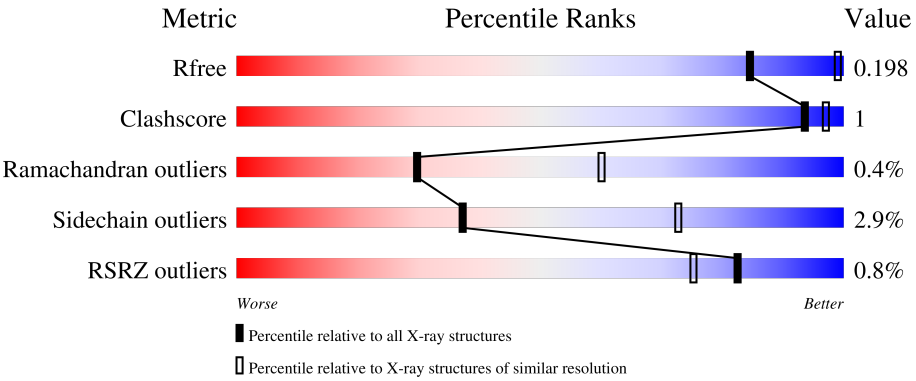
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C	336	95%
2	H	258	2% 93% 6%
3	L	273	97%
4	M	323	93% 7%

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
10	BCB	L	301	X	-	-	-
10	BCB	L	302	X	-	-	-
10	BCB	M	403	X	-	-	-
10	BCB	M	404	X	-	-	-
5	HEC	C	401	X	-	-	-
5	HEC	C	402	X	-	-	-
5	HEC	C	403	X	-	-	-
5	HEC	C	404	X	-	-	-

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 10196 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosynthetic reaction center cytochrome c subunit.

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

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

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

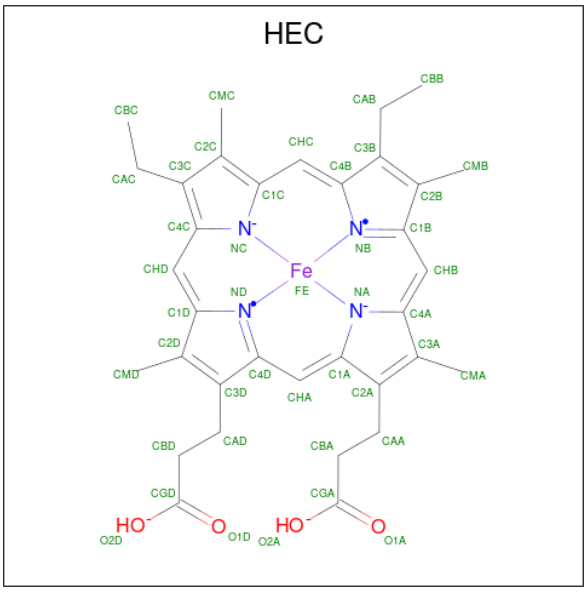
- Molecule 3 is a protein called Reaction center protein L chain.

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

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

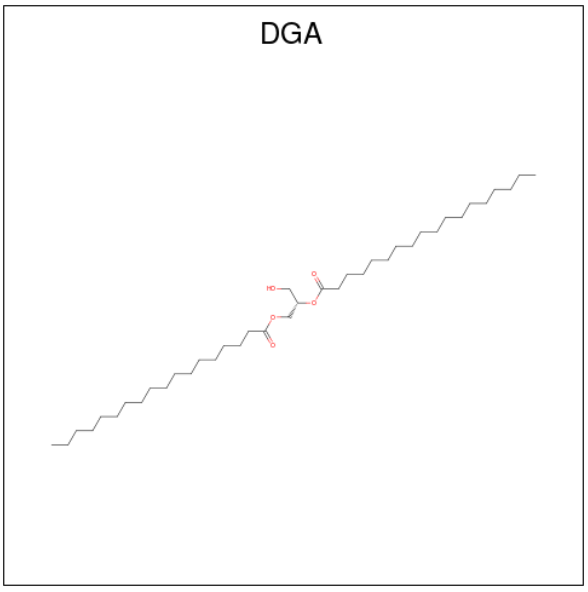
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	323	Total	C	N	O	S	0	0	0
			2555	1702	419	423	11			

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



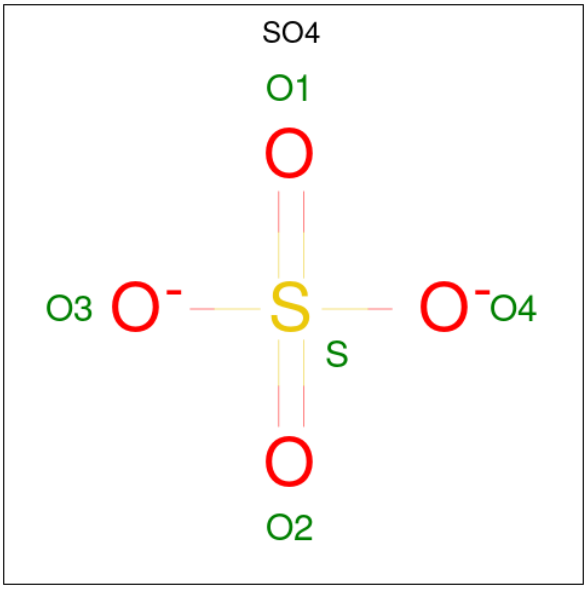
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



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

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



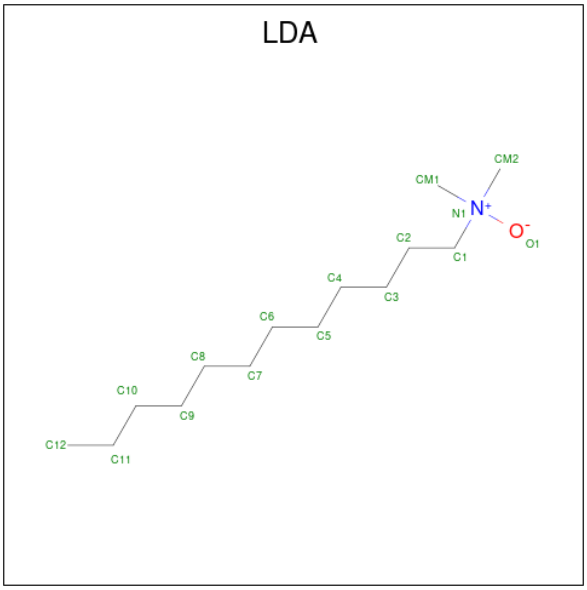
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total O S 5 4 1	0	0
7	H	1	Total O S 5 4 1	0	0
7	H	1	Total O S 5 4 1	0	0
7	H	1	Total O S 5 4 1	0	0
7	H	1	Total O S 5 4 1	0	0
7	M	1	Total O S 5 4 1	0	0
7	M	1	Total O S 5 4 1	0	0
7	M	1	Total O S 5 4 1	0	0
7	M	1	Total O S 5 4 1	0	0
7	M	1	Total O S 5 4 1	0	0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

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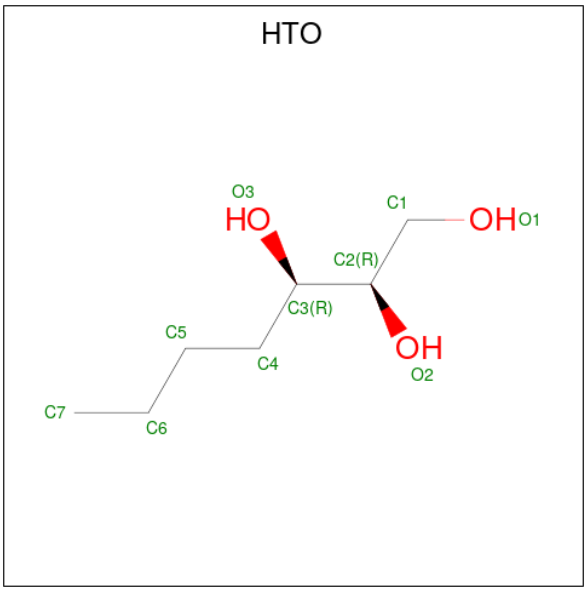
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	M	1	Total O S 5 4 1	0	0

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



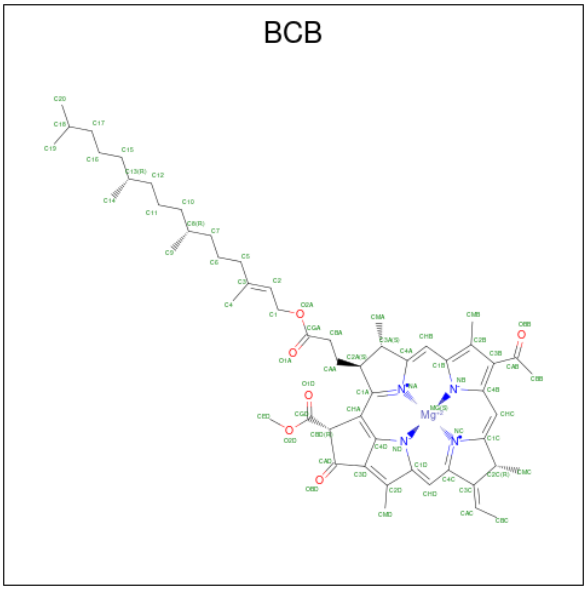
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	H	1	Total C N O 16 14 1 1	0	0
8	H	1	Total C N O 16 14 1 1	0	0
8	H	1	Total C N O 16 14 1 1	0	0
8	L	1	Total C N O 16 14 1 1	0	0

- Molecule 9 is HEPTANE-1,2,3-TRIOL (CCD ID: HTO) (formula: $C_7H_{16}O_3$).



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

- Molecule 10 is BACTERIOCHLOROPHYLL B (CCD ID: BCB) (formula: $C_{55}H_{72}MgN_4O_6$).



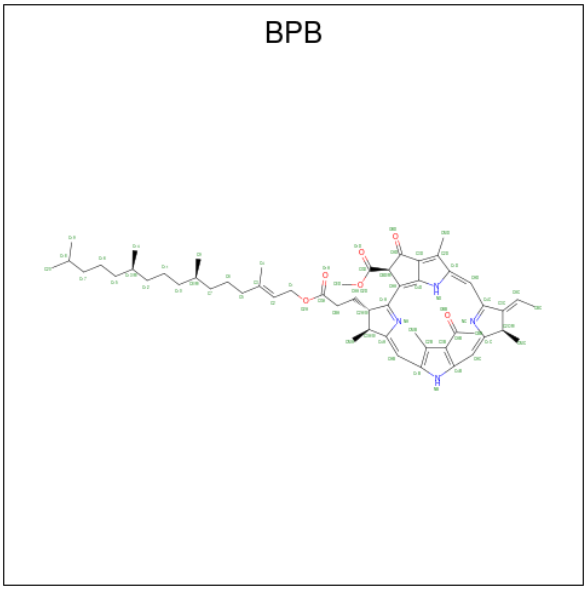
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	L	1	Total C Mg N O 66 55 1 4 6	0	0
10	L	1	Total C Mg N O 66 55 1 4 6	0	0

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

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

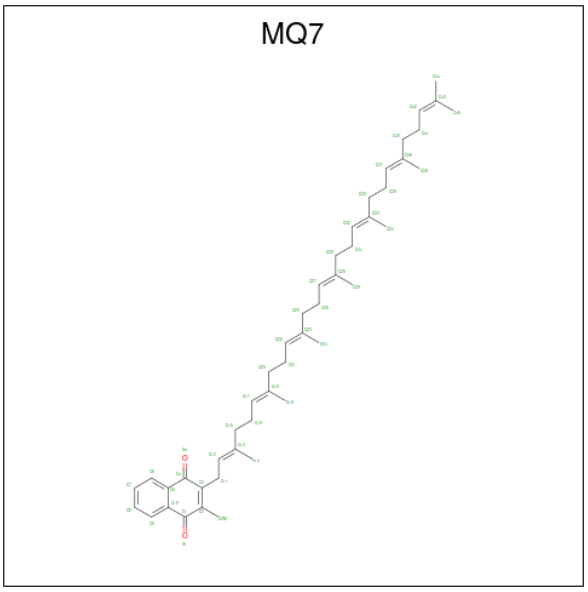


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	L	1	Total	C	N	O	0	0
			65	55	4	6		
11	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 12 is FE (II) ION (CCD ID: FE2) (formula: Fe).

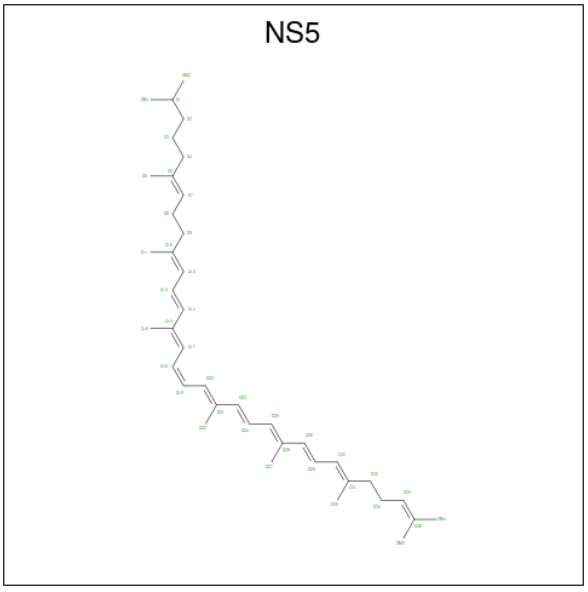
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	M	1	Total	Fe	0	0
			1	1		

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



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

- Molecule 14 is 15-cis-1,2-dihydroneurosporene (CCD ID: NS5) (formula: $C_{40}H_{60}$).



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

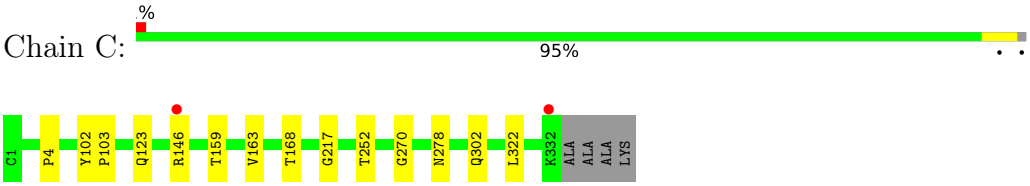
- Molecule 15 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	C	3	Total O 3 3	0	0
15	H	2	Total O 2 2	0	0
15	L	4	Total O 4 4	0	0
15	M	4	Total O 4 4	0	0

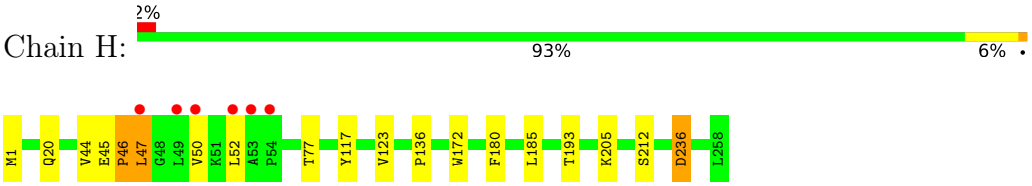
3 Residue-property plots (i)

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.

