



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 05:10 PM EDT

PDB ID : 3G7F / pdb_00003g7f
Title : Crystal structure of Blastochloris viridis heterodimer mutant reaction center
Authors : Ponomarenko, N.S.; Li, L.; Tereshko, V.; Ismagilov, R.F.; Norris Jr., J.R.
Deposited on : 2009-02-09
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

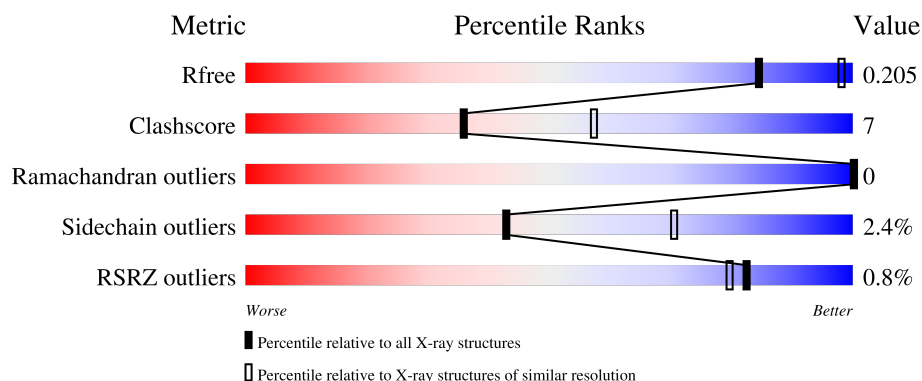
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	
2	H	258	
3	L	273	
4	M	323	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	BPB	M	401	-	-	X	-
5	HEC	C	401	X	-	-	-
5	HEC	C	402	X	-	-	-
5	HEC	C	403	X	-	-	-
5	HEC	C	404	X	-	-	-
6	SO4	C	815	-	-	-	X
6	SO4	C	817	-	-	-	X
6	SO4	L	814	-	-	-	X
6	SO4	M	816	-	-	-	X
6	SO4	M	818	-	-	-	X
6	SO4	M	819	-	-	-	X
7	HTO	L	708	-	-	-	X
7	HTO	L	709	-	-	-	X
9	BCB	L	400	X	-	-	-
9	BCB	L	401	X	-	-	-
9	BCB	M	400	X	-	-	-

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 10922 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
			2598	1637	465	478	18			

- Molecule 2 is a protein called Photosynthetic reaction center H subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	250	Total	C	N	O	S	0	0	0
			1956	1250	335	369	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	216	ASP	GLU	variant	UNP P06008
H	256	ALA	SER	variant	UNP P06008

- Molecule 3 is a protein called Photosynthetic reaction center L subunit.

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

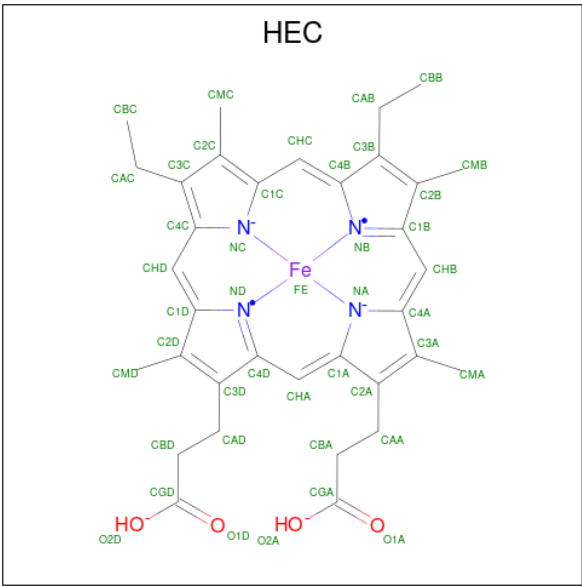
- Molecule 4 is a protein called Photosynthetic reaction center M subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	323	Total	C	N	O	S	0	2	0
			2557	1704	417	424	12			

There is a discrepancy between the modelled and reference sequences:

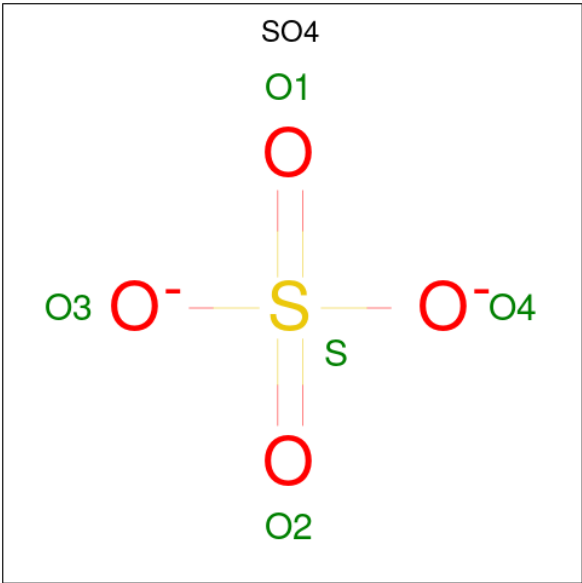
Chain	Residue	Modelled	Actual	Comment	Reference
M	200	LEU	HIS	variant	UNP P06010

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



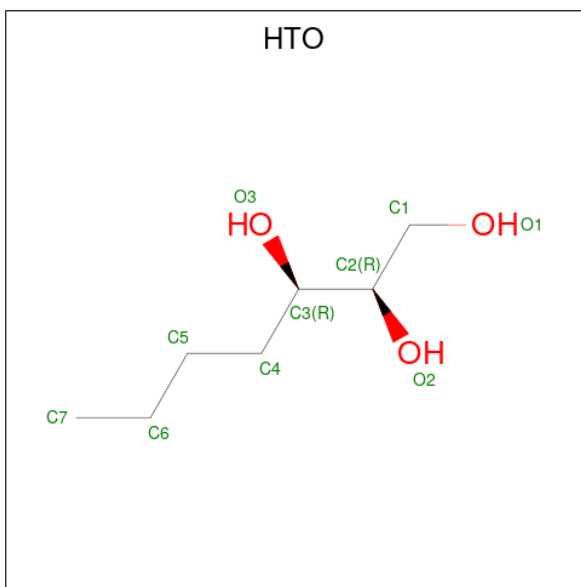
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



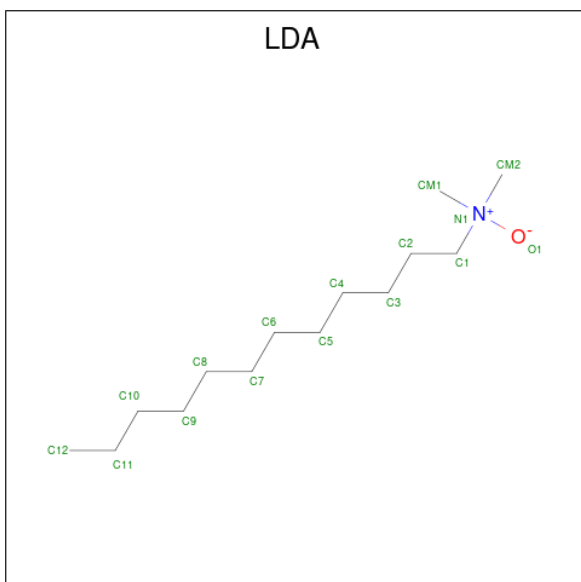
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	H	1	Total O S 5 4 1	0	0
6	H	1	Total O S 5 4 1	0	0
6	H	1	Total O S 5 4 1	0	0
6	H	1	Total O S 5 4 1	0	0
6	L	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
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 HEPTANE-1,2,3-TRIOL (CCD ID: HTO) (formula: C₇H₁₆O₃).



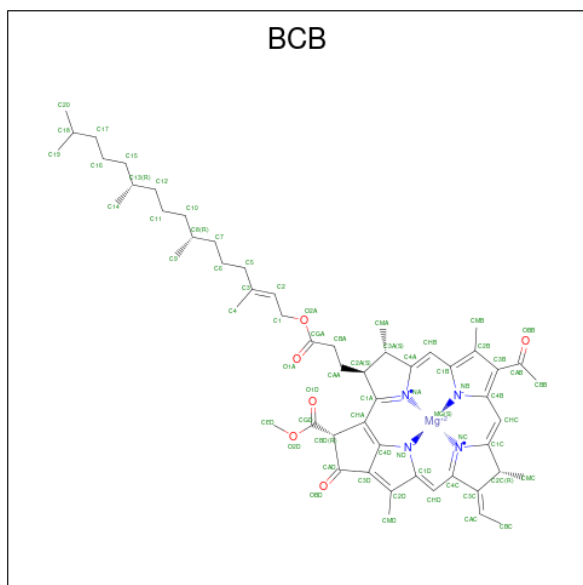
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			10	7	3		
7	C	1	Total	C	O	0	0
			10	7	3		
7	H	1	Total	C	O	0	0
			10	7	3		
7	L	1	Total	C	O	0	0
			10	7	3		
7	L	1	Total	C	O	0	0
			10	7	3		

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



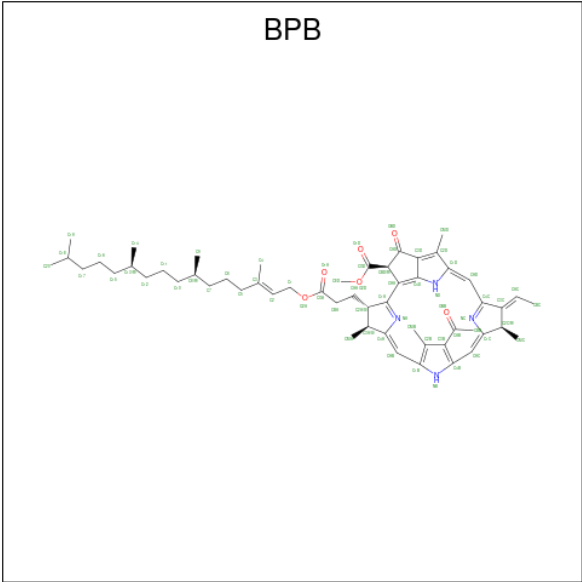
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	H	1	Total	C	N	O	0	0
			16	14	1	1		
8	H	1	Total	C	N	O	0	0
			16	14	1	1		
8	M	1	Total	C	N	O	0	0
			16	14	1	1		
8	M	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 9 is BACTERIOCHLOROPHYLL B (CCD ID: BCB) (formula: $C_{55}H_{72}MgN_4O_6$).



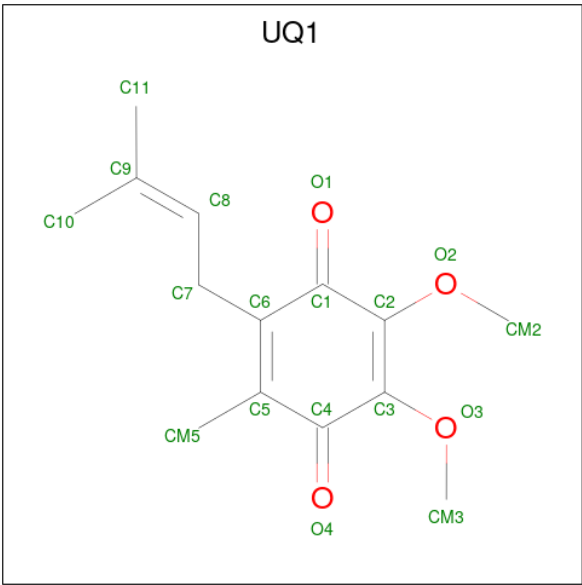
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- Molecule 10 is BACTERIOPHEOPHYTIN B (CCD ID: BPB) (formula: $C_{55}H_{74}N_4O_6$).



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

- Molecule 11 is UBIQUINONE-1 (CCD ID: UQ1) (formula: C₁₄H₁₈O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	L	1	Total	C	O	0	0
			18	14	4		

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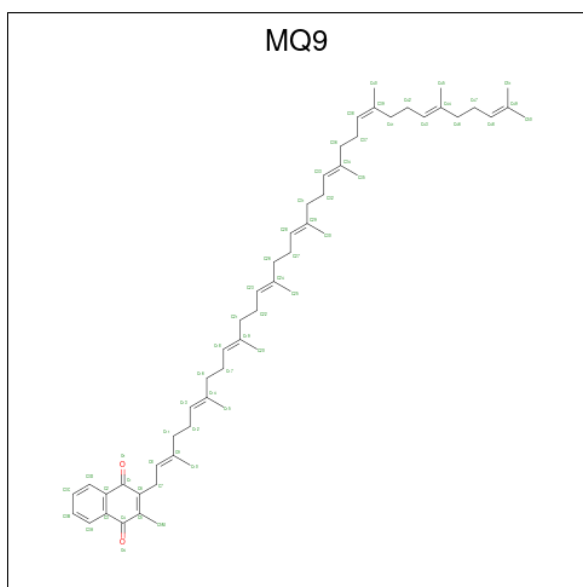
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	M	1	Total	C	O	0	0
			18	14	4		

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

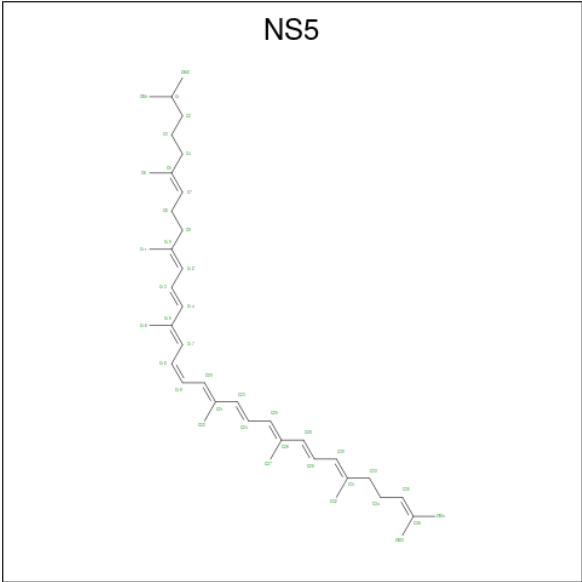
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	M	1	Total	Fe	0	0
			1	1		

- Molecule 13 is MENAQUINONE-9 (CCD ID: MQ9) (formula: C₅₆H₈₀O₂).



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

- Molecule 14 is 15-cis-1,2-dihydroneurosporene (CCD ID: NS5) (formula: C₄₀H₆₀).



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

- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	C	292	Total	O	0	0
			292	292		
15	H	172	Total	O	1	0
			172	172		
15	L	94	Total	O	0	0
			94	94		
15	M	172	Total	O	2	0
			172	172		

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.

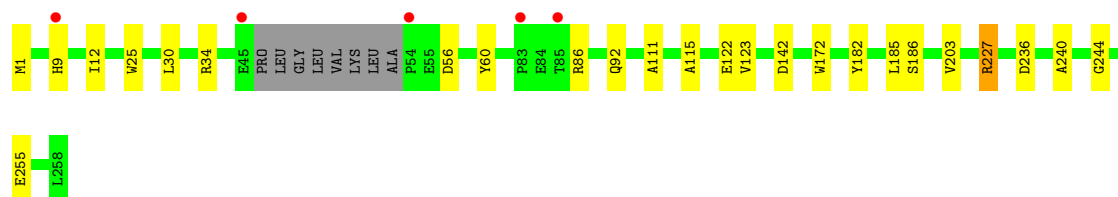
- Molecule 1: Photosynthetic reaction center cytochrome c subunit

Chain C: 



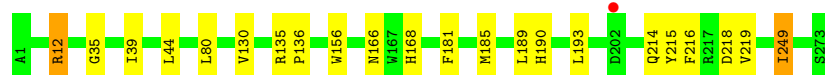
- Molecule 2: Photosynthetic reaction center H subunit

Chain H: 



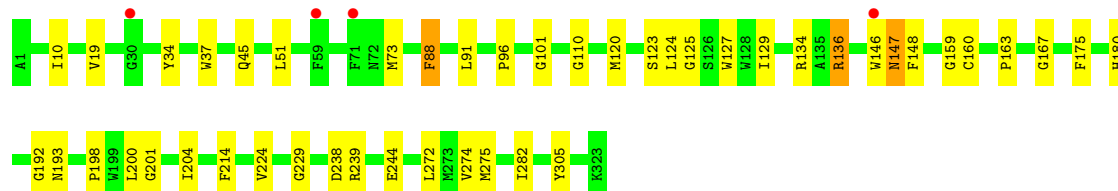
- Molecule 3: Photosynthetic reaction center L subunit

Chain L: 



- Molecule 4: Photosynthetic reaction center M subunit

Chain M: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	220.13Å 220.13Å 112.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 20.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.2 (20.00-2.50) 99.1 (20.00-2.50)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.92 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.176 , 0.206 0.175 , 0.205	Depositor DCC
R_{free} test set	4765 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	34.3	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 49.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10922	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.65% 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: FE2, MQ9, HTO, UQ1, BCB, BPB, FME, HEC, NS5, SO4, 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	0.74	0/2665	0.88	1/3633 (0.0%)
2	H	0.76	0/1991	0.87	1/2718 (0.0%)
3	L	0.77	0/2267	0.90	2/3095 (0.1%)
4	M	0.76	0/2670	0.89	1/3651 (0.0%)
All	All	0.76	0/9593	0.88	5/13097 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	12	ARG	N-CA-CB	-5.39	101.92	110.06
1	C	55	VAL	N-CA-C	5.38	115.59	110.53
4	M	88	PHE	N-CA-C	5.34	117.52	111.11
2	H	12	ILE	N-CA-C	5.09	115.31	110.42
3	L	12	ARG	CG-CD-NE	-5.08	100.82	112.00

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	2598	0	2568	18	0
2	H	1956	0	1944	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	2172	0	2097	21	0
4	M	2557	0	2462	48	0
5	C	172	0	120	3	0
6	C	35	0	0	1	0
6	H	20	0	0	0	0
6	L	5	0	0	0	0
6	M	35	0	0	1	0
7	C	20	0	32	2	0
7	H	10	0	16	1	0
7	L	20	0	32	0	0
8	H	32	0	62	0	0
8	M	32	0	62	3	0
9	L	132	0	144	22	0
9	M	66	0	72	6	0
10	L	65	0	74	5	0
10	M	130	0	148	36	0
11	L	18	0	18	4	0
11	M	18	0	18	0	0
12	M	1	0	0	0	0
13	M	58	0	80	4	0
14	M	40	0	60	4	0
15	C	292	0	0	2	0
15	H	172	0	0	4	0
15	L	94	0	0	0	0
15	M	172	0	0	3	0
All	All	10922	0	10009	147	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 7.

