



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 15, 2023 – 09:14 AM EDT

PDB ID : 1VRN
Title : PHOTOSYNTHETIC REACTION CENTER BLASTOCHLORIS VIRIDIS (ATCC)
Authors : Baxter, R.H.G.; Seagle, B.-L.; Norris, J.R.
Deposited on : 2005-02-23
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

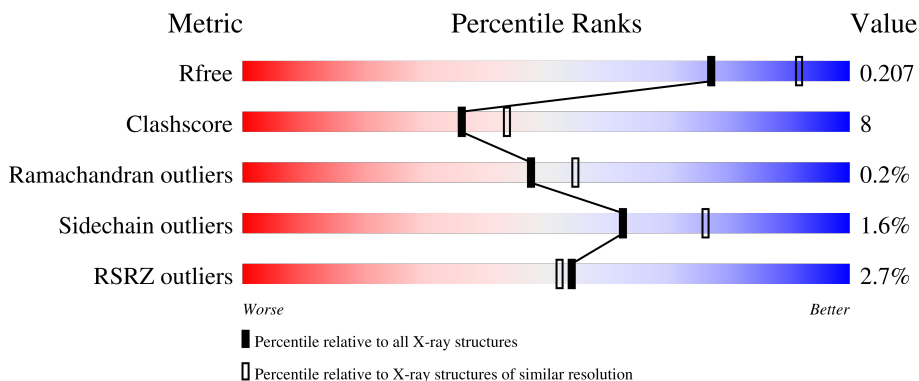
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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

Mol	Chain	Length	Quality of chain
1	C	332	 2% 88% 12%
2	H	258	 5% 84% 16%
3	L	273	 % 84% 16%
4	M	323	 3% 85% 15%

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
6	SO4	H	807	-	-	X	-
8	BCB	M	401	X	-	-	-
9	BPB	M	405	X	-	-	-

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 10747 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	C	332	2603	1640	466	479	18	24	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	258	2018	1292	344	380	2	112	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	1	FME	MET	modified residue	UNP P06008

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	273	2177	1462	351	357	7	5	1	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	M	323	2563	1707	420	424	12	10	1	0

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



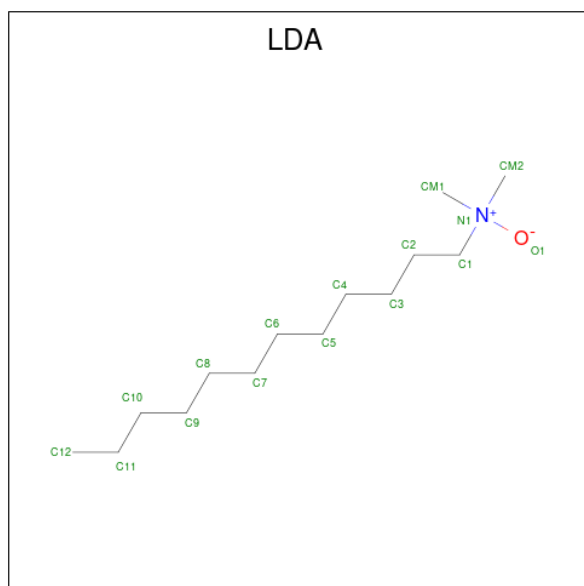
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Fe	N			O
5	C	1	43	34	1	4	4	0	0
5	C	1	43	34	1	4	4	0	0
5	C	1	43	34	1	4	4	0	0
5	C	1	43	34	1	4	4	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 7 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



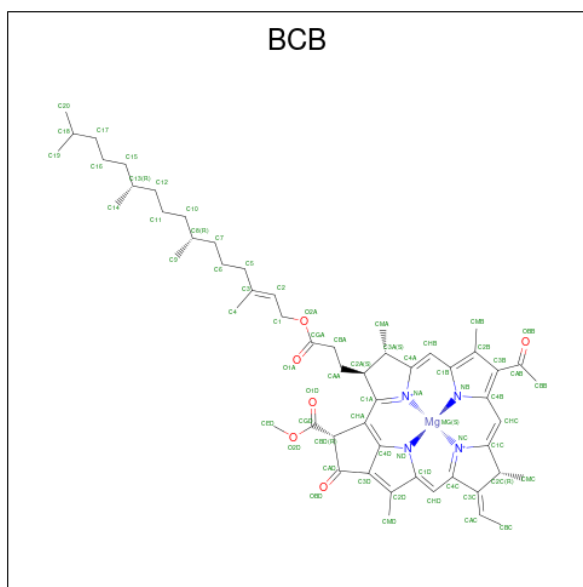
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	H	1	Total C N O 16 14 1 1	0	0
7	H	1	Total C N O 16 14 1 1	0	0
7	L	1	Total C N O 16 14 1 1	0	0
7	L	1	Total C N O 16 14 1 1	0	0

Continued on next page...

Continued from previous page...

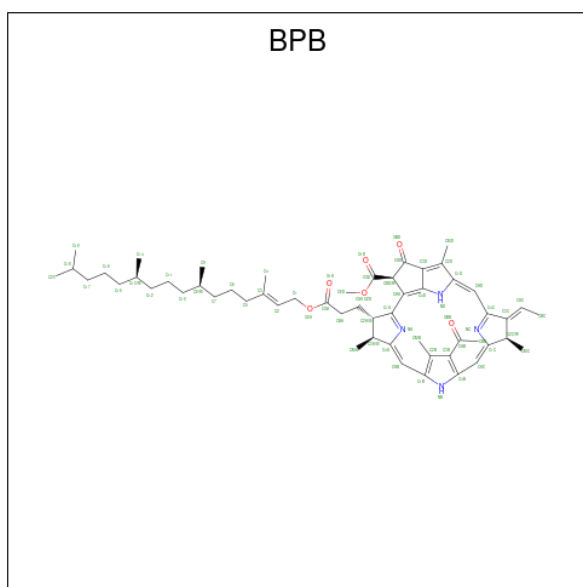
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	M	1	Total	C	N	O	0	0
			16	14	1	1		
7	M	1	Total	C	N	O	4	0
			16	14	1	1		

- Molecule 8 is BACTERIOCHLOROPHYLL B (three-letter code: BCB) (formula: $C_{55}H_{72}MgN_4O_6$).



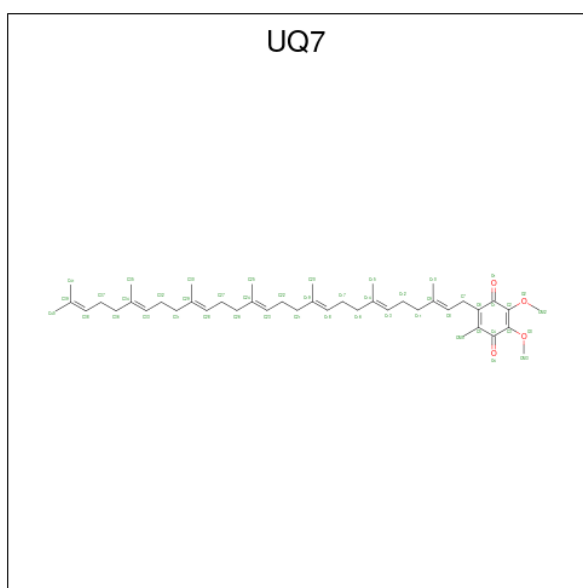
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
8	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
8	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
8	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
8	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 9 is BACTERIOPHEOPHYTIN B (three-letter code: BPB) (formula: $C_{55}H_{74}N_4O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
9	L	1	65	55	4	6	0	0
9	M	1	65	55	4	6	9	0

- Molecule 10 is UBIQUINONE-7 (three-letter code: UQ7) (formula: $C_{44}H_{66}O_4$).

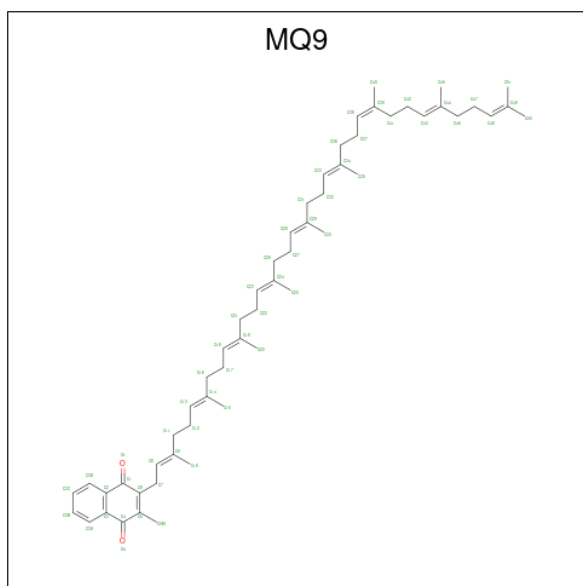


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
10	L	1	48	44	4	0	0

- Molecule 11 is FE (II) ION (three-letter code: FE2) (formula: Fe).

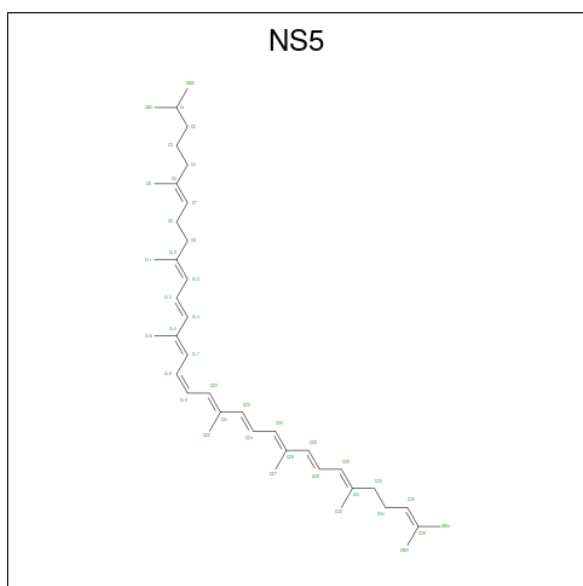
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	M	1	Total	Fe	0	0
			1	1		

- Molecule 12 is MENAQUINONE-9 (three-letter code: MQ9) (formula: $C_{56}H_{80}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	M	1	Total	C	O	0	0
			58	56	2		

- Molecule 13 is 15-cis-1,2-dihydroneurosporene (three-letter code: NS5) (formula: $C_{40}H_{60}$).



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

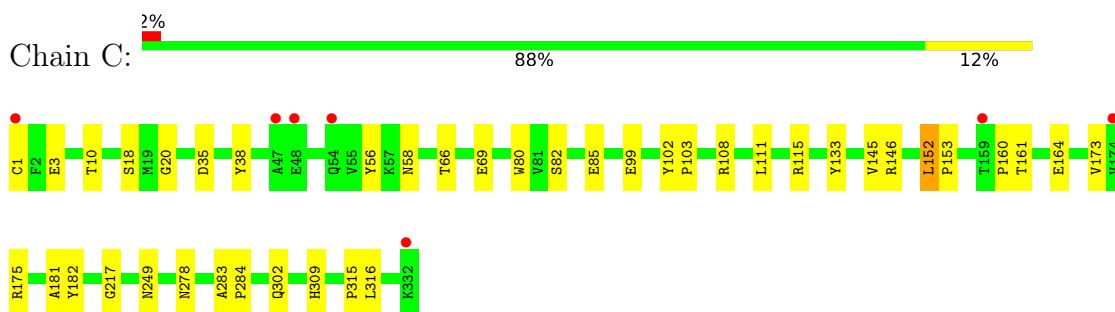
- Molecule 14 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	C	212	Total O 212 212	0	0
14	H	124	Total O 124 124	0	0
14	L	92	Total O 92 92	0	0
14	M	114	Total O 114 114	0	0

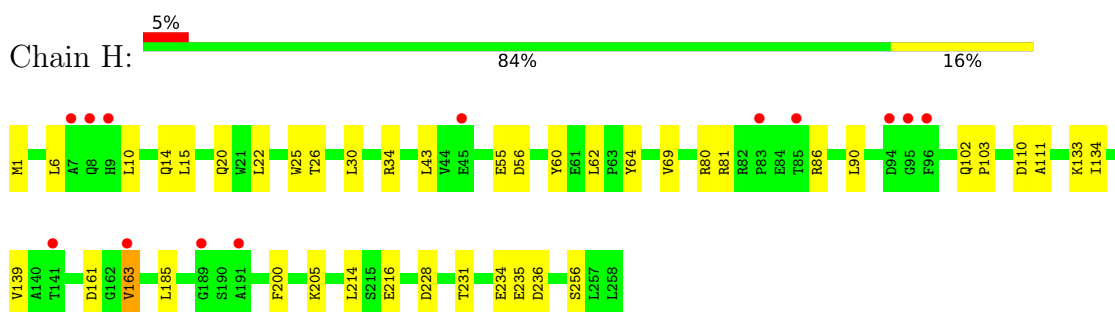
3 Residue-property plots [i](#)

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.

