



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 28, 2026 – 11:49 PM UTC

PDB ID : 2WJN / pdb_00002wjn
Title : Lipidic sponge phase crystal structure of photosynthetic reaction centre from *Blastochloris viridis* (high dose)
Authors : Wohri, A.B.; Wahlgren, W.Y.; Malmerberg, E.; Johansson, L.C.; Neutze, R.; Katona, G.
Deposited on : 2009-05-27
Resolution : 1.86 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

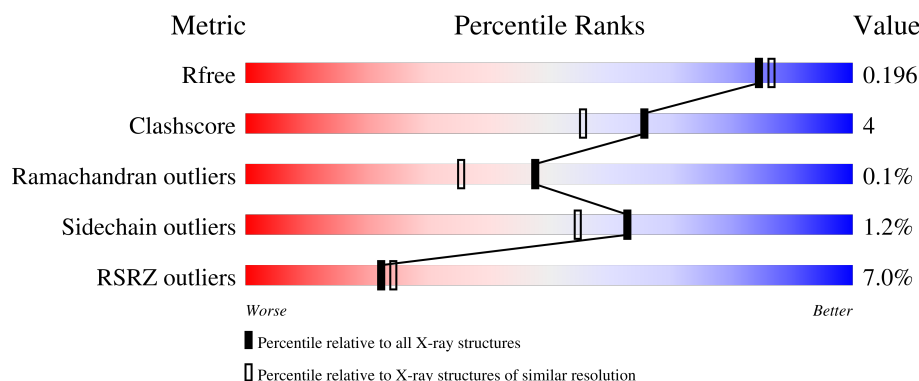
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.86 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	336	4% 94% 5%
2	H	258	11% 81% 13% 6%
3	L	274	11% 96% .
4	M	324	2% 94% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	BCB	L	301	X	-	-	-
6	BCB	L	302	X	-	-	-
6	BCB	M	401	X	-	-	-
6	BCB	M	402	X	-	-	-
8	MPG	L	304	X	-	-	-
8	MPG	L	305	X	-	-	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 10590 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
			2590	1632	464	476	18			

- Molecule 2 is a protein called REACTION CENTER PROTEIN H CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	243	Total	C	N	O	S	0	0	0
			1886	1209	326	349	2			

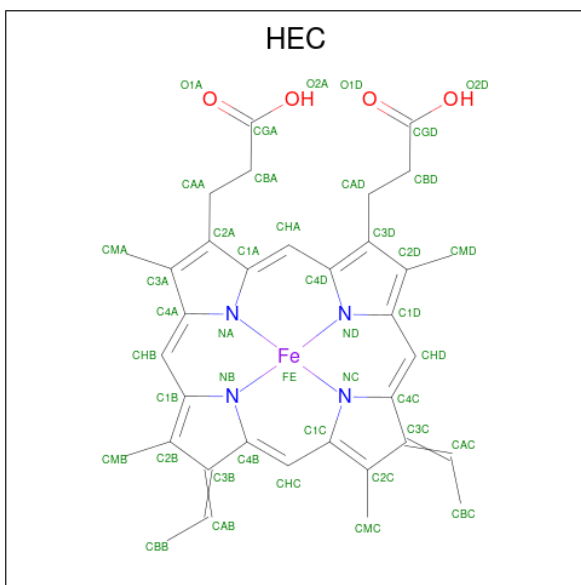
- Molecule 3 is a protein called REACTION CENTER PROTEIN L CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	273	Total	C	N	O	S	0	0	0
			2161	1452	350	352	7			

- Molecule 4 is a protein called REACTION CENTER PROTEIN M CHAIN.

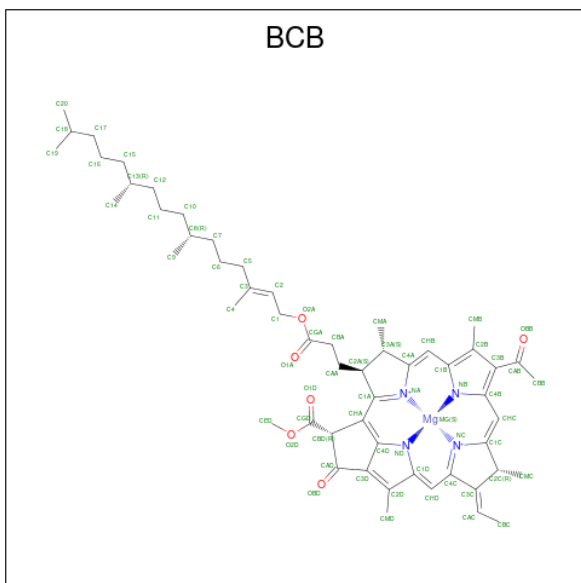
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	323	Total	C	N	O	S	0	0	0
			2548	1697	417	423	11			

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



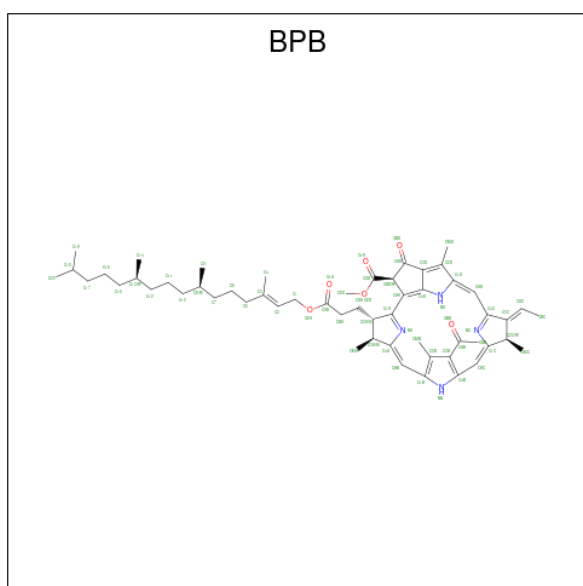
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 6 is BACTERIOCHLOROPHYLL B (CCD ID: BCB) (formula: $\text{C}_{55}\text{H}_{72}\text{MgN}_4\text{O}_6$).



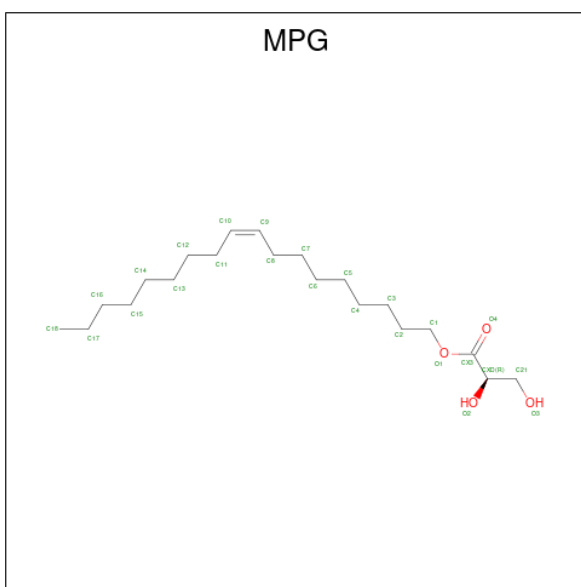
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
6	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
6	M	1	Total 65	C 54	Mg 1	N 4	O 6	0	0
6	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- Molecule 7 is BACTERIOPHEOPHYTIN B (CCD ID: BPB) (formula: $C_{55}H_{74}N_4O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	L	1	Total	C	N	O	0	0
			65	55	4	6		
7	M	1	Total	C	N	O	0	0
			61	51	4	6		

- Molecule 8 is [(Z)-octadec-9-enyl] (2R)-2,3-bis(oxidanyl)propanoate (CCD ID: MPG) (formula: $C_{21}H_{40}O_4$).

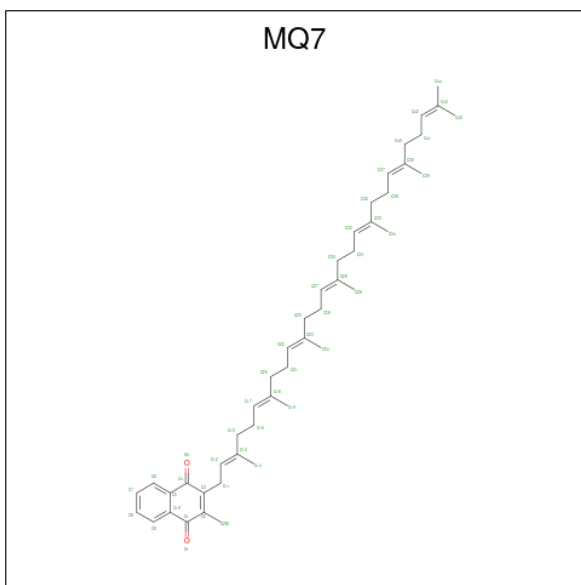


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	L	1	Total C O 21 17 4	0	0
8	L	1	Total C O 25 21 4	0	0
8	M	1	Total C 17 17	0	0

- Molecule 9 is FE (II) ION (CCD ID: FE2) (formula: Fe).

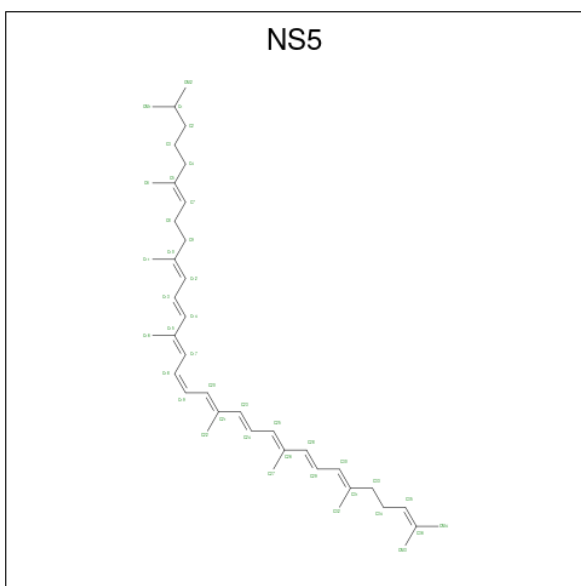
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	L	1	Total Fe 1 1	0	0

- Molecule 10 is MENAQUINONE-7 (CCD ID: MQ7) (formula: C₄₆H₆₄O₂).



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

- Molecule 11 is 15-cis-1,2-dihydroneurosporene (CCD ID: NS5) (formula: C₄₀H₆₀).



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

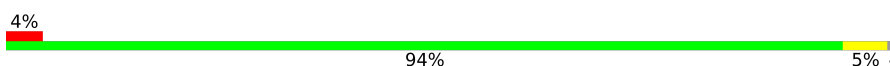
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	C	307	Total 307	O 307	0	0
12	H	149	Total 149	O 149	0	0
12	L	89	Total 89	O 89	0	0
12	M	147	Total 147	O 147	0	0

3 Residue-property plots [i](#)

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

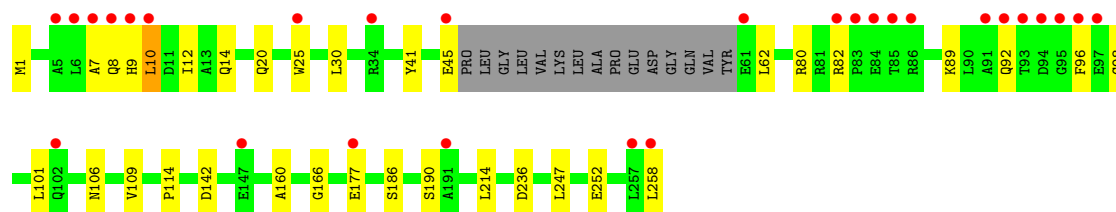
- Molecule 1: PHOTOSYNTHETIC REACTION CENTER CYTOCHROME C SUBUNIT

Chain C: 

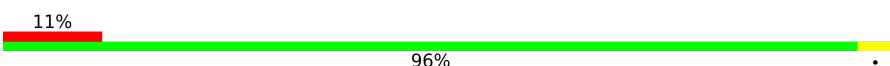


- Molecule 2: REACTION CENTER PROTEIN H CHAIN

Chain H: 

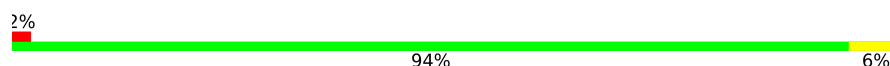


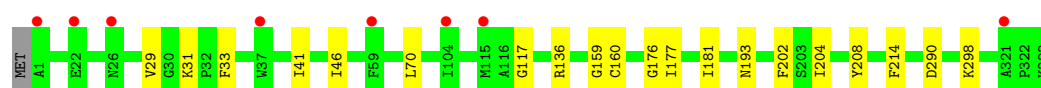
- Molecule 3: REACTION CENTER PROTEIN L CHAIN

Chain L: 



- Molecule 4: REACTION CENTER PROTEIN M CHAIN

Chain M: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	84.76Å 139.43Å 178.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.97 – 1.86 44.97 – 1.86	Depositor EDS
% Data completeness (in resolution range)	99.4 (44.97-1.86) 99.4 (44.97-1.86)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.13 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.171 , 0.193 0.175 , 0.196	Depositor DCC
R_{free} test set	8832 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	32.6	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10590	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% 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

