Full wwPDB X-ray Structure Validation Report (i)

Aug 24, 2026 – 02:53 pm BST

PDB ID	:	9S39 / pdb_00009s39
Title	:	Serial crystallography structure of a photosynthetic reaction center using a go niometer-compatible 96-well chip-based platform
Authors	:	Ghosh, S.; Banacore, A.
Deposited on	:	2025-07-24
Resolution	:	3.30 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

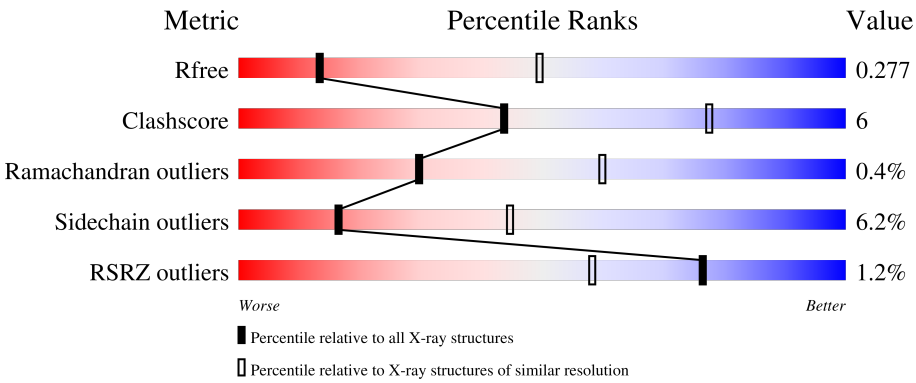
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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

Mol	Chain	Length	Quality of chain
1	C	332	.% 83% 14% .
2	H	242	3% 74% 21% . .
3	L	273	.% 82% 16% .
4	M	323	.% 83% 15% .
5	D	8	62% 38%

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	HEC	C	401	X	-	-	-
6	HEC	C	402	X	-	-	-
6	HEC	C	403	X	-	-	-
6	HEC	C	404	X	-	-	-
7	SO4	H	303	-	-	X	-
8	BCB	L	400	X	-	-	-
8	BCB	L	401	X	-	-	-
8	BCB	M	403	X	-	-	-
8	BCB	M	404	X	-	-	-
9	BPB	L	402	X	-	-	-
9	BPB	M	405	X	-	-	-

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 19384 atoms, of which 9349 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	C	332	5112	1640	2509	466	479	18	0	2	0

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	H	242	3753	1213	1854	324	361	1	0	2	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	?	-	LEU	deletion	UNP P06008
H	?	-	GLY	deletion	UNP P06008
H	?	-	LEU	deletion	UNP P06008
H	?	-	VAL	deletion	UNP P06008
H	?	-	LYS	deletion	UNP P06008
H	?	-	LEU	deletion	UNP P06008
H	?	-	ALA	deletion	UNP P06008
H	?	-	PRO	deletion	UNP P06008

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	L	273	4223	1459	2052	350	355	7	0	1	0

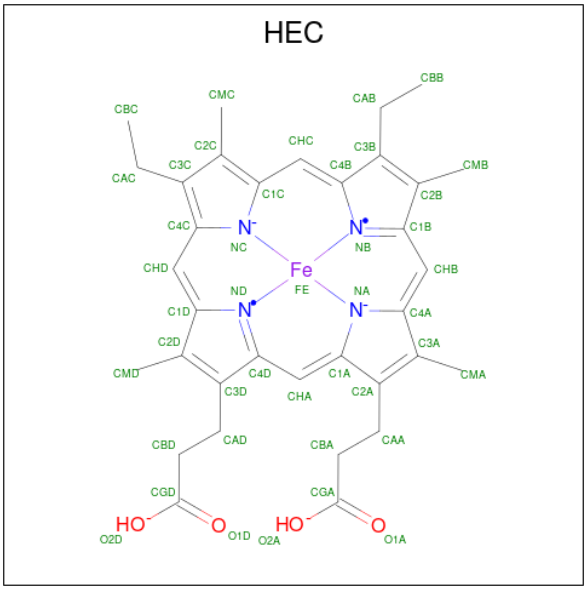
- Molecule 4 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
4	M	323	4945	1702	2390	419	423	11	0	2	0

- Molecule 5 is a protein called FME-TYR-HIS-GLY-ALA-LEU-ALA-GLN.

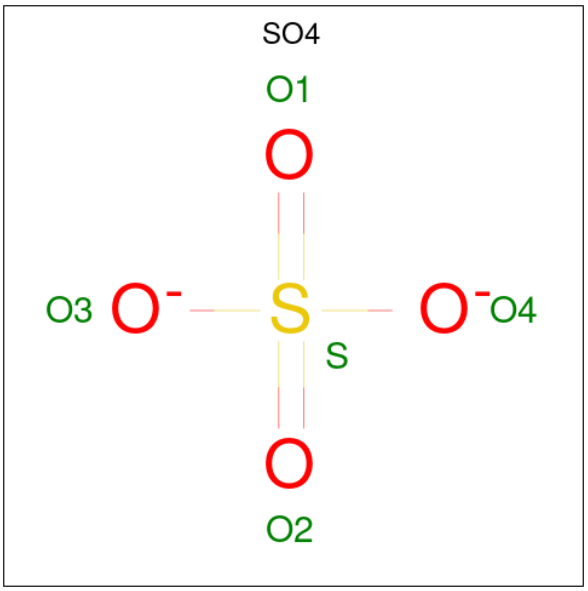
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
5	D	8	118	40	55	11	11	1	0	0	0

- Molecule 6 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



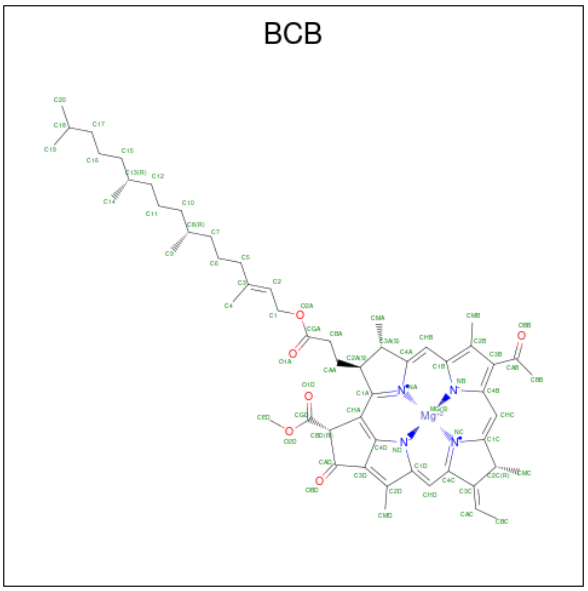
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Fe	H	N	O		
6	C	1	61	34	1	18	4	4	0	0
			Total	C	Fe	H	N	O		
6	C	1	61	34	1	18	4	4	0	0
			Total	C	Fe	H	N	O		
6	C	1	61	34	1	18	4	4	0	0
			Total	C	Fe	H	N	O		
6	C	1	61	34	1	18	4	4	0	0

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O_4S) (labeled as "Ligand of Interest" by depositor).



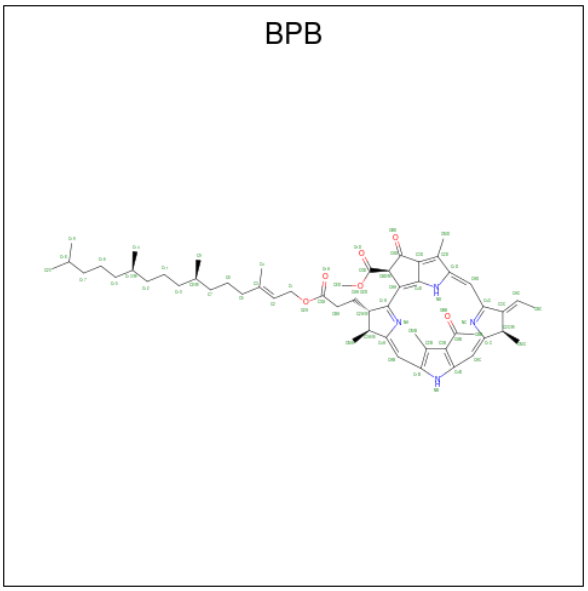
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total O S 5 4 1	0	0
7	C	1	Total O S 5 4 1	0	0
7	H	1	Total O S 5 4 1	0	0
7	H	1	Total O S 5 4 1	0	0
7	H	1	Total O S 5 4 1	0	0
7	M	1	Total O S 5 4 1	0	0
7	M	1	Total O S 5 4 1	0	0
7	M	1	Total O S 5 4 1	0	0

- Molecule 8 is BACTERIOCHLOROPHYLL B (CCD ID: BCB) (formula: $C_{55}H_{72}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	Mg	N	O		
8	L	1	123	55	57	1	4	6	0	0
			Total	C	H	Mg	N	O		
8	L	1	123	55	57	1	4	6	0	0
			Total	C	H	Mg	N	O		
8	M	1	123	55	57	1	4	6	0	0
			Total	C	H	Mg	N	O		
8	M	1	123	55	57	1	4	6	0	0

- Molecule 9 is BACTERIOPHEOPHYTIN B (CCD ID: BPB) (formula: $C_{55}H_{74}N_4O_6$) (labeled as "Ligand of Interest" by depositor).

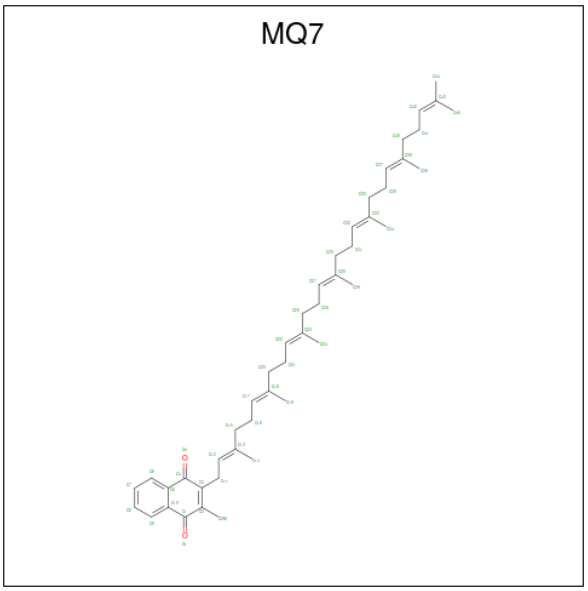


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
9	L	1	123	55	58	4	6	0	0
			Total	C	H	N	O		
9	M	1	123	55	58	4	6	0	0

- Molecule 10 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

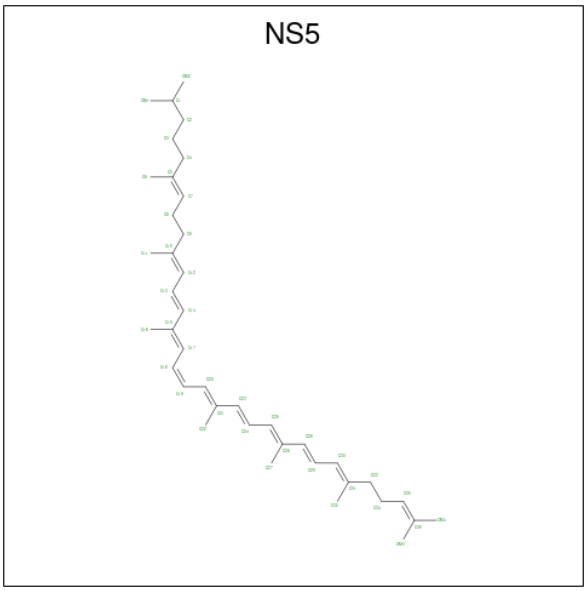
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
10	M	1	1	1	0	0

- Molecule 11 is MENAQUINONE-7 (CCD ID: MQ7) (formula: $C_{46}H_{64}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
11	M	1	85	46	37	2	0	0

- Molecule 12 is 15-cis-1,2-dihydroneurosporene (CCD ID: NS5) (formula: $C_{40}H_{60}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	H		
12	M	1	76	40	36	0	0

- Molecule 13 is water.

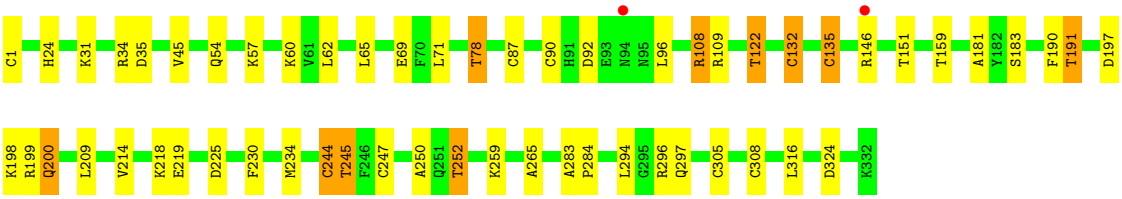
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
13	C	19	19	19	0	0
			Total	O		
13	H	10	10	10	0	0
			Total	O		
13	L	10	10	10	0	0
			Total	O		
13	M	10	10	10	0	0

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.

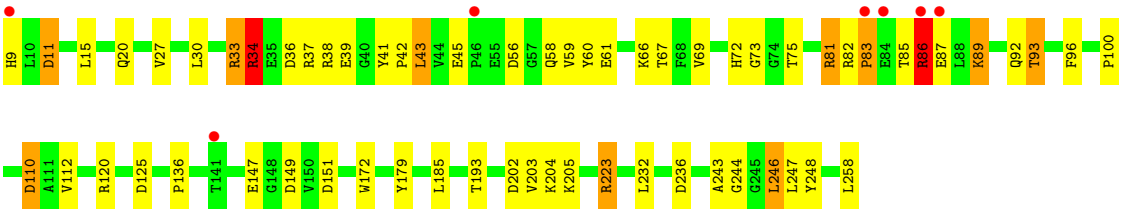
• Molecule 1: Photosynthetic reaction center cytochrome c subunit

Chain C:



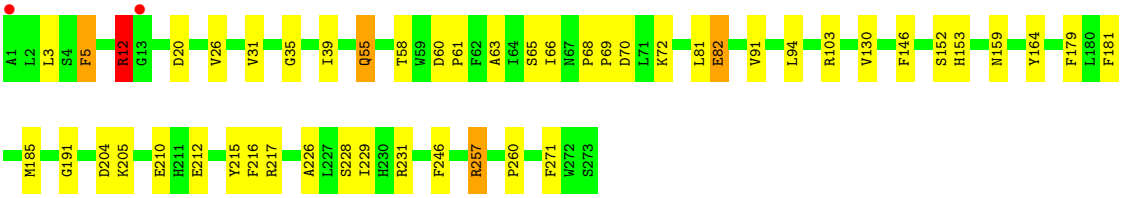
• Molecule 2: Reaction center protein H chain

Chain H:



• Molecule 3: Reaction center protein L chain

Chain L:



• Molecule 4: Reaction center protein M chain

Chain M:

• Molecule 5: FME-TYR-HIS-GLY-ALA-LEU-ALA-GLN

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	226.50Å 226.50Å 113.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.00 – 3.30 60.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	98.9 (60.00-3.30) 99.0 (60.00-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.98 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.100)	Depositor
R, R_{free}	0.246 , 0.296 0.225 , 0.277	Depositor DCC
R_{free} test set	8510 reflections (4.30%)	wwPDB-VP
Wilson B-factor (Å^2)	21.0	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 79.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	19384	wwPDB-VP
Average B, all atoms (Å^2)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.90% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: HEC, NS5, FE2, MQ7, BPB, SO4, FME, BCB

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	0.69	0/2670	1.42	13/3637 (0.4%)
2	H	0.78	3/1942 (0.2%)	1.56	25/2651 (0.9%)
3	L	0.69	0/2259	1.49	25/3084 (0.8%)
4	M	0.72	0/2659	1.46	20/3637 (0.5%)
5	D	0.68	0/54	1.17	1/72 (1.4%)
All	All	0.72	3/9584 (0.0%)	1.48	84/13081 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	5
2	H	0	9
3	L	0	3
4	M	0	4
All	All	0	21

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	58	GLN	C-N	-7.12	1.25	1.33
2	H	59	VAL	N-CA	-6.16	1.38	1.46
2	H	58	GLN	CA-C	-5.96	1.45	1.52

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	122	THR	CA-CB-OG1	-13.29	89.67	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	58	GLN	CA-C-N	-12.92	98.06	120.29
2	H	58	GLN	C-N-CA	-12.92	98.06	120.29
2	H	58	GLN	CA-C-O	11.64	132.76	120.42
2	H	151	ASP	CB-CA-C	9.38	118.88	110.44
1	C	92	ASP	CA-CB-CG	8.59	121.19	112.60
4	M	78[A]	HIS	CA-CB-CG	-7.95	105.85	113.80
2	H	193	THR	CA-CB-OG1	-7.95	97.68	109.60
3	L	212	GLU	N-CA-CB	7.91	121.85	109.82
2	H	223	ARG	CB-CA-C	-7.77	96.23	109.83
1	C	198	LYS	CB-CA-C	7.77	125.32	109.55
3	L	20	ASP	CB-CA-C	-7.71	96.36	110.63
1	C	245	THR	CA-CB-OG1	7.59	120.98	109.60
4	M	182	ASP	CA-CB-CG	7.31	119.91	112.60
4	M	214	PHE	N-CA-CB	7.30	121.07	110.20
1	C	225	ASP	CA-CB-CG	7.04	119.64	112.60
4	M	314	ASP	CA-CB-CG	7.02	119.62	112.60
3	L	271	PHE	CA-CB-CG	7.00	120.81	113.80
1	C	191	THR	CA-CB-OG1	-7.00	99.10	109.60
1	C	190	PHE	CA-CB-CG	-6.88	106.92	113.80
3	L	179	PHE	CA-CB-CG	-6.83	106.97	113.80
4	M	89	PHE	CA-CB-CG	6.65	120.45	113.80
4	M	27	ASP	CA-CB-CG	6.59	119.19	112.60
4	M	164	THR	CA-CB-OG1	-6.57	99.75	109.60
2	H	66	LYS	N-CA-CB	-6.52	100.41	110.85
4	M	290	ASP	CA-CB-CG	6.49	119.09	112.60
3	L	212	GLU	N-CA-C	-6.45	103.15	111.02
2	H	93	THR	OG1-CB-CG2	-6.44	96.42	109.30
4	M	119	PHE	CA-CB-CG	-6.37	107.43	113.80
2	H	147	GLU	CB-CA-C	6.34	120.04	109.89
3	L	130	VAL	N-CA-CB	6.34	117.55	110.51
3	L	146	PHE	CA-CB-CG	6.26	120.06	113.80
2	H	89	LYS	N-CA-CB	-6.25	101.39	110.70
4	M	253	THR	CA-CB-OG1	-6.15	100.38	109.60
3	L	70	ASP	CA-CB-CG	6.11	118.71	112.60
2	H	247	LEU	N-CA-CB	-6.06	102.25	110.67
4	M	274	VAL	N-CA-CB	6.04	118.02	110.47
1	C	197	ASP	CA-CB-CG	5.95	118.55	112.60
2	H	110	ASP	CA-CB-CG	5.94	118.54	112.60
4	M	109	ASP	CA-CB-CG	5.94	118.54	112.60
3	L	164	TYR	CB-CA-C	5.92	120.55	111.02
1	C	135	CYS	CB-CA-C	-5.88	99.79	110.56
2	H	202	ASP	CA-CB-CG	5.84	118.44	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	200	GLN	CB-CA-C	5.71	119.17	109.75
2	H	75	THR	CA-CB-OG1	-5.71	101.04	109.60
3	L	91	VAL	N-CA-CB	5.69	118.28	110.54
3	L	12	ARG	N-CA-CB	5.69	118.65	110.06
4	M	85	PHE	CA-CB-CG	-5.69	108.11	113.80
3	L	210	GLU	CB-CG-CD	5.67	122.24	112.60
2	H	203	VAL	N-CA-CB	-5.64	105.81	111.90
3	L	26	VAL	N-CA-CB	-5.64	105.33	112.15
2	H	34	ARG	CB-CA-C	5.59	120.93	110.70
2	H	39	GLU	CB-CG-CD	5.58	122.08	112.60
3	L	5	PHE	N-CA-CB	-5.58	102.00	111.20
2	H	149	ASP	CA-CB-CG	5.57	118.17	112.60
4	M	142	THR	CA-CB-OG1	-5.55	101.27	109.60
4	M	228	GLY	CA-C-N	5.51	126.10	119.98
4	M	228	GLY	C-N-CA	5.51	126.10	119.98
3	L	82	GLU	CB-CA-C	-5.48	102.78	111.17
3	L	204	ASP	CB-CA-C	5.48	121.75	110.40
1	C	324	ASP	CA-CB-CG	5.47	118.07	112.60
3	L	216	PHE	CA-CB-CG	-5.45	108.35	113.80
1	C	230	PHE	CA-CB-CG	5.43	119.23	113.80
2	H	67	THR	CA-CB-OG1	-5.34	101.58	109.60
3	L	153	HIS	CA-CB-CG	5.31	119.11	113.80
2	H	11	ASP	CA-CB-CG	5.29	117.89	112.60
1	C	24	HIS	CB-CA-C	5.27	115.85	109.85
2	H	85	THR	CA-CB-OG1	-5.24	101.75	109.60
4	M	19	VAL	N-CA-CB	5.22	117.25	110.99
5	D	3	HIS	CA-CB-CG	5.22	119.02	113.80
3	L	146	PHE	CB-CA-C	5.18	116.87	109.26
4	M	71	PHE	CB-CA-C	5.17	119.38	110.79
3	L	205	LYS	N-CA-CB	5.17	117.87	110.06
3	L	215	TYR	N-CA-CB	5.15	117.62	109.94
3	L	246	PHE	CA-CB-CG	5.12	118.92	113.80
2	H	96	PHE	N-CA-CB	-5.11	102.81	110.17
4	M	278	ALA	O-C-N	5.10	127.33	122.07
3	L	60	ASP	CA-CB-CG	5.07	117.67	112.60
2	H	149	ASP	CB-CA-C	5.06	117.98	109.48
3	L	191	GLY	CA-C-N	5.03	125.53	119.94
3	L	191	GLY	C-N-CA	5.03	125.53	119.94
4	M	287	THR	OG1-CB-CG2	-5.02	99.25	109.30
2	H	179	TYR	CB-CA-C	5.01	119.26	109.35
2	H	59	VAL	N-CA-CB	-5.00	101.49	110.95

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	108	ARG	Sidechain
1	C	109	ARG	Sidechain
1	C	199	ARG	Sidechain
1	C	296	ARG	Sidechain
1	C	34	ARG	Sidechain
2	H	120	ARG	Sidechain
2	H	223	ARG	Sidechain
2	H	33	ARG	Sidechain
2	H	34	ARG	Sidechain
2	H	38	ARG	Sidechain
2	H	41	TYR	Peptide
2	H	81	ARG	Sidechain
2	H	82	ARG	Sidechain
2	H	86[A]	ARG	Sidechain
3	L	12	ARG	Sidechain
3	L	217	ARG	Sidechain
3	L	257	ARG	Sidechain
4	M	130	ARG	Sidechain
4	M	136	ARG	Sidechain
4	M	226	ARG	Sidechain
4	M	245	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2603	2509	2587	45	0
2	H	1899	1854	1884	33	0
3	L	2171	2052	2092	16	0
4	M	2555	2390	2443	24	0
5	D	63	55	58	1	0
6	C	172	72	128	35	0
7	C	10	0	0	0	0
7	H	15	0	0	3	0
7	M	15	0	0	0	0
8	L	132	114	144	3	0
8	M	132	114	144	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	L	65	58	74	1	0
9	M	65	58	74	9	0
10	M	1	0	0	0	0
11	M	48	37	64	2	0
12	M	40	36	60	2	0
13	C	19	0	0	0	0
13	H	10	0	0	1	0
13	L	10	0	0	1	0
13	M	10	0	0	0	0
All	All	10035	9349	9752	120	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 6.

