



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 30, 2022 – 12:40 am GMT

PDB ID : 5O64  
Title : From macrocrystals to microcrystals: a strategy for membrane protein serial crystallography  
Authors : Dods, R.; Baath, P.; Branden, G.; Neutze, R.  
Deposited on : 2017-06-05  
Resolution : 3.30 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.3
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

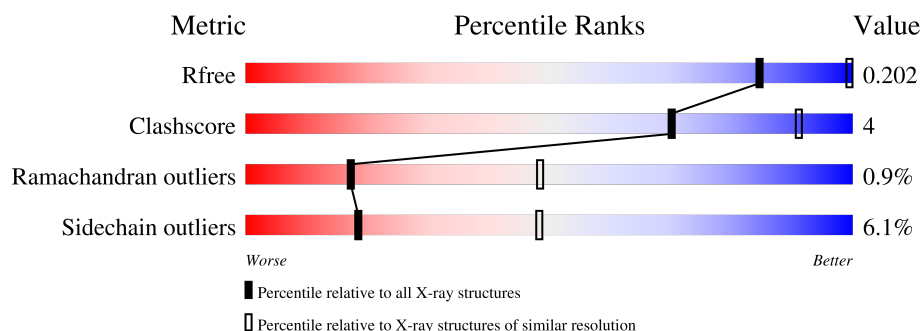
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)

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  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	C	336	87% 11% ..
2	H	258	82% 13% . .
3	L	273	86% 14%
4	M	323	87% 11% .

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
7	SO4	M	408	-	-	X	-

## 2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 10157 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	250	Total	C	N	O	S	0	0	0
			1962	1253	335	372	2			

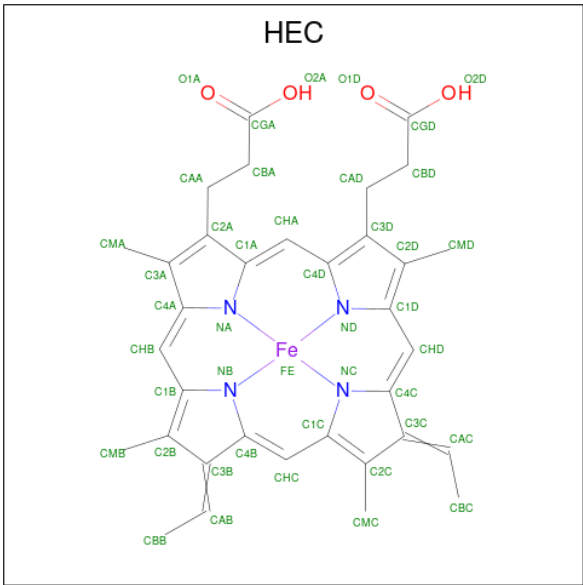
- Molecule 3 is a protein called Reaction center protein L chain.

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.

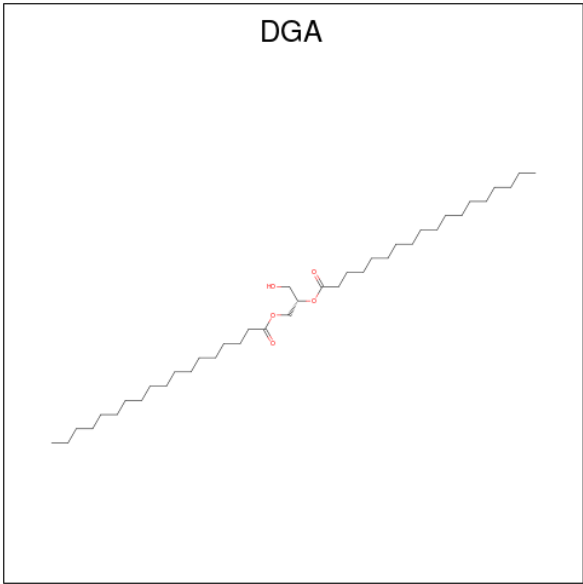
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	323	Total	C	N	O	S	0	0	0
			2555	1702	419	423	11			

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



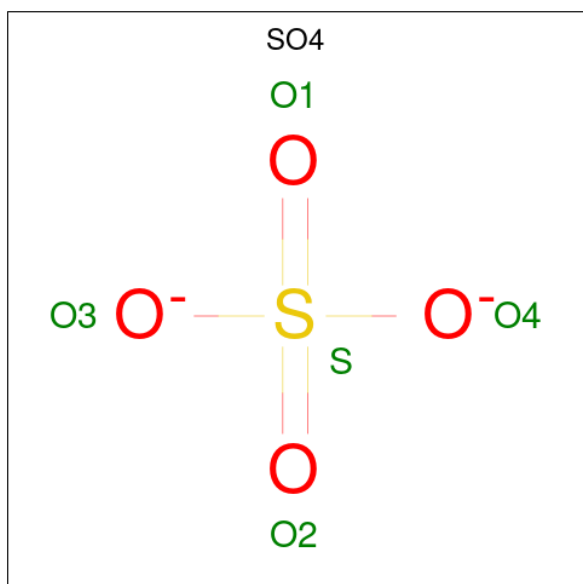
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 6 is DIACYL GLYCEROL (three-letter code: DGA) (formula: C<sub>39</sub>H<sub>76</sub>O<sub>5</sub>).



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

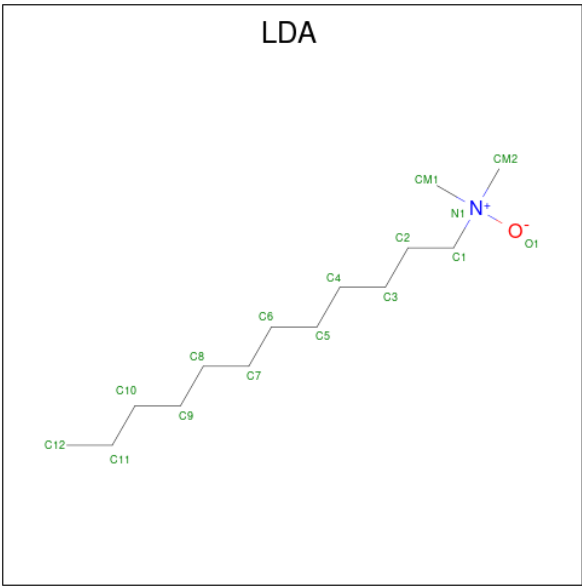
- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

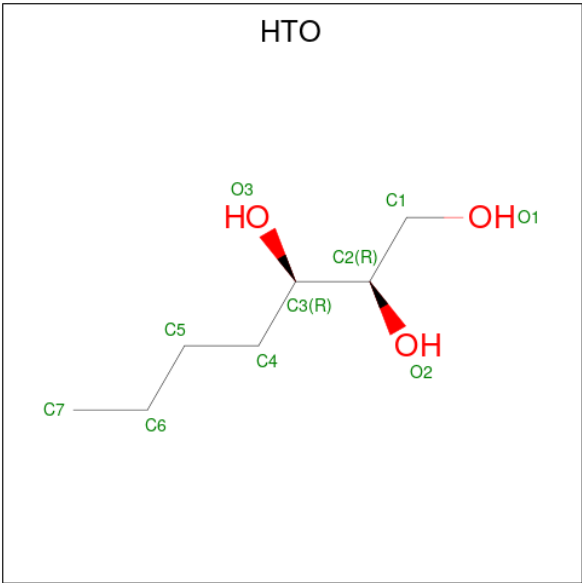
- Molecule 8 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula:

C<sub>14</sub>H<sub>31</sub>NO).



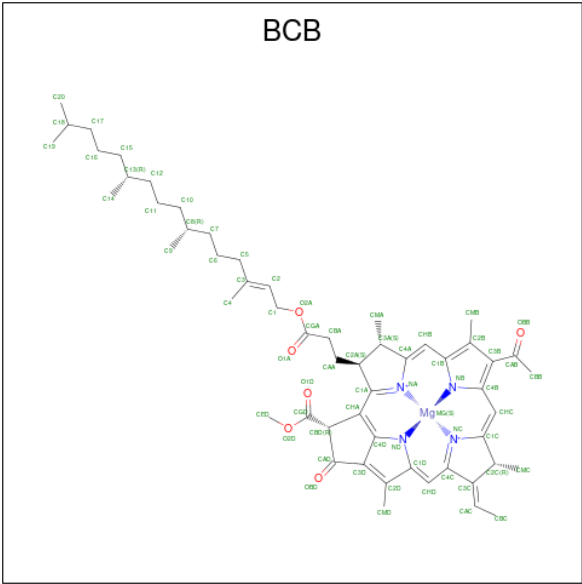
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	H	1	Total	C	N	O	0	0
			16	14	1	1		
8	H	1	Total	C	N	O	0	0
			16	14	1	1		
8	H	1	Total	C	N	O	0	0
			16	14	1	1		
8	M	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 9 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: C<sub>7</sub>H<sub>16</sub>O<sub>3</sub>).

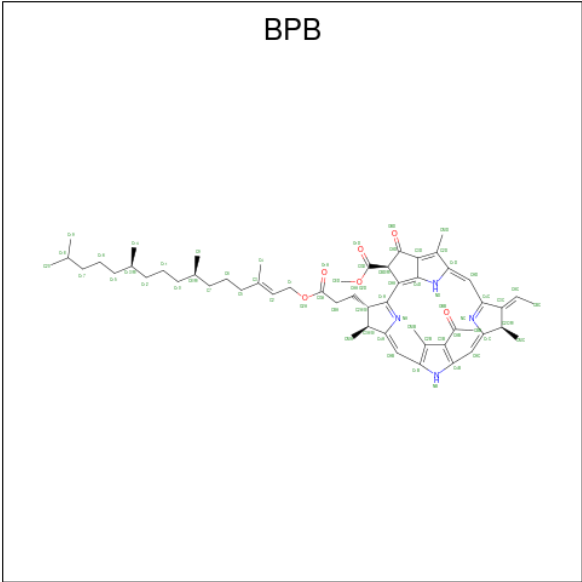


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	H	1	Total	C	O	0	0
			10	7	3		
9	L	1	Total	C	O	0	0
			10	7	3		
9	L	1	Total	C	O	0	0
			10	7	3		

- Molecule 10 is BACTERIOCHLOROPHYLL B (three-letter code: BCB) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>6</sub>).





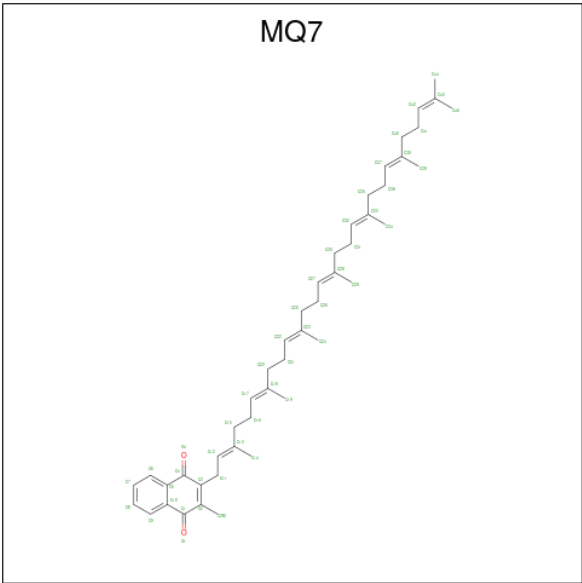


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	L	1	Total	C	N	O	0	0
			65	55	4	6		
11	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 12 is FE (II) ION (three-letter code: FE2) (formula: Fe).

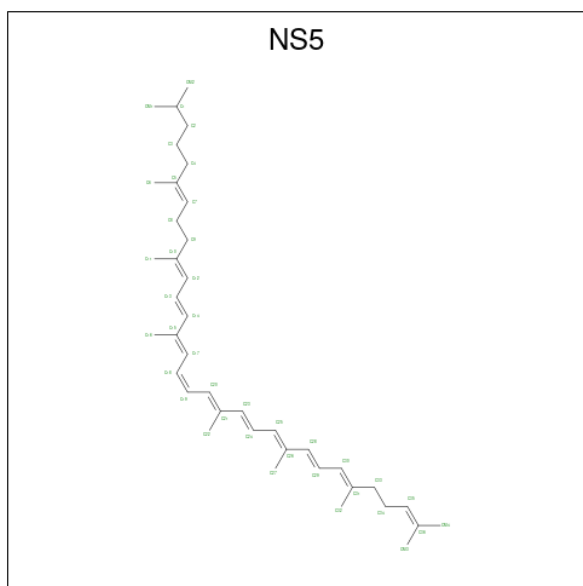
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	M	1	Total	Fe	0	0
			1	1		

- Molecule 13 is MENAQUINONE-7 (three-letter code: MQ7) (formula: C<sub>46</sub>H<sub>64</sub>O<sub>2</sub>).



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

- Molecule 14 is 15-cis-1,2-dihydroneurosporene (three-letter code: NS5) (formula: C<sub>40</sub>H<sub>60</sub>).



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

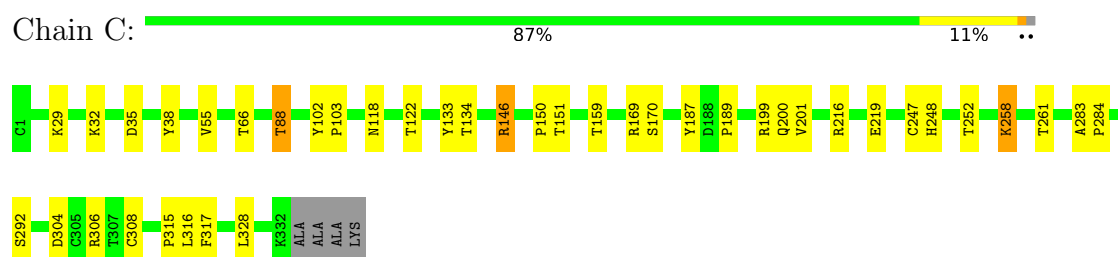
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	C	7	Total	O	0	0
			7	7		
15	H	3	Total	O	0	0
			3	3		
15	L	13	Total	O	0	0
			13	13		
15	M	7	Total	O	0	0
			7	7		

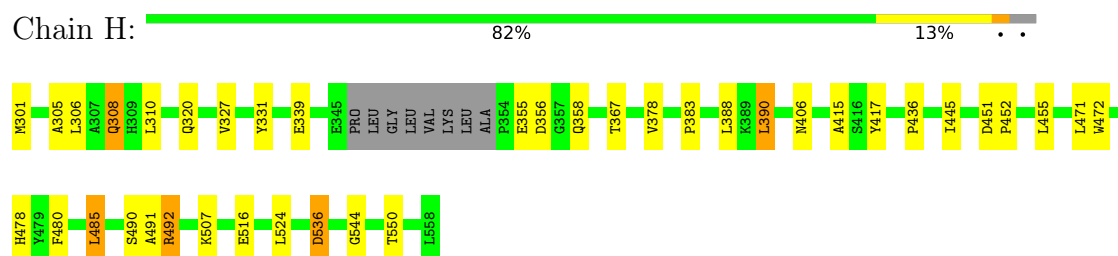
### 3 Residue-property plots

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. 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. 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.

