wwPDB X-ray Structure Validation Summary Report (i)

May 11, 2021 – 06:26 am BST

PDB ID	:	6ZHH
Title	:	Ca2+-ATPase from Listeria Monocytogenes with G4 insertion.
Authors	:	Basse Hansen, S.; Dyla, M.; Neumann, C.; Quistgaard, E.M.H.; Lauwring Andersen, J.; Kjaergaard, M.; Nissen, P.
Deposited on	:	2020-06-23
Resolution	:	3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see references (1)) were used in the production of this report:

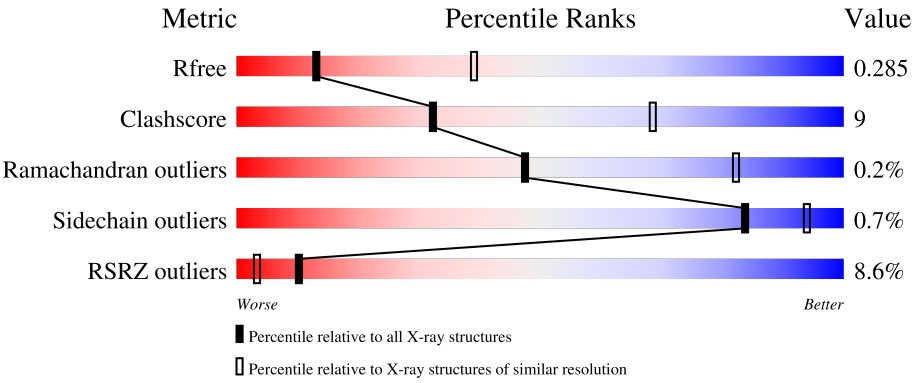
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.18
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.18

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 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	A	911	81% 16% ·
1	B	911	% 79% 18% ·
1	C	911	5% 76% 20% ·
1	D	911	8% 75% 22% ·
1	E	911	17% 74% 22% ·

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Mol	Chain	Length	Quality of chain
1	F	911	
1	G	911	
1	H	911	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 54572 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 Calcium-transporting ATPase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	883	Total	C	N	O	S	0	0	0
			6732	4298	1110	1290	34			
1	B	883	Total	C	N	O	S	0	0	0
			6732	4298	1110	1290	34			
1	C	883	Total	C	N	O	S	0	0	0
			6732	4298	1110	1290	34			
1	D	883	Total	C	N	O	S	0	0	0
			6732	4298	1110	1290	34			
1	E	876	Total	C	N	O	S	0	0	0
			6675	4262	1103	1276	34			
1	F	876	Total	C	N	O	S	0	0	0
			6675	4262	1103	1276	34			
1	G	875	Total	C	N	O	S	0	0	0
			6667	4258	1102	1273	34			
1	H	876	Total	C	N	O	S	0	0	0
			6675	4262	1103	1276	34			

There are 256 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP A0A1C7PY84
A	1	ALA	-	expression tag	UNP A0A1C7PY84
A	40E	GLY	-	insertion	UNP A0A1C7PY84
A	40F	GLY	-	insertion	UNP A0A1C7PY84
A	40G	GLY	-	insertion	UNP A0A1C7PY84
A	40H	GLY	-	insertion	UNP A0A1C7PY84
A	881	ASP	-	expression tag	UNP A0A1C7PY84
A	882	TYR	-	expression tag	UNP A0A1C7PY84
A	883	ASP	-	expression tag	UNP A0A1C7PY84
A	884	ILE	-	expression tag	UNP A0A1C7PY84
A	885	PRO	-	expression tag	UNP A0A1C7PY84
A	886	THR	-	expression tag	UNP A0A1C7PY84
A	887	THR	-	expression tag	UNP A0A1C7PY84

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Chain	Residue	Modelled	Actual	Comment	Reference
A	888	GLU	-	expression tag	UNP A0A1C7PY84
A	889	ASN	-	expression tag	UNP A0A1C7PY84
A	890	LEU	-	expression tag	UNP A0A1C7PY84
A	891	TYR	-	expression tag	UNP A0A1C7PY84
A	892	PHE	-	expression tag	UNP A0A1C7PY84
A	893	GLN	-	expression tag	UNP A0A1C7PY84
A	894	GLY	-	expression tag	UNP A0A1C7PY84
A	895	LEU	-	expression tag	UNP A0A1C7PY84
A	896	GLU	-	expression tag	UNP A0A1C7PY84
A	897	HIS	-	expression tag	UNP A0A1C7PY84
A	898	HIS	-	expression tag	UNP A0A1C7PY84
A	899	HIS	-	expression tag	UNP A0A1C7PY84
A	900	HIS	-	expression tag	UNP A0A1C7PY84
A	901	HIS	-	expression tag	UNP A0A1C7PY84
A	902	HIS	-	expression tag	UNP A0A1C7PY84
A	903	HIS	-	expression tag	UNP A0A1C7PY84
A	904	HIS	-	expression tag	UNP A0A1C7PY84
A	905	HIS	-	expression tag	UNP A0A1C7PY84
A	906	HIS	-	expression tag	UNP A0A1C7PY84
B	0	MET	-	initiating methionine	UNP A0A1C7PY84
B	1	ALA	-	expression tag	UNP A0A1C7PY84
B	40E	GLY	-	insertion	UNP A0A1C7PY84
B	40F	GLY	-	insertion	UNP A0A1C7PY84
B	40G	GLY	-	insertion	UNP A0A1C7PY84
B	40H	GLY	-	insertion	UNP A0A1C7PY84
B	881	ASP	-	expression tag	UNP A0A1C7PY84
B	882	TYR	-	expression tag	UNP A0A1C7PY84
B	883	ASP	-	expression tag	UNP A0A1C7PY84
B	884	ILE	-	expression tag	UNP A0A1C7PY84
B	885	PRO	-	expression tag	UNP A0A1C7PY84
B	886	THR	-	expression tag	UNP A0A1C7PY84
B	887	THR	-	expression tag	UNP A0A1C7PY84
B	888	GLU	-	expression tag	UNP A0A1C7PY84
B	889	ASN	-	expression tag	UNP A0A1C7PY84
B	890	LEU	-	expression tag	UNP A0A1C7PY84
B	891	TYR	-	expression tag	UNP A0A1C7PY84
B	892	PHE	-	expression tag	UNP A0A1C7PY84
B	893	GLN	-	expression tag	UNP A0A1C7PY84
B	894	GLY	-	expression tag	UNP A0A1C7PY84
B	895	LEU	-	expression tag	UNP A0A1C7PY84
B	896	GLU	-	expression tag	UNP A0A1C7PY84
B	897	HIS	-	expression tag	UNP A0A1C7PY84