All (147) 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)
10:M:401:BPB:H4A	10:M:402:BPB:CBB	1.98	0.92
10:M:401:BPB:H4A	10:M:402:BPB:HBBB	1.53	0.90
10:M:402:BPB:CBB	10:M:402:BPB:HHC	2.04	0.88
4:M:204:ILE:HG12	10:M:401:BPB:CHB	2.03	0.87
4:M:120:MET:HE3	4:M:175:PHE:HE1	1.42	0.83
4:M:200:LEU:HD13	4:M:204:ILE:HD12	1.60	0.81
9:M:400:BCB:HHC	9:M:400:BCB:CBB	2.11	0.81
10:M:402:BPB:HBBB	10:M:402:BPB:HHC	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:86:ARG:NH1	15:H:569:HOH:O	2.20	0.74
1:C:123:GLN:H	1:C:123:GLN:HE21	1.35	0.73
10:M:401:BPB:H4A	10:M:402:BPB:CAB	2.19	0.72
9:M:400:BCB:HBB2	14:M:600:NS5:H223	1.76	0.67
3:L:39:ILE:HD12	13:M:501:MQ9:H43	1.76	0.67
4:M:120:MET:CE	4:M:175:PHE:HE1	2.07	0.66
9:M:400:BCB:HHC	9:M:400:BCB:HBB2	1.76	0.66
3:L:168:HIS:CE1	9:L:400:BCB:HMC2	2.31	0.66
4:M:127:TRP:CD1	10:M:402:BPB:HBAA	2.33	0.64
4:M:120:MET:HE3	4:M:175:PHE:CE1	2.31	0.64
4:M:101:GLY:O	15:M:797:HOH:O	2.15	0.63
2:H:122:GLU:OE2	15:H:605:HOH:O	2.16	0.63
3:L:214:GLN:NE2	4:M:19:VAL:H	1.97	0.62
3:L:193:LEU:HD23	11:L:502:UQ1:HM32	1.82	0.62
1:C:221:ARG:NE	1:C:225:ASP:OD2	2.33	0.62
3:L:181:PHE:HB3	10:M:402:BPB:HBBA	1.82	0.62
4:M:200:LEU:HD13	4:M:204:ILE:CD1	2.30	0.62
1:C:123:GLN:H	1:C:123:GLN:NE2	1.98	0.61
10:M:402:BPB:HHC	10:M:402:BPB:HBBA	1.81	0.61
9:L:400:BCB:HMB3	9:L:400:BCB:CBB	2.31	0.61
9:L:400:BCB:H193	13:M:501:MQ9:H252	1.83	0.59
4:M:127:TRP:CD1	10:M:402:BPB:CBA	2.85	0.59
9:L:401:BCB:HMB1	9:L:401:BCB:CBB	2.33	0.58
3:L:185:MET:HE2	3:L:189:LEU:HD11	1.84	0.58
3:L:181:PHE:CD2	10:M:402:BPB:HBB	2.39	0.57
10:M:401:BPB:C4	10:M:402:BPB:HBBB	2.31	0.57
9:L:401:BCB:HMB1	9:L:401:BCB:HBB3	1.86	0.57
10:M:401:BPB:CBB	10:M:401:BPB:HMBB	2.35	0.56
10:M:401:BPB:HMBB	10:M:401:BPB:HBBA	1.88	0.56
9:L:400:BCB:CHB	10:M:401:BPB:CMB	2.84	0.55
4:M:204:ILE:CG1	10:M:401:BPB:CHB	2.82	0.55
9:L:400:BCB:CHB	10:M:401:BPB:HMBB	2.37	0.55
3:L:35:GLY:O	3:L:39:ILE:HG12	2.07	0.55
9:M:400:BCB:HHC	9:M:400:BCB:HBB3	1.87	0.55
1:C:314:LYS:HG2	5:C:404:HEC:HBD2	1.88	0.54
1:C:80:TRP:CD1	1:C:133:TYR:HB2	2.43	0.54
4:M:73:MET:HE1	4:M:88:PHE:CE1	2.42	0.54
9:L:400:BCB:HMB3	9:L:400:BCB:HBB2	1.88	0.54
2:H:227:ARG:NE	2:H:227:ARG:H	2.06	0.53
4:M:200:LEU:CD1	4:M:204:ILE:CD1	2.87	0.53
1:C:18:SER:HB2	3:L:156:TRP:CD1	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:402:BPB:CBB	10:L:402:BPB:HMBB	2.38	0.52
1:C:102:TYR:CG	1:C:103:PRO:HD3	2.44	0.52
4:M:200:LEU:CD1	4:M:204:ILE:HD12	2.36	0.52
1:C:217:GLY:HA2	4:M:167:GLY:O	2.09	0.52
9:M:400:BCB:CBB	14:M:600:NS5:H223	2.38	0.51
1:C:162:HIS:N	6:C:813:SO4:O3	2.42	0.51
2:H:30:LEU:O	2:H:34:ARG:HD2	2.11	0.51
4:M:146:TRP:HZ2	15:M:829:HOH:O	1.92	0.51
2:H:255:GLU:CD	3:L:12:ARG:HH22	2.18	0.51
2:H:115:ALA:HB2	2:H:244:GLY:HA3	1.93	0.51
9:L:401:BCB:OBB	9:L:401:BCB:HHC	2.11	0.50
3:L:166:ASN:OD1	3:L:168:HIS:HB2	2.12	0.50
10:M:402:BPB:CBB	10:M:402:BPB:CHC	2.82	0.50
9:L:400:BCB:HBD	9:L:400:BCB:HAA1	1.94	0.50
3:L:190:HIS:HD1	11:L:502:UQ1:HM33	1.77	0.49
2:H:92:GLN:NE2	15:H:637:HOH:O	2.45	0.49
9:L:400:BCB:H151	10:L:402:BPB:H5A	1.93	0.49
4:M:204:ILE:HG12	10:M:401:BPB:C1B	2.43	0.49
4:M:148:PHE:HE1	10:M:401:BPB:H9B	1.78	0.49
1:C:205:PRO:HB3	7:C:706:HTO:H12	1.93	0.49
2:H:142:ASP:OD1	15:H:551:HOH:O	2.20	0.49
11:L:502:UQ1:HM33	11:L:502:UQ1:O4	2.12	0.49
7:C:707:HTO:H42	15:C:764:HOH:O	2.13	0.49
10:L:402:BPB:HMBB	10:L:402:BPB:HBBA	1.94	0.49
9:L:401:BCB:HMD2	10:M:401:BPB:HBBB	1.95	0.48
10:M:401:BPB:NC	10:M:401:BPB:ND	2.59	0.48
4:M:136:ARG:NH1	15:M:853:HOH:O	2.41	0.48
4:M:282:ILE:HD11	10:M:401:BPB:OBD	2.13	0.48
2:H:25:TRP:HA	2:H:25:TRP:CE3	2.49	0.48
3:L:130:VAL:HG13	3:L:249:ILE:HG12	1.95	0.48
3:L:214:GLN:HE21	4:M:19:VAL:H	1.62	0.48
4:M:160:CYS:C	4:M:163:PRO:HD2	2.38	0.47
3:L:39:ILE:HD11	13:M:501:MQ9:H372	1.97	0.47
4:M:274:VAL:HG12	4:M:275:MET:CE	2.44	0.47
10:M:401:BPB:H16	10:M:401:BPB:H20A	1.75	0.47
13:M:501:MQ9:H403	13:M:501:MQ9:H421	1.75	0.47
10:L:402:BPB:OBB	10:L:402:BPB:HHC	2.15	0.47
4:M:96:PRO:HD3	4:M:110:GLY:HA3	1.96	0.47
4:M:198:PRO:HA	8:M:702:LDA:H112	1.97	0.47
10:M:402:BPB:H9	10:M:402:BPB:H11	1.72	0.46
4:M:147:ASN:C	4:M:147:ASN:HD22	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:127:TRP:CD1	10:M:402:BPB:HBA	2.51	0.46
14:M:600:NS5:H18	14:M:600:NS5:H161	1.81	0.45
4:M:239:ARG:HD3	4:M:244:GLU:HG2	1.99	0.45
8:M:704:LDA:HM11	8:M:704:LDA:H22	1.74	0.45
1:C:145:VAL:O	1:C:146:ARG:HD2	2.17	0.45
4:M:159:GLY:HA3	14:M:600:NS5:H272	1.99	0.45
10:M:402:BPB:CB	10:M:402:BPB:HMC	2.47	0.45
5:C:403:HEC:HBB3	5:C:403:HEC:CMB	2.47	0.45
11:L:502:UQ1:O4	11:L:502:UQ1:CM3	2.65	0.45
4:M:37:TRP:HD1	6:M:805:SO4:O2	1.99	0.45
2:H:56:ASP:HB3	2:H:60:TYR:CE2	2.52	0.44
9:M:400:BCB:CBB	9:M:400:BCB:CHC	2.86	0.44
2:H:172:TRP:HB2	2:H:182:TYR:HB2	1.99	0.44
1:C:188:ASP:OD2	1:C:191:THR:HG23	2.18	0.44
2:H:203:VAL:HG11	4:M:10:ILE:HD11	2.00	0.44
4:M:204:ILE:HD11	10:M:401:BPB:C1B	2.48	0.44
9:L:401:BCB:CBB	9:L:401:BCB:CMB	2.96	0.43
9:L:400:BCB:H203	9:L:400:BCB:H161	1.64	0.43
1:C:105:VAL:HG13	15:C:510:HOH:O	2.17	0.43
1:C:17:LEU:HD21	4:M:305:TYR:CZ	2.54	0.43
5:C:403:HEC:HBB3	5:C:403:HEC:HMB1	2.00	0.43
4:M:192:GLY:O	4:M:193:ASN:HB3	2.19	0.43
4:M:34:TYR:CE2	4:M:45:GLN:HB2	2.53	0.43
9:L:401:BCB:HBA1	9:L:401:BCB:C4A	2.48	0.43
10:M:401:BPB:H14	10:M:401:BPB:H16A	1.64	0.43
2:H:86:ARG:NH2	2:H:111:ALA:O	2.52	0.43
4:M:224:VAL:HG23	4:M:229:GLY:HA3	2.00	0.42
4:M:148:PHE:HE1	10:M:401:BPB:C9	2.32	0.42
4:M:200:LEU:HD11	4:M:204:ILE:HD11	2.01	0.42
3:L:193:LEU:HD22	3:L:216:PHE:HE2	1.84	0.42
9:L:400:BCB:CBB	9:L:400:BCB:CMB	2.97	0.42
9:L:400:BCB:CAD	9:L:401:BCB:HBC1	2.49	0.42
3:L:218:ASP:HB3	4:M:134:ARG:HD2	2.01	0.42
4:M:201:GLY:HA3	8:M:702:LDA:H122	2.02	0.42
9:L:400:BCB:C1B	10:M:401:BPB:C2B	2.97	0.42
2:H:115:ALA:HA	2:H:240:ALA:O	2.20	0.42
3:L:135:ARG:HB3	3:L:136:PRO:HD3	2.02	0.42
9:L:400:BCB:OBB	9:L:400:BCB:HHC	2.19	0.42
9:L:400:BCB:HMB3	10:M:401:BPB:CHB	2.51	0.41
9:L:400:BCB:CMB	10:M:401:BPB:CHB	2.98	0.41
1:C:146:ARG:HD2	1:C:146:ARG:HA	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:402:BPB:NC	10:L:402:BPB:ND	2.68	0.41
1:C:104:TYR:CD1	1:C:104:TYR:C	2.99	0.41
4:M:123:SER:OG	10:M:402:BPB:H1	2.21	0.41
4:M:274:VAL:HG12	4:M:275:MET:HE3	2.02	0.41
7:H:705:HTO:H73	4:M:238:ASP:HB2	2.02	0.41
4:M:275:MET:HA	4:M:275:MET:HE2	2.02	0.41
9:L:400:BCB:H2C	10:M:401:BPB:H43	2.03	0.41
1:C:309:HIS:O	1:C:310:GLN:C	2.64	0.40
3:L:215:TYR:O	3:L:219:VAL:HG23	2.21	0.40
10:M:401:BPB:CBB	10:M:401:BPB:CMB	2.99	0.40
3:L:214:GLN:HG2	4:M:19:VAL:HB	2.03	0.40
4:M:73:MET:HE3	4:M:91:LEU:HB2	2.04	0.40
4:M:146:TRP:CE3	4:M:146:TRP:HA	2.56	0.40
1:C:283:ALA:HB2	1:C:302:GLN:NE2	2.36	0.40
3:L:193:LEU:HD22	3:L:216:PHE:CE2	2.57	0.40
4:M:125:GLY:O	4:M:129:ILE:HG13	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	318 (96%)	12 (4%)	0	100	100
2	H	246/258 (95%)	240 (98%)	6 (2%)	0	100	100
3	L	272/273 (100%)	267 (98%)	5 (2%)	0	100	100
4	M	323/323 (100%)	314 (97%)	9 (3%)	0	100	100
All	All	1171/1190 (98%)	1139 (97%)	32 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	280/282 (99%)	273 (98%)	7 (2%)	42	69
2	H	204/211 (97%)	198 (97%)	6 (3%)	37	65
3	L	219/218 (100%)	216 (99%)	3 (1%)	59	81
4	M	251/249 (101%)	244 (97%)	7 (3%)	38	66
All	All	954/960 (99%)	931 (98%)	23 (2%)	43	70

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1	CYS
1	C	46	LYS
1	C	57	LYS
1	C	123	GLN
1	C	240	LEU
1	C	274	VAL
1	C	316	LEU
2	H	9	HIS
2	H	123	VAL
2	H	185	LEU
2	H	186	SER
2	H	227	ARG
2	H	236	ASP
3	L	44	LEU
3	L	80	LEU
3	L	249	ILE
4	M	51	LEU
4	M	124	LEU
4	M	136	ARG
4	M	147	ASN
4	M	180	HIS
4	M	214	PHE
4	M	272	LEU

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

Mol	Chain	Res	Type
1	C	123	GLN
1	C	206	GLN
2	H	58	GLN
2	H	102	GLN
2	H	220	ASN
2	H	225	GLN
3	L	55	GLN
3	L	158	ASN
3	L	214	GLN
4	M	147	ASN

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	0.83	0	8,9,11	3.01	1 (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
2	FME	H	1	2	-	3/7/9/11	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1	FME	CA-N-CN	-7.98	110.55	122.82

There are no chirality outliers.