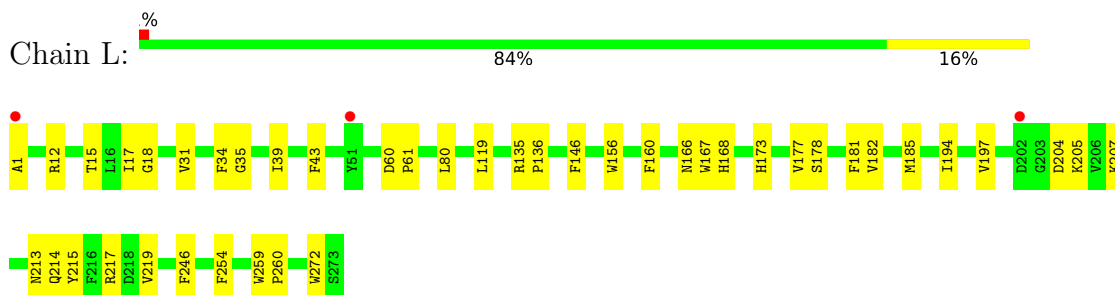
- Molecule 1: Photosynthetic reaction center cytochrome c subunit



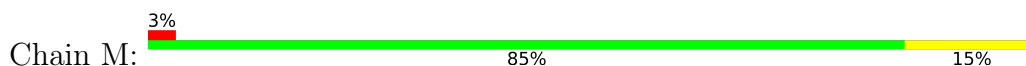
- Molecule 2: Reaction center protein H chain

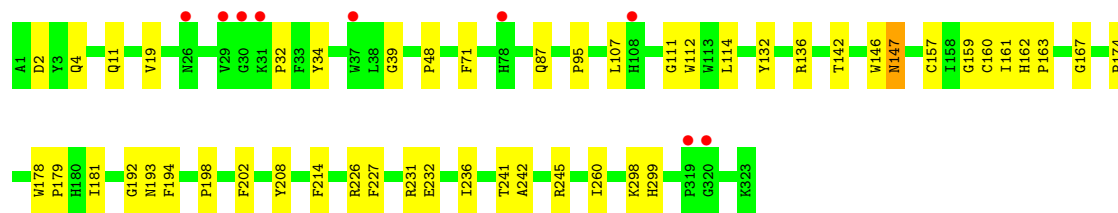


- Molecule 3: Reaction center protein L chain



- Molecule 4: Reaction center protein M chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	219.40Å 219.40Å 112.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.18 – 2.20 20.13 – 2.20	Depositor EDS
% Data completeness (in resolution range)	86.2 (19.18-2.20) 86.2 (20.13-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.15 (at 2.19Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.191 , 0.212 0.186 , 0.207	Depositor DCC
R_{free} test set	6079 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	24.8	Xtrriage
Anisotropy	0.183	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 69.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10747	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: UQ7, SO4, HEC, BCB, BPB, MQ9, FME, FE2, NS5, LDA

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	0.31	0/2670	0.60	1/3637 (0.0%)
2	H	0.29	0/2055	0.56	0/2807
3	L	0.38	0/2265	0.56	0/3092
4	M	0.35	0/2667	0.54	0/3647
All	All	0.34	0/9657	0.56	1/13183 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	249	ASN	N-CA-C	-6.30	93.99	111.00

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	2603	0	2579	23	0
2	H	2018	0	2020	37	0
3	L	2177	0	2102	35	0
4	M	2563	0	2460	42	0
5	C	172	0	120	4	0
6	H	15	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	M	20	0	0	1	0
7	H	32	0	62	8	0
7	L	32	0	62	4	0
7	M	32	0	62	5	0
8	L	132	0	144	10	0
8	M	132	0	144	12	0
9	L	65	0	74	6	0
9	M	65	0	74	8	0
10	L	48	0	66	9	0
11	M	1	0	0	0	0
12	M	58	0	80	2	0
13	M	40	0	60	4	0
14	C	212	0	0	0	0
14	H	124	0	0	1	0
14	L	92	0	0	1	0
14	M	114	0	0	1	0
All	All	10747	0	10109	159	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 8.

All (159) 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:32:PRO:HG3	4:M:48:PRO:HD3	1.46	0.95
9:L:406:BPB:HHC	9:L:406:BPB:HBBB	1.52	0.92
9:M:405:BPB:HHC	9:M:405:BPB:HBBB	1.56	0.87
4:M:114:LEU:HG	13:M:600:NS5:HM43	1.64	0.79
2:H:69:VAL:HG13	3:L:205:LYS:HA	1.66	0.78
8:M:401:BCB:HBB2	8:M:401:BCB:HHC	1.66	0.77
1:C:152:LEU:HD22	1:C:175:ARG:HA	1.66	0.76
2:H:102:GLN:OE1	3:L:12:ARG:HD3	1.91	0.71
10:L:502:UQ7:H171	8:M:401:BCB:H91	1.73	0.70
4:M:71:PHE:HB3	7:M:705:LDA:H61	1.75	0.68
3:L:181:PHE:HB3	9:M:405:BPB:HBBA	1.74	0.68
3:L:214:GLN:NE2	4:M:19:VAL:H	1.91	0.68
1:C:153:PRO:HD3	1:C:160:PRO:HB3	1.77	0.67
9:L:406:BPB:HHC	9:L:406:BPB:CBB	2.24	0.66
2:H:86:ARG:NH2	2:H:111:ALA:HB3	2.11	0.65
8:M:401:BCB:H102	8:M:401:BCB:H142	1.77	0.65
2:H:69:VAL:HG12	14:H:1292:HOH:O	1.95	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:402:BCB:HMB1	8:L:402:BCB:HBB3	1.79	0.64
10:L:502:UQ7:H153	8:M:401:BCB:H101	1.78	0.64
2:H:81:ARG:H	7:H:703:LDA:H112	1.63	0.64
3:L:178:SER:HB3	10:L:502:UQ7:H261	1.79	0.64
9:L:406:BPB:HBBA	4:M:208:TYR:HB3	1.80	0.63
7:L:702:LDA:H72	7:L:702:LDA:H31	1.81	0.62
4:M:231:ARG:HD2	14:M:1383:HOH:O	1.98	0.62
3:L:181:PHE:CD2	9:M:405:BPB:HBB	2.35	0.62
2:H:231:THR:OG1	2:H:234:GLU:HG3	1.99	0.61
6:H:807:SO4:S	7:H:703:LDA:HM23	2.42	0.59
2:H:86:ARG:HH22	2:H:111:ALA:HB3	1.66	0.59
1:C:1:CYS:HB2	14:L:1204:HOH:O	2.03	0.58
6:H:807:SO4:O3	7:H:703:LDA:HM23	2.03	0.58
3:L:181:PHE:HB3	9:M:405:BPB:CBB	2.34	0.57
1:C:145:VAL:O	1:C:146:ARG:HD2	2.03	0.57
4:M:132:TYR:CE1	4:M:142:THR:HG21	2.39	0.56
8:L:404:BCB:HMB1	8:L:404:BCB:HBB2	1.87	0.56
4:M:71:PHE:HB3	7:M:705:LDA:C6	2.35	0.56
7:H:701:LDA:H52	12:M:501:MQ9:H202	1.89	0.55
3:L:182:VAL:HG11	10:L:502:UQ7:H253	1.88	0.55
8:L:404:BCB:HMB1	8:L:404:BCB:CBB	2.36	0.55
4:M:95:PRO:HD3	4:M:174:PRO:HB3	1.88	0.55
9:L:406:BPB:HBB	4:M:208:TYR:CD2	2.41	0.55
2:H:30:LEU:O	2:H:34:ARG:HD2	2.07	0.55
2:H:133:LYS:HG2	2:H:134:ILE:HD12	1.89	0.55
2:H:20:GLN:HG2	4:M:202:PHE:CE2	2.42	0.54
3:L:214:GLN:HE21	4:M:19:VAL:H	1.55	0.54
4:M:112:TRP:CZ3	7:M:705:LDA:H81	2.42	0.54
4:M:162:HIS:HB3	4:M:163:PRO:HD3	1.90	0.54
2:H:139:VAL:HG21	2:H:228:ASP:HB3	1.89	0.54
2:H:6:LEU:HD12	2:H:10:LEU:HD12	1.90	0.54
3:L:135:ARG:HB3	3:L:136:PRO:HD3	1.88	0.54
8:M:403:BCB:H203	9:M:405:BPB:C4	2.38	0.54
8:M:403:BCB:HMB1	8:M:403:BCB:HBB3	1.89	0.53
7:L:702:LDA:H111	4:M:198:PRO:HA	1.91	0.52
8:M:403:BCB:H203	9:M:405:BPB:H4	1.92	0.52
2:H:235:GLU:OE1	4:M:231:ARG:NH2	2.38	0.51
8:M:403:BCB:HMB1	8:M:403:BCB:CBB	2.40	0.51
2:H:81:ARG:N	7:H:703:LDA:H112	2.25	0.51
1:C:18:SER:HB2	3:L:156:TRP:CD1	2.47	0.50
3:L:213:ASN:OD1	10:L:502:UQ7:HM21	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:241:THR:O	4:M:245:ARG:HG3	2.12	0.50
2:H:134:ILE:HD12	2:H:134:ILE:N	2.27	0.50
3:L:177:VAL:HG13	8:L:402:BCB:HMB3	1.93	0.50
4:M:146:TRP:HA	4:M:146:TRP:CE3	2.47	0.50
2:H:6:LEU:HD12	2:H:10:LEU:CD1	2.42	0.50
4:M:157:CYS:HA	4:M:161:ILE:HB	1.93	0.50
2:H:80:ARG:HA	7:H:703:LDA:H101	1.93	0.50
1:C:102:TYR:CG	1:C:103:PRO:HD3	2.47	0.49
4:M:178:TRP:HB2	4:M:179:PRO:HD3	1.94	0.49
1:C:35:ASP:OD2	1:C:316:LEU:HA	2.13	0.49
8:L:402:BCB:HMB1	8:L:402:BCB:CBB	2.43	0.49
4:M:298:LYS:HE3	4:M:299:HIS:NE2	2.28	0.48
1:C:283:ALA:HB3	1:C:284:PRO:HD3	1.96	0.48
8:L:404:BCB:OBB	8:L:404:BCB:HHC	2.13	0.48
3:L:246:PHE:CD1	10:L:502:UQ7:H412	2.49	0.48
1:C:111:LEU:O	1:C:115:ARG:HG3	2.14	0.48
1:C:278:ASN:HB3	1:C:302:GLN:NE2	2.29	0.47
10:L:502:UQ7:H171	8:M:401:BCB:C9	2.43	0.47
9:M:405:BPB:H55	9:M:405:BPB:HMC	1.95	0.47
1:C:80:TRP:CD1	1:C:133:TYR:HB2	2.49	0.47
3:L:43:PHE:CD1	12:M:501:MQ9:H512	2.50	0.47
3:L:167:TRP:HE1	3:L:173:HIS:CD2	2.33	0.47
1:C:161:THR:OG1	1:C:164:GLU:HG3	2.15	0.47
8:L:402:BCB:H11	8:L:404:BCB:H2C	1.97	0.47
2:H:22:LEU:C	2:H:22:LEU:HD13	2.35	0.46
2:H:133:LYS:CG	2:H:134:ILE:HD12	2.45	0.46
3:L:197:VAL:HG13	3:L:207:LYS:HB2	1.95	0.46
4:M:107:LEU:HA	4:M:111:GLY:HA3	1.96	0.46
4:M:192:GLY:O	4:M:193:ASN:HB3	2.14	0.46
3:L:146:PHE:HB3	3:L:156:TRP:CD2	2.50	0.46
2:H:62:LEU:O	7:H:703:LDA:HM13	2.15	0.46
8:M:401:BCB:H142	8:M:401:BCB:C10	2.45	0.46
1:C:66:THR:OG1	1:C:69:GLU:HG3	2.16	0.46
2:H:86:ARG:NH2	2:H:110:ASP:O	2.49	0.46
8:L:404:BCB:H172	9:L:406:BPB:H11A	1.98	0.46
1:C:181:ALA:O	1:C:182:TYR:HB2	2.15	0.46
2:H:26:THR:O	2:H:30:LEU:HB2	2.16	0.45
3:L:35:GLY:O	3:L:39:ILE:HG12	2.16	0.45
5:C:402:HEC:HMB1	5:C:402:HEC:HBB3	1.97	0.45
2:H:90:LEU:HD23	2:H:103:PRO:HA	1.98	0.45
13:M:600:NS5:H29	13:M:600:NS5:H271	1.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:160:CYS:C	4:M:163:PRO:HD2	2.37	0.45
8:M:403:BCB:HHC	8:M:403:BCB:OBB	2.17	0.45
2:H:56:ASP:HB3	2:H:60:TYR:CE2	2.52	0.45
8:M:401:BCB:HHC	8:M:401:BCB:CBB	2.43	0.45
4:M:112:TRP:CH2	7:M:705:LDA:H81	2.52	0.45
7:L:702:LDA:H31	7:L:702:LDA:C7	2.46	0.45
5:C:403:HEC:HBC3	5:C:403:HEC:HMC1	1.99	0.45
1:C:102:TYR:CD2	1:C:103:PRO:HD3	2.52	0.44
2:H:43:LEU:HB3	3:L:1:ALA:H2	1.81	0.44
3:L:17:ILE:HG13	3:L:18:GLY:N	2.32	0.44
2:H:69:VAL:CG1	3:L:204:ASP:O	2.65	0.44
4:M:34:TYR:CD1	4:M:34:TYR:N	2.85	0.44
2:H:256:SER:HA	3:L:15:THR:O	2.18	0.44
2:H:161:ASP:HB3	2:H:214:LEU:HD22	1.99	0.44
2:H:25:TRP:HA	2:H:25:TRP:CE3	2.51	0.44
2:H:216:GLU:H	2:H:216:GLU:CD	2.20	0.44
8:L:402:BCB:OBB	8:L:402:BCB:HHC	2.16	0.44
1:C:10:THR:O	1:C:20:GLY:HA3	2.18	0.43
4:M:132:TYR:CZ	4:M:136:ARG:HD2	2.53	0.43
4:M:178:TRP:O	4:M:181:ILE:HB	2.18	0.43
2:H:161:ASP:CG	2:H:163:VAL:HG13	2.38	0.43
4:M:147:ASN:C	4:M:147:ASN:HD22	2.20	0.43
3:L:60:ASP:OD2	7:L:702:LDA:HM12	2.19	0.43
3:L:214:GLN:HG2	4:M:19:VAL:HB	2.00	0.43
1:C:99:GLU:OE2	1:C:108:ARG:NH2	2.51	0.42
1:C:217:GLY:HA2	4:M:167:GLY:O	2.18	0.42
4:M:227:PHE:HB2	4:M:242:ALA:HB2	2.01	0.42
3:L:215:TYR:O	3:L:219:VAL:HG23	2.20	0.42
2:H:200:PHE:CZ	4:M:226:ARG:HD3	2.54	0.42
3:L:213:ASN:O	3:L:217:ARG:HG3	2.19	0.42
3:L:259:TRP:N	3:L:260:PRO:CD	2.83	0.42
6:M:804:SO4:O4	7:M:704:LDA:HM11	2.19	0.42
1:C:82:SER:HB2	1:C:85:GLU:HB2	2.01	0.42
1:C:309:HIS:CE1	1:C:315:PRO:HD3	2.55	0.42
3:L:166:ASN:OD1	3:L:168:HIS:HB2	2.19	0.42
9:L:406:BPB:CBB	4:M:208:TYR:CD2	3.02	0.42
5:C:401:HEC:HMC1	5:C:401:HEC:HBC3	2.01	0.42
10:L:502:UQ7:H312	10:L:502:UQ7:H352	2.02	0.42
4:M:178:TRP:N	4:M:179:PRO:CD	2.83	0.42
2:H:6:LEU:HB2	2:H:10:LEU:HD12	2.02	0.42
9:M:405:BPB:HBBB	9:M:405:BPB:CHC	2.37	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:10:LEU:HD13	2:H:15:LEU:HD21	2.01	0.42
3:L:194:ILE:HD11	10:L:502:UQ7:HM31	2.01	0.42
4:M:159:GLY:HA3	13:M:600:NS5:H272	2.02	0.42
1:C:173:VAL:HB	4:M:87:GLN:OE1	2.19	0.41
3:L:146:PHE:HB3	3:L:156:TRP:CE3	2.55	0.41
4:M:11:GLN:OE1	4:M:39:GLY:HA3	2.21	0.41
4:M:178:TRP:HA	4:M:178:TRP:CE3	2.55	0.41
2:H:10:LEU:HB2	2:H:14:GLN:OE1	2.21	0.41
4:M:236:ILE:HG12	4:M:260:ILE:HG23	2.01	0.41
1:C:3:GLU:O	3:L:254:PHE:HA	2.20	0.41
2:H:22:LEU:HD13	2:H:22:LEU:O	2.21	0.41
4:M:2:ASP:OD1	4:M:4:GLN:HB2	2.20	0.41
13:M:600:NS5:H22	13:M:600:NS5:H7	2.02	0.41
3:L:60:ASP:HA	3:L:61:PRO:HD3	1.89	0.40
3:L:168:HIS:CE1	8:L:402:BCB:HMC2	2.55	0.40
1:C:56:TYR:HB3	5:C:401:HEC:CGA	2.51	0.40
3:L:17:ILE:HG22	3:L:34:PHE:CE2	2.56	0.40
2:H:64:TYR:CZ	7:H:703:LDA:HM22	2.56	0.40
4:M:232:GLU:O	4:M:236:ILE:HG13	2.21	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	330/332 (99%)	320 (97%)	10 (3%)	0	100	100
2	H	256/258 (99%)	249 (97%)	6 (2%)	1 (0%)	34	37
3	L	272/273 (100%)	267 (98%)	4 (2%)	1 (0%)	34	37
4	M	322/323 (100%)	310 (96%)	12 (4%)	0	100	100
All	All	1180/1186 (100%)	1146 (97%)	32 (3%)	2 (0%)	47	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	55	GLU
3	L	31	VAL