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Chain	Residue	Modelled	Actual	Comment	Reference
B	898	HIS	-	expression tag	UNP A0A1C7PY84
B	899	HIS	-	expression tag	UNP A0A1C7PY84
B	900	HIS	-	expression tag	UNP A0A1C7PY84
B	901	HIS	-	expression tag	UNP A0A1C7PY84
B	902	HIS	-	expression tag	UNP A0A1C7PY84
B	903	HIS	-	expression tag	UNP A0A1C7PY84
B	904	HIS	-	expression tag	UNP A0A1C7PY84
B	905	HIS	-	expression tag	UNP A0A1C7PY84
B	906	HIS	-	expression tag	UNP A0A1C7PY84
C	0	MET	-	initiating methionine	UNP A0A1C7PY84
C	1	ALA	-	expression tag	UNP A0A1C7PY84
C	40E	GLY	-	insertion	UNP A0A1C7PY84
C	40F	GLY	-	insertion	UNP A0A1C7PY84
C	40G	GLY	-	insertion	UNP A0A1C7PY84
C	40H	GLY	-	insertion	UNP A0A1C7PY84
C	881	ASP	-	expression tag	UNP A0A1C7PY84
C	882	TYR	-	expression tag	UNP A0A1C7PY84
C	883	ASP	-	expression tag	UNP A0A1C7PY84
C	884	ILE	-	expression tag	UNP A0A1C7PY84
C	885	PRO	-	expression tag	UNP A0A1C7PY84
C	886	THR	-	expression tag	UNP A0A1C7PY84
C	887	THR	-	expression tag	UNP A0A1C7PY84
C	888	GLU	-	expression tag	UNP A0A1C7PY84
C	889	ASN	-	expression tag	UNP A0A1C7PY84
C	890	LEU	-	expression tag	UNP A0A1C7PY84
C	891	TYR	-	expression tag	UNP A0A1C7PY84
C	892	PHE	-	expression tag	UNP A0A1C7PY84
C	893	GLN	-	expression tag	UNP A0A1C7PY84
C	894	GLY	-	expression tag	UNP A0A1C7PY84
C	895	LEU	-	expression tag	UNP A0A1C7PY84
C	896	GLU	-	expression tag	UNP A0A1C7PY84
C	897	HIS	-	expression tag	UNP A0A1C7PY84
C	898	HIS	-	expression tag	UNP A0A1C7PY84
C	899	HIS	-	expression tag	UNP A0A1C7PY84
C	900	HIS	-	expression tag	UNP A0A1C7PY84
C	901	HIS	-	expression tag	UNP A0A1C7PY84
C	902	HIS	-	expression tag	UNP A0A1C7PY84
C	903	HIS	-	expression tag	UNP A0A1C7PY84
C	904	HIS	-	expression tag	UNP A0A1C7PY84
C	905	HIS	-	expression tag	UNP A0A1C7PY84
C	906	HIS	-	expression tag	UNP A0A1C7PY84
D	0	MET	-	initiating methionine	UNP A0A1C7PY84

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1	ALA	-	expression tag	UNP A0A1C7PY84
D	40E	GLY	-	insertion	UNP A0A1C7PY84
D	40F	GLY	-	insertion	UNP A0A1C7PY84
D	40G	GLY	-	insertion	UNP A0A1C7PY84
D	40H	GLY	-	insertion	UNP A0A1C7PY84
D	881	ASP	-	expression tag	UNP A0A1C7PY84
D	882	TYR	-	expression tag	UNP A0A1C7PY84
D	883	ASP	-	expression tag	UNP A0A1C7PY84
D	884	ILE	-	expression tag	UNP A0A1C7PY84
D	885	PRO	-	expression tag	UNP A0A1C7PY84
D	886	THR	-	expression tag	UNP A0A1C7PY84
D	887	THR	-	expression tag	UNP A0A1C7PY84
D	888	GLU	-	expression tag	UNP A0A1C7PY84
D	889	ASN	-	expression tag	UNP A0A1C7PY84
D	890	LEU	-	expression tag	UNP A0A1C7PY84
D	891	TYR	-	expression tag	UNP A0A1C7PY84
D	892	PHE	-	expression tag	UNP A0A1C7PY84
D	893	GLN	-	expression tag	UNP A0A1C7PY84
D	894	GLY	-	expression tag	UNP A0A1C7PY84
D	895	LEU	-	expression tag	UNP A0A1C7PY84
D	896	GLU	-	expression tag	UNP A0A1C7PY84
D	897	HIS	-	expression tag	UNP A0A1C7PY84
D	898	HIS	-	expression tag	UNP A0A1C7PY84
D	899	HIS	-	expression tag	UNP A0A1C7PY84
D	900	HIS	-	expression tag	UNP A0A1C7PY84
D	901	HIS	-	expression tag	UNP A0A1C7PY84
D	902	HIS	-	expression tag	UNP A0A1C7PY84
D	903	HIS	-	expression tag	UNP A0A1C7PY84
D	904	HIS	-	expression tag	UNP A0A1C7PY84
D	905	HIS	-	expression tag	UNP A0A1C7PY84
D	906	HIS	-	expression tag	UNP A0A1C7PY84
E	0	MET	-	initiating methionine	UNP A0A1C7PY84
E	1	ALA	-	expression tag	UNP A0A1C7PY84
E	40E	GLY	-	insertion	UNP A0A1C7PY84
E	40F	GLY	-	insertion	UNP A0A1C7PY84
E	40G	GLY	-	insertion	UNP A0A1C7PY84
E	40H	GLY	-	insertion	UNP A0A1C7PY84
E	881	ASP	-	expression tag	UNP A0A1C7PY84
E	882	TYR	-	expression tag	UNP A0A1C7PY84
E	883	ASP	-	expression tag	UNP A0A1C7PY84
E	884	ILE	-	expression tag	UNP A0A1C7PY84
E	885	PRO	-	expression tag	UNP A0A1C7PY84

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Chain	Residue	Modelled	Actual	Comment	Reference
E	886	THR	-	expression tag	UNP A0A1C7PY84
E	887	THR	-	expression tag	UNP A0A1C7PY84
E	888	GLU	-	expression tag	UNP A0A1C7PY84
E	889	ASN	-	expression tag	UNP A0A1C7PY84
E	890	LEU	-	expression tag	UNP A0A1C7PY84
E	891	TYR	-	expression tag	UNP A0A1C7PY84
E	892	PHE	-	expression tag	UNP A0A1C7PY84
E	893	GLN	-	expression tag	UNP A0A1C7PY84
E	894	GLY	-	expression tag	UNP A0A1C7PY84
E	895	LEU	-	expression tag	UNP A0A1C7PY84
E	896	GLU	-	expression tag	UNP A0A1C7PY84
E	897	HIS	-	expression tag	UNP A0A1C7PY84
E	898	HIS	-	expression tag	UNP A0A1C7PY84
E	899	HIS	-	expression tag	UNP A0A1C7PY84
E	900	HIS	-	expression tag	UNP A0A1C7PY84
E	901	HIS	-	expression tag	UNP A0A1C7PY84
E	902	HIS	-	expression tag	UNP A0A1C7PY84
E	903	HIS	-	expression tag	UNP A0A1C7PY84
E	904	HIS	-	expression tag	UNP A0A1C7PY84
E	905	HIS	-	expression tag	UNP A0A1C7PY84
E	906	HIS	-	expression tag	UNP A0A1C7PY84
F	0	MET	-	initiating methionine	UNP A0A1C7PY84
F	1	ALA	-	expression tag	UNP A0A1C7PY84
F	40E	GLY	-	insertion	UNP A0A1C7PY84
F	40F	GLY	-	insertion	UNP A0A1C7PY84
F	40G	GLY	-	insertion	UNP A0A1C7PY84
F	40H	GLY	-	insertion	UNP A0A1C7PY84
F	881	ASP	-	expression tag	UNP A0A1C7PY84
F	882	TYR	-	expression tag	UNP A0A1C7PY84
F	883	ASP	-	expression tag	UNP A0A1C7PY84
F	884	ILE	-	expression tag	UNP A0A1C7PY84
F	885	PRO	-	expression tag	UNP A0A1C7PY84
F	886	THR	-	expression tag	UNP A0A1C7PY84
F	887	THR	-	expression tag	UNP A0A1C7PY84
F	888	GLU	-	expression tag	UNP A0A1C7PY84
F	889	ASN	-	expression tag	UNP A0A1C7PY84
F	890	LEU	-	expression tag	UNP A0A1C7PY84
F	891	TYR	-	expression tag	UNP A0A1C7PY84
F	892	PHE	-	expression tag	UNP A0A1C7PY84
F	893	GLN	-	expression tag	UNP A0A1C7PY84
F	894	GLY	-	expression tag	UNP A0A1C7PY84
F	895	LEU	-	expression tag	UNP A0A1C7PY84