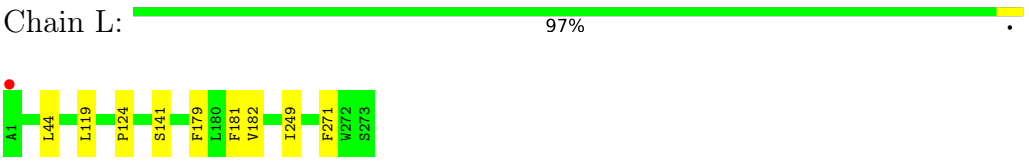
• Molecule 1: Photosynthetic reaction center cytochrome c subunit



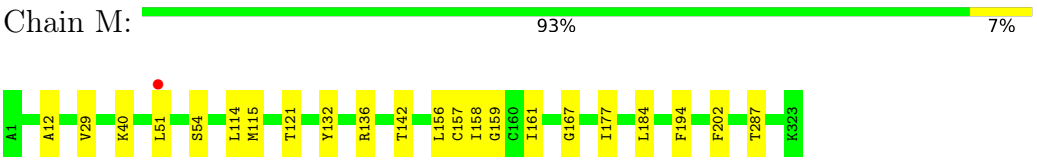
• Molecule 2: Reaction center protein H chain



• Molecule 3: Reaction center protein L chain



• Molecule 4: Reaction center protein M chain



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	226.40Å 226.40Å 113.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.90 – 2.80 36.90 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (36.90-2.80) 99.9 (36.90-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.42 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.165 , 0.196 0.172 , 0.198	Depositor DCC
R_{free} test set	3626 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	102.2	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 59.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	10196	wwPDB-VP
Average B, all atoms (Å^2)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.91% 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: HTO, SO4, HEC, MQ7, LDA, FME, BCB, DGA, FE2, NS5, BPB

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	C	0.65	0/2669	0.89	1/3637 (0.0%)
2	H	0.70	0/2055	0.89	0/2807
3	L	0.66	0/2267	0.88	0/3095
4	M	0.65	0/2659	0.89	0/3637
All	All	0.66	0/9650	0.89	1/13176 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	4	PRO	N-CA-C	5.46	116.42	110.58

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	C	2602	0	2578	6	0
2	H	2018	0	2020	5	0
3	L	2172	0	2097	4	0
4	M	2555	0	2452	10	0
5	C	172	0	120	1	0
6	C	37	0	58	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	5	0	0	0	0
7	H	20	0	0	0	0
7	M	35	0	0	0	0
8	H	48	0	93	0	0
8	L	16	0	31	0	0
9	H	10	0	16	0	0
9	L	10	0	16	0	0
10	L	132	0	144	1	0
10	M	132	0	144	4	0
11	L	65	0	74	2	0
11	M	65	0	74	3	0
12	M	1	0	0	0	0
13	M	48	0	64	0	0
14	M	40	0	60	4	0
15	C	3	0	0	0	0
15	H	2	0	0	0	0
15	L	4	0	0	0	0
15	M	4	0	0	0	0
All	All	10196	0	10041	29	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (29) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:159:GLY:HA3	14:M:406:NS5:H272	1.80	0.63
11:M:405:BPB:HHC	11:M:405:BPB:HBBB	1.82	0.61
10:M:403:BCB:HHC	10:M:403:BCB:HBB2	1.84	0.59
3:L:124:PRO:HD3	11:L:303:BPB:HAC	1.87	0.55
4:M:184:LEU:CD2	10:M:403:BCB:HBC3	2.37	0.54
4:M:121:THR:HG23	4:M:156:LEU:HD21	1.90	0.53
4:M:184:LEU:HD21	10:M:403:BCB:HBC3	1.89	0.53
10:L:302:BCB:HMB3	10:L:302:BCB:HBB2	1.91	0.51
2:H:180:PHE:CE2	4:M:12:ALA:HB2	2.47	0.50
1:C:278:ASN:HB3	1:C:302:GLN:HE21	1.77	0.50
1:C:102:TYR:CG	1:C:103:PRO:HD3	2.49	0.48
11:L:303:BPB:HBBB	11:L:303:BPB:HMB	1.97	0.47
2:H:117:TYR:HB2	2:H:236:ASP:HB3	1.97	0.46
3:L:181:PHE:HB3	11:M:405:BPB:CBB	2.46	0.46
2:H:20:GLN:HG2	4:M:202:PHE:CE2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:157:CYS:HA	4:M:161:ILE:HB	1.97	0.45
3:L:181:PHE:CD2	11:M:405:BPB:HBB	2.51	0.45
2:H:136:PRO:HA	2:H:172:TRP:HA	1.98	0.45
1:C:270:GLY:C	5:C:404:HEC:HBB2	2.42	0.44
1:C:102:TYR:CD2	1:C:103:PRO:HD3	2.53	0.44
2:H:45:GLU:HG3	2:H:46:PRO:HD2	1.99	0.44
3:L:179:PHE:HA	3:L:182:VAL:HG12	2.00	0.44
10:M:403:BCB:HBB3	10:M:404:BCB:H62	1.99	0.43
1:C:163:VAL:HA	1:C:168:THR:HG21	2.01	0.43
14:M:406:NS5:H13	14:M:406:NS5:H111	1.89	0.42
1:C:217:GLY:HA2	4:M:167:GLY:O	2.21	0.41
14:M:406:NS5:H29	14:M:406:NS5:H271	1.86	0.41
4:M:114:LEU:HD11	14:M:406:NS5:H351	2.02	0.41
4:M:132:TYR:CE2	4:M:142:THR:HG21	2.56	0.41

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	330/336 (98%)	316 (96%)	14 (4%)	0	100	100
2	H	256/258 (99%)	244 (95%)	9 (4%)	3 (1%)	10	34
3	L	272/273 (100%)	259 (95%)	12 (4%)	1 (0%)	30	60
4	M	321/323 (99%)	311 (97%)	9 (3%)	1 (0%)	36	66
All	All	1179/1190 (99%)	1130 (96%)	44 (4%)	5 (0%)	30	60

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	47	LEU

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Mol	Chain	Res	Type
3	L	271	PHE
2	H	46	PRO
2	H	50	VAL
4	M	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	C	281/282 (100%)	276 (98%)	5 (2%)	51 82
2	H	212/212 (100%)	202 (95%)	10 (5%)	23 57
3	L	219/218 (100%)	215 (98%)	4 (2%)	51 82
4	M	249/249 (100%)	240 (96%)	9 (4%)	31 66
All	All	961/961 (100%)	933 (97%)	28 (3%)	37 73

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	123	GLN
1	C	146	ARG
1	C	159	THR
1	C	252	THR
1	C	322	LEU
2	H	44	VAL
2	H	47	LEU
2	H	52	LEU
2	H	77	THR
2	H	123	VAL
2	H	185	LEU
2	H	193	THR
2	H	205	LYS
2	H	212	SER
2	H	236	ASP
3	L	44	LEU
3	L	119	LEU

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Mol	Chain	Res	Type
3	L	141	SER
3	L	249	ILE
4	M	29	VAL
4	M	40	LYS
4	M	51	LEU
4	M	54	SER
4	M	115	MET
4	M	136	ARG
4	M	158	ILE
4	M	194	PHE
4	M	287	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	95	ASN
1	C	123	GLN
1	C	206	GLN
1	C	263	GLN
1	C	302	GLN
2	H	8	GLN
2	H	102	GLN
2	H	106	ASN
4	M	147	ASN
4	M	200	HIS

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	$\#\|Z\|>2$
2	FME	H	1	2	8,9,10	0.88	0	7,9,11	3.45	2 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FME	H	1	2	-	3/7/9/11	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	1	FME	CA-N-CN	-8.07	110.41	122.82
2	H	1	FME	CE-SD-CG	2.91	110.40	100.40

There are no chirality outliers.

All (3) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 32 ligands modelled in this entry, 1 is monoatomic - leaving 31 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	SO4	M	409	-	4,4,4	0.36	0	6,6,6	0.32	0
5	HEC	C	402	1	50,50,50	1.37	6 (12%)	68,82,82	1.47	11 (16%)
10	BCB	M	404	4	68,74,74	1.98	14 (20%)	79,115,115	2.95	26 (32%)
10	BCB	L	302	3	68,74,74	1.87	15 (22%)	79,115,115	2.68	25 (31%)
7	SO4	H	705	-	4,4,4	0.33	0	6,6,6	0.22	0
8	LDA	H	706	-	12,15,15	2.08	1 (8%)	14,17,17	0.85	1 (7%)
7	SO4	H	702	-	4,4,4	0.36	0	6,6,6	0.50	0
11	BPB	L	303	-	57,70,70	2.52	16 (28%)	56,101,101	2.21	16 (28%)
8	LDA	L	304	-	12,15,15	2.04	1 (8%)	14,17,17	0.41	0
5	HEC	C	404	1	50,50,50	1.43	6 (12%)	68,82,82	1.47	9 (13%)
9	HTO	L	305	-	9,9,9	0.73	0	10,10,10	0.86	0
13	MQ7	M	402	-	49,49,49	1.55	2 (4%)	60,63,63	1.25	6 (10%)
9	HTO	H	708	-	9,9,9	0.57	0	10,10,10	0.51	0
14	NS5	M	406	-	39,39,39	1.51	2 (5%)	44,46,46	1.87	12 (27%)
10	BCB	M	403	4	68,74,74	1.91	15 (22%)	79,115,115	2.76	22 (27%)
7	SO4	M	411	-	4,4,4	0.40	0	6,6,6	0.25	0
7	SO4	H	704	-	4,4,4	0.29	0	6,6,6	0.25	0
6	DGA	C	405	1	36,36,43	1.30	3 (8%)	38,38,45	1.40	4 (10%)
7	SO4	M	412	-	4,4,4	0.39	0	6,6,6	0.33	0
10	BCB	L	301	3	68,74,74	2.03	16 (23%)	79,115,115	2.90	31 (39%)
7	SO4	H	703	-	4,4,4	0.35	0	6,6,6	0.17	0
5	HEC	C	403	1	50,50,50	1.40	6 (12%)	68,82,82	1.76	14 (20%)
7	SO4	M	408	-	4,4,4	0.28	0	6,6,6	0.18	0
7	SO4	C	406	-	4,4,4	0.40	0	6,6,6	0.32	0
7	SO4	M	407	-	4,4,4	0.29	0	6,6,6	0.51	0
11	BPB	M	405	-	57,70,70	2.64	14 (24%)	56,101,101	2.31	18 (32%)
7	SO4	M	410	-	4,4,4	0.41	0	6,6,6	0.33	0
5	HEC	C	401	1	50,50,50	1.41	4 (8%)	68,82,82	1.63	13 (19%)
8	LDA	H	707	-	12,15,15	2.06	1 (8%)	14,17,17	1.16	1 (7%)
8	LDA	H	701	-	12,15,15	1.98	1 (8%)	14,17,17	0.63	0
7	SO4	M	413	-	4,4,4	0.34	0	6,6,6	0.15	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
5	HEC	C	402	1	1/1/3/7	7/14/54/54	-
10	BCB	M	404	4	3/3/21/26	14/41/137/137	-
10	BCB	L	302	3	3/3/21/26	6/41/137/137	-
8	LDA	H	706	-	-	7/13/13/13	-
11	BPB	L	303	-	-	8/37/105/105	0/5/6/6
8	LDA	L	304	-	-	5/13/13/13	-
5	HEC	C	404	1	1/1/3/7	2/14/54/54	-
13	MQ7	M	402	-	-	0/41/61/61	0/2/2/2
9	HTO	L	305	-	-	5/10/10/10	-
14	NS5	M	406	-	-	6/43/43/43	-
9	HTO	H	708	-	-	1/10/10/10	-
10	BCB	M	403	4	3/3/21/26	16/41/137/137	-
10	BCB	L	301	3	3/3/21/26	7/41/137/137	-
6	DGA	C	405	1	-	15/37/37/45	-
5	HEC	C	403	1	1/1/3/7	4/14/54/54	-
11	BPB	M	405	-	-	7/37/105/105	0/5/6/6
5	HEC	C	401	1	1/1/3/7	8/14/54/54	-
8	LDA	H	707	-	-	10/13/13/13	-
8	LDA	H	701	-	-	3/13/13/13	-

All (123) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	M	405	BPB	C1B-C2B	8.84	1.49	1.39
11	L	303	BPB	C1B-C2B	8.17	1.48	1.39
13	M	402	MQ7	C3-C2	8.00	1.49	1.35
11	L	303	BPB	CAC-C3C	7.52	1.52	1.33
14	M	406	NS5	C35-C36	7.51	1.54	1.32
11	M	405	BPB	CAC-C3C	7.49	1.52	1.33
8	H	706	LDA	O1-N1	-7.13	1.25	1.42
8	H	707	LDA	O1-N1	-7.08	1.25	1.42
8	L	304	LDA	O1-N1	-6.88	1.26	1.42
8	H	701	LDA	O1-N1	-6.77	1.26	1.42
11	M	405	BPB	C1D-C2D	6.35	1.46	1.39
10	M	404	BCB	CAC-C3C	5.90	1.49	1.33
11	L	303	BPB	C1D-C2D	5.73	1.45	1.39
10	L	301	BCB	CAC-C3C	5.67	1.49	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	402	MQ7	C10-C5	5.36	1.49	1.40
11	M	405	BPB	O2A-CGA	5.23	1.48	1.33
11	M	405	BPB	C3D-C2D	5.22	1.48	1.39
10	L	302	BCB	CAC-C3C	5.19	1.47	1.33
11	L	303	BPB	OBD-CAD	5.11	1.29	1.22
10	L	301	BCB	C2C-C3C	-5.08	1.45	1.51
10	L	301	BCB	O2D-CGD	5.04	1.45	1.33
10	M	403	BCB	CAC-C3C	5.02	1.47	1.33
10	L	301	BCB	CHC-C1C	5.01	1.49	1.37
10	M	404	BCB	C3B-C4B	4.92	1.50	1.41
6	C	405	DGA	OG1-CA1	4.92	1.47	1.33
10	L	301	BCB	C1D-ND	-4.89	1.31	1.37
11	L	303	BPB	C4D-CHA	4.87	1.47	1.39
11	M	405	BPB	C4D-CHA	4.85	1.47	1.39
11	M	405	BPB	OBD-CAD	4.81	1.29	1.22
10	M	404	BCB	C2C-C3C	-4.79	1.45	1.51
10	M	404	BCB	O2D-CGD	4.78	1.44	1.33
6	C	405	DGA	OG2-CB1	4.76	1.47	1.34
10	L	301	BCB	C3B-C4B	4.69	1.49	1.41
5	C	401	HEC	FE-ND	4.69	2.09	1.94
5	C	404	HEC	FE-ND	4.64	2.09	1.94
11	M	405	BPB	O2D-CGD	4.63	1.44	1.33
11	L	303	BPB	O2D-CGD	4.55	1.44	1.33
10	L	301	BCB	CHC-C4B	4.54	1.49	1.39
10	L	302	BCB	C2C-C3C	-4.54	1.45	1.51
10	M	404	BCB	CHC-C1C	4.50	1.47	1.37
10	L	302	BCB	O2D-CGD	4.48	1.44	1.33
10	M	403	BCB	C2C-C3C	-4.41	1.46	1.51
11	L	303	BPB	C3B-C2B	4.40	1.47	1.39
10	M	403	BCB	O2A-CGA	4.39	1.46	1.33
5	C	402	HEC	FE-ND	4.36	2.08	1.94
11	L	303	BPB	C3D-C2D	4.35	1.47	1.39
11	M	405	BPB	C3B-C2B	4.35	1.47	1.39
10	L	302	BCB	C3B-C4B	4.27	1.49	1.41
10	M	403	BCB	O2D-CGD	4.27	1.43	1.33
10	M	404	BCB	CHC-C4B	4.24	1.48	1.39
10	M	403	BCB	CHC-C4B	4.20	1.48	1.39
5	C	403	HEC	FE-ND	4.17	2.07	1.94
10	M	403	BCB	CHC-C1C	4.04	1.46	1.37
10	L	301	BCB	OBD-CAD	3.99	1.29	1.22
10	M	403	BCB	C3B-C4B	3.98	1.48	1.41
10	L	302	BCB	CHC-C1C	3.94	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	L	302	BCB	CHC-C4B	3.86	1.48	1.39
10	M	403	BCB	CHD-C1D	3.84	1.45	1.38
10	L	302	BCB	CHD-C1D	3.83	1.45	1.38
11	M	405	BPB	C4C-NC	-3.77	1.26	1.37
10	L	301	BCB	O2A-CGA	3.76	1.44	1.33
11	L	303	BPB	O2A-CGA	3.76	1.44	1.33
10	M	403	BCB	C1D-ND	-3.75	1.33	1.37
10	L	302	BCB	OBD-CAD	3.75	1.28	1.22
5	C	402	HEC	FE-NA	3.69	2.07	1.95
10	L	302	BCB	CHB-C1B	3.65	1.47	1.39
10	L	302	BCB	O2A-CGA	3.61	1.43	1.33
10	M	404	BCB	CHD-C1D	3.60	1.45	1.38
10	M	404	BCB	O2A-CGA	3.60	1.43	1.33
11	L	303	BPB	CHA-CBD	-3.58	1.47	1.51
10	M	404	BCB	OBD-CAD	3.53	1.28	1.22
5	C	401	HEC	FE-NC	3.51	2.07	1.95
10	M	403	BCB	C3D-C2D	3.48	1.48	1.39
5	C	402	HEC	FE-NC	3.48	2.06	1.95
5	C	401	HEC	FE-NA	3.47	2.06	1.95
11	M	405	BPB	C3B-C4B	3.46	1.47	1.41
5	C	404	HEC	FE-NA	3.46	2.06	1.95
10	M	403	BCB	OBD-CAD	3.41	1.28	1.22
10	M	404	BCB	C1D-ND	-3.40	1.33	1.37
10	M	403	BCB	CHB-C1B	3.39	1.47	1.39
11	L	303	BPB	C3B-C4B	3.39	1.47	1.41
10	M	404	BCB	CHB-C1B	3.38	1.47	1.39
5	C	404	HEC	FE-NC	3.37	2.06	1.95
5	C	403	HEC	FE-NA	3.36	2.06	1.95
5	C	403	HEC	FE-NC	3.35	2.06	1.95
11	L	303	BPB	C4C-NC	-3.26	1.27	1.37
11	M	405	BPB	CHA-CBD	-3.24	1.47	1.51
10	M	404	BCB	C3D-C2D	3.22	1.47	1.39
10	L	302	BCB	C3D-C2D	3.18	1.47	1.39
10	L	302	BCB	C1D-ND	-3.17	1.33	1.37
11	L	303	BPB	C3A-C2A	-3.14	1.51	1.54
10	L	301	BCB	CHB-C1B	2.97	1.46	1.39
5	C	404	HEC	FE-NB	2.97	2.04	1.94
5	C	401	HEC	FE-NB	2.95	2.04	1.94
10	L	301	BCB	C3D-C2D	2.94	1.47	1.39
10	M	404	BCB	CHD-C4C	2.93	1.45	1.39
5	C	402	HEC	FE-NB	2.93	2.03	1.94
11	M	405	BPB	C1D-ND	-2.91	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	L	302	BCB	CHD-C4C	2.82	1.45	1.39
5	C	403	HEC	C4B-NB	-2.75	1.35	1.40
10	M	404	BCB	C1B-C2B	2.71	1.49	1.43
10	L	301	BCB	CHD-C1D	2.71	1.43	1.38
10	M	403	BCB	CHD-C4C	2.64	1.45	1.39
5	C	403	HEC	FE-NB	2.55	2.02	1.94
11	L	303	BPB	C1D-ND	-2.52	1.33	1.38
5	C	404	HEC	CAC-C3C	2.46	1.57	1.51
10	L	301	BCB	C1B-NB	-2.42	1.34	1.37
10	L	302	BCB	C1B-C2B	2.38	1.48	1.43
10	M	403	BCB	C1B-NB	-2.33	1.34	1.37
10	L	302	BCB	C3D-C4D	-2.31	1.39	1.44
11	L	303	BPB	CBD-CGD	-2.29	1.49	1.52
5	C	404	HEC	C4B-NB	-2.25	1.36	1.40
11	M	405	BPB	C2-C3	2.24	1.38	1.33
5	C	403	HEC	CAC-C3C	2.21	1.56	1.51
10	L	301	BCB	C3D-C4D	-2.19	1.39	1.44
10	L	301	BCB	CHD-C4C	2.18	1.44	1.39
10	M	403	BCB	C3D-C4D	-2.12	1.39	1.44
14	M	406	NS5	C30-C31	2.10	1.36	1.34
5	C	402	HEC	CBA-CGA	2.09	1.55	1.50
5	C	402	HEC	CAC-C3C	2.07	1.56	1.51
10	L	301	BCB	C1B-C2B	2.06	1.48	1.43
6	C	405	DGA	CG1-CG2	2.02	1.55	1.50
11	L	303	BPB	C3D-C4D	-2.00	1.38	1.41