All (3) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 43 ligands modelled in this entry, 1 is monoatomic - leaving 42 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	HTO	C	707	-	9,9,9	0.82	0	10,10,10	1.00	0
11	UQ1	M	503	-	18,18,18	2.39	2 (11%)	24,25,25	1.30	3 (12%)
5	HEC	C	402	1	50,50,50	1.35	6 (12%)	68,82,82	1.00	4 (5%)
6	SO4	C	809	-	4,4,4	0.25	0	6,6,6	0.17	0
5	HEC	C	403	1	50,50,50	1.45	8 (16%)	68,82,82	1.05	4 (5%)
8	LDA	M	704	-	13,15,15	2.11	2 (15%)	14,17,17	0.60	0
6	SO4	M	819	-	4,4,4	0.23	0	6,6,6	0.10	0
8	LDA	H	703	-	13,15,15	2.16	2 (15%)	14,17,17	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	SO4	M	805	-	4,4,4	0.21	0	6,6,6	0.30	0
6	SO4	L	814	-	4,4,4	0.23	0	6,6,6	0.08	0
9	BCB	L	401	3	68,74,74	1.48	6 (8%)	77,115,115	1.84	13 (16%)
6	SO4	C	813	-	4,4,4	0.28	0	6,6,6	0.47	0
6	SO4	H	807	-	4,4,4	0.22	0	6,6,6	0.24	0
6	SO4	H	806	-	4,4,4	0.27	0	6,6,6	0.28	0
5	HEC	C	401	1	50,50,50	1.35	6 (12%)	68,82,82	1.03	4 (5%)
6	SO4	C	808	-	4,4,4	0.35	0	6,6,6	0.37	0
6	SO4	M	818	-	4,4,4	0.24	0	6,6,6	0.08	0
7	HTO	C	706	-	9,9,9	0.45	0	10,10,10	0.64	0
10	BPB	M	401	-	57,70,70	2.03	12 (21%)	55,101,101	2.36	15 (27%)
7	HTO	H	705	-	9,9,9	0.42	0	10,10,10	0.87	0
8	LDA	M	702	-	13,15,15	2.10	2 (15%)	14,17,17	0.71	0
6	SO4	M	802	-	4,4,4	0.21	0	6,6,6	0.38	0
10	BPB	L	402	-	57,70,70	1.95	10 (17%)	55,101,101	2.06	11 (20%)
8	LDA	H	701	-	13,15,15	1.96	2 (15%)	14,17,17	0.74	0
6	SO4	C	811	-	4,4,4	0.24	0	6,6,6	0.21	0
9	BCB	M	400	4	68,74,74	1.64	7 (10%)	77,115,115	1.68	13 (16%)
11	UQ1	L	502	-	18,18,18	2.31	2 (11%)	24,25,25	1.22	2 (8%)
9	BCB	L	400	3	68,74,74	1.56	8 (11%)	77,115,115	1.94	15 (19%)
14	NS5	M	600	-	39,39,39	1.44	3 (7%)	46,46,46	1.98	12 (26%)
6	SO4	M	801	-	4,4,4	0.29	0	6,6,6	0.34	0
7	HTO	L	709	-	9,9,9	0.23	0	10,10,10	0.75	0
10	BPB	M	402	-	57,70,70	1.86	9 (15%)	55,101,101	2.16	11 (20%)
6	SO4	H	812	-	4,4,4	0.20	0	6,6,6	0.17	0
6	SO4	C	817	-	4,4,4	0.23	0	6,6,6	0.06	0
6	SO4	M	804	-	4,4,4	0.17	0	6,6,6	0.17	0
6	SO4	M	816	-	4,4,4	0.23	0	6,6,6	0.07	0
13	MQ9	M	501	-	59,59,59	1.85	18 (30%)	73,75,75	1.40	16 (21%)
6	SO4	C	815	-	4,4,4	0.23	0	6,6,6	0.07	0
6	SO4	C	810	-	4,4,4	0.22	0	6,6,6	0.20	0
5	HEC	C	404	1	50,50,50	1.23	5 (10%)	68,82,82	1.01	4 (5%)
6	SO4	H	803	-	4,4,4	0.23	0	6,6,6	0.23	0
7	HTO	L	708	-	9,9,9	0.23	0	10,10,10	0.79	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	HTO	C	707	-	-	7/10/10/10	-
11	UQ1	M	503	-	-	0/9/33/33	0/1/1/1
5	HEC	C	402	1	1/1/3/7	7/14/54/54	-
5	HEC	C	403	1	1/1/3/7	4/14/54/54	-
8	LDA	M	704	-	-	9/13/13/13	-
8	LDA	H	703	-	-	8/13/13/13	-
9	BCB	L	401	3	2/2/21/26	4/41/137/137	-
7	HTO	C	706	-	-	3/10/10/10	-
5	HEC	C	401	1	1/1/3/7	6/14/54/54	-
10	BPB	M	401	-	-	17/37/105/105	0/5/6/6
7	HTO	H	705	-	-	7/10/10/10	-
8	LDA	M	702	-	-	5/13/13/13	-
10	BPB	L	402	-	-	5/37/105/105	0/5/6/6
8	LDA	H	701	-	-	8/13/13/13	-
9	BCB	M	400	4	2/2/21/26	10/41/137/137	-
11	UQ1	L	502	-	-	2/9/33/33	0/1/1/1
9	BCB	L	400	3	3/3/21/26	10/41/137/137	-
14	NS5	M	600	-	-	10/43/43/43	-
7	HTO	L	709	-	-	6/10/10/10	-
10	BPB	M	402	-	-	17/37/105/105	0/5/6/6
13	MQ9	M	501	-	-	13/53/73/73	0/2/2/2
5	HEC	C	404	1	1/1/3/7	4/14/54/54	-
7	HTO	L	708	-	-	6/10/10/10	-

All (110) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	L	402	BPB	C1D-C2D	8.78	1.49	1.39
11	L	502	UQ1	C6-C5	8.46	1.50	1.35
11	M	503	UQ1	C6-C5	8.40	1.50	1.35
9	L	401	BCB	CAC-C3C	7.94	1.53	1.33
9	L	400	BCB	CAC-C3C	7.73	1.53	1.33
9	M	400	BCB	CAC-C3C	7.48	1.52	1.33
14	M	600	NS5	C35-C36	6.86	1.53	1.32
10	M	401	BPB	C1D-C2D	6.79	1.47	1.39
8	M	704	LDA	O1-N1	-6.74	1.25	1.42
10	M	402	BPB	C1D-C2D	6.47	1.46	1.39
8	M	702	LDA	O1-N1	-6.36	1.26	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	401	BPB	C1B-C2B	6.35	1.46	1.39
8	H	701	LDA	O1-N1	-5.98	1.27	1.42
8	H	703	LDA	O1-N1	-5.84	1.27	1.42
10	M	402	BPB	C1B-C2B	5.36	1.45	1.39
10	L	402	BPB	C1B-C2B	5.32	1.45	1.39
10	M	401	BPB	O2D-CGD	5.18	1.46	1.33
8	H	703	LDA	C1-N1	-5.08	1.46	1.51
10	M	401	BPB	C3D-C2D	-4.64	1.31	1.39
13	M	501	MQ9	C2-C1	-4.61	1.39	1.48
5	C	403	HEC	FE-NC	4.44	2.09	1.95
9	L	400	BCB	O2D-CGD	4.43	1.44	1.33
9	M	400	BCB	O2A-CGA	4.41	1.46	1.33
9	M	400	BCB	C2C-C3C	-4.24	1.46	1.51
5	C	402	HEC	FE-NC	4.22	2.09	1.95
10	M	402	BPB	O2D-CGD	4.20	1.43	1.33
10	L	402	BPB	O2D-CGD	4.17	1.43	1.33
11	M	503	UQ1	C3-C2	4.13	1.51	1.36
5	C	401	HEC	FE-ND	4.13	2.07	1.94
10	M	402	BPB	O2A-CGA	4.13	1.45	1.33
10	M	402	BPB	C3D-C4D	-4.12	1.35	1.41
9	L	401	BCB	O2A-CGA	4.09	1.45	1.33
9	M	400	BCB	MG-NA	4.01	2.15	2.06
9	L	400	BCB	O2A-CGA	3.99	1.45	1.33
10	M	401	BPB	O2A-CGA	3.99	1.45	1.33
13	M	501	MQ9	C3-C4	-3.97	1.40	1.48
5	C	403	HEC	FE-ND	3.96	2.07	1.94
8	M	702	LDA	C1-N1	-3.92	1.47	1.51
13	M	501	MQ9	C6-C5	3.86	1.42	1.35
9	M	400	BCB	O2D-CGD	3.84	1.42	1.33
10	L	402	BPB	O2A-CGA	3.72	1.44	1.33
13	M	501	MQ9	C8-C9	3.67	1.41	1.33
10	M	401	BPB	C3D-C4D	-3.65	1.36	1.41
8	H	701	LDA	C1-N1	-3.61	1.47	1.51
11	L	502	UQ1	C3-C2	3.55	1.49	1.36
10	L	402	BPB	C3A-C2A	-3.52	1.51	1.54
10	L	402	BPB	C3D-C4D	-3.50	1.36	1.41
9	L	401	BCB	MG-NA	3.39	2.14	2.06
13	M	501	MQ9	C5-C4	-3.36	1.39	1.47
10	M	402	BPB	C2-C3	3.36	1.40	1.33
10	L	402	BPB	C3D-C2D	-3.36	1.33	1.39
8	M	704	LDA	C1-N1	-3.34	1.48	1.51
5	C	401	HEC	FE-NB	3.34	2.05	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	401	BPB	C3A-C2A	-3.33	1.51	1.54
5	C	404	HEC	FE-NC	3.27	2.05	1.95
9	L	401	BCB	O2D-CGD	3.24	1.41	1.33
10	M	402	BPB	C1D-ND	3.24	1.44	1.38
10	M	401	BPB	C1D-ND	3.23	1.44	1.38
13	M	501	MQ9	C28-C29	3.20	1.40	1.33
5	C	404	HEC	FE-NB	3.13	2.04	1.94
13	M	501	MQ9	C13-C14	3.13	1.40	1.33
10	L	402	BPB	C1D-ND	3.11	1.44	1.38
13	M	501	MQ9	C38-C39	3.10	1.40	1.33
5	C	401	HEC	FE-NC	3.10	2.05	1.95
10	M	402	BPB	C3D-C2D	-3.08	1.34	1.39
10	M	401	BPB	C3B-C4B	3.06	1.46	1.41
13	M	501	MQ9	C33-C34	3.05	1.40	1.33
13	M	501	MQ9	C7-C8	-3.03	1.45	1.50
5	C	402	HEC	FE-NA	3.01	2.05	1.95
9	L	400	BCB	C2-C3	2.94	1.39	1.33
5	C	404	HEC	FE-NA	2.92	2.04	1.95
13	M	501	MQ9	C43-C44	2.88	1.39	1.33
9	M	400	BCB	C2-C3	2.84	1.39	1.33
5	C	402	HEC	FE-NB	2.82	2.03	1.94
10	L	402	BPB	C2-C3	2.80	1.39	1.33
13	M	501	MQ9	C23-C24	2.80	1.39	1.33
13	M	501	MQ9	C18-C19	2.74	1.39	1.33
5	C	402	HEC	CAC-C3C	2.70	1.58	1.51
5	C	402	HEC	FE-ND	2.69	2.03	1.94
9	L	400	BCB	MG-ND	-2.66	2.00	2.05
5	C	401	HEC	FE-NA	2.66	2.03	1.95
9	L	401	BCB	C2-C3	2.59	1.39	1.33
9	L	400	BCB	C3B-C4B	2.57	1.46	1.41
5	C	403	HEC	CBA-CGA	2.54	1.56	1.50
10	M	402	BPB	C3A-C2A	-2.51	1.52	1.54
14	M	600	NS5	C4-C5	2.49	1.56	1.51
13	M	501	MQ9	C6-C1	-2.48	1.41	1.47
10	M	401	BPB	C1-C2	-2.40	1.42	1.49
9	M	400	BCB	C4C-C3C	2.39	1.49	1.44
5	C	403	HEC	CBD-CGD	2.39	1.56	1.50
5	C	403	HEC	FE-NA	2.38	2.03	1.95
5	C	403	HEC	CAB-C3B	2.37	1.57	1.51
13	M	501	MQ9	C32-C33	-2.30	1.43	1.50
5	C	402	HEC	CBD-CGD	2.27	1.55	1.50
13	M	501	MQ9	C48-C49	2.26	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	401	BPB	C1A-C2A	2.22	1.54	1.51
9	L	400	BCB	MG-NA	2.20	2.11	2.06
10	M	401	BPB	CHA-CBD	2.17	1.54	1.51
9	L	401	BCB	C2C-C3C	-2.17	1.49	1.51
10	L	402	BPB	C3B-C4B	2.13	1.44	1.41
13	M	501	MQ9	C47-C48	-2.11	1.44	1.50
9	L	400	BCB	C1-C2	-2.08	1.43	1.49
5	C	401	HEC	CBA-CGA	2.06	1.55	1.50
5	C	404	HEC	CAC-C3C	2.06	1.56	1.51
5	C	404	HEC	FE-ND	2.04	2.01	1.94
14	M	600	NS5	C23-C21	2.04	1.50	1.46
5	C	403	HEC	FE-NB	2.04	2.01	1.94
5	C	403	HEC	CAC-C3C	2.03	1.56	1.51
5	C	401	HEC	CBD-CGD	2.03	1.55	1.50
13	M	501	MQ9	C37-C38	-2.02	1.44	1.50