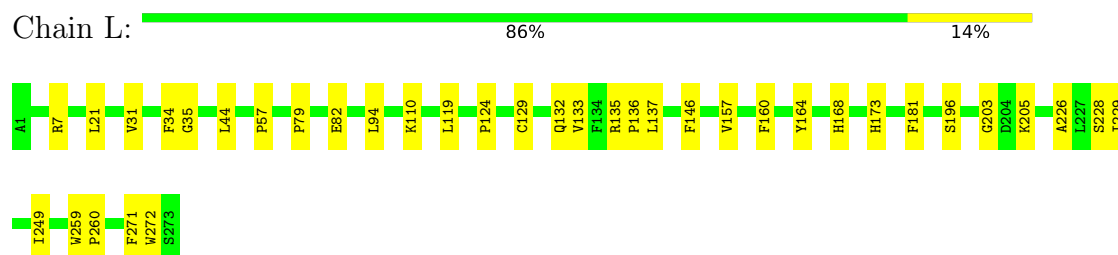
- Molecule 1: Photosynthetic reaction center cytochrome c subunit



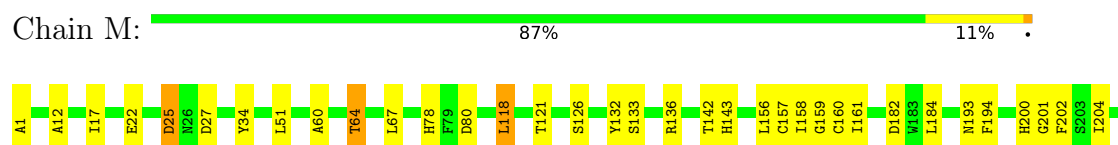
- Molecule 2: Reaction center protein H chain



- Molecule 3: Reaction center protein L chain



- Molecule 4: Reaction center protein M chain





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	226.60Å 226.60Å 113.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.39 – 3.30 46.39 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.39-3.30) 100.0 (46.39-3.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.44 (at 3.32Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.154 , 0.196 0.167 , 0.202	Depositor DCC
$R_{free}$ test set	2294 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	123.8	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10157	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: FME, NS5, LDA, HEC, SO4, BCB, DGA, FE2, HTO, BPB, MQ7

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	0.56	0/2669	0.83	2/3637 (0.1%)
2	H	0.59	0/1997	0.83	1/2725 (0.0%)
3	L	0.59	0/2267	0.77	0/3095
4	M	0.57	0/2659	0.77	3/3637 (0.1%)
All	All	0.58	0/9592	0.80	6/13094 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	485	LEU	CA-CB-CG	5.68	128.36	115.30
4	M	80	ASP	CB-CG-OD1	5.56	123.31	118.30
1	C	146	ARG	NE-CZ-NH1	-5.54	117.53	120.30
1	C	306	ARG	NE-CZ-NH2	-5.36	117.62	120.30
4	M	239	ARG	NE-CZ-NH1	5.10	122.85	120.30
4	M	182	ASP	CB-CG-OD1	5.09	122.88	118.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2602	0	2578	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	1962	0	1950	12	0
3	L	2172	0	2097	17	0
4	M	2555	0	2452	21	0
5	C	172	0	120	7	0
6	C	37	0	58	0	0
7	C	5	0	0	1	0
7	H	15	0	0	0	0
7	M	30	0	0	2	0
8	H	48	0	93	0	0
8	M	16	0	31	0	0
9	H	10	0	16	0	0
9	L	20	0	32	0	0
10	L	132	0	144	7	0
10	M	132	0	144	4	0
11	L	65	0	74	2	0
11	M	65	0	74	2	0
12	M	1	0	0	0	0
13	M	48	0	64	1	0
14	M	40	0	60	4	0
15	C	7	0	0	0	0
15	H	3	0	0	0	0
15	L	13	0	0	0	0
15	M	7	0	0	0	0
All	All	10157	0	9987	73	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 (73) 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)
5:C:401:HEC:HMB1	5:C:401:HEC:HBB3	1.69	0.75
3:L:31:VAL:HG22	13:M:402:MQ7:H401	1.72	0.72
11:L:303:BPB:HBBB	11:L:303:BPB:HMB	1.77	0.67
4:M:159:GLY:HA3	14:M:406:NS5:H272	1.80	0.63
3:L:132:GLN:HE22	3:L:146:PHE:H	1.47	0.61
3:L:133:VAL:O	3:L:137:LEU:HG	2.00	0.60
2:H:480:PHE:CE2	4:M:12:ALA:HB2	2.38	0.59
2:H:320:GLN:HG2	4:M:202:PHE:CE2	2.37	0.59
10:L:302:BCB:HMD2	10:M:404:BCB:HBB3	1.86	0.58
1:C:216:ARG:O	1:C:219:GLU:HG2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:401:HEC:HBC1	5:C:402:HEC:HMA1	1.87	0.56
4:M:160:CYS:SG	14:M:406:NS5:H322	2.46	0.56
4:M:1:ALA:N	7:M:408:SO4:O2	2.38	0.55
2:H:388:LEU:HB3	2:H:390:LEU:HD12	1.89	0.55
4:M:1:ALA:N	7:M:408:SO4:S	2.80	0.55
2:H:415:ALA:HB2	2:H:544:GLY:HA3	1.90	0.54
3:L:181:PHE:HB3	11:M:405:BPB:CBB	2.38	0.54
1:C:102:TYR:CG	1:C:103:PRO:HD3	2.43	0.53
1:C:200:GLN:HE21	1:C:201:VAL:N	2.06	0.53
10:L:302:BCB:HMB1	10:L:302:BCB:HBB2	1.91	0.53
5:C:404:HEC:HHB	5:C:404:HEC:CBD	2.39	0.52
4:M:121:THR:HG23	4:M:156:LEU:HD21	1.91	0.52
2:H:305:ALA:O	2:H:306:LEU:HD23	2.09	0.51
3:L:124:PRO:HD3	11:L:303:BPB:HAC	1.92	0.51
5:C:401:HEC:HBB3	5:C:401:HEC:CMB	2.38	0.51
3:L:168:HIS:CE1	10:L:301:BCB:HMC2	2.46	0.51
1:C:283:ALA:N	1:C:284:PRO:HD2	2.26	0.51
4:M:184:LEU:CD2	10:M:403:BCB:HBC3	2.40	0.51
5:C:404:HEC:HHB	5:C:404:HEC:HBD1	1.94	0.50
2:H:445:ILE:HD13	2:H:451:ASP:HA	1.93	0.50
4:M:184:LEU:HD21	10:M:403:BCB:HBC3	1.92	0.50
2:H:490:SER:O	2:H:492:ARG:N	2.46	0.49
10:M:403:BCB:HHC	10:M:403:BCB:HBB2	1.96	0.48
1:C:258:LYS:HE3	4:M:305:TYR:O	2.14	0.47
3:L:226:ALA:O	3:L:229:ILE:HG22	2.15	0.47
1:C:35:ASP:OD2	1:C:316:LEU:HA	2.17	0.45
3:L:34:PHE:O	3:L:35:GLY:C	2.54	0.45
3:L:157:VAL:HG22	10:L:302:BCB:HBC3	1.99	0.45
5:C:402:HEC:HMB1	5:C:402:HEC:HBB3	1.99	0.45
4:M:132:TYR:CE1	4:M:142:THR:HG21	2.53	0.44
2:H:452:PRO:HD2	2:H:471:LEU:HD11	2.00	0.44
4:M:60:ALA:O	4:M:64:THR:HG23	2.17	0.44
1:C:133:TYR:O	1:C:134:THR:C	2.56	0.44
1:C:308:CYS:O	1:C:315:PRO:HB3	2.18	0.44
4:M:25:ASP:N	4:M:25:ASP:OD1	2.52	0.43
2:H:327:VAL:O	2:H:331:TYR:HB3	2.18	0.43
3:L:94:LEU:HD21	3:L:129:CYS:SG	2.59	0.43
4:M:118:LEU:HD22	14:M:406:NS5:HM33	1.99	0.43
2:H:452:PRO:HA	2:H:455:LEU:HD12	2.01	0.43
5:C:403:HEC:HBC1	5:C:404:HEC:HMA1	2.01	0.42
2:H:417:TYR:HB2	2:H:536:ASP:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:302:BCB:HMD1	4:M:204:ILE:HD13	2.00	0.42
1:C:247:CYS:HA	1:C:261:THR:OG1	2.19	0.42
1:C:169:ARG:N	7:C:406:SO4:O3	2.52	0.42
2:H:436:PRO:HA	2:H:472:TRP:HA	2.01	0.42
1:C:32:LYS:HA	1:C:317:PHE:CE1	2.55	0.42
3:L:196:SER:N	4:M:143:HIS:HD2	2.18	0.42
4:M:200:HIS:CE1	4:M:204:ILE:HD11	2.55	0.42
3:L:132:GLN:NE2	3:L:132:GLN:HA	2.34	0.41
3:L:259:TRP:N	3:L:260:PRO:CD	2.82	0.41
14:M:406:NS5:H18	14:M:406:NS5:H161	1.88	0.41
4:M:239:ARG:HD3	4:M:244:GLU:HG2	2.02	0.41
4:M:157:CYS:HA	4:M:161:ILE:HB	2.01	0.41
1:C:187:TYR:O	1:C:189:PRO:HD3	2.20	0.41
3:L:79:PRO:HG2	3:L:82:GLU:HB2	2.03	0.41
11:M:405:BPB:HHC	11:M:405:BPB:HBBB	2.03	0.41
3:L:135:ARG:HB3	3:L:136:PRO:HD3	2.03	0.40
3:L:164:TYR:CD1	3:L:164:TYR:N	2.89	0.40
10:L:302:BCB:OBD	4:M:201:GLY:HA2	2.21	0.40
1:C:146:ARG:NH1	1:C:150:PRO:HA	2.36	0.40
4:M:34:TYR:CD1	4:M:34:TYR:N	2.89	0.40
3:L:173:HIS:HA	10:L:301:BCB:HED2	2.04	0.40
1:C:118:ASN:ND2	1:C:328:LEU:O	2.48	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	330/336 (98%)	310 (94%)	18 (6%)	2 (1%)	25 57
2	H	246/258 (95%)	223 (91%)	20 (8%)	3 (1%)	13 42
3	L	272/273 (100%)	248 (91%)	21 (8%)	3 (1%)	14 45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	M	321/323 (99%)	301 (94%)	18 (6%)	2 (1%)	25 57
All	All	1169/1190 (98%)	1082 (93%)	77 (7%)	10 (1%)	17 48

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	55	VAL
3	L	57	PRO
3	L	271	PHE
2	H	383	PRO
3	L	203	GLY
4	M	78	HIS
1	C	88	THR
2	H	308	GLN
2	H	491	ALA
4	M	193	ASN

### 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	C	281/282 (100%)	267 (95%)	14 (5%)	24 55
2	H	206/212 (97%)	188 (91%)	18 (9%)	10 34
3	L	219/218 (100%)	209 (95%)	10 (5%)	27 58
4	M	249/249 (100%)	233 (94%)	16 (6%)	17 46
All	All	955/961 (99%)	897 (94%)	58 (6%)	18 48

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	29	LYS
1	C	38	TYR
1	C	66	THR
1	C	88	THR

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Mol	Chain	Res	Type
1	C	122	THR
1	C	151	THR
1	C	159	THR
1	C	170	SER
1	C	199	ARG
1	C	248	HIS
1	C	252	THR
1	C	258	LYS
1	C	292	SER
1	C	304	ASP
2	H	308	GLN
2	H	310	LEU
2	H	339	GLU
2	H	355	GLU
2	H	356	ASP
2	H	358	GLN
2	H	367	THR
2	H	378	VAL
2	H	390	LEU
2	H	406	ASN
2	H	478	HIS
2	H	485	LEU
2	H	492	ARG
2	H	507	LYS
2	H	516	GLU
2	H	524	LEU
2	H	536	ASP
2	H	550	THR
3	L	7	ARG
3	L	21	LEU
3	L	44	LEU
3	L	110	LYS
3	L	119	LEU
3	L	160	PHE
3	L	205	LYS
3	L	228	SER
3	L	249	ILE
3	L	272	TRP
4	M	17	ILE
4	M	22	GLU
4	M	25	ASP
4	M	27	ASP

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Mol	Chain	Res	Type
4	M	51	LEU
4	M	64	THR
4	M	67	LEU
4	M	118	LEU
4	M	126	SER
4	M	133	SER
4	M	136	ARG
4	M	158	ILE
4	M	194	PHE
4	M	214	PHE
4	M	226	ARG
4	M	290	ASP

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	200	GLN
2	H	308	GLN
2	H	392	GLN
2	H	402	GLN
2	H	406	ASN
3	L	132	GLN
3	L	144	HIS
3	L	158	ASN
3	L	239	ASN
4	M	143	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	301	2	8,9,10	0.93	0	7,9,11	3.58	4 (57%)