All (209) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	M	404	BCB	C1C-NC-C4C	-16.14	99.45	106.71
10	M	403	BCB	C1C-NC-C4C	-15.01	99.96	106.71
10	L	301	BCB	C1C-NC-C4C	-14.41	100.23	106.71
10	L	302	BCB	C1C-NC-C4C	-13.63	100.58	106.71
10	L	301	BCB	C2B-C1B-NB	9.52	116.62	110.23
10	M	403	BCB	C2B-C1B-NB	8.51	115.94	110.23
10	L	302	BCB	C2B-C1B-NB	8.02	115.61	110.23
11	M	405	BPB	O2D-CGD-CBD	7.50	120.49	111.00
10	M	404	BCB	C2B-C1B-NB	7.23	115.08	110.23
5	C	403	HEC	CBC-CAC-C3C	7.07	131.92	112.43
11	M	405	BPB	C3D-C4D-ND	6.73	116.90	107.72
10	M	404	BCB	C4D-C3D-CAD	-6.53	100.40	108.10
11	L	303	BPB	C2B-C1B-NB	6.20	113.81	109.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	M	403	BCB	C4D-C3D-CAD	-6.16	100.83	108.10
11	L	303	BPB	C3D-C4D-ND	6.13	116.08	107.72
10	L	302	BCB	C4D-C3D-CAD	-6.05	100.96	108.10
11	L	303	BPB	O2D-CGD-CBD	5.88	118.44	111.00
10	L	301	BCB	C4D-C3D-CAD	-5.66	101.42	108.10
10	L	302	BCB	CMD-C2D-C1D	5.63	134.64	124.71
11	L	303	BPB	CBC-CAC-C3C	-5.49	112.14	126.70
10	M	404	BCB	O2D-CGD-CBD	5.29	120.66	111.27
11	M	405	BPB	CBC-CAC-C3C	-5.26	112.73	126.70
6	C	405	DGA	OG2-CB1-CB2	5.25	122.82	111.50
10	M	404	BCB	C3D-C4D-ND	5.18	118.61	110.24
10	M	403	BCB	C3D-C4D-ND	5.14	118.55	110.24
10	L	301	BCB	C3D-C4D-ND	5.09	118.47	110.24
10	M	403	BCB	CMD-C2D-C1D	4.94	133.42	124.71
10	L	301	BCB	CMD-C2D-C1D	4.93	133.40	124.71
10	L	301	BCB	C1D-ND-C4D	-4.88	102.87	106.33
11	M	405	BPB	C1A-C2A-C3A	-4.87	98.21	102.84
10	L	302	BCB	O2D-CGD-CBD	4.84	119.87	111.27
11	M	405	BPB	C2B-C1B-NB	4.76	112.81	109.53
10	M	404	BCB	C1D-ND-C4D	-4.68	103.01	106.33
10	L	302	BCB	C3D-C4D-ND	4.68	117.81	110.24
5	C	402	HEC	C4B-NB-C1B	4.57	109.80	105.07
10	M	404	BCB	CMD-C2D-C1D	4.44	132.54	124.71
10	L	302	BCB	OBD-CAD-C3D	-4.40	117.92	128.52
11	L	303	BPB	OBD-CAD-C3D	-4.34	120.78	127.98
10	L	301	BCB	C2D-C1D-ND	4.26	113.25	110.10
14	M	406	NS5	C19-C20-C21	-4.26	121.23	127.31
14	M	406	NS5	CM4-C36-C35	-4.24	110.39	122.65
10	M	403	BCB	OBD-CAD-C3D	-4.17	118.50	128.52
10	M	403	BCB	C1D-ND-C4D	-4.16	103.38	106.33
5	C	401	HEC	C4A-NA-C1A	4.08	109.35	105.35
5	C	403	HEC	C4A-NA-C1A	3.99	109.25	105.35
10	L	301	BCB	C4-C3-C5	3.98	121.97	115.27
5	C	401	HEC	C2A-C1A-NA	-3.97	106.46	110.32
5	C	401	HEC	C4B-NB-C1B	3.95	109.16	105.07
5	C	404	HEC	CAD-CBD-CGD	-3.95	105.11	113.60
10	M	404	BCB	CAD-C3D-C2D	3.94	159.79	140.80
14	M	406	NS5	CM3-C36-C35	-3.92	111.32	122.65
5	C	403	HEC	C2A-C1A-NA	-3.90	106.52	110.32
14	M	406	NS5	C34-C35-C36	-3.90	114.42	127.75
5	C	403	HEC	C1D-ND-C4D	3.85	109.05	105.07
5	C	404	HEC	C4B-NB-C1B	3.84	109.04	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	L	301	BCB	O2D-CGD-CBD	3.84	118.09	111.27
10	M	403	BCB	C2C-C1C-CHC	-3.82	114.64	123.64
10	M	403	BCB	CAD-C3D-C2D	3.76	158.96	140.80
10	M	404	BCB	O2D-CGD-O1D	-3.75	116.51	123.84
10	M	403	BCB	O2D-CGD-CBD	3.74	117.91	111.27
5	C	404	HEC	C4A-NA-C1A	3.74	109.01	105.35
11	M	405	BPB	OBD-CAD-C3D	-3.70	121.84	127.98
10	L	301	BCB	OBD-CAD-C3D	-3.67	119.70	128.52
10	L	301	BCB	CHD-C4C-C3C	-3.65	121.32	125.89
10	L	301	BCB	CAD-C3D-C2D	3.65	158.41	140.80
5	C	403	HEC	C4B-NB-C1B	3.65	108.84	105.07
10	L	302	BCB	C2C-C1C-CHC	-3.63	115.08	123.64
8	H	707	LDA	CM1-N1-C1	3.61	117.83	110.23
5	C	402	HEC	C4A-NA-C1A	3.60	108.87	105.35
5	C	404	HEC	C4C-NC-C1C	3.60	108.87	105.35
10	L	302	BCB	CAD-C3D-C2D	3.59	158.13	140.80
6	C	405	DGA	OG2-CG2-CG1	3.58	114.42	106.13
14	M	406	NS5	C18-C17-C15	-3.56	122.24	127.31
10	M	404	BCB	CAA-C2A-C1A	3.50	123.45	111.97
10	M	404	BCB	C2D-C1D-ND	3.48	112.67	110.10
10	L	302	BCB	O1D-CGD-CBD	-3.45	117.43	124.48
6	C	405	DGA	OG1-CA1-CA2	3.42	122.64	111.91
10	L	302	BCB	CMD-C2D-C3D	-3.39	119.82	127.61
10	L	302	BCB	C1D-ND-C4D	-3.38	103.93	106.33
10	M	404	BCB	CHA-C4D-ND	-3.38	125.42	132.50
11	L	303	BPB	CMD-C2D-C3D	-3.32	118.46	124.68
14	M	406	NS5	C18-C19-C20	3.31	130.26	123.47
10	M	404	BCB	C2C-C1C-CHC	-3.30	115.87	123.64
10	M	404	BCB	CHC-C1C-NC	-3.28	119.98	124.51
10	M	404	BCB	C4A-NA-C1A	3.26	108.17	106.71
10	M	404	BCB	CED-O2D-CGD	3.24	123.27	115.94
14	M	406	NS5	C16-C15-C14	3.23	123.17	118.08
5	C	402	HEC	C2A-C1A-NA	-3.23	107.18	110.32
11	M	405	BPB	O2A-CGA-CBA	3.19	121.93	111.91
5	C	401	HEC	C1D-ND-C4D	3.19	108.36	105.07
5	C	401	HEC	C4C-NC-C1C	3.16	108.44	105.35
10	L	301	BCB	O2A-CGA-CBA	3.16	121.81	111.91
10	L	301	BCB	CHB-C4A-NA	3.11	128.81	124.51
11	M	405	BPB	C4D-ND-C1D	-3.09	105.68	108.83
10	L	302	BCB	CHB-C1B-NB	-3.07	121.01	124.26
10	L	301	BCB	CHA-C4D-ND	-3.06	126.09	132.50
11	L	303	BPB	C4D-CHA-CBD	-3.06	107.13	108.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	M	404	BCB	OBD-CAD-C3D	-3.06	121.17	128.52
5	C	402	HEC	C4C-NC-C1C	3.00	108.29	105.35
5	C	401	HEC	CBD-CAD-C3D	-3.00	104.28	112.63
6	C	405	DGA	OG1-CA1-OA1	-2.99	116.06	123.59
10	M	403	BCB	CHA-C4D-ND	-2.98	126.25	132.50
10	L	301	BCB	CED-O2D-CGD	2.98	122.68	115.94
10	M	403	BCB	CBC-CAC-C3C	-2.96	118.05	126.72
10	M	403	BCB	C2D-C1D-ND	2.94	112.27	110.10
10	L	302	BCB	CHB-C4A-NA	2.93	128.57	124.51
11	L	303	BPB	C4D-ND-C1D	-2.93	105.85	108.83
10	M	404	BCB	CHB-C4A-NA	2.92	128.55	124.51
10	M	403	BCB	CHB-C4A-NA	2.92	128.55	124.51
10	L	301	BCB	CMB-C2B-C3B	2.90	133.77	125.93
10	L	301	BCB	O2D-CGD-O1D	-2.89	118.19	123.84
10	M	403	BCB	CMD-C2D-C3D	-2.83	121.09	127.61
5	C	403	HEC	C4C-NC-C1C	2.81	108.10	105.35
10	L	301	BCB	C2C-C1C-CHC	-2.81	117.01	123.64
10	L	301	BCB	C4A-NA-C1A	2.81	107.97	106.71
5	C	401	HEC	CBA-CAA-C2A	-2.80	104.83	112.63
5	C	402	HEC	C1D-ND-C4D	2.80	107.97	105.07
11	L	303	BPB	O1D-CGD-CBD	-2.80	120.08	124.74
10	M	404	BCB	C4B-C3B-C2B	-2.79	103.86	108.36
11	M	405	BPB	O2A-C1-C2	2.79	115.98	108.64
11	M	405	BPB	C5-C3-C2	2.79	126.75	121.12
5	C	404	HEC	C2A-C1A-NA	-2.77	107.62	110.32
10	L	302	BCB	CHA-C4D-ND	-2.77	126.70	132.50
10	L	301	BCB	CHC-C1C-NC	-2.75	120.70	124.51
5	C	401	HEC	CBC-CAC-C3C	2.74	119.98	112.43
10	M	404	BCB	CHC-C4B-C3B	-2.74	122.62	132.35
10	M	403	BCB	CHC-C1C-NC	-2.73	120.74	124.51
10	L	301	BCB	CMD-C2D-C3D	-2.72	121.35	127.61
5	C	404	HEC	CBB-CAB-C3B	-2.71	104.96	112.43
11	L	303	BPB	CMB-C2B-C3B	2.70	129.73	124.68
5	C	403	HEC	C3D-C4D-ND	-2.69	107.75	110.36
11	M	405	BPB	O1D-CGD-CBD	-2.67	120.28	124.74
13	M	402	MQ7	C39-C38-C40	2.67	119.76	115.27
13	M	402	MQ7	C12-C11-C3	-2.66	104.88	112.05
5	C	403	HEC	C2D-C1D-ND	-2.65	106.70	109.84
10	M	404	BCB	CMD-C2D-C3D	-2.65	121.53	127.61
14	M	406	NS5	C6-C5-C7	-2.64	116.91	123.68
10	L	302	BCB	CHD-C4C-C3C	-2.64	122.59	125.89
10	M	403	BCB	CHC-C4B-C3B	-2.63	122.98	132.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	L	302	BCB	CHC-C4B-C3B	-2.63	122.99	132.35
10	L	302	BCB	CED-O2D-CGD	2.62	121.86	115.94
10	M	404	BCB	CHD-C4C-C3C	-2.62	122.62	125.89
10	M	404	BCB	CHB-C1B-NB	-2.62	121.49	124.26
10	L	301	BCB	C5-C3-C2	-2.61	115.83	121.12
13	M	402	MQ7	C2M-C2-C3	-2.61	120.15	124.40
10	M	404	BCB	C1D-CHD-C4C	-2.60	120.45	126.06
11	M	405	BPB	CMD-C2D-C3D	-2.60	119.82	124.68
13	M	402	MQ7	C29-C28-C30	2.59	119.63	115.27
8	H	706	LDA	CM2-N1-C1	2.57	115.63	110.23
10	L	302	BCB	CBC-CAC-C3C	-2.56	119.24	126.72
14	M	406	NS5	C14-C15-C17	-2.55	115.02	118.94
5	C	401	HEC	C3D-C4D-ND	-2.55	107.89	110.36
13	M	402	MQ7	C2M-C2-C1	2.54	120.48	116.27
11	L	303	BPB	CMA-C3A-C4A	-2.53	108.83	114.38
11	M	405	BPB	C3D-CAD-CBD	2.53	110.93	107.61
5	C	402	HEC	C2B-C1B-NB	-2.52	106.86	109.88
5	C	403	HEC	CBA-CAA-C2A	-2.51	105.66	112.63
11	L	303	BPB	C3D-CAD-CBD	2.47	110.85	107.61
10	M	403	BCB	CHD-C4C-C3C	-2.47	122.81	125.89
10	M	403	BCB	O2A-CGA-CBA	2.44	119.57	111.91
10	M	404	BCB	O2A-CGA-O1A	-2.43	117.46	123.59
5	C	404	HEC	C1D-ND-C4D	2.42	107.58	105.07
13	M	402	MQ7	O4-C4-C3	-2.42	116.67	120.56
11	M	405	BPB	C1-O2A-CGA	2.42	122.78	116.44
5	C	402	HEC	CAC-C3C-C2C	2.40	130.70	126.86
5	C	401	HEC	CAA-C2A-C3A	-2.38	123.44	127.88
5	C	403	HEC	O2D-CGD-CBD	2.38	121.68	114.03
10	L	301	BCB	O2A-CGA-O1A	-2.38	117.60	123.59
5	C	404	HEC	CBD-CAD-C3D	2.37	119.22	112.63
11	M	405	BPB	O2D-CGD-O1D	-2.37	119.21	123.84
5	C	403	HEC	CHB-C4A-NA	2.36	126.99	124.44
11	L	303	BPB	CMC-C2C-C1C	-2.35	110.42	114.36
11	M	405	BPB	C3B-C4B-NB	2.34	111.54	108.04
5	C	402	HEC	CBA-CAA-C2A	-2.34	106.13	112.63
5	C	401	HEC	C3B-C4B-NB	-2.31	107.60	110.17
10	L	301	BCB	CHC-C4B-C3B	-2.30	124.15	132.35
10	L	302	BCB	C2D-C1D-ND	2.30	111.80	110.10
10	L	301	BCB	CAA-C2A-C1A	2.29	119.49	111.97
10	L	301	BCB	C3C-C4C-NC	2.28	113.06	110.57
10	M	403	BCB	C2A-C1A-CHA	-2.26	119.90	123.86
14	M	406	NS5	C11-C10-C9	2.26	119.07	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	403	HEC	O1D-CGD-CBD	-2.26	115.83	123.08
10	L	302	BCB	CHC-C1C-NC	-2.26	121.39	124.51
11	L	303	BPB	C4A-C3A-C2A	-2.25	100.69	102.84
10	L	301	BCB	C1-C2-C3	-2.25	122.15	126.04
5	C	402	HEC	C3B-C4B-NB	-2.23	107.68	110.17
11	L	303	BPB	C3B-C4B-NB	2.22	111.36	108.04
5	C	402	HEC	O2A-CGA-CBA	2.21	121.14	114.03
10	M	403	BCB	C4-C3-C5	2.21	118.98	115.27
11	L	303	BPB	CBA-CAA-C2A	-2.20	107.39	113.81
11	M	405	BPB	O2A-CGA-O1A	-2.16	118.15	123.59
14	M	406	NS5	C8-C9-C10	-2.15	105.90	112.98
5	C	402	HEC	C3D-C4D-ND	-2.12	108.30	110.36
5	C	403	HEC	C1D-C2D-C3D	2.11	109.18	106.96
10	L	301	BCB	C4B-C3B-C2B	-2.11	104.96	108.36
10	L	302	BCB	C1D-CHD-C4C	-2.11	121.50	126.06
10	L	301	BCB	CHB-C1B-C2B	-2.10	121.31	127.24
10	M	404	BCB	C1-O2A-CGA	2.10	121.95	116.44
10	L	302	BCB	C2A-C1A-CHA	-2.09	120.20	123.86
5	C	403	HEC	CHD-C1D-ND	2.08	126.94	124.37
11	M	405	BPB	CMA-C3A-C4A	-2.07	109.84	114.38
10	M	403	BCB	CMB-C2B-C1B	2.07	128.51	125.37
10	L	301	BCB	CHB-C1B-NB	-2.06	122.08	124.26
5	C	401	HEC	CAC-C3C-C2C	2.05	130.14	126.86
10	L	302	BCB	C1-O2A-CGA	2.04	121.79	116.44
5	C	404	HEC	C3B-C4B-NB	-2.04	107.90	110.17
5	C	401	HEC	C2D-C1D-ND	-2.02	107.45	109.84
10	L	302	BCB	C6-C5-C3	-2.01	108.19	113.45
14	M	406	NS5	C4-C5-C7	2.00	125.17	121.12