All (127) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	M	402	BPB	O2D-CGD-CBD	9.17	121.03	110.95
10	L	402	BPB	O2D-CGD-CBD	8.89	120.71	110.95
10	M	401	BPB	O2D-CGD-CBD	8.79	120.60	110.95
10	M	401	BPB	C3D-C4D-ND	-7.76	97.75	107.71
9	L	401	BCB	C4A-NA-C1A	7.74	110.21	106.68
9	L	400	BCB	C4A-NA-C1A	7.21	109.97	106.68
9	L	400	BCB	C1C-NC-C4C	7.06	109.90	106.68
10	M	402	BPB	C3D-C4D-ND	-6.50	99.38	107.71
9	M	400	BCB	C4A-NA-C1A	6.26	109.54	106.68
10	L	402	BPB	C3D-C4D-ND	-6.20	99.75	107.71
9	L	401	BCB	O2D-CGD-CBD	5.88	121.50	111.23
10	M	402	BPB	CMD-C2D-C3D	5.53	135.74	124.68
10	M	401	BPB	C4D-CHA-CBD	-5.30	105.91	108.45
10	M	401	BPB	C1-C2-C3	-5.15	117.76	126.20
9	M	400	BCB	O2D-CGD-CBD	5.15	120.22	111.23
9	L	401	BCB	C1C-NC-C4C	5.07	108.99	106.68
10	L	402	BPB	CMD-C2D-C3D	5.02	134.72	124.68
14	M	600	NS5	C34-C35-C36	-4.84	111.50	127.64
9	L	400	BCB	O2D-CGD-CBD	4.83	119.67	111.23
14	M	600	NS5	C19-C20-C21	-4.77	120.59	127.28
10	M	401	BPB	CMD-C2D-C3D	4.40	133.48	124.68
14	M	600	NS5	CM4-C36-C35	-3.92	110.90	122.66
14	M	600	NS5	CM3-C36-C35	-3.85	111.09	122.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	M	600	NS5	C29-C30-C31	-3.85	122.28	127.69
10	M	402	BPB	O1D-CGD-CBD	-3.72	119.08	124.72
10	M	402	BPB	O2A-CGA-CBA	3.72	123.18	111.83
14	M	600	NS5	C18-C17-C15	-3.68	122.12	127.28
14	M	600	NS5	C13-C12-C10	-3.68	122.52	127.69
9	L	400	BCB	C1-C2-C3	-3.59	120.31	126.20
9	L	401	BCB	C1D-ND-C4D	3.55	108.80	106.31
9	M	400	BCB	CHA-C4D-ND	3.54	139.86	132.55
9	L	401	BCB	CHA-C4D-ND	3.53	139.84	132.55
9	M	400	BCB	C1D-ND-C4D	3.46	108.74	106.31
10	M	401	BPB	O1D-CGD-CBD	-3.39	119.59	124.72
9	L	400	BCB	CHA-C4D-ND	3.29	139.34	132.55
10	M	401	BPB	C2B-C1B-NB	-3.21	107.11	109.43
10	L	402	BPB	O1D-CGD-CBD	-3.12	119.98	124.72
9	L	400	BCB	O2A-CGA-CBA	3.12	121.34	111.83
9	M	400	BCB	O1D-CGD-CBD	-3.11	118.38	124.52
9	L	401	BCB	O2D-CGD-O1D	-3.08	117.86	123.85
13	M	501	MQ9	C25-C24-C26	3.06	120.55	115.23
9	L	400	BCB	C1D-ND-C4D	3.04	108.44	106.31
9	L	401	BCB	C4-C3-C5	3.02	120.48	115.23
14	M	600	NS5	C6-C5-C4	2.99	120.42	115.23
9	M	400	BCB	C1-C2-C3	-2.93	121.40	126.20
9	L	400	BCB	C4-C3-C5	2.90	120.27	115.23
10	M	402	BPB	C4-C3-C2	-2.84	116.34	123.63
9	M	400	BCB	C4-C3-C5	2.81	120.11	115.23
5	C	404	HEC	C1D-ND-C4D	2.77	108.49	105.21
9	L	401	BCB	C1-C2-C3	-2.76	121.68	126.20
9	L	400	BCB	C3A-C2A-C1A	2.74	105.44	101.34
10	M	401	BPB	CGD-CBD-CAD	-2.70	102.10	110.85
5	C	403	HEC	C4B-NB-C1B	2.69	108.40	105.21
5	C	403	HEC	C1D-ND-C4D	2.68	108.38	105.21
13	M	501	MQ9	C32-C33-C34	-2.67	121.52	127.62
10	M	402	BPB	CAA-C2A-C3A	-2.62	105.92	113.00
11	M	503	UQ1	CM5-C5-C6	-2.61	120.16	124.45
9	M	400	BCB	CBC-CAC-C3C	-2.61	119.63	126.70
9	L	401	BCB	O2A-CGA-CBA	2.60	119.76	111.83
10	L	402	BPB	O2A-CGA-CBA	2.59	119.74	111.83
5	C	402	HEC	C1D-ND-C4D	2.59	108.27	105.21
11	M	503	UQ1	C7-C6-C5	-2.59	120.46	124.89
9	L	400	BCB	C2A-C1A-CHA	2.58	128.35	123.87
5	C	404	HEC	CAD-CBD-CGD	-2.58	106.82	113.67
9	M	400	BCB	C1C-NC-C4C	2.58	107.86	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	M	400	BCB	O2A-CGA-CBA	2.57	119.68	111.83
14	M	600	NS5	C32-C31-C33	2.56	119.68	115.23
10	M	401	BPB	C6-C5-C3	-2.55	107.25	113.47
9	L	400	BCB	CBC-CAC-C3C	-2.54	119.82	126.70
13	M	501	MQ9	C35-C34-C36	2.54	119.63	115.23
10	L	402	BPB	CMA-C3A-C4A	-2.53	109.16	114.61
13	M	501	MQ9	C22-C23-C24	-2.53	121.84	127.62
5	C	401	HEC	C1D-ND-C4D	2.50	108.17	105.21
5	C	401	HEC	C4B-NB-C1B	2.44	108.10	105.21
9	L	400	BCB	C6-C7-C8	-2.41	107.95	115.97
10	M	401	BPB	CED-O2D-CGD	2.40	121.36	115.92
13	M	501	MQ9	C42-C43-C44	-2.40	122.13	127.62
5	C	403	HEC	C3D-C4D-ND	-2.38	108.06	110.35
10	L	402	BPB	O2D-CGD-O1D	-2.36	119.25	123.85
10	M	401	BPB	C6-C7-C8	-2.33	108.21	115.97
13	M	501	MQ9	C40-C39-C38	-2.33	117.64	123.63
11	L	502	UQ1	CM5-C5-C6	-2.31	120.66	124.45
10	L	402	BPB	O2A-CGA-O1A	-2.31	117.86	123.63
13	M	501	MQ9	C17-C18-C19	-2.29	122.37	127.62
10	L	402	BPB	C1-C2-C3	-2.29	122.44	126.20
5	C	404	HEC	C3D-C4D-ND	-2.28	108.15	110.35
13	M	501	MQ9	C40-C39-C41	2.26	119.16	115.23
13	M	501	MQ9	C15-C14-C16	2.26	119.15	115.23
9	L	400	BCB	O1D-CGD-CBD	-2.26	120.07	124.52
9	L	401	BCB	CBC-CAC-C3C	-2.24	120.62	126.70
14	M	600	NS5	C11-C10-C9	2.24	119.11	115.23
13	M	501	MQ9	C20-C19-C21	2.24	119.11	115.23
10	M	401	BPB	O2A-CGA-CBA	2.23	118.65	111.83
5	C	402	HEC	C3D-C4D-ND	-2.23	108.20	110.35
11	L	502	UQ1	CM3-O3-C3	2.22	124.28	116.47
5	C	402	HEC	C4B-NB-C1B	2.20	107.82	105.21
5	C	401	HEC	C2A-C1A-NA	-2.20	108.20	110.32
13	M	501	MQ9	C37-C38-C39	-2.19	122.62	127.62
5	C	403	HEC	C2A-C1A-NA	-2.18	108.22	110.32
10	L	402	BPB	C7-C6-C5	-2.18	107.45	113.26
13	M	501	MQ9	C30-C29-C31	2.18	119.01	115.23
9	L	401	BCB	C2D-C1D-ND	-2.18	107.97	110.13
13	M	501	MQ9	C7-C8-C9	-2.18	123.08	126.83
9	L	401	BCB	C2B-C1B-NB	-2.17	108.08	110.33
10	M	402	BPB	CAA-CBA-CGA	-2.16	107.08	113.21
9	M	400	BCB	C3A-C2A-C1A	2.14	104.55	101.34
5	C	404	HEC	CHA-C4D-ND	2.14	126.73	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	L	400	BCB	CED-O2D-CGD	2.14	120.77	115.92
9	M	400	BCB	C2B-C1B-NB	-2.12	108.13	110.33
11	M	503	UQ1	C11-C9-C10	2.11	119.44	114.59
13	M	501	MQ9	C51-C49-C50	2.11	119.44	114.59
5	C	402	HEC	C2A-C1A-NA	-2.10	108.29	110.32
10	M	401	BPB	C4-C3-C5	2.10	118.87	115.23
14	M	600	NS5	C6-C5-C7	-2.08	118.27	123.63
10	M	401	BPB	O2D-CGD-O1D	-2.08	119.79	123.85
13	M	501	MQ9	C47-C48-C49	-2.08	120.71	127.64
10	M	402	BPB	C4-C3-C5	2.08	118.83	115.23
10	M	401	BPB	C1-O2A-CGA	2.08	121.67	116.65
9	M	400	BCB	C2D-C1D-ND	-2.06	108.08	110.13
9	L	401	BCB	O1D-CGD-CBD	-2.06	120.46	124.52
10	M	402	BPB	C2B-C1B-NB	-2.04	107.95	109.43
5	C	401	HEC	C3D-C4D-ND	-2.04	108.38	110.35
10	L	402	BPB	C4-C3-C5	2.04	118.77	115.23
10	M	402	BPB	O2D-CGD-O1D	-2.04	119.88	123.85
9	L	400	BCB	O2A-CGA-O1A	-2.03	118.56	123.63
14	M	600	NS5	C12-C13-C14	-2.02	117.35	123.20
13	M	501	MQ9	C5M-C5-C6	-2.00	121.16	124.45

All (11) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	C	401	HEC	NA
5	C	402	HEC	NA
5	C	403	HEC	NA
5	C	404	HEC	NA
9	L	400	BCB	ND
9	L	400	BCB	NC
9	L	400	BCB	NA
9	L	401	BCB	NC
9	L	401	BCB	NA
9	M	400	BCB	NC
9	M	400	BCB	NA

All (168) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	707	HTO	O1-C1-C2-O2
7	C	707	HTO	O1-C1-C2-C3
7	C	707	HTO	O3-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
7	H	705	HTO	O2-C2-C3-C4
7	L	708	HTO	O1-C1-C2-O2
7	L	708	HTO	O1-C1-C2-C3
7	L	709	HTO	C1-C2-C3-O3
8	H	701	LDA	C2-C1-N1-CM1
8	H	701	LDA	C2-C1-N1-CM2
8	M	702	LDA	C2-C1-N1-CM1
8	M	704	LDA	C2-C1-N1-O1
8	M	704	LDA	C2-C1-N1-CM1
8	M	704	LDA	C2-C1-N1-CM2
9	L	401	BCB	C2C-C3C-CAC-CBC
9	M	400	BCB	C2C-C3C-CAC-CBC
10	M	401	BPB	C4-C3-C5-C6
10	M	401	BPB	C2C-C3C-CAC-CBC
10	M	401	BPB	CAD-CBD-CGD-O1D
10	M	401	BPB	CAD-CBD-CGD-O2D
10	M	402	BPB	C1A-C2A-CAA-CBA
13	M	501	MQ9	C37-C38-C39-C41
13	M	501	MQ9	C42-C43-C44-C45
13	M	501	MQ9	C42-C43-C44-C46
13	M	501	MQ9	C47-C48-C49-C50
13	M	501	MQ9	C47-C48-C49-C51
14	M	600	NS5	C34-C35-C36-CM3
5	C	403	HEC	C2B-C3B-CAB-CBB
14	M	600	NS5	C34-C35-C36-CM4
14	M	600	NS5	C3-C4-C5-C6
10	M	401	BPB	C2-C3-C5-C6
13	M	501	MQ9	C38-C39-C41-C42
14	M	600	NS5	C2-C3-C4-C5
13	M	501	MQ9	C37-C38-C39-C40
5	C	403	HEC	C4B-C3B-CAB-CBB
14	M	600	NS5	C3-C4-C5-C7
13	M	501	MQ9	C34-C36-C37-C38
13	M	501	MQ9	C44-C46-C47-C48
5	C	403	HEC	C4C-C3C-CAC-CBC
5	C	403	HEC	C2C-C3C-CAC-CBC
10	M	401	BPB	C14-C13-C15-C16
10	M	402	BPB	C11-C10-C8-C9
7	C	706	HTO	O3-C3-C4-C5
14	M	600	NS5	C31-C33-C34-C35
11	L	502	UQ1	C2-C3-O3-CM3
10	M	402	BPB	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
9	L	400	BCB	C5-C6-C7-C8
10	M	402	BPB	C10-C11-C12-C13
10	M	401	BPB	C13-C15-C16-C17
10	M	402	BPB	C13-C15-C16-C17
10	M	401	BPB	C3-C5-C6-C7
10	M	401	BPB	C5-C6-C7-C8
10	M	402	BPB	C16-C17-C18-C20
7	H	705	HTO	O1-C1-C2-O2
8	H	703	LDA	C6-C7-C8-C9
8	H	701	LDA	C4-C5-C6-C7
8	H	703	LDA	C4-C5-C6-C7
5	C	404	HEC	C2B-C3B-CAB-CBB
8	M	704	LDA	C7-C8-C9-C10
8	M	704	LDA	C5-C6-C7-C8
10	M	402	BPB	C3A-C2A-CAA-CBA
10	M	402	BPB	C3-C5-C6-C7
13	M	501	MQ9	C17-C18-C19-C20
10	M	402	BPB	C16-C17-C18-C19
8	H	701	LDA	C3-C4-C5-C6
8	M	704	LDA	C1-C2-C3-C4
10	M	401	BPB	C2A-CAA-CBA-CGA
9	M	400	BCB	C16-C17-C18-C19
9	L	400	BCB	C15-C16-C17-C18
10	M	401	BPB	C10-C11-C12-C13
8	H	701	LDA	C6-C7-C8-C9
8	M	704	LDA	C2-C3-C4-C5
8	H	701	LDA	C1-C2-C3-C4
9	M	400	BCB	C16-C17-C18-C20
5	C	402	HEC	C2B-C3B-CAB-CBB
8	H	703	LDA	C7-C8-C9-C10
9	M	400	BCB	C11-C12-C13-C15
7	C	707	HTO	C2-C3-C4-C5
7	H	705	HTO	C2-C3-C4-C5
8	H	701	LDA	C7-C8-C9-C10
7	H	705	HTO	O3-C3-C4-C5
10	L	402	BPB	O2A-C1-C2-C3
7	L	709	HTO	C4-C5-C6-C7
8	M	704	LDA	N1-C1-C2-C3
7	C	707	HTO	C4-C5-C6-C7
10	L	402	BPB	C8-C10-C11-C12
9	M	400	BCB	C11-C12-C13-C14
5	C	404	HEC	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
10	M	401	BPB	C12-C13-C15-C16
10	M	402	BPB	C11-C10-C8-C7
7	L	708	HTO	O3-C3-C4-C5
7	H	705	HTO	C1-C2-C3-C4
7	L	709	HTO	C1-C2-C3-C4
7	C	706	HTO	O2-C2-C3-C4
9	L	400	BCB	C4-C3-C5-C6
10	L	402	BPB	C4-C3-C5-C6
7	C	706	HTO	C2-C3-C4-C5
8	M	704	LDA	C11-C10-C9-C8
13	M	501	MQ9	C39-C41-C42-C43
5	C	401	HEC	C2C-C3C-CAC-CBC
5	C	402	HEC	C3D-CAD-CBD-CGD
5	C	401	HEC	C2B-C3B-CAB-CBB
9	L	400	BCB	C16-C17-C18-C20
8	M	702	LDA	C11-C10-C9-C8
9	L	400	BCB	C2-C3-C5-C6
5	C	402	HEC	C4B-C3B-CAB-CBB
7	C	707	HTO	C1-C2-C3-O3
7	L	708	HTO	C1-C2-C3-O3
8	H	703	LDA	C2-C1-N1-CM1
8	H	703	LDA	C2-C1-N1-CM2
8	M	702	LDA	C2-C1-N1-CM2
10	L	402	BPB	C2-C3-C5-C6
7	L	708	HTO	C3-C4-C5-C6
9	L	400	BCB	C12-C13-C15-C16
9	M	400	BCB	C6-C7-C8-C10
10	M	402	BPB	C12-C13-C15-C16
7	L	708	HTO	C2-C3-C4-C5
10	M	401	BPB	C15-C16-C17-C18
8	H	701	LDA	C2-C1-N1-O1
8	H	703	LDA	C2-C1-N1-O1
8	M	702	LDA	C2-C1-N1-O1
9	L	400	BCB	CAD-CBD-CGD-O2D
7	H	705	HTO	O2-C2-C3-O3
9	L	400	BCB	CAD-CBD-CGD-O1D
14	M	600	NS5	C23-C24-C25-C26
9	L	401	BCB	C15-C16-C17-C18
9	L	400	BCB	C14-C13-C15-C16
9	M	400	BCB	C6-C7-C8-C9
8	H	703	LDA	C5-C6-C7-C8
9	L	400	BCB	C16-C17-C18-C19