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	281/281 (100%)	278 (99%)	3 (1%)	73 85
2	H	212/212 (100%)	208 (98%)	4 (2%)	57 71
3	L	219/218 (100%)	214 (98%)	5 (2%)	50 63
4	M	250/249 (100%)	247 (99%)	3 (1%)	71 83
All	All	962/960 (100%)	947 (98%)	15 (2%)	62 76

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	38	TYR
1	C	58	ASN
1	C	152	LEU
2	H	163	VAL
2	H	185	LEU
2	H	205	LYS
2	H	236	ASP
3	L	80	LEU
3	L	119	LEU
3	L	160	PHE
3	L	185	MET
3	L	272	TRP
4	M	147	ASN
4	M	194	PHE
4	M	214	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	54	GLN
1	C	58	ASN
1	C	94	ASN
1	C	127	GLN
1	C	206	GLN
2	H	8	GLN
2	H	58	GLN
3	L	214	GLN
4	M	147	ASN

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	0.65	0	7,9,11	2.29	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	-	1/7/9/11	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1	FME	CA-N-CN	-4.17	116.40	122.82
2	H	1	FME	O1-CN-N	-3.85	115.12	125.27

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	1	FME	O1-CN-N-CA

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 27 ligands modelled in this entry, 1 is monoatomic - leaving 26 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	$\# Z > 2$
6	SO4	H	806	-	4,4,4	0.38	0	6,6,6	0.15	0
7	LDA	H	703	-	12,15,15	2.25	1 (8%)	14,17,17	0.53	0
7	LDA	H	701	-	12,15,15	2.12	1 (8%)	14,17,17	0.52	0
9	BPB	M	405	-	49,70,70	1.30	7 (14%)	47,101,101	1.97	6 (12%)
5	HEC	C	403	1	32,50,50	1.52	2 (6%)	24,82,82	0.92	0
6	SO4	M	805	-	4,4,4	0.50	0	6,6,6	0.33	0
5	HEC	C	402	1	32,50,50	1.50	2 (6%)	24,82,82	1.03	1 (4%)
7	LDA	L	706	-	12,15,15	2.30	1 (8%)	14,17,17	0.58	0
7	LDA	L	702	-	12,15,15	2.36	1 (8%)	14,17,17	0.53	0
7	LDA	M	705	-	12,15,15	2.42	1 (8%)	14,17,17	0.53	0

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	1.49	2 (6%)	24,82,82	1.24	2 (8%)
6	SO4	H	807	-	4,4,4	0.65	0	6,6,6	0.33	0
8	BCB	L	402	3	54,74,74	1.46	7 (12%)	52,115,115	2.07	12 (23%)
8	BCB	L	404	3	54,74,74	1.67	11 (20%)	52,115,115	2.77	14 (26%)
13	NS5	M	600	-	39,39,39	0.53	0	44,46,46	0.88	3 (6%)
6	SO4	M	803	-	4,4,4	0.59	0	6,6,6	0.44	0
8	BCB	M	401	4	54,74,74	1.54	10 (18%)	52,115,115	2.24	11 (21%)
9	BPB	L	406	-	49,70,70	1.34	7 (14%)	47,101,101	2.06	7 (14%)
6	SO4	M	801	-	4,4,4	0.57	0	6,6,6	0.21	0
6	SO4	H	802	-	4,4,4	0.46	0	6,6,6	0.15	0
6	SO4	M	804	-	4,4,4	0.55	0	6,6,6	0.33	0
8	BCB	M	403	4	54,74,74	1.44	9 (16%)	52,115,115	2.11	10 (19%)
7	LDA	M	704	-	12,15,15	2.37	1 (8%)	14,17,17	0.56	0
5	HEC	C	401	1	32,50,50	1.48	2 (6%)	24,82,82	0.86	0
12	MQ9	M	501	-	59,59,59	1.54	10 (16%)	72,75,75	1.03	6 (8%)
10	UQ7	L	502	-	48,48,48	1.67	10 (20%)	58,61,61	1.22	7 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	LDA	H	703	-	-	0/13/13/13	-
7	LDA	H	701	-	-	1/13/13/13	-
9	BPB	M	405	-	2/2/18/23	4/37/105/105	0/5/6/6
5	HEC	C	403	1	-	3/10/54/54	-
5	HEC	C	402	1	-	4/10/54/54	-
7	LDA	L	706	-	-	1/13/13/13	-
7	LDA	L	702	-	-	2/13/13/13	-
7	LDA	M	705	-	-	0/13/13/13	-
5	HEC	C	404	1	-	1/10/54/54	-
8	BCB	L	402	3	-	5/37/177/177	-
8	BCB	L	404	3	-	5/37/177/177	-
13	NS5	M	600	-	-	14/43/43/43	-
8	BCB	M	401	4	1/1/31/36	5/37/177/177	-
9	BPB	L	406	-	-	5/37/105/105	0/5/6/6
8	BCB	M	403	4	-	4/37/177/177	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	LDA	M	704	-	-	0/13/13/13	-
5	HEC	C	401	1	-	2/10/54/54	-
12	MQ9	M	501	-	-	4/53/73/73	0/2/2/2
10	UQ7	L	502	-	-	12/45/69/69	0/1/1/1

All (85) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	705	LDA	O1-N1	-8.37	1.22	1.42
7	M	704	LDA	O1-N1	-8.20	1.23	1.42
7	L	702	LDA	O1-N1	-8.14	1.23	1.42
7	L	706	LDA	O1-N1	-7.95	1.23	1.42
7	H	703	LDA	O1-N1	-7.73	1.24	1.42
7	H	701	LDA	O1-N1	-7.29	1.25	1.42
8	M	403	BCB	C4C-NC	6.16	1.40	1.35
8	M	401	BCB	C4C-NC	6.02	1.40	1.35
8	L	402	BCB	C4C-NC	5.76	1.40	1.35
8	L	404	BCB	C4C-NC	5.69	1.40	1.35
5	C	403	HEC	C2B-C3B	-4.86	1.35	1.40
5	C	404	HEC	C2B-C3B	-4.86	1.35	1.40
5	C	401	HEC	C3C-C2C	-4.85	1.35	1.40
9	M	405	BPB	C3A-C2A	-4.83	1.50	1.54
5	C	404	HEC	C3C-C2C	-4.81	1.35	1.40
8	L	404	BCB	O2A-CGA	4.76	1.47	1.33
5	C	402	HEC	C3C-C2C	-4.67	1.35	1.40
5	C	401	HEC	C2B-C3B	-4.65	1.35	1.40
5	C	402	HEC	C2B-C3B	-4.64	1.35	1.40
5	C	403	HEC	C3C-C2C	-4.57	1.36	1.40
9	L	406	BPB	C3A-C2A	-4.52	1.50	1.54
8	M	401	BCB	C3A-C2A	-3.88	1.51	1.54
10	L	502	UQ7	C7-C8	-3.80	1.45	1.50
8	L	402	BCB	C3A-C2A	-3.77	1.51	1.54
9	L	406	BPB	O2D-CGD	3.77	1.42	1.33
8	L	402	BCB	O2D-CGD	3.65	1.42	1.33
8	M	403	BCB	C3A-C2A	-3.63	1.51	1.54
8	L	404	BCB	O2D-CGD	3.56	1.41	1.33
8	M	401	BCB	O2D-CGD	3.47	1.41	1.33
8	L	404	BCB	C3A-C2A	-3.46	1.51	1.54
8	L	404	BCB	C1-C2	-3.32	1.39	1.49
9	M	405	BPB	O2D-CGD	3.29	1.41	1.33
8	M	401	BCB	O2A-CGA	3.04	1.42	1.33
8	M	403	BCB	O2D-CGD	3.03	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	404	BCB	O2D-CED	-3.01	1.38	1.45
9	L	406	BPB	O2A-CGA	2.96	1.42	1.33
10	L	502	UQ7	C13-C14	2.85	1.39	1.33
12	M	501	MQ9	C43-C44	2.82	1.39	1.33
12	M	501	MQ9	C33-C34	2.82	1.39	1.33
8	M	401	BCB	O2D-CED	-2.80	1.38	1.45
9	L	406	BPB	C2-C3	2.80	1.39	1.33
10	L	502	UQ7	C33-C34	2.78	1.39	1.33
10	L	502	UQ7	C8-C9	2.77	1.39	1.33
12	M	501	MQ9	C28-C29	2.76	1.39	1.33
10	L	502	UQ7	C28-C29	2.75	1.39	1.33
10	L	502	UQ7	C23-C24	2.74	1.39	1.33
10	L	502	UQ7	C18-C19	2.73	1.39	1.33
9	M	405	BPB	O2A-CGA	2.72	1.41	1.33
10	L	502	UQ7	O3-CM3	-2.72	1.38	1.45
12	M	501	MQ9	C38-C39	2.69	1.39	1.33
12	M	501	MQ9	C8-C9	2.65	1.39	1.33
12	M	501	MQ9	C23-C24	2.61	1.39	1.33
10	L	502	UQ7	C38-C39	2.61	1.39	1.32
8	M	403	BCB	C2-C3	2.59	1.39	1.33
9	M	405	BPB	C2-C3	2.54	1.39	1.33
12	M	501	MQ9	C18-C19	2.54	1.39	1.33
12	M	501	MQ9	C48-C49	2.53	1.39	1.32
8	L	404	BCB	C2-C3	2.53	1.39	1.33
9	M	405	BPB	CAC-C3C	2.52	1.39	1.33
8	L	404	BCB	C3B-C4B	2.51	1.46	1.40
8	M	403	BCB	C3B-C4B	2.51	1.46	1.40
8	M	401	BCB	C3B-C4B	2.50	1.46	1.40
8	M	401	BCB	C2-C3	2.49	1.39	1.33
12	M	501	MQ9	C13-C14	2.44	1.38	1.33
8	M	401	BCB	C1-C2	-2.43	1.41	1.49
10	L	502	UQ7	O2-CM2	-2.41	1.39	1.45
8	L	402	BCB	C3B-C4B	2.38	1.46	1.40
8	M	403	BCB	O2A-CGA	2.35	1.40	1.33
8	L	402	BCB	C1-C2	-2.31	1.42	1.49
8	L	402	BCB	C2-C3	2.31	1.38	1.33
8	L	404	BCB	CHA-CBD	2.31	1.55	1.52
9	L	406	BPB	CAC-C3C	2.30	1.39	1.33
9	L	406	BPB	C3B-C2B	-2.24	1.35	1.39
9	L	406	BPB	O2D-CED	-2.22	1.40	1.45
9	M	405	BPB	O2D-CED	-2.22	1.40	1.45
8	L	404	BCB	CHD-C4C	2.18	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	403	BCB	O2D-CED	-2.18	1.40	1.45
8	L	404	BCB	CAC-C3C	2.17	1.38	1.33
9	M	405	BPB	C3B-C2B	-2.16	1.35	1.39
8	M	401	BCB	C3B-C2B	-2.11	1.35	1.39
8	M	403	BCB	CHD-C4C	2.07	1.41	1.37
8	L	402	BCB	O2D-CED	-2.06	1.40	1.45
12	M	501	MQ9	C32-C33	-2.05	1.43	1.50
8	M	401	BCB	CHD-C4C	2.04	1.41	1.37
8	M	403	BCB	CAC-C3C	2.01	1.38	1.33