All (120) 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)
2:H:56:ASP:O	2:H:60:TYR:CD1	1.65	1.46
1:C:135:CYS:SG	6:C:402:HEC:CAC	2.27	1.21
1:C:90:CYS:SG	6:C:401:HEC:CAC	2.30	1.20
2:H:86[A]:ARG:HG2	2:H:86[A]:ARG:HH21	1.05	1.18
1:C:87:CYS:SG	6:C:401:HEC:CAB	2.34	1.15
2:H:56:ASP:O	2:H:60:TYR:HD1	0.76	1.11
1:C:247:CYS:SG	6:C:403:HEC:CAC	2.43	1.07
2:H:86[A]:ARG:HG2	2:H:86[A]:ARG:NH2	1.65	1.03
1:C:244:CYS:SG	6:C:403:HEC:CAB	2.48	1.01
1:C:308:CYS:SG	6:C:404:HEC:CAC	2.49	0.99
1:C:305:CYS:SG	6:C:404:HEC:CAB	2.55	0.95
1:C:305:CYS:SG	6:C:404:HEC:HBB3	2.08	0.93
2:H:86[A]:ARG:NH2	2:H:86[A]:ARG:CG	2.32	0.92
2:H:56:ASP:C	2:H:60:TYR:CD1	2.49	0.89
1:C:305:CYS:SG	6:C:404:HEC:CBB	2.64	0.86
1:C:87:CYS:SG	6:C:401:HEC:CBB	2.65	0.85
1:C:135:CYS:SG	6:C:402:HEC:C3C	2.66	0.83
1:C:90:CYS:SG	6:C:401:HEC:C3C	2.68	0.82
2:H:56:ASP:HB3	2:H:60:TYR:CE1	2.15	0.80
1:C:132:CYS:SG	6:C:402:HEC:CAB	2.70	0.80
1:C:135:CYS:SG	6:C:402:HEC:CBC	2.72	0.76
2:H:34:ARG:NH1	7:H:303:SO4:O1	2.20	0.75
9:M:405:BPB:HHC	9:M:405:BPB:HBBB	1.68	0.74
4:M:160:CYS:SG	12:M:406:NS5:H322	2.29	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:86[A]:ARG:CZ	2:H:86[A]:ARG:CB	2.63	0.70
2:H:93:THR:HG22	2:H:100:PRO:O	1.93	0.69
1:C:87:CYS:SG	6:C:401:HEC:HAB	2.32	0.69
1:C:132:CYS:SG	6:C:402:HEC:CBB	2.82	0.68
1:C:247:CYS:SG	6:C:403:HEC:CBC	2.82	0.68
1:C:132:CYS:SG	6:C:402:HEC:HBB3	2.35	0.67
1:C:78:THR:HG23	6:C:401:HEC:HMC3	1.79	0.65
9:M:405:BPB:C7	9:M:405:BPB:H4	2.26	0.64
1:C:135:CYS:SG	6:C:402:HEC:HBC3	2.37	0.64
1:C:244:CYS:SG	6:C:403:HEC:CBB	2.86	0.63
3:L:181:PHE:HB3	9:M:405:BPB:HBBA	1.80	0.63
9:M:405:BPB:H4	9:M:405:BPB:H7A	1.80	0.63
2:H:86[A]:ARG:CZ	2:H:86[A]:ARG:HB3	2.27	0.62
6:C:401:HEC:HMB1	6:C:401:HEC:HBB3	1.80	0.62
1:C:247:CYS:SG	6:C:403:HEC:C3C	2.88	0.61
4:M:283:LEU:O	4:M:287:THR:HG21	2.01	0.61
3:L:55:GLN:HE21	3:L:81:LEU:HD11	1.66	0.60
2:H:56:ASP:CB	2:H:60:TYR:CE1	2.84	0.59
2:H:20:GLN:HG2	4:M:202:PHE:CE2	2.37	0.59
1:C:90:CYS:SG	6:C:401:HEC:CBC	2.91	0.59
4:M:275:MET:HG2	9:M:405:BPB:HBCA	1.83	0.59
8:M:403:BCB:HHC	8:M:403:BCB:HBB2	1.86	0.58
2:H:9:HIS:N	5:D:8:GLN:O	2.37	0.58
1:C:247:CYS:SG	6:C:403:HEC:HBC3	2.44	0.57
4:M:283:LEU:O	4:M:287:THR:CG2	2.53	0.57
1:C:183:SER:HB3	1:C:234:MET:HE3	1.87	0.56
1:C:90:CYS:SG	6:C:401:HEC:HAC	2.42	0.56
2:H:34:ARG:NH1	7:H:303:SO4:S	2.80	0.55
8:L:401:BCB:HMD2	8:M:404:BCB:HBB3	1.89	0.55
12:M:406:NS5:C7	12:M:406:NS5:H113	2.37	0.55
4:M:78[A]:HIS:N	4:M:78[A]:HIS:CD2	2.75	0.54
1:C:87:CYS:SG	6:C:401:HEC:HBB3	2.45	0.54
4:M:157:CYS:HA	4:M:161:ILE:HB	1.90	0.54
2:H:34:ARG:NH1	7:H:303:SO4:O4	2.41	0.53
3:L:231:ARG:HD3	4:M:5:THR:O	2.08	0.53
8:M:404:BCB:HBB2	8:M:404:BCB:HMB3	1.90	0.53
2:H:37:ARG:HD2	2:H:61:GLU:HG3	1.90	0.52
2:H:86[A]:ARG:NH2	2:H:86[A]:ARG:HA	2.24	0.52
2:H:86[A]:ARG:NH2	2:H:86[A]:ARG:CB	2.73	0.50
1:C:250:ALA:H	3:L:159:ASN:HD21	1.59	0.50
1:C:308:CYS:SG	6:C:404:HEC:CBC	3.00	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:66:ILE:HD13	9:M:405:BPB:H9A	1.93	0.50
3:L:5:PHE:HB3	4:M:239:ARG:HH21	1.77	0.49
1:C:308:CYS:SG	6:C:404:HEC:HAC	2.49	0.49
3:L:35:GLY:CA	3:L:103:ARG:HD2	2.42	0.49
4:M:102:MET:HE1	4:M:169:TRP:CZ2	2.48	0.49
3:L:181:PHE:CD2	9:M:405:BPB:HBB	2.47	0.48
4:M:257:ASN:HA	11:M:402:MQ7:H143	1.95	0.48
2:H:27:VAL:HG11	4:M:269:PHE:CE1	2.49	0.48
2:H:56:ASP:O	2:H:60:TYR:CE1	2.52	0.47
2:H:86[A]:ARG:NH2	2:H:86[A]:ARG:CA	2.78	0.47
2:H:136:PRO:HA	2:H:172:TRP:HA	1.95	0.47
3:L:103:ARG:NH1	13:L:501:HOH:O	2.42	0.47
2:H:11:ASP:HB2	13:H:403:HOH:O	2.15	0.46
1:C:45:VAL:HG21	1:C:69:GLU:HA	1.97	0.46
2:H:125:ASP:HB2	2:H:232:LEU:HD21	1.95	0.46
4:M:101:GLY:HA2	4:M:167:GLY:O	2.16	0.46
1:C:305:CYS:SG	6:C:404:HEC:C3B	3.03	0.46
2:H:89:LYS:HB3	2:H:110:ASP:HB3	1.98	0.46
8:L:400:BCB:H2C	8:M:404:BCB:H2C	1.98	0.46
1:C:283:ALA:N	1:C:284:PRO:CD	2.79	0.46
1:C:308:CYS:SG	6:C:404:HEC:C3C	3.04	0.45
1:C:244:CYS:SG	6:C:403:HEC:HAB	2.50	0.45
6:C:401:HEC:CBB	6:C:401:HEC:HMB1	2.45	0.45
1:C:252:THR:HG21	4:M:293:TYR:CE2	2.53	0.44
4:M:69:ILE:HG22	4:M:73:MET:SD	2.56	0.44
2:H:56:ASP:CA	2:H:60:TYR:CE1	3.00	0.44
4:M:11:GLN:HE21	4:M:13:ARG:HH12	1.65	0.44
2:H:56:ASP:C	2:H:60:TYR:CE1	2.94	0.43
9:M:405:BPB:HHC	9:M:405:BPB:CBB	2.44	0.43
3:L:68:PRO:HB2	3:L:69:PRO:HD2	2.01	0.43
4:M:235:GLN:NE2	4:M:242:ALA:HB3	2.32	0.43
8:L:401:BCB:CMD	8:M:404:BCB:HBB3	2.48	0.43
9:M:405:BPB:H55	9:M:405:BPB:HMC	2.00	0.43
1:C:214:VAL:HA	1:C:219:GLU:HG3	2.01	0.43
2:H:43:LEU:HD22	3:L:3:LEU:HA	2.00	0.42
4:M:102:MET:HG2	4:M:167:GLY:HA2	2.01	0.42
4:M:250:TRP:CD1	11:M:402:MQ7:C3	3.03	0.42
3:L:58:THR:HG21	3:L:63:ALA:HB3	2.02	0.42
1:C:245:THR:HG22	3:L:159:ASN:HD22	1.84	0.42
2:H:33:ARG:NH1	2:H:36:ASP:OD2	2.49	0.42
2:H:244:GLY:O	2:H:248:TYR:HB2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:152:SER:HA	4:M:305:TYR:OH	2.20	0.41
1:C:62:LEU:HB3	1:C:65:LEU:HD13	2.00	0.41
1:C:265:ALA:HB2	4:M:312:THR:HG21	2.03	0.41
2:H:86[A]:ARG:CZ	2:H:86[A]:ARG:HA	2.50	0.41
3:L:226:ALA:O	3:L:229:ILE:HG22	2.19	0.41
1:C:35:ASP:HB3	1:C:316:LEU:HA	2.02	0.41
2:H:243:ALA:O	2:H:246:LEU:HB2	2.20	0.41
9:L:402:BPB:NC	9:L:402:BPB:ND	2.69	0.41
1:C:181:ALA:O	3:L:260:PRO:HB2	2.20	0.40
1:C:244:CYS:SG	6:C:403:HEC:HBB3	2.59	0.40
6:C:401:HEC:CBB	6:C:401:HEC:CMB	3.00	0.40
1:C:259:LYS:NZ	4:M:304:ASP:OD1	2.53	0.40
1:C:265:ALA:HB2	4:M:312:THR:CG2	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	330/332 (99%)	312 (94%)	18 (6%)	0	100	100
2	H	238/242 (98%)	224 (94%)	12 (5%)	2 (1%)	16	45
3	L	271/273 (99%)	259 (96%)	11 (4%)	1 (0%)	30	60
4	M	321/323 (99%)	309 (96%)	10 (3%)	2 (1%)	21	52
5	D	6/8 (75%)	6 (100%)	0	0	100	100
All	All	1166/1178 (99%)	1110 (95%)	51 (4%)	5 (0%)	30	60

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	66[A]	ILE

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Mol	Chain	Res	Type
2	H	73	GLY
4	M	192	GLY
4	M	193	ASN
2	H	83	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	281/281 (100%)	259 (92%)	22 (8%)	11	36
2	H	202/202 (100%)	183 (91%)	19 (9%)	8	30
3	L	218/218 (100%)	207 (95%)	11 (5%)	22	50
4	M	249/249 (100%)	242 (97%)	7 (3%)	38	62
5	D	4/4 (100%)	4 (100%)	0	100	100
All	All	954/954 (100%)	895 (94%)	59 (6%)	16	45

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1	CYS
1	C	31	LYS
1	C	54	GLN
1	C	57	LYS
1	C	60	LYS
1	C	71	LEU
1	C	78	THR
1	C	96	LEU
1	C	108	ARG
1	C	122	THR
1	C	132	CYS
1	C	146[A]	ARG
1	C	151	THR
1	C	159	THR
1	C	191	THR

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Mol	Chain	Res	Type
1	C	200	GLN
1	C	209	LEU
1	C	218	LYS
1	C	244	CYS
1	C	252	THR
1	C	294	LEU
1	C	297	GLN
2	H	15	LEU
2	H	30	LEU
2	H	42	PRO
2	H	43	LEU
2	H	45	GLU
2	H	69	VAL
2	H	72	HIS
2	H	81	ARG
2	H	83	PRO
2	H	86[A]	ARG
2	H	87[A]	GLU
2	H	92	GLN
2	H	112	VAL
2	H	185	LEU
2	H	204	LYS
2	H	205	LYS
2	H	236	ASP
2	H	246	LEU
2	H	258	LEU
3	L	12	ARG
3	L	31	VAL
3	L	39	ILE
3	L	55	GLN
3	L	61	PRO
3	L	72	LYS
3	L	82	GLU
3	L	94	LEU
3	L	185	MET
3	L	228	SER
3	L	257	ARG
4	M	66	ILE
4	M	71	PHE
4	M	85	PHE
4	M	194	PHE
4	M	214	PHE

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Mol	Chain	Res	Type
4	M	298	LYS
4	M	323	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	54	GLN
1	C	263	GLN
1	C	280	ASN
1	C	302	GLN
2	H	229	GLN
3	L	55	GLN
3	L	159	ASN
3	L	183	ASN
4	M	4	GLN
4	M	11	GLN
4	M	45	GLN
4	M	87	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	FME	D	1	5	8,9,10	0.52	0	7,9,11	1.48	1 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	FME	D	1	5	-	2/7/9/11	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	1	FME	O-C-CA	-3.56	115.44	124.78

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	1	FME	CA-CB-CG-SD
5	D	1	FME	C-CA-CB-CG

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 21 ligands modelled in this entry, 1 is monoatomic - leaving 20 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	SO4	C	406	-	4,4,4	0.35	0	6,6,6	0.30	0
8	BCB	M	403	4	68,74,74	1.20	7 (10%)	79,115,115	1.94	14 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	SO4	C	405	-	4,4,4	0.28	0	6,6,6	0.20	0
12	NS5	M	406	-	39,39,39	1.72	5 (12%)	44,46,46	1.79	9 (20%)
8	BCB	L	400	3	68,74,74	1.50	13 (19%)	79,115,115	1.76	10 (12%)
7	SO4	H	302	-	4,4,4	0.26	0	6,6,6	0.43	0
11	MQ7	M	402	-	49,49,49	0.67	1 (2%)	60,63,63	0.80	1 (1%)
6	HEC	C	403	1	50,50,50	2.39	16 (32%)	68,82,82	2.08	21 (30%)
6	HEC	C	404	1	50,50,50	1.85	9 (18%)	68,82,82	2.19	29 (42%)
6	HEC	C	401	1	50,50,50	2.22	16 (32%)	68,82,82	1.94	19 (27%)
9	BPB	L	402	-	57,70,70	1.03	5 (8%)	56,101,101	1.38	5 (8%)
7	SO4	M	409	-	4,4,4	0.36	0	6,6,6	0.19	0
6	HEC	C	402	1	50,50,50	2.27	15 (30%)	68,82,82	1.97	25 (36%)
8	BCB	M	404	4	68,74,74	1.74	10 (14%)	79,115,115	1.94	15 (18%)
9	BPB	M	405	-	57,70,70	1.32	5 (8%)	56,101,101	1.58	9 (16%)
7	SO4	M	407	-	4,4,4	0.34	0	6,6,6	0.22	0
7	SO4	H	303	-	4,4,4	0.30	0	6,6,6	0.12	0
7	SO4	M	408	-	4,4,4	0.31	0	6,6,6	0.32	0
8	BCB	L	401	3	68,74,74	1.31	9 (13%)	79,115,115	1.48	15 (18%)
7	SO4	H	301	-	4,4,4	0.34	0	6,6,6	0.20	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
12	NS5	M	406	-	-	7/43/43/43	-
8	BCB	L	400	3	2/2/26/26	9/41/137/137	-
6	HEC	C	402	1	1/1/7/7	9/14/54/54	-
8	BCB	M	404	4	2/2/26/26	11/41/137/137	-
9	BPB	M	405	-	1/1/23/23	18/37/105/105	0/5/6/6
8	BCB	M	403	4	3/3/26/26	22/41/137/137	-
8	BCB	L	401	3	2/2/26/26	11/41/137/137	-
6	HEC	C	403	1	1/1/7/7	5/14/54/54	-
11	MQ7	M	402	-	-	3/41/61/61	0/2/2/2
6	HEC	C	404	1	1/1/7/7	9/14/54/54	-
6	HEC	C	401	1	1/1/7/7	7/14/54/54	-
9	BPB	L	402	-	1/1/23/23	6/37/105/105	0/5/6/6

All (111) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	401	HEC	FE-NB	8.55	2.21	1.94
8	M	404	BCB	MG-NB	8.34	2.22	2.05
6	C	403	HEC	FE-ND	7.42	2.17	1.94
6	C	403	HEC	FE-NC	6.61	2.17	1.95
6	C	402	HEC	FE-ND	6.02	2.13	1.94
6	C	404	HEC	FE-ND	5.82	2.12	1.94
6	C	402	HEC	FE-NB	5.68	2.12	1.94
6	C	402	HEC	C3B-C2B	5.58	1.48	1.36
6	C	403	HEC	C3B-C2B	5.54	1.48	1.36
12	M	406	NS5	C25-C26	5.50	1.43	1.35
9	M	405	BPB	C1B-C2B	5.49	1.45	1.39
12	M	406	NS5	C17-C15	5.10	1.42	1.35
6	C	404	HEC	C3B-C2B	5.09	1.47	1.36
8	M	404	BCB	C3B-C4B	4.95	1.50	1.41
8	L	400	BCB	MG-NB	4.94	2.15	2.05
6	C	401	HEC	FE-NA	4.85	2.11	1.95
6	C	404	HEC	FE-NA	4.70	2.11	1.95
8	L	400	BCB	C4D-ND	-4.62	1.31	1.37
6	C	402	HEC	FE-NC	4.54	2.10	1.95
12	M	406	NS5	C20-C21	4.42	1.41	1.35
8	L	401	BCB	C3B-C4B	4.30	1.49	1.41
6	C	403	HEC	C4A-C3A	-4.23	1.37	1.45
6	C	401	HEC	C3B-C2B	4.21	1.45	1.36
9	L	402	BPB	C4D-CHA	4.20	1.46	1.39
8	L	401	BCB	MG-NB	4.17	2.14	2.05
6	C	402	HEC	FE-NA	4.17	2.09	1.95
6	C	401	HEC	FE-NC	4.09	2.09	1.95
8	L	401	BCB	CHC-C4B	4.07	1.48	1.39
9	M	405	BPB	C4D-CHA	4.06	1.46	1.39
6	C	402	HEC	C3C-C2C	3.94	1.49	1.38
8	M	404	BCB	MG-NA	-3.83	1.97	2.06
6	C	404	HEC	CHB-C4A	3.73	1.45	1.38
6	C	403	HEC	FE-NB	3.73	2.06	1.94
8	M	403	BCB	CHC-C4B	3.68	1.47	1.39
8	L	400	BCB	MG-ND	-3.67	1.98	2.05
8	M	404	BCB	MG-ND	-3.53	1.98	2.05
8	M	404	BCB	C1B-NB	3.52	1.42	1.37
8	M	403	BCB	C3B-C4B	3.49	1.47	1.41
8	L	400	BCB	C3B-C4B	3.44	1.47	1.41
6	C	403	HEC	CHA-C1A	3.39	1.45	1.38
6	C	402	HEC	CHB-C4A	3.38	1.44	1.38
9	M	405	BPB	C3D-C2D	3.38	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	403	HEC	CHD-C1D	3.37	1.45	1.38
6	C	403	HEC	C1A-C2A	-3.33	1.39	1.45
11	M	402	MQ7	C3-C2	3.22	1.41	1.35
6	C	401	HEC	C4D-C3D	-3.18	1.39	1.45
8	M	404	BCB	C4D-ND	-3.16	1.33	1.37
6	C	402	HEC	C4B-NB	-3.12	1.34	1.40
9	M	405	BPB	C3A-C2A	-3.11	1.51	1.54
6	C	402	HEC	C1A-C2A	-3.09	1.39	1.45
6	C	401	HEC	CHD-C1D	3.06	1.44	1.38
6	C	403	HEC	CHB-C4A	3.02	1.44	1.38
6	C	401	HEC	C1C-C2C	-3.01	1.36	1.43
8	M	403	BCB	C3D-C4D	-2.97	1.37	1.44
8	L	400	BCB	CHC-C4B	2.94	1.46	1.39
6	C	404	HEC	C4B-NB	-2.91	1.35	1.40
9	L	402	BPB	C1B-C2B	2.89	1.42	1.39
8	L	400	BCB	CHB-C1B	2.85	1.45	1.39
6	C	403	HEC	CHA-C4D	2.84	1.45	1.39
6	C	403	HEC	C3C-C2C	2.82	1.46	1.38
6	C	403	HEC	C4C-NC	-2.81	1.34	1.39
6	C	404	HEC	FE-NB	2.81	2.03	1.94
8	L	400	BCB	MG-NA	-2.77	1.99	2.06
6	C	401	HEC	C1A-C2A	-2.77	1.40	1.45
8	L	401	BCB	C4B-NB	2.75	1.41	1.37
6	C	402	HEC	CHC-C4B	2.69	1.44	1.38
9	M	405	BPB	CBD-CGD	-2.67	1.48	1.52
6	C	402	HEC	CAB-C3B	-2.65	1.44	1.51
8	M	404	BCB	CHC-C4B	2.65	1.45	1.39
8	M	403	BCB	CHD-C1D	2.62	1.43	1.38
8	M	404	BCB	C4B-NB	2.60	1.41	1.37
8	L	400	BCB	C3D-C4D	-2.58	1.38	1.44
8	M	403	BCB	CHB-C1B	2.57	1.45	1.39
6	C	401	HEC	CAB-C3B	-2.57	1.44	1.51
8	L	400	BCB	C1D-C2D	-2.52	1.40	1.45
9	L	402	BPB	CBD-CGD	-2.51	1.49	1.52
8	L	401	BCB	C1D-C2D	-2.51	1.40	1.45
6	C	403	HEC	FE-NA	2.49	2.03	1.95
8	M	404	BCB	C1D-ND	2.49	1.40	1.37
12	M	406	NS5	C18-C17	-2.47	1.35	1.43
8	L	400	BCB	C4C-C3C	-2.46	1.39	1.44
6	C	403	HEC	C1C-C2C	-2.45	1.37	1.43
6	C	402	HEC	C4C-NC	-2.45	1.35	1.39
6	C	401	HEC	C4C-NC	-2.45	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	401	HEC	C3C-C2C	2.44	1.45	1.38
6	C	401	HEC	FE-ND	2.43	2.02	1.94
8	L	401	BCB	MG-NC	2.42	2.12	2.06
6	C	401	HEC	C4A-C3A	-2.41	1.40	1.45
8	L	401	BCB	CHB-C1B	2.37	1.44	1.39
6	C	404	HEC	C1A-C2A	-2.35	1.41	1.45
6	C	403	HEC	CHC-C4B	2.33	1.43	1.38
8	M	404	BCB	C3D-C2D	2.31	1.45	1.39
6	C	401	HEC	O2A-CGA	-2.28	1.23	1.30
6	C	402	HEC	C4A-C3A	-2.27	1.40	1.45
8	L	401	BCB	C4C-C3C	-2.27	1.40	1.44
6	C	402	HEC	CHA-C1A	2.25	1.42	1.38
6	C	404	HEC	FE-NC	2.25	2.02	1.95
6	C	401	HEC	CHC-C4B	2.24	1.43	1.38
8	M	403	BCB	MG-ND	2.24	2.10	2.05
8	M	403	BCB	C4B-NB	2.21	1.40	1.37
9	L	402	BPB	C1D-C2D	2.21	1.42	1.39
6	C	401	HEC	C1D-ND	-2.20	1.36	1.40
12	M	406	NS5	C24-C23	2.19	1.40	1.34
6	C	402	HEC	C1B-C2B	-2.18	1.40	1.44
8	L	400	BCB	OBB-CAB	-2.15	1.18	1.23
9	L	402	BPB	C3A-C2A	-2.12	1.52	1.54
8	L	400	BCB	CAA-C2A	-2.11	1.50	1.54
8	L	400	BCB	O2A-CGA	2.08	1.39	1.33
6	C	404	HEC	C3C-C2C	2.07	1.44	1.38
8	L	401	BCB	O2D-CGD	2.05	1.38	1.33
6	C	403	HEC	C4A-NA	-2.04	1.35	1.39