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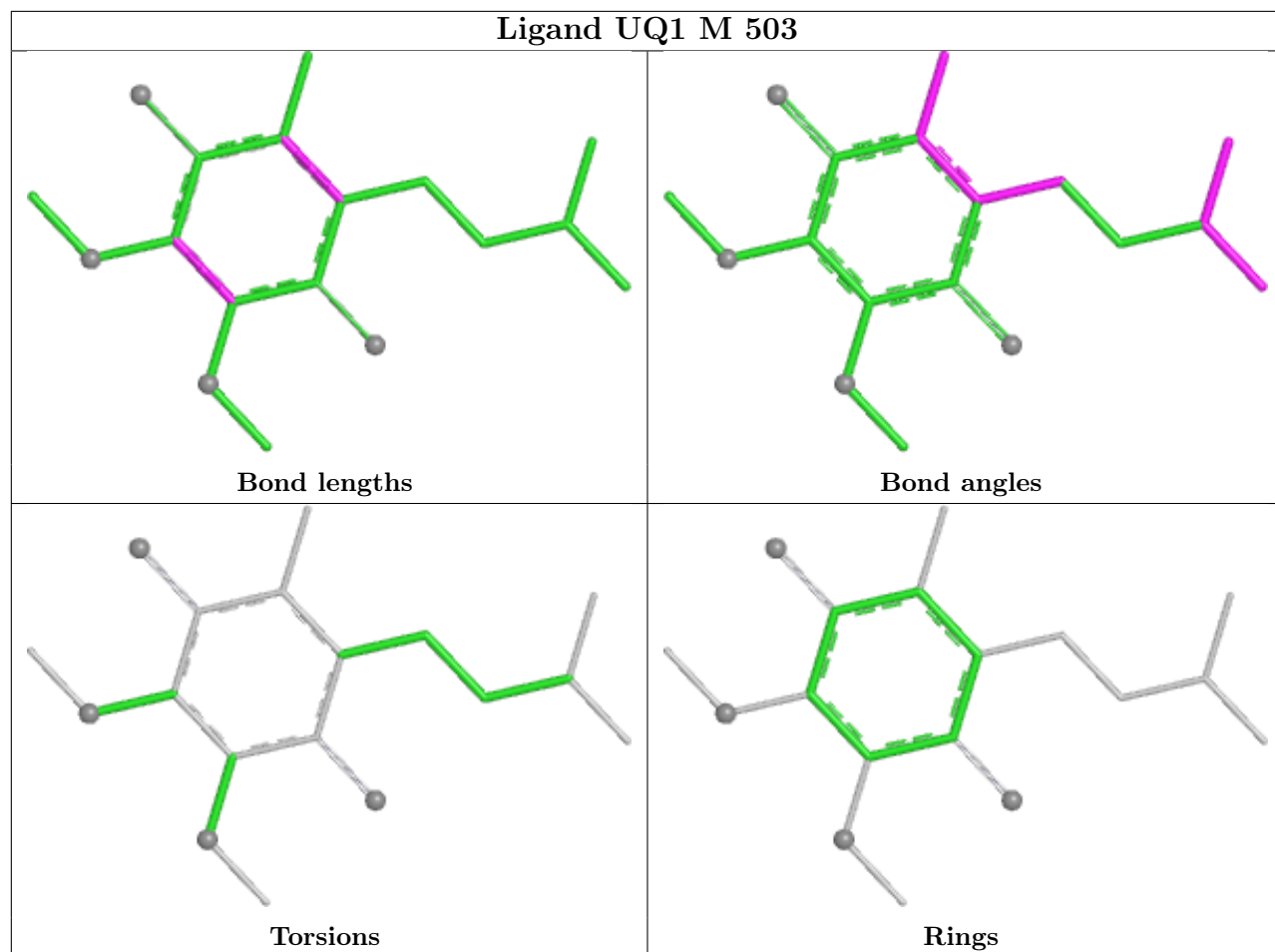
Mol	Chain	Res	Type	Atoms
5	C	404	HEC	C2C-C3C-CAC-CBC
7	L	709	HTO	C3-C4-C5-C6
10	M	402	BPB	C2-C1-O2A-CGA
14	M	600	NS5	C7-C8-C9-C10
13	M	501	MQ9	C40-C39-C41-C42
5	C	404	HEC	C4C-C3C-CAC-CBC
5	C	401	HEC	CAA-CBA-CGA-O2A
5	C	401	HEC	CAA-CBA-CGA-O1A
5	C	401	HEC	C4C-C3C-CAC-CBC
11	L	502	UQ1	C1-C2-O2-CM2
8	H	703	LDA	C1-C2-C3-C4
5	C	402	HEC	CAA-CBA-CGA-O1A
10	M	402	BPB	C14-C13-C15-C16
13	M	501	MQ9	C35-C34-C36-C37
10	M	402	BPB	C6-C7-C8-C10
5	C	402	HEC	CAA-CBA-CGA-O2A
9	M	400	BCB	C4-C3-C5-C6
10	M	402	BPB	C6-C7-C8-C9
10	M	402	BPB	C5-C6-C7-C8
5	C	401	HEC	C4B-C3B-CAB-CBB
14	M	600	NS5	C11-C10-C9-C8
9	L	401	BCB	C16-C17-C18-C20
7	C	707	HTO	O2-C2-C3-O3
7	L	709	HTO	O2-C2-C3-O3
10	M	401	BPB	CHA-CBD-CGD-O1D
10	M	401	BPB	CHA-CBD-CGD-O2D
8	M	702	LDA	C3-C4-C5-C6
10	L	402	BPB	C3A-C2A-CAA-CBA
9	M	400	BCB	C3-C5-C6-C7
10	M	401	BPB	C11-C10-C8-C9
10	M	402	BPB	C2C-C3C-CAC-CBC
5	C	402	HEC	CAD-CBD-CGD-O2D
10	M	401	BPB	C11-C10-C8-C7
9	L	401	BCB	C16-C17-C18-C19
5	C	402	HEC	CAD-CBD-CGD-O1D
14	M	600	NS5	C12-C10-C9-C8
7	L	709	HTO	O2-C2-C3-C4
9	M	400	BCB	C5-C6-C7-C8
7	H	705	HTO	C4-C5-C6-C7

There are no ring outliers.

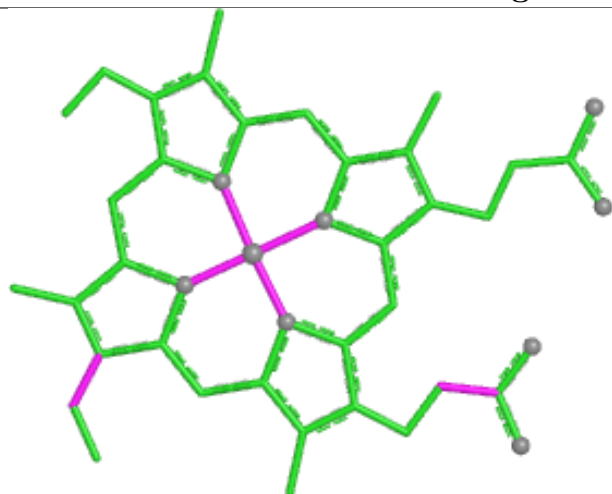
18 monomers are involved in 81 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	707	HTO	1	0
5	C	403	HEC	2	0
8	M	704	LDA	1	0
6	M	805	SO4	1	0
9	L	401	BCB	7	0
6	C	813	SO4	1	0
7	C	706	HTO	1	0
10	M	401	BPB	24	0
7	H	705	HTO	1	0
8	M	702	LDA	2	0
10	L	402	BPB	5	0
9	M	400	BCB	6	0
11	L	502	UQ1	4	0
9	L	400	BCB	16	0
14	M	600	NS5	4	0
10	M	402	BPB	16	0
13	M	501	MQ9	4	0
5	C	404	HEC	1	0

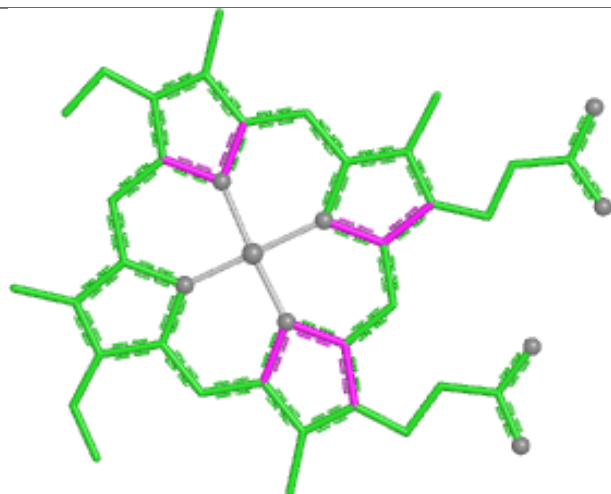
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