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	301	2	-	3/7/9/11	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	301	FME	CA-N-CN	-7.86	110.73	122.82
2	H	301	FME	CE-SD-CG	4.05	114.32	100.40
2	H	301	FME	O-C-CA	-2.28	118.81	124.78
2	H	301	FME	O1-CN-N	-2.11	119.71	125.27

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	301	FME	O1-CN-N-CA
2	H	301	FME	O-C-CA-CB
2	H	301	FME	CB-CG-SD-CE

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

Of 31 ligands modelled in this entry, 1 is monoatomic - leaving 30 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
5	HEC	C	404	1	32,50,50	1.59	4 (12%)	24,82,82	1.55	5 (20%)
7	SO4	M	411	-	4,4,4	0.39	0	6,6,6	0.32	0
7	SO4	H	602	-	4,4,4	0.49	0	6,6,6	0.50	0
10	BCB	L	302	-	54,74,74	2.36	16 (29%)	52,115,115	2.62	14 (26%)
9	HTO	L	304	-	9,9,9	1.23	2 (22%)	10,10,10	1.40	2 (20%)
8	LDA	H	601	-	12,15,15	2.09	1 (8%)	14,17,17	0.55	0
8	LDA	H	605	-	12,15,15	2.13	1 (8%)	14,17,17	0.84	1 (7%)
10	BCB	M	404	-	54,74,74	2.40	13 (24%)	52,115,115	2.48	13 (25%)
6	DGA	C	405	1	36,36,43	1.46	3 (8%)	38,38,45	1.71	6 (15%)
7	SO4	M	410	-	4,4,4	0.37	0	6,6,6	0.27	0
7	SO4	H	603	-	4,4,4	0.40	0	6,6,6	0.35	0
5	HEC	C	401	1	32,50,50	1.66	2 (6%)	24,82,82	1.93	5 (20%)
9	HTO	H	607	-	9,9,9	0.83	0	10,10,10	1.26	2 (20%)
5	HEC	C	402	1	32,50,50	1.59	4 (12%)	24,82,82	1.83	7 (29%)
14	NS5	M	406	-	39,39,39	1.65	4 (10%)	44,46,46	2.39	16 (36%)
7	SO4	M	408	-	4,4,4	0.41	0	6,6,6	0.28	0
7	SO4	H	604	-	4,4,4	0.33	0	6,6,6	0.19	0
11	BPB	M	405	-	49,70,70	2.27	10 (20%)	47,101,101	2.18	10 (21%)
11	BPB	L	303	-	49,70,70	2.12	10 (20%)	47,101,101	1.84	9 (19%)
10	BCB	M	403	-	54,74,74	2.41	15 (27%)	52,115,115	2.49	12 (23%)
10	BCB	L	301	-	54,74,74	2.36	14 (25%)	52,115,115	2.30	15 (28%)
7	SO4	C	406	-	4,4,4	0.44	0	6,6,6	0.46	0
8	LDA	H	606	-	12,15,15	1.94	1 (8%)	14,17,17	0.50	0
7	SO4	M	409	-	4,4,4	0.32	0	6,6,6	0.74	0
7	SO4	M	407	-	4,4,4	0.36	0	6,6,6	0.58	0
9	HTO	L	305	-	9,9,9	0.72	0	10,10,10	0.67	0
8	LDA	M	413	-	12,15,15	2.10	1 (8%)	14,17,17	0.40	0
13	MQ7	M	402	-	49,49,49	1.48	3 (6%)	60,63,63	1.22	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	HEC	C	403	1	32,50,50	1.75	4 (12%)	24,82,82	1.56	4 (16%)
7	SO4	M	412	-	4,4,4	0.45	0	6,6,6	0.38	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	404	1	-	4/10/54/54	-
10	BCB	L	302	-	-	8/37/177/177	-
9	HTO	L	304	-	-	2/10/10/10	-
8	LDA	H	601	-	-	4/13/13/13	-
8	LDA	H	605	-	-	7/13/13/13	-
10	BCB	M	404	-	-	9/37/177/177	-
6	DGA	C	405	1	-	21/37/37/45	-
5	HEC	C	401	1	-	4/10/54/54	-
9	HTO	H	607	-	-	4/10/10/10	-
5	HEC	C	402	1	-	3/10/54/54	-
14	NS5	M	406	-	-	13/43/43/43	-
11	BPB	M	405	-	-	16/37/105/105	0/5/6/6
11	BPB	L	303	-	-	10/37/105/105	0/5/6/6
10	BCB	M	403	-	-	13/37/177/177	-
10	BCB	L	301	-	-	9/37/177/177	-
8	LDA	H	606	-	-	4/13/13/13	-
9	HTO	L	305	-	-	3/10/10/10	-
8	LDA	M	413	-	-	5/13/13/13	-
13	MQ7	M	402	-	-	2/41/61/61	0/2/2/2
5	HEC	C	403	1	-	0/10/54/54	-

All (108) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	404	BCB	C1A-CHA	8.63	1.49	1.39
13	M	402	MQ7	C3-C2	8.00	1.49	1.35
10	L	301	BCB	C1A-CHA	7.98	1.48	1.39
14	M	406	NS5	C35-C36	7.74	1.54	1.32
11	M	405	BPB	CAC-C3C	7.74	1.53	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	L	303	BPB	CAC-C3C	7.69	1.53	1.33
8	H	605	LDA	O1-N1	-7.31	1.25	1.42
10	M	403	BCB	C1A-CHA	7.15	1.47	1.39
8	H	601	LDA	O1-N1	-7.14	1.25	1.42
8	M	413	LDA	O1-N1	-7.07	1.25	1.42
8	H	606	LDA	O1-N1	-6.63	1.26	1.42
10	L	302	BCB	C1A-CHA	6.27	1.46	1.39
11	M	405	BPB	O2A-CGA	6.07	1.51	1.33
5	C	401	HEC	C2B-C3B	-6.03	1.34	1.40
5	C	403	HEC	C2B-C3B	-5.97	1.34	1.40
10	M	404	BCB	CAC-C3C	5.69	1.47	1.33
10	M	403	BCB	CHD-C4C	5.69	1.47	1.37
10	L	301	BCB	CAC-C3C	5.62	1.47	1.33
6	C	405	DGA	OG2-CB1	5.60	1.50	1.34
10	L	301	BCB	O2D-CGD	5.56	1.46	1.33
10	L	302	BCB	CHD-C4C	5.44	1.46	1.37
10	M	403	BCB	CAC-C3C	5.42	1.47	1.33
11	M	405	BPB	C3D-C2D	5.32	1.49	1.39
10	L	302	BCB	CAC-C3C	5.29	1.46	1.33
5	C	402	HEC	C2B-C3B	-5.20	1.35	1.40
10	M	404	BCB	C3B-C2B	5.14	1.48	1.39
11	M	405	BPB	OBD-CAD	5.04	1.29	1.22
13	M	402	MQ7	C10-C5	5.00	1.49	1.40
6	C	405	DGA	OG1-CA1	4.93	1.47	1.33
11	L	303	BPB	O2D-CGD	4.92	1.45	1.33
11	L	303	BPB	C3B-C2B	4.92	1.48	1.39
10	M	403	BCB	O2D-CGD	4.91	1.45	1.33
10	M	403	BCB	C3D-C2D	4.88	1.48	1.39
10	M	404	BCB	CHD-C4C	4.83	1.45	1.37
5	C	404	HEC	C2B-C3B	-4.81	1.35	1.40
11	L	303	BPB	OBD-CAD	4.73	1.28	1.22
10	M	404	BCB	O2D-CGD	4.70	1.44	1.33
10	M	403	BCB	C3A-C2A	-4.68	1.50	1.54
10	L	301	BCB	OBD-CAD	4.66	1.28	1.22
10	M	403	BCB	O2A-CGA	4.66	1.47	1.33
10	L	302	BCB	C3B-C2B	4.59	1.47	1.39
11	M	405	BPB	O2D-CGD	4.57	1.44	1.33
10	L	302	BCB	CHA-CBD	-4.55	1.47	1.52
10	L	301	BCB	C3B-C2B	4.53	1.47	1.39
10	M	404	BCB	CHA-CBD	-4.46	1.47	1.52
10	L	302	BCB	OBD-CAD	4.42	1.28	1.22
11	L	303	BPB	C3D-C2D	4.40	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	L	301	BCB	CHC-C4B	4.35	1.49	1.40
5	C	401	HEC	C3C-C2C	-4.33	1.36	1.40
10	M	404	BCB	O2A-CGA	4.29	1.45	1.33
10	L	301	BCB	O2A-CGA	4.27	1.45	1.33
10	M	404	BCB	C3D-C2D	4.25	1.47	1.39
5	C	403	HEC	C3C-C2C	-4.25	1.36	1.40
10	L	301	BCB	CHD-C4C	4.14	1.44	1.37
10	M	404	BCB	OBD-CAD	4.04	1.28	1.22
10	L	302	BCB	CBD-CGD	-4.01	1.47	1.52
10	L	302	BCB	O2D-CGD	4.00	1.43	1.33
11	M	405	BPB	CHA-CBD	-3.98	1.47	1.52
10	M	403	BCB	OBD-CAD	3.96	1.27	1.22
10	L	302	BCB	C3D-C2D	3.96	1.46	1.39
10	L	302	BCB	CHC-C4B	3.95	1.48	1.40
10	L	302	BCB	O2A-CGA	3.94	1.44	1.33
11	L	303	BPB	O2A-CGA	3.93	1.44	1.33
5	C	402	HEC	C3C-C2C	-3.92	1.36	1.40
10	M	403	BCB	CHA-CBD	-3.82	1.47	1.52
10	M	404	BCB	CHC-C4B	3.75	1.48	1.40
10	L	302	BCB	C3B-C4B	3.74	1.49	1.40
10	M	404	BCB	C3B-C4B	3.71	1.49	1.40
10	L	301	BCB	C3D-C2D	3.69	1.46	1.39
11	L	303	BPB	C4C-NC	-3.66	1.26	1.37
11	M	405	BPB	C3B-C2B	3.62	1.45	1.39
11	M	405	BPB	C4C-NC	-3.58	1.26	1.37
10	L	301	BCB	CHA-CBD	-3.58	1.48	1.52
10	L	302	BCB	CHB-C1B	3.57	1.48	1.40
11	L	303	BPB	CHA-CBD	-3.51	1.48	1.52
5	C	404	HEC	C3C-C2C	-3.49	1.37	1.40
10	M	403	BCB	CHC-C4B	3.44	1.47	1.40
10	L	302	BCB	CHD-C1D	3.44	1.47	1.40
10	M	403	BCB	CHB-C1B	3.35	1.47	1.40
10	L	301	BCB	C3B-C4B	3.33	1.48	1.40
10	M	403	BCB	C3B-C2B	3.29	1.45	1.39
10	L	301	BCB	CHB-C1B	3.21	1.47	1.40
10	M	403	BCB	CHD-C1D	3.21	1.47	1.40
10	M	403	BCB	C3B-C4B	3.11	1.48	1.40
10	L	301	BCB	C3A-C2A	-3.03	1.51	1.54
10	M	404	BCB	CHB-C1B	2.81	1.46	1.40
14	M	406	NS5	C30-C31	2.77	1.37	1.34
14	M	406	NS5	C23-C21	2.65	1.51	1.45
10	M	403	BCB	CBD-CGD	-2.54	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	404	BCB	CHD-C1D	2.48	1.45	1.40
5	C	404	HEC	C3C-C4C	2.48	1.47	1.43
5	C	402	HEC	CBA-CGA	2.44	1.56	1.50
10	L	302	BCB	C4C-NC	2.42	1.37	1.35
10	L	301	BCB	CHD-C1D	2.34	1.45	1.40
5	C	404	HEC	CBA-CGA	2.31	1.56	1.50
6	C	405	DGA	CG1-CG2	2.31	1.55	1.50
5	C	403	HEC	C3C-C4C	2.28	1.47	1.43
11	L	303	BPB	C3A-C2A	-2.26	1.52	1.54
9	L	304	HTO	C4-C3	2.26	1.56	1.52
9	L	304	HTO	C3-C2	2.25	1.58	1.52
11	L	303	BPB	CBD-CGD	-2.25	1.49	1.52
5	C	402	HEC	C3C-C4C	2.16	1.47	1.43
14	M	406	NS5	C29-C30	2.12	1.50	1.43
10	L	302	BCB	C3A-C2A	-2.08	1.52	1.54
11	M	405	BPB	C1-C2	2.07	1.55	1.49
5	C	403	HEC	CBD-CGD	2.06	1.55	1.50
13	M	402	MQ7	C11-C12	2.02	1.53	1.50
11	M	405	BPB	C2-C3	2.02	1.37	1.33