All (172) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	M	404	BCB	C1C-NC-C4C	-9.31	102.52	106.71
8	M	403	BCB	CHD-C1D-ND	-7.64	117.43	124.45
8	L	400	BCB	C1C-NC-C4C	-7.38	103.39	106.71
8	L	400	BCB	CHC-C4B-NB	-6.99	116.86	124.26
6	C	404	HEC	CBB-CAB-C3B	6.48	130.30	112.43
12	M	406	NS5	C18-C19-C20	5.96	135.68	123.47
6	C	403	HEC	CHA-C4D-ND	-5.87	118.04	124.42
6	C	403	HEC	CHB-C1B-NB	-5.78	118.14	124.42
9	L	402	BPB	C4D-CHA-CBD	-5.65	105.96	108.52
8	M	403	BCB	C1C-NC-C4C	-5.58	104.20	106.71
6	C	401	HEC	CBC-CAC-C3C	5.54	127.71	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	M	404	BCB	CHD-C1D-ND	-5.45	119.45	124.45
9	M	405	BPB	C1A-C2A-C3A	-5.21	97.88	102.84
8	M	403	BCB	CMD-C2D-C1D	5.21	133.89	124.71
6	C	401	HEC	CHB-C1B-NB	-5.19	118.78	124.42
8	L	401	BCB	CHD-C1D-ND	-5.02	119.84	124.45
6	C	403	HEC	CBC-CAC-C3C	4.89	125.91	112.43
12	M	406	NS5	C18-C17-C15	4.80	134.16	127.31
6	C	402	HEC	CHA-C4D-ND	-4.79	119.22	124.42
6	C	402	HEC	CBC-CAC-C3C	4.66	125.27	112.43
8	M	403	BCB	CHC-C4B-NB	-4.64	119.35	124.26
8	M	404	BCB	CHC-C4B-NB	-4.62	119.36	124.26
9	M	405	BPB	C2B-C1B-NB	-4.62	106.34	109.53
6	C	401	HEC	CBA-CAA-C2A	-4.54	100.03	112.63
6	C	404	HEC	CBD-CAD-C3D	4.48	125.08	112.63
6	C	403	HEC	CAD-CBD-CGD	4.33	122.91	113.60
6	C	403	HEC	CAB-C3B-C2B	4.29	134.86	127.53
6	C	401	HEC	C4A-CHB-C1B	4.17	135.04	126.06
6	C	402	HEC	CAC-C3C-C2C	4.15	133.51	126.86
9	M	405	BPB	C1-C2-C3	4.14	133.20	126.04
6	C	404	HEC	CAC-C3C-C2C	4.09	133.42	126.86
6	C	404	HEC	CBC-CAC-C3C	4.01	123.49	112.43
6	C	403	HEC	CHA-C4D-C3D	3.97	130.68	124.84
8	L	400	BCB	O2A-C1-C2	3.94	118.98	108.64
6	C	404	HEC	CHA-C4D-ND	-3.93	120.14	124.42
9	L	402	BPB	CMA-C3A-C4A	-3.86	105.93	114.38
8	M	404	BCB	C3C-C4C-NC	3.85	114.78	110.57
8	L	400	BCB	CHD-C1D-ND	-3.72	121.04	124.45
6	C	404	HEC	CHB-C1B-NB	-3.71	120.38	124.42
8	M	404	BCB	O2D-CGD-CBD	3.67	117.79	111.27
8	M	403	BCB	C2C-C1C-CHC	-3.64	115.06	123.64
8	M	403	BCB	C6-C5-C3	3.63	122.96	113.45
12	M	406	NS5	C22-C21-C20	-3.62	117.85	122.92
8	L	401	BCB	CHC-C1C-NC	3.59	129.48	124.51
6	C	402	HEC	C1C-CHC-C4B	3.59	134.84	126.34
8	M	403	BCB	CHD-C1D-C2D	3.56	132.96	125.48
6	C	404	HEC	CHB-C4A-NA	-3.53	120.62	124.44
6	C	404	HEC	CAB-C3B-C2B	3.49	133.50	127.53
8	M	403	BCB	O2D-CGD-CBD	3.38	117.28	111.27
6	C	404	HEC	CAD-C3D-C4D	3.37	130.55	124.66
6	C	402	HEC	C1B-C2B-C3B	-3.37	103.41	106.96
6	C	401	HEC	CHD-C1D-ND	-3.35	120.24	124.37
8	M	404	BCB	C2C-C1C-CHC	-3.34	115.78	123.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	401	HEC	C2B-C1B-NB	3.30	113.83	109.88
6	C	401	HEC	C4C-NC-C1C	3.30	108.58	105.35
8	M	403	BCB	C4B-C3B-C2B	-3.29	103.06	108.36
8	L	401	BCB	C2C-C1C-CHC	-3.25	115.98	123.64
8	M	404	BCB	CHB-C1B-NB	-3.24	120.82	124.26
8	L	401	BCB	CMD-C2D-C1D	3.20	130.35	124.71
6	C	402	HEC	CHB-C1B-NB	-3.19	120.95	124.42
12	M	406	NS5	C14-C15-C17	-3.19	114.04	118.94
6	C	404	HEC	CHD-C1D-ND	-3.19	120.44	124.37
8	L	400	BCB	C3C-C4C-NC	3.18	114.05	110.57
6	C	404	HEC	CAD-C3D-C2D	-3.14	122.03	127.88
6	C	403	HEC	C4B-C3B-C2B	-3.13	102.34	106.90
6	C	403	HEC	CAD-C3D-C4D	3.11	130.09	124.66
8	M	403	BCB	C4D-CHA-C1A	3.06	124.97	121.25
6	C	401	HEC	CHB-C4A-NA	-3.03	121.16	124.44
6	C	402	HEC	CBA-CAA-C2A	-3.03	104.22	112.63
9	L	402	BPB	C2B-C1B-NB	-3.01	107.45	109.53
8	M	404	BCB	C2B-C1B-NB	3.01	112.25	110.23
8	L	400	BCB	CMD-C2D-C1D	2.99	129.98	124.71
6	C	403	HEC	C1C-CHC-C4B	2.95	133.34	126.34
6	C	402	HEC	CAD-C3D-C4D	2.93	129.78	124.66
6	C	401	HEC	CAD-CBD-CGD	2.93	119.91	113.60
8	M	404	BCB	C3D-C2D-C1D	-2.91	101.85	105.83
6	C	401	HEC	C1B-C2B-C3B	-2.91	103.90	106.96
12	M	406	NS5	C25-C24-C23	2.90	132.26	123.22
6	C	404	HEC	C1C-CHC-C4B	2.86	133.13	126.34
6	C	404	HEC	C4C-C3C-C2C	-2.84	102.42	106.89
6	C	403	HEC	CAC-C3C-C2C	2.84	131.41	126.86
6	C	404	HEC	C3C-C4C-NC	2.83	113.31	110.15
12	M	406	NS5	C16-C15-C14	2.80	122.49	118.08
6	C	402	HEC	CAC-C3C-C4C	-2.80	121.03	124.92
6	C	403	HEC	C4C-CHD-C1D	2.79	132.96	126.34
8	L	401	BCB	CHD-C1D-C2D	2.79	131.32	125.48
6	C	402	HEC	O1A-CGA-CBA	-2.78	114.15	123.08
6	C	404	HEC	C1D-ND-C4D	-2.78	102.20	105.07
6	C	403	HEC	C1A-CHA-C4D	2.77	132.03	126.06
8	M	404	BCB	CAA-C2A-C1A	2.77	121.05	111.97
6	C	404	HEC	C2D-C1D-ND	2.77	113.12	109.84
6	C	402	HEC	C1C-C2C-C3C	-2.73	103.64	106.83
6	C	402	HEC	C4B-NB-C1B	2.71	107.87	105.07
6	C	404	HEC	C4A-CHB-C1B	2.71	131.90	126.06
8	L	401	BCB	CHB-C1B-NB	-2.68	121.42	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	L	401	BCB	C4D-CHA-C1A	2.66	124.49	121.25
12	M	406	NS5	C23-C21-C20	2.65	123.00	118.94
6	C	403	HEC	C2B-C1B-NB	2.60	113.00	109.88
8	M	403	BCB	CHC-C1C-NC	2.58	128.08	124.51
8	L	400	BCB	C4-C3-C5	2.58	119.61	115.27
9	M	405	BPB	C4-C3-C2	-2.57	117.07	123.68
6	C	402	HEC	CHD-C1D-ND	-2.57	121.20	124.37
6	C	401	HEC	C4C-CHD-C1D	2.57	132.43	126.34
9	M	405	BPB	C2D-C1D-ND	-2.56	107.76	109.53
8	M	404	BCB	C2D-C1D-ND	2.52	111.96	110.10
6	C	404	HEC	C4B-C3B-C2B	-2.51	103.23	106.90
6	C	402	HEC	C4C-CHD-C1D	2.51	132.28	126.34
8	L	400	BCB	C2C-C1C-CHC	-2.49	117.77	123.64
6	C	403	HEC	O2D-CGD-CBD	2.49	122.03	114.03
6	C	404	HEC	CMD-C2D-C1D	2.47	128.80	125.04
6	C	403	HEC	CHB-C1B-C2B	2.47	128.83	124.98
6	C	404	HEC	C1A-CHA-C4D	2.46	131.37	126.06
6	C	402	HEC	C1A-CHA-C4D	2.46	131.36	126.06
9	M	405	BPB	C5-C3-C2	2.46	126.08	121.12
8	M	404	BCB	CHC-C1C-NC	2.44	127.89	124.51
6	C	404	HEC	C3D-C4D-ND	2.43	112.70	110.36
8	M	403	BCB	C4-C3-C5	2.42	119.35	115.27
12	M	406	NS5	C19-C18-C17	2.42	128.44	123.47
8	L	401	BCB	CMD-C2D-C3D	-2.42	122.05	127.61
6	C	403	HEC	C4C-C3C-C2C	-2.41	103.09	106.89
6	C	404	HEC	C4C-CHD-C1D	2.40	132.03	126.34
6	C	402	HEC	C4C-NC-C1C	2.39	107.69	105.35
8	M	404	BCB	CHB-C4A-NA	2.39	127.82	124.51
6	C	402	HEC	CHA-C4D-C3D	2.38	128.34	124.84
8	M	403	BCB	CMD-C2D-C3D	-2.36	122.17	127.61
8	L	401	BCB	CHB-C4A-NA	2.34	127.75	124.51
8	M	404	BCB	O2D-CGD-O1D	-2.34	119.27	123.84
6	C	402	HEC	C1A-C2A-C3A	2.33	110.17	107.13
8	L	401	BCB	CHA-C1A-NA	-2.33	121.06	126.40
9	M	405	BPB	OBD-CAD-CBD	-2.32	122.42	125.82
12	M	406	NS5	C13-C14-C15	2.30	132.87	126.42
6	C	404	HEC	CHB-C4A-C3A	2.29	130.29	125.48
9	L	402	BPB	CED-O2D-CGD	2.29	121.12	115.94
6	C	402	HEC	C2A-C1A-NA	-2.29	108.09	110.32
6	C	403	HEC	CHD-C1D-ND	-2.28	121.57	124.37
6	C	402	HEC	O2A-CGA-CBA	2.27	121.33	114.03
8	L	400	BCB	C4B-C3B-C2B	-2.27	104.71	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	404	HEC	CHB-C1B-C2B	2.26	128.52	124.98
8	L	401	BCB	CHC-C4B-NB	-2.26	121.87	124.26
8	L	401	BCB	C4A-NA-C1A	2.26	107.72	106.71
6	C	402	HEC	C2B-C1B-NB	2.24	112.57	109.88
6	C	403	HEC	CHD-C4C-NC	-2.24	119.72	123.85
8	M	403	BCB	CHA-C1A-NA	-2.22	121.31	126.40
6	C	401	HEC	C1D-C2D-C3D	2.22	109.29	106.96
11	M	402	MQ7	C15-C16-C17	2.21	119.16	111.88
6	C	401	HEC	CBB-CAB-C3B	2.21	118.52	112.43
6	C	403	HEC	O1D-CGD-CBD	-2.20	116.00	123.08
6	C	401	HEC	C1C-CHC-C4B	2.19	131.53	126.34
6	C	401	HEC	CBD-CAD-C3D	-2.18	106.56	112.63
6	C	401	HEC	O1D-CGD-CBD	-2.18	116.07	123.08
6	C	401	HEC	CHC-C4B-NB	-2.17	121.70	124.37
8	L	400	BCB	C2A-C3A-C4A	-2.16	98.37	101.87
6	C	401	HEC	O2D-CGD-CBD	2.14	120.91	114.03
9	M	405	BPB	OBB-CAB-C3B	2.14	123.78	119.99
9	L	402	BPB	C1A-C2A-C3A	-2.13	100.82	102.84
6	C	402	HEC	CAB-C3B-C2B	2.11	131.14	127.53
8	L	401	BCB	C4B-C3B-C2B	-2.10	104.98	108.36
6	C	404	HEC	C4B-NB-C1B	2.10	107.24	105.07
6	C	402	HEC	CBB-CAB-C3B	2.10	118.22	112.43
6	C	404	HEC	CMA-C3A-C4A	2.09	128.39	124.71
6	C	404	HEC	CHC-C1C-NC	-2.08	120.01	123.85
6	C	402	HEC	CHC-C1C-NC	-2.08	120.03	123.85
9	M	405	BPB	C4D-CHA-CBD	-2.06	107.58	108.52
6	C	402	HEC	CMC-C2C-C3C	2.05	130.05	125.61
8	L	401	BCB	C4D-C3D-CAD	2.04	110.51	108.10
6	C	401	HEC	CHD-C4C-C3C	2.04	129.82	125.36
6	C	404	HEC	C1D-C2D-C3D	-2.03	104.82	106.96
6	C	403	HEC	C3B-C4B-NB	2.03	112.42	110.17
6	C	404	HEC	C2A-C1A-NA	2.02	112.29	110.32
6	C	403	HEC	CMC-C2C-C3C	2.02	129.98	125.61
8	L	401	BCB	O1D-CGD-CBD	-2.02	120.36	124.48
8	M	404	BCB	C17-C16-C15	-2.00	104.04	113.24

All (15) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	C	401	HEC	NA
6	C	402	HEC	NA
6	C	403	HEC	NA

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Mol	Chain	Res	Type	Atom
6	C	404	HEC	NA
8	L	400	BCB	NC
8	L	400	BCB	NA
8	L	401	BCB	NC
8	L	401	BCB	NA
8	M	403	BCB	NC
8	M	403	BCB	ND
8	M	403	BCB	NA
8	M	404	BCB	NC
8	M	404	BCB	NA
9	L	402	BPB	C13
9	M	405	BPB	C13

All (117) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	M	403	BCB	C11-C10-C8-C9
8	M	404	BCB	C2A-CAA-CBA-CGA
8	M	404	BCB	CAD-CBD-CGD-O1D
8	M	404	BCB	CAD-CBD-CGD-O2D
9	M	405	BPB	C1-C2-C3-C4
9	M	405	BPB	C1-C2-C3-C5
9	M	405	BPB	C4C-C3C-CAC-CBC
12	M	406	NS5	C9-C10-C12-C13
12	M	406	NS5	C11-C10-C12-C13
6	C	404	HEC	C2C-C3C-CAC-CBC
6	C	402	HEC	C4C-C3C-CAC-CBC
6	C	403	HEC	C2B-C3B-CAB-CBB
6	C	403	HEC	C4B-C3B-CAB-CBB
6	C	402	HEC	C2B-C3B-CAB-CBB
6	C	402	HEC	C2C-C3C-CAC-CBC
6	C	402	HEC	C4B-C3B-CAB-CBB
6	C	401	HEC	C4C-C3C-CAC-CBC
6	C	403	HEC	C4C-C3C-CAC-CBC
6	C	404	HEC	C4C-C3C-CAC-CBC
6	C	401	HEC	C4B-C3B-CAB-CBB
6	C	401	HEC	C2B-C3B-CAB-CBB
6	C	404	HEC	C2B-C3B-CAB-CBB
6	C	404	HEC	C4B-C3B-CAB-CBB
6	C	403	HEC	C2C-C3C-CAC-CBC
8	M	403	BCB	C3-C5-C6-C7
6	C	401	HEC	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
8	L	400	BCB	C4-C3-C5-C6
8	M	403	BCB	C4-C3-C5-C6
8	L	400	BCB	C2-C3-C5-C6
8	M	403	BCB	C2-C3-C5-C6
8	M	403	BCB	CBD-CGD-O2D-CED
9	L	402	BPB	C8-C10-C11-C12
9	M	405	BPB	C2-C3-C5-C6
9	M	405	BPB	C11-C10-C8-C9
8	M	403	BCB	C5-C6-C7-C8
9	M	405	BPB	C13-C15-C16-C17
6	C	404	HEC	C2D-C3D-CAD-CBD
12	M	406	NS5	CM1-C1-C2-C3
8	M	403	BCB	C11-C12-C13-C14
9	M	405	BPB	C14-C13-C15-C16
9	M	405	BPB	C10-C11-C12-C13
6	C	404	HEC	C4D-C3D-CAD-CBD
8	L	400	BCB	C14-C13-C15-C16
12	M	406	NS5	CM2-C1-C2-C3
6	C	404	HEC	C3D-CAD-CBD-CGD
8	M	403	BCB	C16-C17-C18-C19
8	M	404	BCB	C13-C15-C16-C17
8	M	403	BCB	C4B-C3B-CAB-CBB
8	L	400	BCB	C12-C13-C15-C16
8	L	401	BCB	C11-C12-C13-C15
9	L	402	BPB	C11-C12-C13-C15
9	M	405	BPB	C11-C10-C8-C7
9	M	405	BPB	C11-C12-C13-C15
9	M	405	BPB	C5-C6-C7-C8
8	L	401	BCB	C14-C13-C15-C16
8	M	403	BCB	C6-C7-C8-C9
9	L	402	BPB	C11-C12-C13-C14
9	M	405	BPB	C8-C10-C11-C12
8	M	403	BCB	C6-C7-C8-C10
8	M	403	BCB	C12-C13-C15-C16
8	M	404	BCB	C11-C12-C13-C15
9	M	405	BPB	C4-C3-C5-C6
11	M	402	MQ7	C37-C38-C40-C41
8	L	400	BCB	CHA-CBD-CGD-O1D
9	M	405	BPB	O1A-CGA-O2A-C1
11	M	402	MQ7	C39-C38-C40-C41
8	M	404	BCB	C11-C12-C13-C14
9	M	405	BPB	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
9	M	405	BPB	CBA-CGA-O2A-C1
8	L	400	BCB	CAD-CBD-CGD-O1D
9	M	405	BPB	C2C-C3C-CAC-CBC
8	M	403	BCB	C10-C11-C12-C13
8	M	403	BCB	C11-C10-C8-C7
9	M	405	BPB	C6-C7-C8-C10
8	M	403	BCB	C2B-C3B-CAB-CBB
8	M	403	BCB	C16-C17-C18-C20
8	M	403	BCB	C14-C13-C15-C16
8	M	404	BCB	C3-C5-C6-C7
8	M	403	BCB	C11-C12-C13-C15
8	L	400	BCB	C15-C16-C17-C18
8	L	401	BCB	C13-C15-C16-C17
8	L	401	BCB	C8-C10-C11-C12
6	C	402	HEC	CAA-CBA-CGA-O1A
8	L	400	BCB	C16-C17-C18-C20
9	L	402	BPB	O2A-C1-C2-C3
6	C	401	HEC	CAA-CBA-CGA-O1A
6	C	402	HEC	CAA-CBA-CGA-O2A
12	M	406	NS5	C6-C5-C7-C8
12	M	406	NS5	C1-C2-C3-C4
8	L	401	BCB	C3-C5-C6-C7
8	L	401	BCB	C16-C17-C18-C19
6	C	401	HEC	CAA-CBA-CGA-O2A
6	C	404	HEC	CAD-CBD-CGD-O2D
8	M	403	BCB	C1-C2-C3-C4
8	L	401	BCB	C11-C12-C13-C14
8	M	404	BCB	O1A-CGA-O2A-C1
8	M	403	BCB	CAD-CBD-CGD-O2D
9	L	402	BPB	CAD-CBD-CGD-O2D
12	M	406	NS5	C13-C14-C15-C17
6	C	402	HEC	CAD-CBD-CGD-O2D
6	C	402	HEC	CAD-CBD-CGD-O1D
8	L	400	BCB	C16-C17-C18-C19
6	C	402	HEC	C3D-CAD-CBD-CGD
8	L	401	BCB	CHA-CBD-CGD-O2D
8	M	404	BCB	CHA-CBD-CGD-O2D
6	C	404	HEC	CAD-CBD-CGD-O1D
9	L	402	BPB	C12-C13-C15-C16
8	L	401	BCB	C11-C10-C8-C9
8	M	404	BCB	CBA-CGA-O2A-C1
8	M	403	BCB	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
8	M	404	BCB	C5-C6-C7-C8
8	L	401	BCB	C11-C10-C8-C7
8	L	401	BCB	C12-C13-C15-C16
6	C	401	HEC	CAD-CBD-CGD-O2D
8	M	403	BCB	C2B-C3B-CAB-OBB
11	M	402	MQ7	C13-C15-C16-C17
6	C	403	HEC	CAA-CBA-CGA-O2A

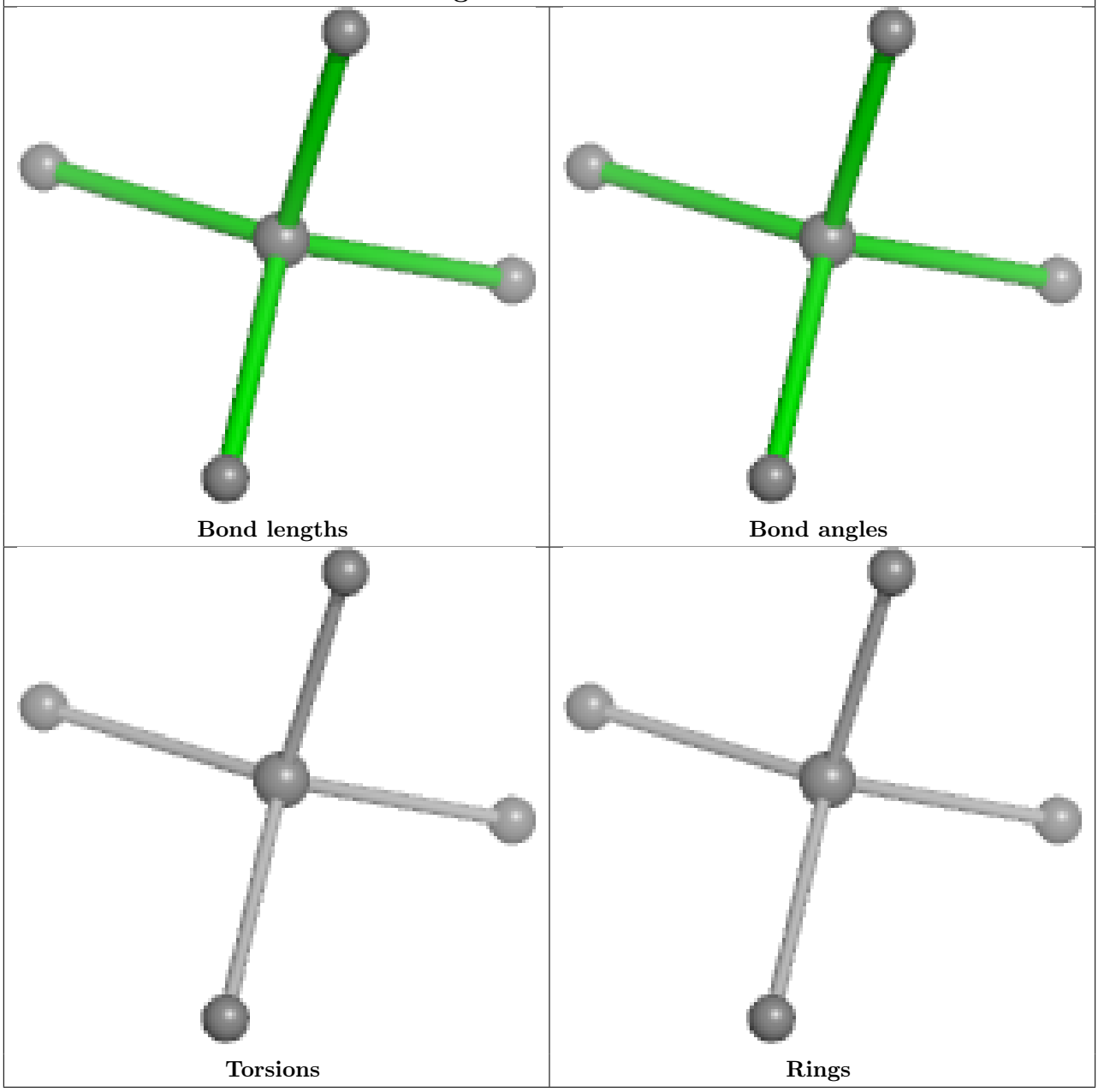
There are no ring outliers.