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Chain	Residue	Modelled	Actual	Comment	Reference
F	896	GLU	-	expression tag	UNP A0A1C7PY84
F	897	HIS	-	expression tag	UNP A0A1C7PY84
F	898	HIS	-	expression tag	UNP A0A1C7PY84
F	899	HIS	-	expression tag	UNP A0A1C7PY84
F	900	HIS	-	expression tag	UNP A0A1C7PY84
F	901	HIS	-	expression tag	UNP A0A1C7PY84
F	902	HIS	-	expression tag	UNP A0A1C7PY84
F	903	HIS	-	expression tag	UNP A0A1C7PY84
F	904	HIS	-	expression tag	UNP A0A1C7PY84
F	905	HIS	-	expression tag	UNP A0A1C7PY84
F	906	HIS	-	expression tag	UNP A0A1C7PY84
G	0	MET	-	initiating methionine	UNP A0A1C7PY84
G	1	ALA	-	expression tag	UNP A0A1C7PY84
G	40E	GLY	-	insertion	UNP A0A1C7PY84
G	40F	GLY	-	insertion	UNP A0A1C7PY84
G	40G	GLY	-	insertion	UNP A0A1C7PY84
G	40H	GLY	-	insertion	UNP A0A1C7PY84
G	881	ASP	-	expression tag	UNP A0A1C7PY84
G	882	TYR	-	expression tag	UNP A0A1C7PY84
G	883	ASP	-	expression tag	UNP A0A1C7PY84
G	884	ILE	-	expression tag	UNP A0A1C7PY84
G	885	PRO	-	expression tag	UNP A0A1C7PY84
G	886	THR	-	expression tag	UNP A0A1C7PY84
G	887	THR	-	expression tag	UNP A0A1C7PY84
G	888	GLU	-	expression tag	UNP A0A1C7PY84
G	889	ASN	-	expression tag	UNP A0A1C7PY84
G	890	LEU	-	expression tag	UNP A0A1C7PY84
G	891	TYR	-	expression tag	UNP A0A1C7PY84
G	892	PHE	-	expression tag	UNP A0A1C7PY84
G	893	GLN	-	expression tag	UNP A0A1C7PY84
G	894	GLY	-	expression tag	UNP A0A1C7PY84
G	895	LEU	-	expression tag	UNP A0A1C7PY84
G	896	GLU	-	expression tag	UNP A0A1C7PY84
G	897	HIS	-	expression tag	UNP A0A1C7PY84
G	898	HIS	-	expression tag	UNP A0A1C7PY84
G	899	HIS	-	expression tag	UNP A0A1C7PY84
G	900	HIS	-	expression tag	UNP A0A1C7PY84
G	901	HIS	-	expression tag	UNP A0A1C7PY84
G	902	HIS	-	expression tag	UNP A0A1C7PY84
G	903	HIS	-	expression tag	UNP A0A1C7PY84
G	904	HIS	-	expression tag	UNP A0A1C7PY84
G	905	HIS	-	expression tag	UNP A0A1C7PY84

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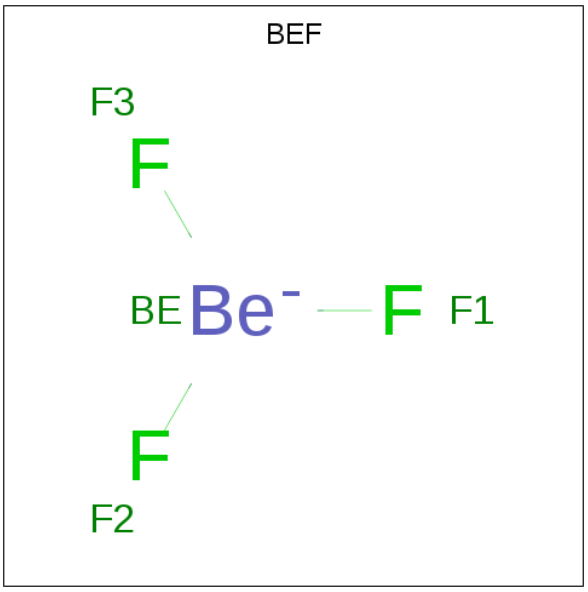
Chain	Residue	Modelled	Actual	Comment	Reference
G	906	HIS	-	expression tag	UNP A0A1C7PY84
H	0	MET	-	initiating methionine	UNP A0A1C7PY84
H	1	ALA	-	expression tag	UNP A0A1C7PY84
H	40E	GLY	-	insertion	UNP A0A1C7PY84
H	40F	GLY	-	insertion	UNP A0A1C7PY84
H	40G	GLY	-	insertion	UNP A0A1C7PY84
H	40H	GLY	-	insertion	UNP A0A1C7PY84
H	881	ASP	-	expression tag	UNP A0A1C7PY84
H	882	TYR	-	expression tag	UNP A0A1C7PY84
H	883	ASP	-	expression tag	UNP A0A1C7PY84
H	884	ILE	-	expression tag	UNP A0A1C7PY84
H	885	PRO	-	expression tag	UNP A0A1C7PY84
H	886	THR	-	expression tag	UNP A0A1C7PY84
H	887	THR	-	expression tag	UNP A0A1C7PY84
H	888	GLU	-	expression tag	UNP A0A1C7PY84
H	889	ASN	-	expression tag	UNP A0A1C7PY84
H	890	LEU	-	expression tag	UNP A0A1C7PY84
H	891	TYR	-	expression tag	UNP A0A1C7PY84
H	892	PHE	-	expression tag	UNP A0A1C7PY84
H	893	GLN	-	expression tag	UNP A0A1C7PY84
H	894	GLY	-	expression tag	UNP A0A1C7PY84
H	895	LEU	-	expression tag	UNP A0A1C7PY84
H	896	GLU	-	expression tag	UNP A0A1C7PY84
H	897	HIS	-	expression tag	UNP A0A1C7PY84
H	898	HIS	-	expression tag	UNP A0A1C7PY84
H	899	HIS	-	expression tag	UNP A0A1C7PY84
H	900	HIS	-	expression tag	UNP A0A1C7PY84
H	901	HIS	-	expression tag	UNP A0A1C7PY84
H	902	HIS	-	expression tag	UNP A0A1C7PY84
H	903	HIS	-	expression tag	UNP A0A1C7PY84
H	904	HIS	-	expression tag	UNP A0A1C7PY84
H	905	HIS	-	expression tag	UNP A0A1C7PY84
H	906	HIS	-	expression tag	UNP A0A1C7PY84

- Molecule 2 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF_3) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Be F 4 1 3	0	0
2	B	1	Total Be F 4 1 3	0	0
2	C	1	Total Be F 4 1 3	0	0
2	D	1	Total Be F 4 1 3	0	0
2	E	1	Total Be F 4 1 3	0	0
2	F	1	Total Be F 4 1 3	0	0
2	G	1	Total Be F 4 1 3	0	0
2	H	1	Total Be F 4 1 3	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0

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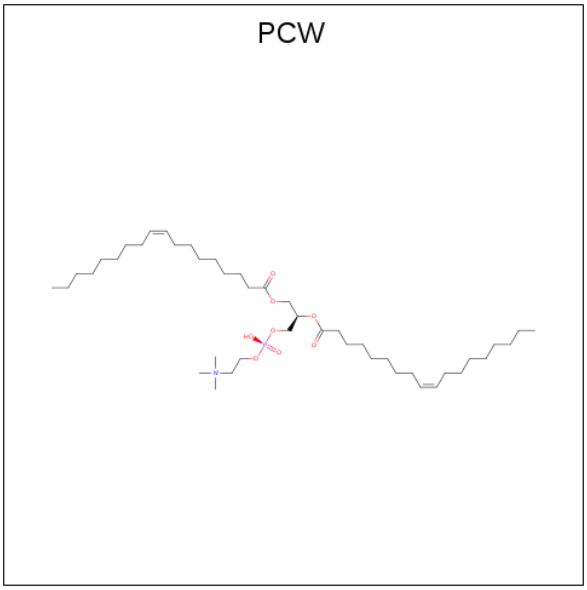
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total Mg 1 1	0	0
3	E	1	Total Mg 1 1	0	0
3	F	1	Total Mg 1 1	0	0
3	G	1	Total Mg 1 1	0	0
3	H	1	Total Mg 1 1	0	0