All (127) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	M	403	BCB	C4D-C3D-CAD	-10.81	100.39	116.53
10	M	404	BCB	C4D-C3D-CAD	-10.57	100.74	116.53
10	L	302	BCB	C4D-C3D-CAD	-10.21	101.29	116.53
10	L	301	BCB	C4D-C3D-CAD	-9.52	102.32	116.53
10	L	302	BCB	O2D-CGD-CBD	8.09	121.24	111.00
11	M	405	BPB	O2D-CGD-CBD	7.03	119.90	111.00
14	M	406	NS5	C27-C26-C28	-6.83	107.31	118.08
11	L	303	BPB	O2D-CGD-CBD	6.70	119.49	111.00
10	M	403	BCB	C3D-CAD-CBD	6.70	116.42	107.61
6	C	405	DGA	OG2-CB1-CB2	6.58	125.68	111.50
11	M	405	BPB	C1A-C2A-C3A	-6.52	96.63	102.84
10	M	404	BCB	O2D-CGD-CBD	6.51	119.24	111.00
14	M	406	NS5	C28-C26-C25	6.47	128.86	118.94
10	L	302	BCB	CHA-C1A-C2A	-6.37	118.35	133.31
10	M	403	BCB	CHA-C1A-C2A	-6.07	119.05	133.31
10	M	403	BCB	O2D-CGD-CBD	6.07	118.68	111.00
10	L	302	BCB	C3D-CAD-CBD	5.76	115.19	107.61
5	C	401	HEC	CBD-CAD-C3D	-5.43	103.36	112.62
10	L	301	BCB	CHA-C1A-C2A	-5.28	120.91	133.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	M	405	BPB	CBC-CAC-C3C	-5.22	112.84	126.70
11	L	303	BPB	CBC-CAC-C3C	-5.21	112.89	126.70
10	M	404	BCB	C3D-CAD-CBD	5.16	114.40	107.61
10	L	301	BCB	CMB-C2B-C3B	4.99	134.01	124.68
10	M	404	BCB	CHA-C1A-C2A	-4.97	121.63	133.31
14	M	406	NS5	C24-C25-C26	-4.88	120.34	127.31
10	M	404	BCB	CMB-C2B-C3B	4.75	133.56	124.68
5	C	401	HEC	CBA-CAA-C2A	-4.52	104.98	112.60
14	M	406	NS5	CM4-C36-C35	-4.48	109.69	122.65
11	M	405	BPB	O2A-C1-C2	4.36	120.08	108.64
10	L	301	BCB	C3D-CAD-CBD	4.27	113.23	107.61
6	C	405	DGA	OG2-CG2-CG1	4.23	115.94	106.13
10	L	302	BCB	CMD-C2D-C3D	-4.09	117.02	124.68
5	C	402	HEC	CBA-CAA-C2A	-4.06	105.75	112.60
10	L	301	BCB	O2D-CGD-CBD	4.02	116.09	111.00
11	M	405	BPB	C1-O2A-CGA	4.02	126.99	116.44
6	C	405	DGA	OG1-CA1-OA1	-3.94	113.65	123.59
5	C	402	HEC	CMB-C2B-C1B	-3.89	122.49	128.46
5	C	403	HEC	C1D-C2D-C3D	3.85	109.67	107.00
10	L	301	BCB	C4-C3-C5	3.70	121.50	115.27
6	C	405	DGA	OG1-CA1-CA2	3.64	123.34	111.91
11	M	405	BPB	CMA-C3A-C4A	-3.60	106.48	114.38
10	L	302	BCB	CMB-C2B-C3B	3.52	131.26	124.68
10	M	404	BCB	C1-O2A-CGA	3.50	125.62	116.44
14	M	406	NS5	CM3-C36-C35	-3.45	112.67	122.65
14	M	406	NS5	C18-C17-C15	-3.41	122.44	127.31
11	L	303	BPB	CMD-C2D-C3D	-3.35	118.40	124.68
13	M	402	MQ7	C24-C23-C25	3.30	120.83	115.27
5	C	404	HEC	C1D-C2D-C3D	3.30	109.29	107.00
10	M	403	BCB	CBC-CAC-C3C	-3.29	117.98	126.70
14	M	406	NS5	C19-C20-C21	-3.22	122.71	127.31
10	M	404	BCB	O2D-CGD-O1D	-3.19	117.59	123.84
11	L	303	BPB	CMA-C3A-C4A	-3.14	107.50	114.38
10	M	403	BCB	CHC-C1C-C2C	-3.07	114.19	122.60
11	L	303	BPB	CMB-C2B-C3B	3.05	130.38	124.68
10	L	302	BCB	O1D-CGD-CBD	-3.05	119.66	124.74
14	M	406	NS5	C34-C35-C36	-3.03	117.39	127.75
14	M	406	NS5	C14-C15-C17	-3.00	114.34	118.94
5	C	403	HEC	CBA-CAA-C2A	-2.98	107.57	112.60
10	L	302	BCB	C1-O2A-CGA	2.95	124.19	116.44
11	M	405	BPB	O2D-CGD-O1D	-2.95	118.07	123.84
10	L	301	BCB	CED-O2D-CGD	2.95	122.61	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	M	404	BCB	CBC-CAC-C3C	-2.94	118.90	126.70
5	C	404	HEC	CMB-C2B-C1B	-2.92	123.97	128.46
14	M	406	NS5	C6-C5-C7	-2.92	116.19	123.68
10	M	403	BCB	O2A-CGA-CBA	2.88	120.96	111.91
10	M	404	BCB	CHD-C4C-C3C	-2.87	121.95	130.10
10	L	302	BCB	CBC-CAC-C3C	-2.84	119.17	126.70
5	C	402	HEC	C1D-C2D-C3D	2.84	108.97	107.00
14	M	406	NS5	C16-C15-C14	2.81	122.51	118.08
10	L	302	BCB	CHC-C1C-C2C	-2.80	114.94	122.60
10	L	301	BCB	CHD-C4C-C3C	-2.78	122.22	130.10
10	L	301	BCB	CMD-C2D-C3D	-2.78	119.48	124.68
11	M	405	BPB	CMD-C2D-C3D	-2.76	119.52	124.68
14	M	406	NS5	C18-C19-C20	2.74	129.09	123.47
10	L	301	BCB	O2A-CGA-CBA	2.72	120.45	111.91
10	M	403	BCB	CMD-C2D-C3D	-2.71	119.60	124.68
10	M	403	BCB	CMB-C2B-C3B	2.68	129.70	124.68
5	C	402	HEC	O2A-CGA-CBA	2.65	122.55	114.03
11	L	303	BPB	O1D-CGD-CBD	-2.63	120.36	124.74
10	M	404	BCB	CHC-C1C-C2C	-2.62	115.41	122.60
14	M	406	NS5	C4-C5-C7	2.62	126.42	121.12
5	C	403	HEC	O2D-CGD-CBD	2.59	122.35	114.03
10	L	302	BCB	CMA-C3A-C4A	-2.54	108.81	114.38
11	L	303	BPB	C3D-CAD-CBD	2.54	110.95	107.61
9	H	607	HTO	O3-C3-C2	-2.53	104.53	109.72
10	M	403	BCB	CMA-C3A-C4A	-2.51	108.87	114.38
10	L	302	BCB	O2D-CGD-O1D	-2.46	119.02	123.84
5	C	401	HEC	CMB-C2B-C1B	-2.45	124.69	128.46
5	C	404	HEC	O1D-CGD-CBD	-2.43	115.26	123.08
10	L	301	BCB	C1-C2-C3	-2.41	121.88	126.04
10	L	302	BCB	CHD-C4C-C3C	-2.40	123.29	130.10
5	C	404	HEC	CBD-CAD-C3D	2.39	116.70	112.62
10	L	301	BCB	C5-C3-C2	-2.36	116.33	121.12
10	L	301	BCB	CBC-CAC-C3C	-2.36	120.43	126.70
10	L	301	BCB	CHC-C1C-C2C	-2.36	116.14	122.60
5	C	401	HEC	CMC-C2C-C1C	-2.36	124.84	128.46
10	M	404	BCB	CMD-C2D-C3D	-2.35	120.28	124.68
10	L	301	BCB	O2A-CGA-O1A	-2.35	117.66	123.59
5	C	403	HEC	CMC-C2C-C1C	-2.35	124.86	128.46
6	C	405	DGA	OG2-CB1-OB1	-2.32	118.10	123.70
13	M	402	MQ7	C45-C43-C44	2.30	119.68	114.60
10	M	404	BCB	C16-C15-C13	-2.30	108.49	115.92
10	M	403	BCB	CHD-C4C-C3C	-2.29	123.60	130.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	401	HEC	C1D-C2D-C3D	2.27	108.58	107.00
5	C	404	HEC	CMC-C2C-C1C	-2.27	124.97	128.46
10	M	404	BCB	CED-O2D-CGD	2.24	121.01	115.94
11	L	303	BPB	C1A-C2A-C3A	-2.23	100.72	102.84
9	L	304	HTO	C1-C2-C3	2.21	117.91	113.11
10	M	403	BCB	O1D-CGD-CBD	-2.21	121.06	124.74
5	C	402	HEC	CMD-C2D-C1D	-2.20	125.08	128.46
14	M	406	NS5	C32-C31-C30	2.18	128.23	122.59
13	M	402	MQ7	C39-C38-C40	2.18	118.93	115.27
13	M	402	MQ7	C2M-C2-C3	-2.14	120.91	124.40
14	M	406	NS5	C12-C13-C14	-2.13	116.56	123.22
14	M	406	NS5	C11-C10-C9	2.13	118.85	115.27
13	M	402	MQ7	C40-C38-C37	-2.12	116.82	121.12
11	M	405	BPB	C3D-CAD-CBD	2.12	110.40	107.61
11	L	303	BPB	O2A-C1-C2	2.12	114.20	108.64
10	L	302	BCB	C5-C3-C2	-2.12	116.83	121.12
6	C	405	DGA	CG3-CG2-CG1	-2.11	106.57	112.63
5	C	402	HEC	CMB-C2B-C3B	2.10	128.29	125.82
11	M	405	BPB	O2A-CGA-CBA	2.07	118.39	111.91
13	M	402	MQ7	C12-C11-C3	-2.05	106.52	112.05
9	H	607	HTO	O3-C3-C4	2.03	113.58	109.15
9	L	304	HTO	C4-C3-C2	2.02	118.14	113.35
8	H	605	LDA	O1-N1-C1	-2.02	104.32	109.27
5	C	402	HEC	CAD-CBD-CGD	-2.01	108.13	113.76

There are no chirality outliers.

All (141) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	401	HEC	C2A-CAA-CBA-CGA
5	C	404	HEC	C2D-C3D-CAD-CBD
5	C	404	HEC	C4D-C3D-CAD-CBD
6	C	405	DGA	OG1-CG1-CG2-OG2
6	C	405	DGA	OG1-CG1-CG2-CG3
8	H	606	LDA	N1-C1-C2-C3
9	H	607	HTO	O1-C1-C2-O2
9	H	607	HTO	O3-C3-C4-C5
9	L	305	HTO	O2-C2-C3-C4
10	L	301	BCB	C2C-C3C-CAC-CBC
10	L	302	BCB	C2C-C3C-CAC-CBC
10	L	302	BCB	C4C-C3C-CAC-CBC
10	L	302	BCB	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
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	C2C-C3C-CAC-CBC
10	M	404	BCB	CAD-CBD-CGD-O1D
11	L	303	BPB	C2C-C3C-CAC-CBC
11	M	405	BPB	CBD-CGD-O2D-CED
11	M	405	BPB	C2C-C3C-CAC-CBC
11	L	303	BPB	CBD-CGD-O2D-CED
11	L	303	BPB	O1D-CGD-O2D-CED
10	M	403	BCB	O1D-CGD-O2D-CED
14	M	406	NS5	C34-C35-C36-CM3
10	L	302	BCB	O1D-CGD-O2D-CED
11	M	405	BPB	O1D-CGD-O2D-CED
10	M	404	BCB	C2A-CAA-CBA-CGA
6	C	405	DGA	OA1-CA1-OG1-CG1
6	C	405	DGA	CA2-CA1-OG1-CG1
14	M	406	NS5	C28-C29-C30-C31
6	C	405	DGA	CG1-CG2-OG2-CB1
10	L	301	BCB	CBD-CGD-O2D-CED
10	L	301	BCB	C4-C3-C5-C6
10	L	301	BCB	C2-C3-C5-C6
14	M	406	NS5	C27-C26-C28-C29
14	M	406	NS5	C25-C26-C28-C29
11	M	405	BPB	C5-C6-C7-C8
11	M	405	BPB	C10-C11-C12-C13
11	L	303	BPB	C15-C16-C17-C18
11	M	405	BPB	C15-C16-C17-C18
10	M	403	BCB	C13-C15-C16-C17
9	H	607	HTO	O1-C1-C2-C3
14	M	406	NS5	C31-C33-C34-C35
10	L	301	BCB	C13-C15-C16-C17
10	M	403	BCB	C8-C10-C11-C12
10	L	301	BCB	C15-C16-C17-C18
13	M	402	MQ7	C24-C23-C25-C26
6	C	405	DGA	CBB-CAB-CB9-CB8
8	H	601	LDA	C6-C7-C8-C9
14	M	406	NS5	C34-C35-C36-CM4
6	C	405	DGA	CA5-CA6-CA7-CA8
8	M	413	LDA	C6-C7-C8-C9
6	C	405	DGA	CA1-CA2-CA3-CA4
10	L	301	BCB	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
6	C	405	DGA	CA2-CA3-CA4-CA5
11	L	303	BPB	C8-C10-C11-C12
11	M	405	BPB	O2A-C1-C2-C3
8	H	601	LDA	C4-C5-C6-C7
6	C	405	DGA	CCB-CDB-CEB-CFB
8	M	413	LDA	C5-C6-C7-C8
13	M	402	MQ7	C22-C23-C25-C26
8	H	606	LDA	C6-C7-C8-C9
6	C	405	DGA	CB9-CAB-CBB-CCB
11	L	303	BPB	C4-C3-C5-C6
8	H	606	LDA	C1-C2-C3-C4
8	H	601	LDA	C9-C10-C11-C12
6	C	405	DGA	CB4-CB5-CB6-CB7
9	L	305	HTO	O2-C2-C3-O3
8	H	605	LDA	C7-C8-C9-C10
10	M	403	BCB	C6-C7-C8-C10
11	M	405	BPB	C11-C12-C13-C15
10	L	302	BCB	C14-C13-C15-C16
10	M	403	BCB	C6-C7-C8-C9
8	H	605	LDA	N1-C1-C2-C3
11	L	303	BPB	C10-C11-C12-C13
10	L	302	BCB	C3A-C2A-CAA-CBA
8	M	413	LDA	C2-C3-C4-C5
9	L	304	HTO	O1-C1-C2-O2
6	C	405	DGA	CB2-CB3-CB4-CB5
6	C	405	DGA	CA7-CA8-CA9-CAA
8	H	605	LDA	C9-C10-C11-C12
11	L	303	BPB	C2-C3-C5-C6
10	M	404	BCB	C13-C15-C16-C17
9	L	304	HTO	O2-C2-C3-C4
8	M	413	LDA	C11-C10-C9-C8
10	L	302	BCB	C12-C13-C15-C16
10	M	403	BCB	C11-C12-C13-C15
11	L	303	BPB	CAD-CBD-CGD-O2D
11	M	405	BPB	CAD-CBD-CGD-O2D
6	C	405	DGA	CG3-CG2-OG2-CB1
14	M	406	NS5	CM1-C1-C2-C3
14	M	406	NS5	C2-C3-C4-C5
6	C	405	DGA	CB5-CB6-CB7-CB8
10	M	403	BCB	C11-C12-C13-C14
10	M	403	BCB	C10-C11-C12-C13
9	H	607	HTO	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
8	H	605	LDA	C2-C3-C4-C5
5	C	402	HEC	C3D-CAD-CBD-CGD
6	C	405	DGA	CAB-CBB-CCB-CDB
8	M	413	LDA	C1-C2-C3-C4
10	M	404	BCB	O1D-CGD-O2D-CED
11	L	303	BPB	O2A-C1-C2-C3
8	H	605	LDA	C11-C10-C9-C8
10	M	403	BCB	C4-C3-C5-C6
8	H	605	LDA	C6-C7-C8-C9
11	M	405	BPB	O1A-CGA-O2A-C1
11	M	405	BPB	C11-C12-C13-C14
14	M	406	NS5	CM2-C1-C2-C3
11	M	405	BPB	CBA-CGA-O2A-C1
11	M	405	BPB	C16-C17-C18-C20
8	H	605	LDA	C4-C5-C6-C7
8	H	606	LDA	C3-C4-C5-C6
5	C	404	HEC	CAD-CBD-CGD-O1D
9	L	305	HTO	C1-C2-C3-O3
5	C	404	HEC	CAD-CBD-CGD-O2D
14	M	406	NS5	C32-C31-C33-C34
6	C	405	DGA	OB1-CB1-OG2-CG2
10	M	403	BCB	C2-C3-C5-C6
6	C	405	DGA	CDB-CEB-CFB-CGB
11	M	405	BPB	C3-C5-C6-C7
14	M	406	NS5	C30-C31-C33-C34
11	M	405	BPB	C14-C13-C15-C16
10	L	302	BCB	CAD-CBD-CGD-O2D
10	M	404	BCB	CAD-CBD-CGD-O2D
10	L	301	BCB	C16-C17-C18-C19
6	C	405	DGA	CA8-CA9-CAA-CBA
5	C	401	HEC	CAA-CBA-CGA-O2A
5	C	402	HEC	CAD-CBD-CGD-O2D
14	M	406	NS5	C7-C8-C9-C10
10	M	404	BCB	O2A-C1-C2-C3
5	C	401	HEC	CAA-CBA-CGA-O1A
6	C	405	DGA	CB2-CB1-OG2-CG2
5	C	402	HEC	CAD-CBD-CGD-O1D
14	M	406	NS5	C23-C24-C25-C26
5	C	401	HEC	CAD-CBD-CGD-O2D
10	L	301	BCB	CAD-CBD-CGD-O1D
10	M	404	BCB	C6-C7-C8-C10
11	M	405	BPB	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
10	M	404	BCB	C15-C16-C17-C18
8	H	601	LDA	C3-C4-C5-C6