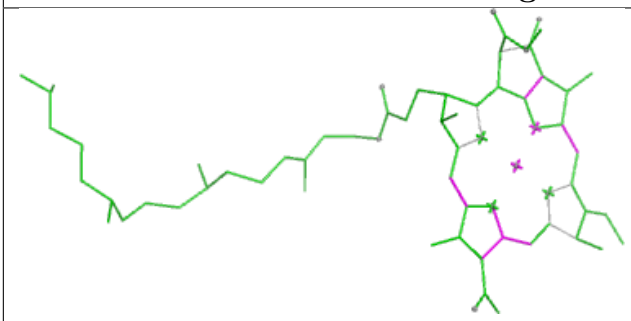
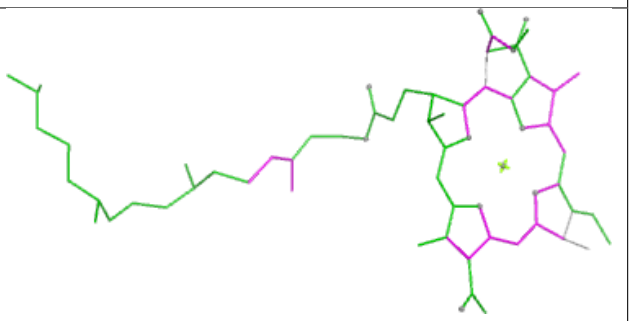
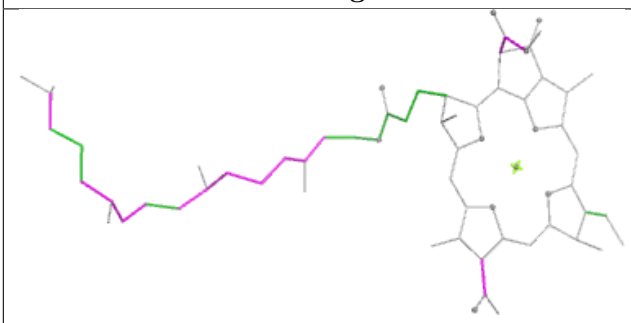
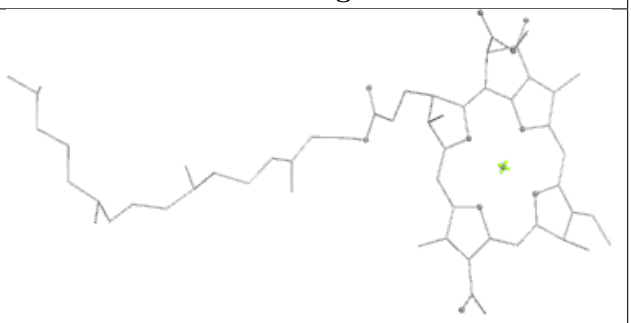
13 monomers are involved in 57 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	M	403	BCB	1	0
12	M	406	NS5	2	0
8	L	400	BCB	1	0
11	M	402	MQ7	2	0
6	C	403	HEC	8	0
6	C	404	HEC	8	0
6	C	401	HEC	12	0
9	L	402	BPB	1	0
6	C	402	HEC	7	0
8	M	404	BCB	4	0
9	M	405	BPB	9	0
7	H	303	SO4	3	0
8	L	401	BCB	2	0

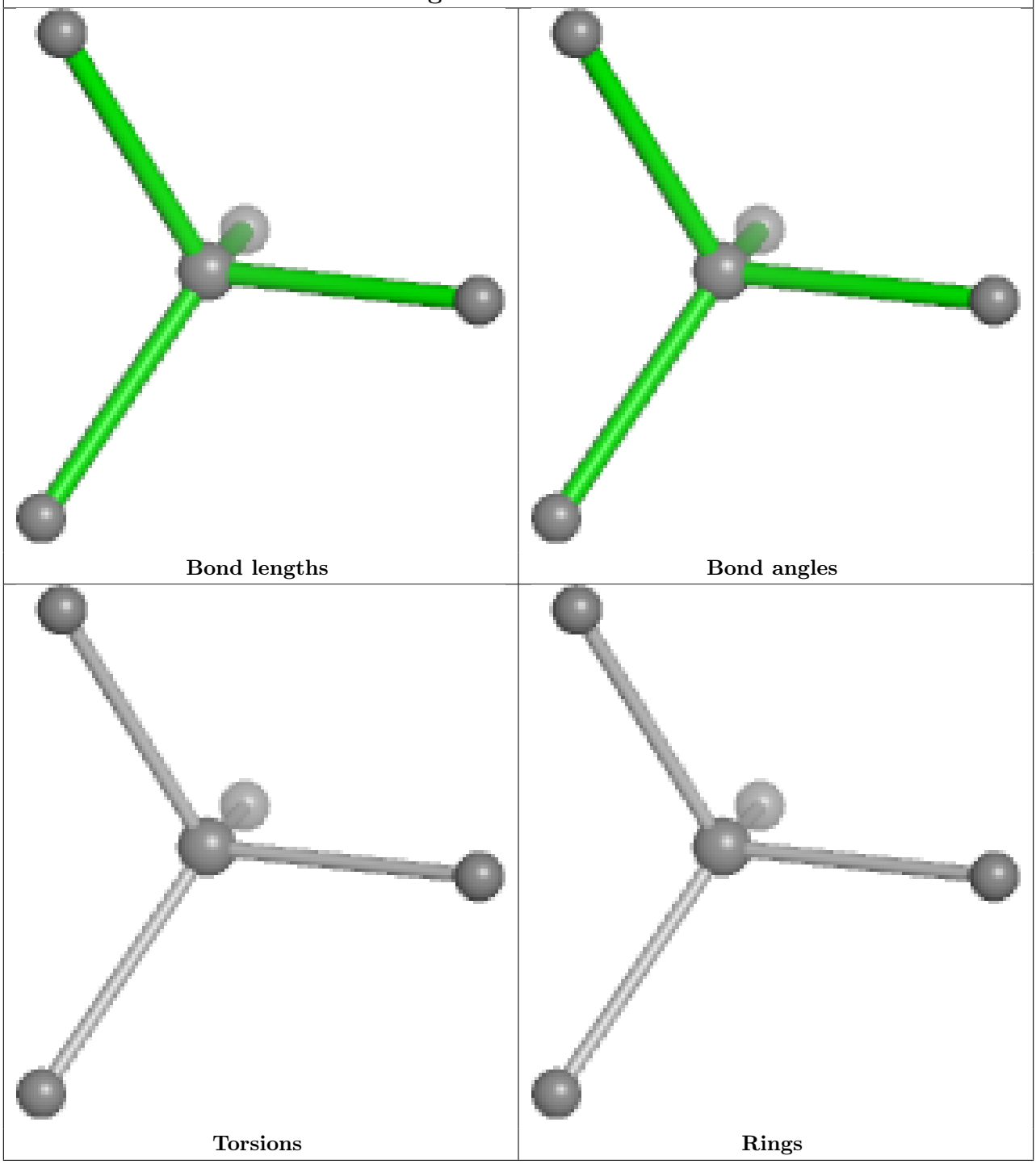
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand SO4 C 406