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	C	0.99	2/2657 (0.1%)	0.98	3/3624 (0.1%)
2	H	0.88	0/1919	0.86	1/2621 (0.0%)
3	L	0.99	1/2248 (0.0%)	0.93	0/3069
4	M	1.03	0/2652	0.94	3/3630 (0.1%)
All	All	0.98	3/9476 (0.0%)	0.93	7/12944 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	272	ARG	CG-CD	-5.33	1.36	1.52
3	L	166	ASN	N-CA	-5.25	1.40	1.46
1	C	240	LEU	CA-C	-5.17	1.45	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	108	ARG	NE-CZ-NH2	-8.20	111.82	119.20
2	H	12	ILE	N-CA-C	6.33	116.50	110.42
4	M	160	CYS	N-CA-C	5.88	121.32	114.62
1	C	108	ARG	NE-CZ-NH1	5.55	127.05	121.50
4	M	31	LYS	CA-C-N	-5.09	114.71	119.85
4	M	31	LYS	C-N-CA	-5.09	114.71	119.85
1	C	227	TYR	CA-CB-CG	5.02	122.93	113.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2590	0	2553	9	0
2	H	1886	0	1880	24	0
3	L	2161	0	2089	10	0
4	M	2548	0	2432	14	0
5	C	172	0	120	1	0
6	L	132	0	144	5	0
6	M	131	0	140	3	0
7	L	65	0	74	8	0
7	M	61	0	63	13	0
8	L	46	0	67	3	0
8	M	17	0	31	0	0
9	L	1	0	0	0	0
10	M	48	0	64	0	0
11	M	40	0	60	10	0
12	C	307	0	0	3	0
12	H	149	0	0	4	0
12	L	89	0	0	0	0
12	M	147	0	0	0	0
All	All	10590	0	9717	74	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 (74) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:403:BPB:H14A	11:M:405:NS5:HM43	1.37	1.07
7:M:403:BPB:C14	11:M:405:NS5:HM43	1.94	0.97
7:M:403:BPB:HHC	7:M:403:BPB:HBBB	1.47	0.97
7:L:303:BPB:HHC	7:L:303:BPB:HBBB	1.50	0.92
3:L:16:LEU:HD13	3:L:106:GLU:HG2	1.53	0.91
2:H:142:ASP:OD1	12:H:301:HOH:O	1.91	0.89
1:C:48:GLU:O	12:C:501:HOH:O	2.04	0.74
7:M:403:BPB:H14A	11:M:405:NS5:CM4	2.17	0.73
1:C:49:GLY:HA3	12:C:501:HOH:O	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:117:GLY:HA3	11:M:405:NS5:H92	1.75	0.69
7:L:303:BPB:HHC	7:L:303:BPB:CBB	2.23	0.65
6:M:401:BCB:HBB2	6:M:401:BCB:HHC	1.79	0.65
2:H:96:PHE:HD2	2:H:98:GLY:H	1.39	0.64
2:H:258:LEU:HB2	3:L:17:ILE:HG22	1.83	0.60
6:L:301:BCB:HMB1	6:L:301:BCB:HBB3	1.82	0.60
7:M:403:BPB:C14	11:M:405:NS5:CM4	2.77	0.60
8:L:305:MPG:O2	8:L:305:MPG:HX32	2.01	0.59
2:H:177:GLU:OE1	12:H:302:HOH:O	2.17	0.59
7:M:403:BPB:H14B	11:M:405:NS5:HM43	1.83	0.59
7:M:403:BPB:HBBB	7:M:403:BPB:CHC	2.27	0.59
3:L:181:PHE:CD2	7:M:403:BPB:HBB	2.39	0.58
3:L:181:PHE:HB3	7:M:403:BPB:HBBA	1.84	0.57
6:M:401:BCB:HHC	6:M:401:BCB:CBB	2.35	0.57
1:C:301:PRO:HG2	5:C:402:HEC:HBD1	1.87	0.56
8:L:305:MPG:O2	8:L:305:MPG:C1	2.54	0.55
2:H:142:ASP:CG	12:H:301:HOH:O	2.44	0.54
4:M:177:ILE:HD11	11:M:405:NS5:H273	1.90	0.53
4:M:70:LEU:HD21	11:M:405:NS5:H323	1.89	0.53
2:H:96:PHE:CD2	2:H:98:GLY:N	2.63	0.52
4:M:159:GLY:HA3	11:M:405:NS5:C11	2.40	0.52
3:L:16:LEU:N	3:L:16:LEU:CD1	2.73	0.52
2:H:106:ASN:HB3	2:H:109:VAL:HG22	1.93	0.51
7:M:403:BPB:HHC	7:M:403:BPB:CBB	2.32	0.51
1:C:309:HIS:CE1	1:C:315:PRO:HD3	2.45	0.51
2:H:9:HIS:HE1	4:M:298:LYS:HG3	1.76	0.51
2:H:92:GLN:HA	2:H:101:LEU:HD23	1.92	0.51
7:L:303:BPB:HBBA	4:M:208:TYR:HB3	1.93	0.50
7:L:303:BPB:HBB	4:M:208:TYR:CD2	2.47	0.50
2:H:10:LEU:HA	2:H:14:GLN:OE1	2.13	0.48
7:L:303:BPB:CBB	7:L:303:BPB:CHC	2.91	0.47
3:L:181:PHE:HB3	7:M:403:BPB:CBB	2.46	0.46
3:L:259:TRP:N	3:L:260:PRO:CD	2.79	0.46
6:L:302:BCB:C14	7:L:303:BPB:H20B	2.46	0.45
4:M:41:ILE:HD12	4:M:41:ILE:C	2.42	0.45
1:C:77:ILE:HD11	1:C:111:LEU:HD21	1.98	0.45
1:C:17:LEU:O	3:L:159:ASN:HB2	2.16	0.45
2:H:252:GLU:CG	12:H:428:HOH:O	2.64	0.44
4:M:33:PHE:CE2	4:M:46:ILE:HD12	2.52	0.44
3:L:116:HIS:CD2	8:L:304:MPG:H32C	2.53	0.44
6:M:402:BCB:HMB3	6:M:402:BCB:CBB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:9:HIS:CE1	4:M:298:LYS:HG3	2.53	0.43
1:C:323:LYS:HE2	12:C:744:HOH:O	2.18	0.43
2:H:9:HIS:CE1	4:M:298:LYS:HE3	2.54	0.43
7:M:403:BPB:CHC	7:M:403:BPB:CBB	2.95	0.43
2:H:41:TYR:CD2	2:H:62:LEU:HD21	2.54	0.43
1:C:153:PRO:HD3	1:C:160:PRO:HB3	2.01	0.42
6:L:302:BCB:H143	7:L:303:BPB:H20B	2.01	0.42
2:H:166:GLY:HA3	2:H:186:SER:O	2.20	0.42
2:H:80:ARG:O	2:H:80:ARG:HG3	2.19	0.42
2:H:20:GLN:HG2	4:M:202:PHE:CE2	2.55	0.41
6:L:302:BCB:HMD1	4:M:204:ILE:HD13	2.03	0.41
7:L:303:BPB:NC	7:L:303:BPB:ND	2.67	0.41
2:H:96:PHE:CE2	2:H:98:GLY:N	2.88	0.41
2:H:160:ALA:HB3	2:H:214:LEU:HD23	2.03	0.41
1:C:80:TRP:CD1	1:C:133:TYR:HB2	2.56	0.41
7:M:403:BPB:HMC	7:M:403:BPB:HBCA	2.02	0.41
4:M:176:GLY:H	11:M:405:NS5:C23	2.34	0.41
3:L:16:LEU:N	3:L:16:LEU:HD12	2.35	0.41
6:L:301:BCB:HBD	6:L:301:BCB:HAA1	2.02	0.41
2:H:7:ALA:O	2:H:8:GLN:CB	2.69	0.41
2:H:25:TRP:CE3	2:H:25:TRP:HA	2.56	0.40
2:H:80:ARG:HD3	2:H:82:ARG:HG2	2.02	0.40
2:H:89:LYS:HB3	2:H:89:LYS:HE2	1.88	0.40
2:H:114:PRO:HG3	2:H:247:LEU:HD22	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	330/336 (98%)	321 (97%)	9 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	239/258 (93%)	234 (98%)	5 (2%)	0	100	100
3	L	271/274 (99%)	264 (97%)	7 (3%)	0	100	100
4	M	321/324 (99%)	313 (98%)	7 (2%)	1 (0%)	36	25
All	All	1161/1192 (97%)	1132 (98%)	28 (2%)	1 (0%)	48	35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
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	278/282 (99%)	278 (100%)	0	100	100
2	H	194/212 (92%)	189 (97%)	5 (3%)	40	25
3	L	216/219 (99%)	215 (100%)	1 (0%)	81	77
4	M	247/250 (99%)	242 (98%)	5 (2%)	48	36
All	All	935/963 (97%)	924 (99%)	11 (1%)	63	55

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

Mol	Chain	Res	Type
2	H	10	LEU
2	H	30	LEU
2	H	45	GLU
2	H	190	SER
2	H	236	ASP
3	L	44	LEU
4	M	29	VAL
4	M	136	ARG
4	M	181	ILE
4	M	214	PHE

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Mol	Chain	Res	Type
4	M	290	ASP

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	84	GLN
1	C	120	ASN
2	H	8	GLN
2	H	9	HIS
2	H	178	HIS
2	H	220	ASN
3	L	183	ASN
3	L	239	ASN
4	M	45	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FME	H	1	2	8,9,10	0.87	1 (12%)	8,9,11	2.37	2 (25%)

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	-	5/7/9/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1	FME	CN-N	2.19	1.40	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1	FME	CA-N-CN	-5.77	113.94	122.82
2	H	1	FME	O1-CN-N	-2.67	118.43	125.32

There are no chirality outliers.

All (5) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 1 is monoatomic - leaving 15 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
8	MPG	L	305	-	24,24,24	1.67	1 (4%)	24,25,25	1.37	5 (20%)
8	MPG	M	406	-	16,16,24	0.35	0	15,15,25	0.46	0
6	BCB	L	301	-	60,74,74	2.53	14 (23%)	59,115,115	2.95	17 (28%)
5	HEC	C	401	1	46,50,50	2.19	9 (19%)	58,82,82	1.85	11 (18%)
8	MPG	L	304	-	20,20,24	1.79	1 (5%)	20,21,25	2.16	7 (35%)
7	BPB	M	403	-	53,66,70	2.49	15 (28%)	50,96,101	2.16	17 (34%)
6	BCB	L	302	-	60,74,74	2.67	18 (30%)	59,115,115	2.24	13 (22%)
5	HEC	C	403	1	46,50,50	1.96	11 (23%)	58,82,82	1.52	8 (13%)
6	BCB	M	401	-	59,73,74	2.52	17 (28%)	57,113,115	2.33	11 (19%)
6	BCB	M	402	-	60,74,74	2.48	16 (26%)	59,115,115	2.66	19 (32%)
7	BPB	L	303	-	57,70,70	2.24	13 (22%)	55,101,101	2.25	14 (25%)
5	HEC	C	402	1	46,50,50	2.20	12 (26%)	58,82,82	1.94	13 (22%)
10	MQ7	M	404	-	49,49,49	1.64	4 (8%)	61,63,63	1.16	7 (11%)
11	NS5	M	405	-	39,39,39	2.09	5 (12%)	46,46,46	2.57	20 (43%)
5	HEC	C	404	1	46,50,50	2.20	13 (28%)	58,82,82	1.59	10 (17%)

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
8	MPG	L	305	-	1/1/2/4	15/25/25/25	-
8	MPG	M	406	-	-	4/14/14/25	-
6	BCB	L	301	-	2/2/21/26	6/37/137/137	-
8	MPG	L	304	-	1/1/2/4	9/21/21/25	-
5	HEC	C	401	1	-	6/14/54/54	-
7	BPB	M	403	-	-	8/33/101/105	0/5/6/6
6	BCB	L	302	-	2/2/21/26	5/37/137/137	-
6	BCB	M	402	-	3/3/21/26	4/37/137/137	-
6	BCB	M	401	-	2/2/20/26	4/36/136/137	-
5	HEC	C	403	1	-	4/14/54/54	-
7	BPB	L	303	-	-	5/37/105/105	0/5/6/6
5	HEC	C	402	1	-	9/14/54/54	-
10	MQ7	M	404	-	-	3/41/61/61	0/2/2/2
11	NS5	M	405	-	-	10/43/43/43	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	HEC	C	404	1	-	4/14/54/54	-

All (149) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	403	BPB	C1B-C2B	9.91	1.50	1.39
10	M	404	MQ7	C3-C2	8.09	1.49	1.35
6	L	301	BCB	C1B-C2B	8.08	1.48	1.39
7	L	303	BPB	C1B-C2B	7.93	1.48	1.39
8	L	304	MPG	O1-CX3	7.49	1.49	1.33
5	C	401	HEC	CAC-C3C	7.47	1.59	1.35
8	L	305	MPG	O1-CX3	7.43	1.48	1.33
6	M	401	BCB	C1B-C2B	7.36	1.47	1.39
6	M	401	BCB	CHC-C1C	7.35	1.47	1.38
11	M	405	NS5	C35-C36	7.22	1.54	1.32
6	L	302	BCB	C1A-CHA	7.22	1.48	1.40
6	L	302	BCB	CHC-C1C	7.16	1.47	1.38
5	C	402	HEC	CAC-C3C	7.16	1.58	1.35
6	M	402	BCB	C1B-C2B	7.12	1.47	1.39
5	C	404	HEC	CAC-C3C	7.10	1.58	1.35
6	L	301	BCB	OBD-CAD	7.02	1.31	1.22
6	M	401	BCB	C1A-CHA	7.01	1.48	1.40
6	M	402	BCB	CHC-C1C	6.94	1.47	1.38
11	M	405	NS5	C29-C28	6.87	1.52	1.34
6	L	302	BCB	C1B-C2B	6.81	1.47	1.39
6	L	301	BCB	CHC-C1C	6.75	1.46	1.38
7	M	403	BPB	C1D-C2D	6.54	1.46	1.39
5	C	402	HEC	CAB-C3B	6.32	1.55	1.35
5	C	404	HEC	CAB-C3B	6.19	1.55	1.35
6	M	402	BCB	OBD-CAD	6.09	1.30	1.22
11	M	405	NS5	C9-C8	-6.07	1.33	1.53
6	M	402	BCB	CHC-C4B	6.05	1.49	1.39
6	L	301	BCB	CHC-C4B	6.04	1.49	1.39
5	C	401	HEC	CAB-C3B	5.91	1.54	1.35
5	C	403	HEC	CAC-C3C	5.88	1.54	1.35
5	C	403	HEC	CAB-C3B	5.84	1.54	1.35
7	L	303	BPB	C1D-C2D	5.83	1.45	1.39
6	L	302	BCB	CHC-C4B	5.82	1.49	1.39
6	L	302	BCB	CHB-C4A	-5.69	1.31	1.38
6	L	302	BCB	OBD-CAD	5.62	1.29	1.22
6	L	302	BCB	C1D-C2D	5.60	1.45	1.39
6	L	301	BCB	C1D-C2D	5.53	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	303	BPB	C3B-C4B	5.36	1.50	1.41
10	M	404	MQ7	C10-C5	5.34	1.49	1.40
7	M	403	BPB	C3A-C2A	-5.28	1.50	1.54
5	C	401	HEC	C3D-C2D	5.26	1.52	1.38
6	M	402	BCB	CHA-CBD	-5.13	1.45	1.51
6	M	402	BCB	C1D-C2D	4.89	1.45	1.39
7	L	303	BPB	C4D-CHA	4.79	1.46	1.39
5	C	404	HEC	C3D-C2D	4.68	1.51	1.38
5	C	402	HEC	C3D-C2D	4.66	1.51	1.38
6	M	402	BCB	C1A-CHA	4.63	1.45	1.40
6	M	401	BCB	CHB-C1B	4.61	1.47	1.39
6	M	401	BCB	CHC-C4B	4.57	1.47	1.39
7	L	303	BPB	C3D-C2D	4.50	1.47	1.39
7	M	403	BPB	OBD-CAD	4.50	1.28	1.22
6	M	401	BCB	C3A-C2A	-4.48	1.50	1.54
6	M	402	BCB	C3D-C2D	4.45	1.47	1.39
7	L	303	BPB	C3B-C2B	4.39	1.47	1.39
5	C	403	HEC	C3D-C2D	4.36	1.50	1.38
6	L	302	BCB	C3D-C2D	4.33	1.47	1.39
6	L	302	BCB	C3B-C4B	4.33	1.48	1.41
6	M	401	BCB	C3B-C4B	4.32	1.48	1.41
5	C	401	HEC	CMA-C3A	4.30	1.59	1.50
6	M	401	BCB	C3D-C2D	4.28	1.46	1.39
6	L	301	BCB	C1A-CHA	4.26	1.44	1.40
7	M	403	BPB	C3D-C2D	4.25	1.46	1.39
6	L	301	BCB	CHD-C4C	4.16	1.47	1.39
6	M	402	BCB	C3B-C2B	4.14	1.46	1.39
7	M	403	BPB	C3B-C4B	4.11	1.48	1.41
6	L	301	BCB	C3D-C2D	4.01	1.46	1.39
6	L	301	BCB	C3B-C2B	4.00	1.46	1.39
6	L	301	BCB	O2D-CGD	3.98	1.43	1.33
5	C	401	HEC	CBB-CAB	-3.96	1.34	1.49
6	M	401	BCB	O2D-CGD	3.93	1.42	1.33
6	M	401	BCB	CBD-CGD	-3.91	1.47	1.52
6	L	302	BCB	C3B-C2B	3.86	1.46	1.39
7	M	403	BPB	C4D-CHA	3.76	1.45	1.39
7	M	403	BPB	O2A-CGA	3.61	1.43	1.33
6	M	402	BCB	O2D-CGD	3.60	1.42	1.33
7	L	303	BPB	OBD-CAD	3.60	1.27	1.22
7	L	303	BPB	CBD-CGD	-3.57	1.48	1.52
5	C	402	HEC	CMB-C2B	3.57	1.58	1.50
6	L	302	BCB	CHB-C1B	3.57	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	401	HEC	CBC-CAC	-3.56	1.36	1.49
6	L	302	BCB	CHD-C4C	3.55	1.46	1.39
6	L	301	BCB	C3A-C2A	-3.53	1.51	1.54
6	M	401	BCB	C1D-C2D	3.49	1.43	1.39
5	C	402	HEC	CMA-C3A	3.48	1.57	1.50
5	C	404	HEC	CBB-CAB	-3.47	1.36	1.49
7	L	303	BPB	OBB-CAB	3.41	1.32	1.22
6	L	302	BCB	CBD-CGD	-3.40	1.48	1.52
7	L	303	BPB	O2A-CGA	3.38	1.43	1.33
6	L	302	BCB	O2D-CGD	3.36	1.41	1.33
5	C	404	HEC	CMB-C2B	3.33	1.57	1.50
6	M	402	BCB	C3B-C4B	3.32	1.46	1.41
7	M	403	BPB	CBD-CGD	-3.29	1.48	1.52
7	M	403	BPB	C4C-NC	-3.22	1.27	1.37
6	M	401	BCB	C3D-C4D	-3.20	1.36	1.41
6	M	401	BCB	OBD-CAD	3.18	1.26	1.22
5	C	403	HEC	CMB-C2B	3.16	1.57	1.50
6	L	302	BCB	C3A-C2A	-3.15	1.52	1.54
5	C	402	HEC	CBC-CAC	-3.15	1.37	1.49
5	C	403	HEC	CBC-CAC	-3.14	1.37	1.49
7	M	403	BPB	O2D-CGD	3.11	1.40	1.33
5	C	403	HEC	CBB-CAB	-3.11	1.38	1.49
5	C	402	HEC	CMD-C2D	3.09	1.57	1.50
5	C	402	HEC	CBB-CAB	-3.09	1.38	1.49
11	M	405	NS5	C29-C30	3.08	1.52	1.43
5	C	404	HEC	C3C-C4C	-3.08	1.40	1.46
5	C	404	HEC	CBC-CAC	-3.06	1.38	1.49
5	C	404	HEC	CMD-C2D	3.01	1.56	1.50
7	M	403	BPB	C3B-C2B	2.92	1.44	1.39
7	L	303	BPB	O2D-CGD	2.84	1.40	1.33
7	M	403	BPB	C1D-ND	-2.80	1.33	1.38
6	M	402	BCB	O2A-CGA	2.79	1.41	1.33
5	C	401	HEC	CMB-C2B	2.78	1.56	1.50
7	M	403	BPB	CBB-CAB	-2.72	1.41	1.49
6	M	401	BCB	CHD-C4C	2.69	1.44	1.39
5	C	403	HEC	CMD-C2D	2.68	1.56	1.50
6	M	402	BCB	C3A-C2A	-2.67	1.52	1.54
5	C	403	HEC	CMC-C2C	2.66	1.56	1.50
5	C	404	HEC	CMA-C3A	2.66	1.56	1.50
5	C	404	HEC	CHD-C1D	-2.65	1.33	1.39
5	C	403	HEC	CMA-C3A	2.64	1.56	1.50
5	C	402	HEC	C4A-NA	2.64	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	301	BCB	CHB-C1B	2.63	1.43	1.39
6	L	302	BCB	O2A-CGA	2.52	1.40	1.33
5	C	404	HEC	CAA-C2A	2.52	1.57	1.51
6	L	301	BCB	C3B-C4B	2.51	1.45	1.41
6	M	401	BCB	O2A-CGA	2.50	1.40	1.33
6	L	302	BCB	CHD-C1D	2.49	1.43	1.39
5	C	404	HEC	CMC-C2C	2.47	1.55	1.50
10	M	404	MQ7	O4-C4	2.45	1.28	1.23
6	L	302	BCB	MG-ND	-2.43	2.01	2.05
6	M	402	BCB	CHD-C4C	2.43	1.44	1.39
6	L	301	BCB	MG-NB	-2.37	2.01	2.05
5	C	401	HEC	O2D-CGD	-2.33	1.23	1.30
6	M	401	BCB	C3B-C2B	2.32	1.43	1.39
6	M	401	BCB	MG-ND	-2.31	2.01	2.05
7	L	303	BPB	CBB-CAB	-2.28	1.43	1.49
11	M	405	NS5	C28-C26	2.28	1.50	1.46
7	M	403	BPB	OBB-CAB	2.26	1.29	1.22
7	L	303	BPB	C4B-NB	-2.26	1.34	1.38
6	M	402	BCB	CHB-C1B	2.20	1.43	1.39
5	C	404	HEC	C3B-C2B	-2.20	1.33	1.41
5	C	402	HEC	CAA-C2A	2.12	1.56	1.51
5	C	403	HEC	C4B-NB	-2.11	1.35	1.39
5	C	402	HEC	C4B-NB	-2.10	1.35	1.39
6	M	402	BCB	CHB-C4A	-2.08	1.36	1.38
5	C	402	HEC	C3B-C4B	2.08	1.49	1.46
5	C	401	HEC	C1C-NC	-2.07	1.35	1.39
5	C	403	HEC	C4D-C3D	2.05	1.48	1.44
10	M	404	MQ7	O1-C1	2.04	1.27	1.23