All (16) chirality outliers are listed below:

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

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Mol	Chain	Res	Type	Atom
10	M	403	BCB	NA
10	M	403	BCB	NC
10	M	403	BCB	ND
10	M	404	BCB	NA
10	M	404	BCB	NC
10	M	404	BCB	ND

All (131) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	405	DGA	OG1-CG1-CG2-OG2
6	C	405	DGA	OG1-CG1-CG2-CG3
8	H	706	LDA	C2-C1-N1-O1
8	H	706	LDA	C2-C1-N1-CM1
8	H	706	LDA	C2-C1-N1-CM2
8	H	707	LDA	C2-C1-N1-O1
8	H	707	LDA	C2-C1-N1-CM1
8	H	707	LDA	N1-C1-C2-C3
9	L	305	HTO	O2-C2-C3-C4
10	L	301	BCB	C2-C3-C5-C6
10	L	301	BCB	C4-C3-C5-C6
10	L	302	BCB	C2C-C3C-CAC-CBC
10	M	403	BCB	C2B-C3B-CAB-OBB
10	M	403	BCB	C2B-C3B-CAB-CBB
10	M	403	BCB	C4B-C3B-CAB-OBB
10	M	403	BCB	C4B-C3B-CAB-CBB
10	M	403	BCB	C2C-C3C-CAC-CBC
10	M	403	BCB	C4C-C3C-CAC-CBC
10	M	403	BCB	CBD-CGD-O2D-CED
10	M	404	BCB	CHA-CBD-CGD-O1D
10	M	404	BCB	CHA-CBD-CGD-O2D
10	M	404	BCB	CAD-CBD-CGD-O1D
10	M	404	BCB	CAD-CBD-CGD-O2D
11	L	303	BPB	C2C-C3C-CAC-CBC
11	M	405	BPB	C2C-C3C-CAC-CBC
14	M	406	NS5	C34-C35-C36-CM3
10	M	403	BCB	O1D-CGD-O2D-CED
10	M	404	BCB	C2A-CAA-CBA-CGA
14	M	406	NS5	C34-C35-C36-CM4
5	C	402	HEC	C2C-C3C-CAC-CBC
5	C	402	HEC	C2B-C3B-CAB-CBB
11	L	303	BPB	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
5	C	401	HEC	C2C-C3C-CAC-CBC
5	C	403	HEC	C2C-C3C-CAC-CBC
14	M	406	NS5	C31-C33-C34-C35
5	C	401	HEC	C2B-C3B-CAB-CBB
5	C	402	HEC	C4C-C3C-CAC-CBC
6	C	405	DGA	CA2-CA1-OG1-CG1
11	M	405	BPB	CBA-CGA-O2A-C1
5	C	403	HEC	C4C-C3C-CAC-CBC
11	M	405	BPB	O1A-CGA-O2A-C1
6	C	405	DGA	OA1-CA1-OG1-CG1
5	C	401	HEC	C4C-C3C-CAC-CBC
10	L	301	BCB	C13-C15-C16-C17
10	M	404	BCB	C15-C16-C17-C18
10	M	403	BCB	C5-C6-C7-C8
11	M	405	BPB	C15-C16-C17-C18
5	C	401	HEC	C2A-CAA-CBA-CGA
10	L	302	BCB	C12-C13-C15-C16
5	C	402	HEC	C4B-C3B-CAB-CBB
8	H	707	LDA	C6-C7-C8-C9
11	L	303	BPB	C2-C3-C5-C6
10	M	404	BCB	C14-C13-C15-C16
11	L	303	BPB	O1D-CGD-O2D-CED
8	H	707	LDA	C4-C5-C6-C7
8	L	304	LDA	C2-C3-C4-C5
8	H	706	LDA	C3-C4-C5-C6
8	H	706	LDA	C6-C7-C8-C9
6	C	405	DGA	CCB-CDB-CEB-CFB
11	L	303	BPB	C4-C3-C5-C6
9	H	708	HTO	O1-C1-C2-O2
8	L	304	LDA	C5-C6-C7-C8
8	H	701	LDA	C6-C7-C8-C9
10	M	404	BCB	C12-C13-C15-C16
8	L	304	LDA	C1-C2-C3-C4
10	L	302	BCB	C14-C13-C15-C16
6	C	405	DGA	CBB-CAB-CB9-CB8
10	M	404	BCB	C13-C15-C16-C17
5	C	401	HEC	C4B-C3B-CAB-CBB
6	C	405	DGA	CAB-CBB-CCB-CDB
9	L	305	HTO	C4-C5-C6-C7
5	C	404	HEC	C2B-C3B-CAB-CBB
10	M	403	BCB	C8-C10-C11-C12
8	L	304	LDA	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
8	L	304	LDA	C3-C4-C5-C6
8	H	707	LDA	C2-C3-C4-C5
8	H	706	LDA	N1-C1-C2-C3
8	H	707	LDA	C11-C10-C9-C8
11	L	303	BPB	C8-C10-C11-C12
6	C	405	DGA	CB9-CAB-CBB-CCB
9	L	305	HTO	O3-C3-C4-C5
5	C	402	HEC	C3D-CAD-CBD-CGD
5	C	403	HEC	C2B-C3B-CAB-CBB
10	L	301	BCB	C15-C16-C17-C18
10	M	403	BCB	C3-C5-C6-C7
11	L	303	BPB	CAD-CBD-CGD-O2D
8	H	706	LDA	C1-C2-C3-C4
8	H	707	LDA	C2-C1-N1-CM2
9	L	305	HTO	C2-C3-C4-C5
10	L	301	BCB	C2C-C3C-CAC-CBC
10	L	301	BCB	CAD-CBD-CGD-O1D
10	M	404	BCB	C10-C11-C12-C13
10	M	403	BCB	C11-C10-C8-C7
10	L	302	BCB	C4C-C3C-CAC-CBC
10	L	302	BCB	C13-C15-C16-C17
10	M	404	BCB	C5-C6-C7-C8
6	C	405	DGA	CBB-CCB-CDB-CEB
6	C	405	DGA	CB6-CB7-CB8-CB9
10	M	404	BCB	C8-C10-C11-C12
5	C	404	HEC	C4B-C3B-CAB-CBB
6	C	405	DGA	CA7-CA8-CA9-CAA
10	M	403	BCB	C11-C10-C8-C9
8	H	701	LDA	C4-C5-C6-C7
5	C	403	HEC	C4B-C3B-CAB-CBB
6	C	405	DGA	CG3-CG2-OG2-CB1
8	H	707	LDA	C3-C4-C5-C6
11	L	303	BPB	O2A-C1-C2-C3
8	H	707	LDA	C1-C2-C3-C4
11	M	405	BPB	C10-C11-C12-C13
6	C	405	DGA	CA6-CA7-CA8-CA9
11	M	405	BPB	C16-C17-C18-C20
10	M	403	BCB	C4-C3-C5-C6
10	M	403	BCB	C11-C12-C13-C14
9	L	305	HTO	O1-C1-C2-O2
8	H	701	LDA	C9-C10-C11-C12
14	M	406	NS5	C3-C4-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	M	406	NS5	C7-C8-C9-C10
10	M	403	BCB	C2-C3-C5-C6
11	M	405	BPB	CAD-CBD-CGD-O2D
10	M	404	BCB	C16-C17-C18-C20
5	C	401	HEC	CAA-CBA-CGA-O2A
10	M	404	BCB	O2A-C1-C2-C3
10	L	302	BCB	CHA-CBD-CGD-O2D
5	C	401	HEC	CAA-CBA-CGA-O1A
5	C	402	HEC	CAA-CBA-CGA-O1A
5	C	402	HEC	CAA-CBA-CGA-O2A
10	L	301	BCB	C6-C7-C8-C10
6	C	405	DGA	CEB-CFB-CGB-CHB
6	C	405	DGA	CG1-CG2-OG2-CB1
5	C	401	HEC	CAD-CBD-CGD-O2D
14	M	406	NS5	C20-C21-C23-C24

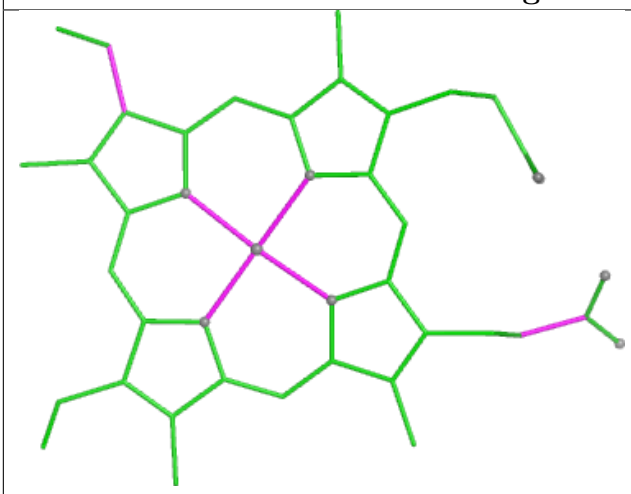
There are no ring outliers.

7 monomers are involved in 15 short contacts:

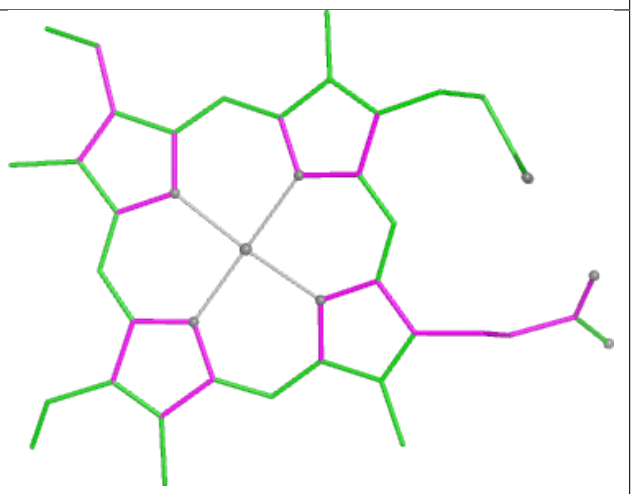
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	M	404	BCB	1	0
10	L	302	BCB	1	0
11	L	303	BPB	2	0
5	C	404	HEC	1	0
14	M	406	NS5	4	0
10	M	403	BCB	4	0
11	M	405	BPB	3	0

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.