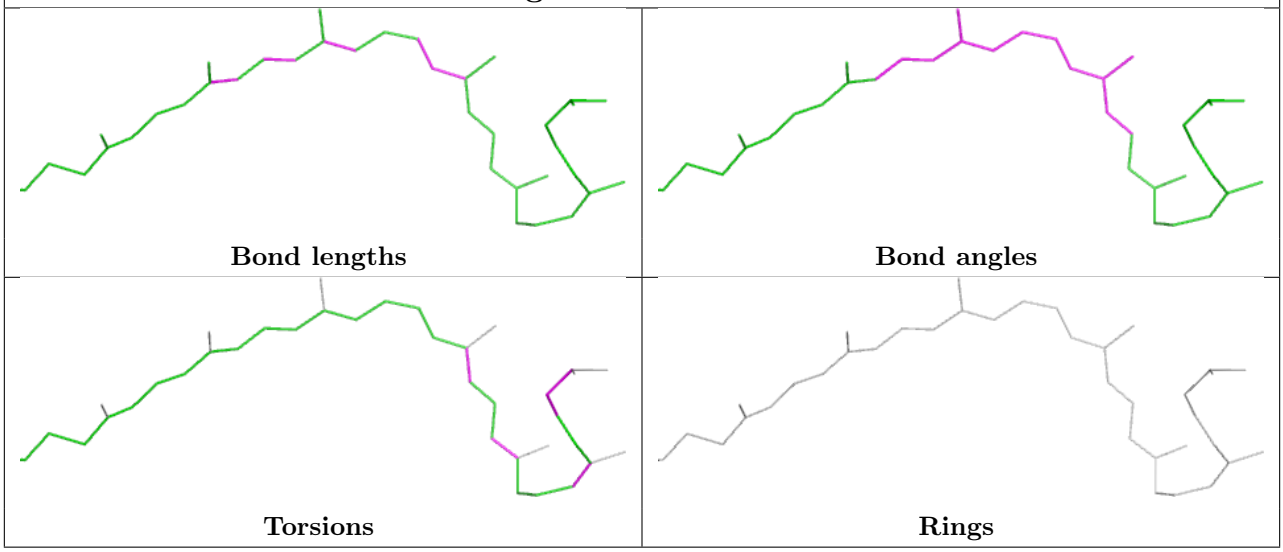


Ligand BCB M 403	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

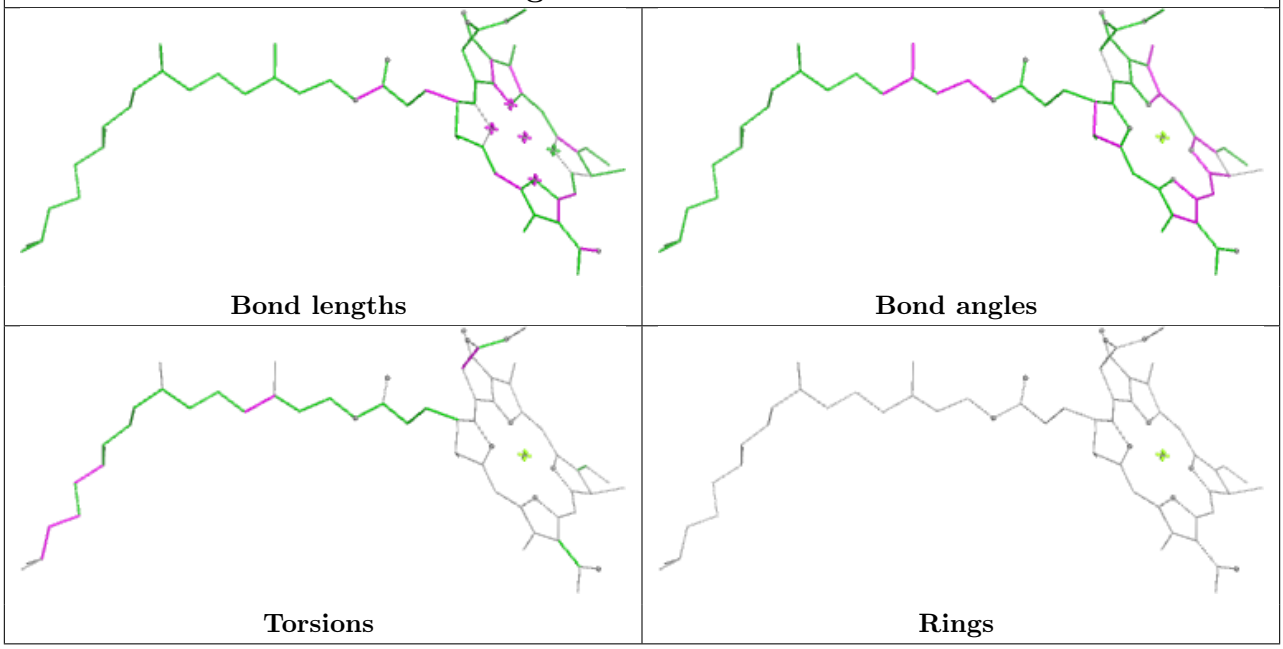
Ligand SO4 C 405



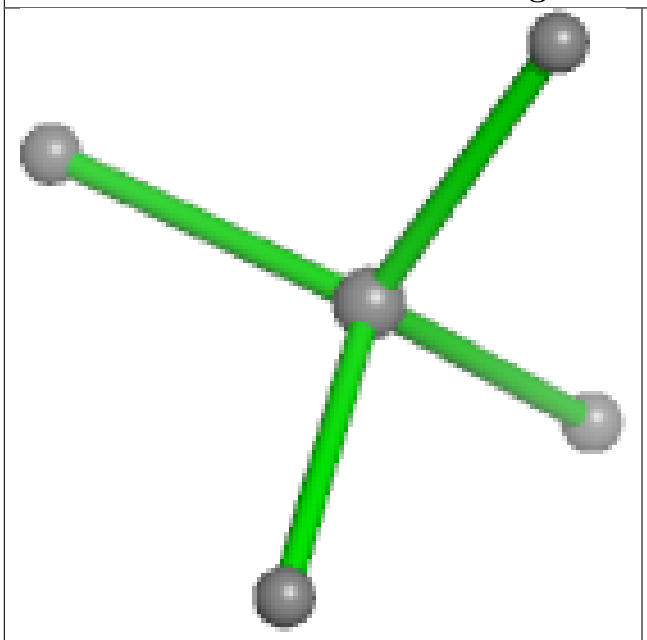
Ligand NS5 M 406



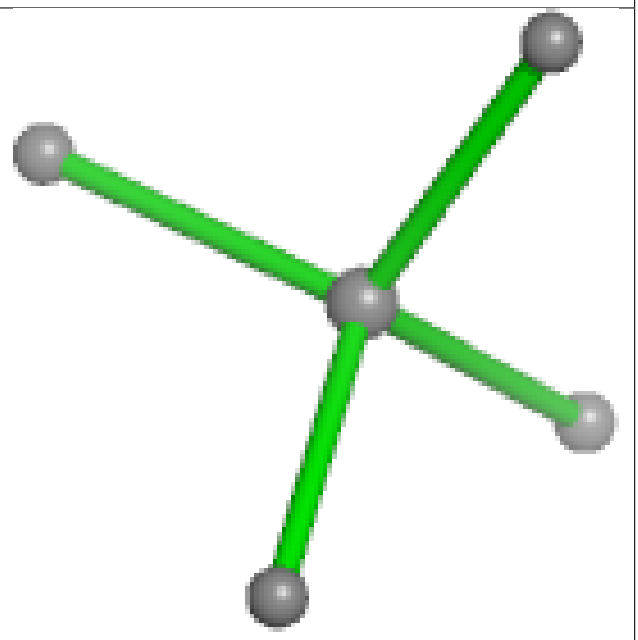
Ligand BCB L 400



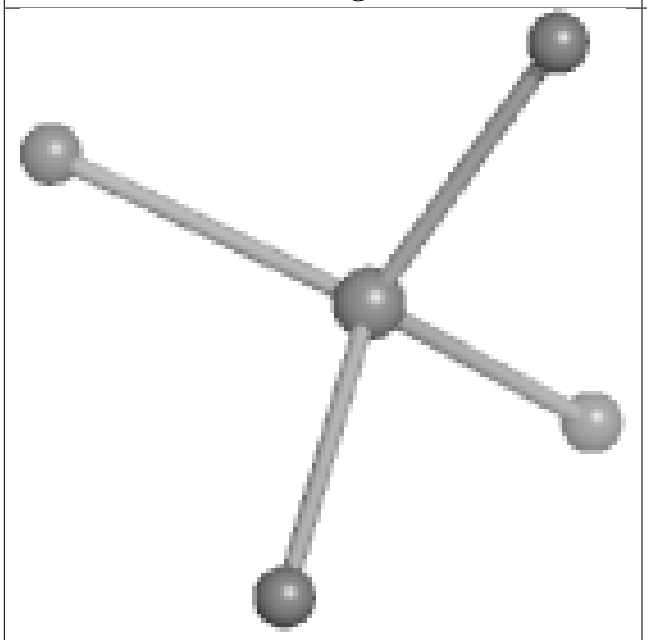
Ligand SO4 H 302



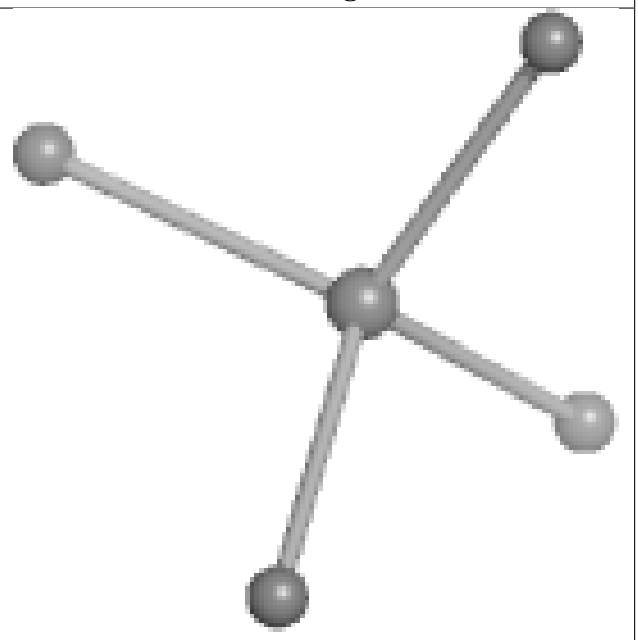
Bond lengths



Bond angles

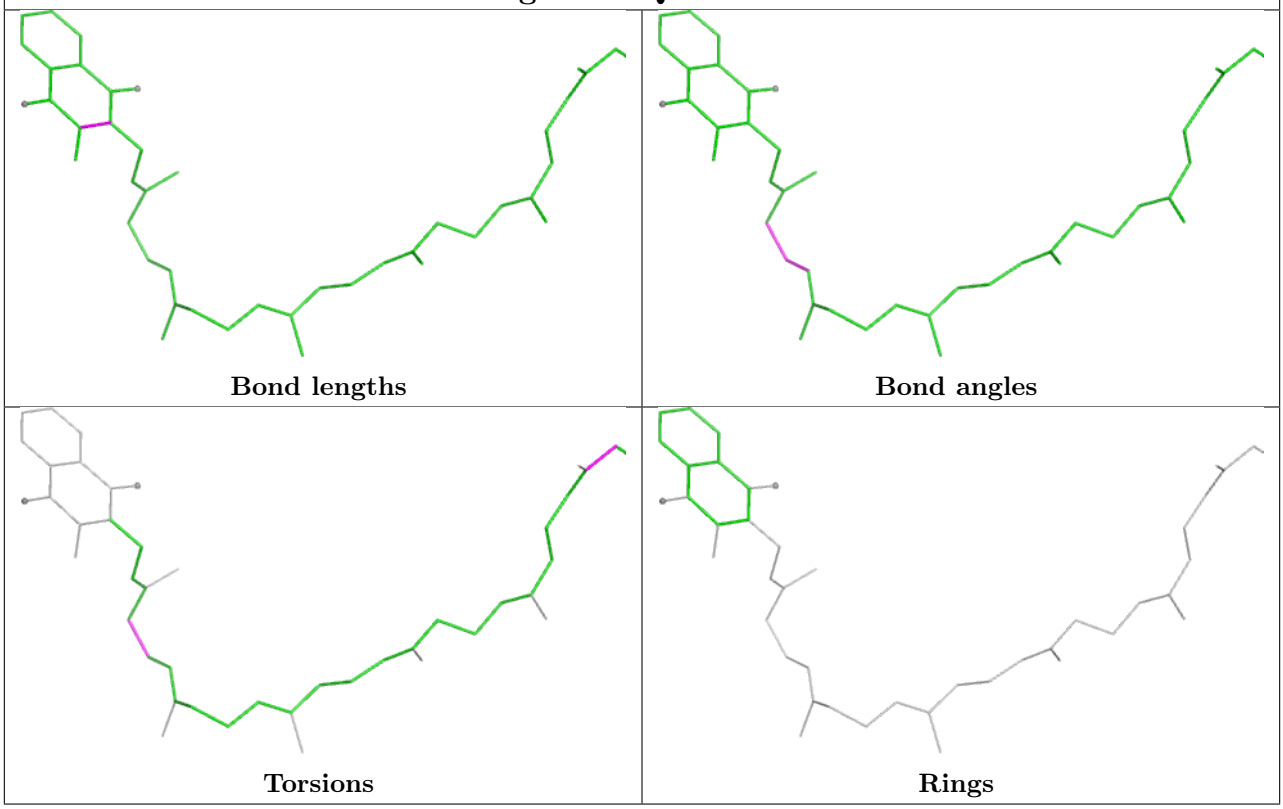


Torsions

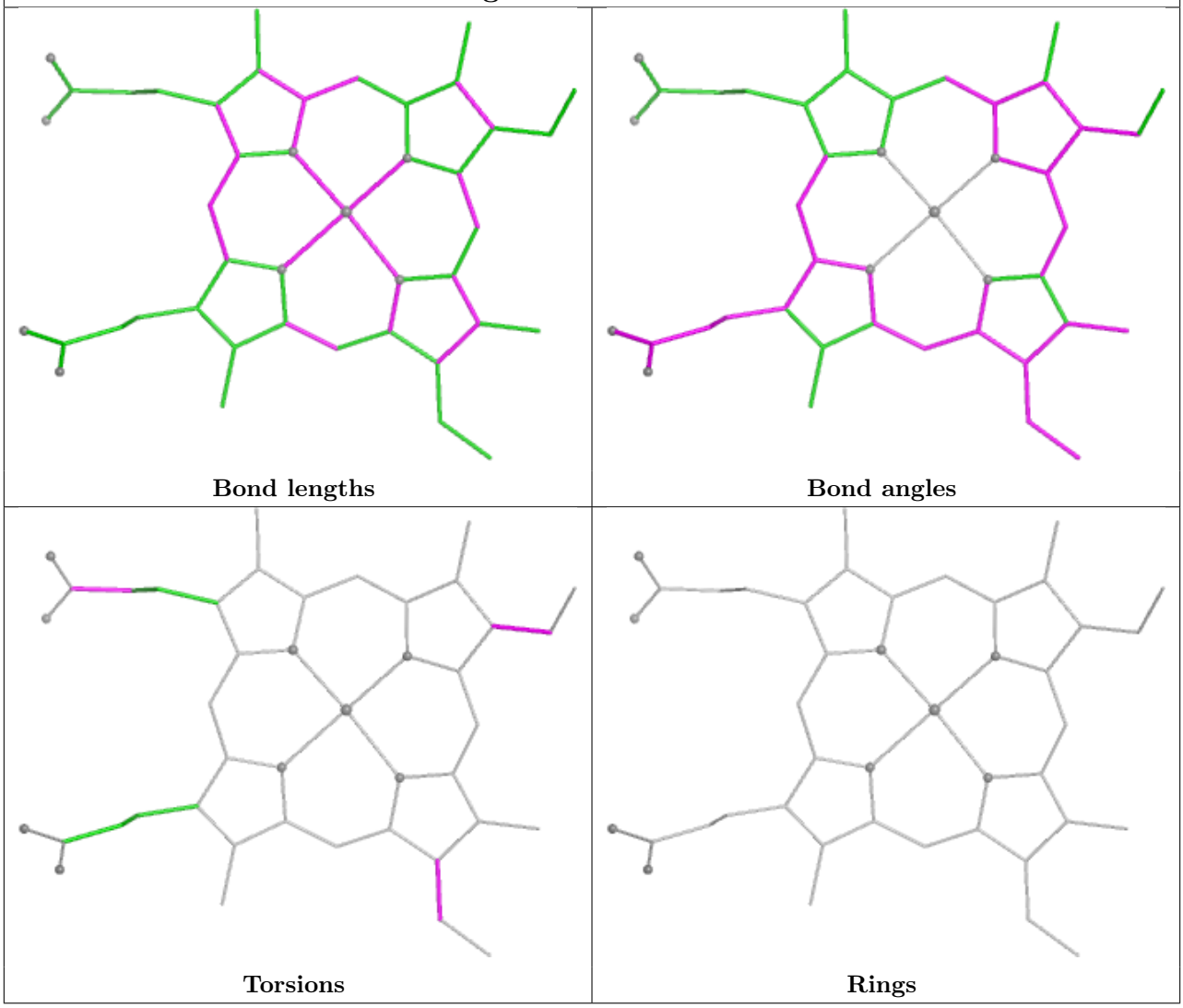


Rings

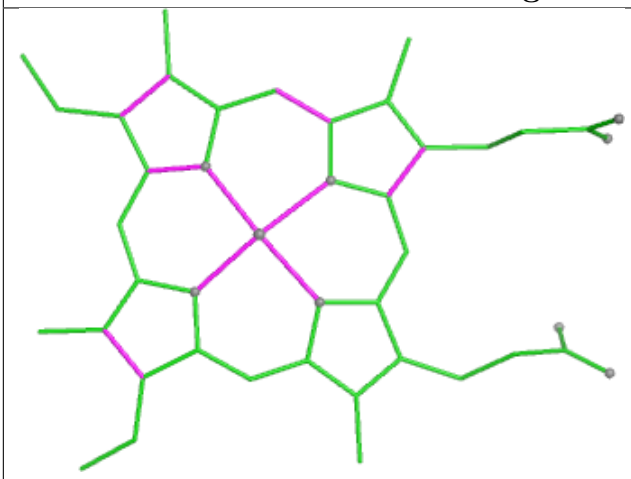
Ligand MQ7 M 402



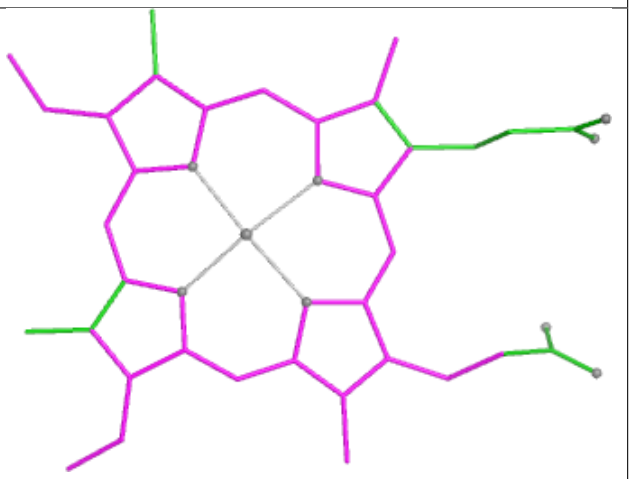
Ligand HEC C 403



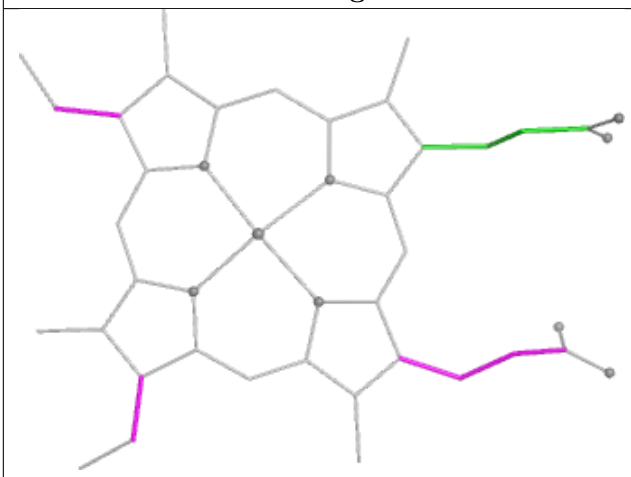
Ligand HEC C 404



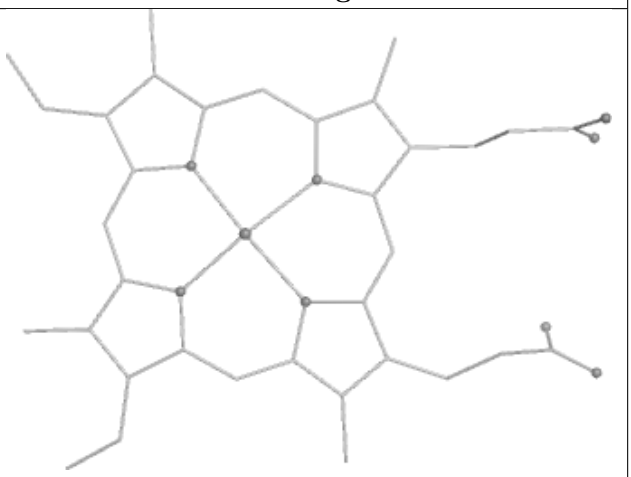
Bond lengths



Bond angles

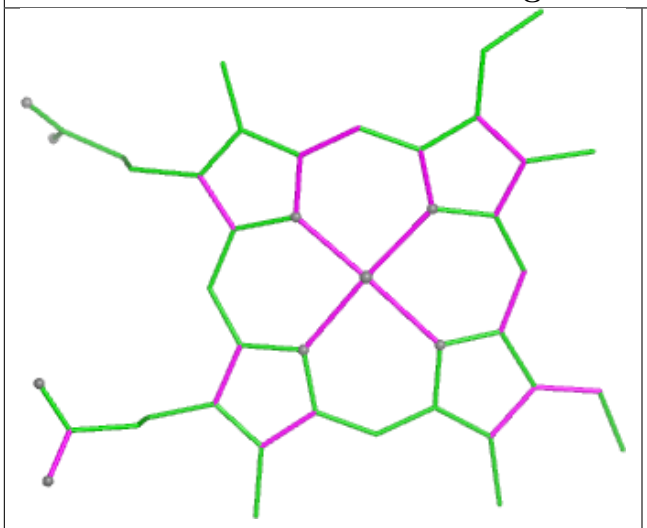


Torsions

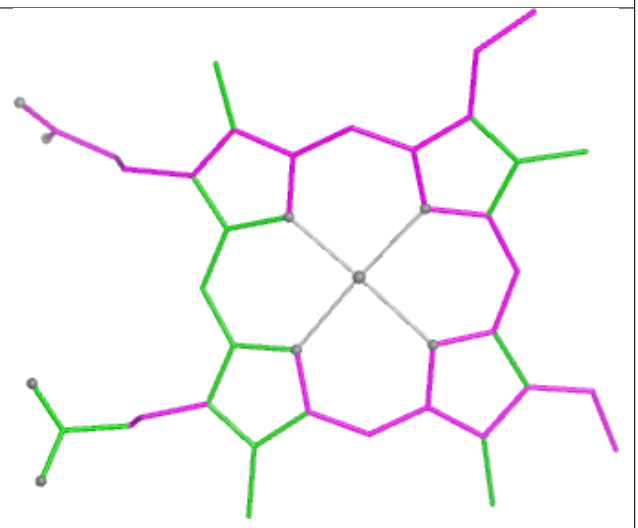


Rings

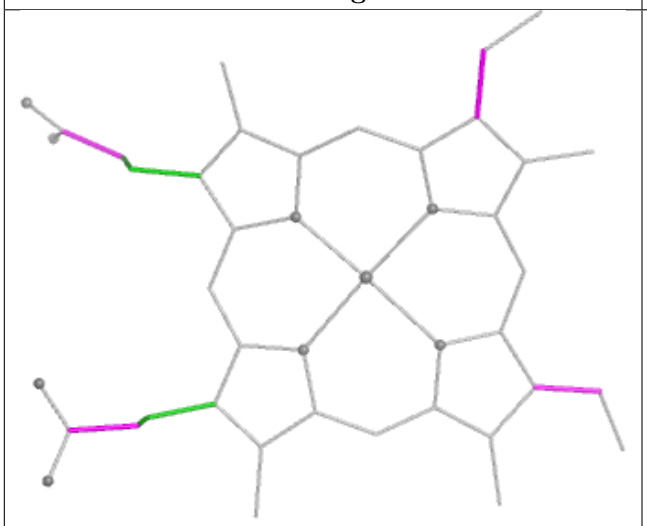
Ligand HEC C 401



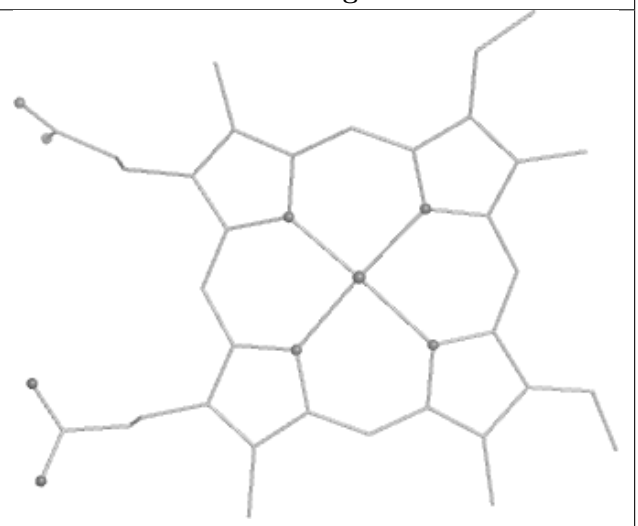
Bond lengths



Bond angles

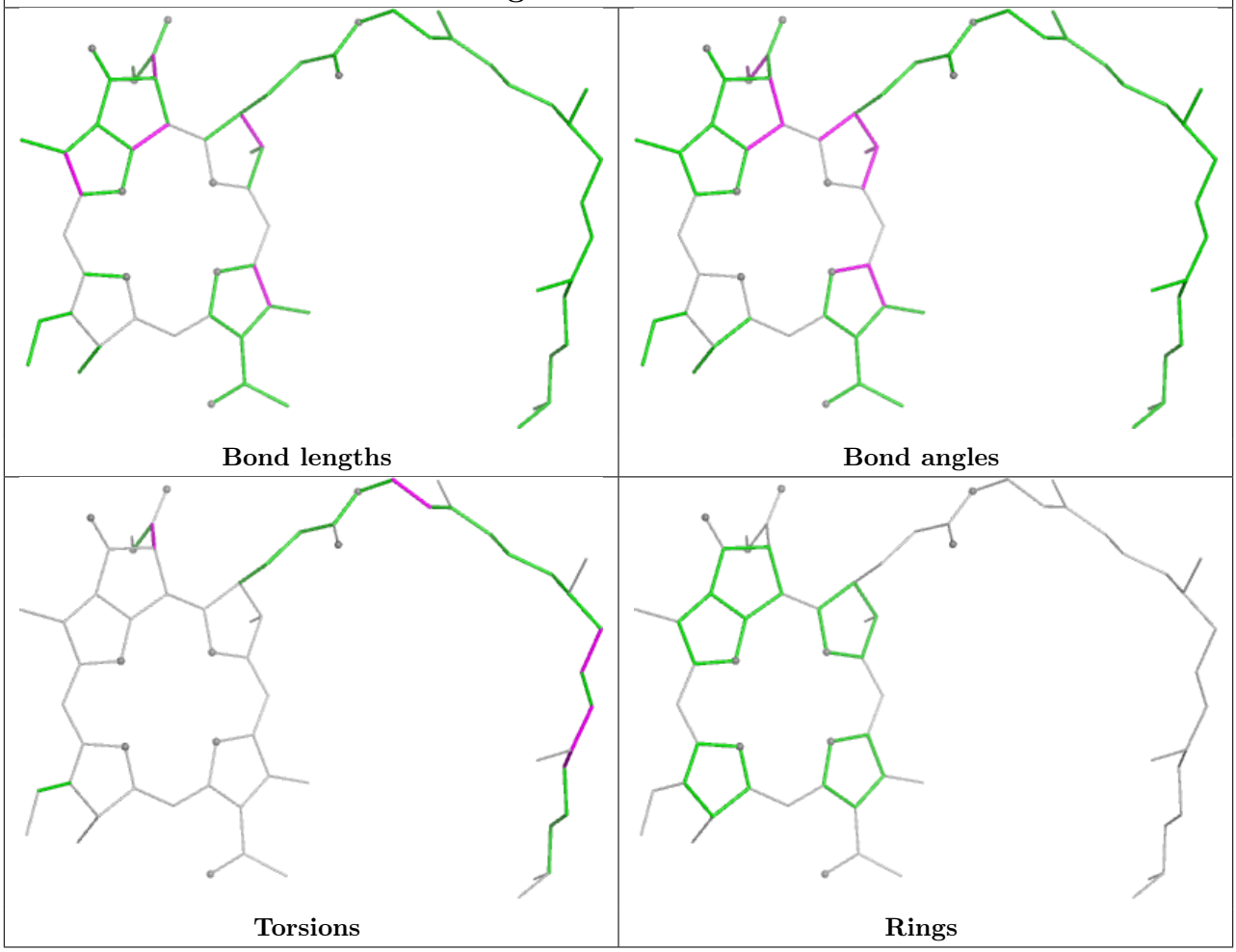


Torsions

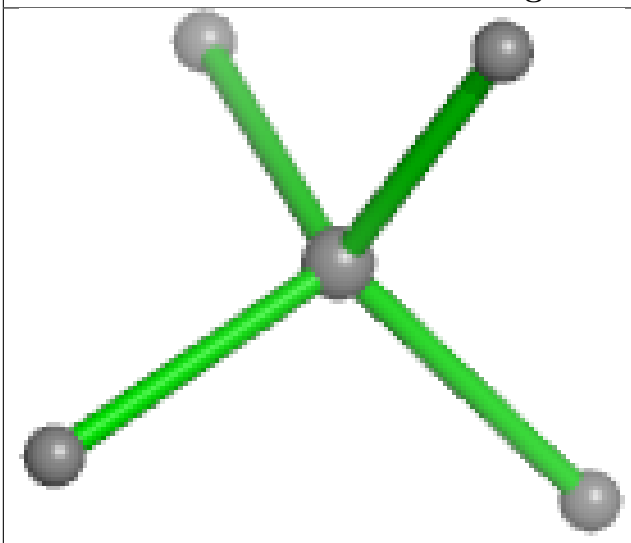


Rings

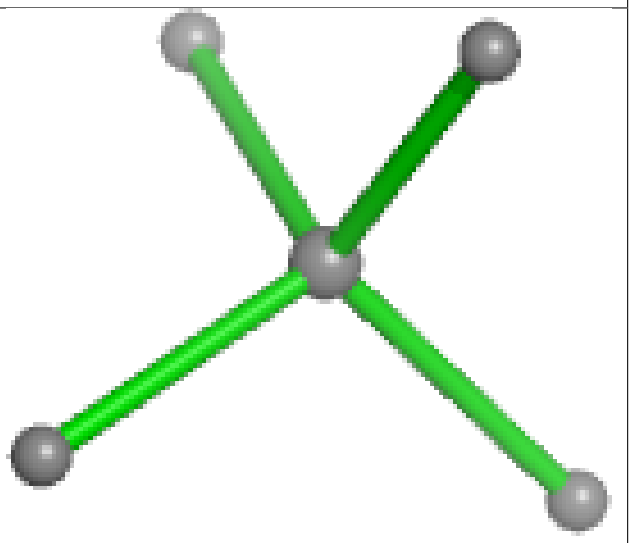
Ligand BPB L 402



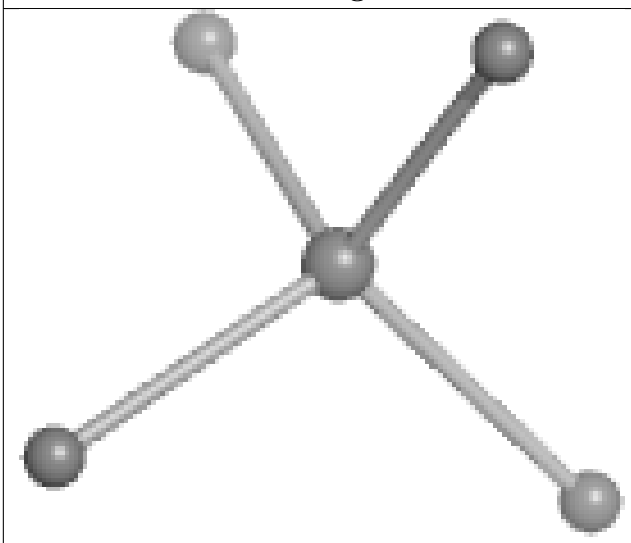
Ligand SO4 M 409



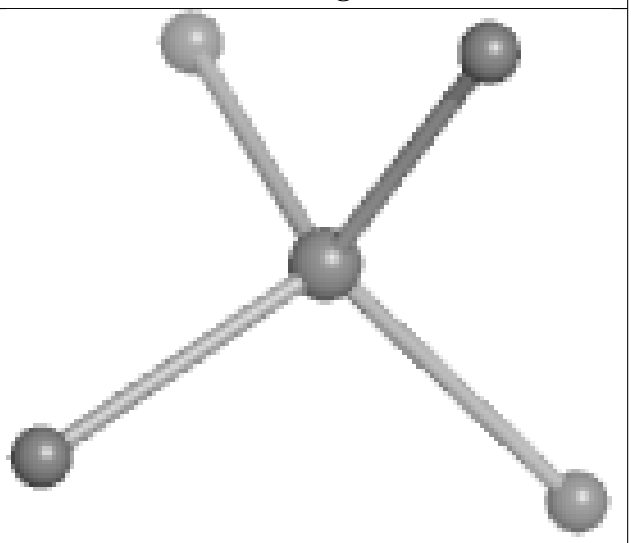
Bond lengths



Bond angles

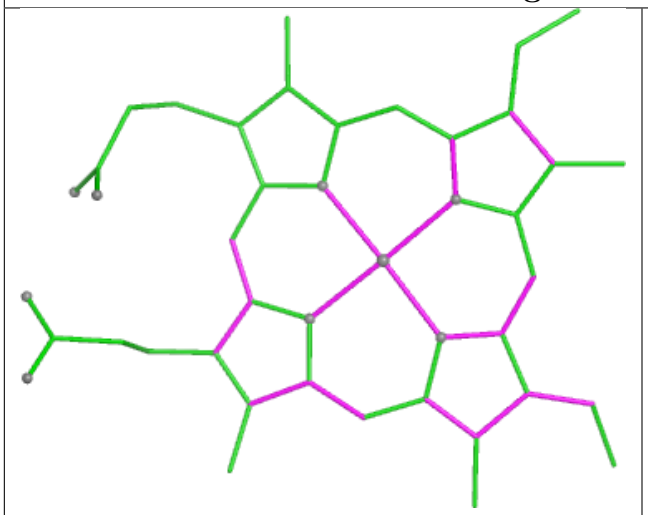


Torsions

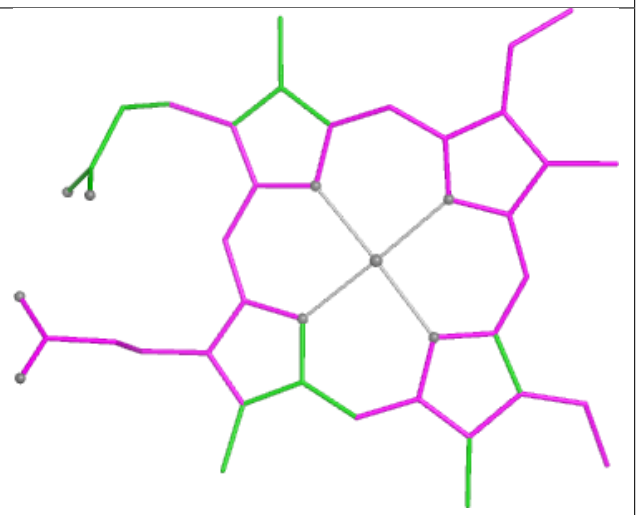


Rings

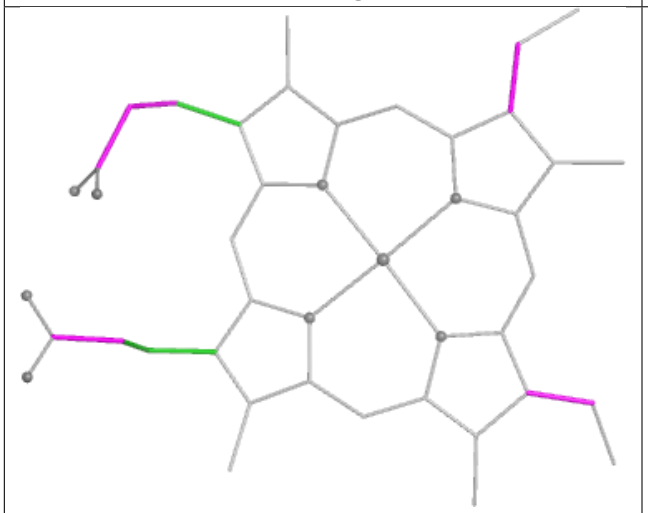
Ligand HEC C 402



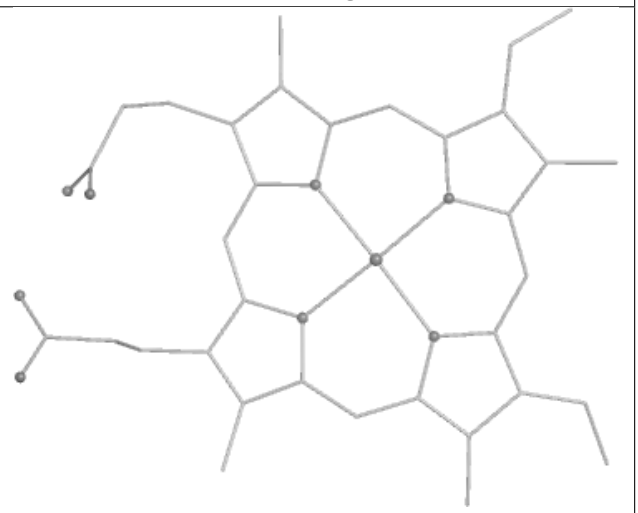
Bond lengths



Bond angles

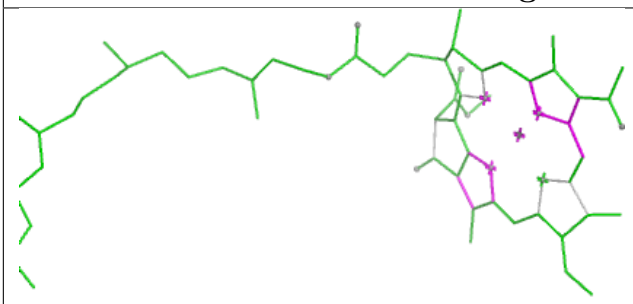


Torsions



Rings

Ligand BCB M 404



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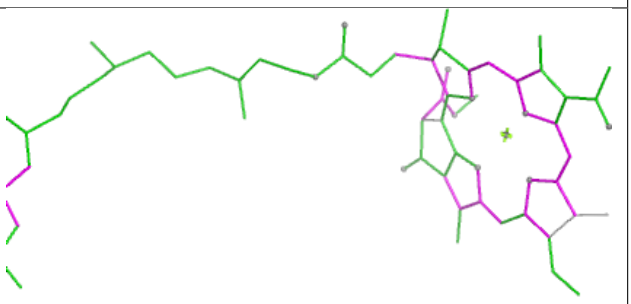

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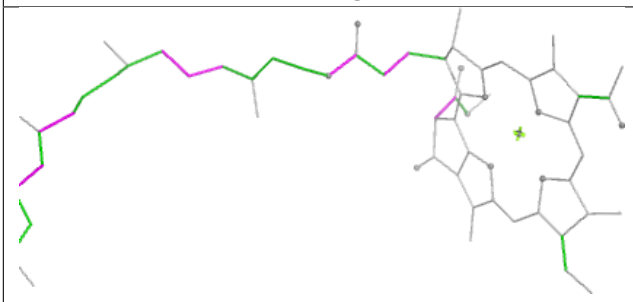
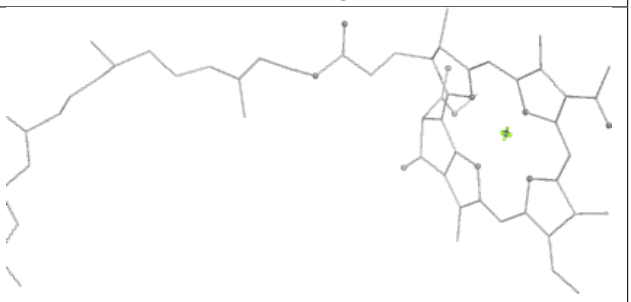
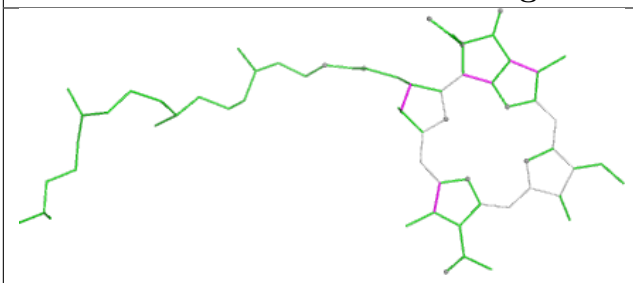