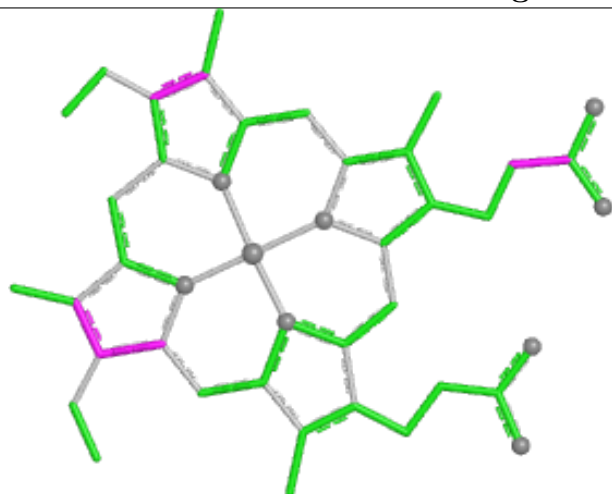
There are no ring outliers.

14 monomers are involved in 29 short contacts:

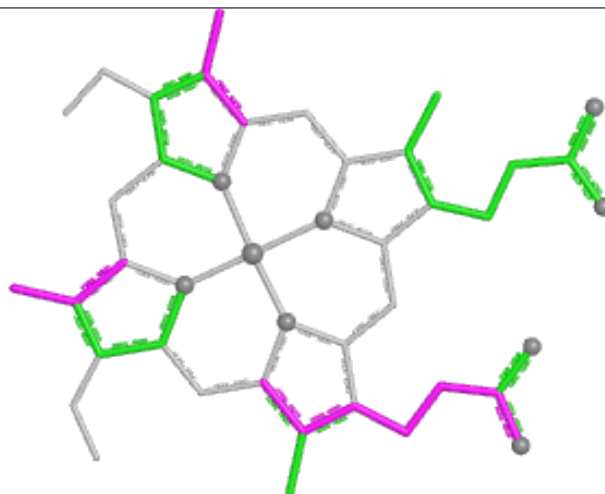
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	404	HEC	3	0
10	L	302	BCB	5	0
10	M	404	BCB	1	0
5	C	401	HEC	3	0
5	C	402	HEC	2	0
14	M	406	NS5	4	0
7	M	408	SO4	2	0
11	M	405	BPB	2	0
11	L	303	BPB	2	0
10	M	403	BCB	3	0
10	L	301	BCB	2	0
7	C	406	SO4	1	0
13	M	402	MQ7	1	0
5	C	403	HEC	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

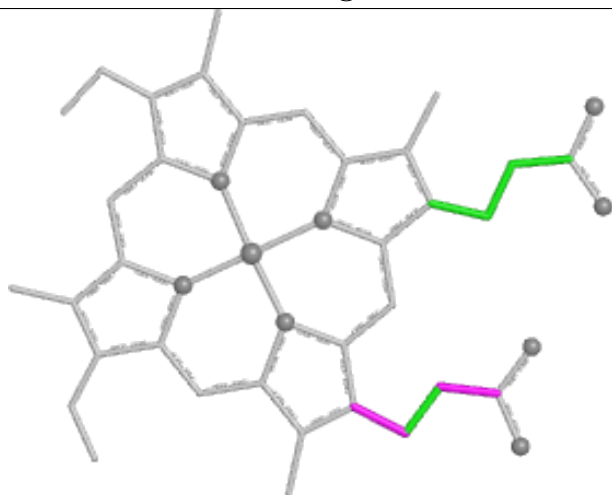
## Ligand HEC C 404



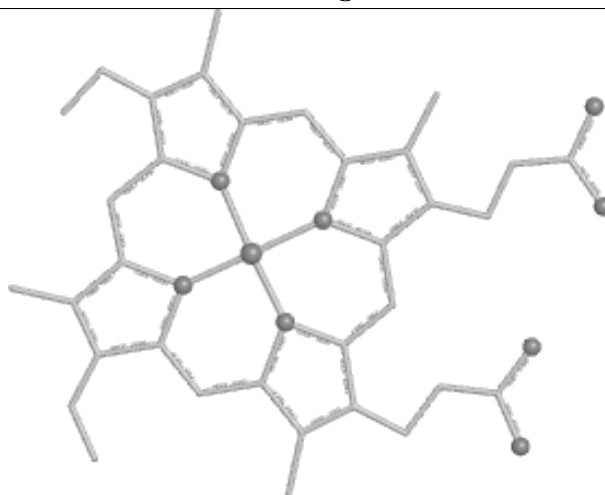
Bond lengths



Bond angles

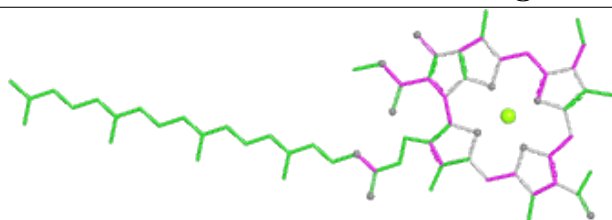


Torsions

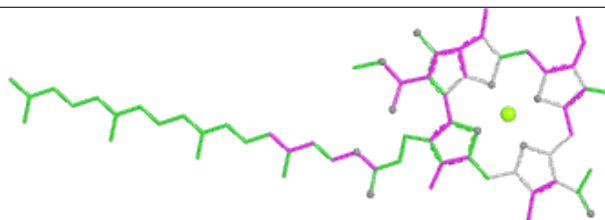


Rings

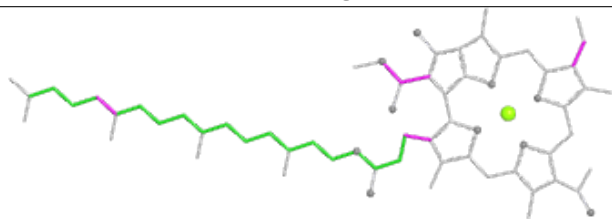
## Ligand BCB L 302



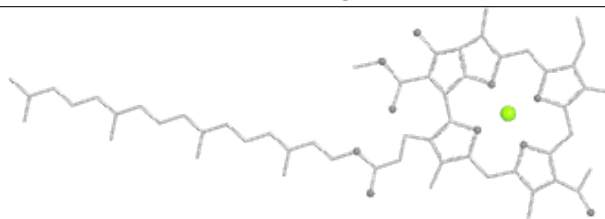
Bond lengths



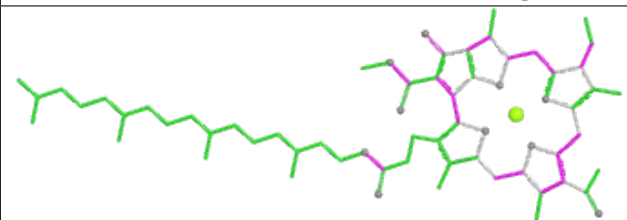
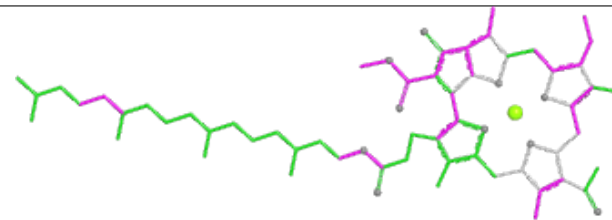
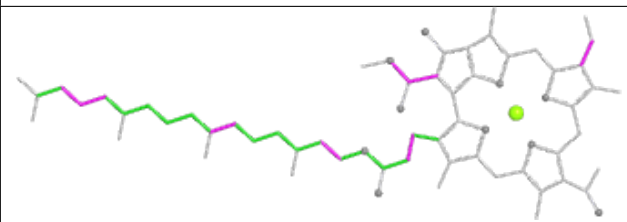
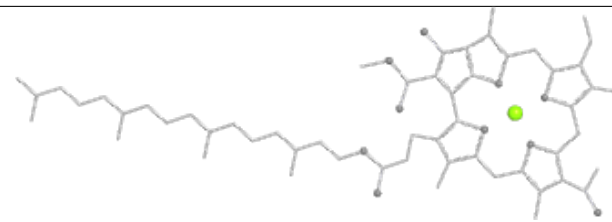
Bond angles

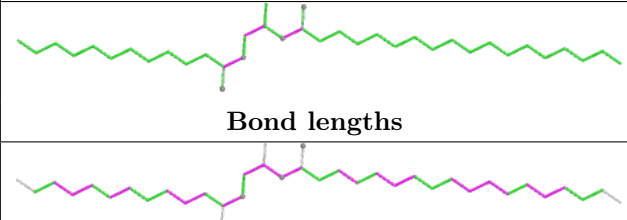
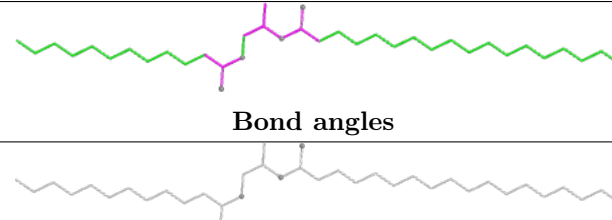
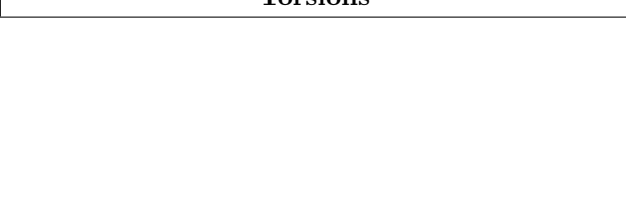
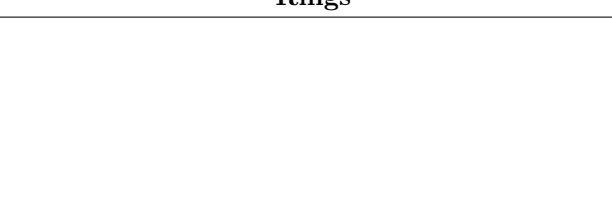


Torsions

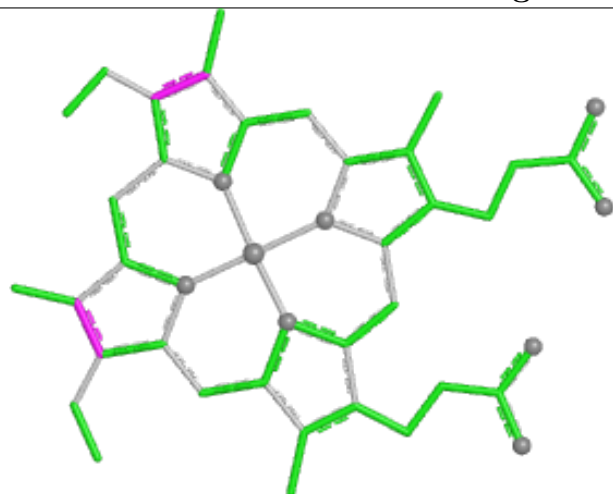


Rings

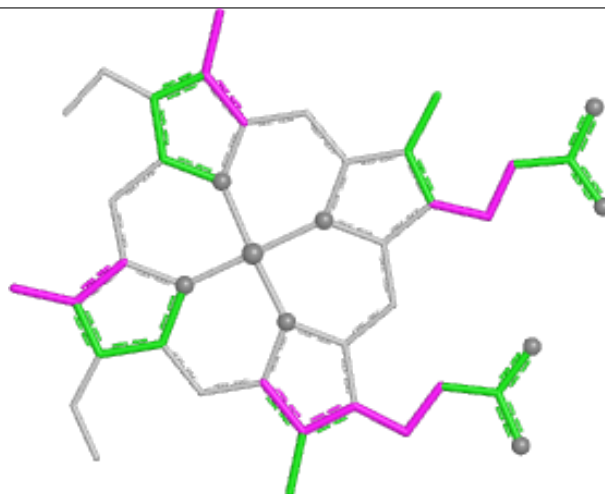
Ligand BCB M 404	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand DGA C 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