All (172) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	301	BCB	C1B-CHB-C4A	12.83	129.57	121.32
6	M	401	BCB	C4B-CHC-C1C	8.48	126.78	121.32
6	M	402	BCB	C4B-CHC-C1C	8.14	126.56	121.32
6	L	301	BCB	C4B-CHC-C1C	8.09	126.53	121.32
6	M	402	BCB	C1B-CHB-C4A	7.79	126.33	121.32
6	L	301	BCB	OBD-CAD-C3D	-7.21	116.65	127.89
5	C	401	HEC	CBC-CAC-C3C	-7.05	113.35	127.43
6	M	401	BCB	C1B-CHB-C4A	6.59	125.56	121.32
6	M	402	BCB	O2D-CGD-CBD	6.59	118.19	110.95
7	L	303	BPB	C3D-C4D-ND	6.50	116.04	107.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	402	HEC	CBC-CAC-C3C	-6.32	114.81	127.43
5	C	401	HEC	CBB-CAB-C3B	-6.29	114.86	127.43
6	L	301	BCB	O2D-CGD-CBD	6.07	117.62	110.95
11	M	405	NS5	C29-C28-C26	-6.00	109.90	126.36
6	L	302	BCB	C1B-CHB-C4A	5.93	125.14	121.32
6	L	302	BCB	C3D-CAD-CBD	5.92	115.40	107.61
6	L	302	BCB	O2D-CGD-CBD	5.82	117.34	110.95
6	M	401	BCB	CHA-C1A-C2A	-5.81	119.67	133.31
6	L	302	BCB	C4B-CHC-C1C	5.78	125.04	121.32
7	M	403	BPB	C3D-C4D-ND	5.73	115.06	107.71
6	M	401	BCB	C3D-CAD-CBD	5.72	115.14	107.61
6	M	402	BCB	O2D-CGD-O1D	-5.70	112.76	123.85
5	C	403	HEC	CBB-CAB-C3B	-5.61	116.22	127.43
5	C	404	HEC	CBB-CAB-C3B	-5.59	116.25	127.43
6	M	402	BCB	C3D-CAD-CBD	5.46	114.80	107.61
7	M	403	BPB	O2D-CGD-CBD	5.42	116.90	110.95
11	M	405	NS5	C19-C18-C17	5.33	134.43	123.52
6	M	402	BCB	OBD-CAD-C3D	-5.23	119.73	127.89
7	L	303	BPB	C2B-C1B-NB	5.21	113.20	109.43
11	M	405	NS5	C22-C21-C20	5.19	131.23	122.82
11	M	405	NS5	C34-C35-C36	-5.19	110.34	127.64
7	M	403	BPB	OBD-CAD-C3D	-5.18	119.82	127.89
6	L	301	BCB	C1-C2-C3	-5.12	117.80	126.20
6	L	301	BCB	C3D-CAD-CBD	4.99	114.18	107.61
6	L	302	BCB	OBD-CAD-C3D	-4.96	120.16	127.89
7	L	303	BPB	O2D-CGD-CBD	4.91	116.35	110.95
6	M	402	BCB	C3D-C4D-CHA	4.83	115.88	108.54
5	C	402	HEC	CBB-CAB-C3B	-4.73	117.98	127.43
7	L	303	BPB	C2D-C1D-ND	4.70	112.83	109.43
7	L	303	BPB	C4D-ND-C1D	-4.66	103.29	108.87
6	L	302	BCB	CHA-C1A-C2A	-4.64	122.42	133.31
6	M	401	BCB	O2D-CGD-CBD	4.57	115.97	110.95
6	M	402	BCB	CHA-C1A-C2A	-4.56	122.60	133.31
7	L	303	BPB	OBD-CAD-C3D	-4.56	120.78	127.89
5	C	402	HEC	C4B-NB-C1B	4.54	113.23	105.82
5	C	402	HEC	C4D-ND-C1D	4.51	113.18	105.82
6	L	301	BCB	CHA-C1A-C2A	-4.51	122.73	133.31
8	L	304	MPG	C1-O1-CX3	4.40	126.23	116.53
7	M	403	BPB	C2D-C1D-ND	4.37	112.59	109.43
8	L	304	MPG	O1-CX3-CXD	4.34	121.82	111.78
6	L	302	BCB	CMB-C2B-C3B	4.32	133.32	124.68
6	L	301	BCB	C4-C3-C5	4.26	122.63	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	401	BCB	CMB-C2B-C3B	4.20	133.08	124.68
6	L	301	BCB	C3D-C4D-CHA	4.14	114.83	108.54
5	C	403	HEC	CHC-C4B-NB	4.02	128.83	124.45
5	C	404	HEC	C4D-ND-C1D	3.99	112.33	105.82
11	M	405	NS5	C18-C19-C20	3.93	131.57	123.52
11	M	405	NS5	CM4-C36-C35	-3.92	110.89	122.66
8	L	304	MPG	O2-CXD-CX3	3.92	119.65	109.45
6	M	401	BCB	OBD-CAD-C3D	-3.89	121.83	127.89
6	L	302	BCB	C3D-C4D-CHA	3.88	114.44	108.54
7	M	403	BPB	C2B-C1B-NB	3.86	112.22	109.43
6	L	301	BCB	C4D-CHA-CBD	-3.85	105.09	108.97
11	M	405	NS5	C18-C17-C15	-3.84	121.89	127.28
11	M	405	NS5	C24-C25-C26	-3.78	121.98	127.28
7	M	403	BPB	C4D-CHA-CBD	-3.75	106.66	108.45
11	M	405	NS5	C13-C12-C10	-3.67	122.53	127.69
7	L	303	BPB	C1-C2-C3	-3.67	120.19	126.20
8	L	304	MPG	O4-CX3-CXD	-3.62	114.81	123.56
7	M	403	BPB	C4D-ND-C1D	-3.59	104.58	108.87
8	L	304	MPG	O2-CXD-C21	3.58	117.46	109.97
6	M	402	BCB	C4D-CHA-CBD	-3.57	105.36	108.97
6	L	302	BCB	O1D-CGD-CBD	-3.57	119.31	124.72
11	M	405	NS5	C16-C15-C14	-3.57	112.64	118.09
11	M	405	NS5	CM3-C36-C35	-3.55	111.99	122.66
5	C	403	HEC	CBC-CAC-C3C	-3.55	120.34	127.43
5	C	404	HEC	CBC-CAC-C3C	-3.54	120.36	127.43
7	L	303	BPB	OBB-CAB-C3B	3.53	125.89	119.99
6	M	402	BCB	CMB-C2B-C3B	3.50	131.68	124.68
6	M	401	BCB	C3D-C4D-CHA	3.50	113.86	108.54
5	C	403	HEC	C4D-ND-C1D	3.50	111.53	105.82
7	L	303	BPB	CED-O2D-CGD	3.48	123.82	115.92
6	M	401	BCB	C4D-ND-C1D	-3.44	102.61	105.22
7	L	303	BPB	C3D-CAD-CBD	3.40	112.09	107.61
7	M	403	BPB	CBB-CAB-C3B	-3.34	110.33	120.34
5	C	401	HEC	CBD-CAD-C3D	-3.29	103.44	112.53
10	M	404	MQ7	C26-C27-C28	-3.29	120.10	127.62
5	C	401	HEC	CHD-C4C-NC	3.24	127.98	124.45
6	M	402	BCB	C1-O2A-CGA	3.15	124.28	116.65
8	L	305	MPG	O2-CXD-CX3	3.14	117.61	109.45
5	C	401	HEC	C2A-C1A-NA	-3.13	107.30	110.32
5	C	402	HEC	CMC-C2C-C1C	-3.03	120.81	125.42
7	M	403	BPB	OBB-CAB-C3B	3.02	125.04	119.99
6	M	402	BCB	C4-C3-C5	2.99	120.42	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	403	BPB	C3D-CAD-CBD	2.98	111.53	107.61
5	C	403	HEC	C4B-NB-C1B	2.98	110.67	105.82
11	M	405	NS5	C23-C21-C20	-2.95	114.36	119.01
5	C	404	HEC	C4B-NB-C1B	2.95	110.64	105.82
7	L	303	BPB	CBB-CAB-C3B	-2.91	111.62	120.34
6	L	301	BCB	O2D-CGD-O1D	-2.91	118.18	123.85
11	M	405	NS5	C8-C7-C5	-2.89	121.01	127.62
7	L	303	BPB	CMA-C3A-C4A	-2.86	108.46	114.61
8	L	305	MPG	O1-C1-C2	2.84	118.43	108.61
5	C	402	HEC	CHD-C1D-ND	2.80	128.95	123.86
5	C	402	HEC	O2D-CGD-CBD	2.78	122.79	114.00
8	L	305	MPG	O3-C21-CXD	-2.78	105.10	111.95
6	L	301	BCB	C1A-CHA-C4D	2.75	123.58	118.98
11	M	405	NS5	C16-C15-C17	2.74	127.25	122.82
6	L	302	BCB	CHC-C1C-C2C	-2.74	115.36	122.69
11	M	405	NS5	C11-C10-C9	2.73	119.97	115.23
6	M	402	BCB	C4D-ND-C1D	-2.73	103.15	105.22
6	L	301	BCB	CHD-C4C-C3C	-2.69	121.99	130.04
11	M	405	NS5	C30-C29-C28	-2.68	115.45	123.20
8	L	304	MPG	O3-C21-CXD	-2.67	105.37	111.95
5	C	404	HEC	CHA-C4D-ND	2.61	128.60	123.86
5	C	404	HEC	C3D-C4D-ND	-2.61	107.26	110.15
5	C	402	HEC	O1D-CGD-CBD	-2.58	114.90	123.09
6	M	401	BCB	CHC-C1C-C2C	-2.58	115.78	122.69
7	M	403	BPB	O2D-CGD-O1D	-2.57	118.85	123.85
10	M	404	MQ7	C11-C3-C2	-2.54	120.54	124.89
5	C	403	HEC	C2A-C1A-NA	-2.53	107.88	110.32
6	M	402	BCB	C1A-CHA-C4D	2.53	123.20	118.98
5	C	404	HEC	C4C-NC-C1C	-2.50	101.75	105.82
5	C	401	HEC	C4D-ND-C1D	2.47	109.86	105.82
6	M	402	BCB	CMD-C2D-C3D	-2.47	119.75	124.68
5	C	402	HEC	C2B-C1B-NB	-2.46	106.20	110.14
7	L	303	BPB	O2A-CGA-O1A	-2.46	117.48	123.63
11	M	405	NS5	C22-C21-C23	-2.45	114.35	118.09
5	C	401	HEC	CMD-C2D-C1D	2.45	129.14	125.42
5	C	401	HEC	C4A-NA-C1A	2.44	109.81	105.82
5	C	401	HEC	C4C-NC-C1C	2.41	109.75	105.82
7	M	403	BPB	C1-C2-C3	-2.40	122.27	126.20
5	C	402	HEC	O1A-CGA-CBA	-2.39	115.51	123.09
7	L	303	BPB	O2D-CGD-O1D	-2.39	119.19	123.85
11	M	405	NS5	C24-C23-C21	-2.38	119.85	126.36
8	L	305	MPG	O1-CX3-CXD	2.38	117.28	111.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	M	405	NS5	C6-C5-C4	2.37	119.33	115.23
5	C	404	HEC	C2B-C1B-NB	-2.35	106.37	110.14
7	M	403	BPB	C4-C3-C5	2.34	119.29	115.23
5	C	402	HEC	CHC-C4B-NB	2.34	127.00	124.45
6	M	402	BCB	CHD-C4C-C3C	-2.32	123.10	130.04
5	C	401	HEC	CMC-C2C-C1C	-2.28	121.95	125.42
5	C	403	HEC	C3D-C4D-ND	-2.27	107.63	110.15
6	L	302	BCB	C1A-CHA-C4D	2.27	122.77	118.98
6	M	402	BCB	C1-C2-C3	-2.26	122.49	126.20
6	M	401	BCB	C3D-C4D-ND	2.26	116.56	112.94
5	C	401	HEC	C2B-C1B-NB	-2.25	106.53	110.14
6	L	301	BCB	OBD-CAD-CBD	2.25	129.13	125.82
10	M	404	MQ7	C45-C43-C44	2.25	119.76	114.59
6	L	302	BCB	CMA-C3A-C4A	-2.23	109.80	114.61
7	M	403	BPB	CMA-C3A-C4A	-2.22	109.83	114.61
10	M	404	MQ7	C44-C43-C42	-2.21	116.01	122.66
5	C	403	HEC	CHD-C4C-NC	2.21	126.86	124.45
5	C	404	HEC	CHD-C1D-ND	2.20	127.84	123.86
8	L	305	MPG	O2-CXD-C21	2.15	114.47	109.97
10	M	404	MQ7	C39-C38-C40	2.14	118.94	115.23
5	C	402	HEC	CMC-C2C-C3C	2.13	131.56	126.55
6	M	402	BCB	O1D-CGD-CBD	2.11	127.93	124.72
6	L	301	BCB	CHC-C1C-C2C	-2.11	117.04	122.69
6	M	402	BCB	CHC-C1C-C2C	-2.10	117.05	122.69
7	M	403	BPB	CMB-C2B-C3B	2.09	128.85	124.68
10	M	404	MQ7	C19-C18-C20	2.08	118.84	115.23
7	M	403	BPB	OBB-CAB-CBB	2.08	124.62	120.19
6	L	302	BCB	C1-O2A-CGA	2.08	121.68	116.65
10	M	404	MQ7	C34-C33-C35	2.07	118.82	115.23
6	L	301	BCB	C15-C13-C12	-2.07	101.60	112.07
5	C	402	HEC	C1D-CHD-C4C	2.06	131.02	124.66
7	M	403	BPB	C7-C6-C5	-2.06	107.78	113.26
5	C	404	HEC	O2A-CGA-CBA	2.05	120.49	114.00
6	L	301	BCB	CED-O2D-CGD	2.04	120.55	115.92
11	M	405	NS5	C12-C13-C14	-2.03	117.31	123.20
8	L	304	MPG	O1-C1-C2	2.01	115.57	108.61