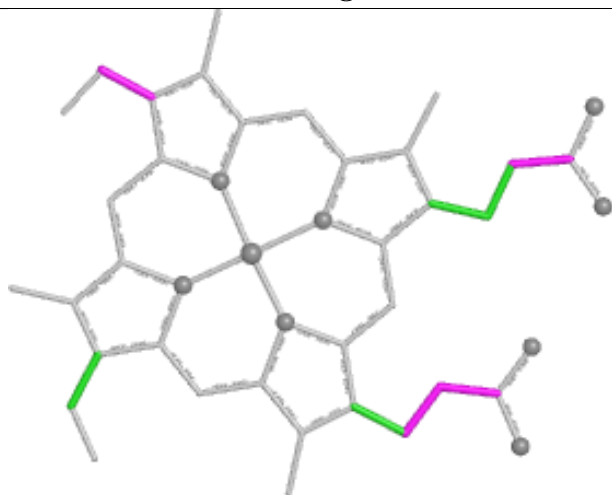
Ligand HEC C 402



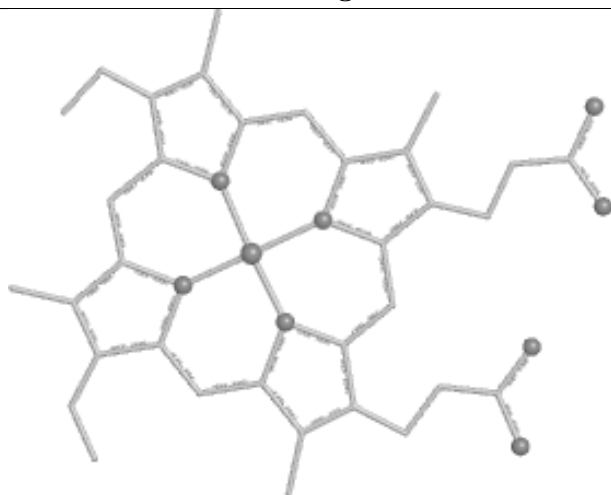
Bond lengths



Bond angles

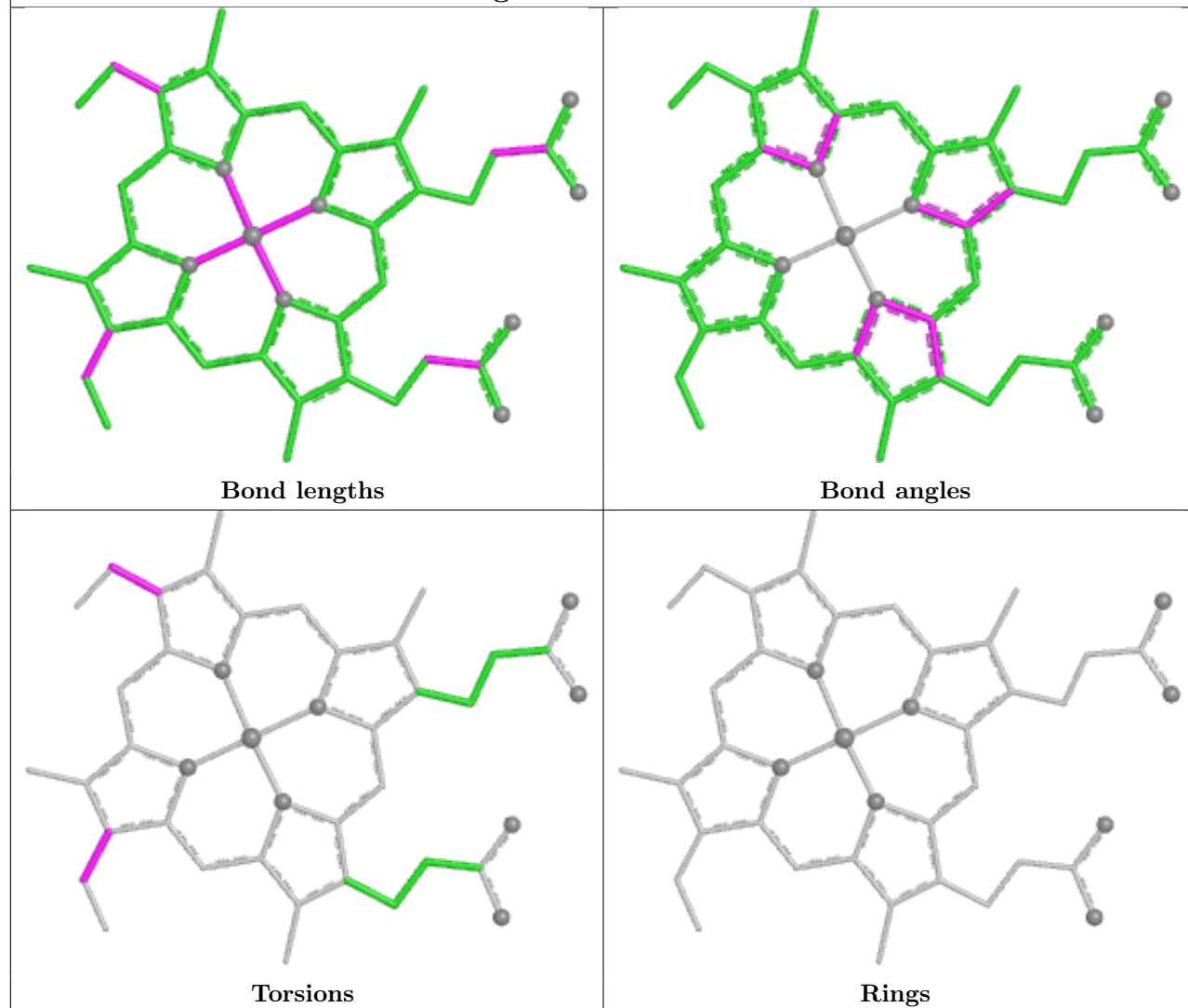


Torsions

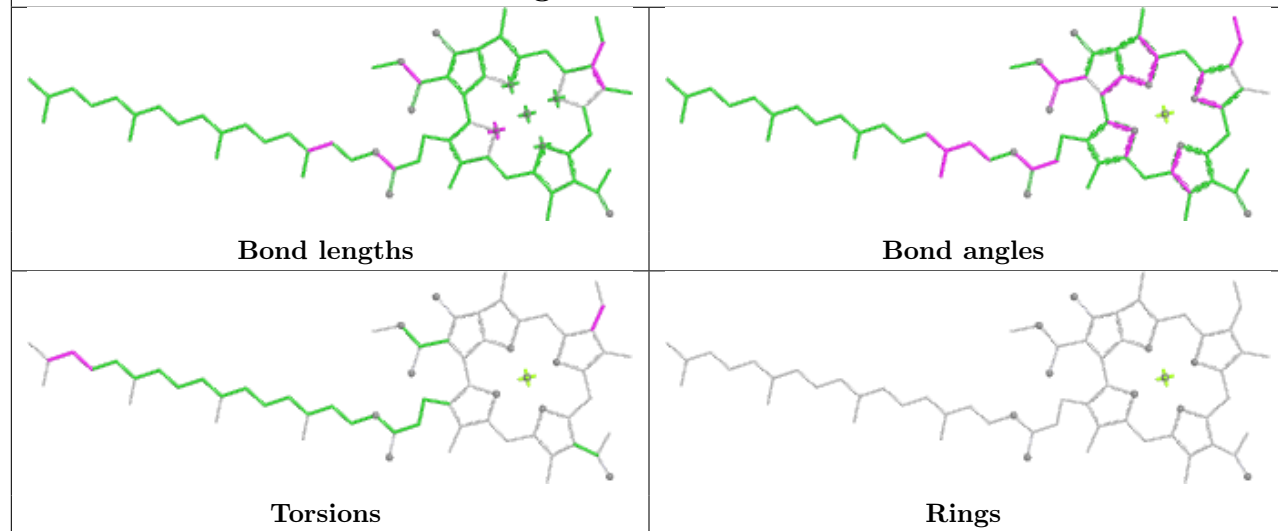


Rings

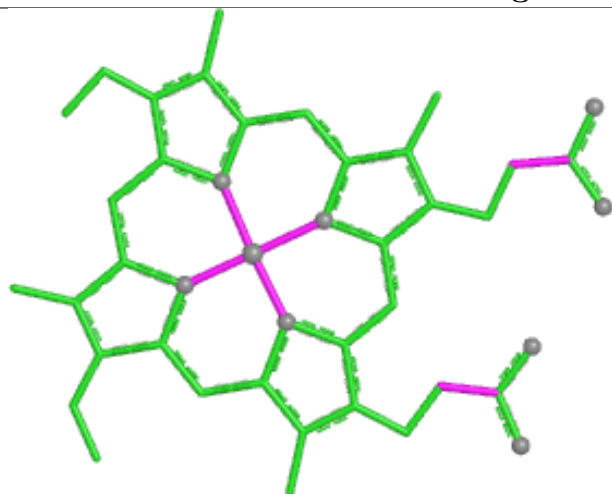
Ligand HEC C 403



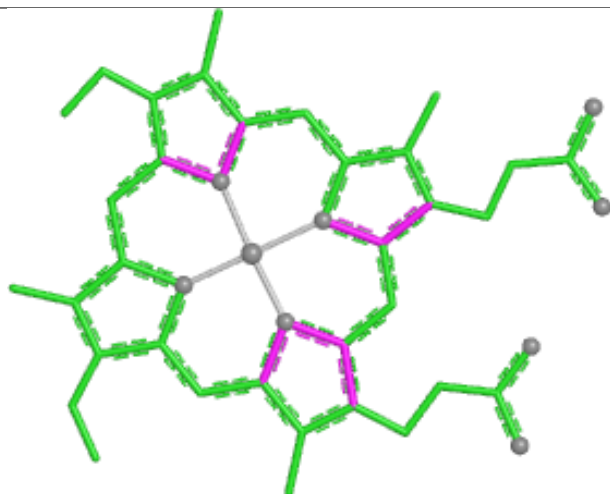
Ligand BCB L 401



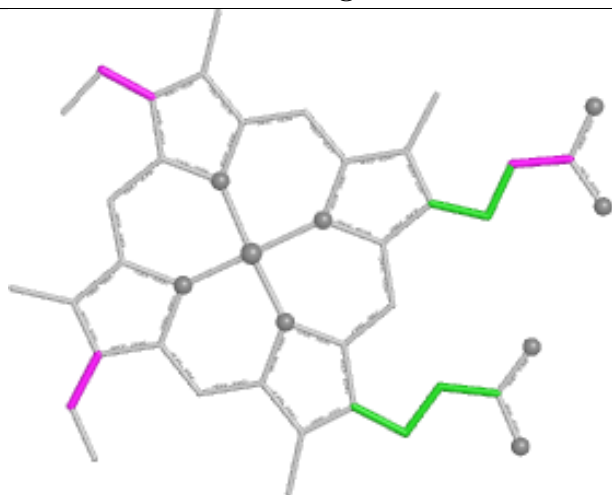
Ligand HEC C 401



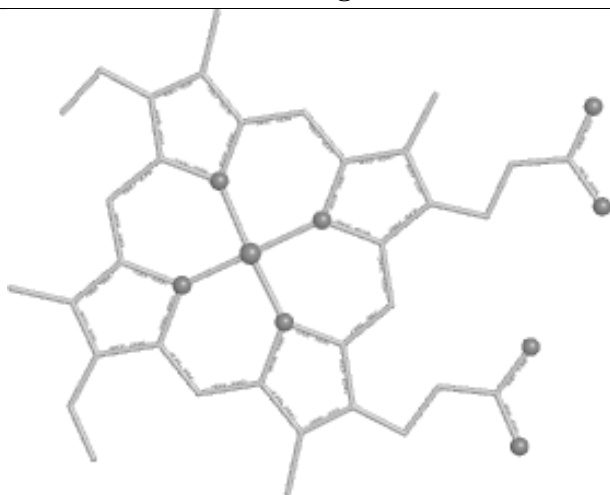
Bond lengths



Bond angles

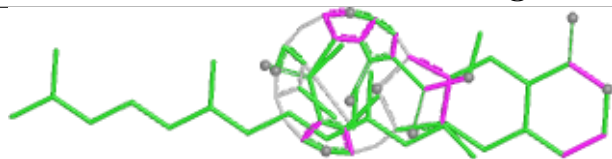


Torsions

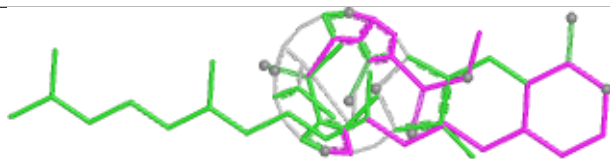


Rings

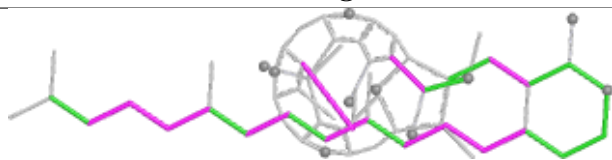
Ligand BPB M 401



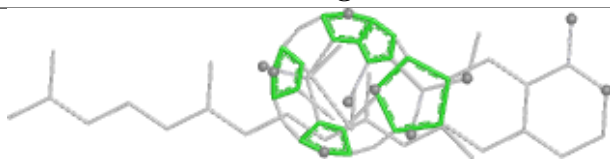
Bond lengths



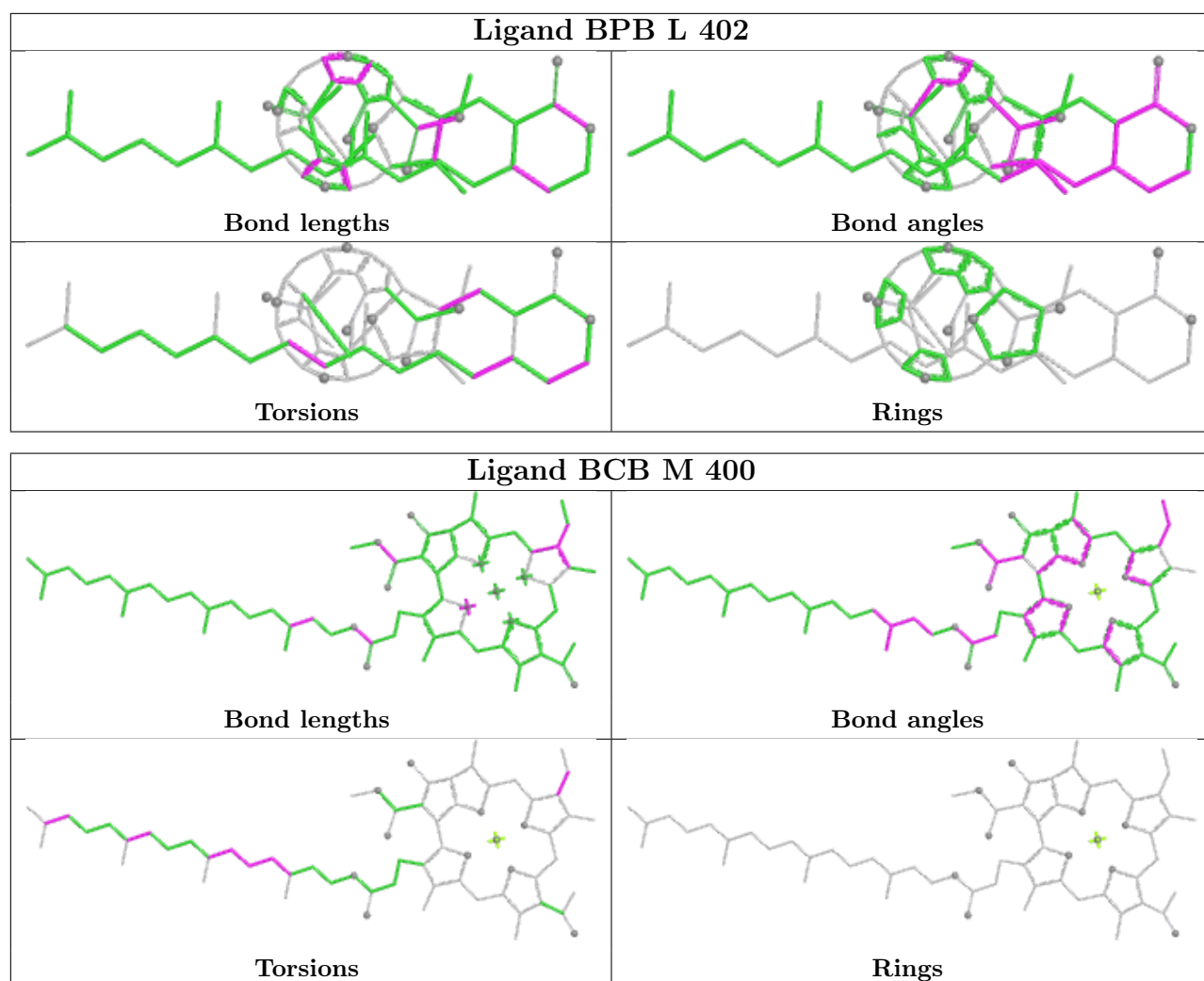
Bond angles



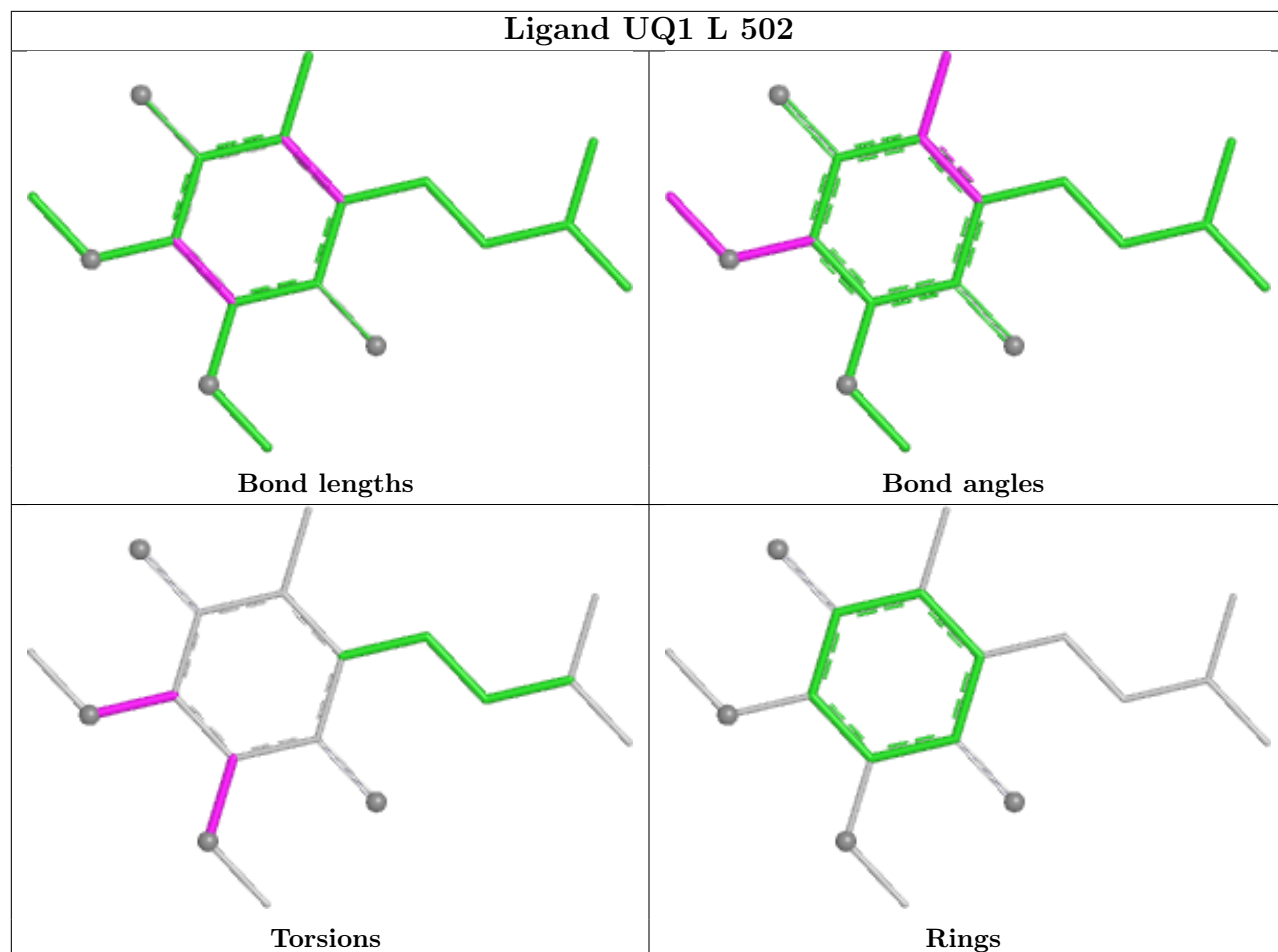
Torsions



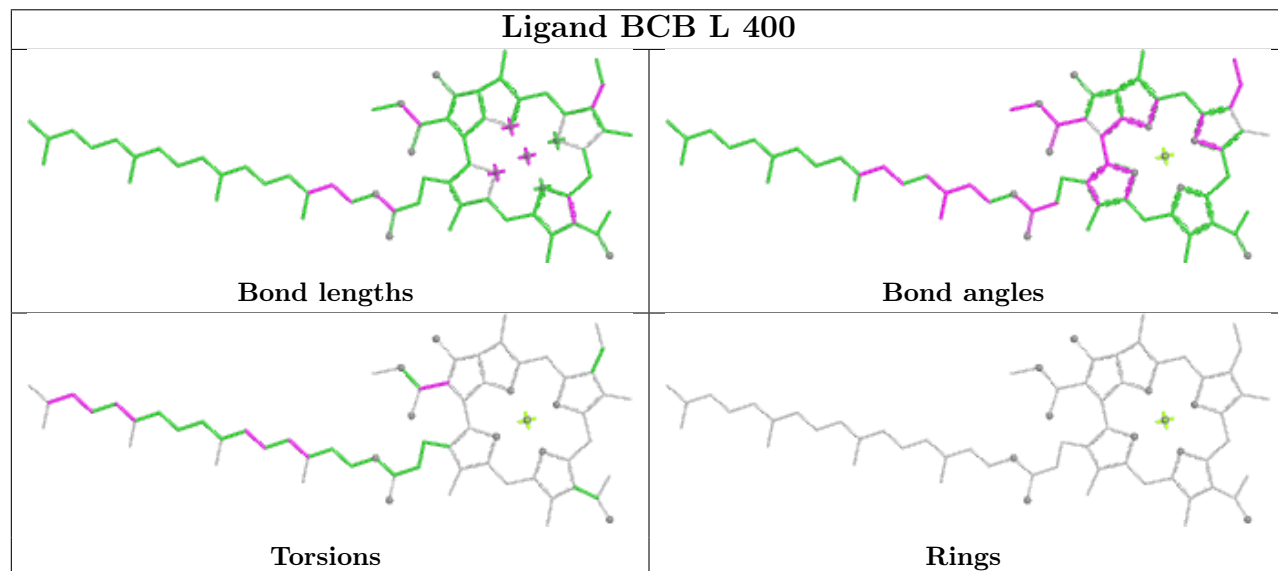
Rings

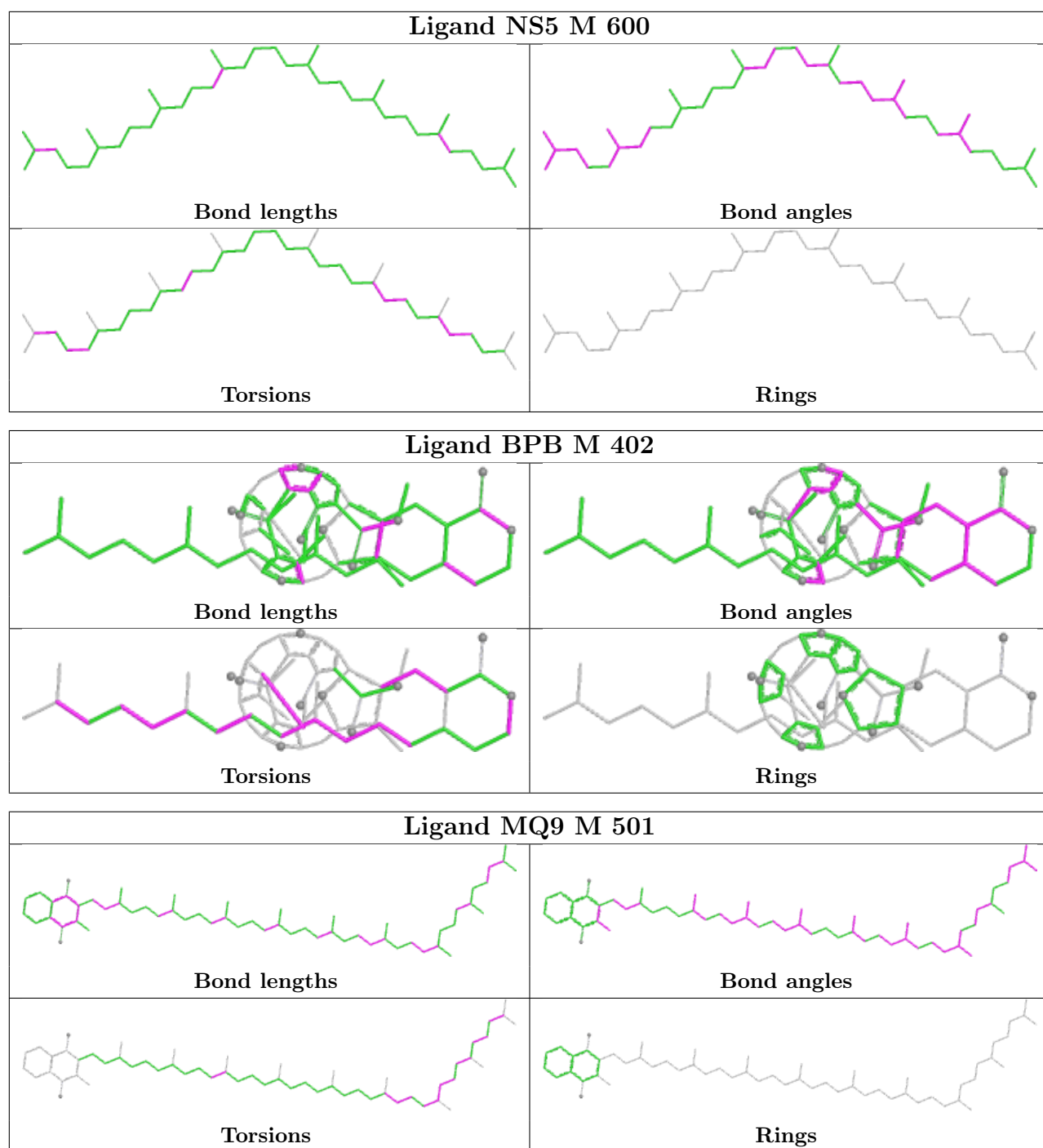


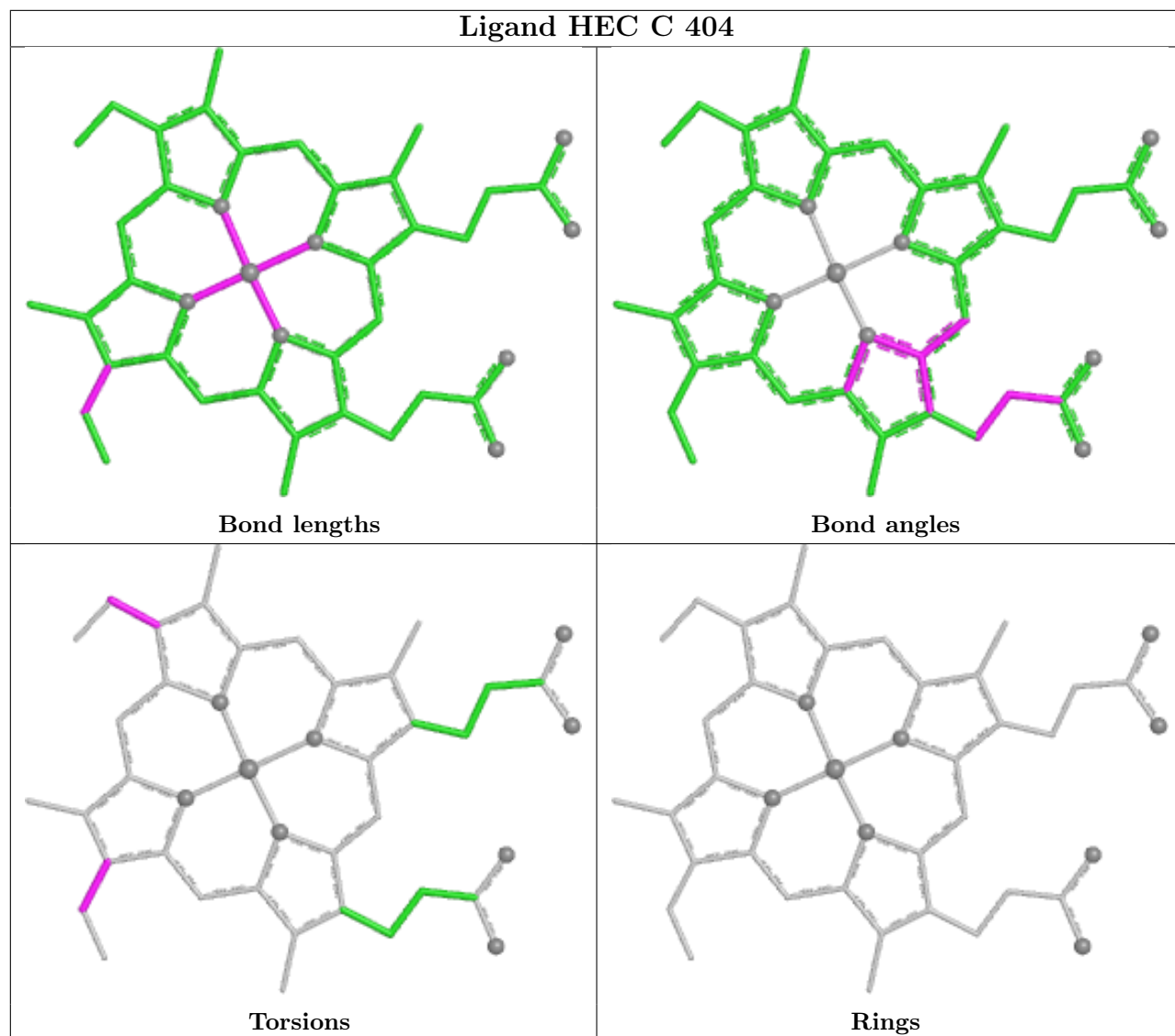
Ligand UQ1 L 502



Ligand BCB L 400







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	332/336 (98%)	-0.56	0 100 100	21, 31, 49, 61	0
2	H	249/258 (96%)	-0.41	5 (2%) 65 61	18, 32, 50, 60	0
3	L	273/273 (100%)	-0.71	1 (0%) 88 86	20, 26, 41, 47	1 (0%)
4	M	323/323 (100%)	-0.58	4 (1%) 76 73	17, 28, 45, 50	2 (0%)
All	All	1177/1190 (98%)	-0.57	10 (0%) 82 80	17, 29, 46, 61	3 (0%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	85	THR	4.5
2	H	9	HIS	2.9
2	H	83	PRO	2.5
2	H	45	GLU	2.4
4	M	146	TRP	2.3
3	L	202	ASP	2.3
4	M	30	GLY	2.2
4	M	71	PHE	2.2
2	H	54	PRO	2.2
4	M	59	PHE	2.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FME	H	1	10/11	0.95	0.08	36,38,49,53	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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
6	SO4	M	816	5/5	-0.41	2.74	2,2,2,2	5
6	SO4	L	814	5/5	-0.28	2.40	2,2,2,2	5
6	SO4	M	819	5/5	-0.20	2.54	2,2,2,2	5
6	SO4	C	817	5/5	-0.19	2.65	2,2,2,2	5
6	SO4	M	818	5/5	-0.15	2.39	2,2,2,2	5
7	HTO	L	708	10/10	-0.11	1.91	2,2,2,2	10
6	SO4	C	815	5/5	-0.08	2.50	2,2,2,2	5
7	HTO	L	709	10/10	0.11	2.71	2,2,2,2	10
11	UQ1	M	503	18/18	0.63	0.34	93,94,95,95	0
10	BPB	M	401	65/65	0.77	0.25	28,39,45,47	65
14	NS5	M	600	40/40	0.82	0.19	35,45,74,74	4
11	UQ1	L	502	18/18	0.83	0.15	45,46,49,50	0
8	LDA	M	704	16/16	0.84	0.21	55,58,68,69	0
7	HTO	C	707	10/10	0.86	0.20	50,54,57,57	0