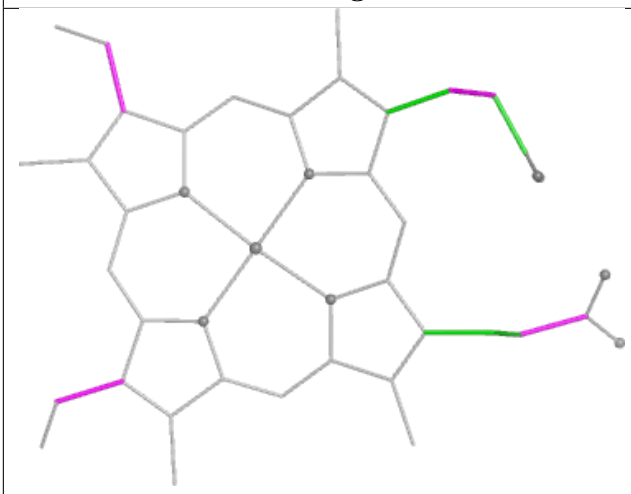
Ligand HEC C 402



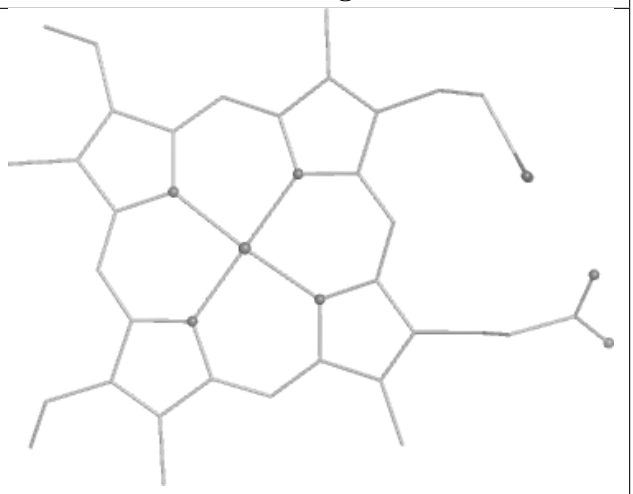
Bond lengths



Bond angles

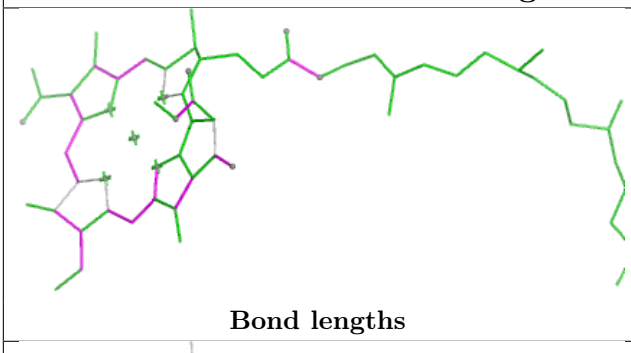


Torsions

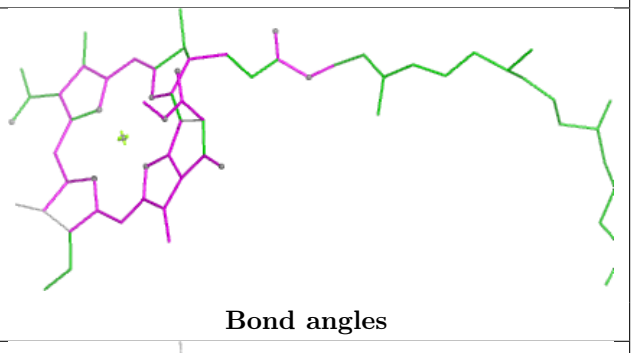


Rings

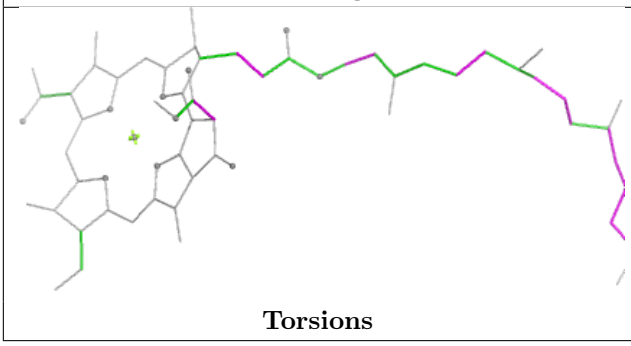
Ligand BCB M 404



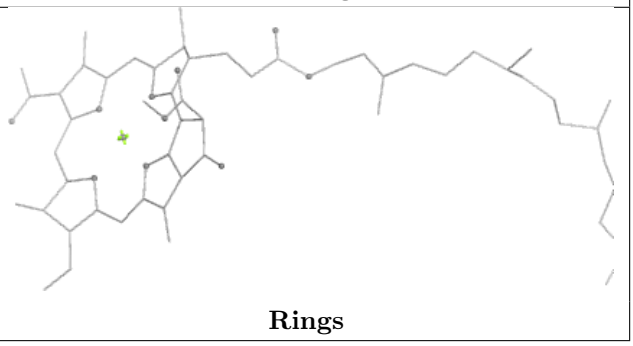
Bond lengths



Bond angles

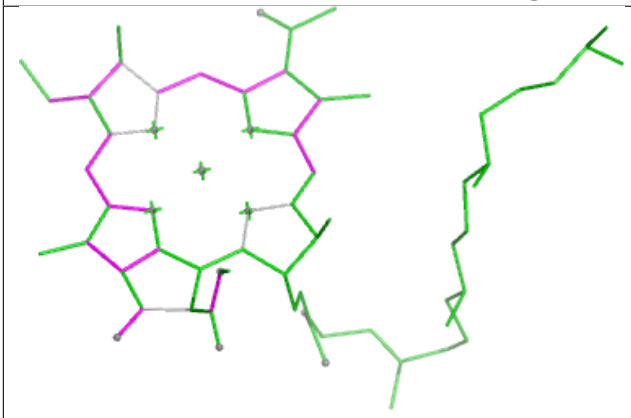


Torsions

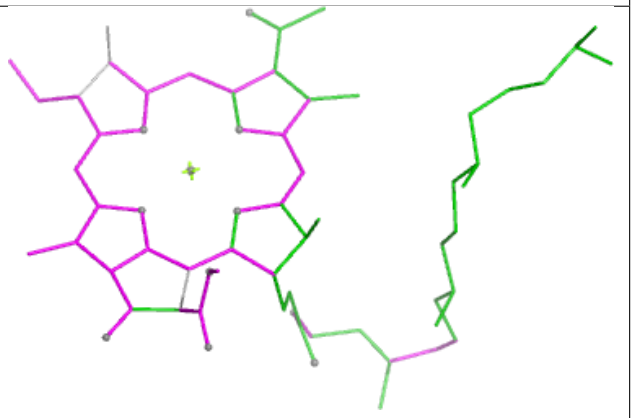


Rings

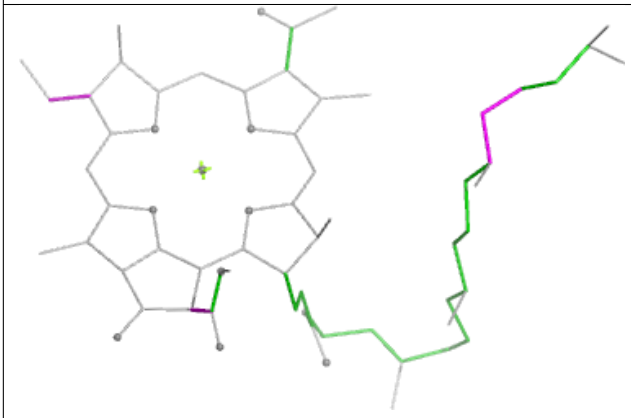
Ligand BCB L 302



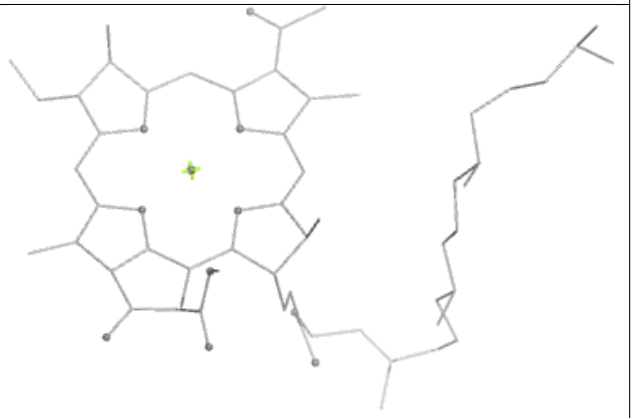
Bond lengths



Bond angles

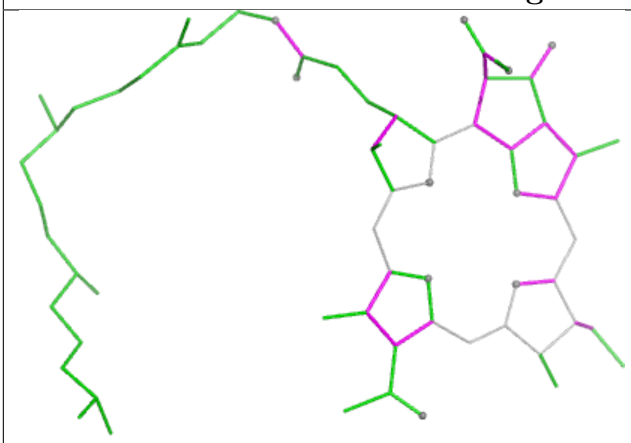


Torsions

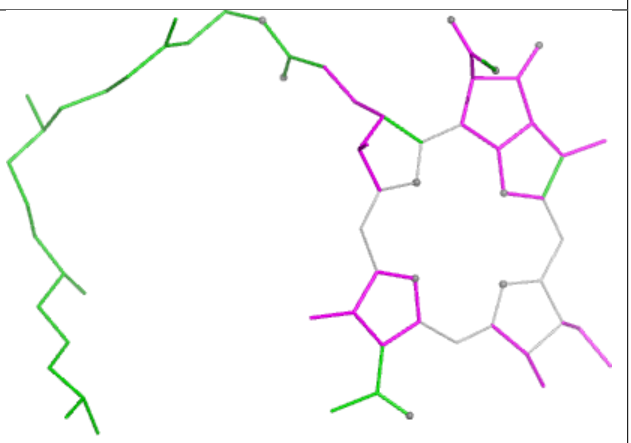


Rings

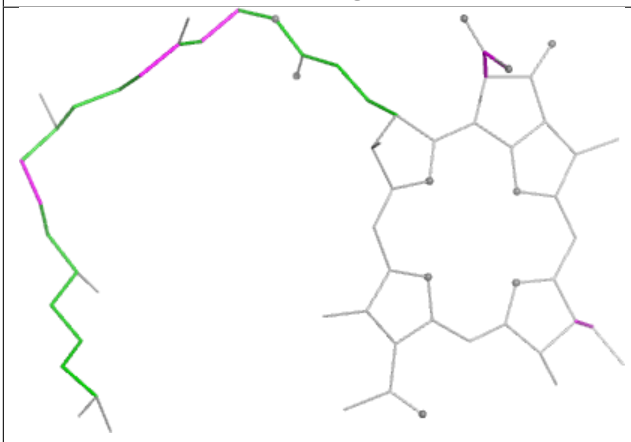
Ligand BPB L 303



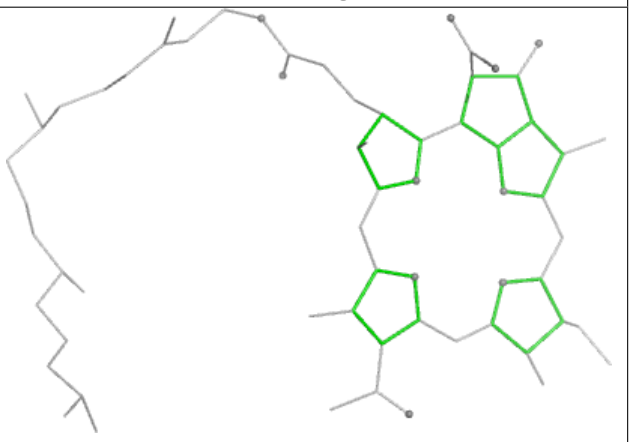
Bond lengths



Bond angles

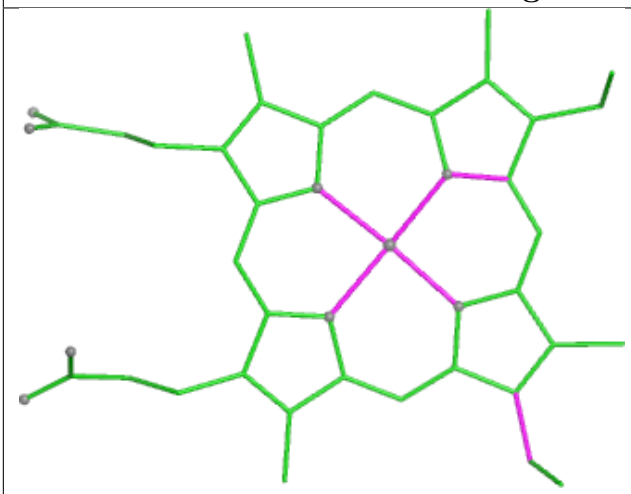


Torsions

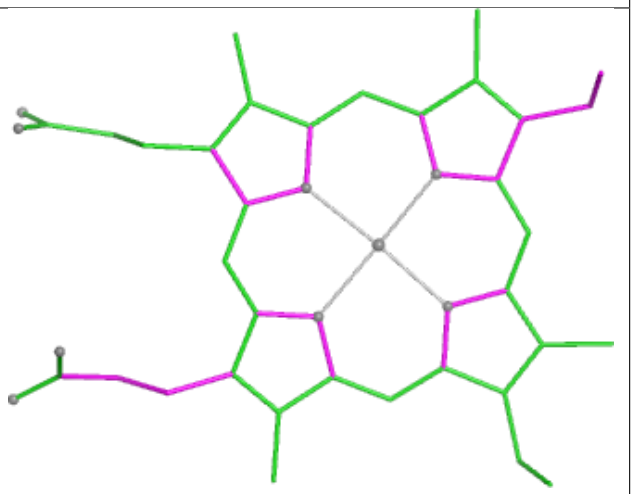


Rings

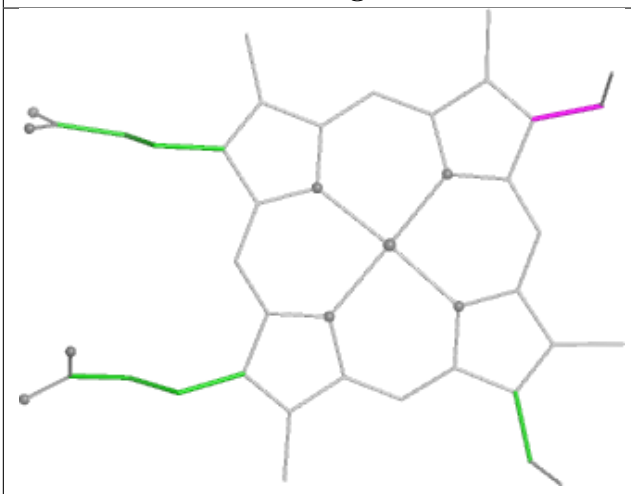
Ligand HEC C 404



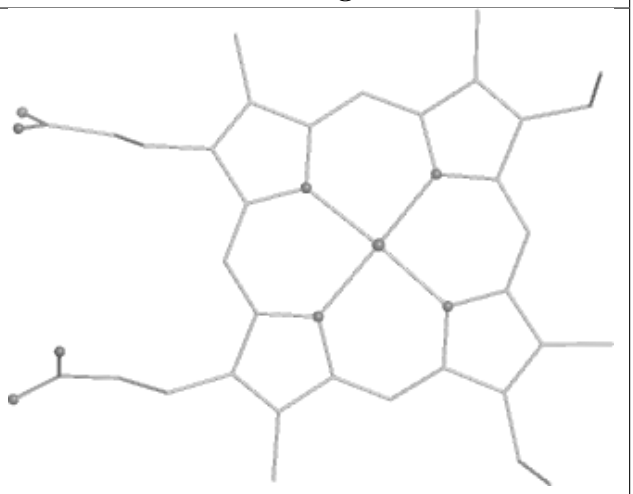
Bond lengths



Bond angles

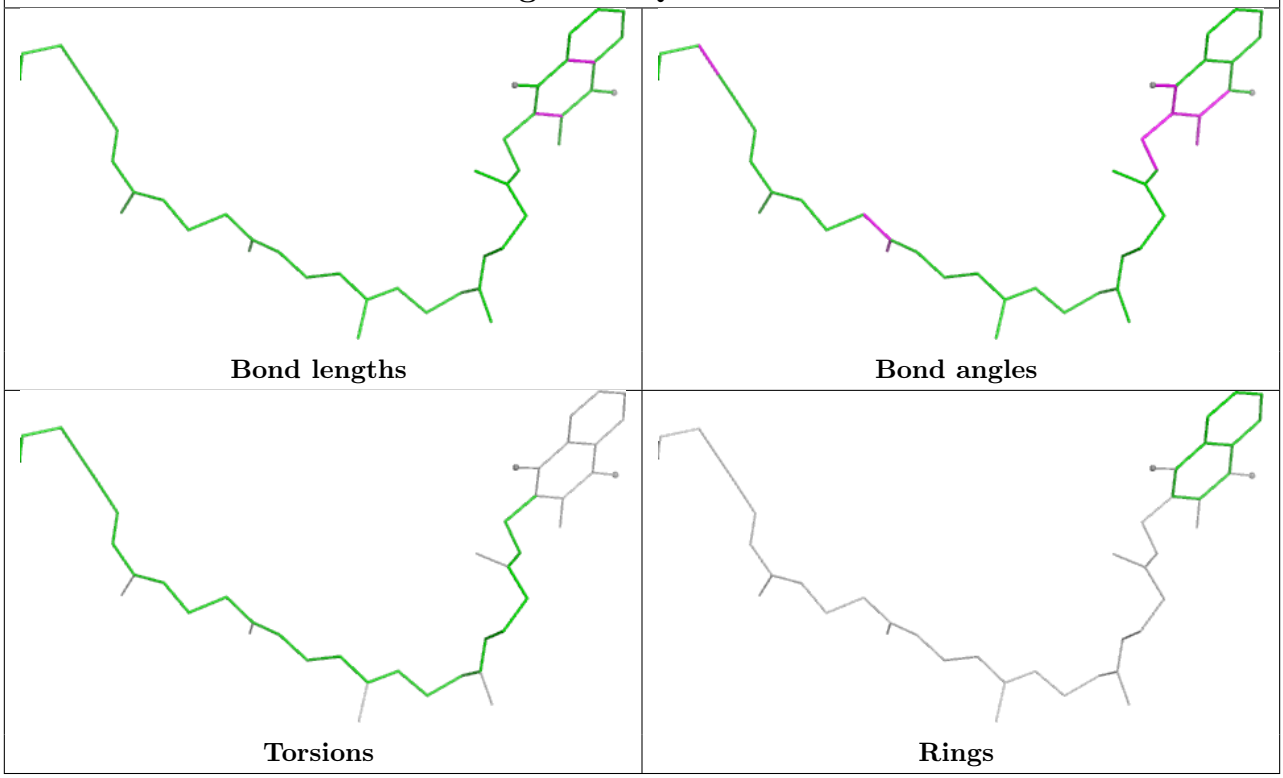


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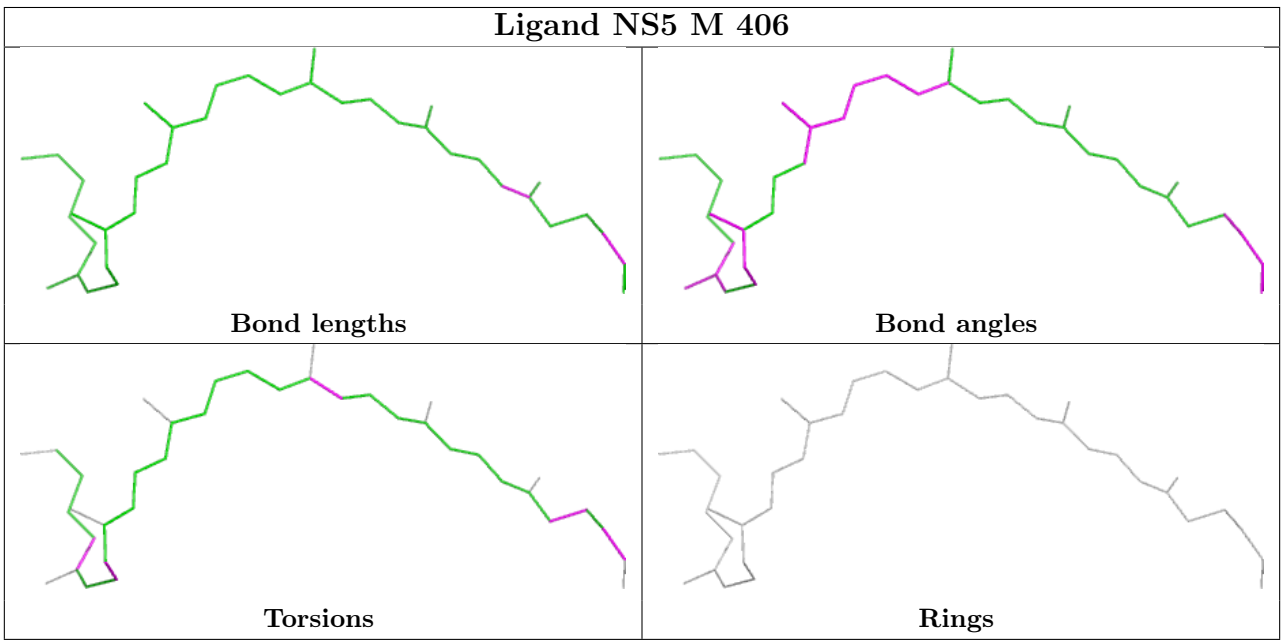