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L	404	BCB	C1-C2-C3	9.83	143.04	126.04
8	L	404	BCB	O2D-CGD-CBD	9.38	122.88	111.00
9	M	405	BPB	O2D-CGD-CBD	9.36	122.85	111.00
8	M	401	BCB	O2D-CGD-CBD	9.24	122.70	111.00
9	L	406	BPB	O2D-CGD-CBD	9.22	122.67	111.00
8	M	403	BCB	O2D-CGD-CBD	8.57	121.86	111.00
8	L	402	BCB	O2D-CGD-CBD	7.64	120.67	111.00
8	M	403	BCB	C4D-C3D-CAD	-6.86	106.29	116.53
8	M	401	BCB	C4D-C3D-CAD	-6.75	106.46	116.53
8	L	402	BCB	C4D-C3D-CAD	-6.66	106.59	116.53
8	L	404	BCB	C4D-C3D-CAD	-6.62	106.64	116.53
8	M	401	BCB	O1D-CGD-CBD	-5.86	114.98	124.74
8	L	404	BCB	O1D-CGD-CBD	-5.74	115.17	124.74
9	M	405	BPB	O1D-CGD-CBD	-5.74	115.18	124.74
9	L	406	BPB	O1D-CGD-CBD	-5.73	115.20	124.74
8	L	404	BCB	C5-C3-C2	5.59	132.43	121.12
8	M	403	BCB	O1D-CGD-CBD	-5.32	115.88	124.74
8	L	402	BCB	O1D-CGD-CBD	-5.06	116.31	124.74
8	L	404	BCB	C4-C3-C2	-4.45	112.27	123.68
9	L	406	BPB	C1-C2-C3	4.20	133.30	126.04
8	M	401	BCB	OBD-CAD-CBD	-3.61	120.52	125.82
5	C	404	HEC	CBD-CAD-C3D	3.61	118.78	112.62
8	L	402	BCB	O2A-CGA-CBA	3.59	123.18	111.91
9	M	405	BPB	OBD-CAD-CBD	-3.49	120.71	125.82
8	L	404	BCB	C4C-CHD-C1D	3.45	128.01	118.67
8	M	403	BCB	OBD-CAD-CBD	-3.43	120.79	125.82
8	M	403	BCB	CMC-C2C-C1C	-3.35	108.73	114.36
8	L	402	BCB	C4C-CHD-C1D	3.35	127.73	118.67
9	L	406	BPB	OBD-CAD-CBD	-3.32	120.94	125.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L	402	BCB	OBD-CAD-CBD	-3.31	120.97	125.82
8	M	401	BCB	CMC-C2C-C1C	-3.30	108.82	114.36
8	M	401	BCB	C4C-CHD-C1D	3.30	127.59	118.67
5	C	402	HEC	CBD-CAD-C3D	3.24	118.14	112.62
8	M	403	BCB	C4C-CHD-C1D	3.15	127.19	118.67
9	L	406	BPB	O2A-CGA-CBA	3.13	121.72	111.91
8	L	404	BCB	OBD-CAD-CBD	-3.12	121.25	125.82
12	M	501	MQ9	C37-C38-C39	3.12	135.17	127.66
8	L	402	BCB	O2A-CGA-O1A	-3.05	115.90	123.59
8	L	404	BCB	CMC-C2C-C1C	-2.91	109.47	114.36
8	M	403	BCB	CMB-C2B-C3B	2.89	130.08	124.68
10	L	502	UQ7	C17-C18-C19	2.76	134.31	127.66
8	L	404	BCB	O2A-CGA-CBA	2.76	120.56	111.91
8	L	404	BCB	CMA-C3A-C4A	-2.75	108.36	114.38
8	M	403	BCB	CMD-C2D-C3D	2.64	129.62	124.68
8	M	401	BCB	CMA-C3A-C4A	-2.63	108.61	114.38
10	L	502	UQ7	C12-C11-C9	-2.63	104.32	112.98
8	L	402	BCB	CMC-C2C-C1C	-2.58	110.03	114.36
8	M	401	BCB	CHA-C1A-C2A	-2.57	127.27	133.31
12	M	501	MQ9	C32-C33-C34	2.57	133.85	127.66
8	L	404	BCB	CHA-C1A-C2A	-2.55	127.31	133.31
9	M	405	BPB	C5-C3-C2	2.55	126.28	121.12
12	M	501	MQ9	C7-C8-C9	2.54	131.02	126.79
10	L	502	UQ7	C25-C24-C26	-2.51	111.04	115.27
9	L	406	BPB	O2A-CGA-O1A	-2.47	117.36	123.59
13	M	600	NS5	C19-C18-C17	2.47	128.53	123.47
9	M	405	BPB	O2A-CGA-CBA	2.29	119.10	111.91
8	M	403	BCB	O2A-CGA-CBA	2.27	119.03	111.91
13	M	600	NS5	C16-C15-C14	-2.27	114.51	118.08
8	M	401	BCB	CMD-C2D-C3D	2.24	128.87	124.68
10	L	502	UQ7	C7-C8-C9	2.24	130.51	126.79
12	M	501	MQ9	C45-C44-C46	-2.22	111.53	115.27
8	L	404	BCB	CMB-C2B-C3B	2.21	128.82	124.68
10	L	502	UQ7	C37-C36-C34	2.21	120.24	112.98
8	L	404	BCB	CED-O2D-CGD	2.15	120.81	115.94
8	L	402	BCB	CMD-C2D-C3D	2.13	128.66	124.68
10	L	502	UQ7	CM3-O3-C3	2.13	124.01	116.47
13	M	600	NS5	C19-C20-C21	-2.12	124.28	127.31
9	M	405	BPB	CMD-C2D-C3D	2.10	128.62	124.68
9	L	406	BPB	CMD-C2D-C3D	2.10	128.60	124.68
8	L	402	BCB	CMB-C2B-C3B	2.09	128.59	124.68
12	M	501	MQ9	C30-C29-C31	-2.08	111.77	115.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	404	HEC	CMB-C2B-C1B	-2.07	125.29	128.46
8	L	402	BCB	CHA-C1A-C2A	-2.06	128.47	133.31
8	M	401	BCB	C15-C13-C12	2.04	122.86	112.13
10	L	502	UQ7	C26-C27-C28	2.02	118.53	111.88
8	M	403	BCB	CHA-C1A-C2A	-2.02	128.56	133.31
12	M	501	MQ9	C37-C36-C34	2.02	119.61	112.98
8	M	401	BCB	C1-C2-C3	2.02	129.53	126.04
8	L	402	BCB	CED-O2D-CGD	2.01	120.48	115.94

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	M	401	BCB	C8
9	M	405	BPB	C13
9	M	405	BPB	C8

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	M	403	BCB	CAD-CBD-CGD-O1D
8	M	403	BCB	CAD-CBD-CGD-O2D
9	L	406	BPB	O2A-C1-C2-C3
13	M	600	NS5	C13-C14-C15-C16
13	M	600	NS5	C22-C21-C23-C24
10	L	502	UQ7	C31-C32-C33-C34
8	L	402	BCB	C4-C3-C5-C6
10	L	502	UQ7	C30-C29-C31-C32
8	L	402	BCB	C2-C3-C5-C6
10	L	502	UQ7	C28-C29-C31-C32
10	L	502	UQ7	C19-C21-C22-C23
8	L	404	BCB	CBA-CGA-O2A-C1
8	L	404	BCB	O1A-CGA-O2A-C1
8	M	403	BCB	C2A-CAA-CBA-CGA
13	M	600	NS5	C34-C35-C36-CM4
13	M	600	NS5	C3-C4-C5-C7
8	L	404	BCB	C2-C1-O2A-CGA
8	L	402	BCB	C15-C16-C17-C18
13	M	600	NS5	C3-C4-C5-C6
9	M	405	BPB	CBA-CGA-O2A-C1
10	L	502	UQ7	C15-C14-C16-C17
8	M	401	BCB	C11-C12-C13-C15
7	L	702	LDA	N1-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	L	702	LDA	C3-C4-C5-C6
13	M	600	NS5	C7-C8-C9-C10
10	L	502	UQ7	C13-C14-C16-C17
9	M	405	BPB	O1A-CGA-O2A-C1
7	L	706	LDA	C7-C8-C9-C10
10	L	502	UQ7	C25-C24-C26-C27
8	M	401	BCB	CAD-CBD-CGD-O2D
9	L	406	BPB	CAD-CBD-CGD-O2D
13	M	600	NS5	C11-C10-C12-C13
10	L	502	UQ7	C23-C24-C26-C27
8	L	402	BCB	C16-C17-C18-C20
10	L	502	UQ7	C20-C19-C21-C22
13	M	600	NS5	C20-C21-C23-C24
8	L	402	BCB	CAD-CBD-CGD-O1D
9	L	406	BPB	C4C-C3C-CAC-CBC
5	C	404	HEC	C2D-C3D-CAD-CBD
10	L	502	UQ7	C18-C19-C21-C22
8	M	401	BCB	C3-C5-C6-C7
13	M	600	NS5	C2-C3-C4-C5
13	M	600	NS5	C32-C31-C33-C34
8	M	403	BCB	O2A-C1-C2-C3
5	C	403	HEC	CAD-CBD-CGD-O2D
5	C	401	HEC	CAA-CBA-CGA-O2A
5	C	402	HEC	CAD-CBD-CGD-O2D
10	L	502	UQ7	C35-C34-C36-C37
13	M	600	NS5	C13-C14-C15-C17
5	C	401	HEC	CAA-CBA-CGA-O1A
5	C	403	HEC	CAD-CBD-CGD-O1D
12	M	501	MQ9	C45-C44-C46-C47
5	C	402	HEC	CAA-CBA-CGA-O2A
10	L	502	UQ7	C33-C34-C36-C37
8	L	404	BCB	CAD-CBD-CGD-O2D
12	M	501	MQ9	C35-C34-C36-C37
5	C	402	HEC	CAD-CBD-CGD-O1D
9	M	405	BPB	O2A-C1-C2-C3
5	C	402	HEC	CAA-CBA-CGA-O1A
7	H	701	LDA	C4-C5-C6-C7
8	M	401	BCB	C4-C3-C5-C6
13	M	600	NS5	C30-C31-C33-C34
8	L	404	BCB	CHA-CBD-CGD-O1D
8	M	401	BCB	CHA-CBD-CGD-O2D
12	M	501	MQ9	C40-C39-C41-C42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	M	405	BPB	C6-C7-C8-C10
12	M	501	MQ9	C46-C47-C48-C49
9	L	406	BPB	C2-C3-C5-C6
13	M	600	NS5	C12-C10-C9-C8
9	L	406	BPB	C4-C3-C5-C6
5	C	403	HEC	CAA-CBA-CGA-O2A
13	M	600	NS5	C6-C5-C7-C8

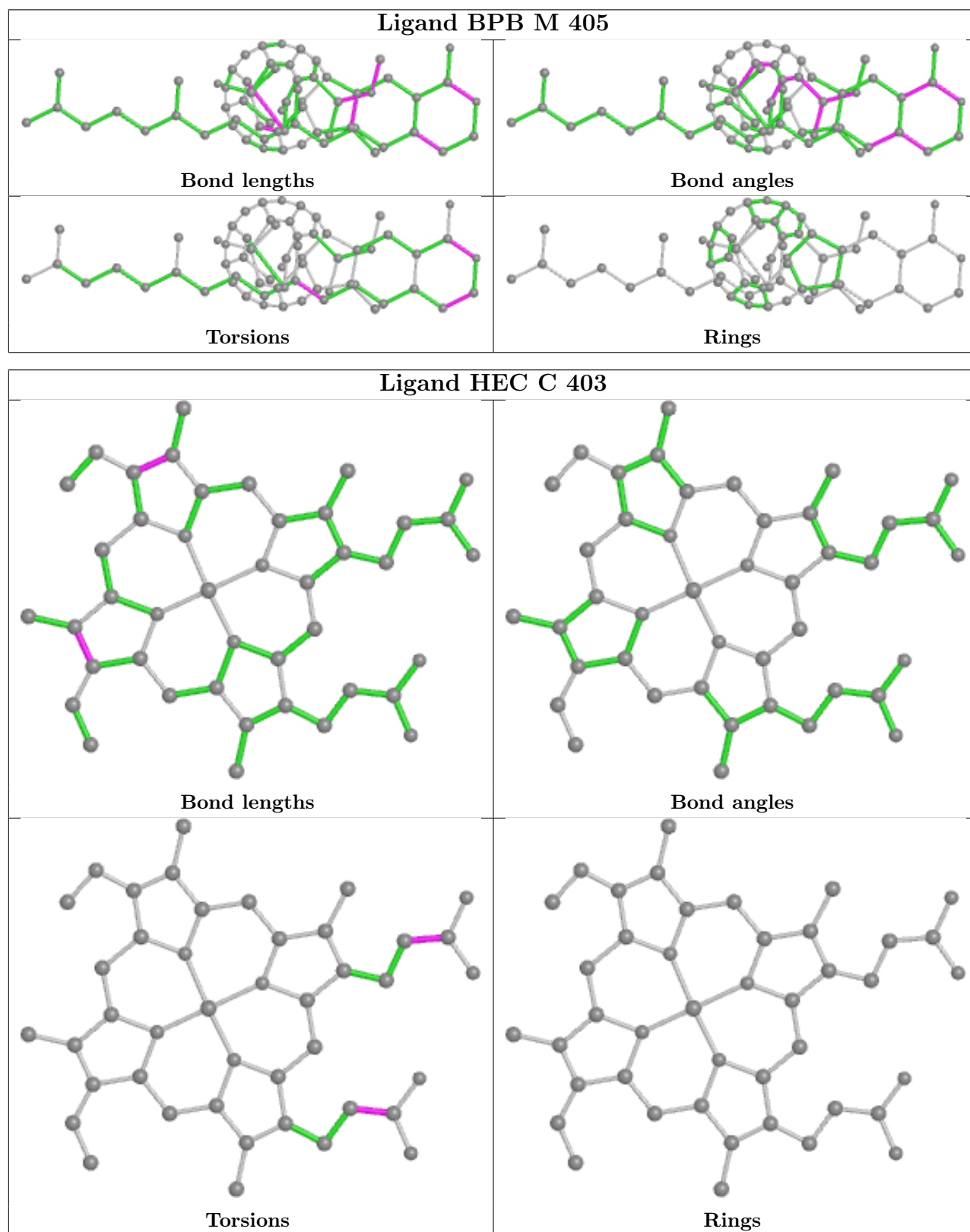
There are no ring outliers.

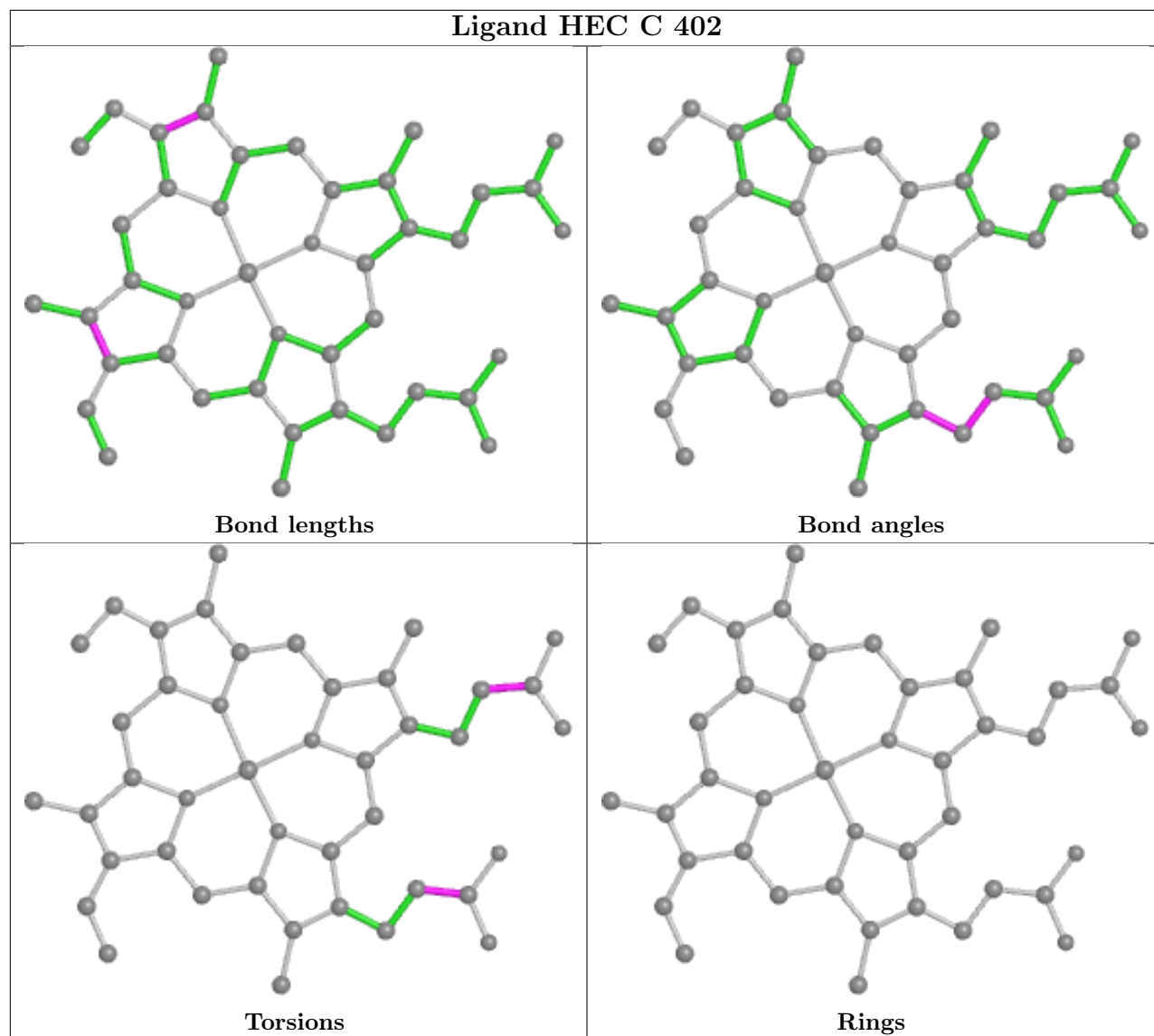
19 monomers are involved in 65 short contacts:

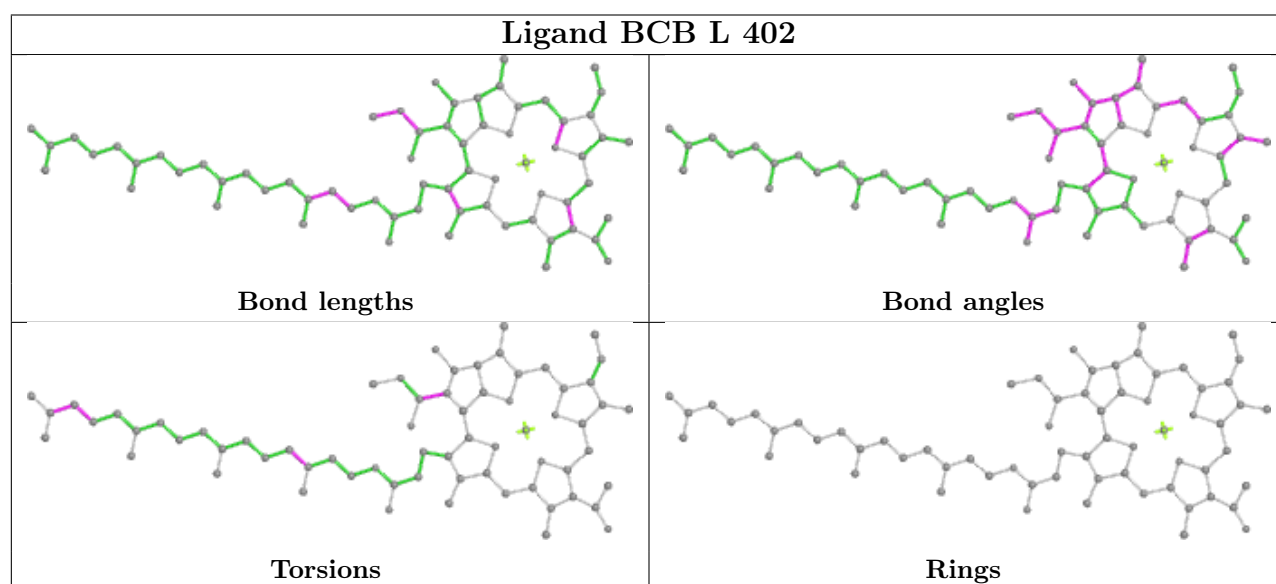
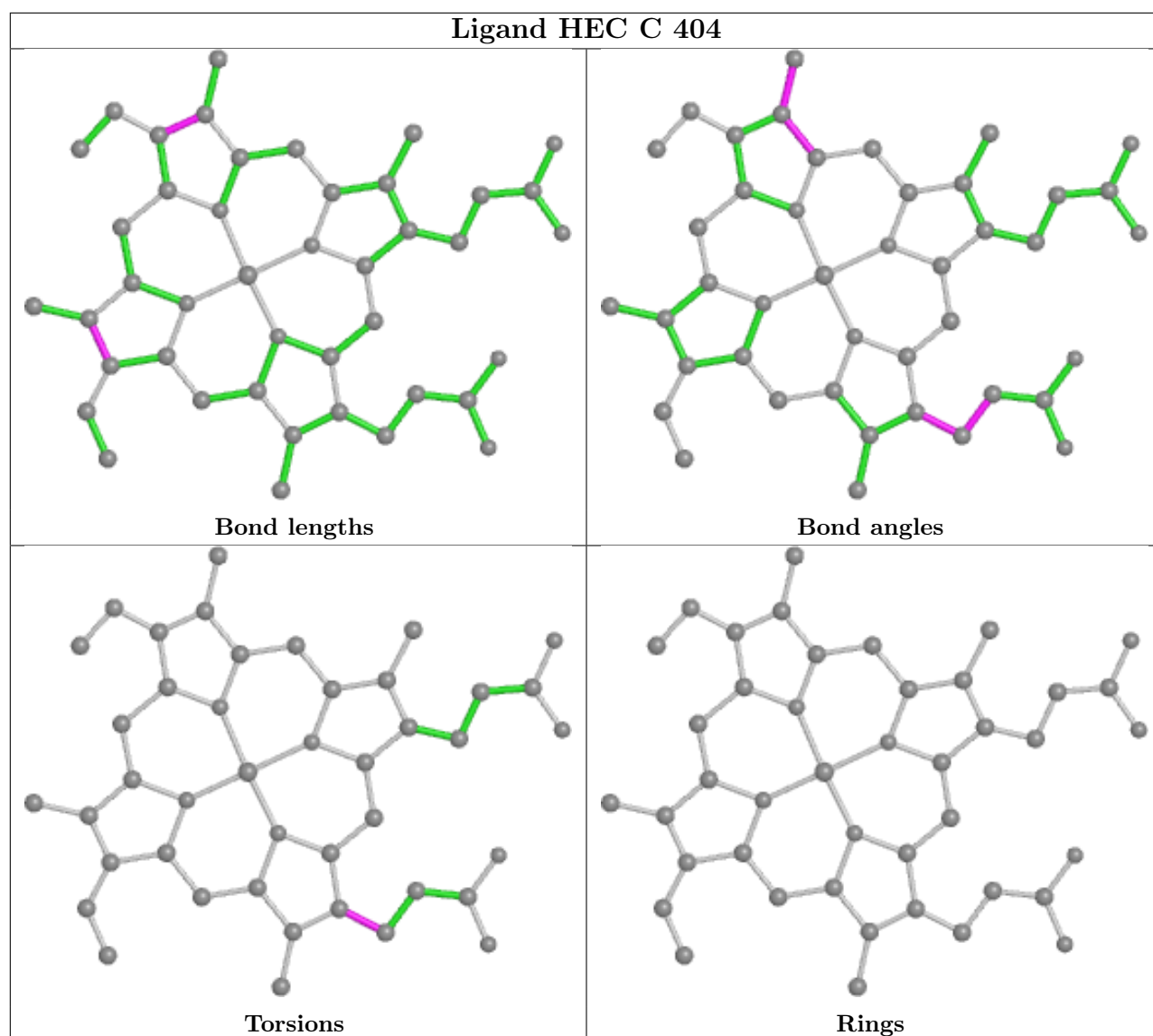
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	H	703	LDA	7	0
7	H	701	LDA	1	0
9	M	405	BPB	8	0
5	C	403	HEC	1	0
5	C	402	HEC	1	0
7	L	702	LDA	4	0
7	M	705	LDA	4	0
6	H	807	SO4	2	0
8	L	402	BCB	6	0
8	L	404	BCB	5	0
13	M	600	NS5	4	0
8	M	401	BCB	7	0
9	L	406	BPB	6	0
6	M	804	SO4	1	0
8	M	403	BCB	5	0
7	M	704	LDA	1	0
5	C	401	HEC	2	0
12	M	501	MQ9	2	0
10	L	502	UQ7	9	0

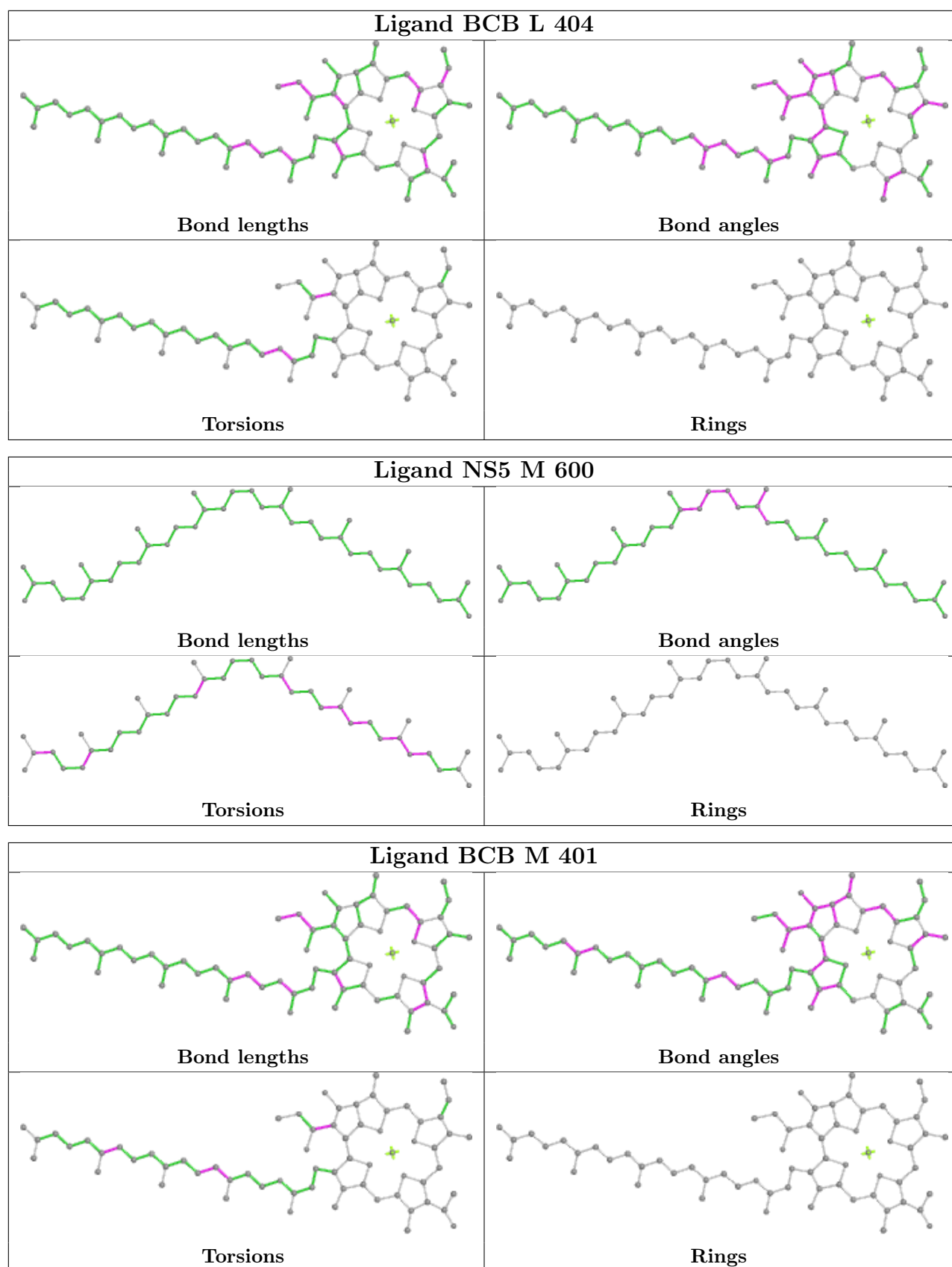
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

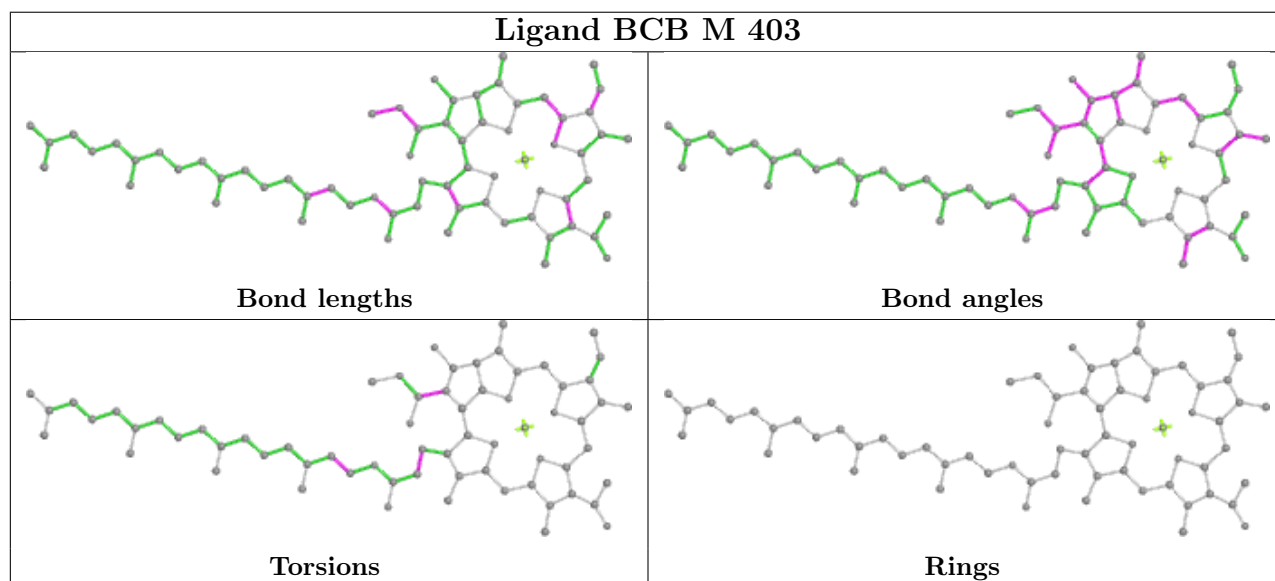
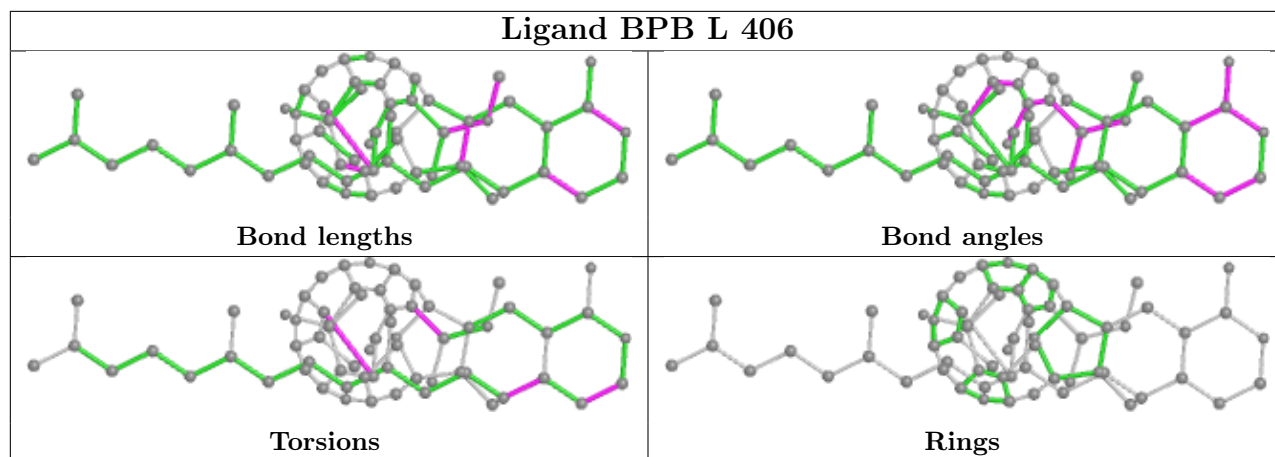
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