6	SO4	C	808	5/5	0.86	0.14	55,56,57,58	5
6	SO4	C	810	5/5	0.86	0.22	46,47,47,47	5
6	SO4	C	813	5/5	0.86	0.15	39,39,41,41	5
7	HTO	C	706	10/10	0.87	0.18	45,50,51,51	0
8	LDA	M	702	16/16	0.91	0.15	47,57,67,67	0
6	SO4	C	811	5/5	0.91	0.19	42,43,44,44	5
6	SO4	C	809	5/5	0.91	0.15	66,67,67,68	5
6	SO4	H	812	5/5	0.92	0.20	47,47,48,48	5
6	SO4	H	803	5/5	0.92	0.15	67,68,68,69	0
10	BPB	M	402	65/65	0.92	0.13	21,27,97,99	0
7	HTO	H	705	10/10	0.93	0.10	41,42,44,45	0
6	SO4	H	807	5/5	0.93	0.13	64,65,66,66	5
9	BCB	M	400	66/66	0.94	0.10	23,27,85,86	0
6	SO4	M	805	5/5	0.94	0.10	48,49,49,50	5
8	LDA	H	703	16/16	0.95	0.13	47,53,60,62	0
6	SO4	H	806	5/5	0.95	0.10	48,49,50,50	5
8	LDA	H	701	16/16	0.95	0.08	36,41,47,48	0
13	MQ9	M	501	58/58	0.96	0.08	16,22,74,75	0

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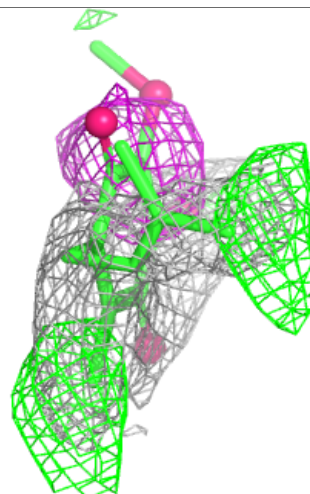
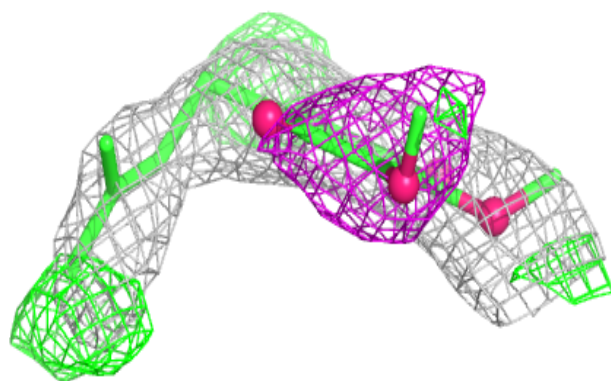
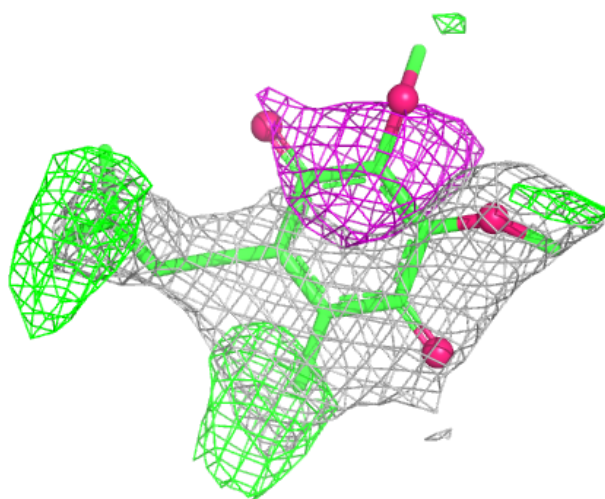
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	SO4	M	804	5/5	0.97	0.15	53,54,55,56	0
10	BPB	L	402	65/65	0.97	0.05	14,20,28,29	0
9	BCB	L	400	66/66	0.97	0.06	23,26,33,38	0
9	BCB	L	401	66/66	0.97	0.05	18,24,40,44	0
5	HEC	C	402	43/43	0.98	0.07	26,30,37,39	0
6	SO4	M	802	5/5	0.98	0.06	47,48,49,50	0
5	HEC	C	403	43/43	0.99	0.05	14,21,27,31	0
5	HEC	C	404	43/43	0.99	0.06	21,24,34,41	0
6	SO4	M	801	5/5	0.99	0.06	29,29,32,32	0
5	HEC	C	401	43/43	0.99	0.06	30,33,45,51	0
12	FE2	M	500	1/1	1.00	0.01	21,21,21,21	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.

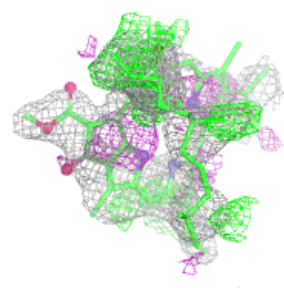
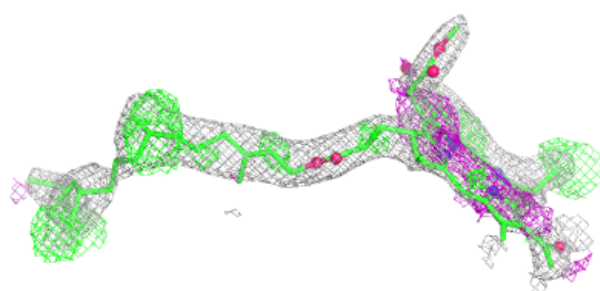
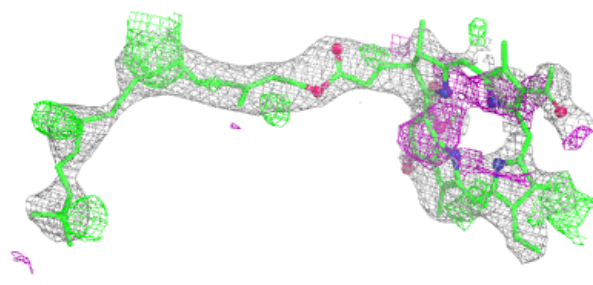
Electron density around UQ1 M 503:

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

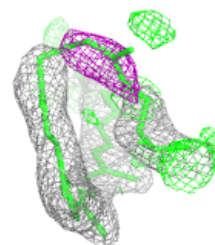
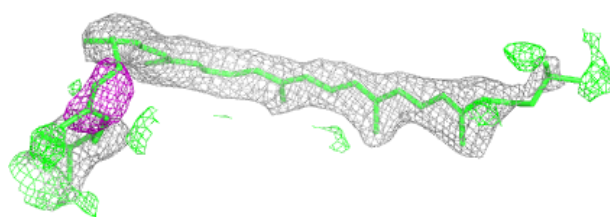
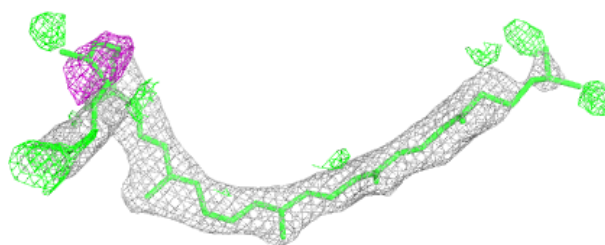


Electron density around BPB M 401:

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

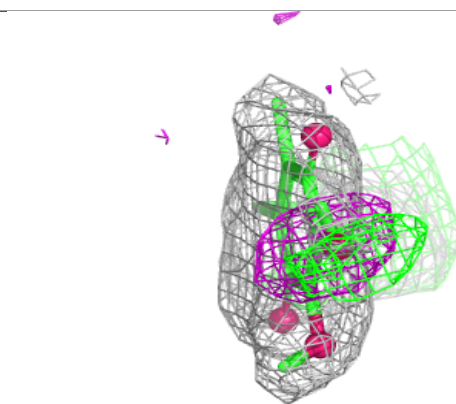
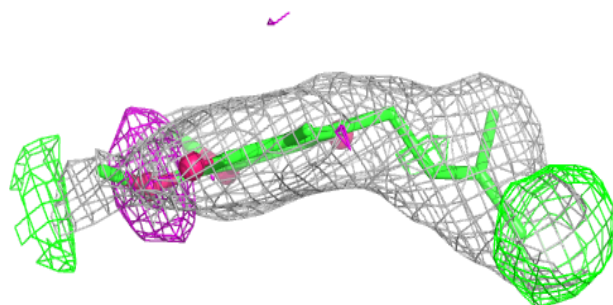
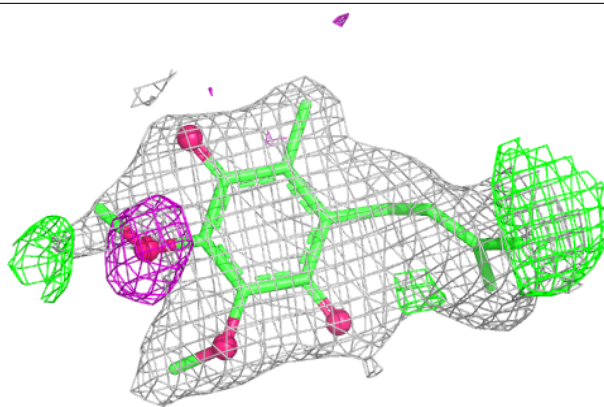
**Electron density around NS5 M 600:**

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

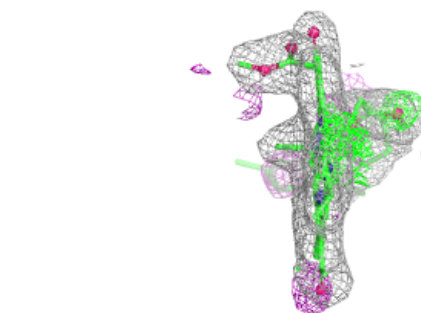
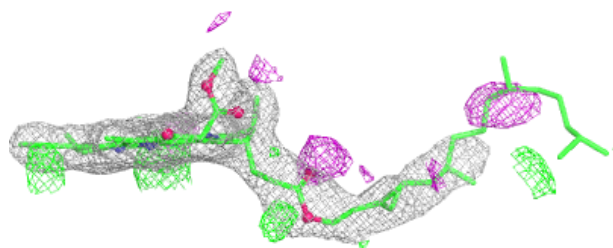
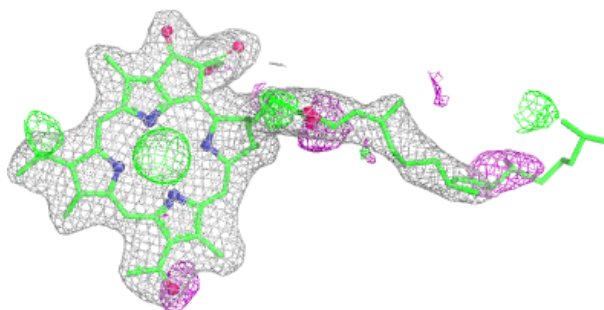


Electron density around UQ1 L 502:

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

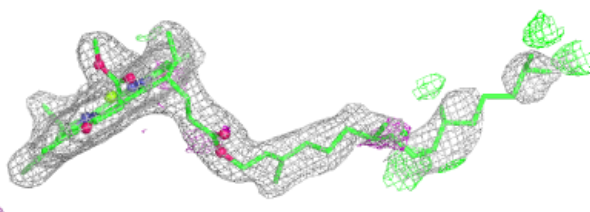
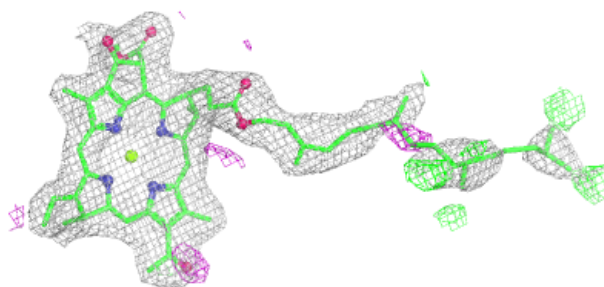
**Electron density around BPB M 402:**

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

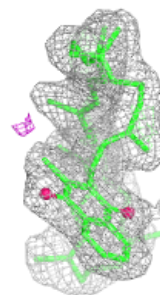
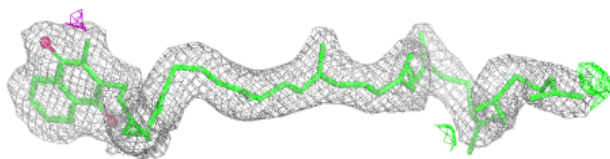
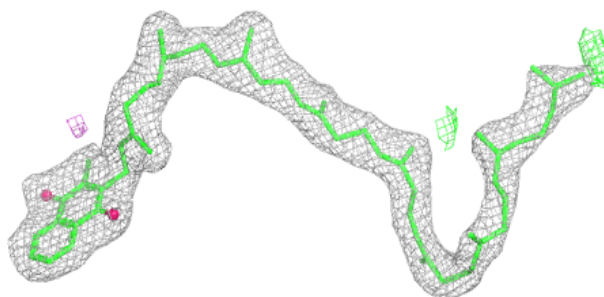


Electron density around BCB M 400:

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

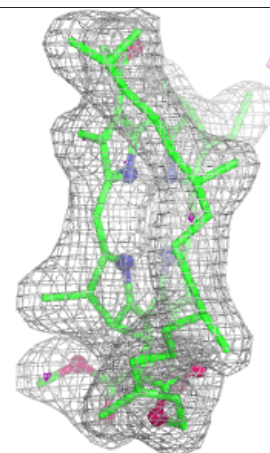
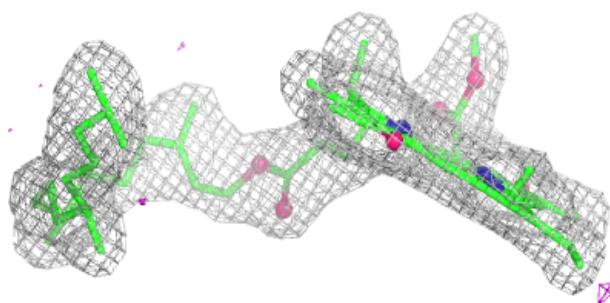
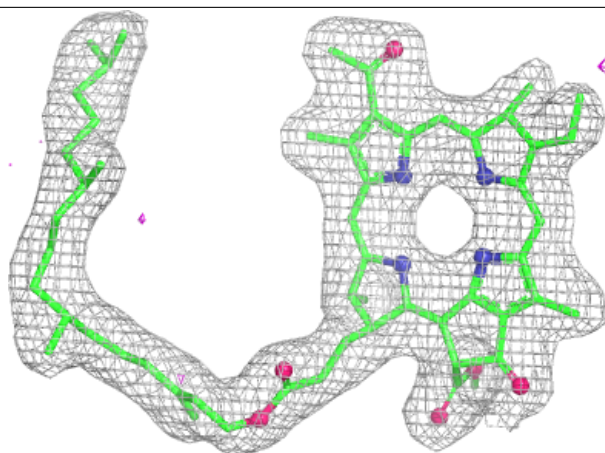
**Electron density around MQ9 M 501:**

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



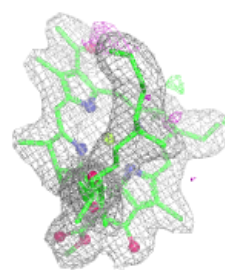
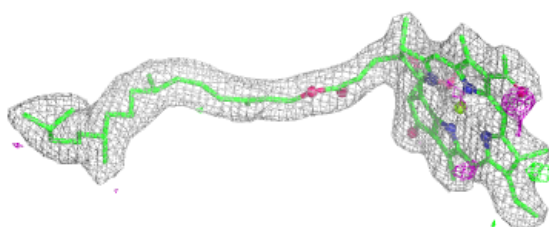
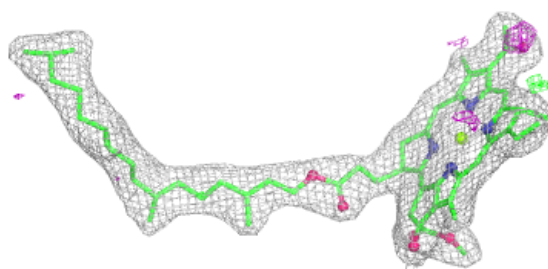
Electron density around BPB L 402:

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

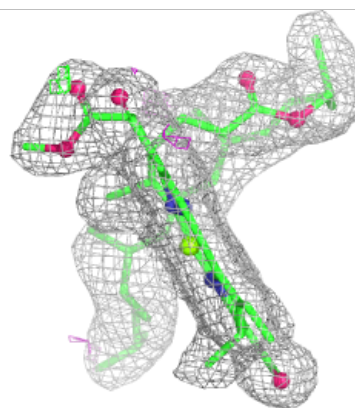
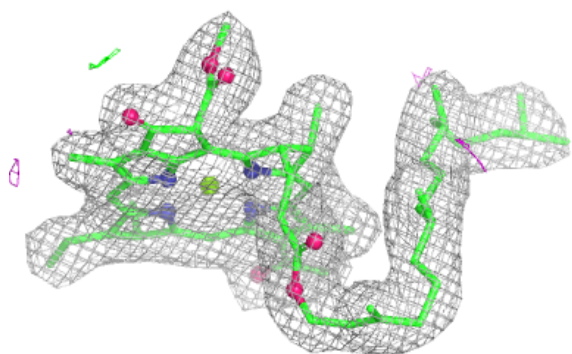
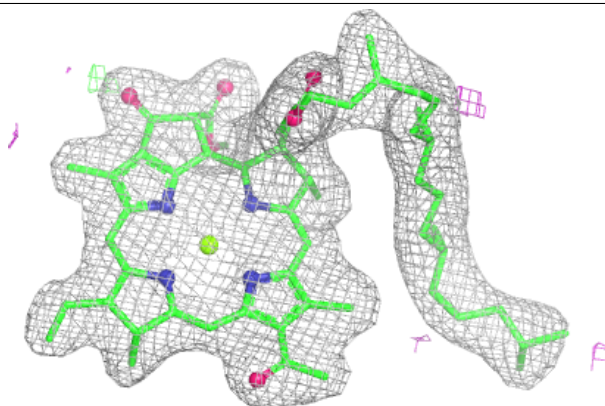


Electron density around BCB L 400:

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

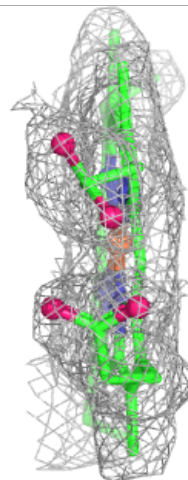
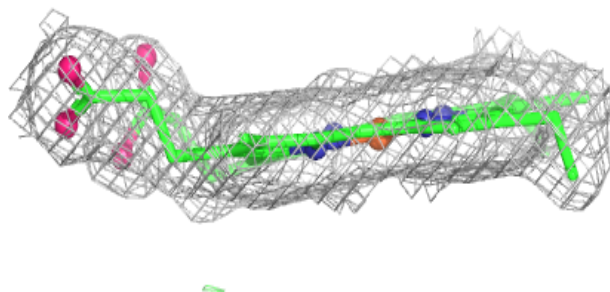
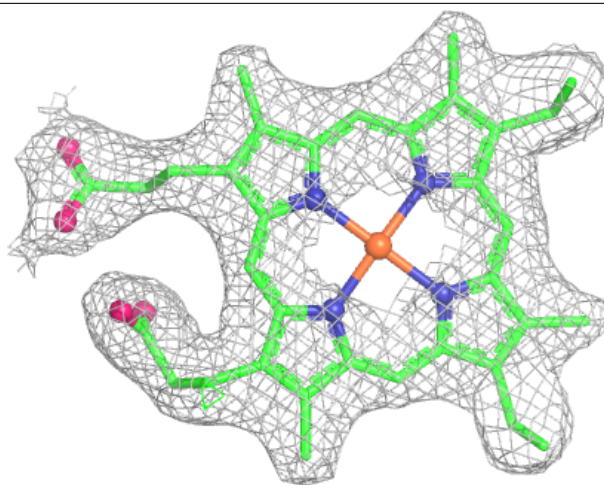
**Electron density around BCB L 401:**

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



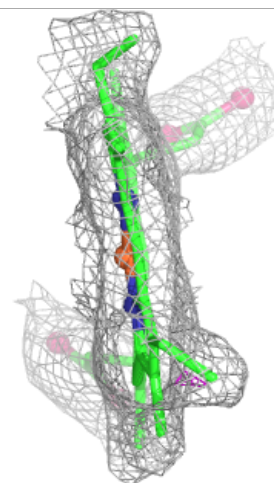
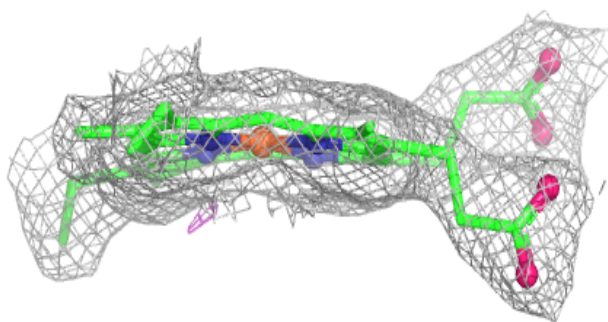
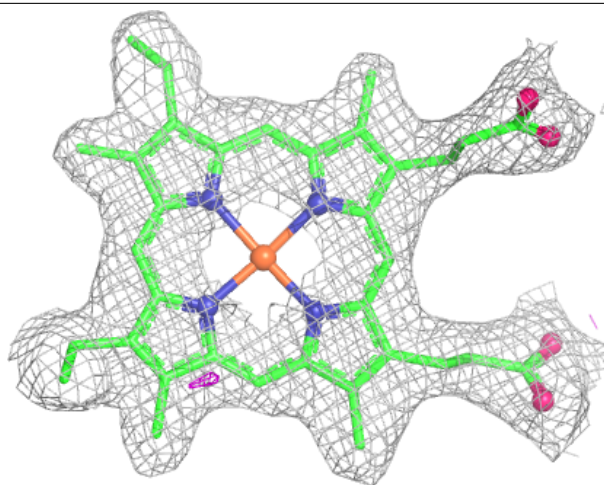
Electron density around HEC C 402:

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



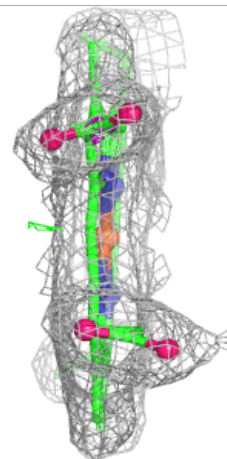
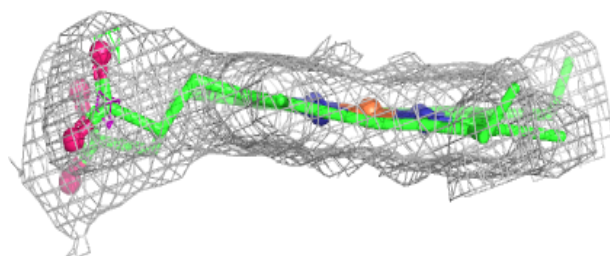
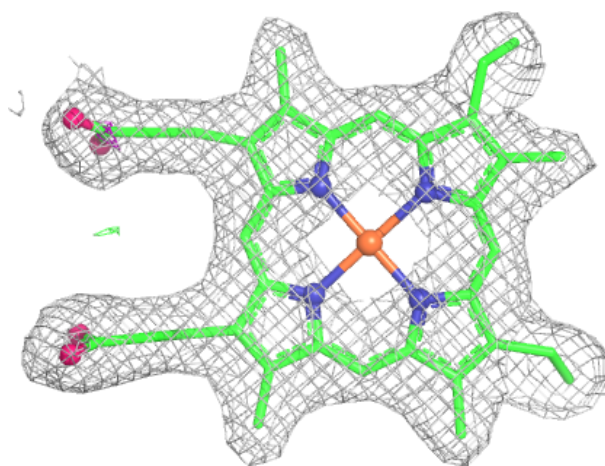
Electron density around HEC C 403:

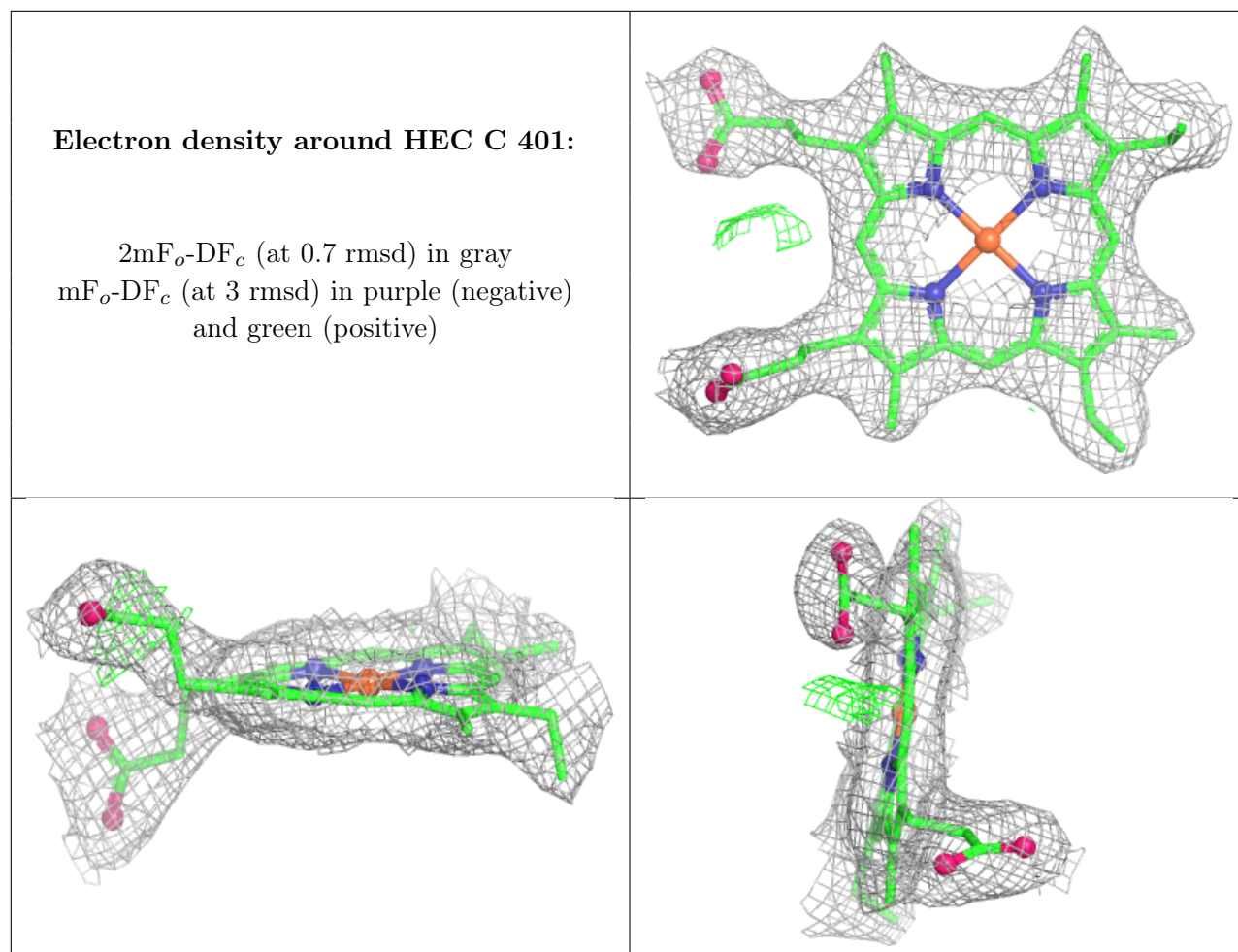
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC C 404:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.