Rings

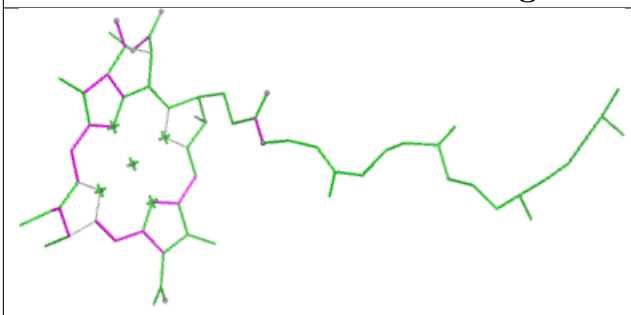
Ligand MQ7 M 402



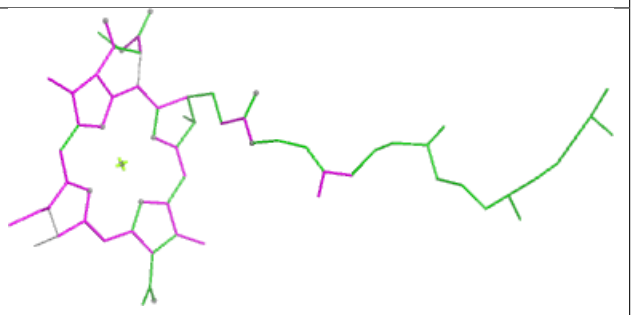
Ligand NS5 M 406



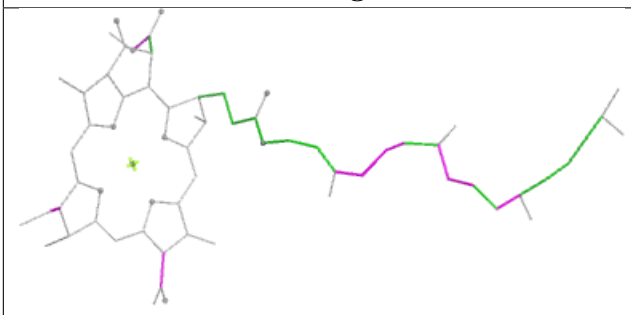
Ligand BCB M 403



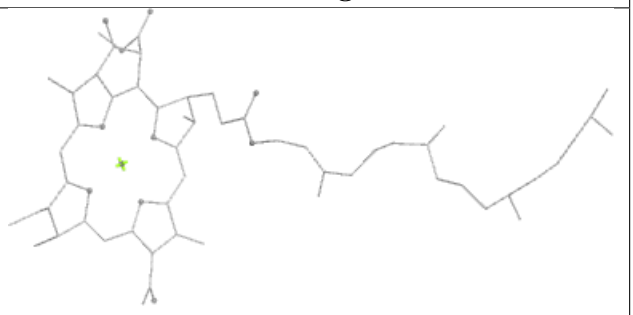
Bond lengths



Bond angles

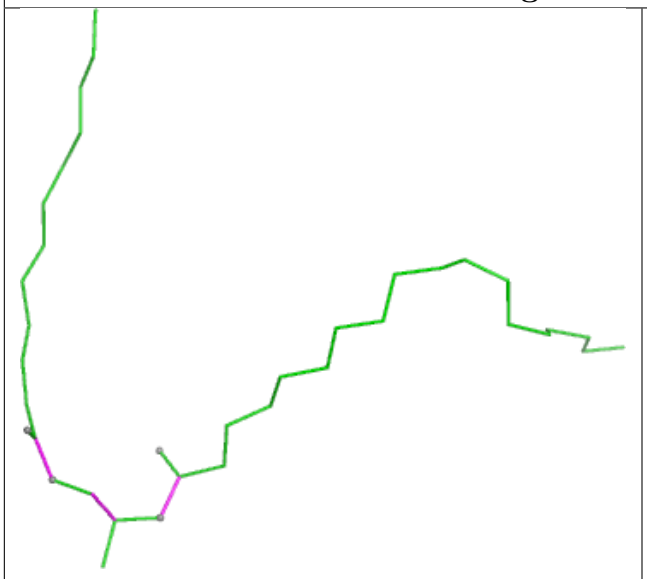


Torsions

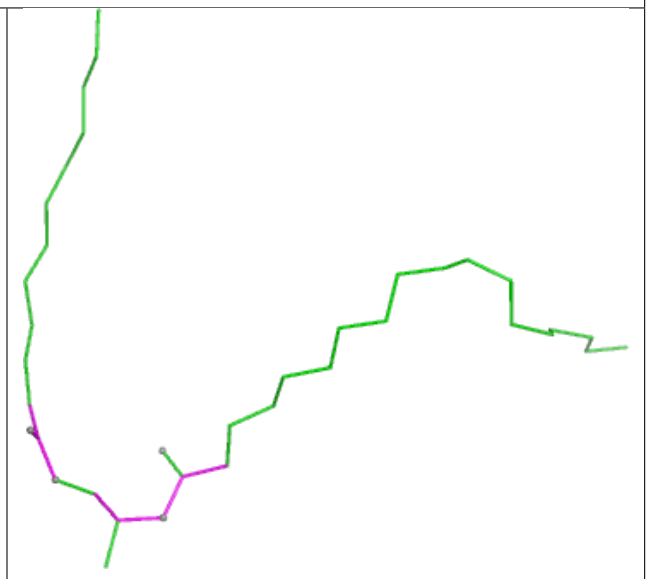


Rings

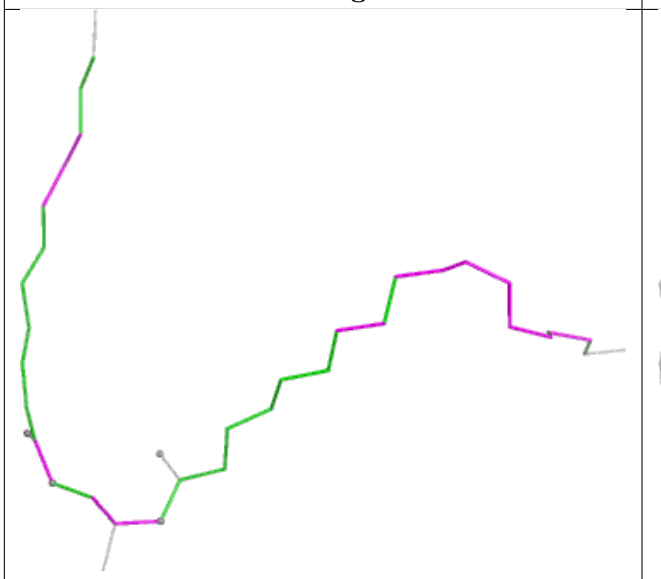
Ligand DGA C 405



Bond lengths



Bond angles

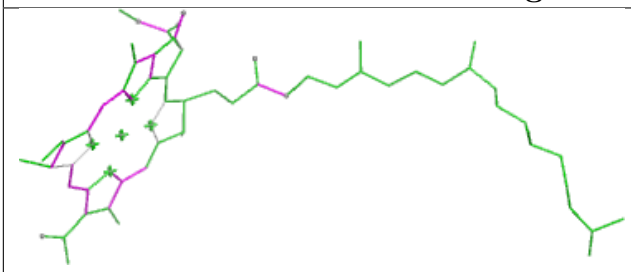


Torsions

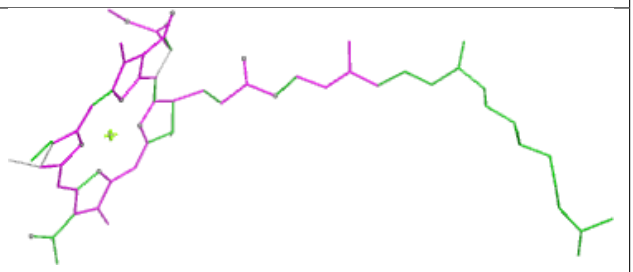


Rings

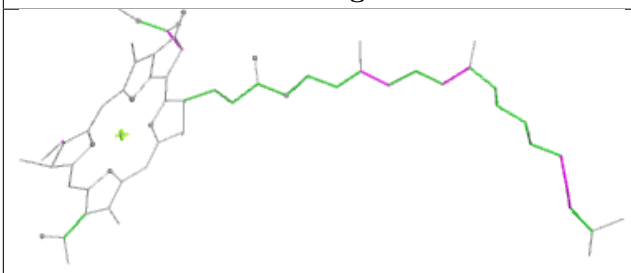
Ligand BCB L 301



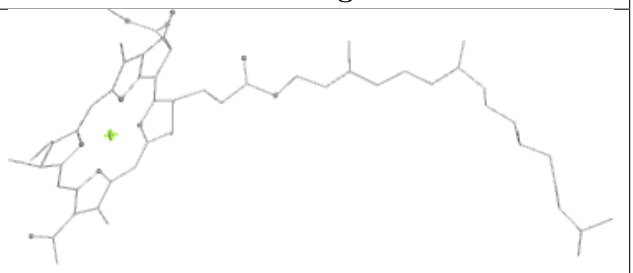
Bond lengths



Bond angles

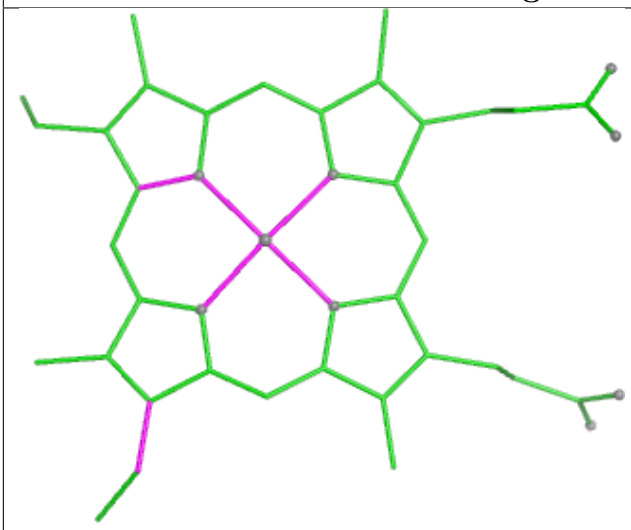


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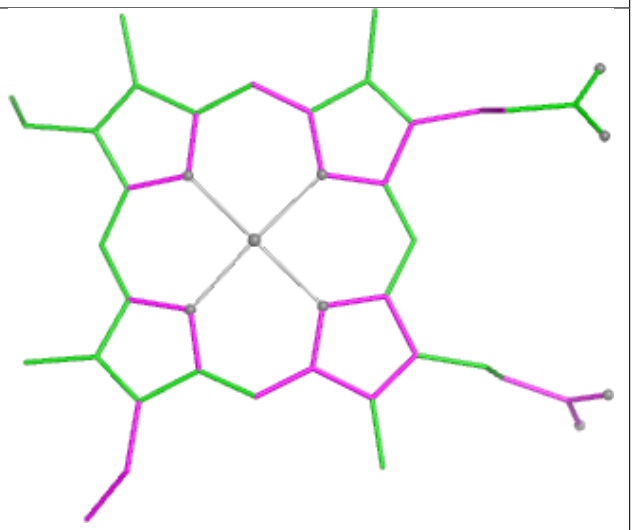