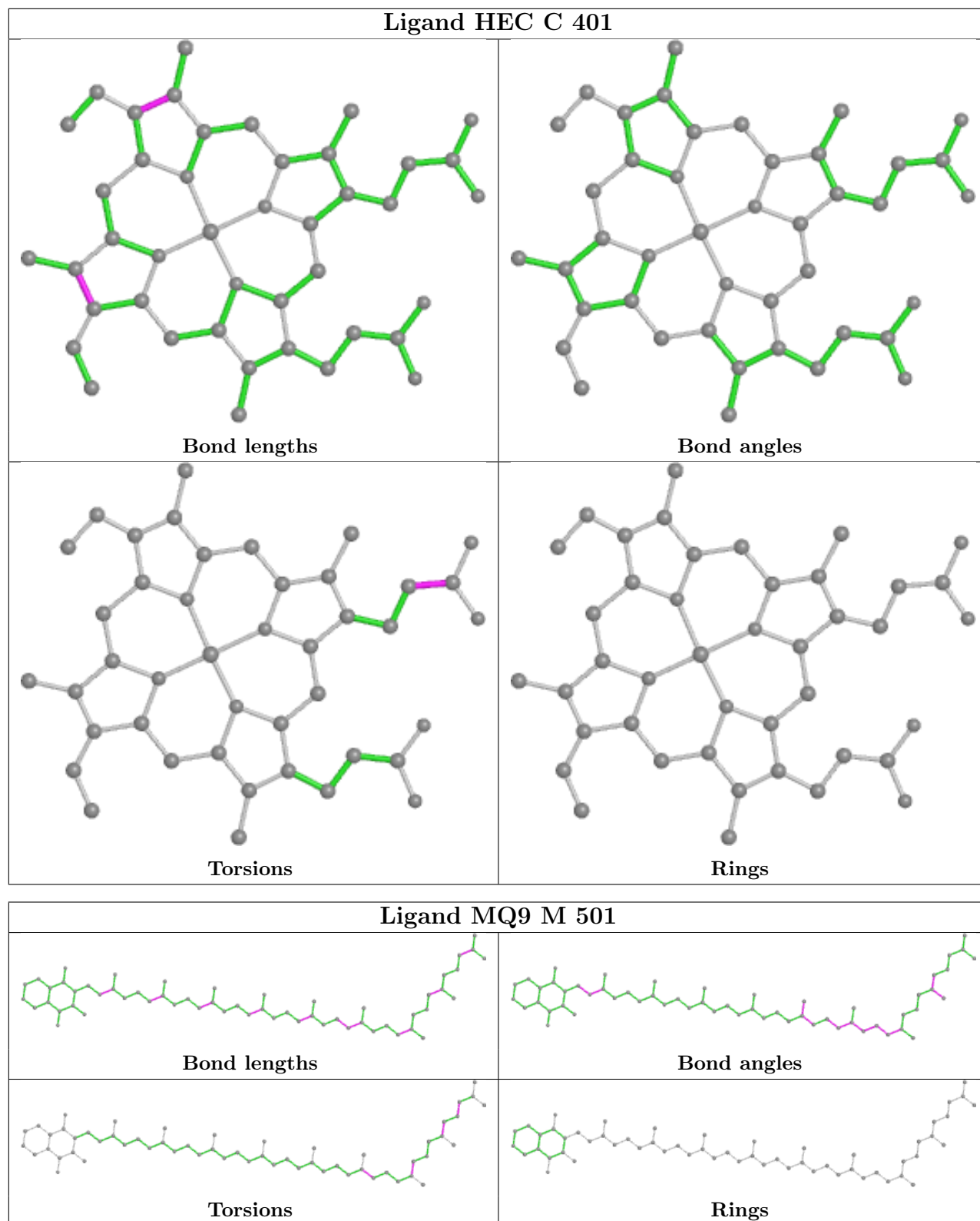


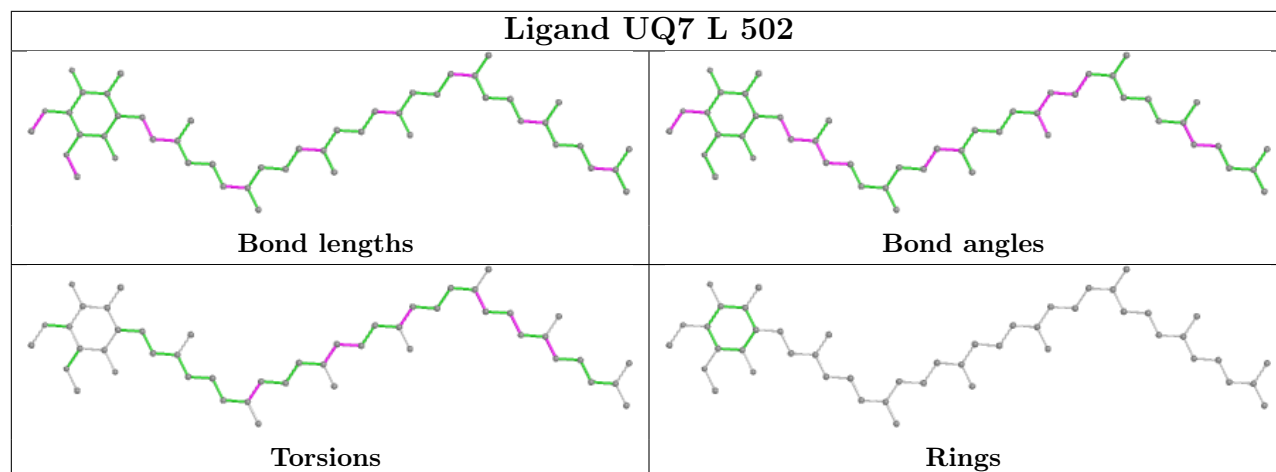












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	C	332/332 (100%)	-0.40	7 (2%) 63 61	16, 27, 44, 59	9 (2%)
2	H	248/258 (96%)	-0.17	13 (5%) 27 26	19, 32, 49, 58	20 (8%)
3	L	273/273 (100%)	-0.68	3 (1%) 80 79	16, 23, 35, 52	5 (1%)
4	M	323/323 (100%)	-0.54	9 (2%) 53 51	16, 26, 44, 58	7 (2%)
All	All	1176/1186 (99%)	-0.46	32 (2%) 54 52	16, 27, 45, 59	41 (3%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	85	THR	5.1
2	H	45	GLU	4.7
2	H	8	GLN	4.1
1	C	332	LYS	4.1
1	C	47	ALA	3.9
2	H	96	PHE	3.9
4	M	30	GLY	3.9
1	C	1	CYS	3.8
2	H	9	HIS	3.7
4	M	319	PRO	3.7
4	M	320	GLY	3.5
2	H	95	GLY	3.2
4	M	29	VAL	2.9
4	M	108	HIS	2.8
2	H	189	GLY	2.7
2	H	83	PRO	2.7
2	H	7	ALA	2.7
3	L	202	ASP	2.6
3	L	1	ALA	2.5
2	H	141	THR	2.4
4	M	78	HIS	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	191	ALA	2.4
1	C	159	THR	2.4
4	M	26	ASN	2.4
4	M	37	TRP	2.3
2	H	94	ASP	2.3
1	C	54	GLN	2.2
3	L	51	TYR	2.1
1	C	174	VAL	2.1
2	H	163	VAL	2.0
1	C	48	GLU	2.0
4	M	31	LYS	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FME	H	1	10/11	0.96	0.08	28,32,49,55	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
10	UQ7	L	502	48/48	0.65	0.34	23,36,44,44	48
7	LDA	L	706	16/16	0.68	0.33	48,58,69,69	0
7	LDA	L	702	16/16	0.73	0.26	29,50,54,54	0
13	NS5	M	600	40/40	0.78	0.20	24,35,65,66	0
7	LDA	H	703	16/16	0.80	0.22	38,48,61,62	0
7	LDA	M	704	16/16	0.82	0.18	52,54,65,65	0

Continued on next page...

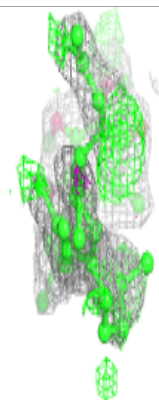
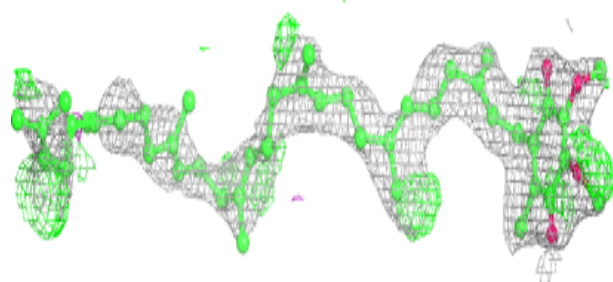
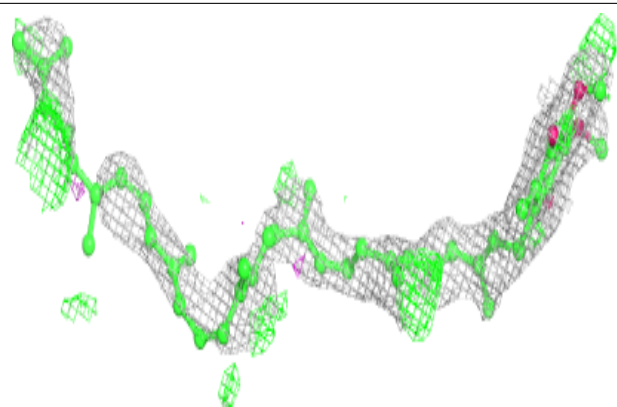
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	LDA	M	705	16/16	0.83	0.22	57,60,62,63	4
7	LDA	H	701	16/16	0.89	0.15	23,36,50,52	0
12	MQ9	M	501	58/58	0.90	0.15	15,20,62,64	0
8	BCB	M	401	66/66	0.92	0.13	15,22,68,71	0
6	SO4	H	807	5/5	0.93	0.20	31,32,32,38	5
9	BPB	M	405	65/65	0.94	0.11	14,24,57,59	9
8	BCB	L	404	66/66	0.96	0.08	10,16,41,48	0
6	SO4	M	803	5/5	0.96	0.12	46,47,53,55	0
8	BCB	M	403	66/66	0.96	0.11	12,18,40,41	0
9	BPB	L	406	65/65	0.96	0.11	14,18,23,26	0
6	SO4	M	805	5/5	0.96	0.23	55,57,59,60	0
6	SO4	H	806	5/5	0.96	0.26	58,61,63,63	0
5	HEC	C	402	43/43	0.96	0.13	18,27,32,34	0
8	BCB	L	402	66/66	0.96	0.12	13,17,23,30	0
5	HEC	C	404	43/43	0.97	0.10	14,21,33,43	0
6	SO4	H	802	5/5	0.97	0.14	57,59,60,61	0
5	HEC	C	401	43/43	0.97	0.11	23,30,37,39	0
5	HEC	C	403	43/43	0.98	0.09	14,19,22,26	0
6	SO4	M	801	5/5	0.99	0.10	31,32,33,38	0
6	SO4	M	804	5/5	0.99	0.07	40,41,42,44	0
11	FE2	M	500	1/1	1.00	0.02	17,17,17,17	0

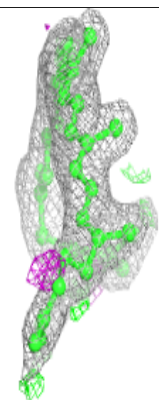
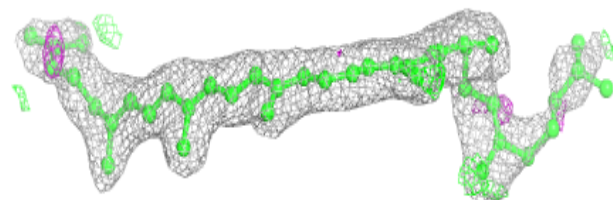
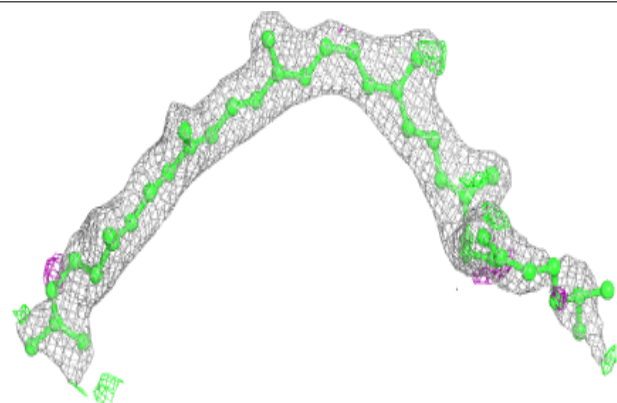
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UQ7 L 502:

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

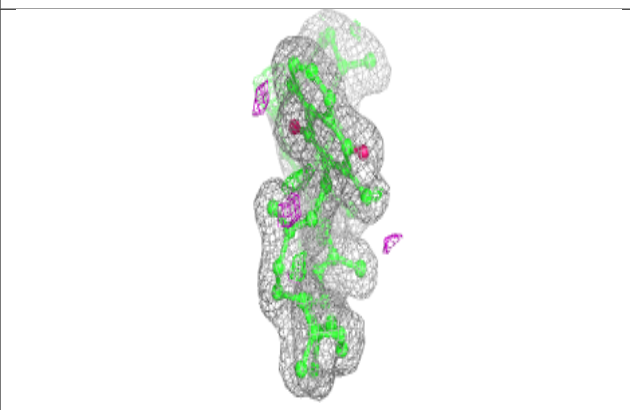
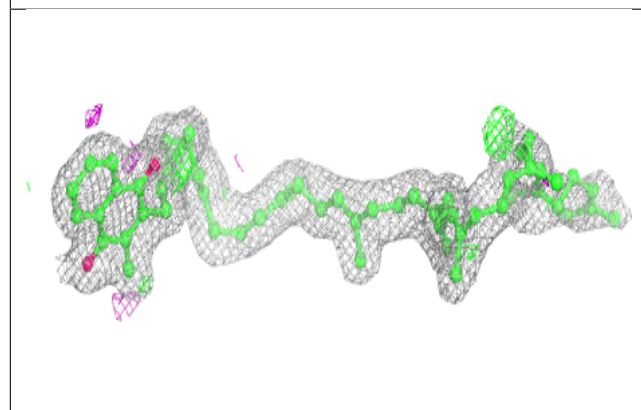
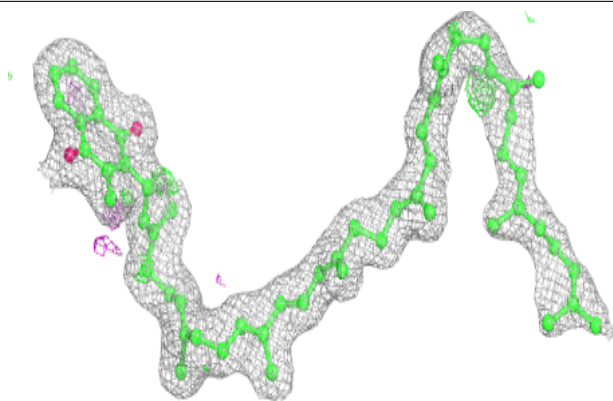
**Electron density around NS5 M 600:**

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

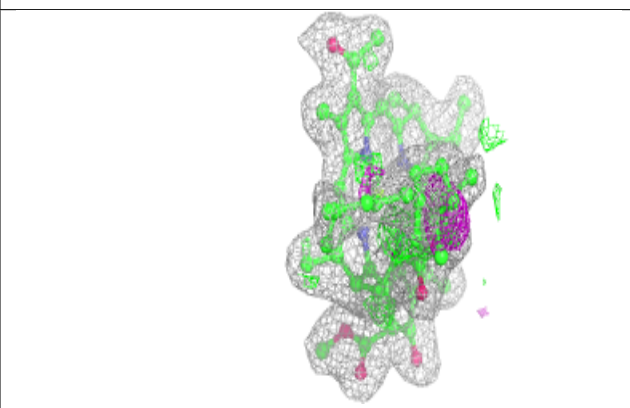
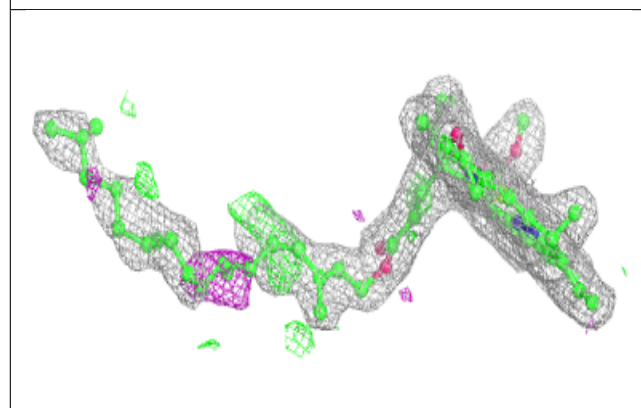
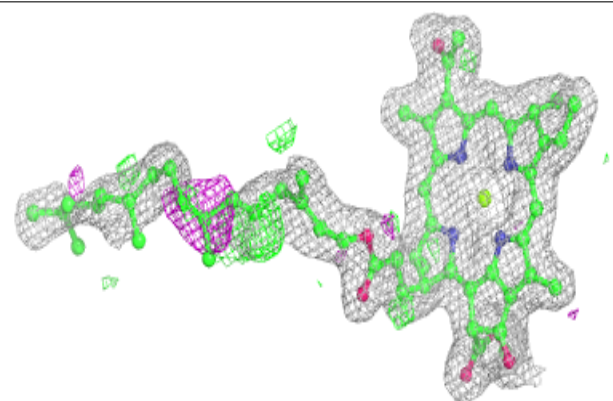


Electron density around MQ9 M 501:

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

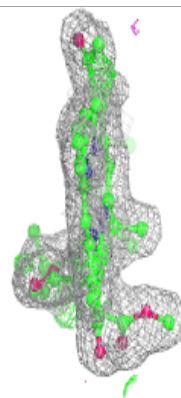
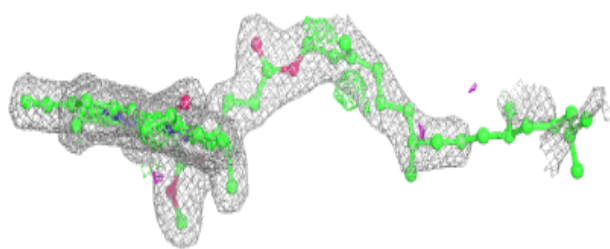
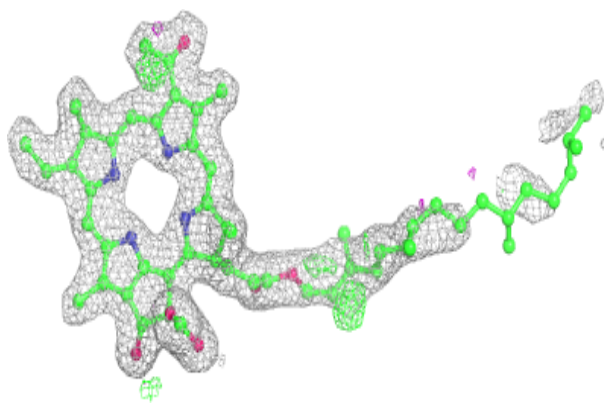
**Electron density around BCB M 401:**

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

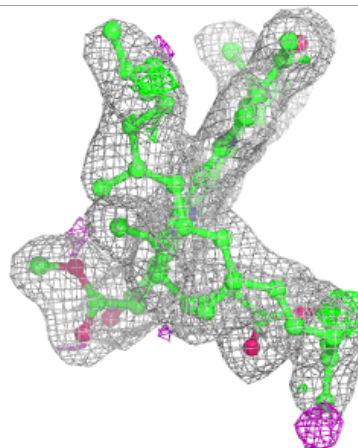
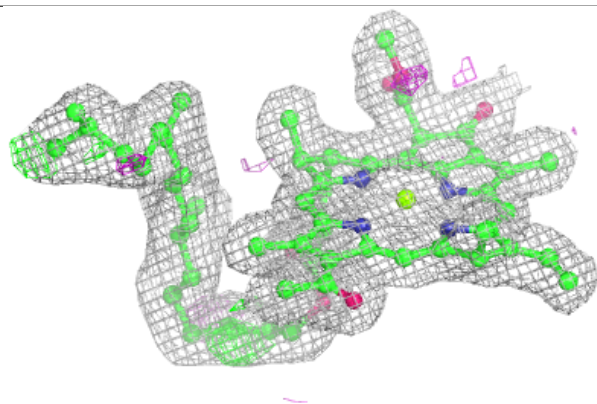
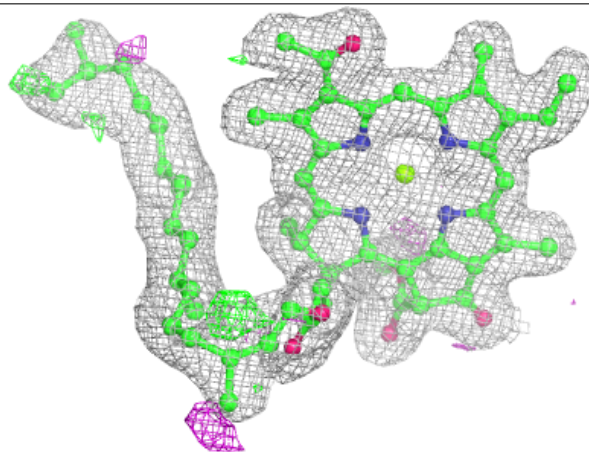


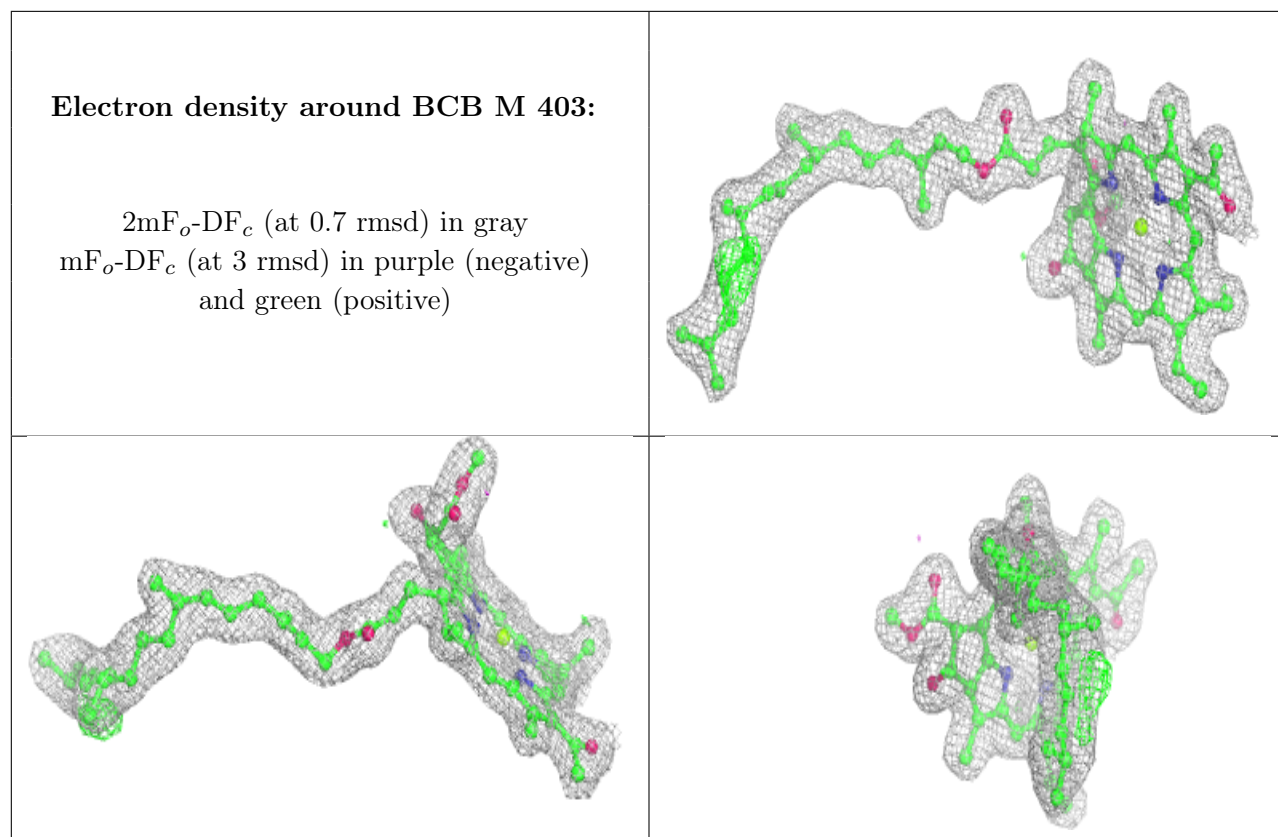
Electron density around BPB M 405:

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

**Electron density around BCB L 404:**

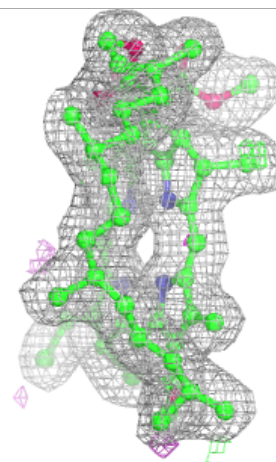
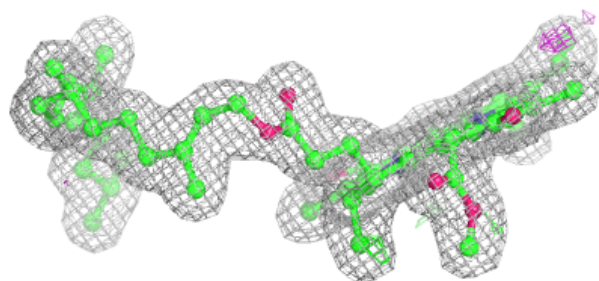
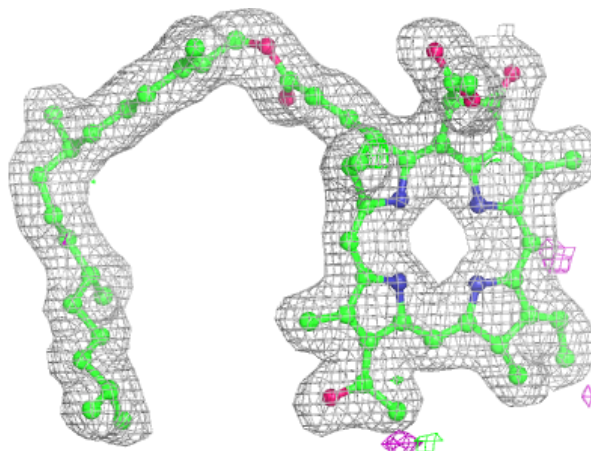
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