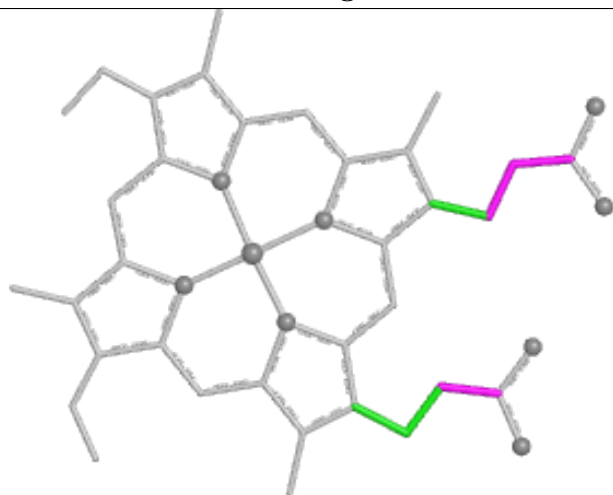
## Ligand HEC C 401



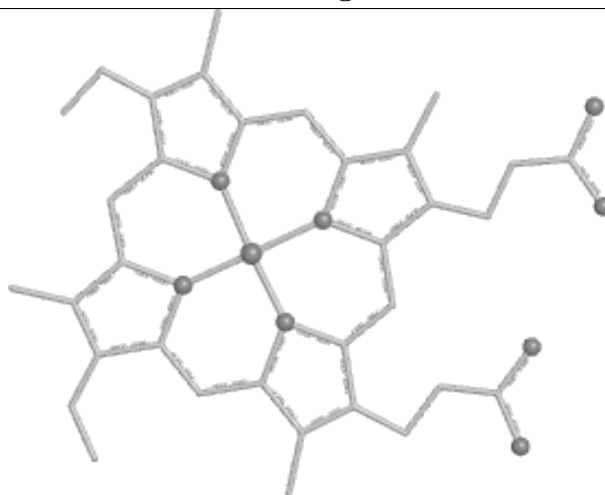
Bond lengths



Bond angles

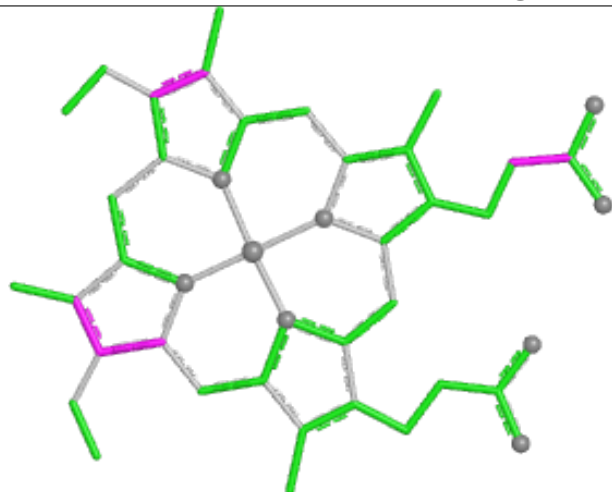


Torsions

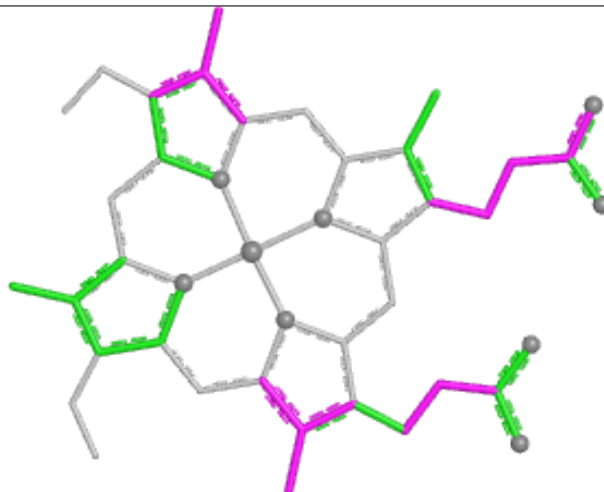


Rings

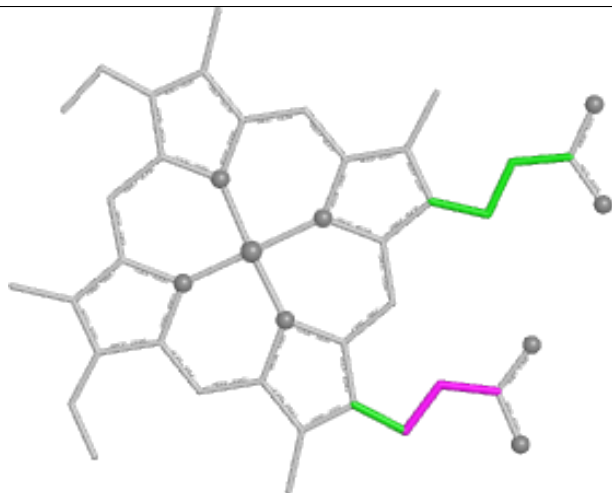
## Ligand HEC C 402



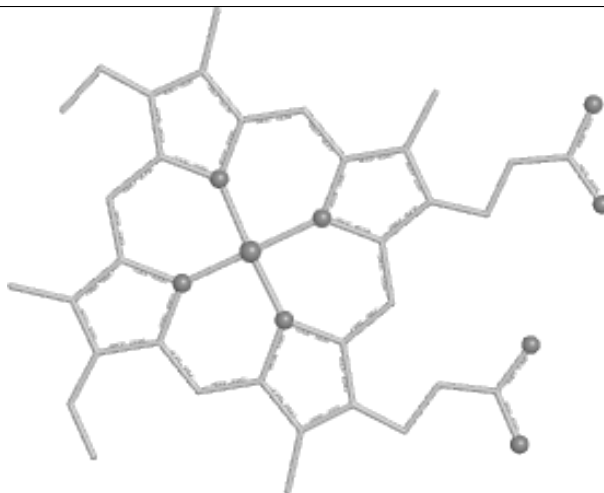
Bond lengths



Bond angles

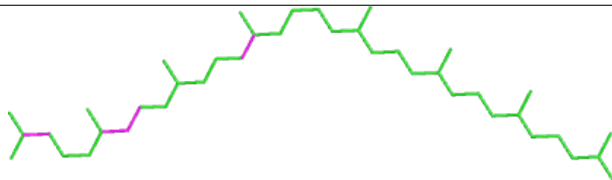


Torsions

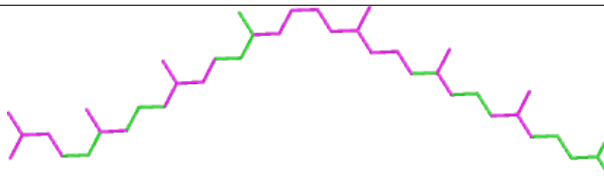


Rings

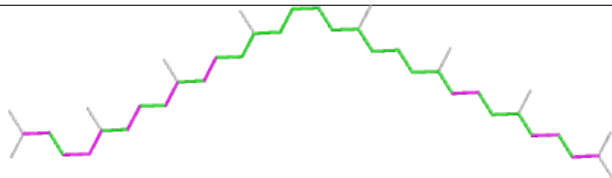
## Ligand NS5 M 406



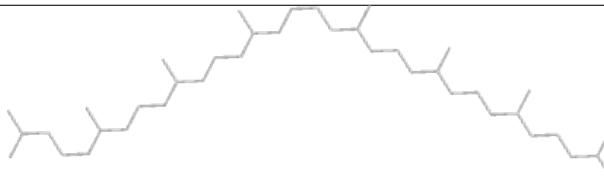
Bond lengths



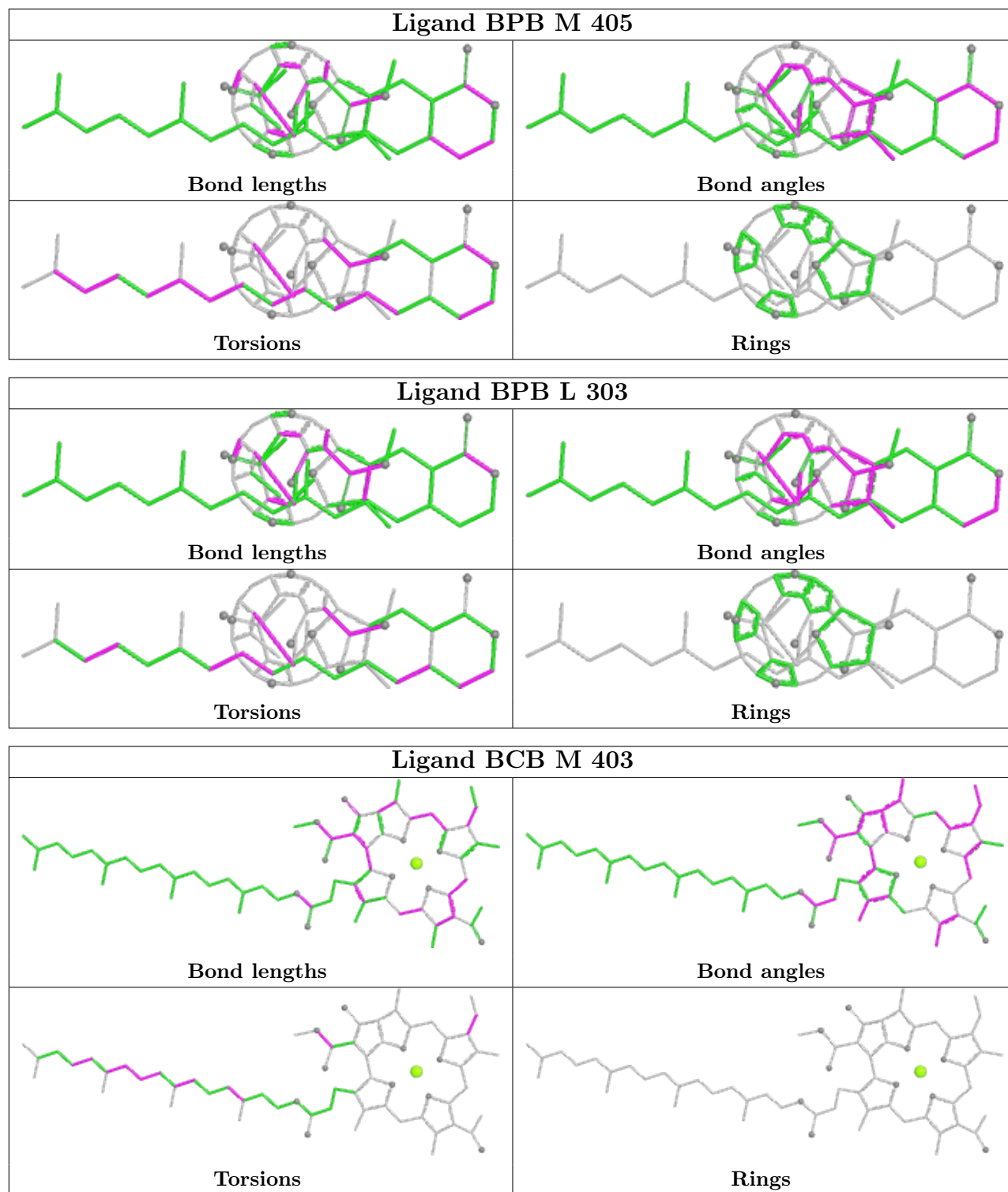
Bond angles

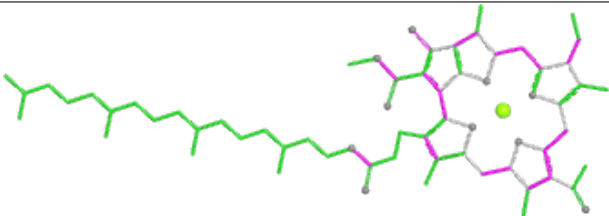
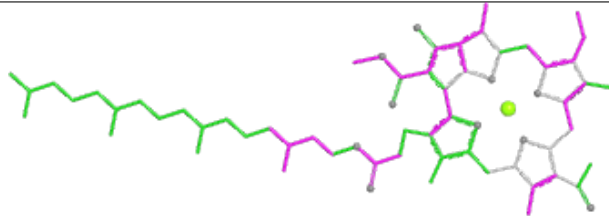
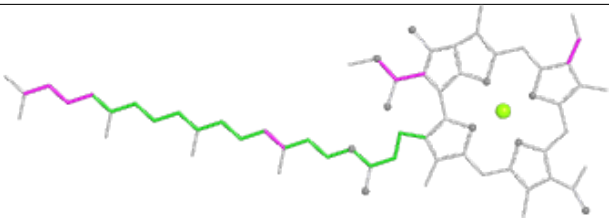
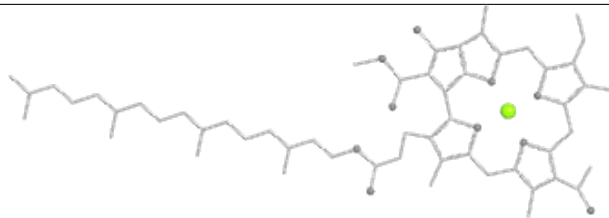
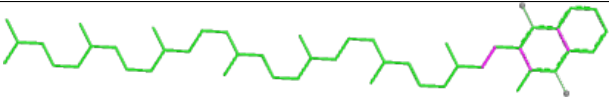
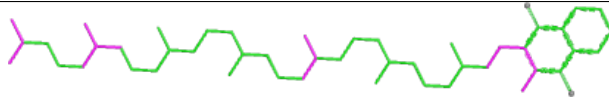
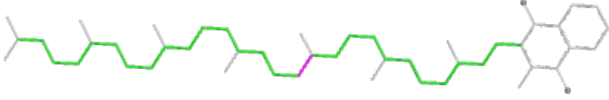
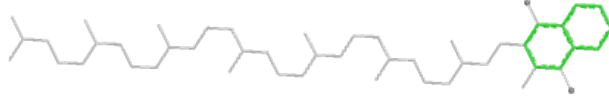