All (11) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	L	301	BCB	NC
6	L	301	BCB	NA

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Mol	Chain	Res	Type	Atom
6	L	302	BCB	NC
6	L	302	BCB	NA
6	M	401	BCB	NC
6	M	401	BCB	NA
6	M	402	BCB	NC
6	M	402	BCB	NA
6	M	402	BCB	ND
8	L	304	MPG	CXD
8	L	305	MPG	CXD

All (96) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	401	HEC	C2B-C3B-CAB-CBB
5	C	401	HEC	C4B-C3B-CAB-CBB
5	C	401	HEC	C2C-C3C-CAC-CBC
5	C	401	HEC	C4C-C3C-CAC-CBC
5	C	402	HEC	C2B-C3B-CAB-CBB
5	C	402	HEC	C4B-C3B-CAB-CBB
5	C	402	HEC	C2C-C3C-CAC-CBC
5	C	402	HEC	C4C-C3C-CAC-CBC
5	C	403	HEC	C2B-C3B-CAB-CBB
5	C	403	HEC	C4B-C3B-CAB-CBB
5	C	403	HEC	C2C-C3C-CAC-CBC
5	C	403	HEC	C4C-C3C-CAC-CBC
5	C	404	HEC	C2B-C3B-CAB-CBB
5	C	404	HEC	C4B-C3B-CAB-CBB
5	C	404	HEC	C2C-C3C-CAC-CBC
5	C	404	HEC	C4C-C3C-CAC-CBC
6	M	402	BCB	CAD-CBD-CGD-O1D
6	M	402	BCB	CAD-CBD-CGD-O2D
7	L	303	BPB	C2C-C3C-CAC-CBC
7	M	403	BPB	C2C-C3C-CAC-CBC
8	L	304	MPG	CXD-CX3-O1-C1
8	L	304	MPG	O3-C21-CXD-O2
8	L	304	MPG	O1-CX3-CXD-C21
8	L	305	MPG	CXD-CX3-O1-C1
8	L	305	MPG	O3-C21-CXD-O2
8	L	305	MPG	O1-CX3-CXD-C21
8	L	305	MPG	O4-CX3-CXD-C21
11	M	405	NS5	C25-C26-C28-C29
11	M	405	NS5	C27-C26-C28-C29

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Mol	Chain	Res	Type	Atoms
11	M	405	NS5	C26-C28-C29-C30
11	M	405	NS5	C28-C29-C30-C31
8	L	305	MPG	O4-CX3-O1-C1
11	M	405	NS5	C34-C35-C36-CM4
8	L	304	MPG	O4-CX3-O1-C1
11	M	405	NS5	C2-C3-C4-C5
6	L	301	BCB	C4-C3-C5-C6
11	M	405	NS5	C11-C10-C9-C8
6	L	301	BCB	C2-C3-C5-C6
11	M	405	NS5	C12-C10-C9-C8
6	M	401	BCB	C11-C10-C8-C9
7	M	403	BPB	C11-C10-C8-C9
7	M	403	BPB	C10-C11-C12-C13
6	M	402	BCB	C2A-CAA-CBA-CGA
6	L	301	BCB	C15-C16-C17-C18
8	L	304	MPG	O1-C1-C2-C3
7	M	403	BPB	C8-C10-C11-C12
8	L	304	MPG	O3-C21-CXD-CX3
8	L	305	MPG	C14-C15-C16-C17
7	L	303	BPB	C16-C17-C18-C19
6	L	302	BCB	C16-C17-C18-C20
6	L	302	BCB	C16-C17-C18-C19
7	L	303	BPB	C16-C17-C18-C20
8	L	305	MPG	C11-C12-C13-C14
6	M	401	BCB	C15-C16-C17-C18
8	L	304	MPG	C10-C11-C12-C13
6	L	302	BCB	C11-C12-C13-C15
6	M	401	BCB	C2-C3-C5-C6
6	L	302	BCB	C11-C12-C13-C14
8	L	305	MPG	C10-C11-C12-C13
8	M	406	MPG	C3-C4-C5-C6
8	L	304	MPG	C2-C3-C4-C5
6	M	401	BCB	C4-C3-C5-C6
7	L	303	BPB	O2A-C1-C2-C3
8	M	406	MPG	C10-C11-C12-C13
8	L	305	MPG	C3-C4-C5-C6
7	M	403	BPB	C11-C10-C8-C7
8	L	305	MPG	C12-C13-C14-C15
8	L	305	MPG	C4-C5-C6-C7
8	L	305	MPG	O1-C1-C2-C3
8	L	305	MPG	C5-C6-C7-C8
5	C	402	HEC	C3D-CAD-CBD-CGD

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Mol	Chain	Res	Type	Atoms
7	M	403	BPB	C14-C13-C15-C16
6	L	301	BCB	CAD-CBD-CGD-O2D
6	L	301	BCB	CAD-CBD-CGD-O1D
8	M	406	MPG	C13-C14-C15-C16
11	M	405	NS5	C1-C2-C3-C4
6	L	301	BCB	C16-C17-C18-C20
7	L	303	BPB	C8-C10-C11-C12
5	C	402	HEC	CAA-CBA-CGA-O1A
10	M	404	MQ7	C39-C38-C40-C41
10	M	404	MQ7	C37-C38-C40-C41
10	M	404	MQ7	C38-C40-C41-C42
5	C	402	HEC	CAD-CBD-CGD-O1D
7	M	403	BPB	C12-C13-C15-C16
5	C	402	HEC	CAD-CBD-CGD-O2D
5	C	402	HEC	CAA-CBA-CGA-O2A
6	M	402	BCB	CHA-CBD-CGD-O1D
11	M	405	NS5	C20-C21-C23-C24
5	C	401	HEC	CAA-CBA-CGA-O2A
8	L	304	MPG	C6-C7-C8-C9
5	C	401	HEC	CAA-CBA-CGA-O1A
8	M	406	MPG	C7-C8-C9-C10
8	L	305	MPG	C13-C14-C15-C16
8	L	305	MPG	C9-C10-C11-C12
7	M	403	BPB	C6-C7-C8-C10
6	L	302	BCB	C15-C16-C17-C18

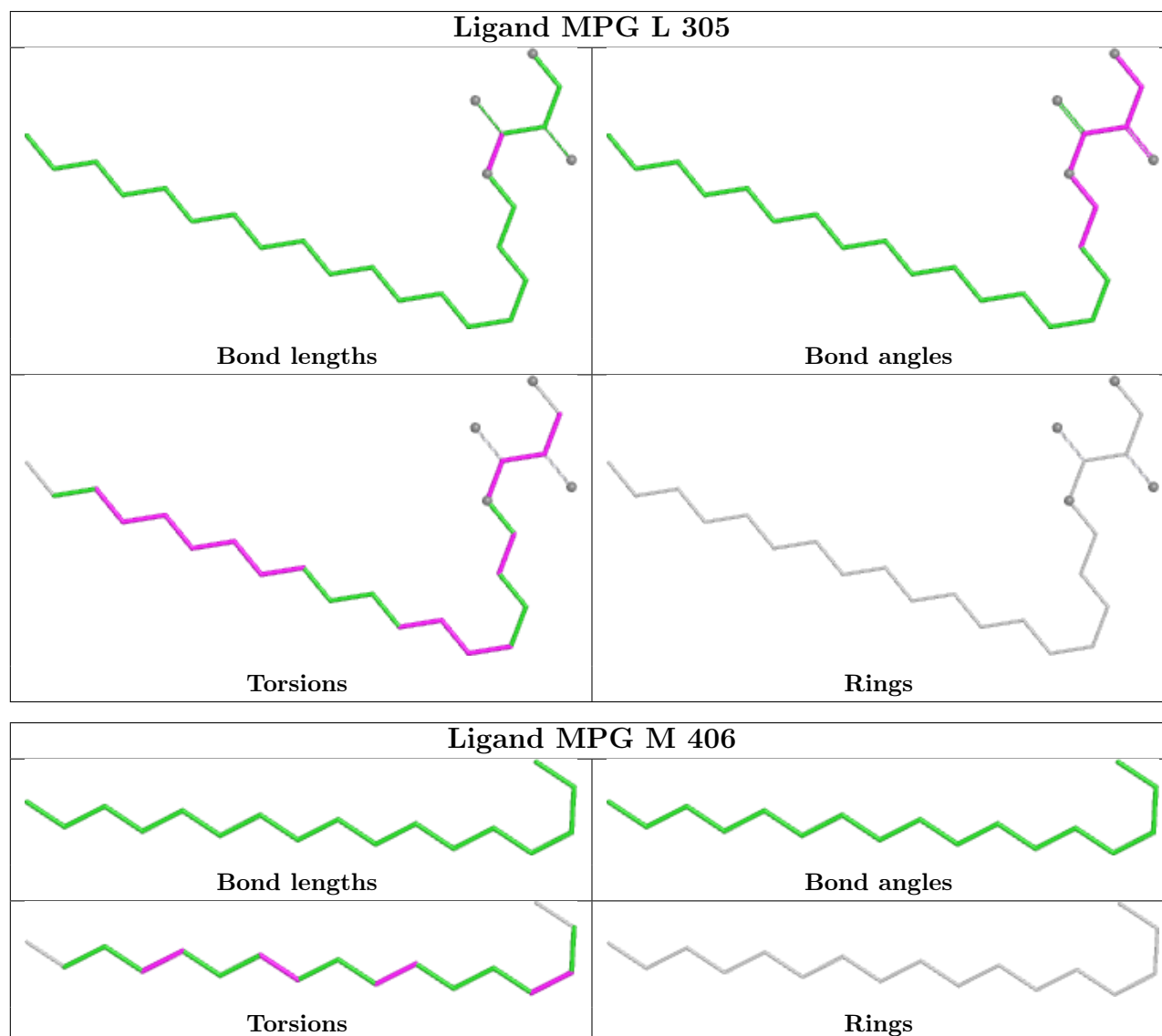
There are no ring outliers.

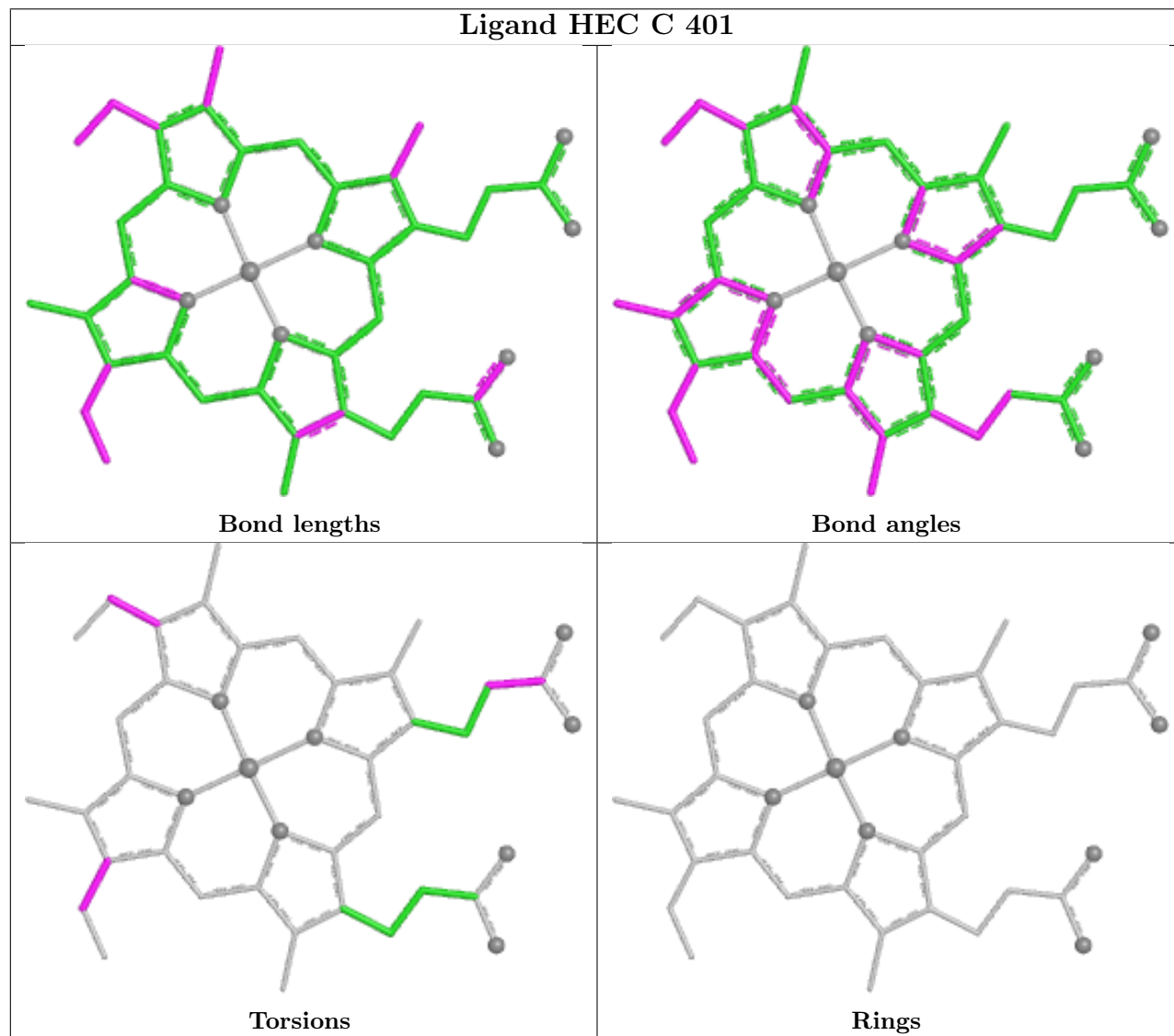
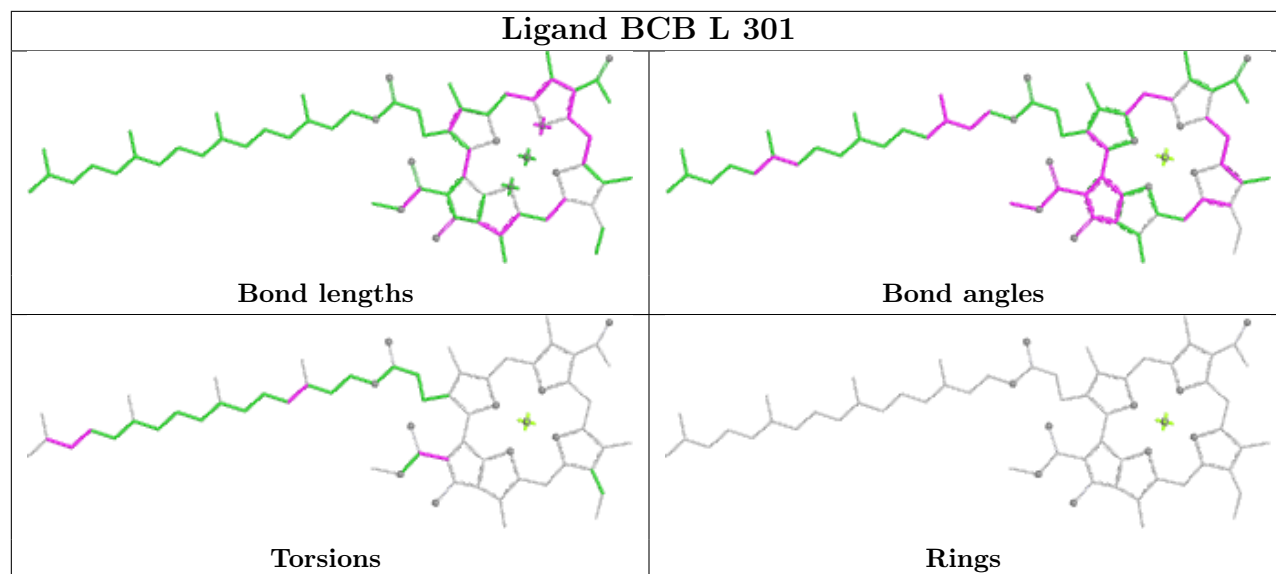
10 monomers are involved in 36 short contacts:

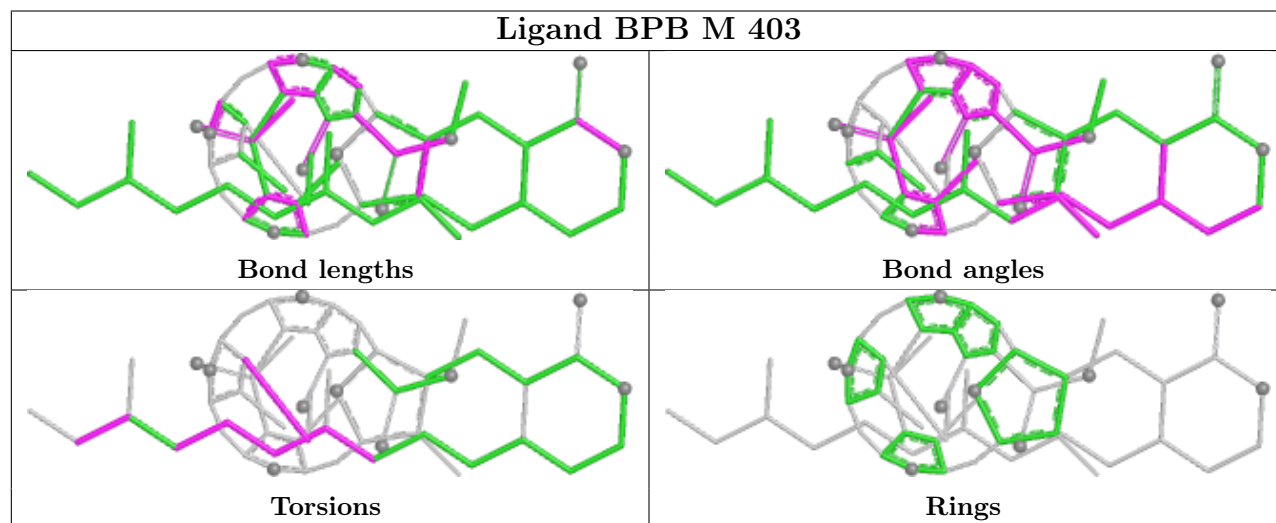
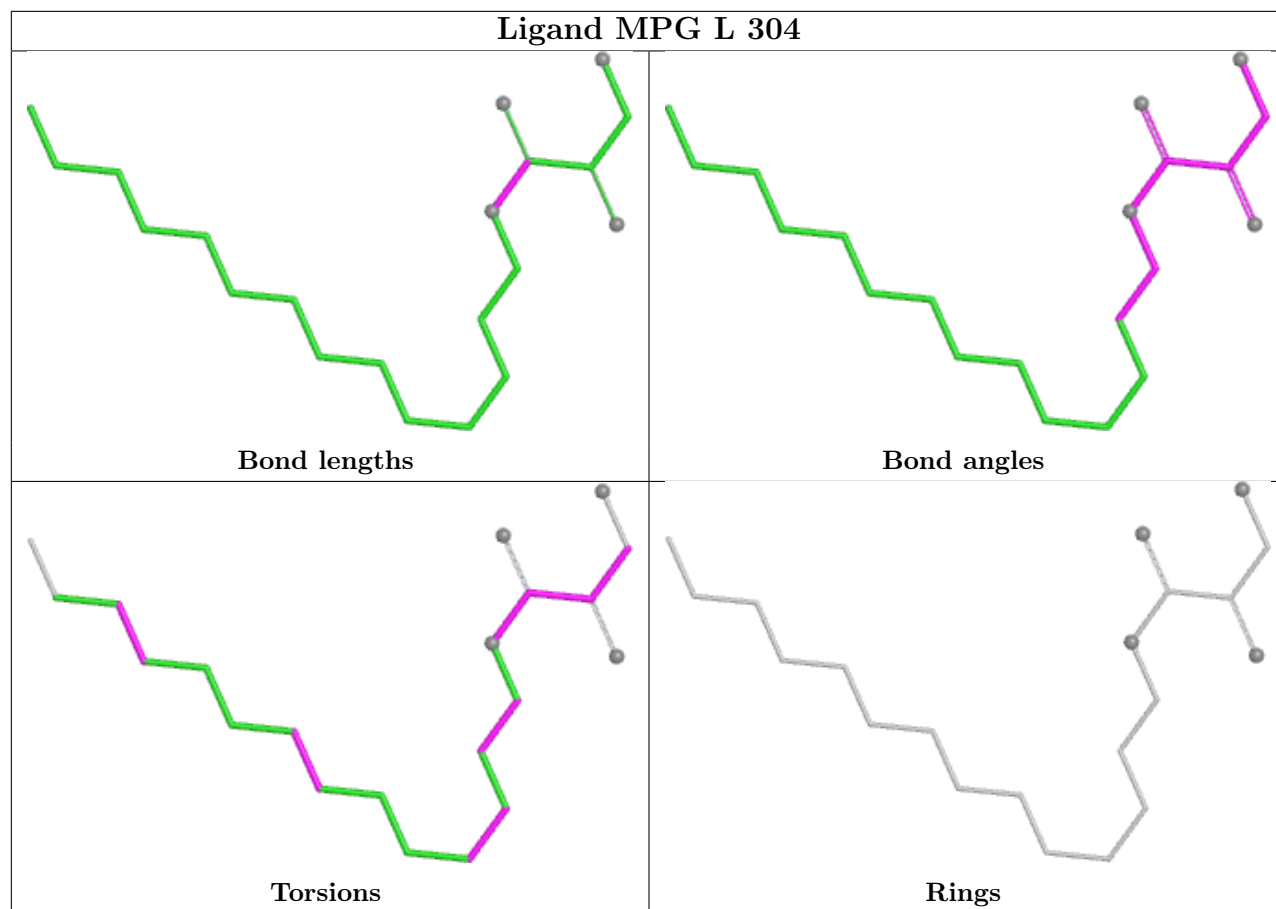
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	L	305	MPG	2	0
6	L	301	BCB	2	0
8	L	304	MPG	1	0
7	M	403	BPB	13	0
6	L	302	BCB	3	0
6	M	401	BCB	2	0
6	M	402	BCB	1	0
7	L	303	BPB	8	0
5	C	402	HEC	1	0
11	M	405	NS5	10	0

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

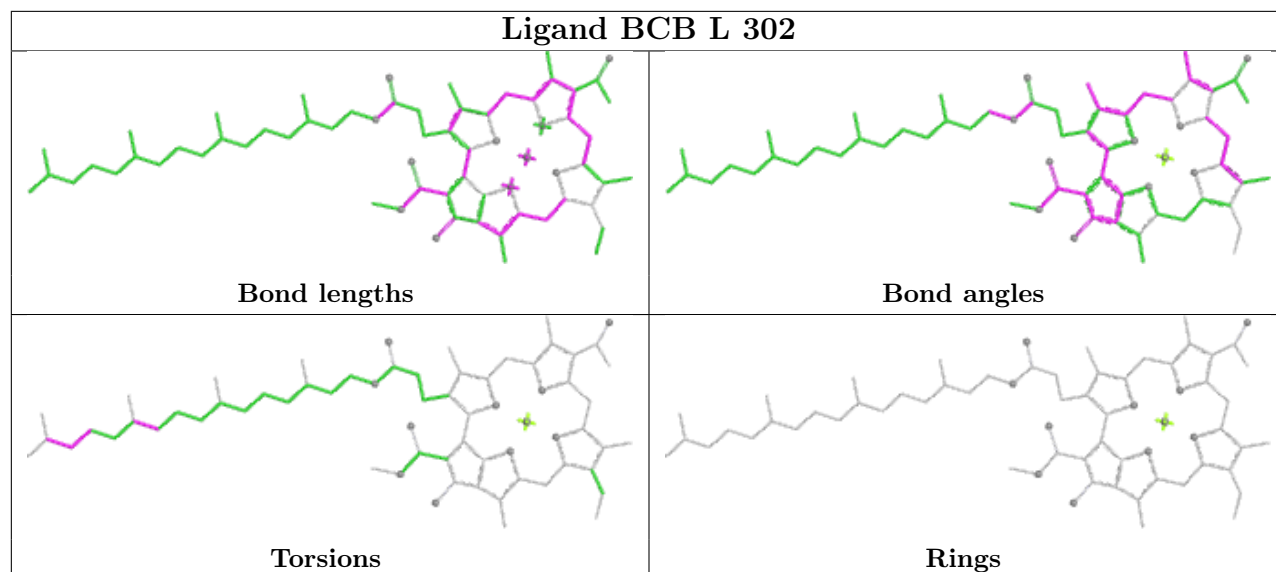
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.