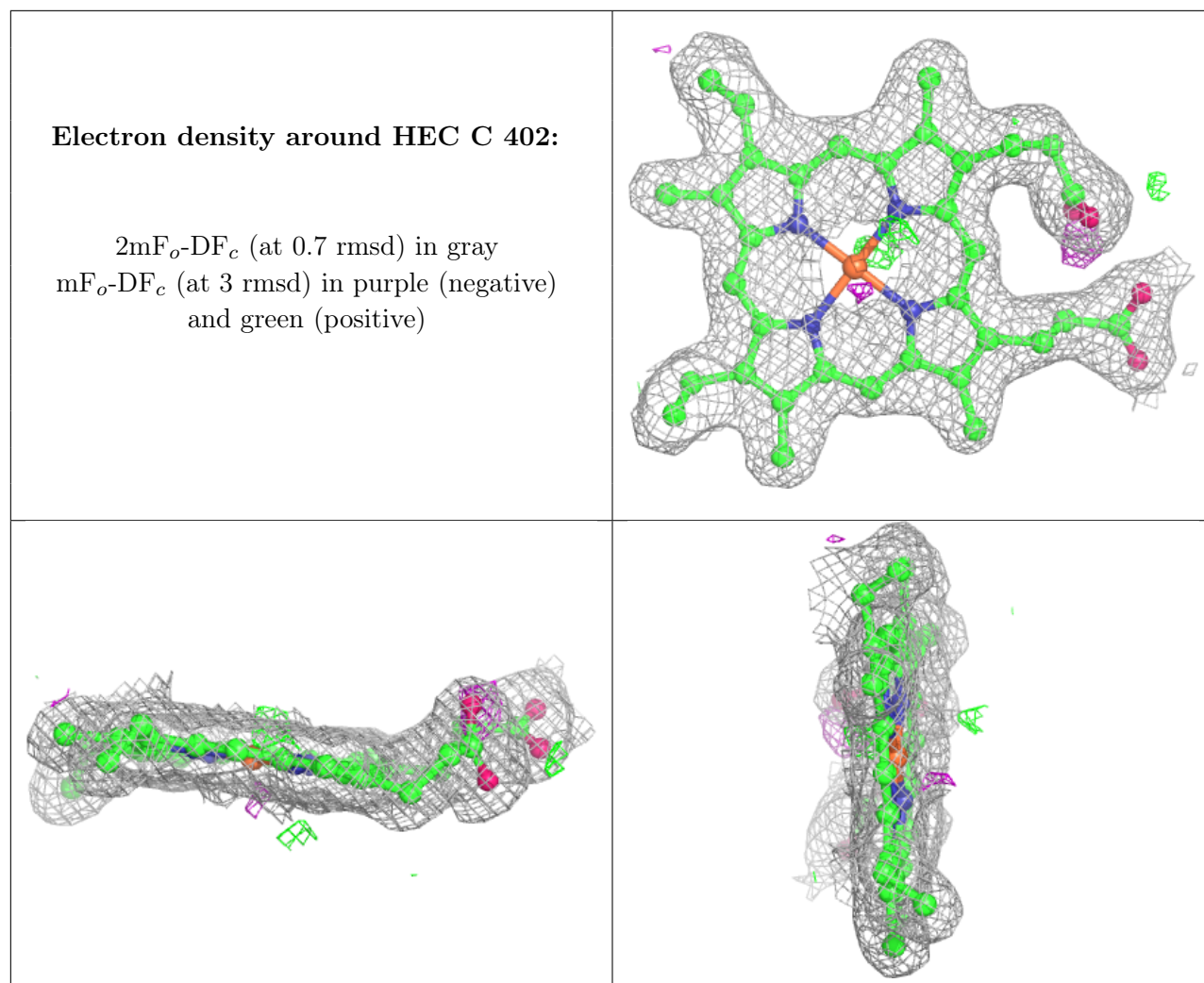




Electron density around BPB L 406:

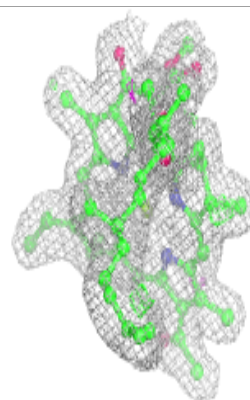
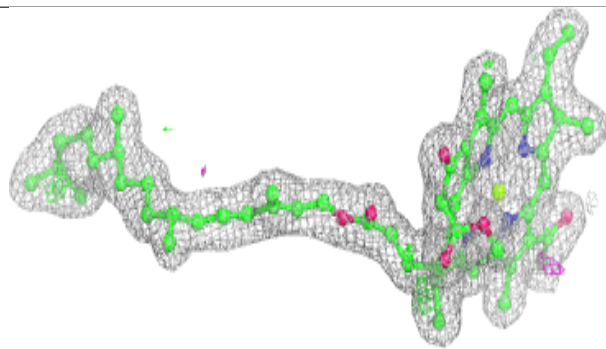
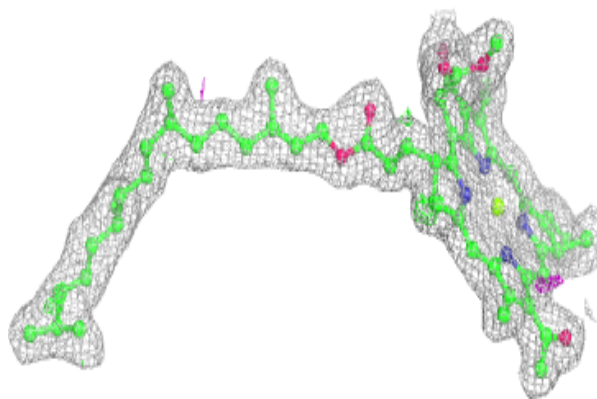
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

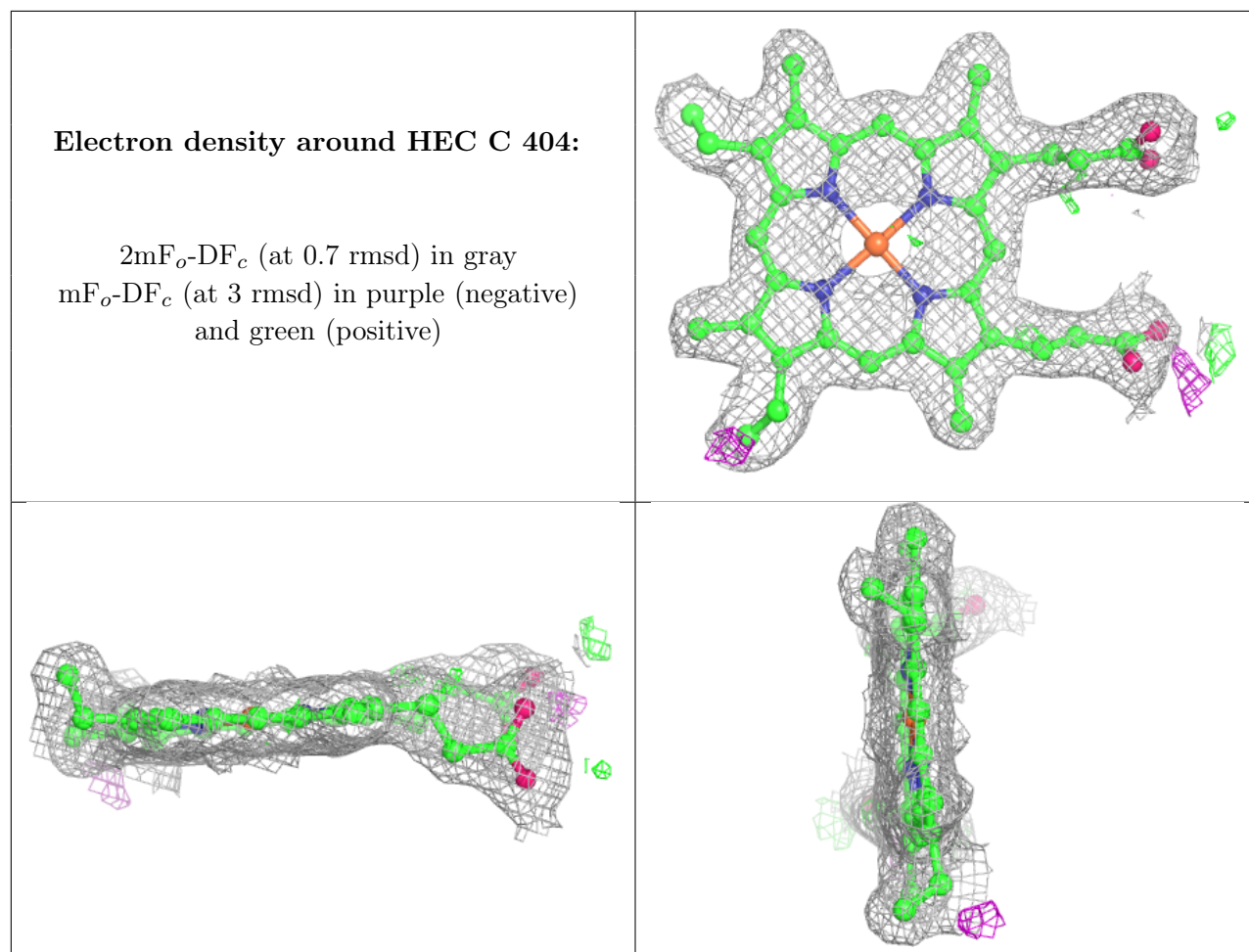




Electron density around BCB L 402:

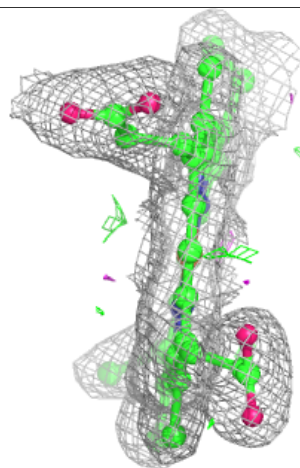
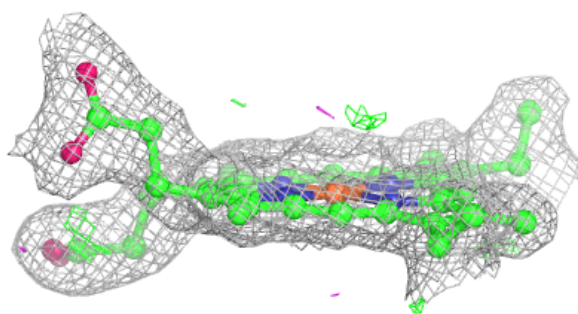
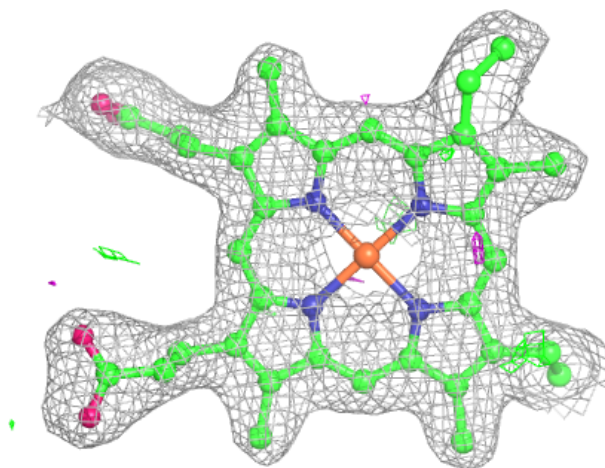
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

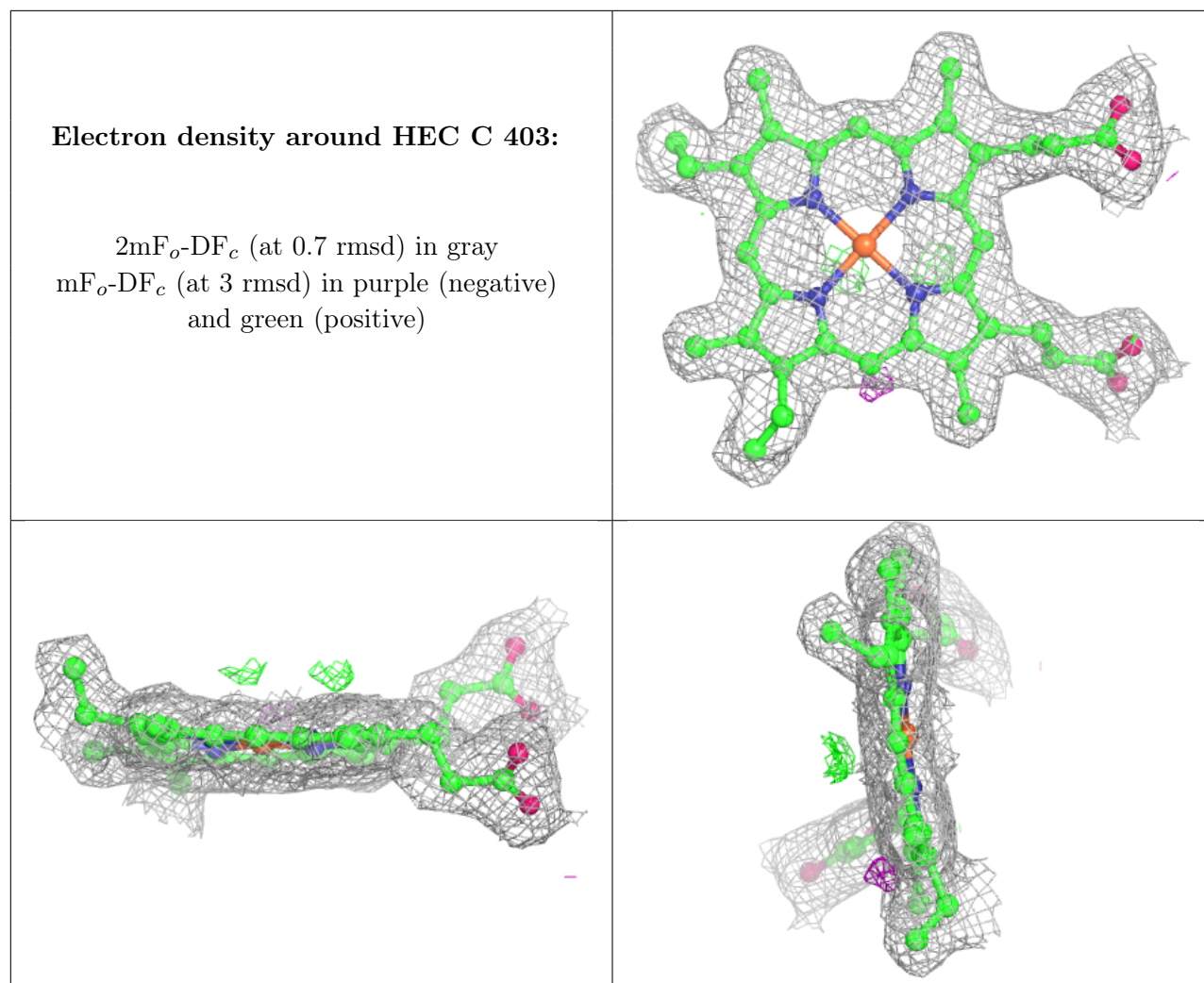




Electron density around HEC C 401:

$2mF_o-DF_c$ (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.