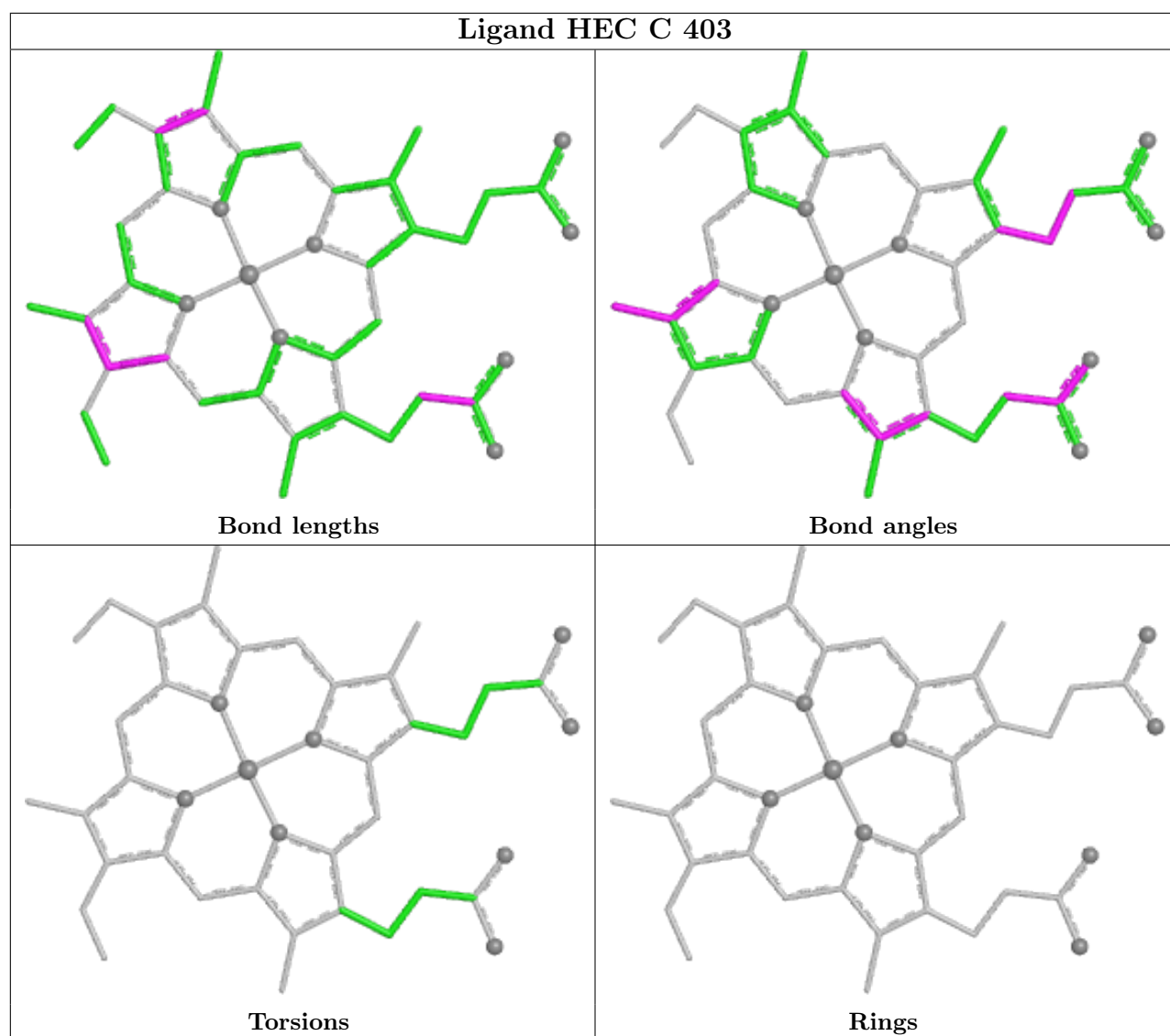
Torsions



Rings



Ligand BCB L 301	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand MQ7 M 402	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>



## 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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

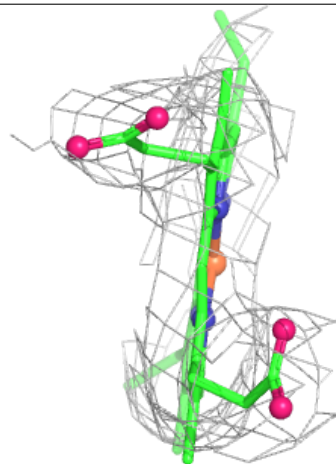
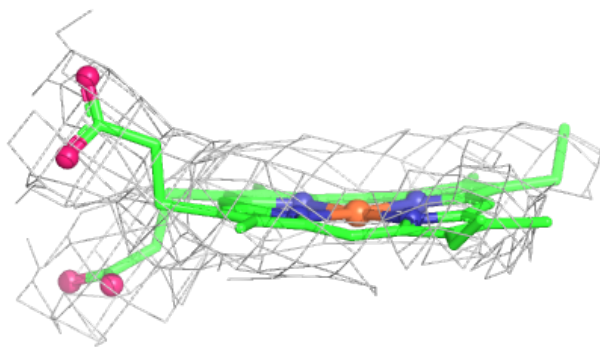
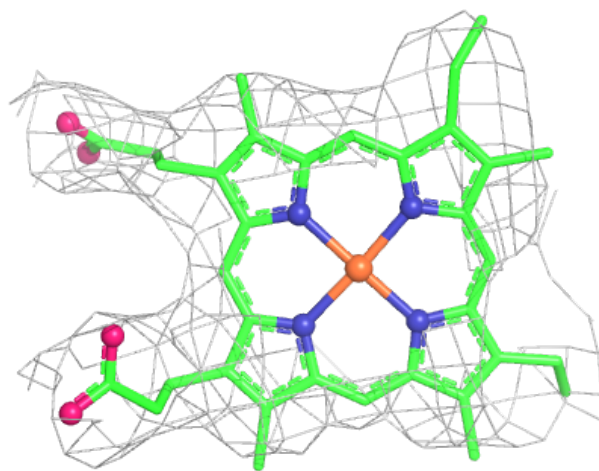
### 6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

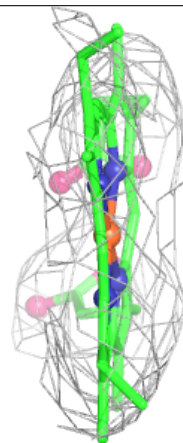
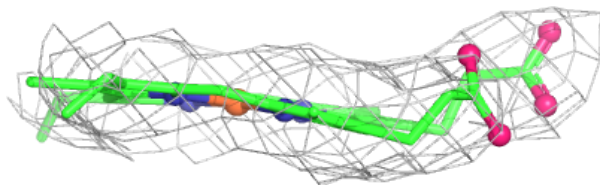
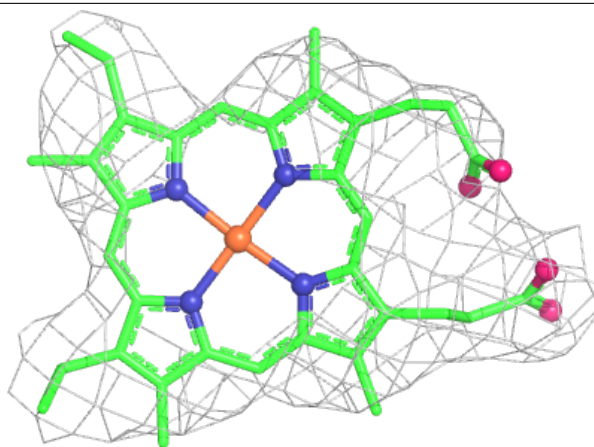
**Electron density around HEC C 401:**

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



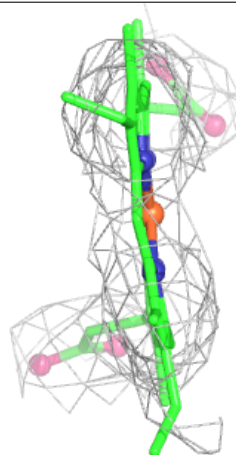
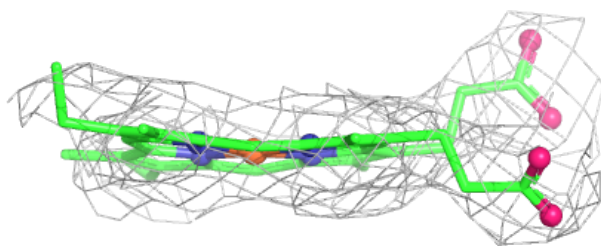
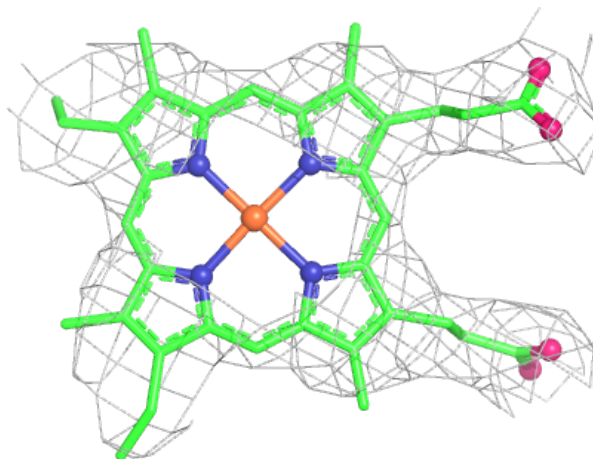
**Electron density around HEC C 402:**

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



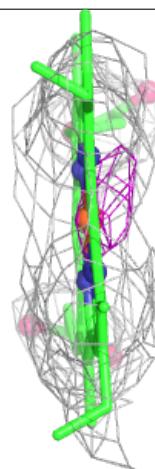
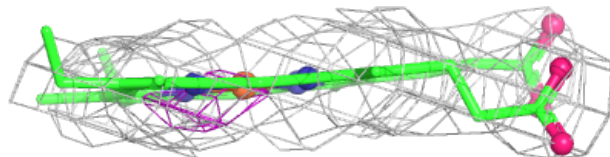
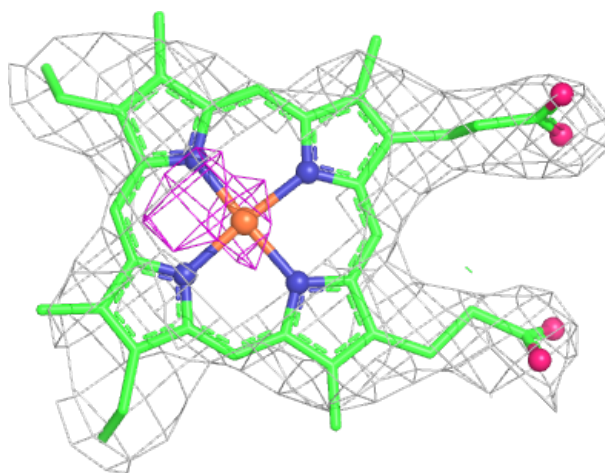
**Electron density around HEC C 403:**

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



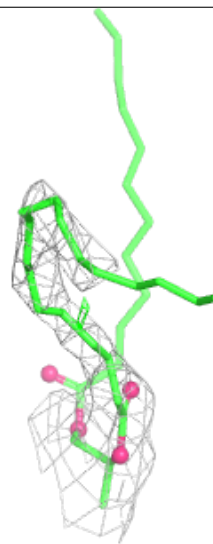
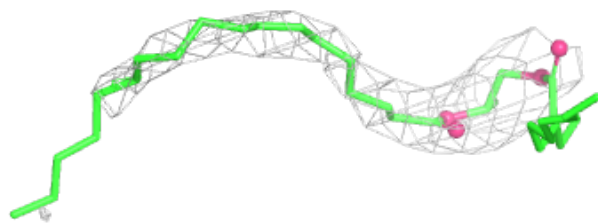
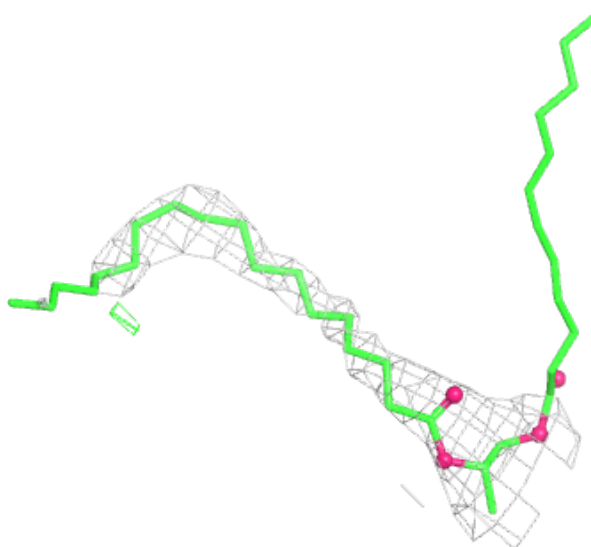
**Electron density around HEC C 404:**