- Molecule 4 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula: $C_{44}H_{85}NO_8P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P 54 44 1 8 1	0	0
4	A	1	Total C N O P 54 44 1 8 1	0	0
4	B	1	Total C N O P 54 44 1 8 1	0	0
4	B	1	Total C N O P 54 44 1 8 1	0	0
4	B	1	Total C N O P 54 44 1 8 1	0	0
4	B	1	Total C N O P 54 44 1 8 1	0	0

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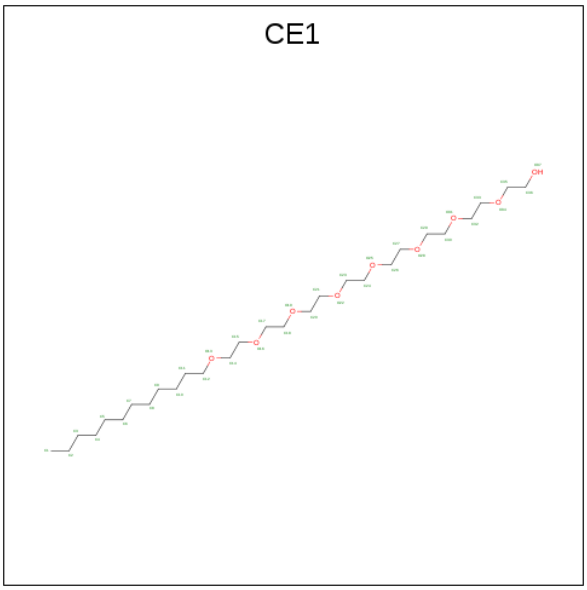
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N O P 54 44 1 8 1	0	0
4	B	1	Total C N O P 54 44 1 8 1	0	0
4	B	1	Total C N O P 54 44 1 8 1	0	0
4	C	1	Total C N O P 54 44 1 8 1	0	0
4	C	1	Total C N O P 54 44 1 8 1	0	0
4	C	1	Total C N O P 54 44 1 8 1	0	0
4	C	1	Total C N O P 54 44 1 8 1	0	0
4	C	1	Total C N O P 54 44 1 8 1	0	0
4	D	1	Total C N O P 54 44 1 8 1	0	0

- Molecule 5 is O-DODECANYL OCTAETHYLENE GLYCOL (three-letter code: CE1) (formula: $C_{28}H_{58}O_9$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C O 15 14 1	0	0
5	D	1	Total C 12 12	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total C 12 12	0	0
5	D	1	Total C 12 12	0	0
5	D	1	Total C 12 12	0	0
5	D	1	Total C 11 11	0	0
5	D	1	Total C 12 12	0	0

- Molecule 6 is water.

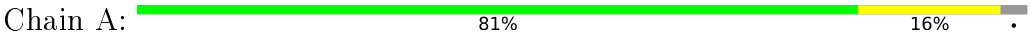
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total O 2 2	0	0
6	B	2	Total O 2 2	0	0
6	C	2	Total O 2 2	0	0
6	D	2	Total O 2 2	0	0
6	E	2	Total O 2 2	0	0
6	F	2	Total O 2 2	0	0
6	G	2	Total O 2 2	0	0
6	H	2	Total O 2 2	0	0

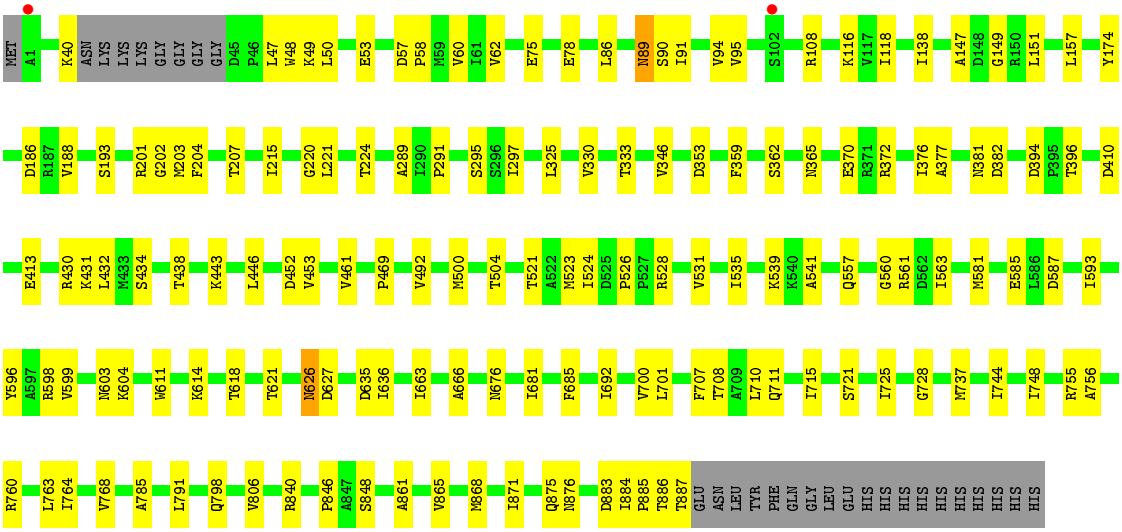
3 Residue-property plots (i)

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: Calcium-transporting ATPase

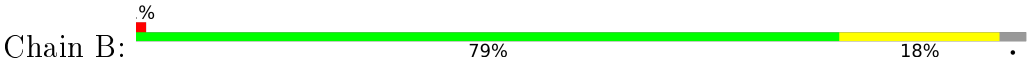
Chain A:

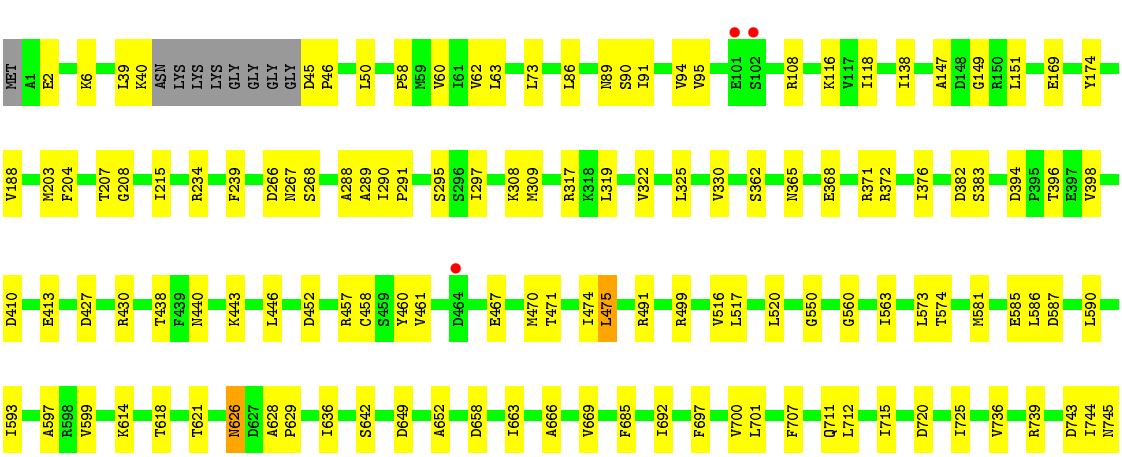


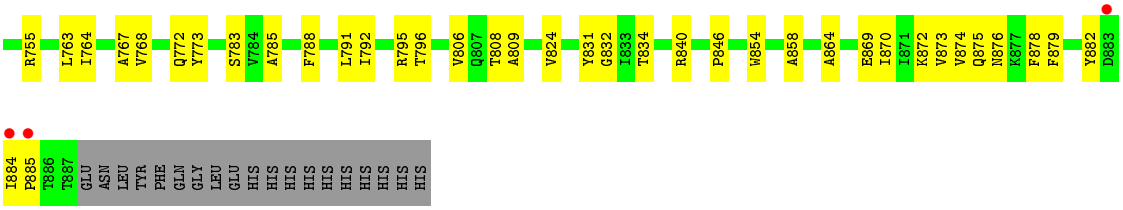


- Molecule 1: Calcium-transporting ATPase

Chain B:

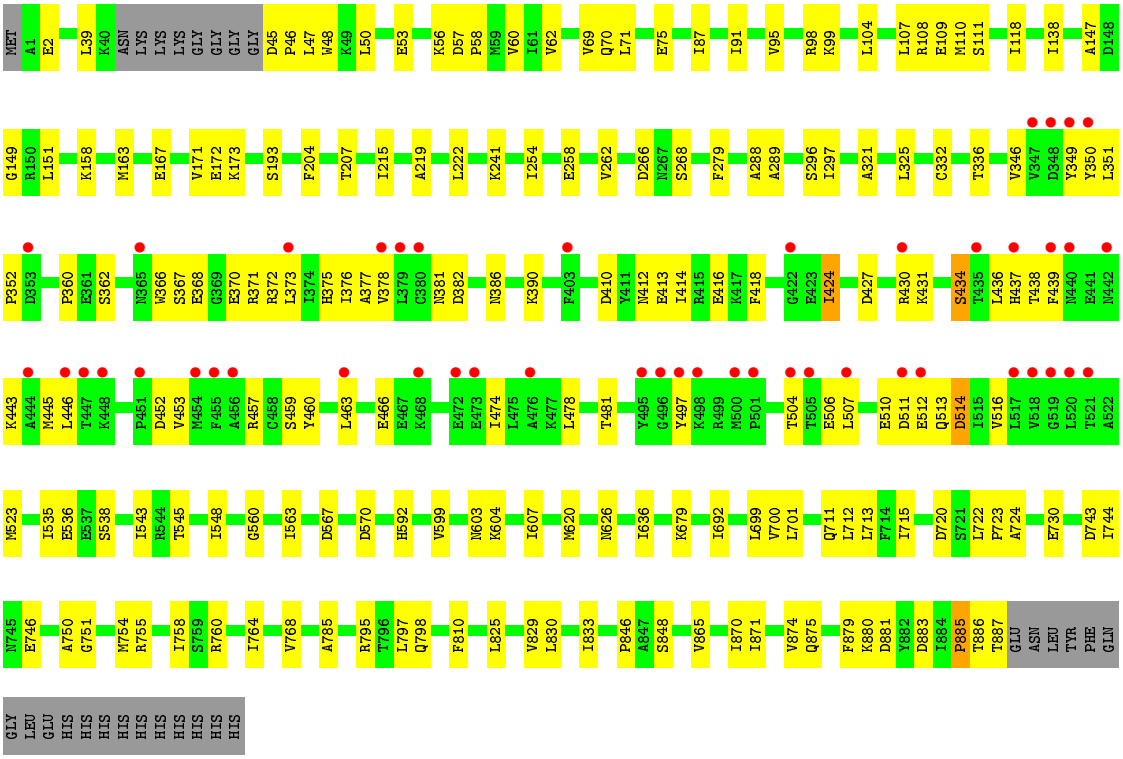






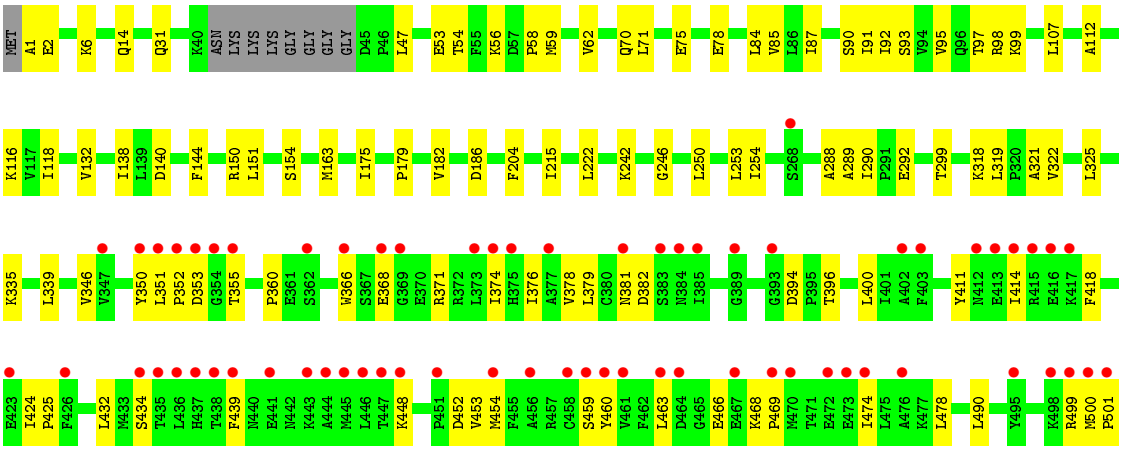
• Molecule 1: Calcium-transporting ATPase

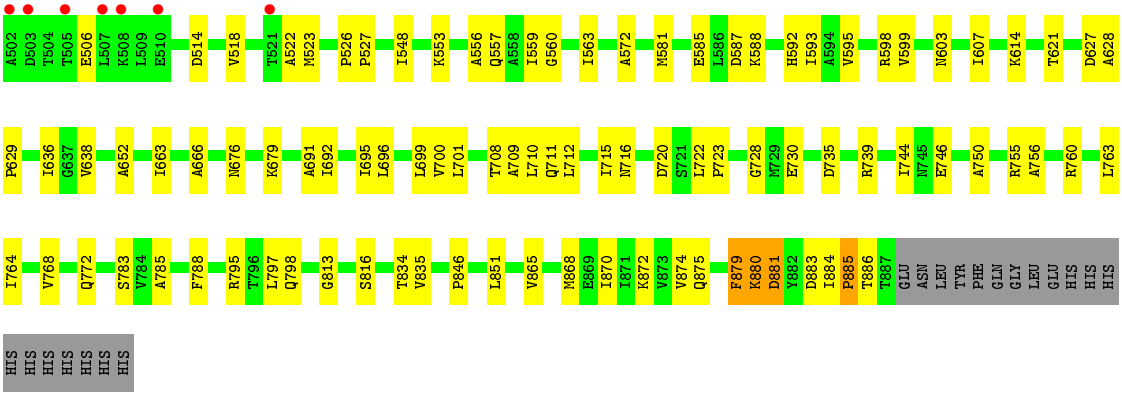
Chain C:



• Molecule 1: Calcium-transporting ATPase

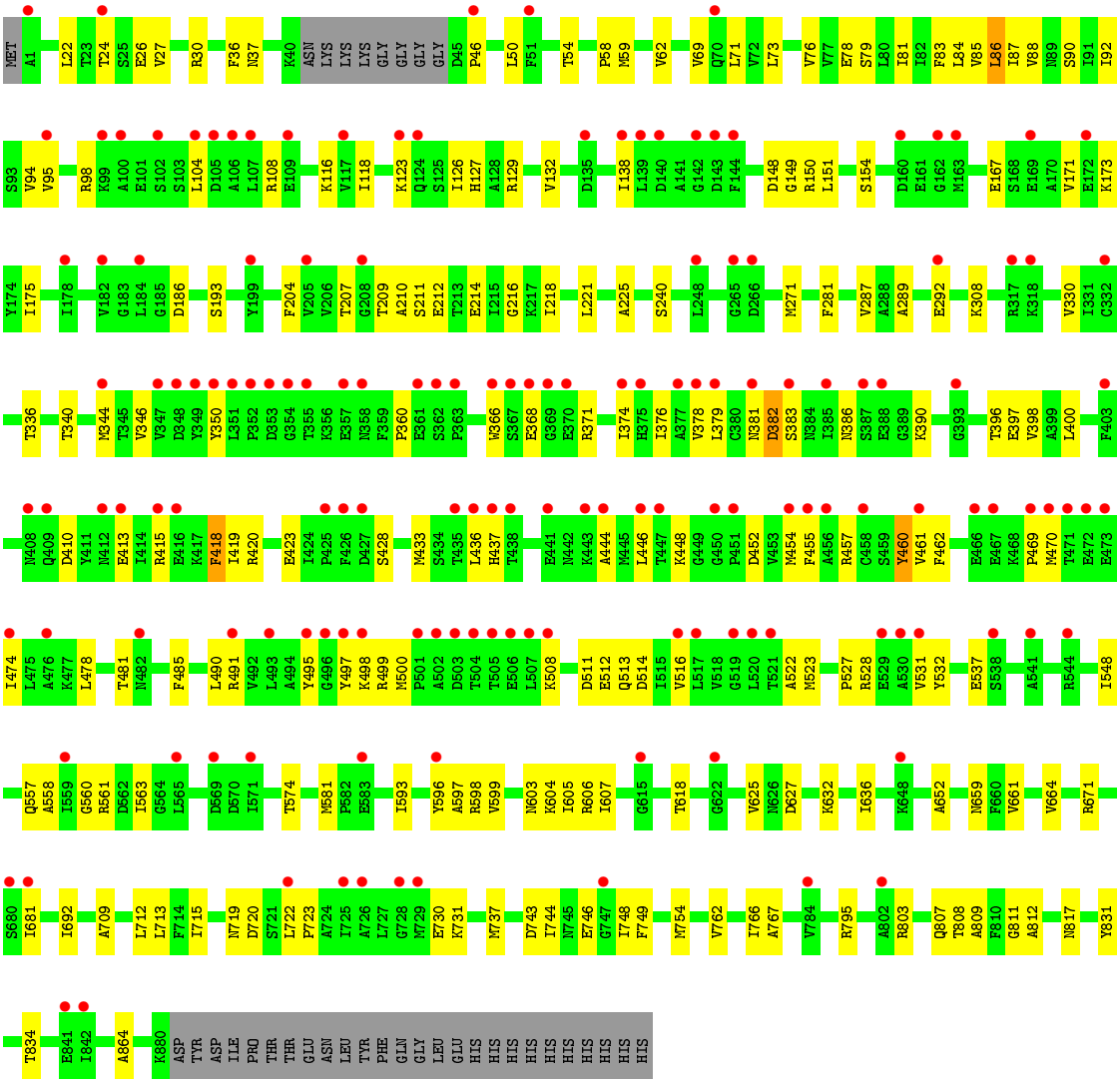
Chain D:



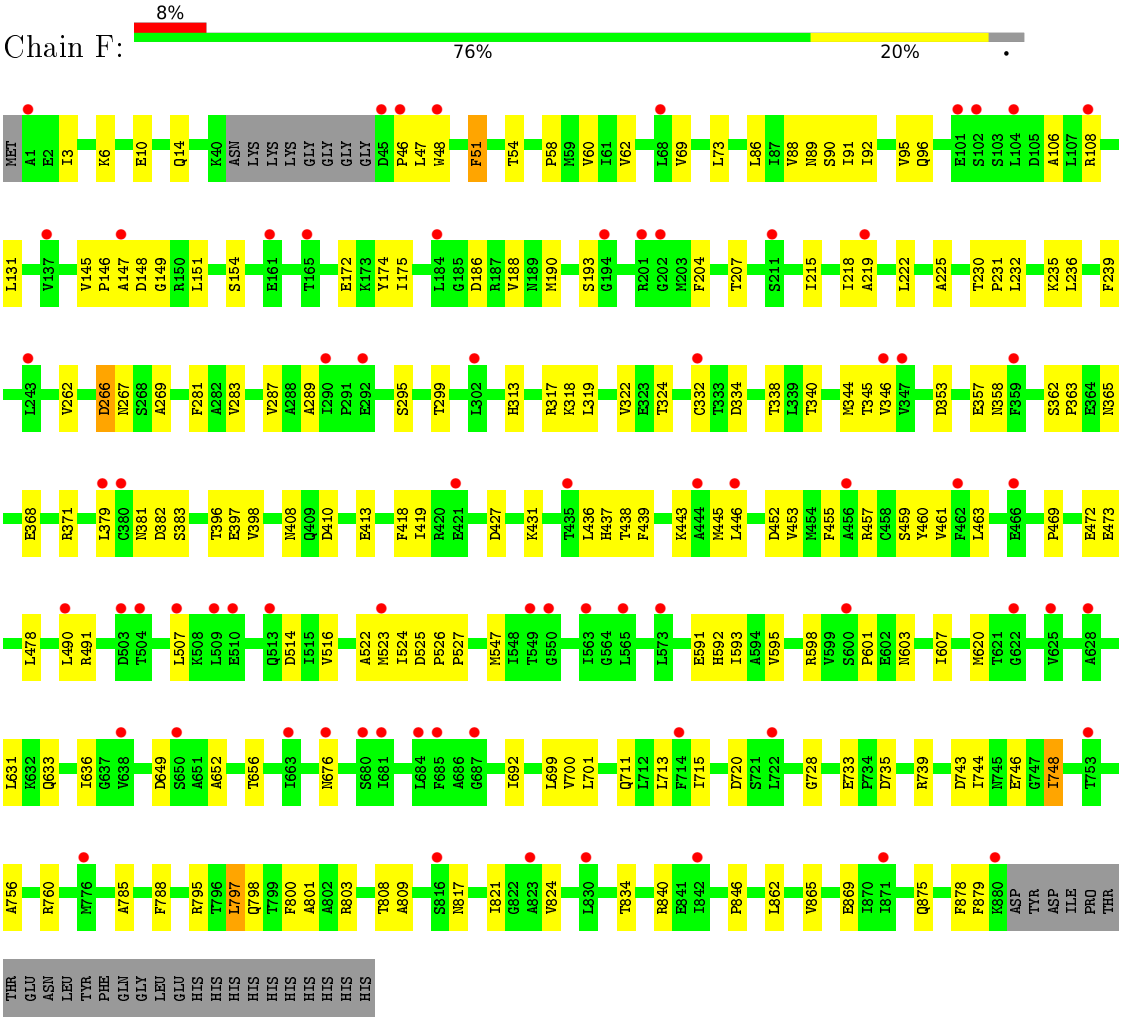


• Molecule 1: Calcium-transporting ATPase

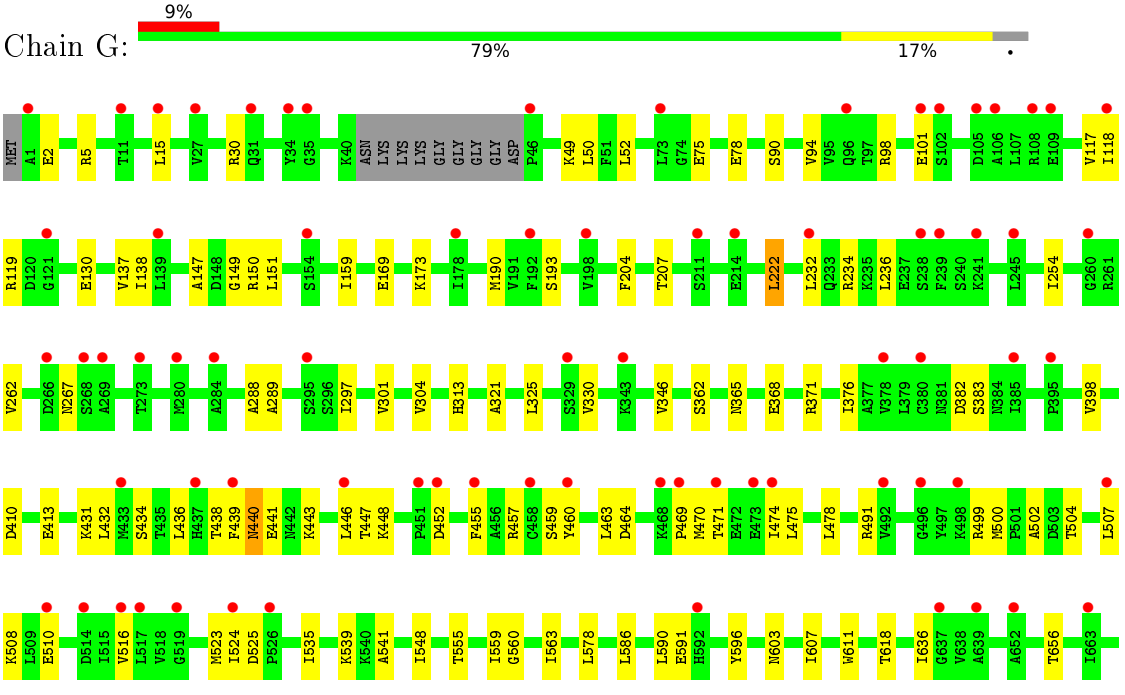
Chain E:

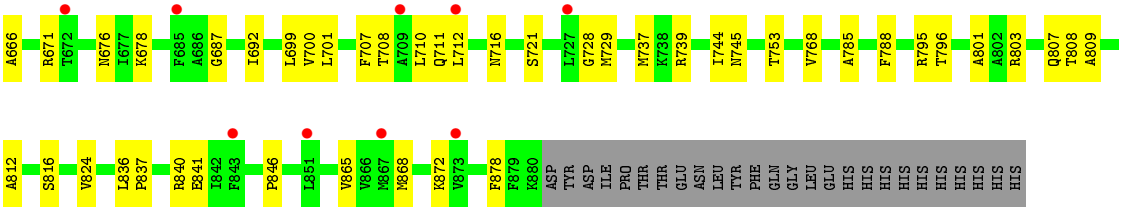


• Molecule 1: Calcium-transporting ATPase



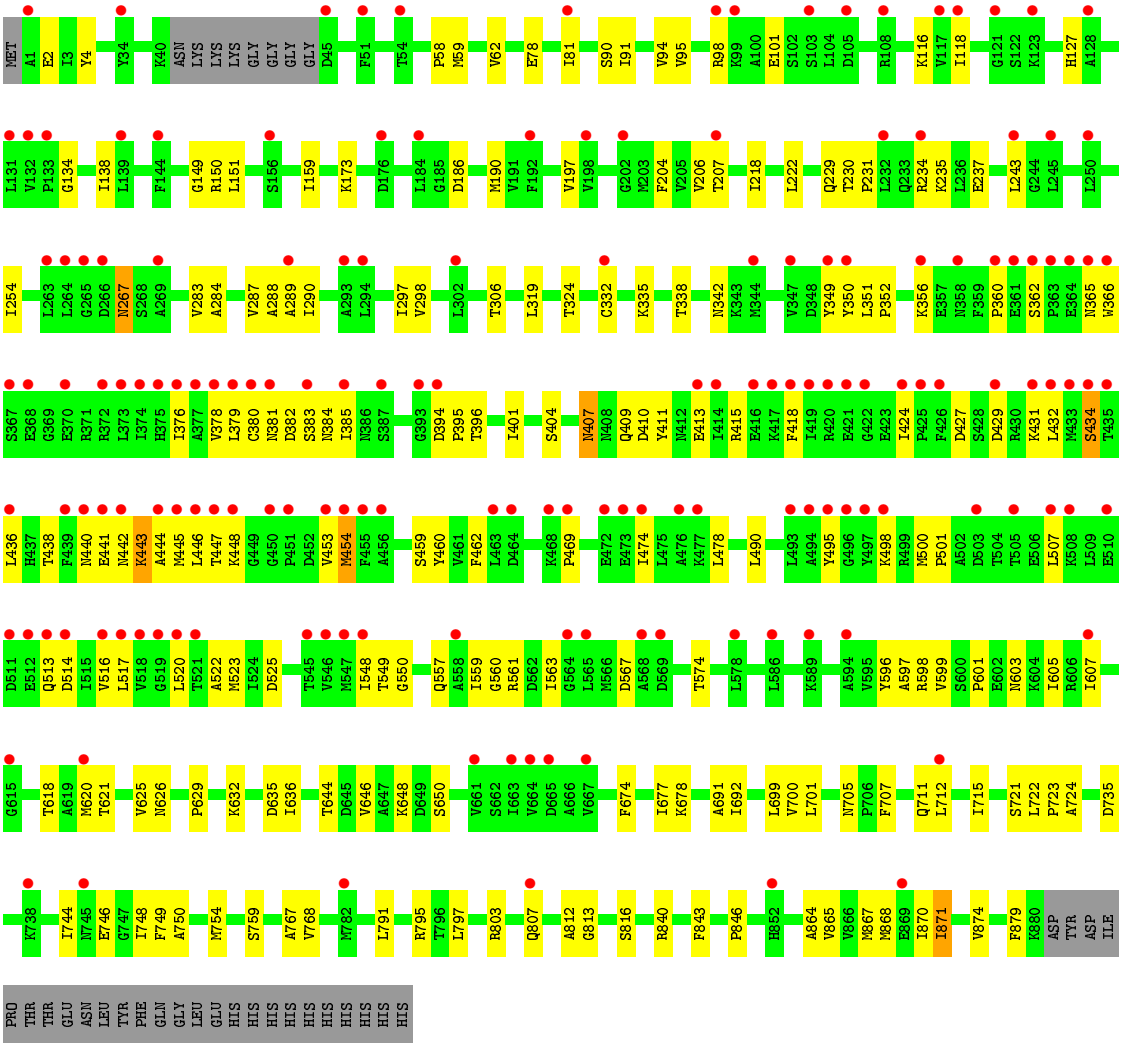
• Molecule 1: Calcium-transporting ATPase





• Molecule 1: Calcium-transporting ATPase

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	74.06Å 188.50Å 350.01Å 90.00° 91.94° 90.00°	Depositor
Resolution (Å)	49.58 – 3.00 49.58 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.1 (49.58-3.00) 96.0 (49.58-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.35 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.255 , 0.285 0.255 , 0.285	Depositor DCC
R_{free} test set	1999 reflections (1.09%)	wwPDB-VP
Wilson B-factor (Å^2)	67.1	Xtriage
Anisotropy	0.274	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 60.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.066 for h,-k,-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	54572	wwPDB-VP
Average B, all atoms (Å^2)	128.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.68 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7655e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CE1, MG, BEF, PCW

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	A	0.42	0/6832	0.65	0/9248
1	B	0.42	0/6832	0.65	2/9248 (0.0%)
1	C	0.40	0/6832	0.64	3/9248 (0.0%)
1	D	0.39	0/6832	0.63	0/9248
1	E	0.31	0/6773	0.55	1/9165 (0.0%)
1	F	0.32	0/6773	0.54	1/9165 (0.0%)
1	G	0.30	0/6765	0.53	1/9153 (0.0%)
1	H	0.31	0/6773	0.54	0/9165
All	All	0.36	0/54412	0.59	8/73640 (0.0%)

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	797	LEU	CA-CB-CG	6.22	129.60	115.30
1	C	825	LEU	CA-CB-CG	6.03	129.18	115.30
1	B	520	LEU	CA-CB-CG	5.88	128.82	115.30
1	B	475	LEU	CA-CB-CG	5.64	128.27	115.30
1	E	86	LEU	CA-CB-CG	5.36	127.63	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6732	0	6905	93	0
1	B	6732	0	6905	113	0
1	C	6732	0	6905	139	0
1	D	6732	0	6905	137	0
1	E	6675	0	6856	131	0
1	F	6675	0	6856	116	0
1	G	6667	0	6853	97	0
1	H	6675	0	6856	137	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
2	E	4	0	0	0	0
2	F	4	0	0	0	0
2	G	4	0	0	0	0
2	H	4	0	0	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	108	0	168	3	0
4	B	378	0	588	18	0
4	C	270	0	420	21	0
4	D	54	0	81	4	0
5	C	15	0	27	0	0
5	D	71	0	136	10	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
6	C	2	0	0	0	0
6	D	2	0	0	1	0
6	E	2	0	0	0	0
6	F	2	0	0	0	0
6	G	2	0	0	0	0
6	H	2	0	0	0	0
All	All	54572	0	56461	971	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 9.