Torsions

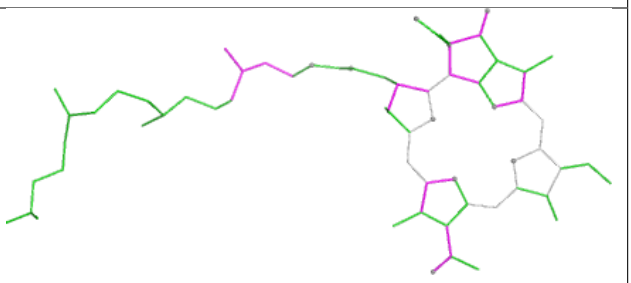


Rings

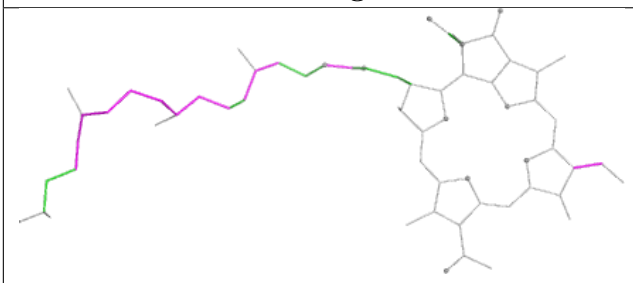
Ligand BPB M 405



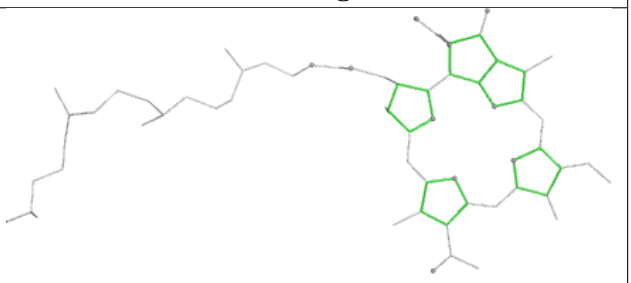
Bond lengths



Bond angles

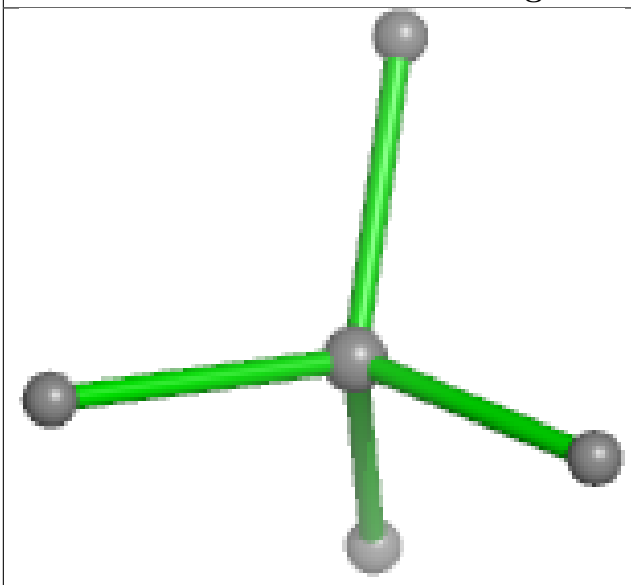


Torsions

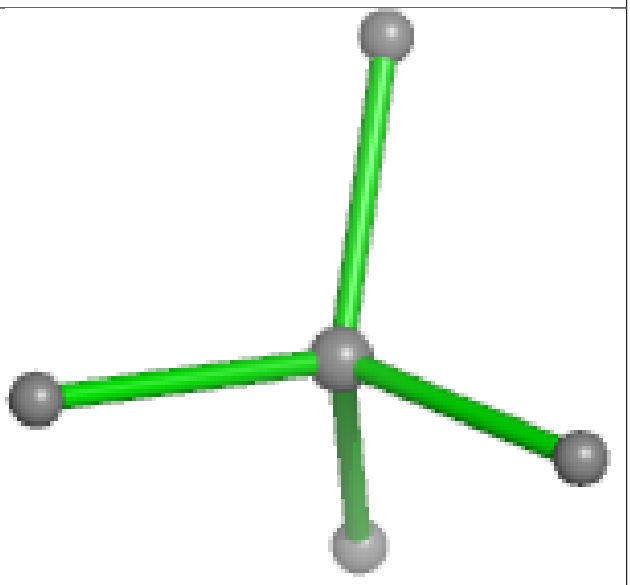


Rings

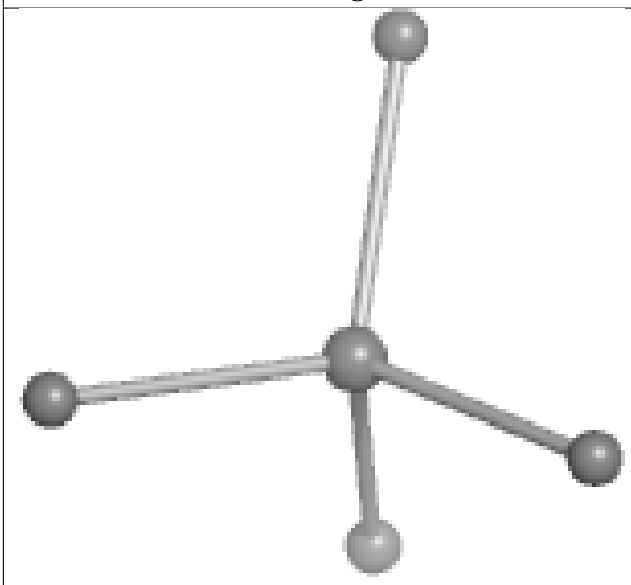
Ligand SO4 M 407



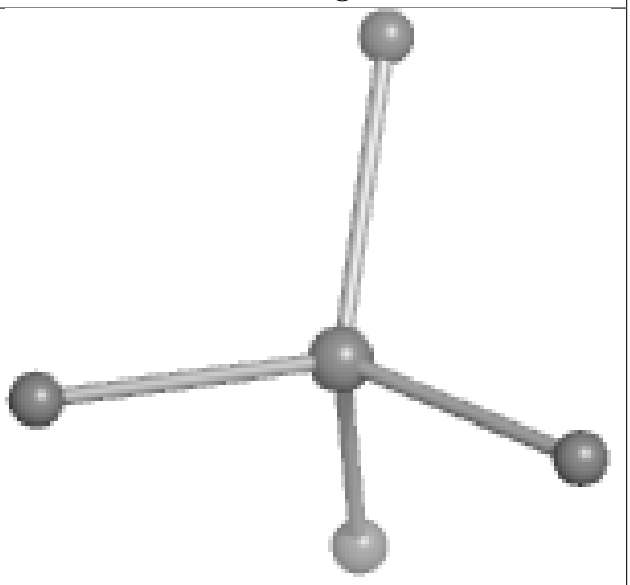
Bond lengths



Bond angles

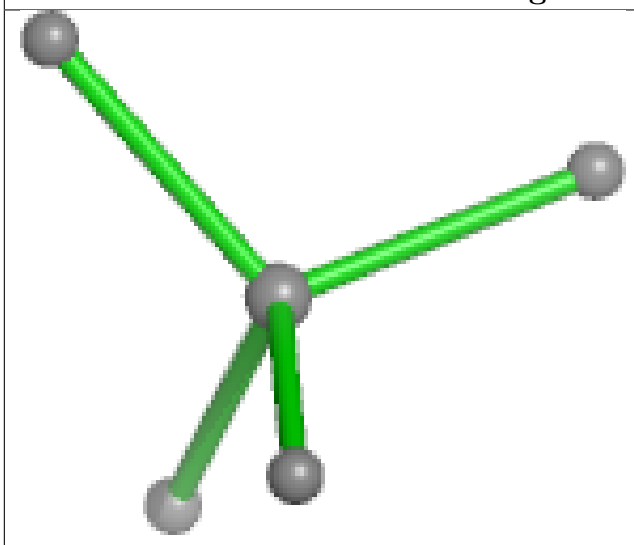


Torsions



Rings

Ligand SO4 H 303



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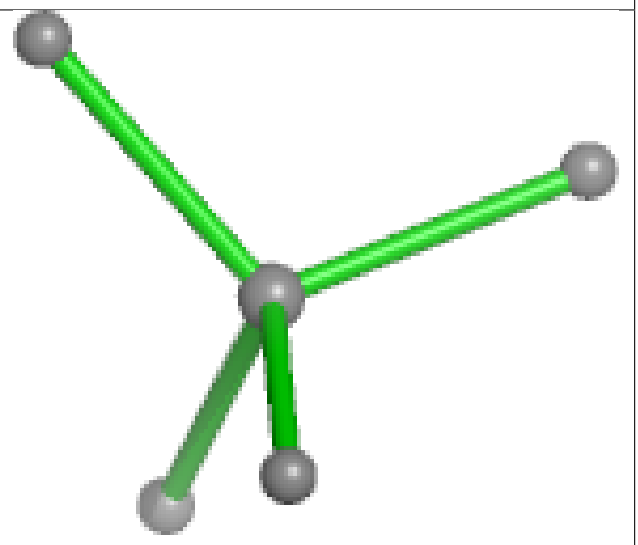
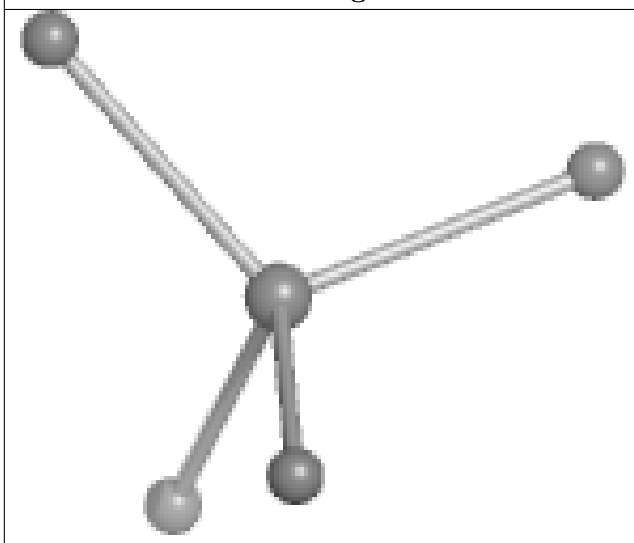
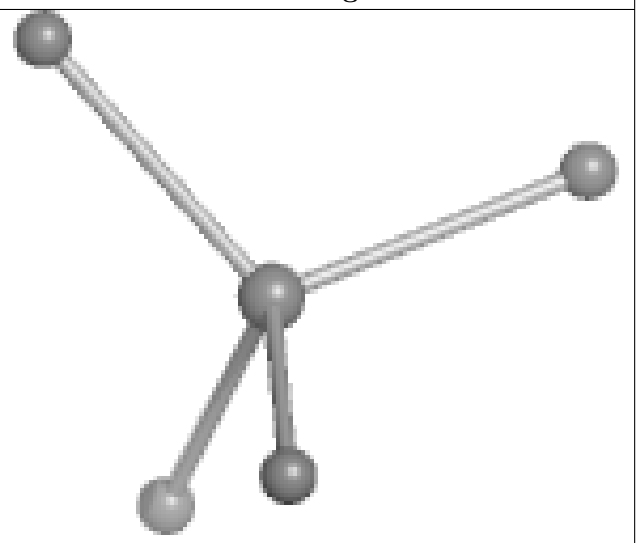


Bond angles

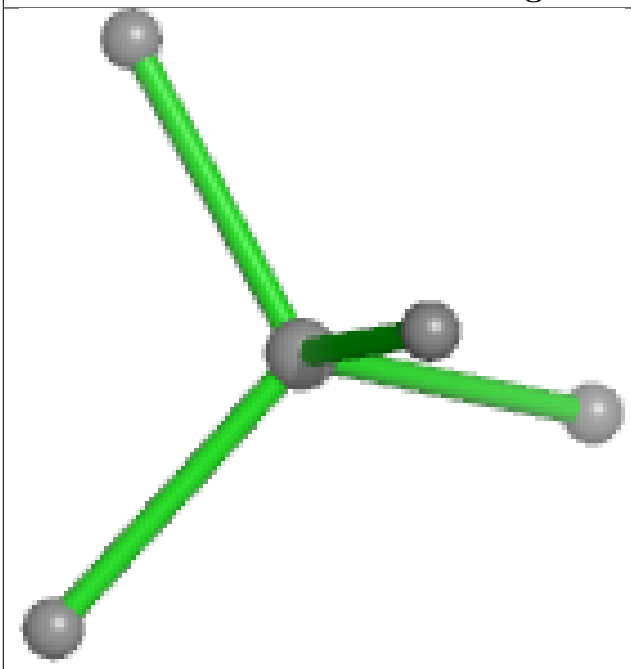


Torsions

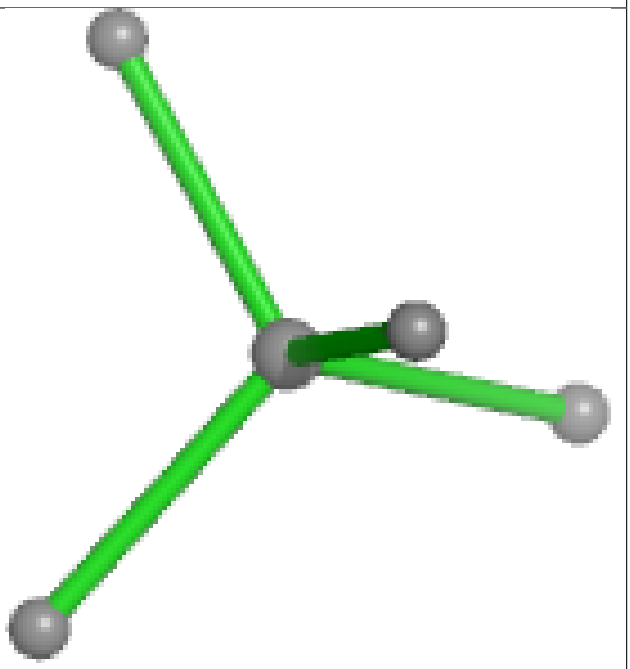


Rings

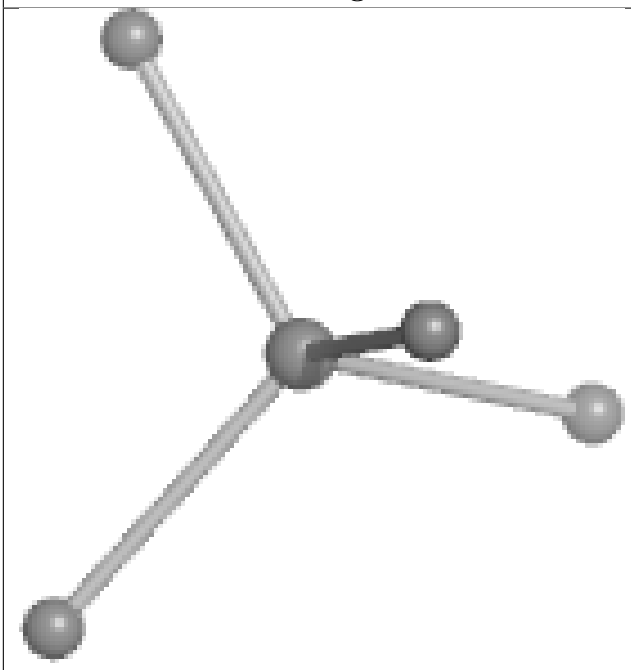
Ligand SO4 M 408



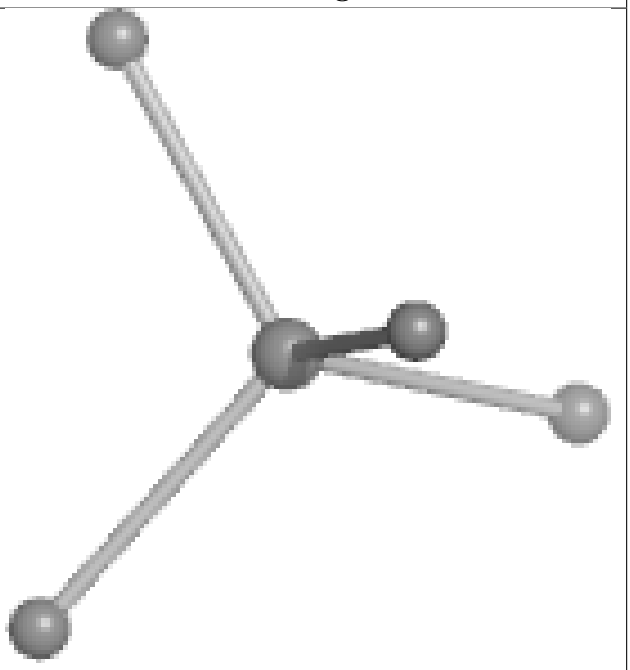
Bond lengths



Bond angles

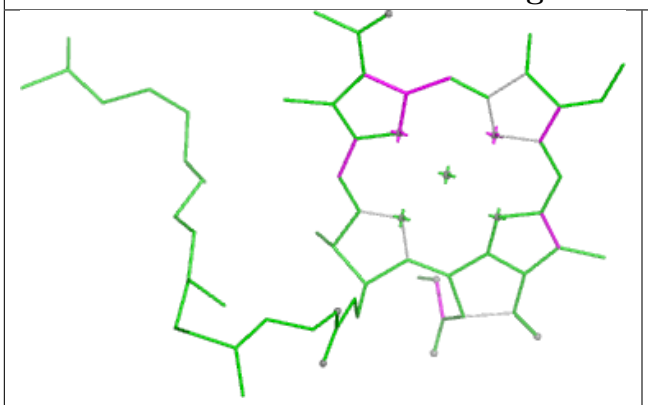


Torsions

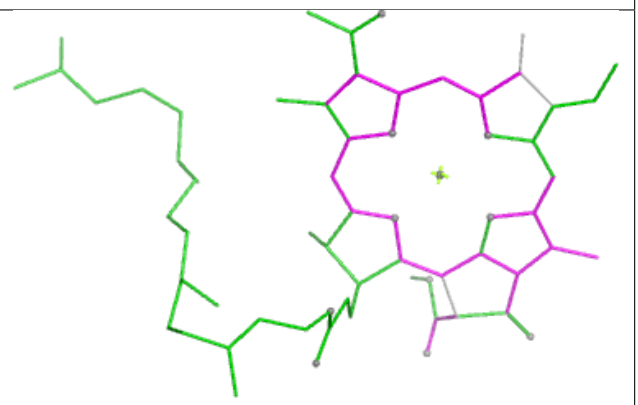


Rings

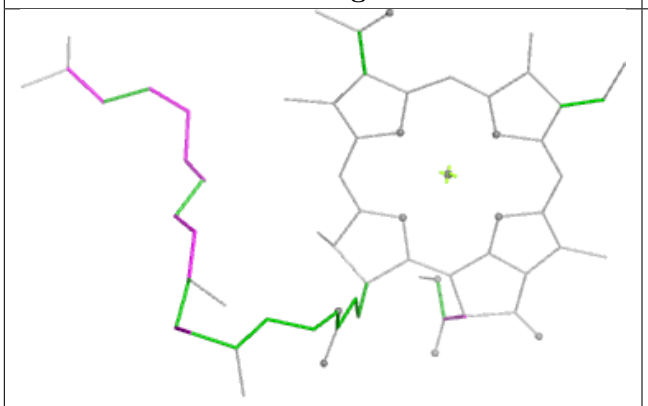
Ligand BCB L 401



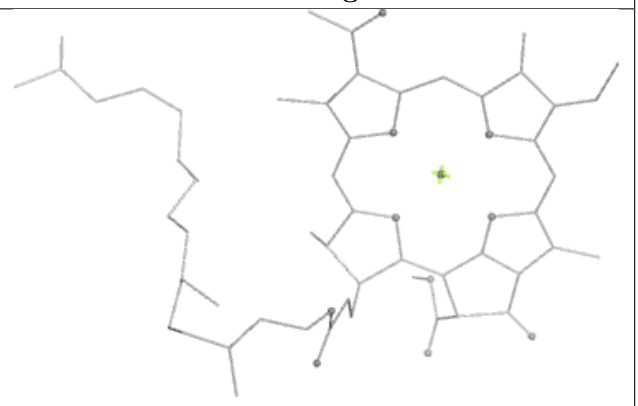
Bond lengths



Bond angles

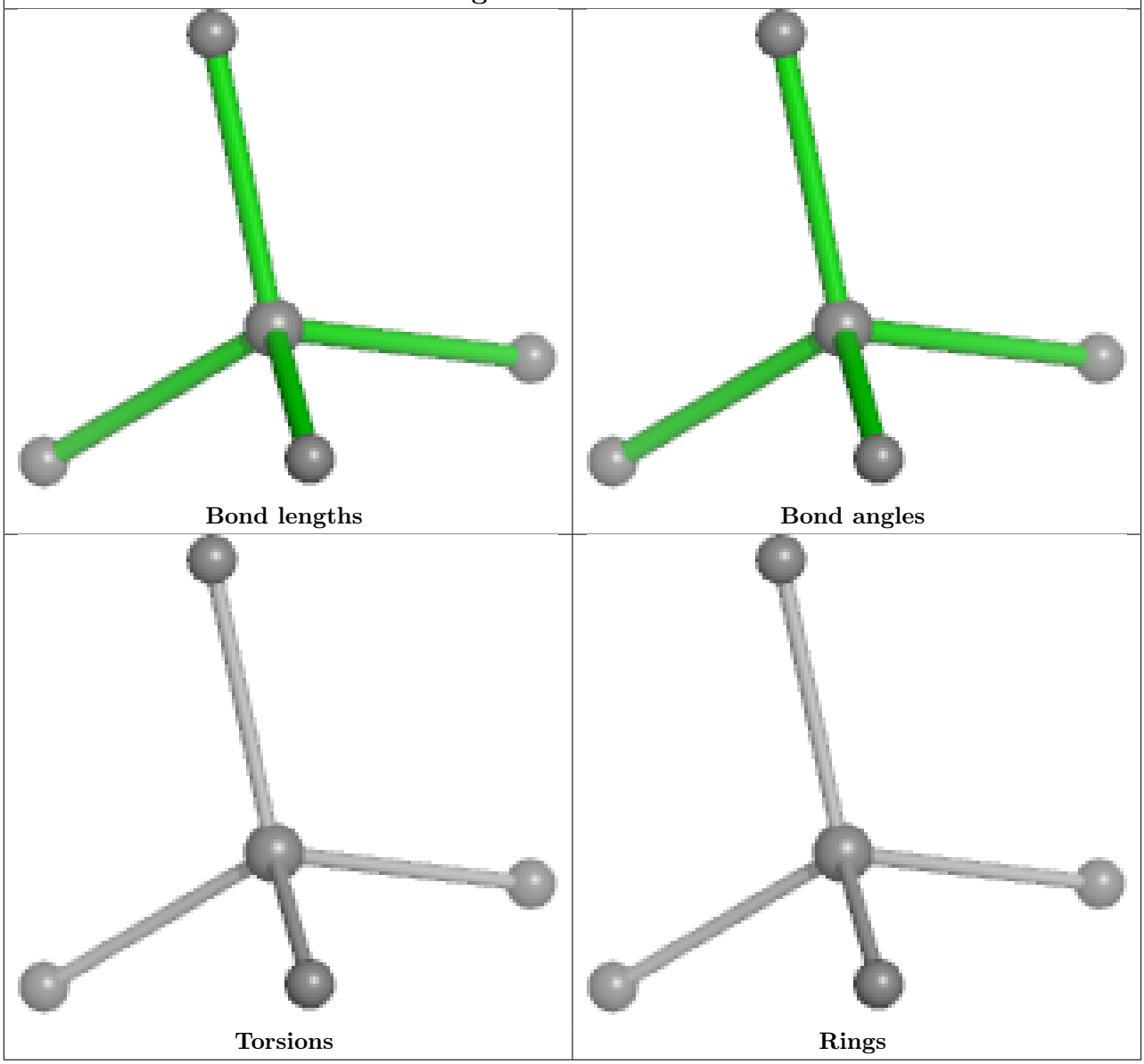


Torsions



Rings

Ligand SO4 H 301



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	46:PRO	C	55:GLU	N	13.88

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	C	332/332 (100%)	-0.41	2 (0%)	85	73	33, 96, 132, 174	2 (0%)
2	H	242/242 (100%)	-0.04	7 (2%)	53	35	55, 108, 157, 254	1 (0%)
3	L	273/273 (100%)	-0.36	2 (0%)	84	70	61, 90, 127, 140	0
4	M	323/323 (100%)	-0.36	3 (0%)	81	65	44, 92, 125, 167	1 (0%)
5	D	7/8 (87%)	0.08	0	100	100	104, 111, 171, 182	0
All	All	1177/1178 (99%)	-0.31	14 (1%)	76	58	33, 95, 136, 254	4 (0%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	86[A]	ARG	6.7
1	C	94[A]	ASN	5.7
4	M	78[A]	HIS	5.5
4	M	89	PHE	4.3
2	H	9	HIS	3.9
2	H	141	THR	3.0
2	H	87[A]	GLU	2.8
3	L	13	GLY	2.6
3	L	1	ALA	2.6
1	C	146[A]	ARG	2.5
4	M	227	PHE	2.4
2	H	46	PRO	2.4
2	H	83	PRO	2.2
2	H	84	GLU	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
5	FME	D	1	10/11	0.94	0.18	105,117,126,127	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