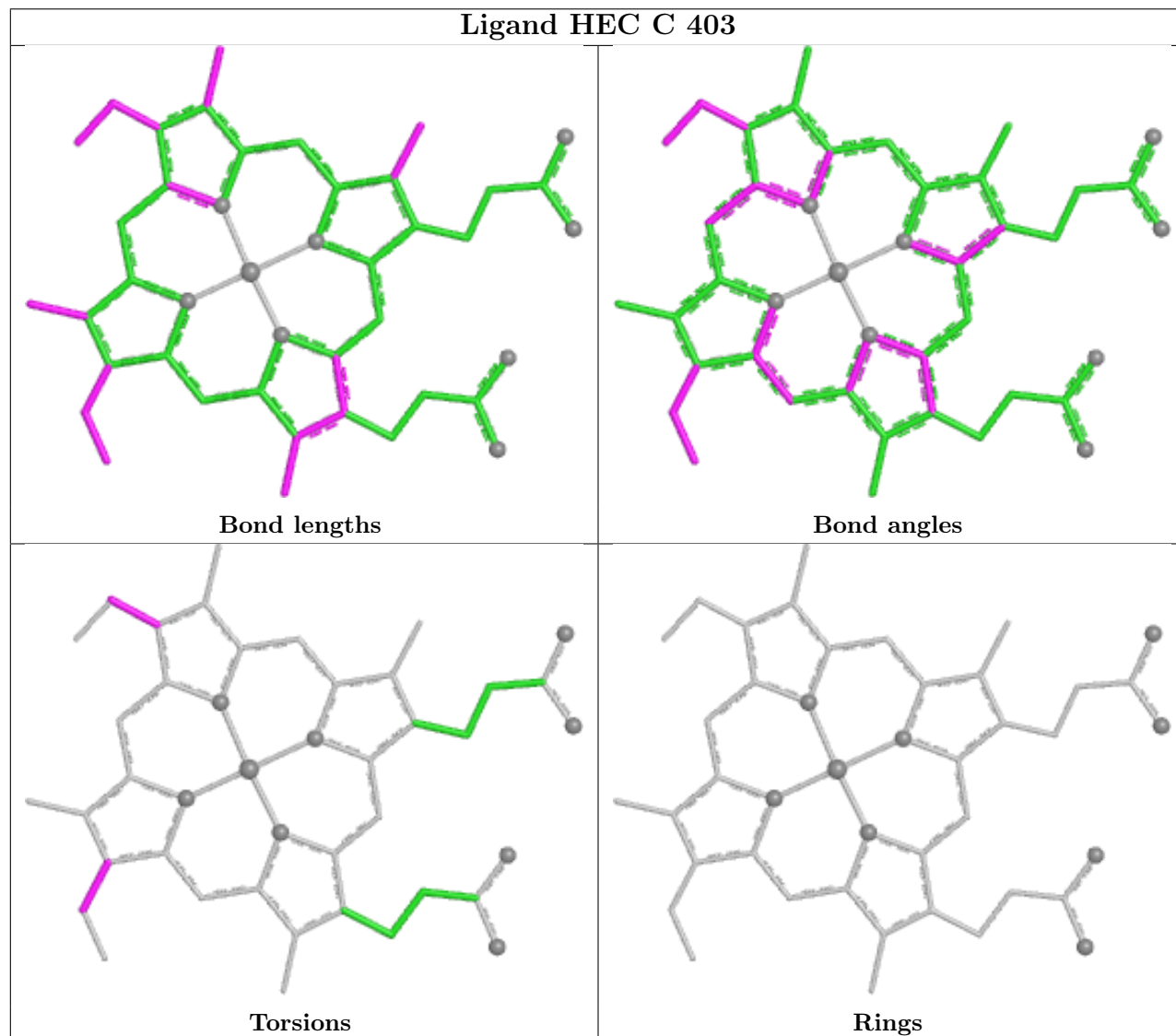


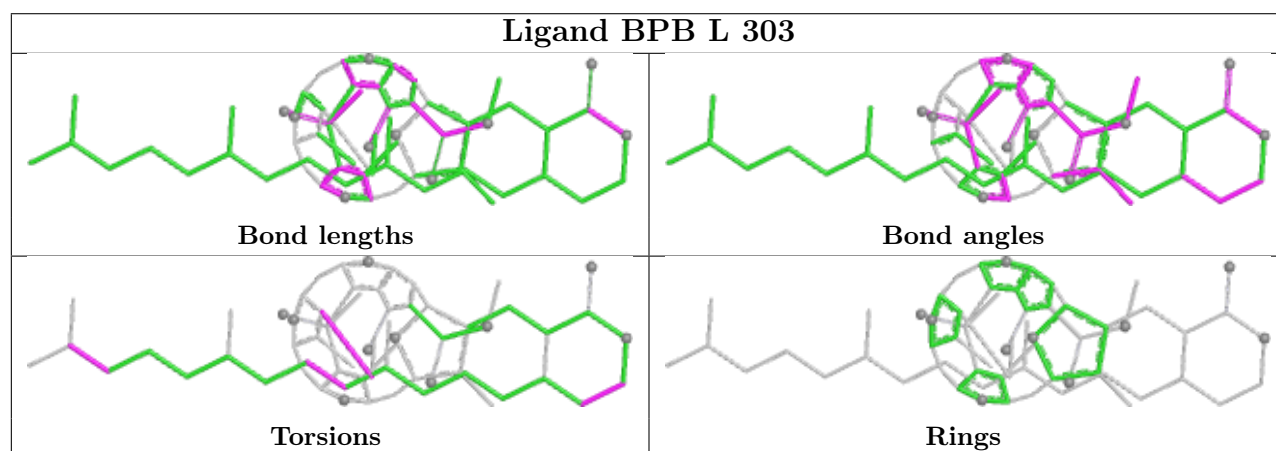
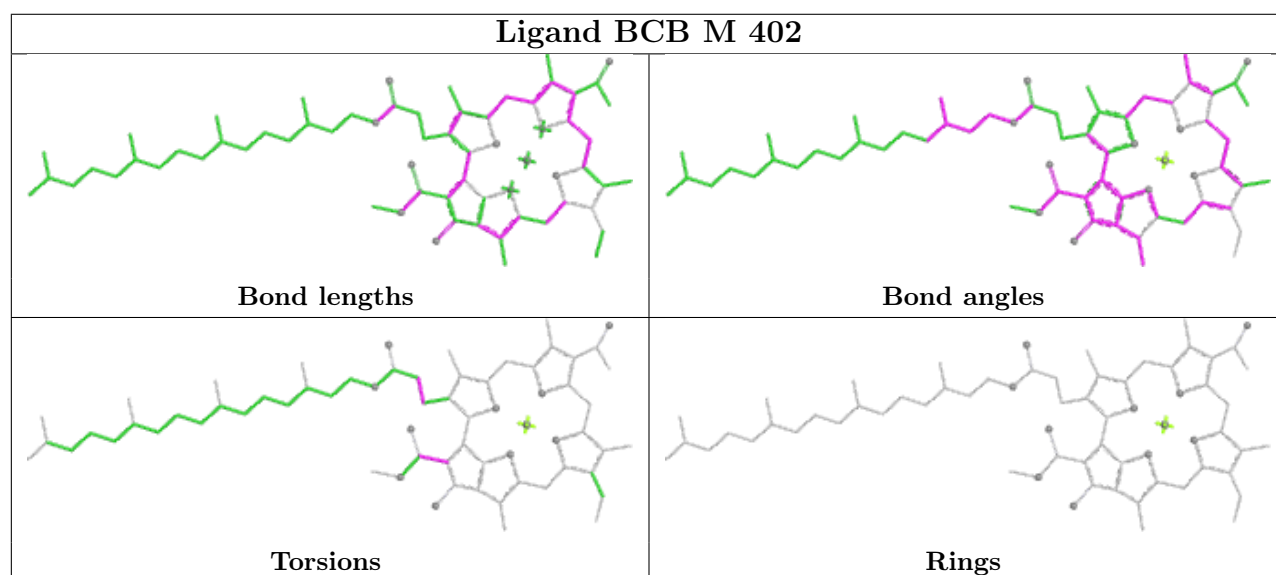
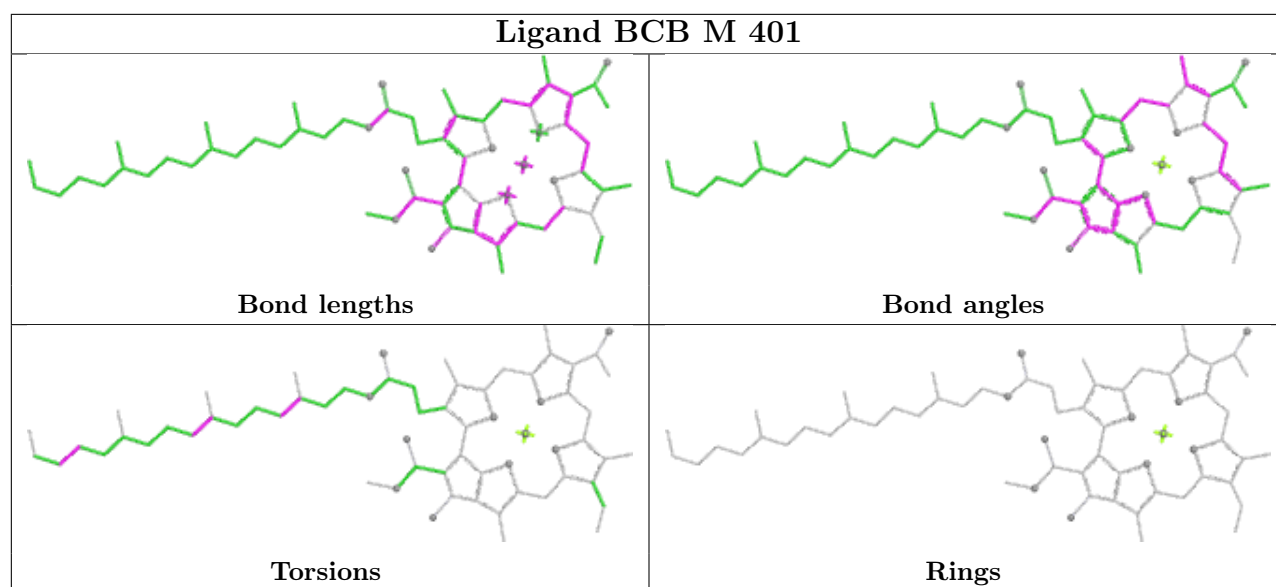


Ligand BCB L 302

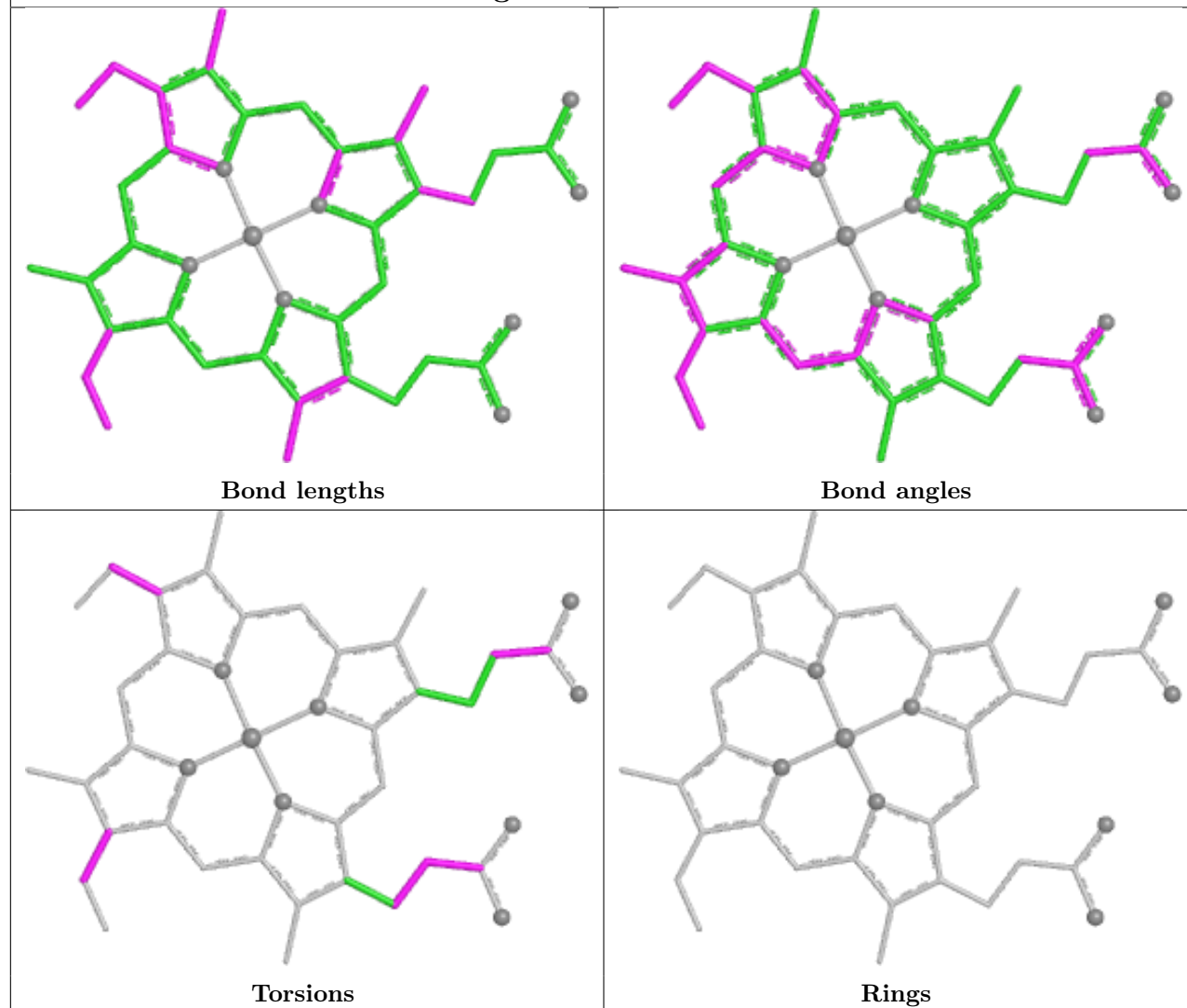


Ligand HEC C 403

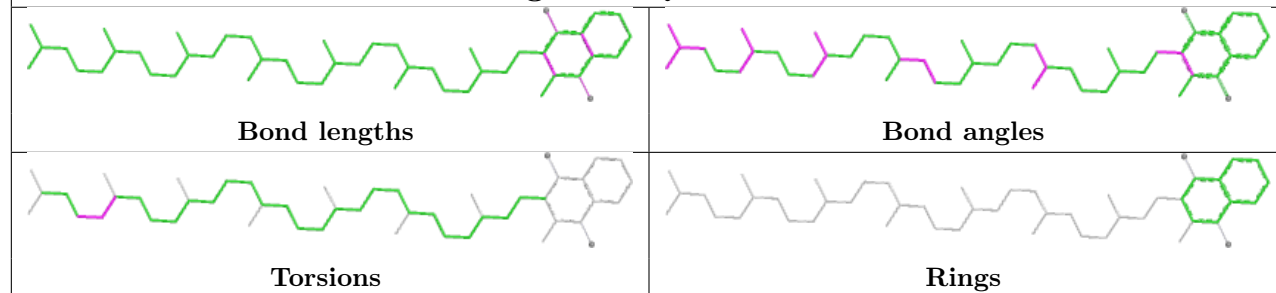


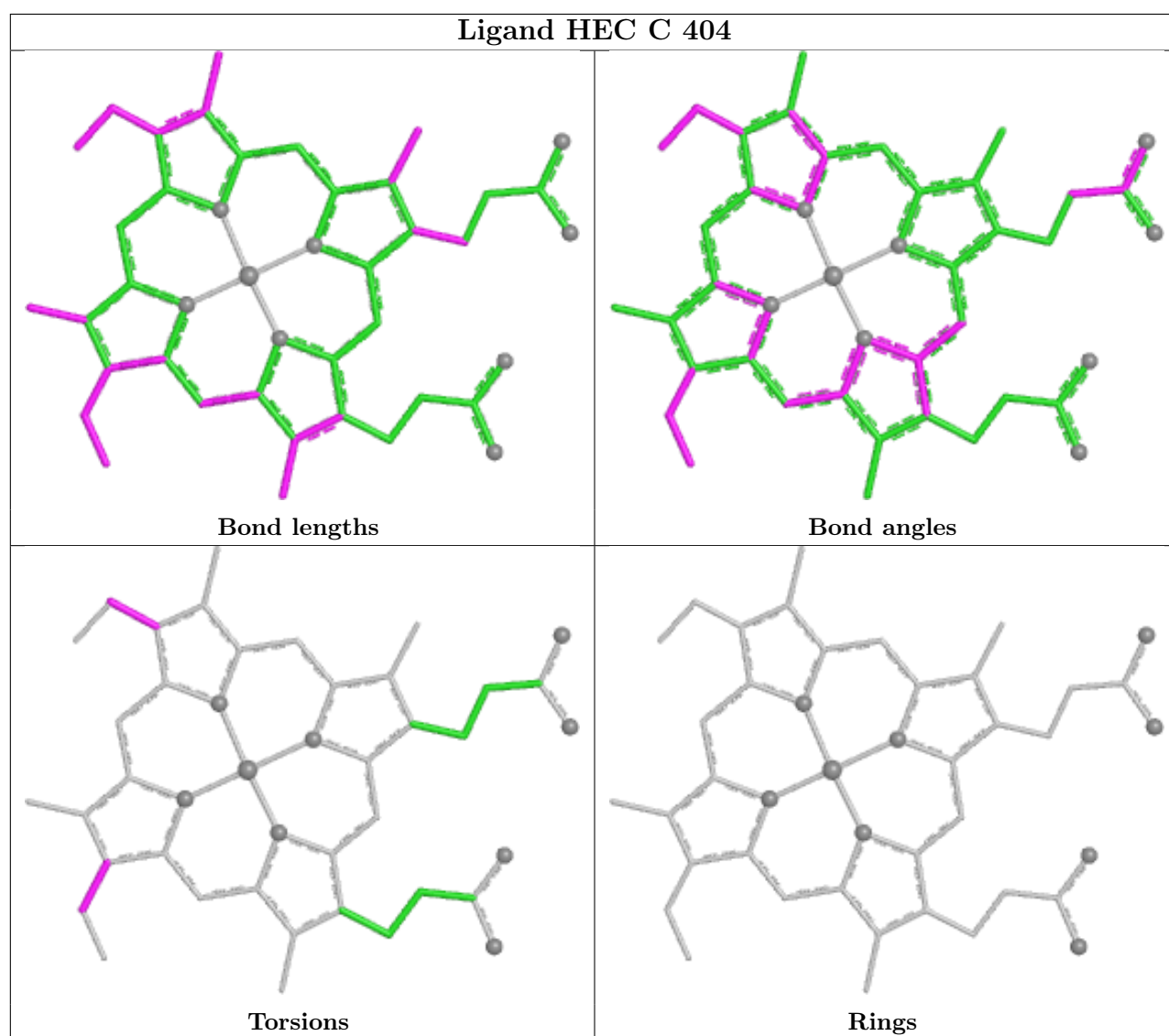
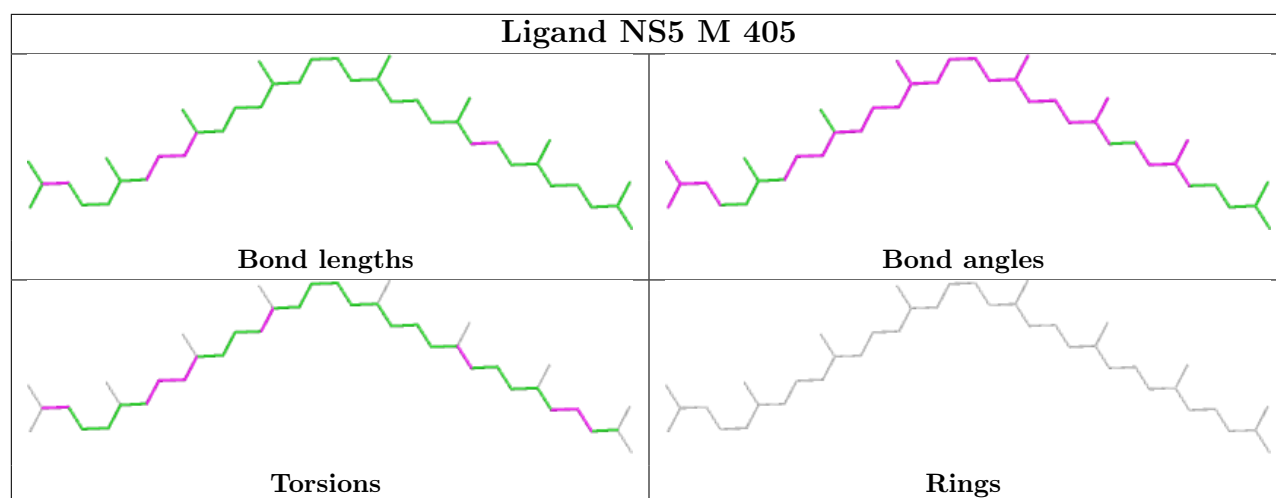