Rings

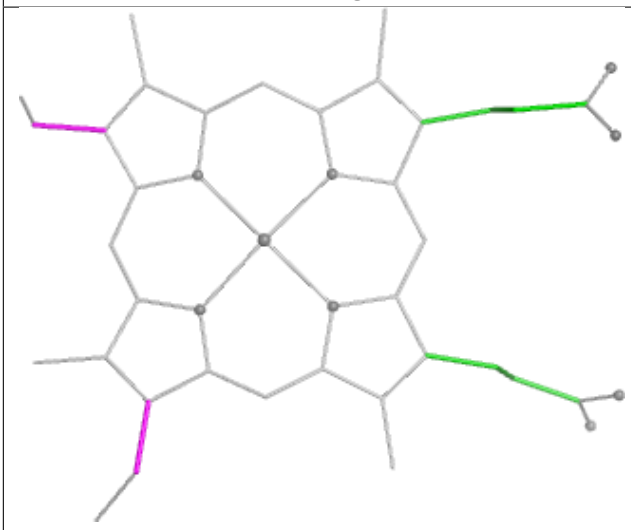
Ligand HEC C 403



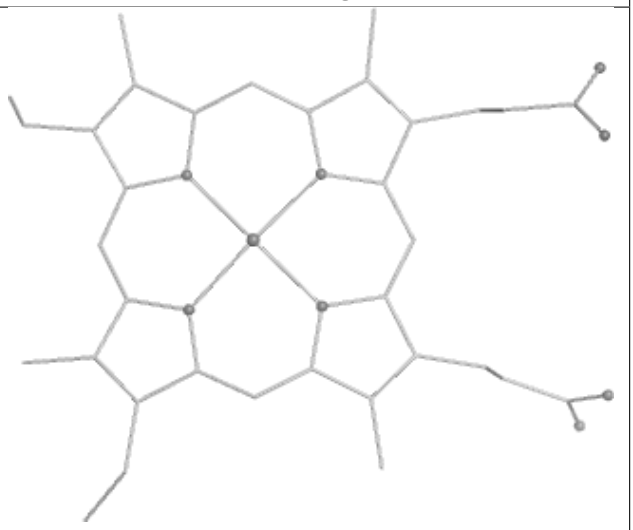
Bond lengths



Bond angles

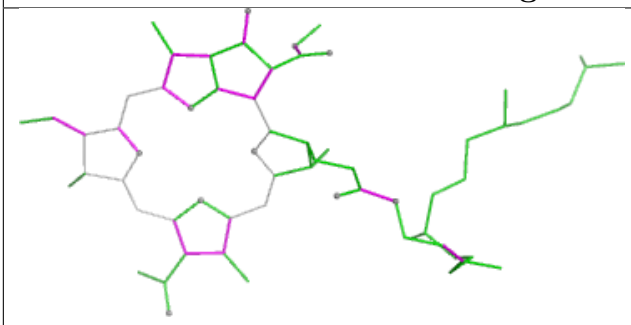


Torsions

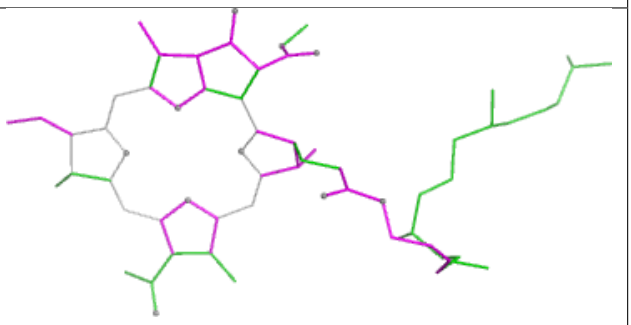


Rings

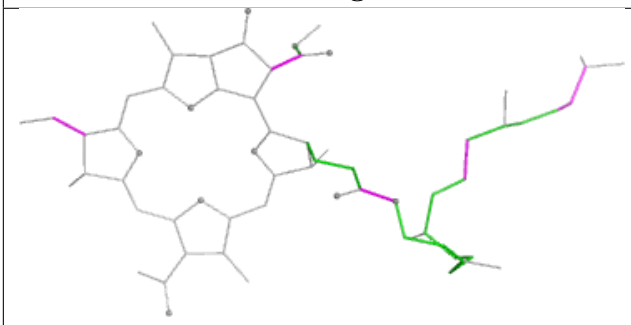
Ligand BPB M 405



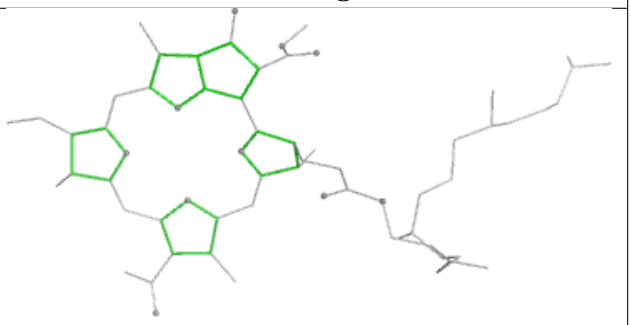
Bond lengths



Bond angles

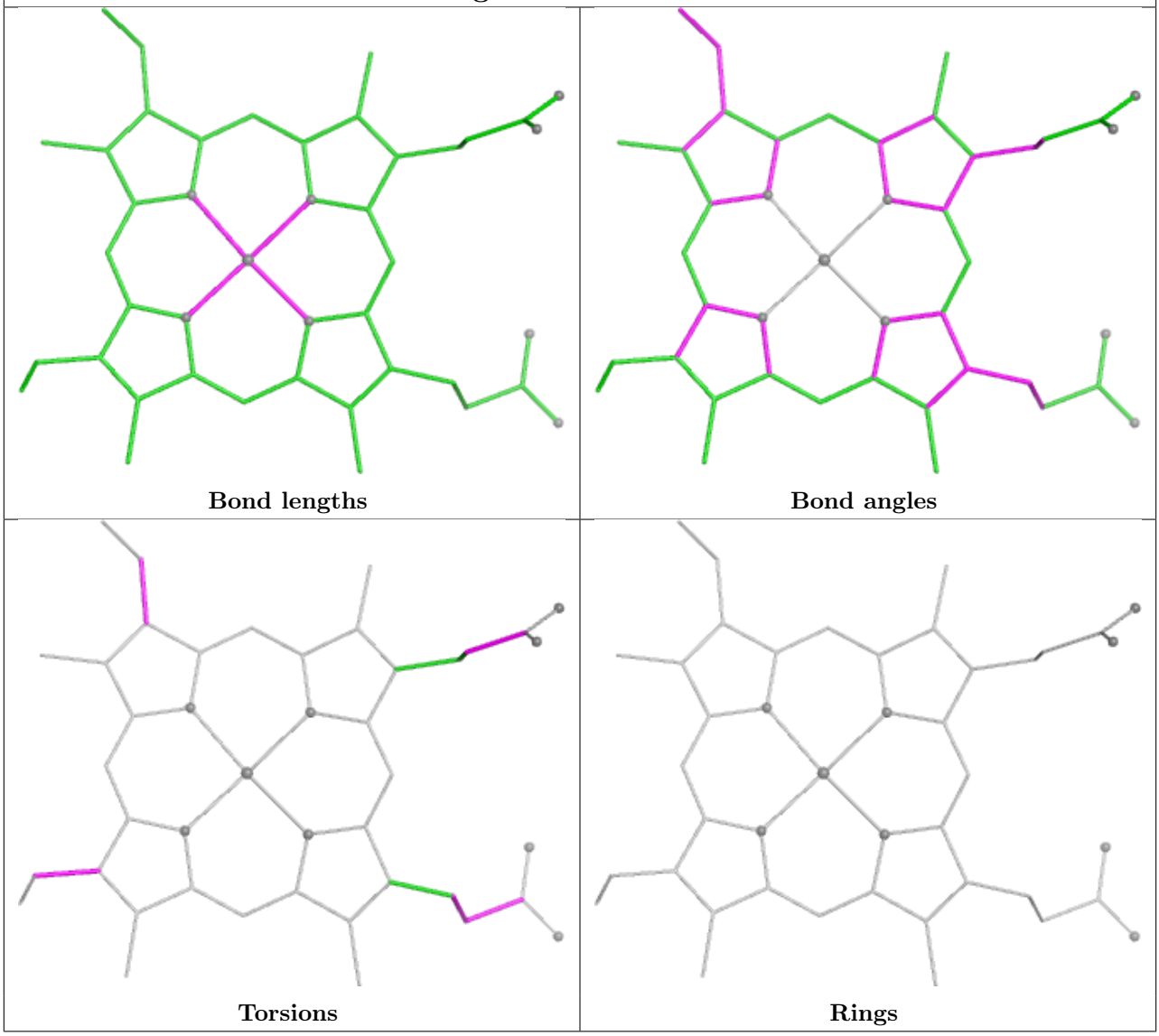


Torsions



Rings

Ligand HEC C 401



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	C	332/336 (98%)	-0.63	2 (0%)	85	80	73, 92, 119, 156	0
2	H	257/258 (99%)	-0.25	6 (2%)	61	51	80, 104, 152, 211	0
3	L	273/273 (100%)	-0.48	1 (0%)	88	84	75, 91, 117, 139	1 (0%)
4	M	323/323 (100%)	-0.44	1 (0%)	90	86	73, 90, 117, 149	0
All	All	1185/1190 (99%)	-0.46	10 (0%)	82	75	73, 93, 128, 211	1 (0%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	52	LEU	4.8
2	H	50	VAL	4.6
2	H	53	ALA	3.5
2	H	54	PRO	3.1
3	L	1	ALA	2.9
1	C	332	LYS	2.6
2	H	49	LEU	2.5
2	H	47	LEU	2.3
4	M	51	LEU	2.3
1	C	146	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
2	FME	H	1	10/11	0.95	0.12	93,105,115,130	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

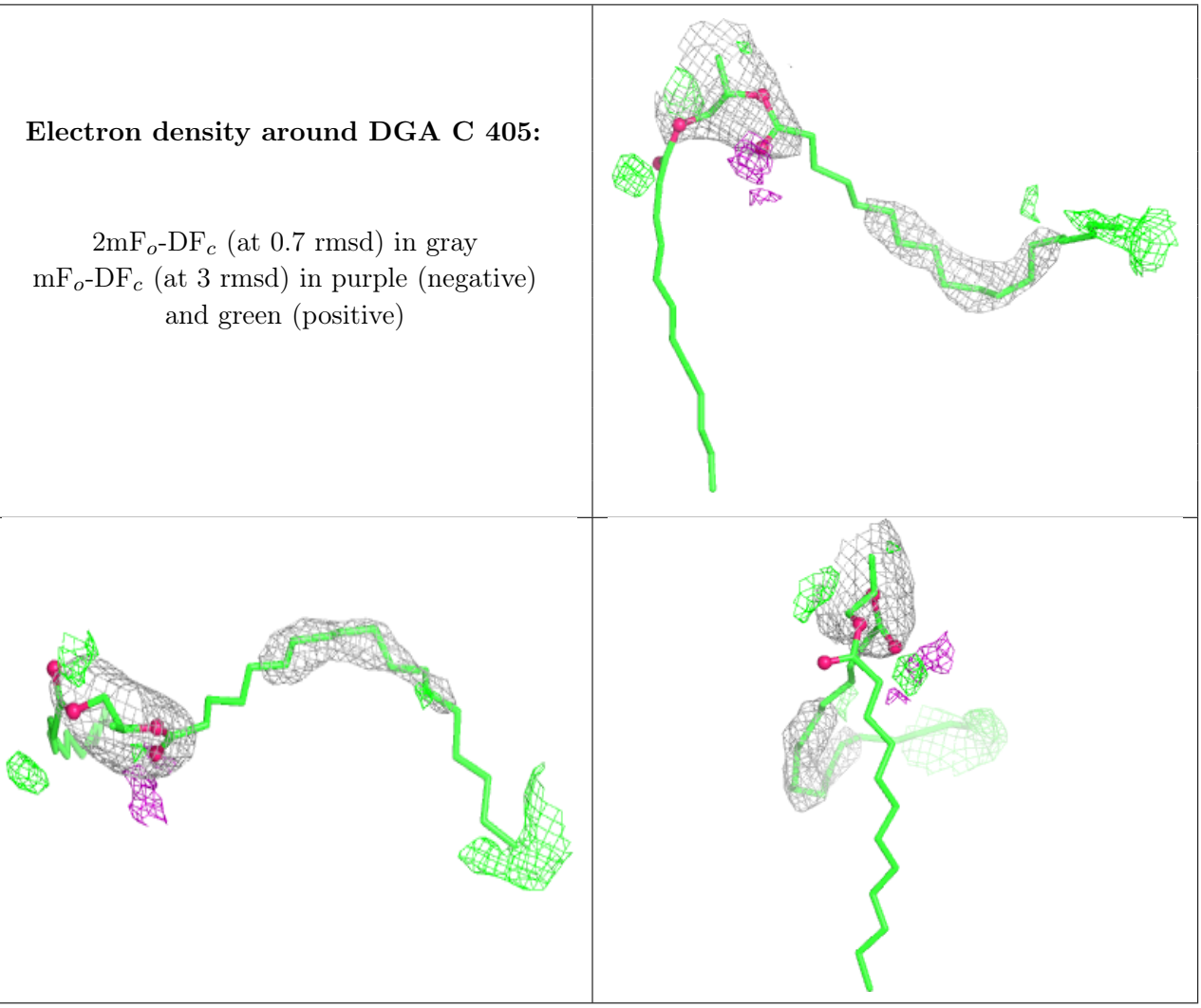
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	HTO	L	305	10/10	0.67	0.34	109,132,143,144	0
7	SO4	H	703	5/5	0.68	0.10	182,184,190,202	0
7	SO4	M	413	5/5	0.72	0.08	222,237,243,256	0
7	SO4	M	411	5/5	0.72	0.08	148,174,187,192	0
7	SO4	M	412	5/5	0.74	0.11	158,161,185,212	0
7	SO4	M	410	5/5	0.75	0.07	148,154,167,181	0
7	SO4	C	406	5/5	0.80	0.08	145,159,166,179	0
7	SO4	M	408	5/5	0.83	0.09	121,121,131,153	0
6	DGA	C	405	37/44	0.88	0.23	112,146,180,185	0
9	HTO	H	708	10/10	0.90	0.21	116,128,142,144	0
8	LDA	L	304	16/16	0.90	0.31	120,143,167,172	0
11	BPB	M	405	65/65	0.95	0.14	82,95,176,184	0
14	NS5	M	406	40/40	0.95	0.18	84,100,141,143	0
8	LDA	H	707	16/16	0.96	0.14	108,126,144,147	0
7	SO4	M	407	5/5	0.96	0.06	98,111,122,123	0
8	LDA	H	706	16/16	0.96	0.16	106,123,191,192	0
7	SO4	H	704	5/5	0.97	0.18	90,94,108,109	5
10	BCB	M	403	66/66	0.97	0.11	78,88,170,180	0
7	SO4	H	705	5/5	0.97	0.04	115,115,127,127	5
13	MQ7	M	402	48/48	0.97	0.11	80,88,125,148	0
7	SO4	H	702	5/5	0.97	0.07	105,115,122,126	0
8	LDA	H	701	16/16	0.98	0.12	89,103,119,119	0
10	BCB	M	404	66/66	0.98	0.11	61,76,107,113	0
11	BPB	L	303	65/65	0.98	0.09	78,84,92,98	0
7	SO4	M	409	5/5	0.98	0.05	85,93,99,100	0
10	BCB	L	301	66/66	0.98	0.10	67,77,93,111	0
10	BCB	L	302	66/66	0.98	0.09	72,80,112,115	0
5	HEC	C	404	43/43	0.99	0.06	75,84,101,123	0
5	HEC	C	401	43/43	0.99	0.06	88,96,110,124	0
5	HEC	C	402	43/43	0.99	0.06	83,95,105,131	0
5	HEC	C	403	43/43	0.99	0.05	70,79,90,93	0
12	FE2	M	401	1/1	1.00	0.04	91,91,91,91	0

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

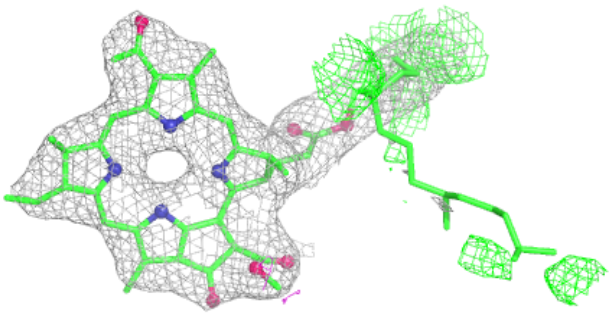
Electron density around DGA C 405:

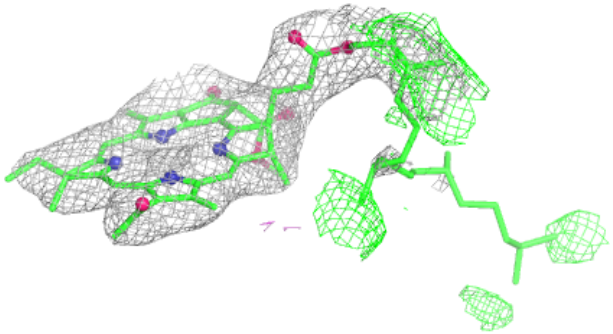
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

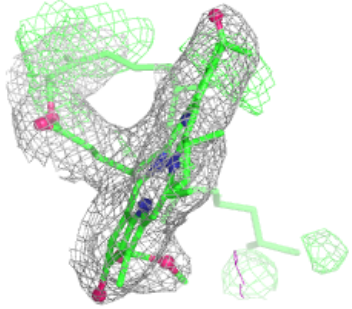


Electron density around BPB M 405:

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

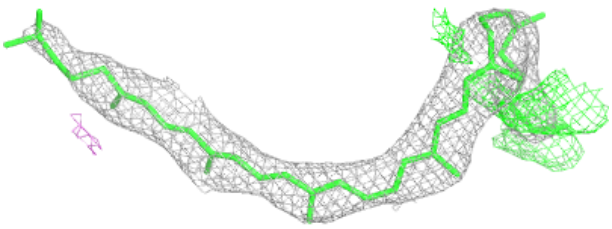


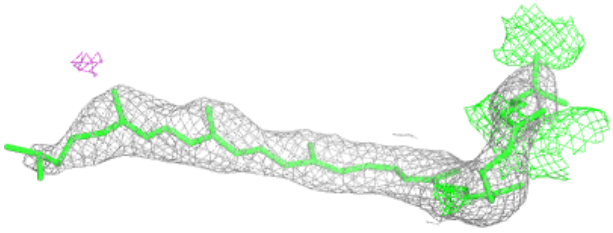


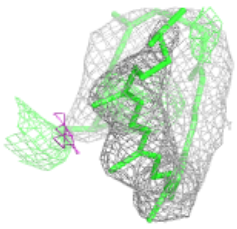


Electron density around NS5 M 406:

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

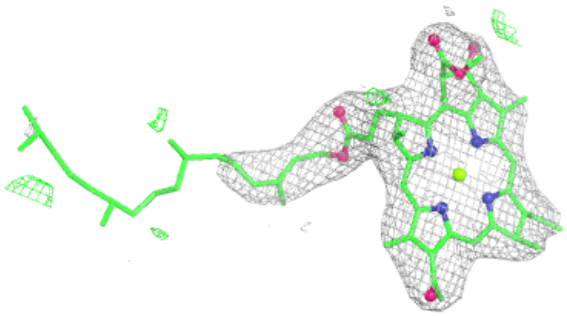


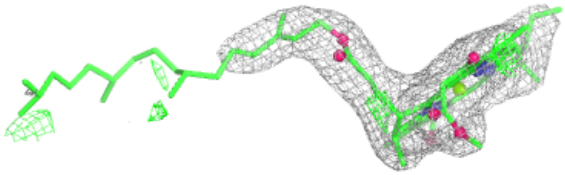


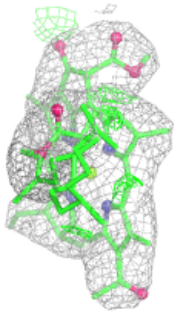


Electron density around BCB M 403:

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

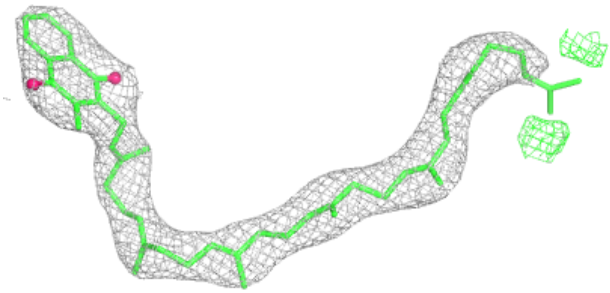


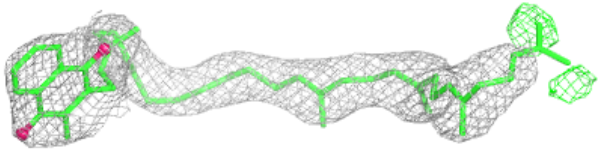


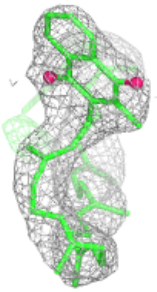


Electron density around MQ7 M 402:

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

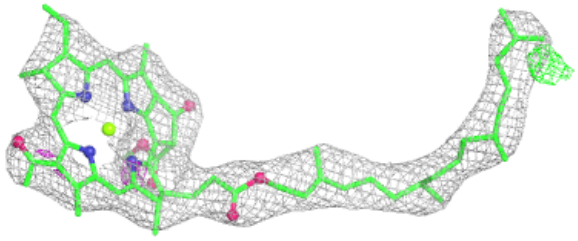


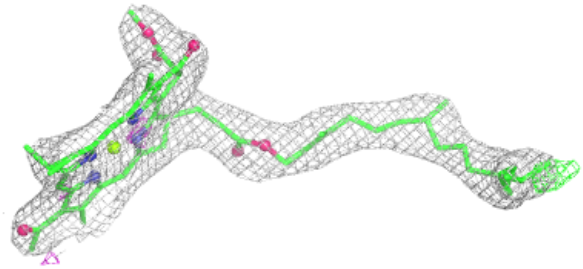


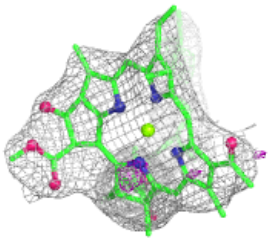


Electron density around BCB M 404:

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

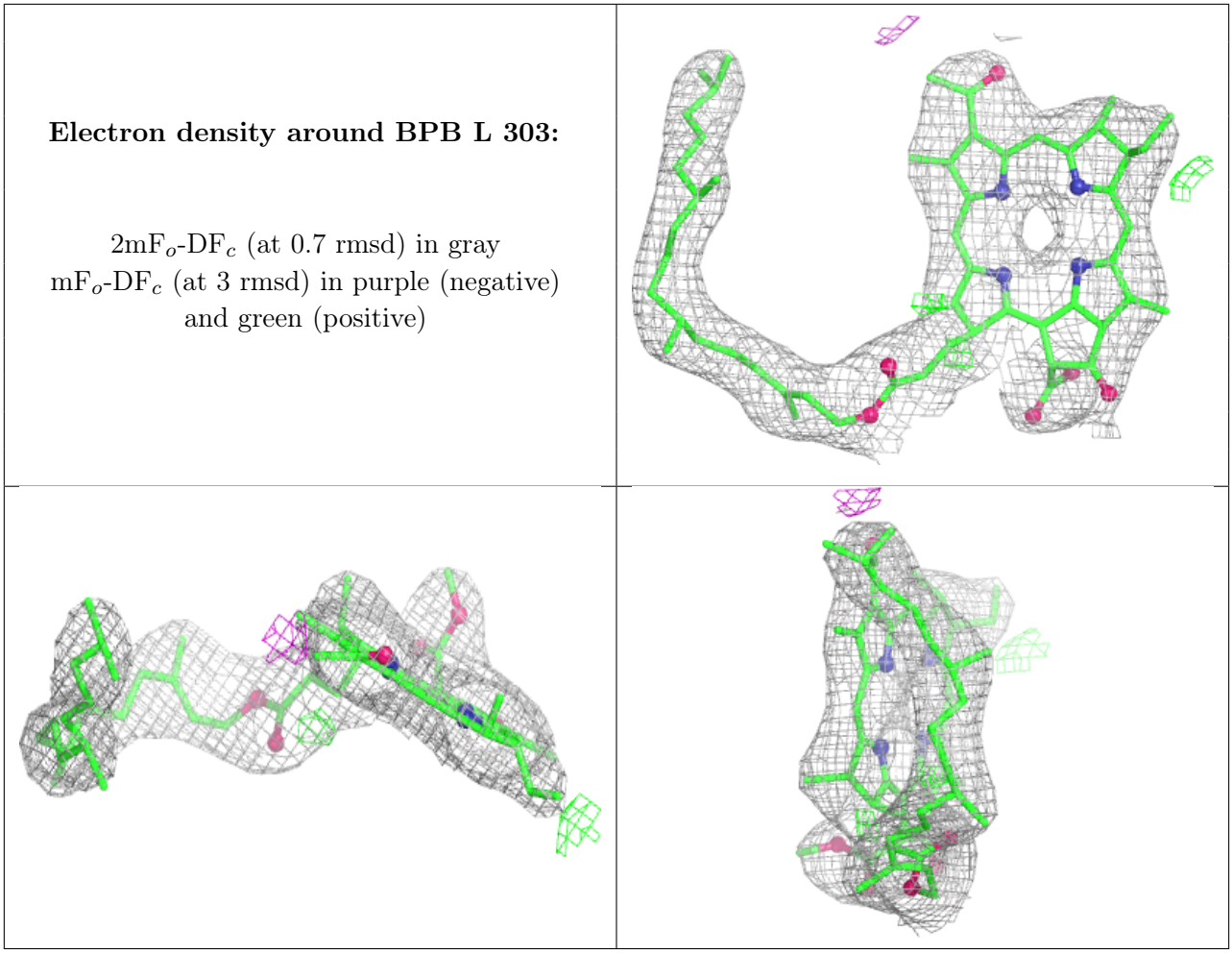






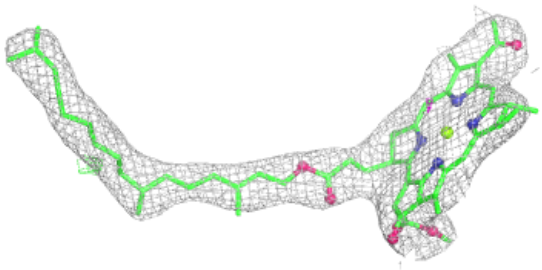
Electron density around BPB L 303:

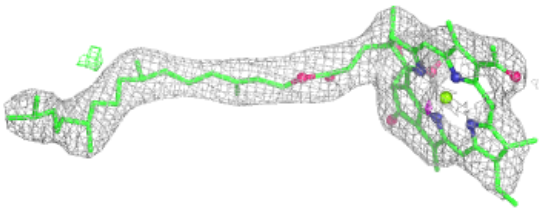
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around BCB L 301:

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

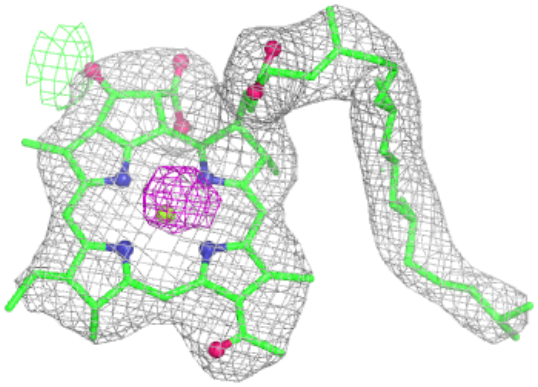


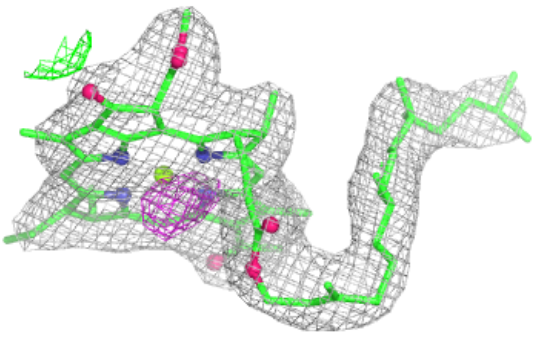


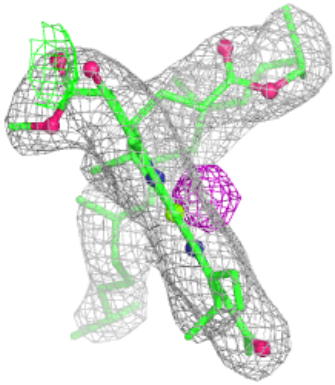


Electron density around BCB L 302:

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

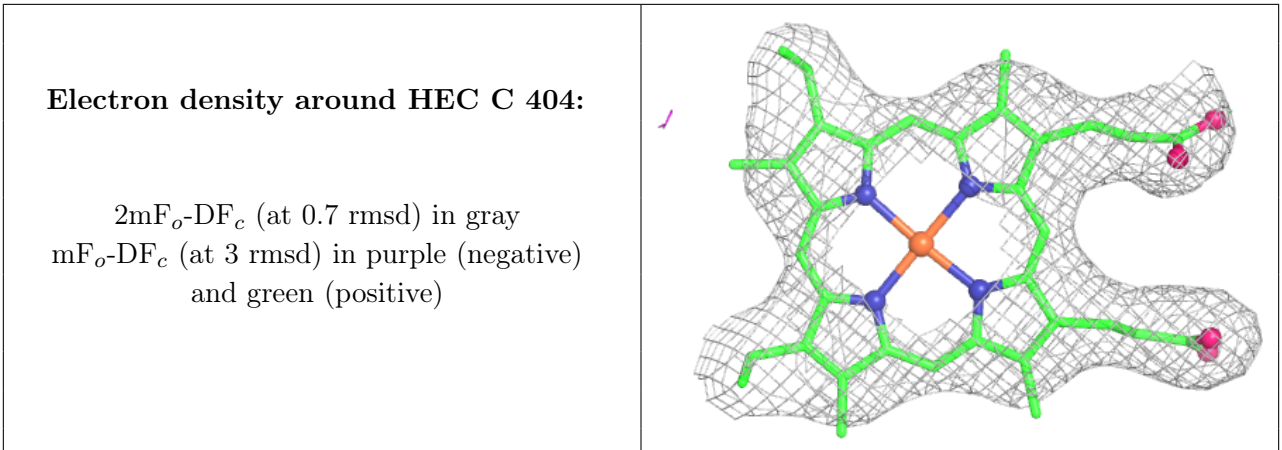


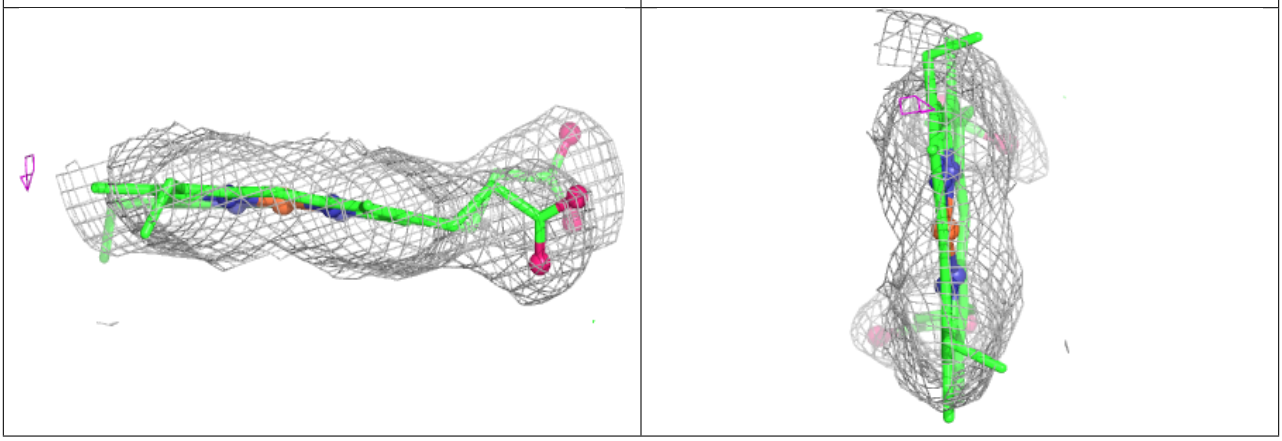




Electron density around HEC C 404:

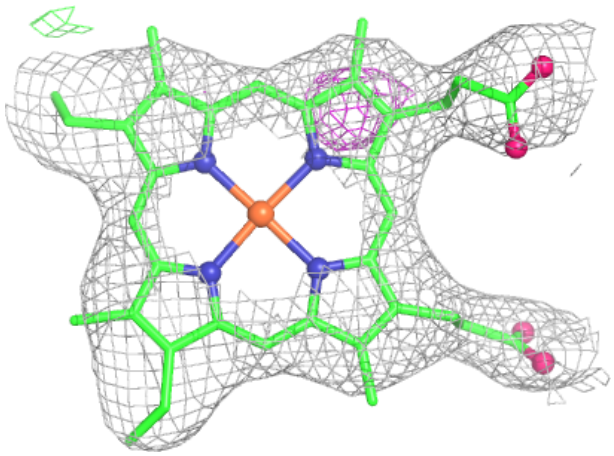
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

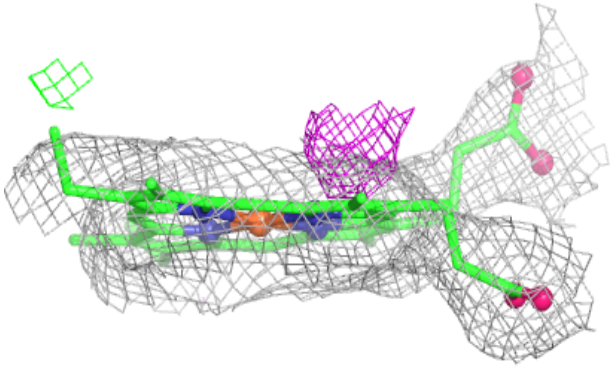




Electron density around HEC C 401:

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

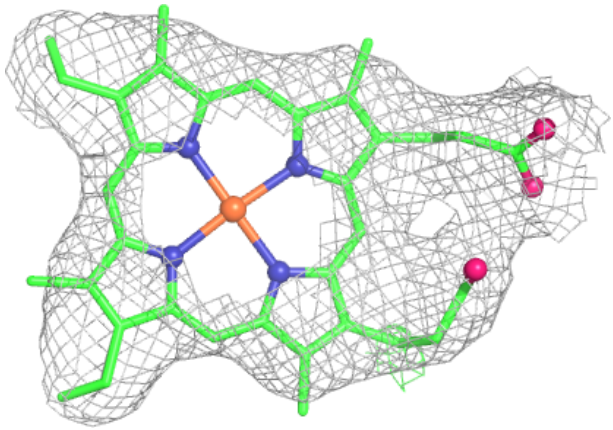


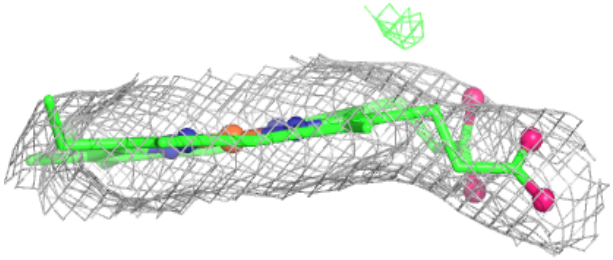


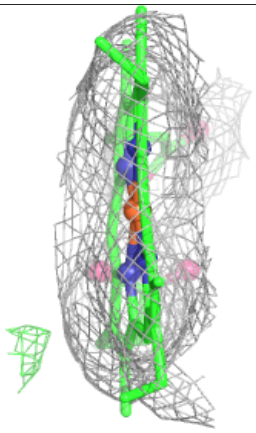


Electron density around HEC C 402:

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

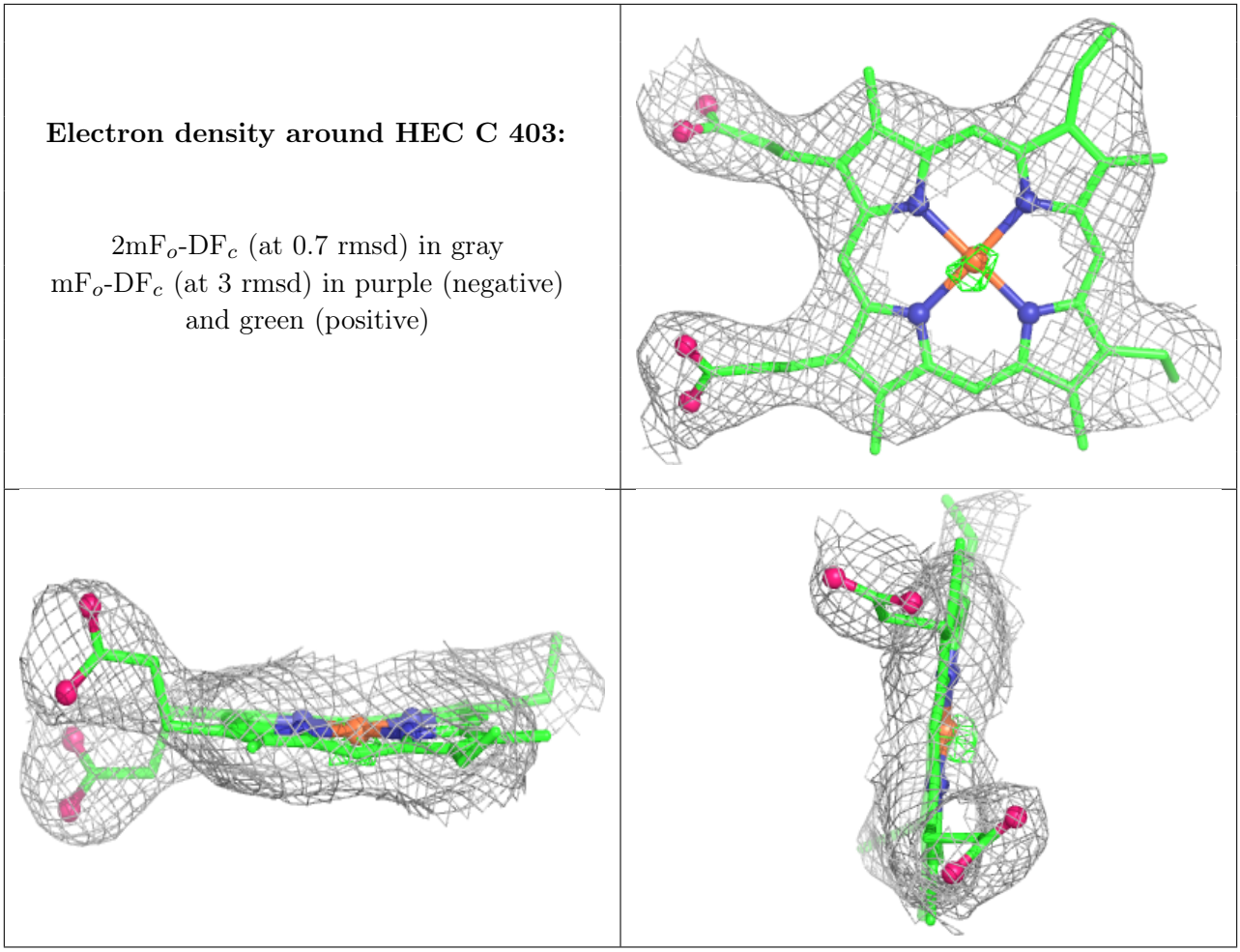






Electron density around HEC C 403:

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



6.5 Other polymers (i)

There are no such residues in this entry.