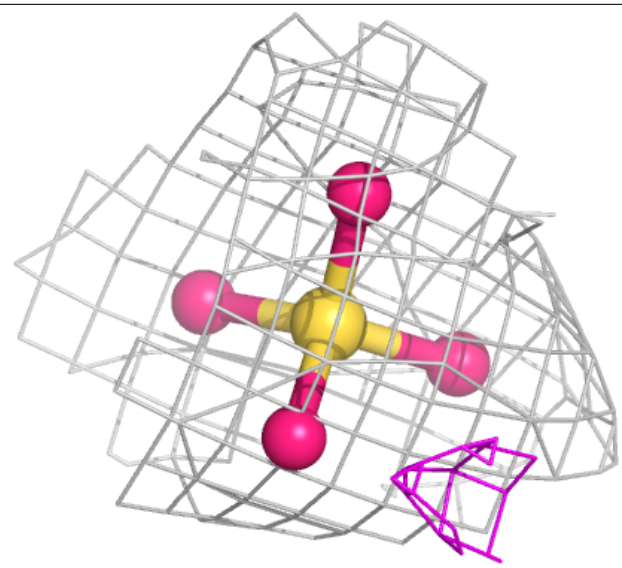
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

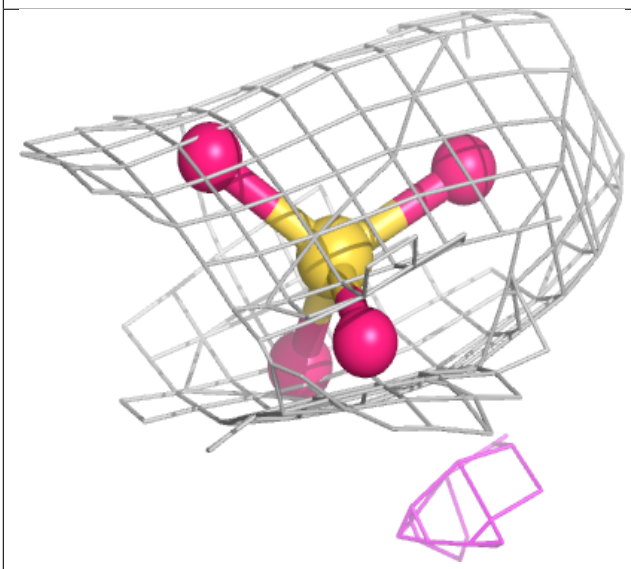
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	SO4	C	406	5/5	0.63	0.13	121,172,217,276	0
7	SO4	M	409	5/5	0.65	0.12	112,189,214,237	0
7	SO4	C	405	5/5	0.71	0.11	130,159,198,258	0
7	SO4	H	302	5/5	0.82	0.16	112,125,150,180	0
7	SO4	H	301	5/5	0.88	0.17	106,113,143,145	0
7	SO4	H	303	5/5	0.93	0.10	76,190,221,256	0
12	NS5	M	406	40/40	0.95	0.22	68,115,174,176	0
9	BPB	M	405	65/65	0.96	0.13	69,103,170,184	0
11	MQ7	M	402	48/48	0.96	0.14	63,83,124,140	0
8	BCB	M	403	66/66	0.96	0.13	56,104,168,173	0
9	BPB	L	402	65/65	0.97	0.10	59,87,97,102	0
7	SO4	M	407	5/5	0.97	0.06	106,112,138,182	0
8	BCB	L	401	66/66	0.97	0.10	61,83,105,118	0
7	SO4	M	408	5/5	0.97	0.07	83,102,121,133	0
8	BCB	L	400	66/66	0.98	0.08	58,79,101,111	0
8	BCB	M	404	66/66	0.98	0.09	44,79,126,143	0
6	HEC	C	401	43/43	0.98	0.08	69,97,132,148	0
6	HEC	C	403	43/43	0.99	0.07	58,71,88,95	0
6	HEC	C	404	43/43	0.99	0.06	52,74,104,116	0
6	HEC	C	402	43/43	0.99	0.06	44,88,109,117	0
10	FE2	M	401	1/1	1.00	0.02	72,72,72,72	0

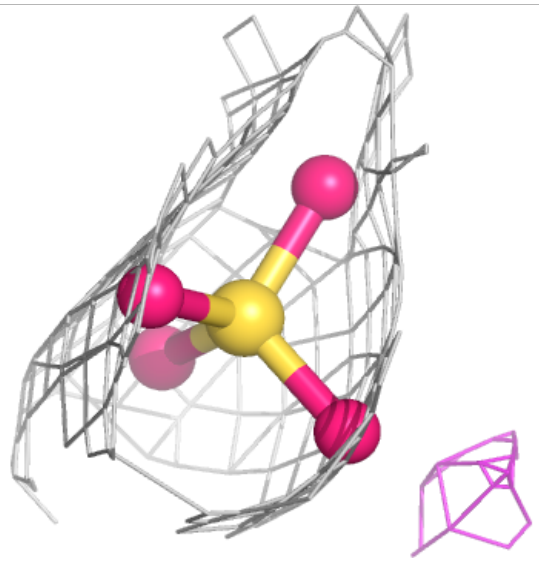
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SO4 C 406:

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

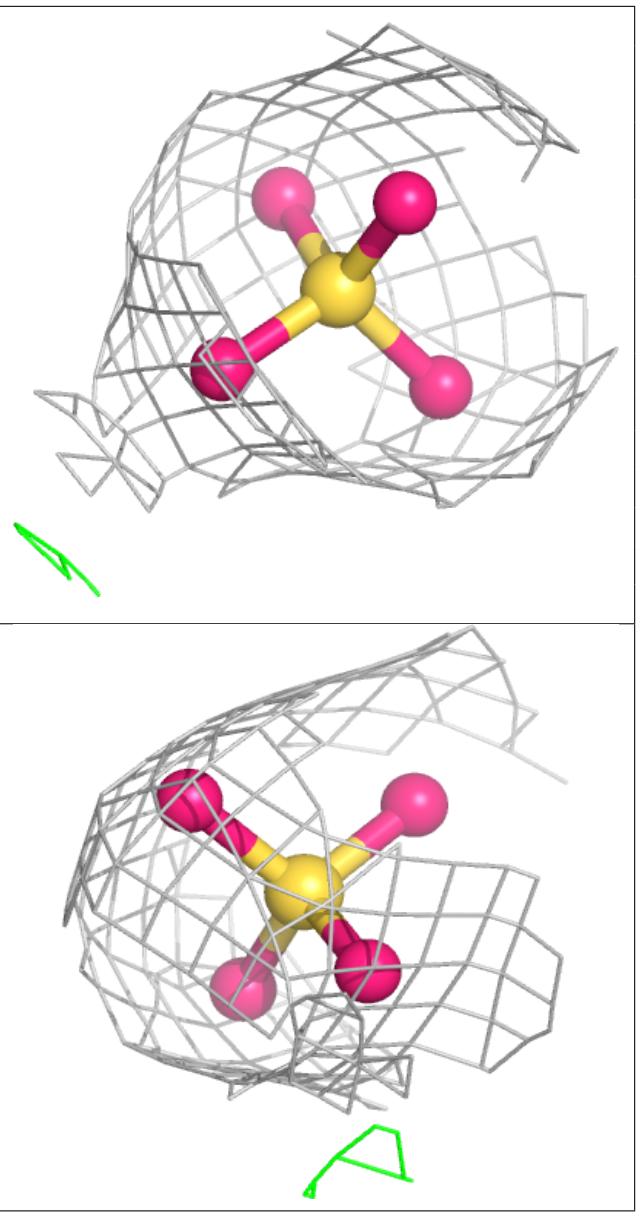






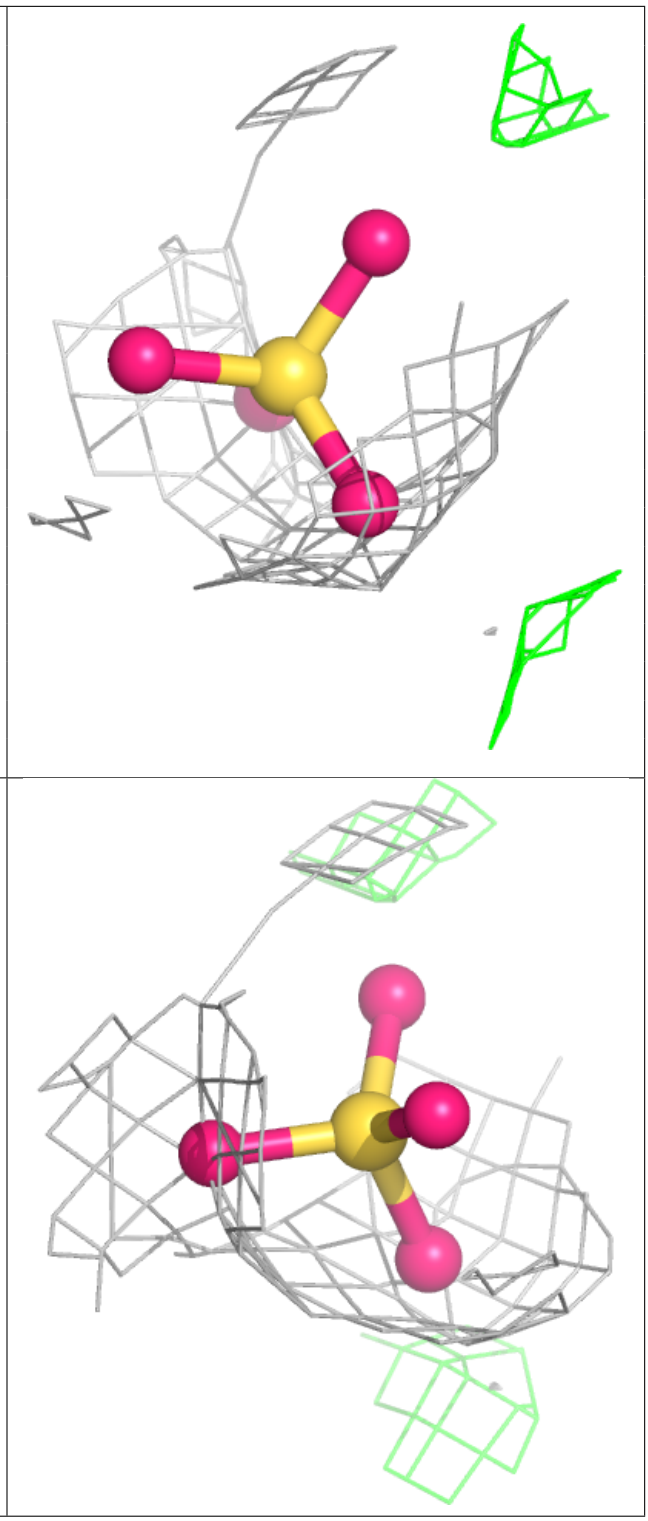
Electron density around SO4 M 409:

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



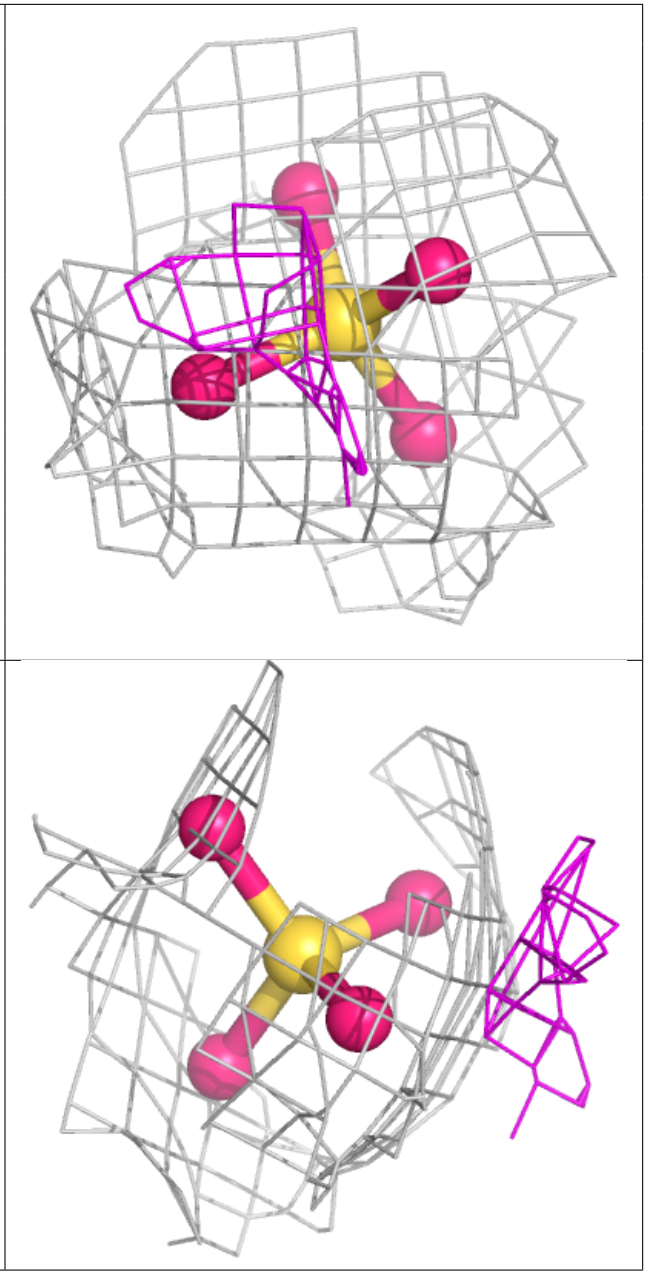
Electron density around SO4 C 405:

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



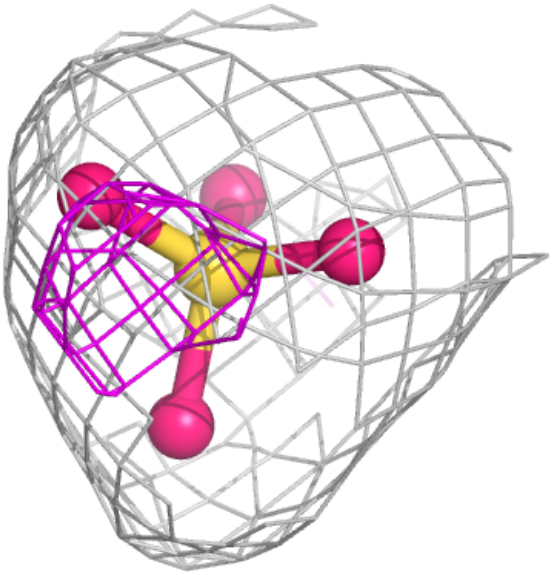
Electron density around SO4 H 302:

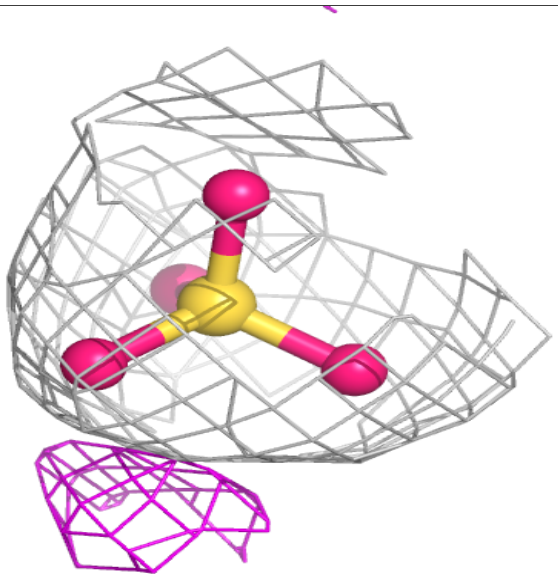
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

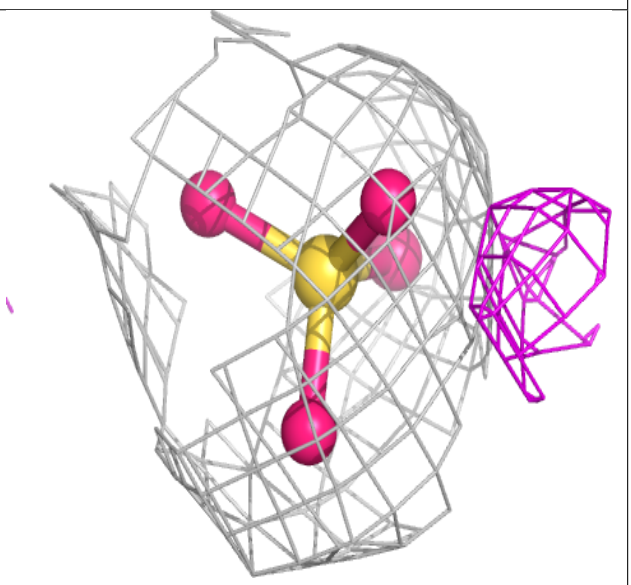


Electron density around SO4 H 301:

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

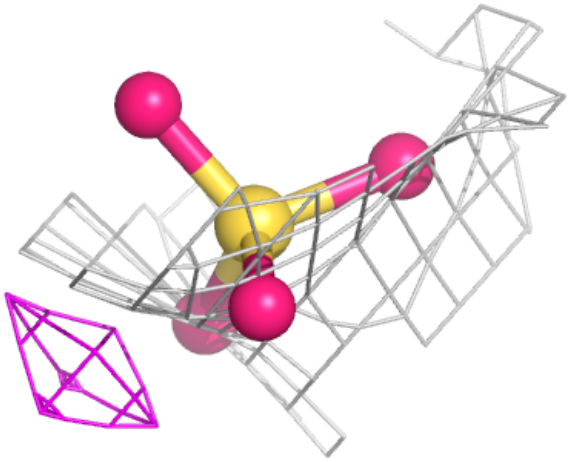


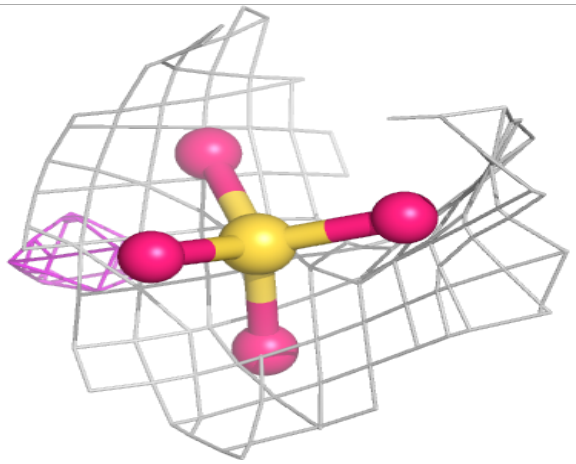


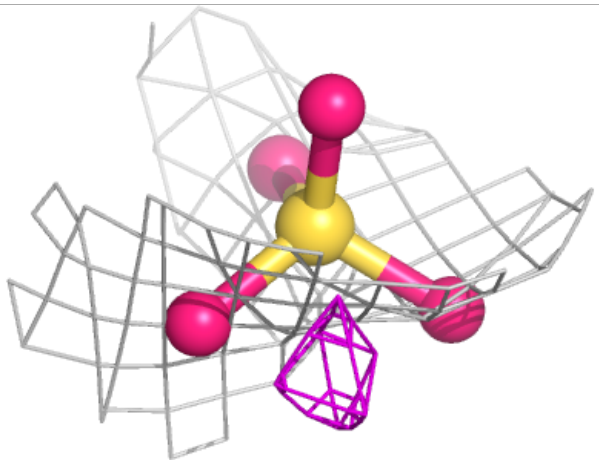


Electron density around SO4 H 303:

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

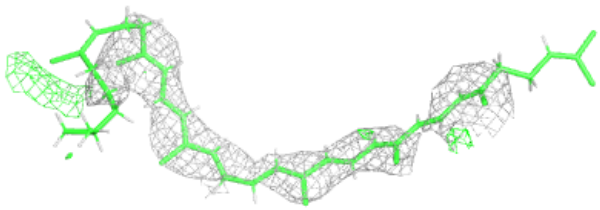


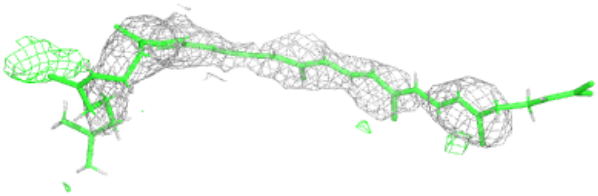


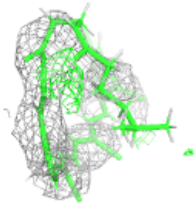


Electron density around NS5 M 406:

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

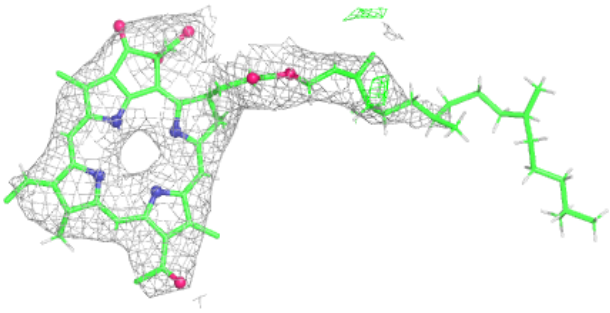


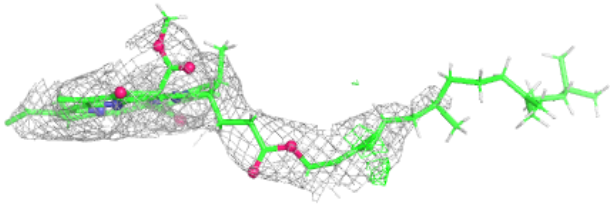


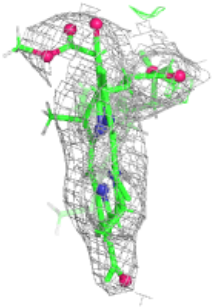


Electron density around BPB M 405:

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

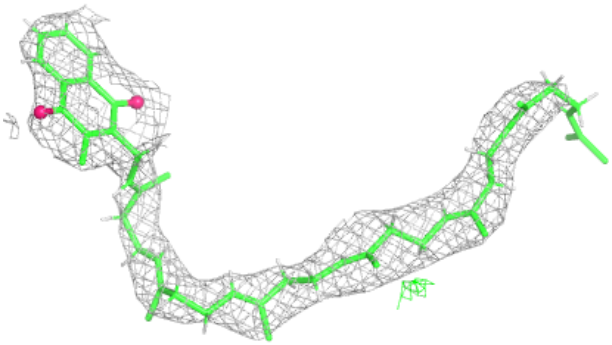


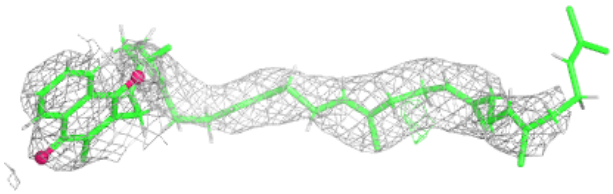


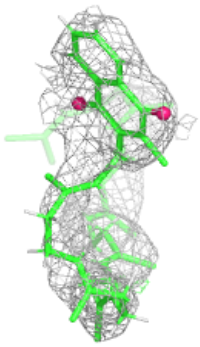


Electron density around MQ7 M 402:

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

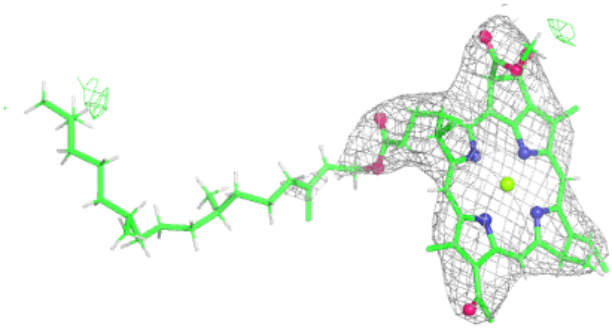


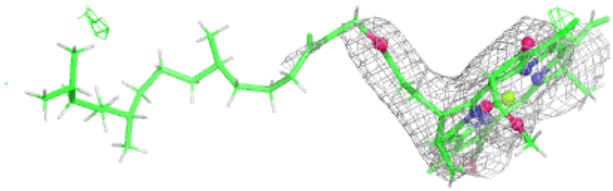




Electron density around BCB M 403:

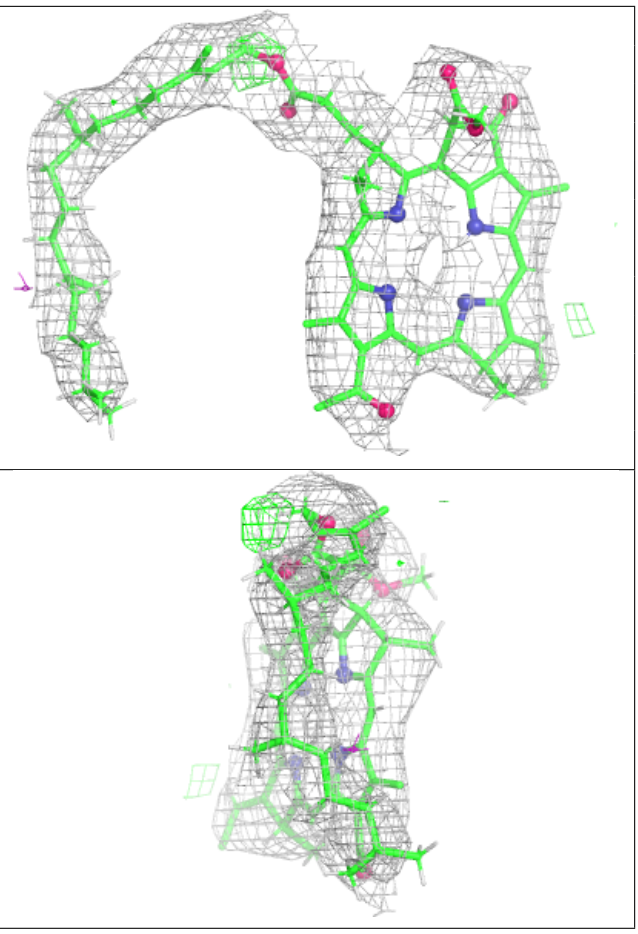
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

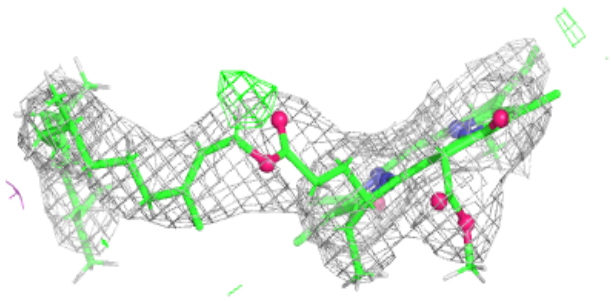




Electron density around BPB L 402:

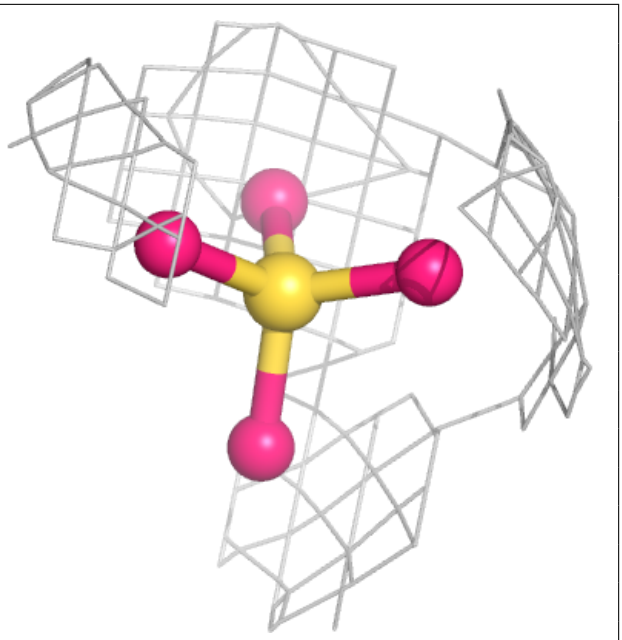
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

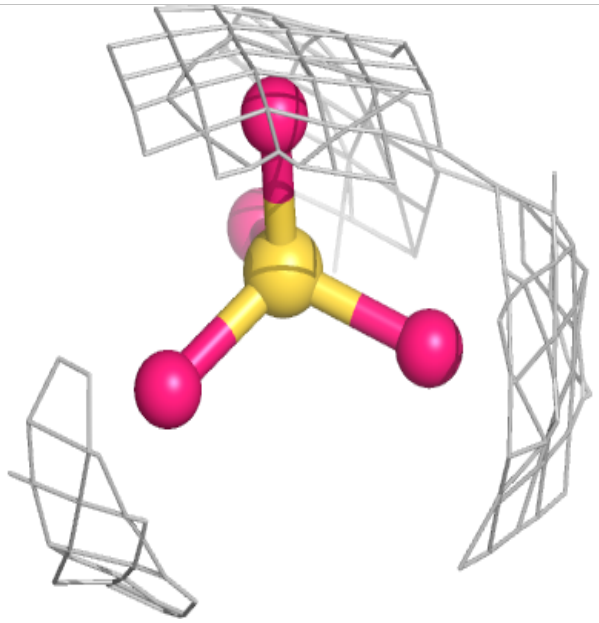


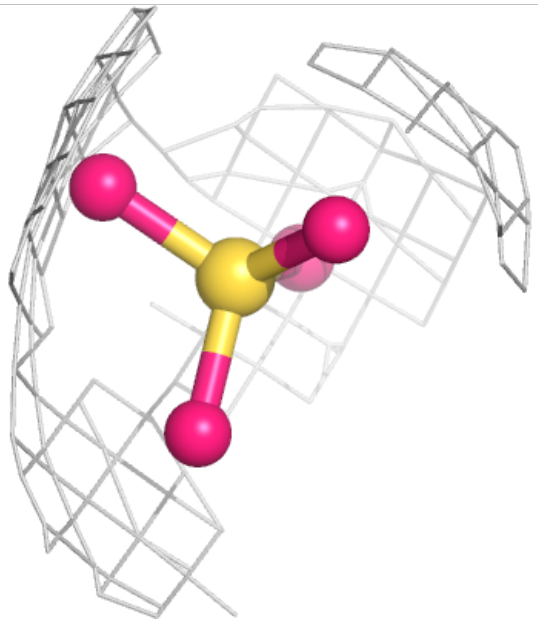


Electron density around SO4 M 407:

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

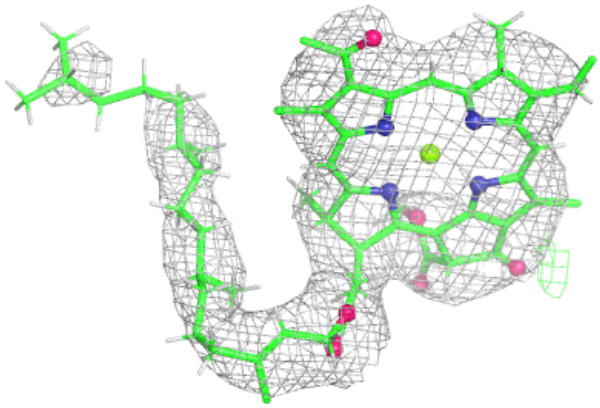


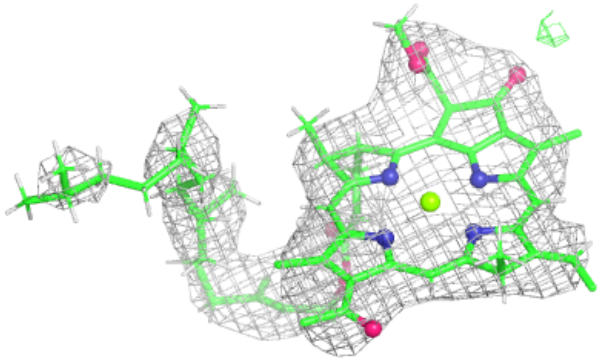


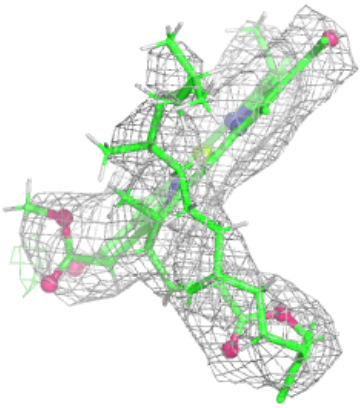


Electron density around BCB L 401:

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

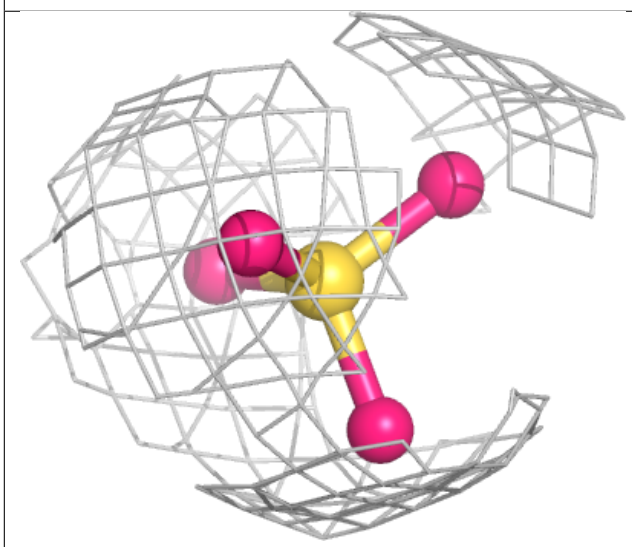


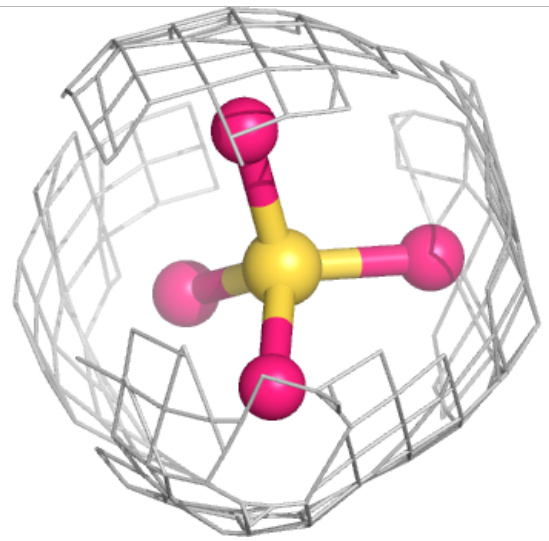


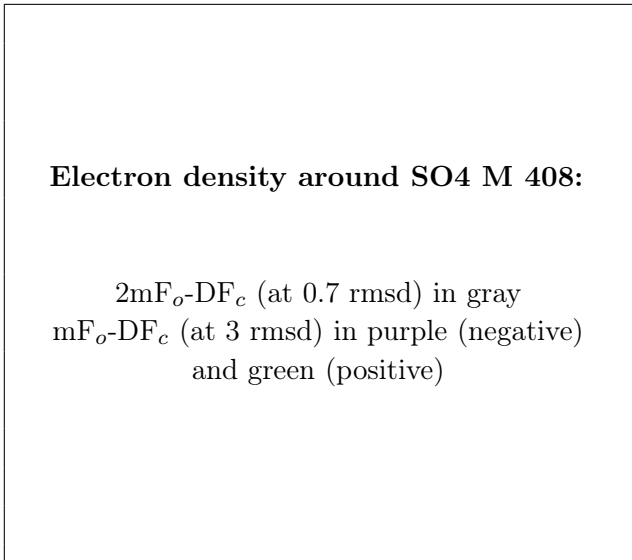


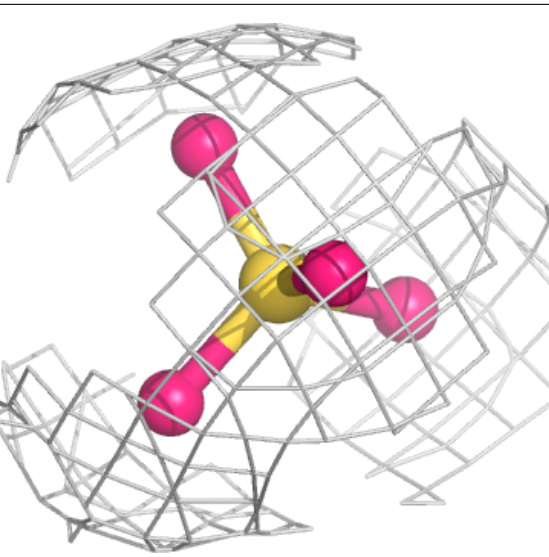
Electron density around SO4 M 408:

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



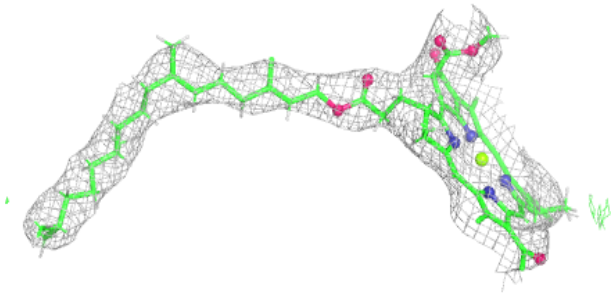


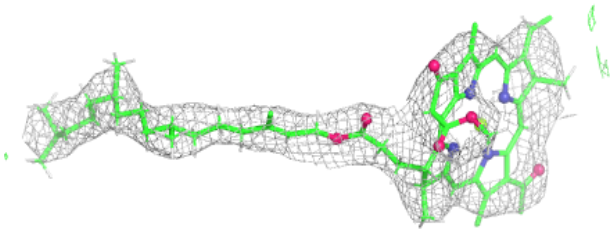


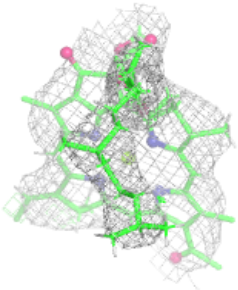


Electron density around BCB L 400:

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

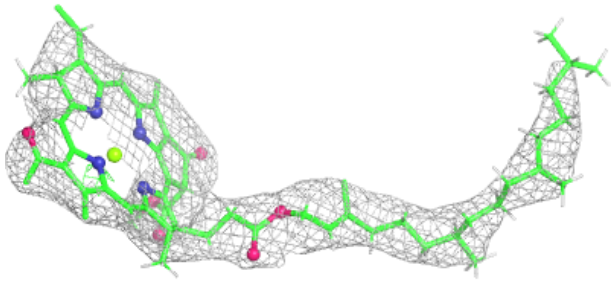


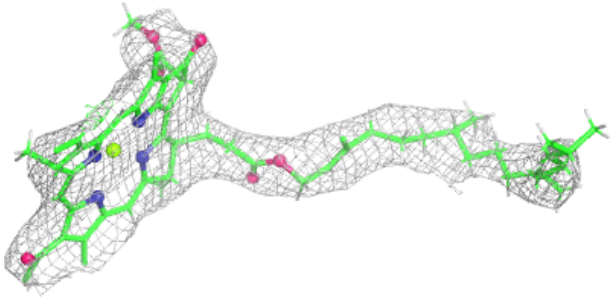


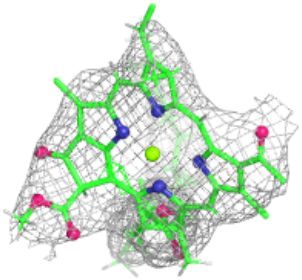


Electron density around BCB M 404:

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

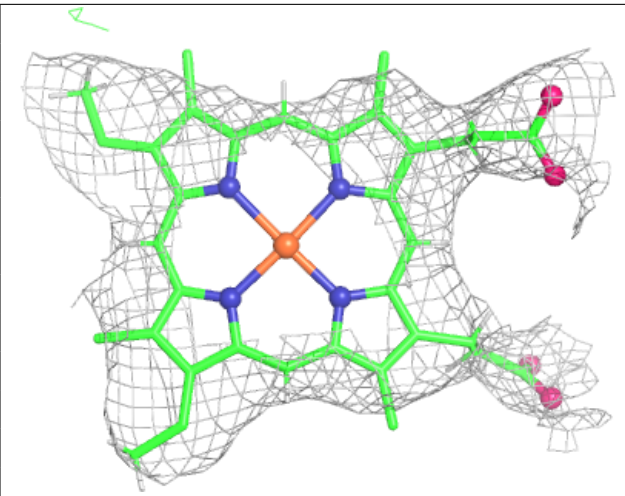


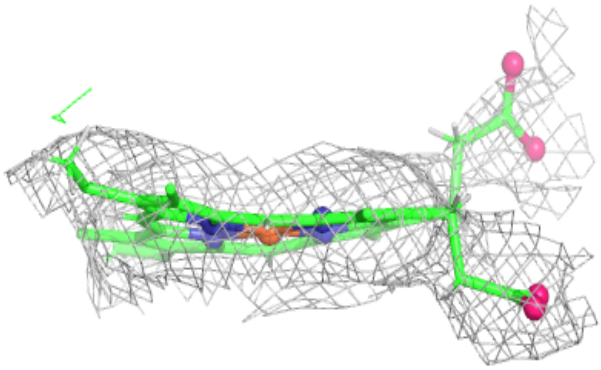


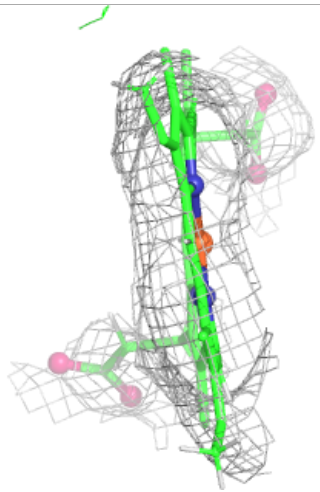


Electron density around HEC C 401:

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

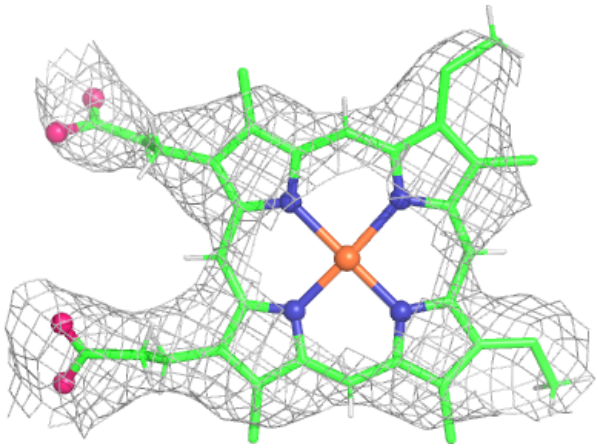


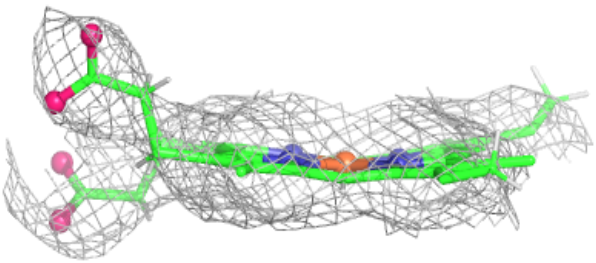


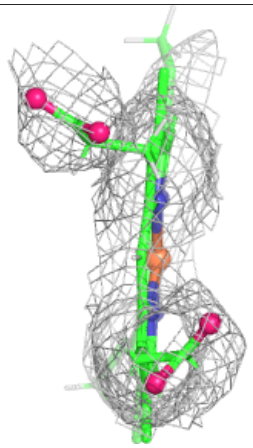


Electron density around HEC C 403:

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

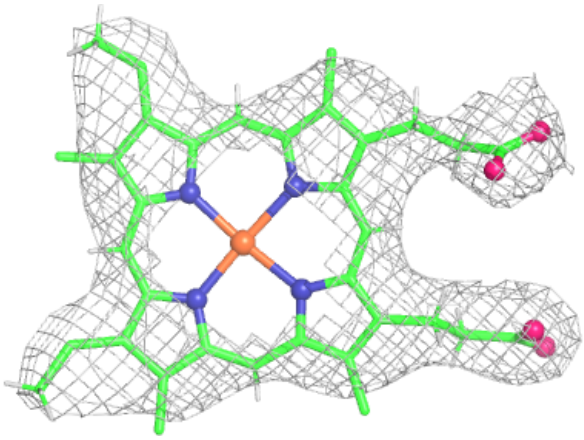


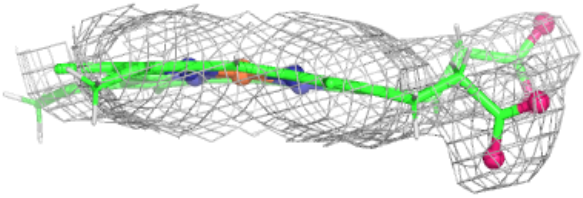


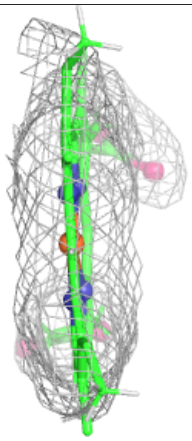


Electron density around HEC C 404:

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

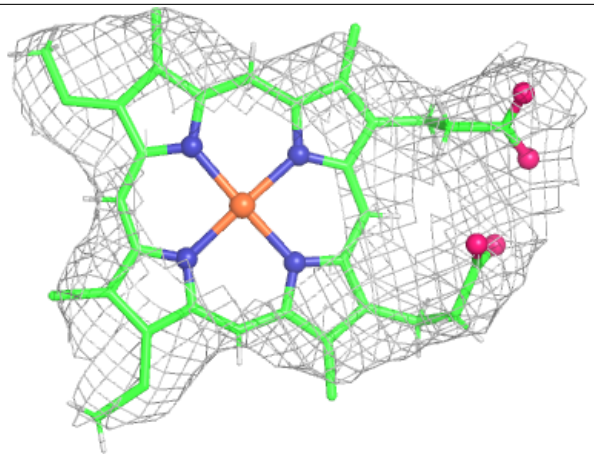


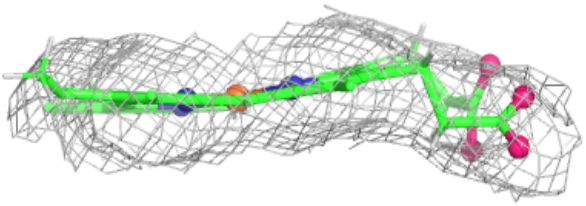


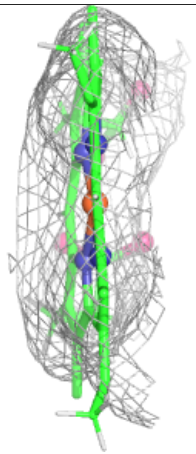


Electron density around HEC C 402:

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

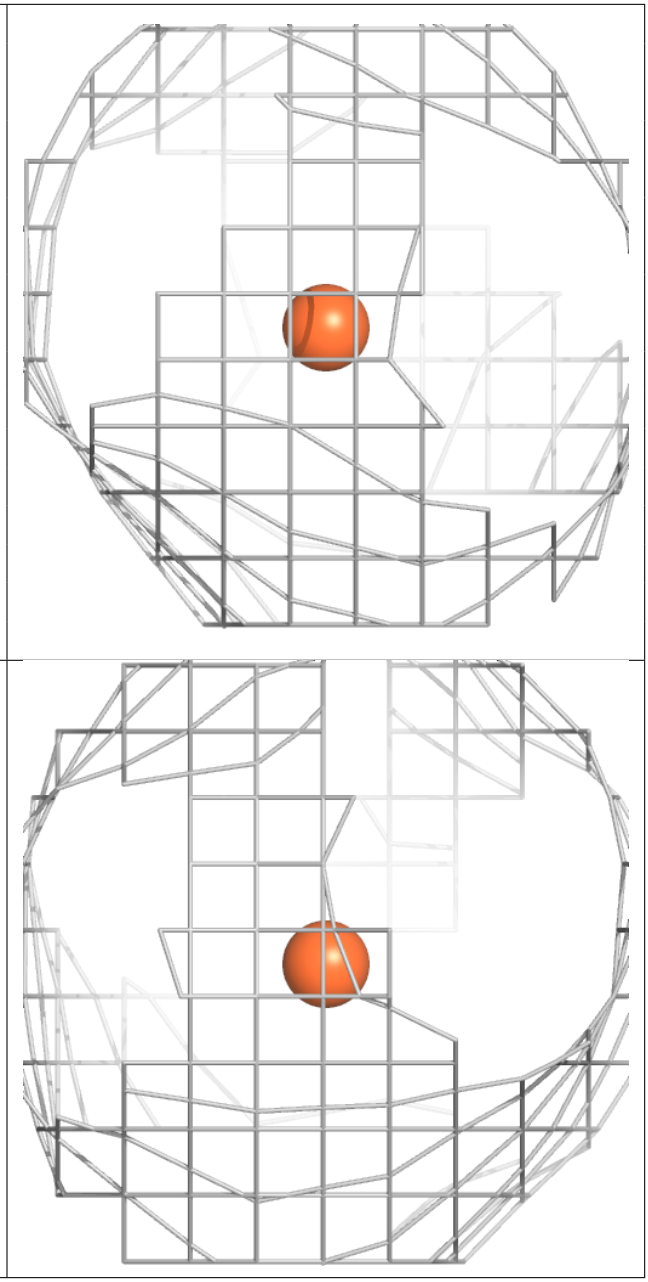






Electron density around FE2 M 401:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.