Ligand HEC C 402



Ligand MQ7 M 404





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	332/336 (98%)	0.72	15 (4%) 38 41	31, 35, 44, 69	0
2	H	242/258 (93%)	1.02	28 (11%) 9 9	28, 35, 48, 65	0
3	L	273/274 (99%)	0.99	31 (11%) 10 9	31, 35, 46, 59	0
4	M	323/324 (99%)	0.36	8 (2%) 58 62	32, 35, 44, 52	0
All	All	1170/1192 (98%)	0.75	82 (7%) 22 24	28, 35, 46, 69	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1	CYS	6.0
2	H	83	PRO	5.5
3	L	59	TRP	5.0
2	H	9	HIS	4.7
2	H	7	ALA	4.6
2	H	84	GLU	4.5
2	H	94	ASP	4.5
1	C	2	PHE	4.4
2	H	96	PHE	4.3
3	L	269	ILE	4.2
3	L	51	TYR	4.2
2	H	85	THR	4.0
3	L	63	ALA	4.0
3	L	1	ALA	4.0
3	L	60	ASP	3.9
3	L	265	TRP	3.8
3	L	272	TRP	3.5
2	H	25	TRP	3.4
3	L	271	PHE	3.4
1	C	47	ALA	3.3
2	H	8	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
2	H	91	ALA	3.3
3	L	62	PHE	3.3
2	H	82	ARG	3.1
3	L	203	GLY	3.0
3	L	53	ALA	3.0
3	L	61	PRO	2.9
2	H	191	ALA	2.9
1	C	84	GLN	2.9
4	M	104	ILE	2.9
2	H	93	THR	2.9
3	L	264	GLY	2.9
4	M	115	MET	2.8
3	L	263	TRP	2.8
4	M	22	GLU	2.8
1	C	48	GLU	2.8
3	L	58	THR	2.7
3	L	20	ASP	2.7
1	C	64	ASN	2.7
1	C	332	LYS	2.7
2	H	95	GLY	2.7
2	H	258	LEU	2.7
3	L	222	TYR	2.6
2	H	102	GLN	2.6
3	L	202	ASP	2.6
1	C	214	VAL	2.6
4	M	1	ALA	2.6
4	M	37	TRP	2.6
3	L	267	LEU	2.5
2	H	92	GLN	2.4
2	H	61	GLU	2.4
2	H	97	GLU	2.4
4	M	321	ALA	2.4
1	C	58	ASN	2.3
1	C	5	PRO	2.3
3	L	273	SER	2.3
3	L	81	LEU	2.3
2	H	45	GLU	2.3
2	H	5	ALA	2.2
2	H	177	GLU	2.2
1	C	212	VAL	2.2
1	C	46	LYS	2.2
1	C	213	GLY	2.2

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Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	L	55	GLN	2.2
3	L	215	TYR	2.2
4	M	59	PHE	2.2
2	H	34	ARG	2.2
2	H	147	GLU	2.2
1	C	57	LYS	2.2
2	H	10	LEU	2.1
2	H	86	ARG	2.1
3	L	165	LEU	2.1
3	L	82	GLU	2.1
3	L	64	ILE	2.1
3	L	255	TRP	2.1
3	L	57	PRO	2.1
2	H	257	LEU	2.1
3	L	219	VAL	2.0
2	H	6	LEU	2.0
1	C	68	ALA	2.0
3	L	224	ILE	2.0
4	M	26	ASN	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	0.68	0.21	33,40,56,58	0

6.3 Carbohydrates [i](#)

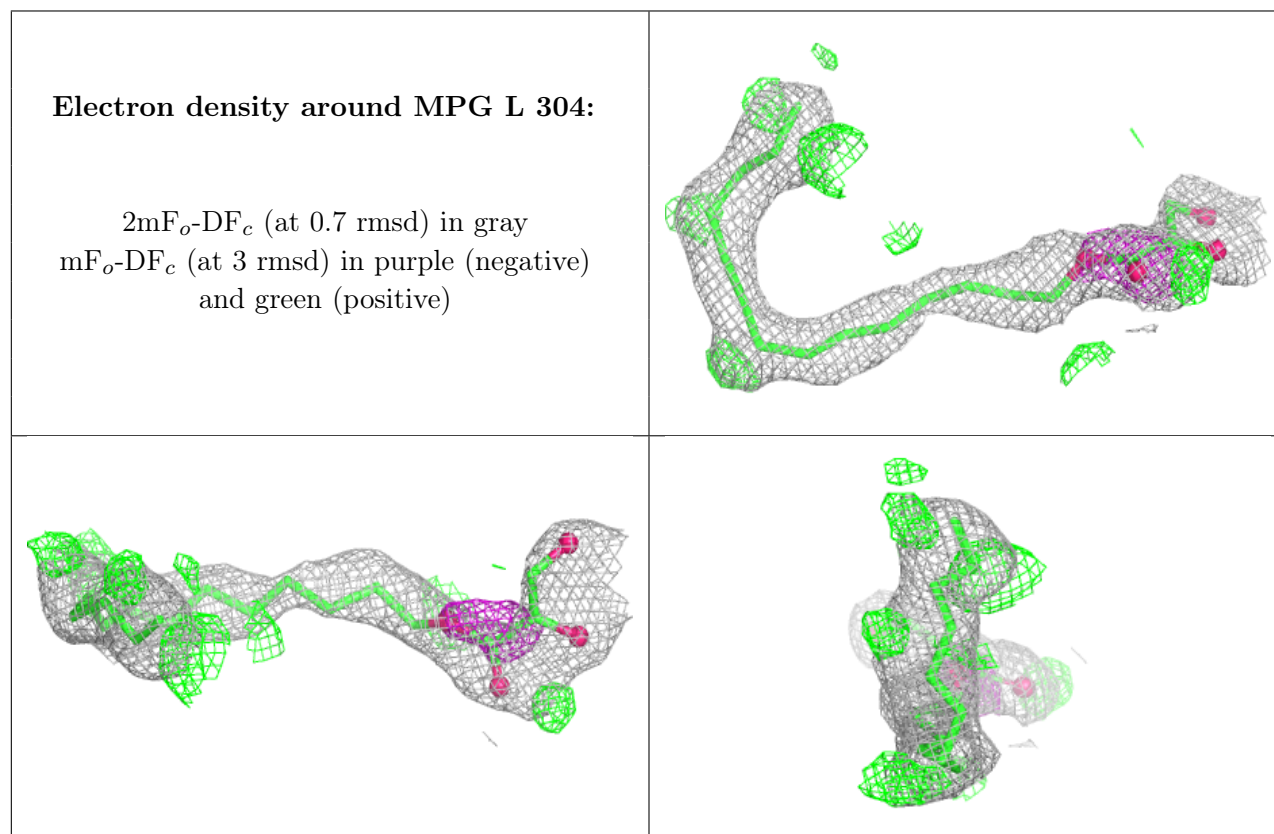
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

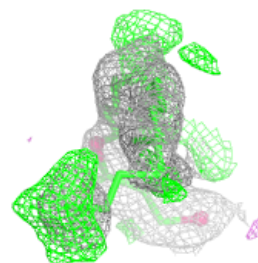
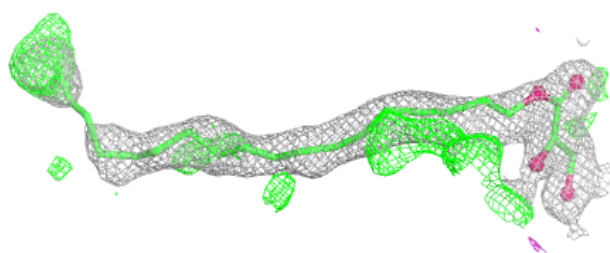
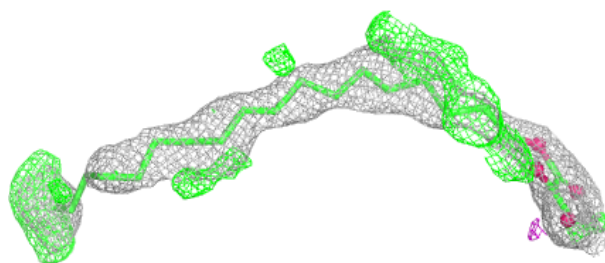
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	MPG	L	304	21/25	0.77	0.23	56,63,69,71	0
8	MPG	L	305	25/25	0.79	0.28	36,47,54,54	25
8	MPG	M	406	17/25	0.82	0.25	62,64,65,65	0
11	NS5	M	405	40/40	0.82	0.24	42,62,77,77	0
10	MQ7	M	404	48/48	0.94	0.12	28,34,53,57	0
7	BPB	M	403	61/65	0.95	0.10	17,28,59,62	0
6	BCB	M	401	65/66	0.95	0.12	23,27,73,75	0
7	BPB	L	303	65/65	0.95	0.10	22,31,37,40	0
6	BCB	L	301	66/66	0.96	0.09	19,26,38,42	0
6	BCB	M	402	66/66	0.96	0.09	20,26,37,39	0
6	BCB	L	302	66/66	0.96	0.10	22,27,51,56	0
5	HEC	C	404	43/43	0.97	0.09	20,27,36,48	0
5	HEC	C	401	43/43	0.97	0.10	28,32,37,41	0
5	HEC	C	402	43/43	0.97	0.09	27,30,37,38	0
5	HEC	C	403	43/43	0.98	0.08	21,25,27,29	0
9	FE2	L	306	1/1	1.00	0.08	27,27,27,27	0

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

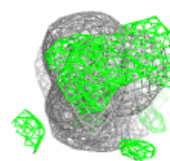
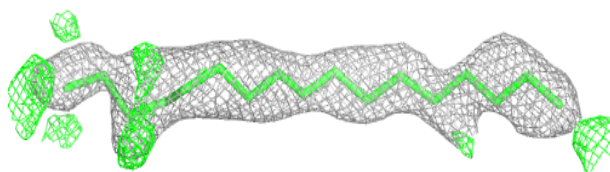
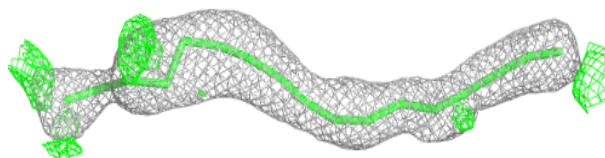


Electron density around MPG L 305:

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

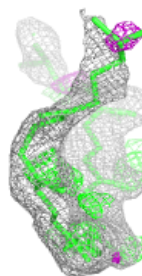
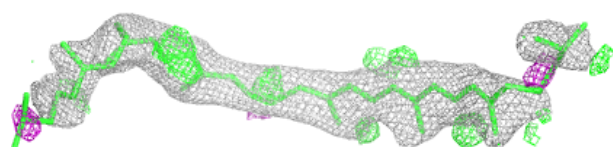
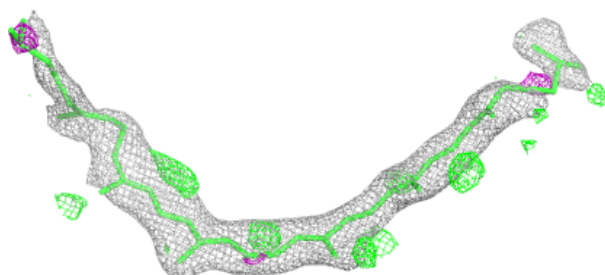
**Electron density around MPG M 406:**

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

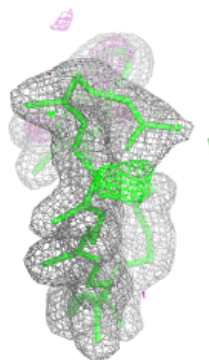
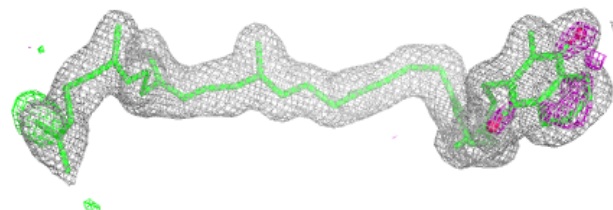
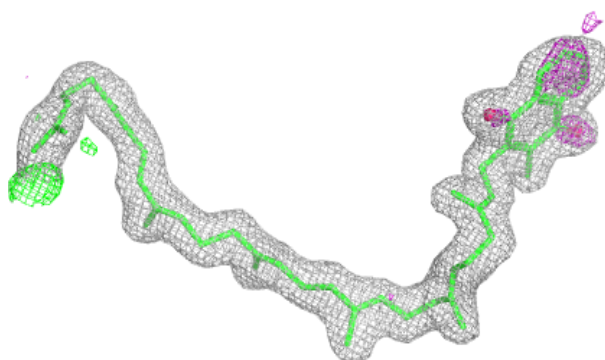


Electron density around NS5 M 405:

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

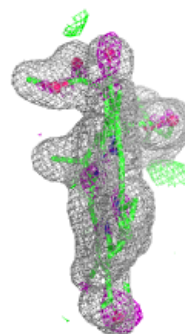
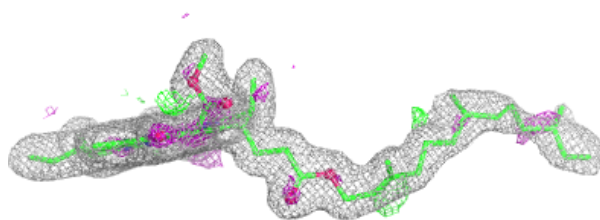
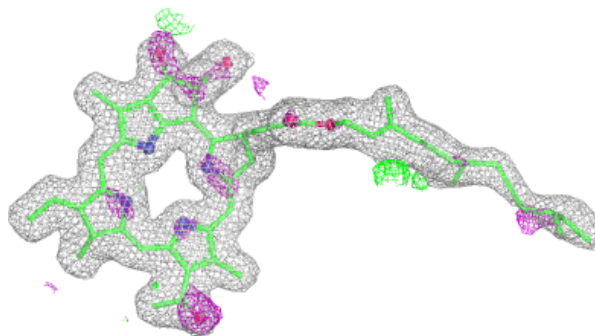
**Electron density around MQ7 M 404:**

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

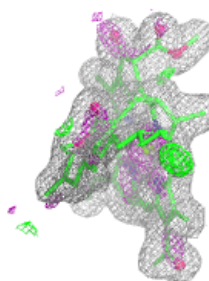
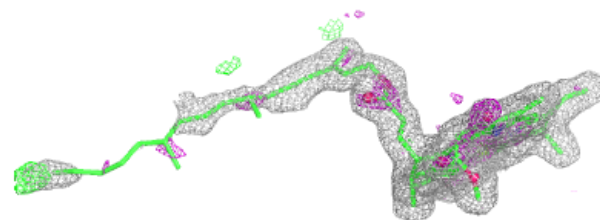
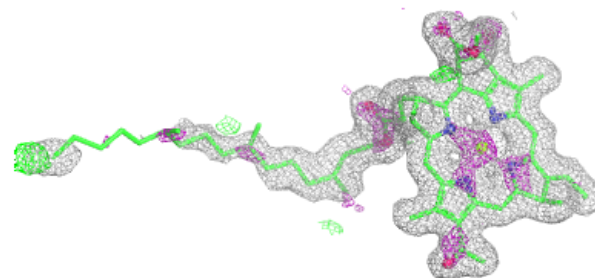


Electron density around BPB M 403:

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

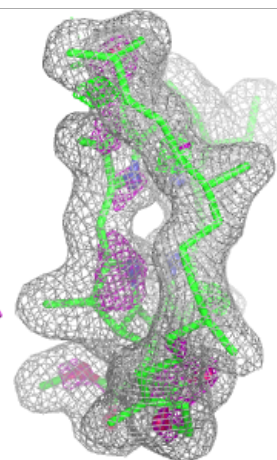
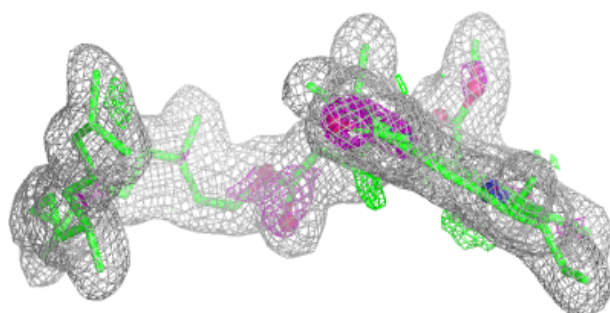
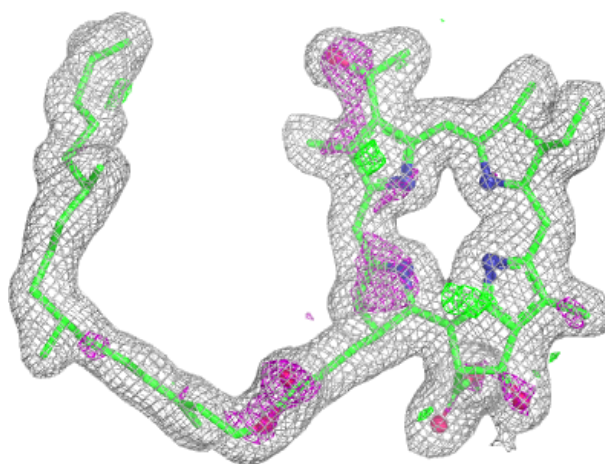
**Electron density around BCB M 401:**

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



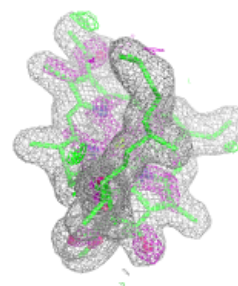
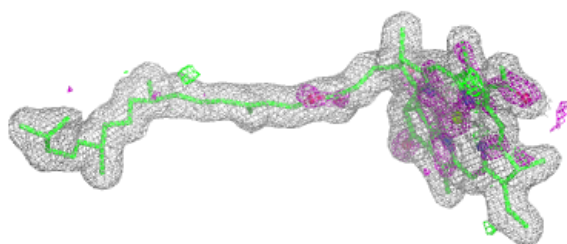
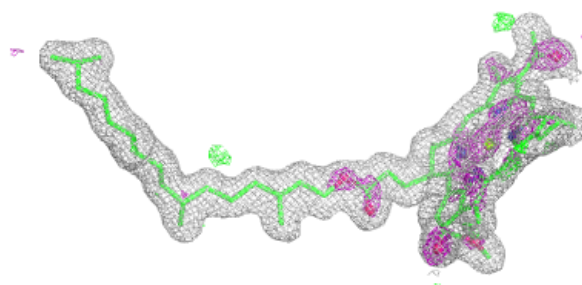
Electron density around BPB L 303:

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

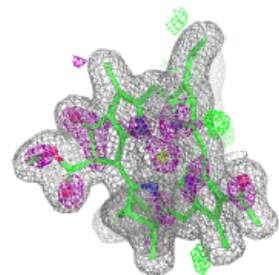
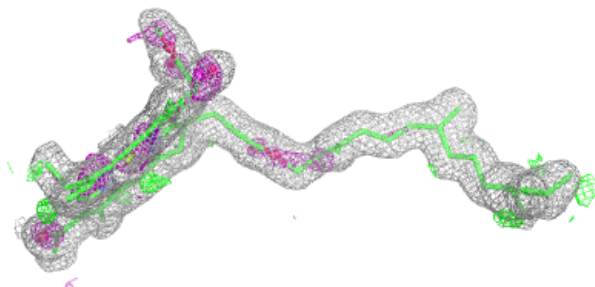
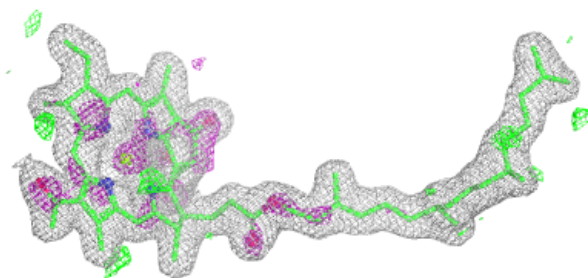


Electron density around BCB L 301:

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and green (positive)

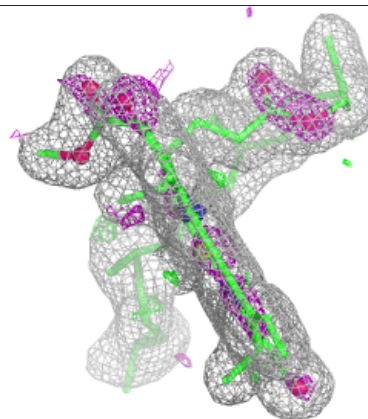
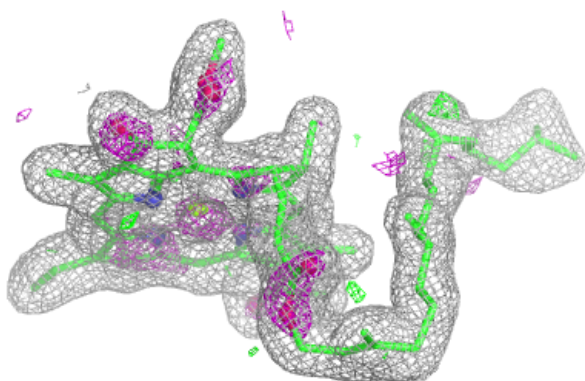
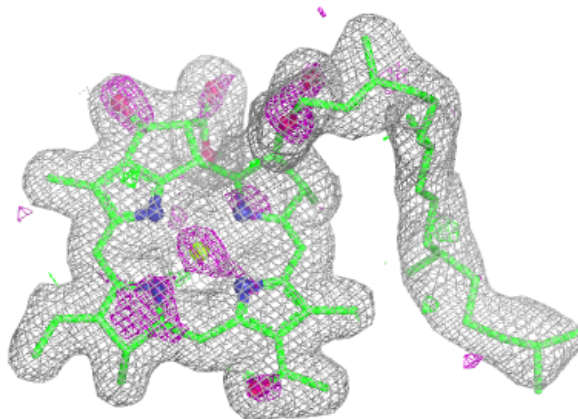
**Electron density around BCB M 402:**

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



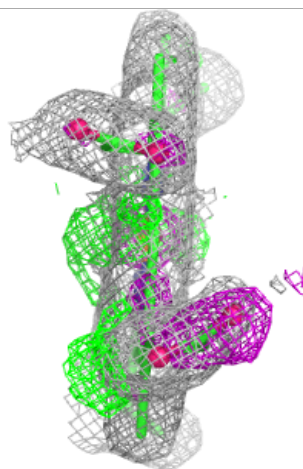
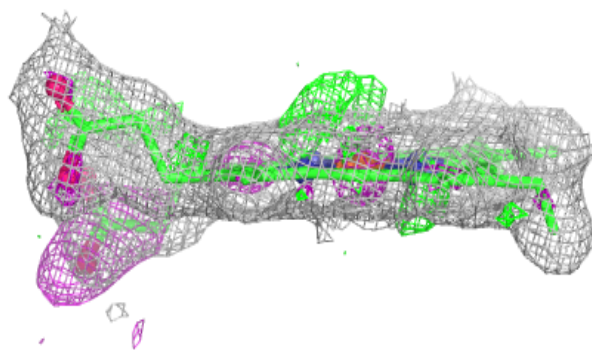
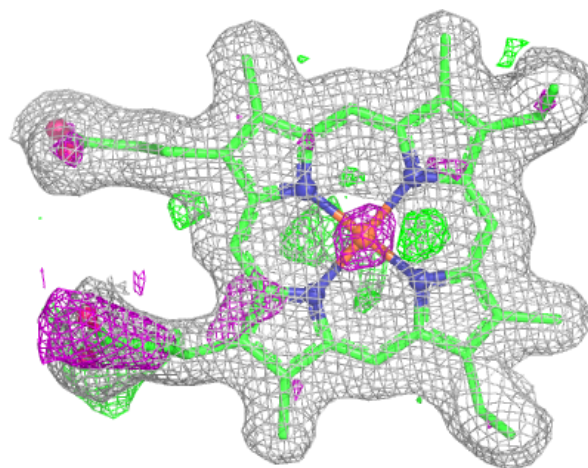
Electron density around BCB L 302:

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



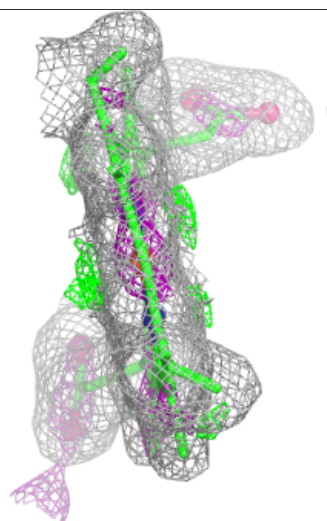
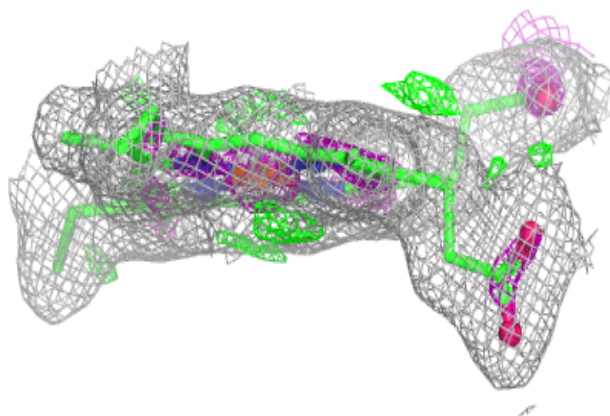
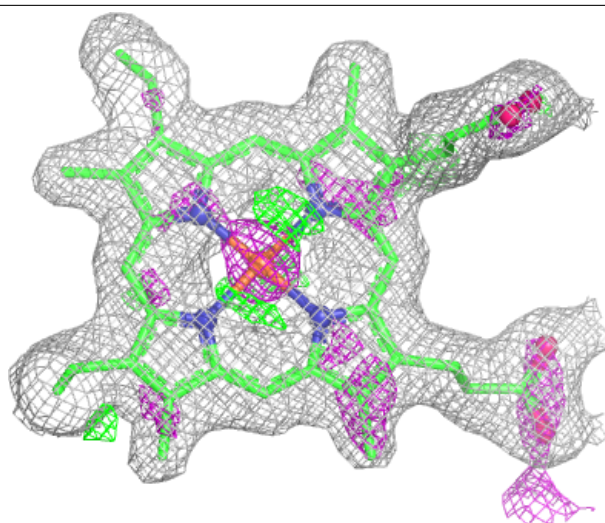
Electron density around HEC C 404:

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



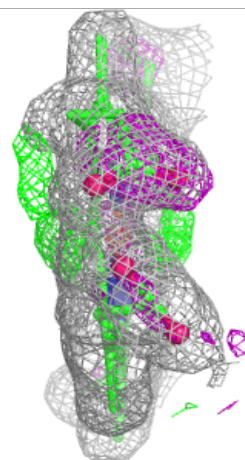
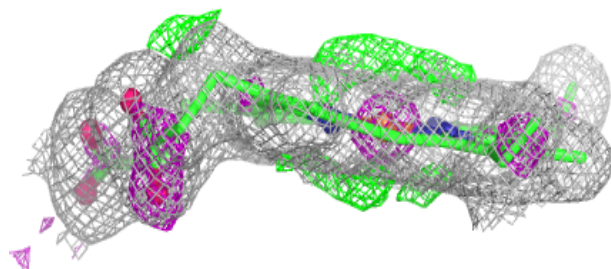
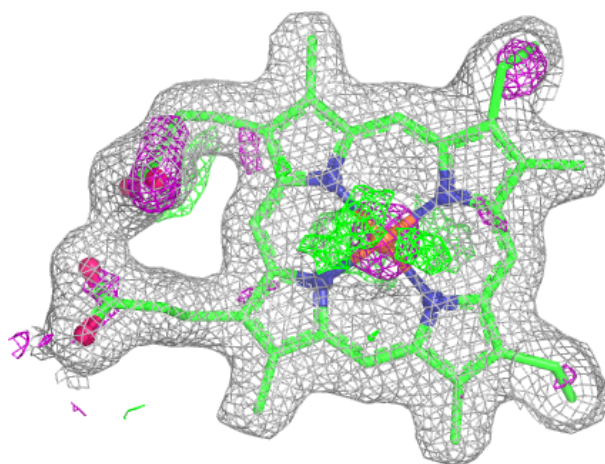
Electron density around HEC C 401:

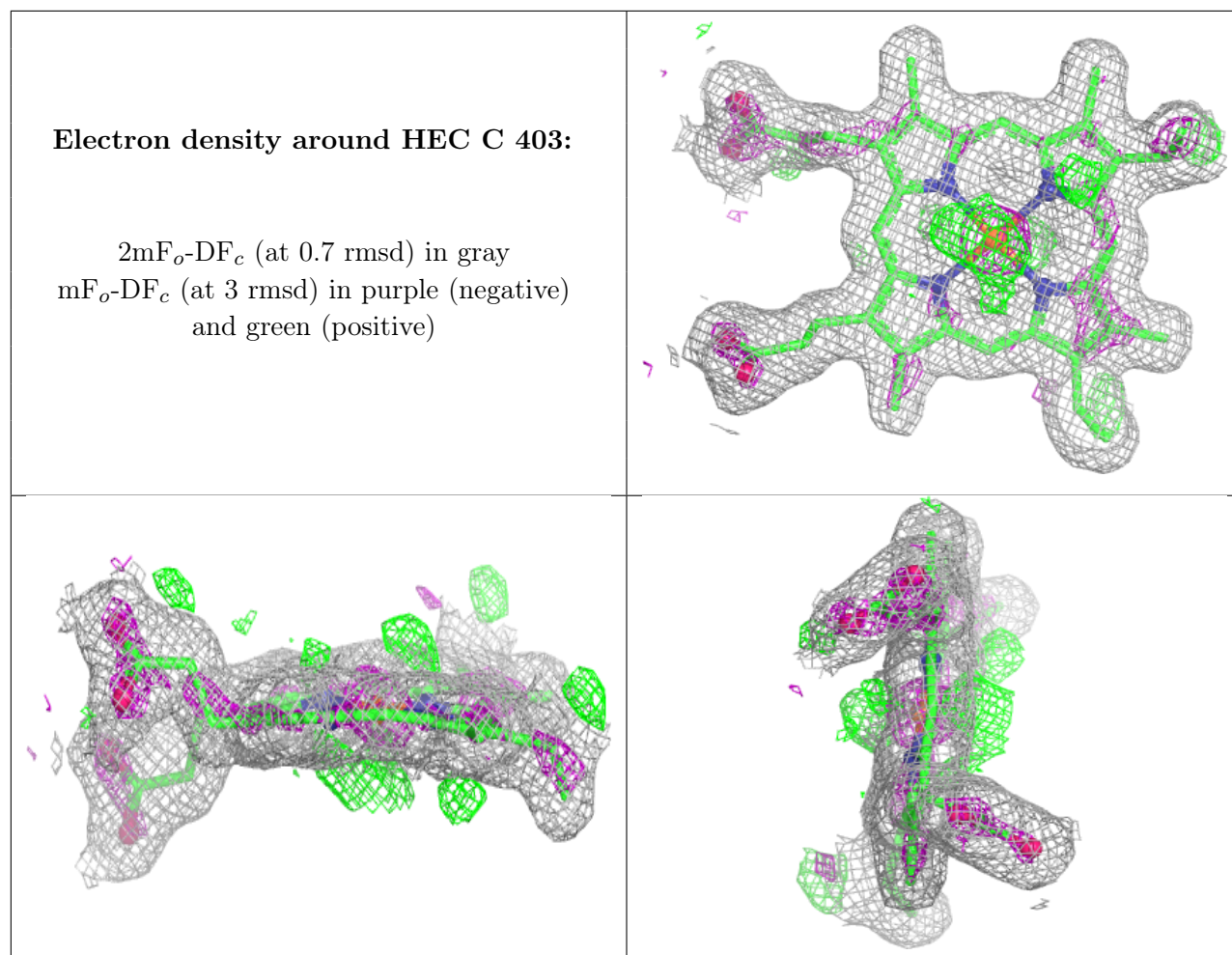
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC C 402:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.