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



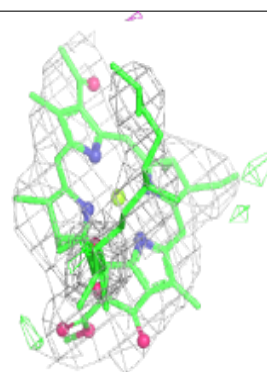
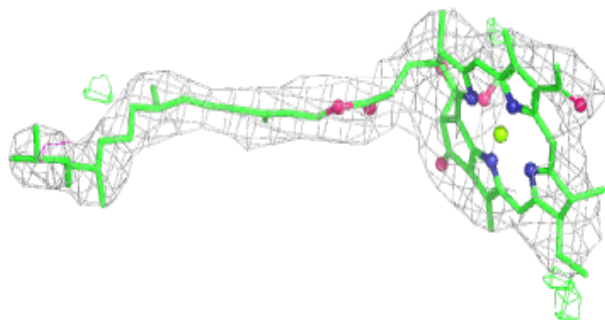
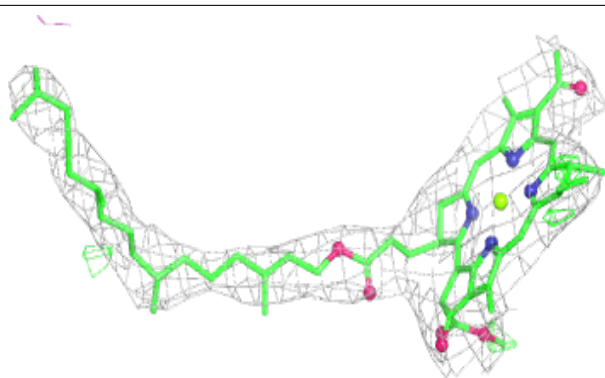
**Electron density around DGA C 405:**

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

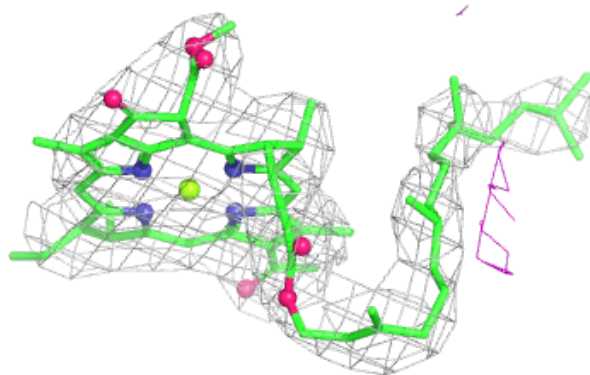
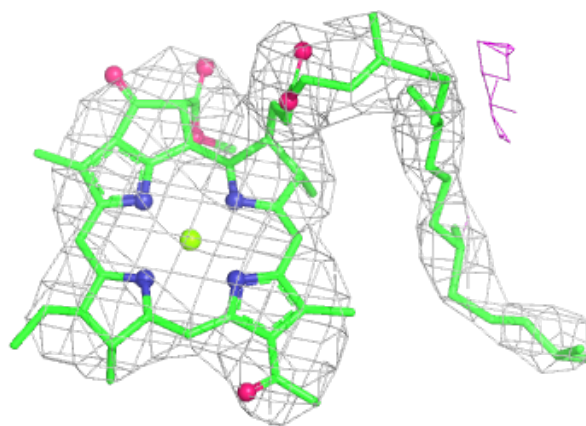


**Electron density around BCB L 301:**

$2mF_o-DF_c$  (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:**

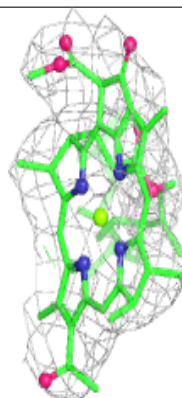
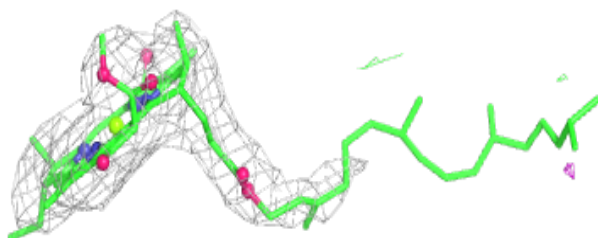
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



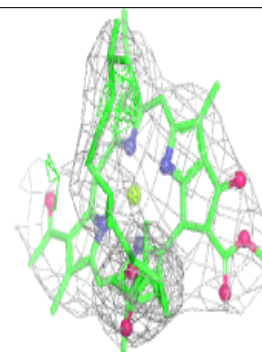
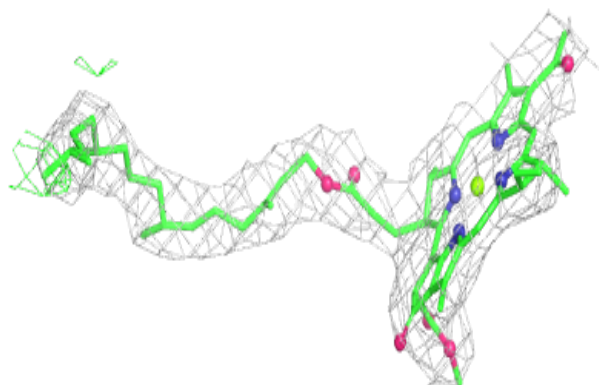
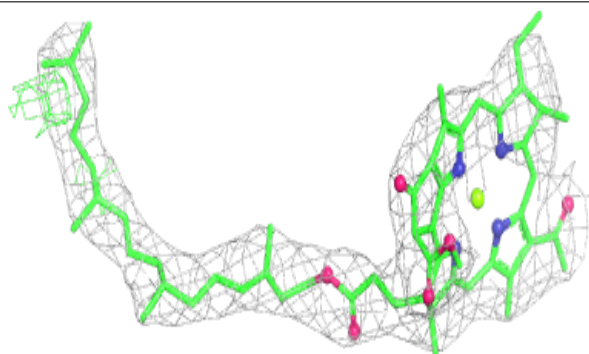


**Electron density around BCB M 403:**

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

**Electron density around BCB M 404:**

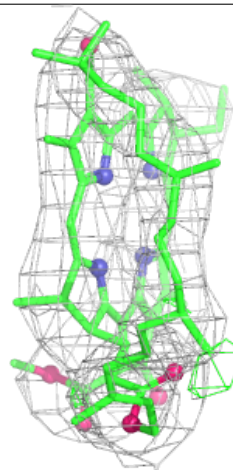
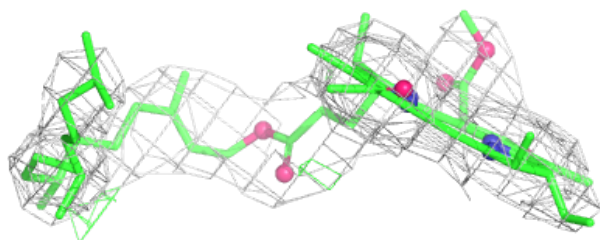
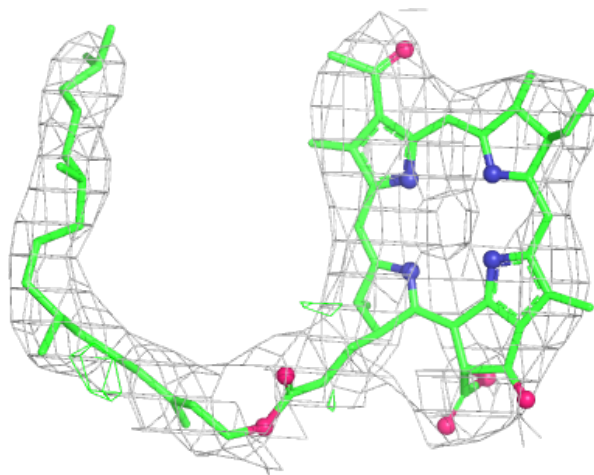
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





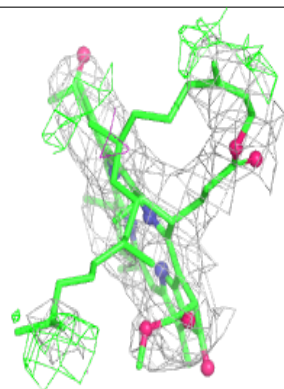
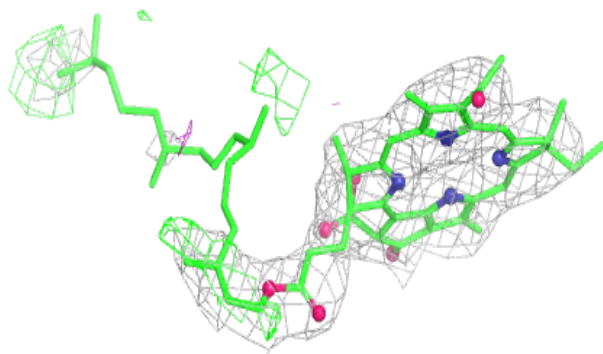
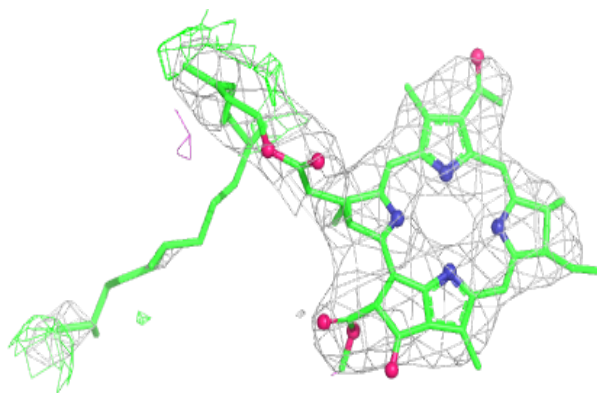
**Electron density around BPB L 303:**

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

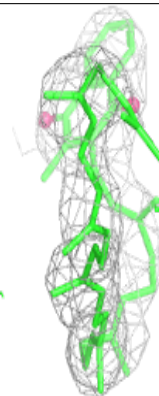
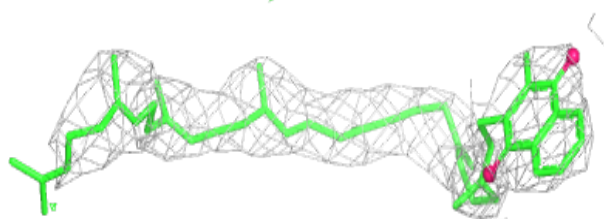
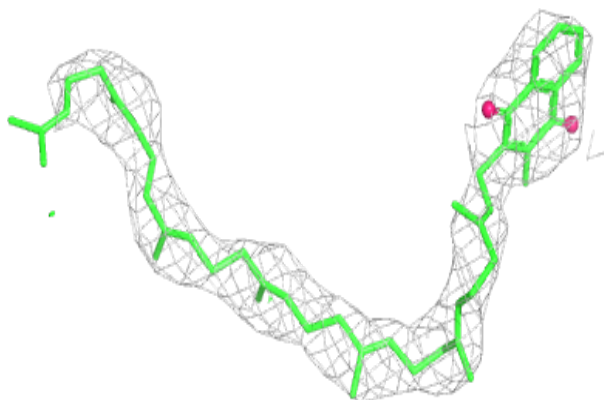


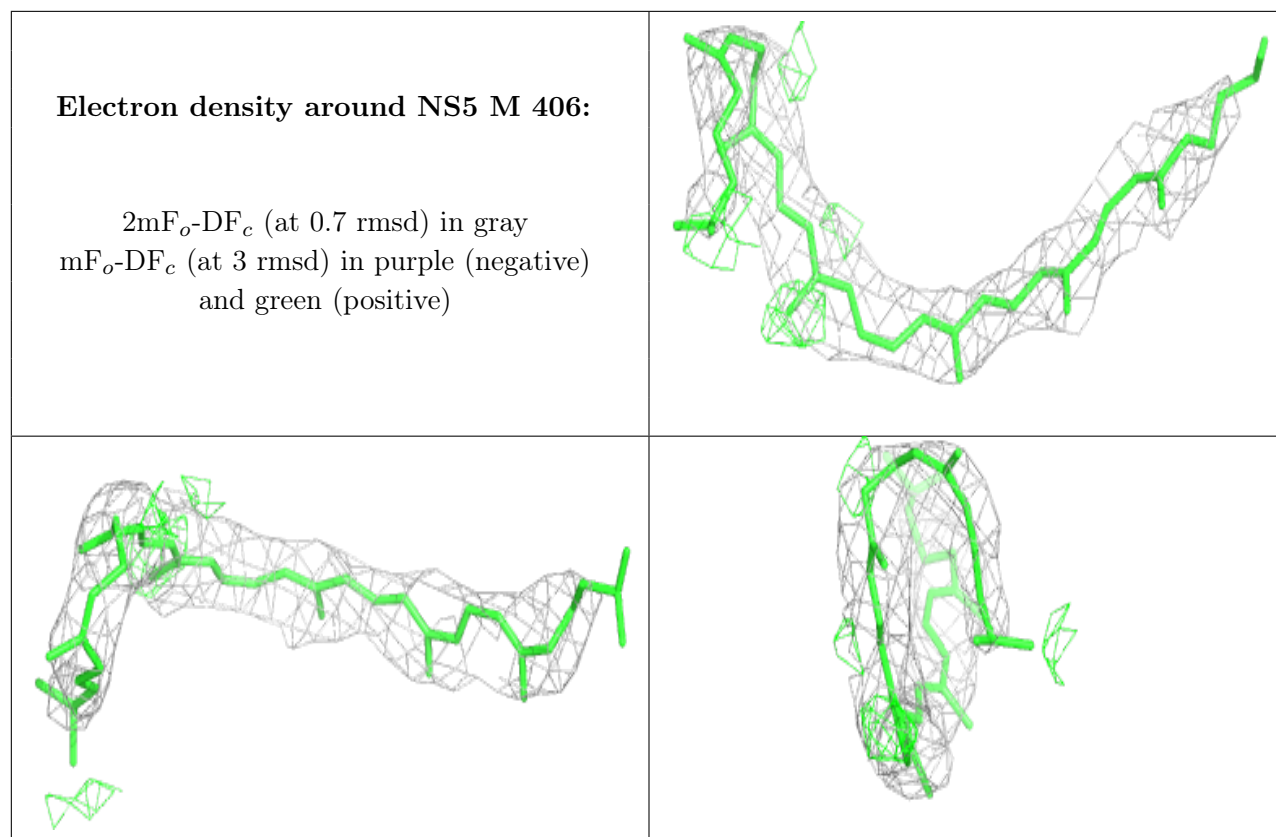
**Electron density around BPB M 405:**

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

**Electron density around 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)





## 6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.