The worst 5 of 971 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)
1:E:46:PRO:HG2	1:E:98:ARG:HH12	1.34	0.92
1:A:875:GLN:HB2	1:A:885:PRO:HB3	1.57	0.87
1:C:241:LYS:HE2	4:C:1004:PCW:H41	1.61	0.81
1:C:366:TRP:HE1	1:C:371:ARG:HB3	1.44	0.81
1:C:325:LEU:HG	1:C:636:ILE:HD13	1.63	0.81

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	A	879/911 (96%)	842 (96%)	37 (4%)	0	100	100
1	B	879/911 (96%)	844 (96%)	33 (4%)	2 (0%)	47	82
1	C	879/911 (96%)	836 (95%)	41 (5%)	2 (0%)	47	82
1	D	879/911 (96%)	838 (95%)	38 (4%)	3 (0%)	41	76
1	E	872/911 (96%)	843 (97%)	28 (3%)	1 (0%)	51	85
1	F	872/911 (96%)	830 (95%)	40 (5%)	2 (0%)	47	82
1	G	871/911 (96%)	838 (96%)	32 (4%)	1 (0%)	51	85
1	H	872/911 (96%)	830 (95%)	38 (4%)	4 (0%)	29	68
All	All	7003/7288 (96%)	6701 (96%)	287 (4%)	15 (0%)	47	82

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	267	ASN
1	C	885	PRO
1	D	879	PHE
1	D	885	PRO

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Mol	Chain	Res	Type
1	H	442	ASN

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	727/750 (97%)	723 (99%)	4 (1%)	86 95
1	B	727/750 (97%)	725 (100%)	2 (0%)	92 97
1	C	727/750 (97%)	722 (99%)	5 (1%)	84 94
1	D	727/750 (97%)	718 (99%)	9 (1%)	71 90
1	E	720/750 (96%)	714 (99%)	6 (1%)	81 93
1	F	720/750 (96%)	715 (99%)	5 (1%)	84 94
1	G	719/750 (96%)	715 (99%)	4 (1%)	86 95
1	H	720/750 (96%)	713 (99%)	7 (1%)	76 91
All	All	5787/6000 (96%)	5745 (99%)	42 (1%)	84 94

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	266	ASP
1	H	382	ASP
1	F	382	ASP
1	G	434	SER
1	H	429	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	437	HIS
1	D	557	GLN
1	F	233	GLN
1	D	592	HIS

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Mol	Chain	Res	Type
1	B	229	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 38 ligands modelled in this entry, 8 are monoatomic - leaving 30 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	BEF	E	1001	1	0,3,3	0.00	-	-		
4	PCW	B	1006	-	53,53,53	0.99	2 (3%)	59,61,61	0.99	3 (5%)
5	CE1	C	1007	-	14,14,36	0.55	0	13,13,35	0.95	1 (7%)
5	CE1	D	1009	-	11,11,36	0.42	0	10,10,35	0.75	0
4	PCW	C	1004	-	53,53,53	0.95	3 (5%)	59,61,61	1.05	5 (8%)
4	PCW	A	1004	-	53,53,53	0.93	2 (3%)	59,61,61	1.07	5 (8%)
4	PCW	C	1008	-	53,53,53	0.99	2 (3%)	59,61,61	1.10	5 (8%)
4	PCW	C	1006	-	53,53,53	1.00	3 (5%)	59,61,61	1.09	6 (10%)
4	PCW	B	1004	-	53,53,53	0.98	4 (7%)	59,61,61	1.00	5 (8%)
4	PCW	A	1003	-	53,53,53	0.83	2 (3%)	59,61,61	1.01	4 (6%)
2	BEF	F	1001	1	0,3,3	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	PCW	B	1005	-	53,53,53	0.85	2 (3%)	59,61,61	1.11	5 (8%)
4	PCW	B	1008	-	53,53,53	1.10	4 (7%)	59,61,61	1.06	4 (6%)
2	BEF	H	1001	1	0,3,3	0.00	-	-		
5	CE1	D	1004	-	11,11,36	0.54	0	10,10,35	0.72	0
4	PCW	B	1007	-	53,53,53	1.07	4 (7%)	59,61,61	1.06	4 (6%)
2	BEF	B	1001	1	0,3,3	0.00	-	-		
5	CE1	D	1007	-	11,11,36	0.40	0	10,10,35	0.90	0
5	CE1	D	1005	-	11,11,36	0.30	0	10,10,35	0.89	0
2	BEF	A	1001	1	0,3,3	0.00	-	-		
4	PCW	D	1003	1	53,53,53	1.04	4 (7%)	59,61,61	1.02	5 (8%)
4	PCW	B	1009	-	53,53,53	0.99	5 (9%)	59,61,61	1.01	4 (6%)
5	CE1	D	1008	-	10,10,36	0.64	0	9,9,35	0.62	0
4	PCW	B	1003	-	53,53,53	1.07	5 (9%)	59,61,61	1.05	6 (10%)
2	BEF	D	1001	1	0,3,3	0.00	-	-		
4	PCW	C	1003	-	53,53,53	0.85	2 (3%)	59,61,61	1.07	6 (10%)
5	CE1	D	1006	-	11,11,36	0.83	0	10,10,35	0.84	0
4	PCW	C	1005	-	53,53,53	1.09	5 (9%)	59,61,61	1.05	5 (8%)
2	BEF	C	1001	1	0,3,3	0.00	-	-		
2	BEF	G	1001	1	0,3,3	0.00	-	-		

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
4	PCW	B	1006	-	-	30/57/57/57	-
5	CE1	C	1007	-	-	6/12/12/34	-
5	CE1	D	1009	-	-	5/9/9/34	-
4	PCW	C	1004	-	-	32/57/57/57	-
4	PCW	A	1004	-	-	28/57/57/57	-
4	PCW	C	1008	-	-	31/57/57/57	-
4	PCW	C	1006	-	-	36/57/57/57	-
4	PCW	B	1004	-	-	33/57/57/57	-
4	PCW	A	1003	-	-	27/57/57/57	-
4	PCW	B	1005	-	-	31/57/57/57	-
4	PCW	B	1008	-	-	31/57/57/57	-
5	CE1	D	1004	-	-	5/9/9/34	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PCW	B	1007	-	-	30/57/57/57	-
5	CE1	D	1007	-	-	1/9/9/34	-
5	CE1	D	1005	-	-	3/9/9/34	-
4	PCW	D	1003	1	-	26/57/57/57	-
4	PCW	B	1009	-	-	29/57/57/57	-
5	CE1	D	1008	-	-	5/8/8/34	-
4	PCW	B	1003	-	-	25/57/57/57	-
4	PCW	C	1003	-	-	22/57/57/57	-
5	CE1	D	1006	-	-	4/9/9/34	-
4	PCW	C	1005	-	-	29/57/57/57	-

The worst 5 of 49 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1005	PCW	P-O4P	4.43	1.77	1.59
4	B	1008	PCW	P-O4P	4.43	1.77	1.59
4	B	1007	PCW	P-O4P	4.36	1.76	1.59
4	C	1008	PCW	P-O4P	4.29	1.76	1.59
4	C	1006	PCW	P-O4P	4.28	1.76	1.59

The worst 5 of 73 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	1003	PCW	O1P-P-O2P	3.23	128.19	112.24
4	B	1006	PCW	O1P-P-O2P	3.12	127.67	112.24
4	D	1003	PCW	O4P-P-O2P	-3.12	96.89	109.07
4	B	1003	PCW	O1P-P-O2P	3.10	127.55	112.24
4	B	1008	PCW	O1P-P-O2P	3.07	127.43	112.24

There are no chirality outliers.

5 of 469 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1003	PCW	O4P-C4-C5-N
4	A	1003	PCW	C4-O4P-P-O1P
4	A	1003	PCW	C4-O4P-P-O2P
4	A	1003	PCW	C4-O4P-P-O3P
4	A	1004	PCW	O4P-C4-C5-N

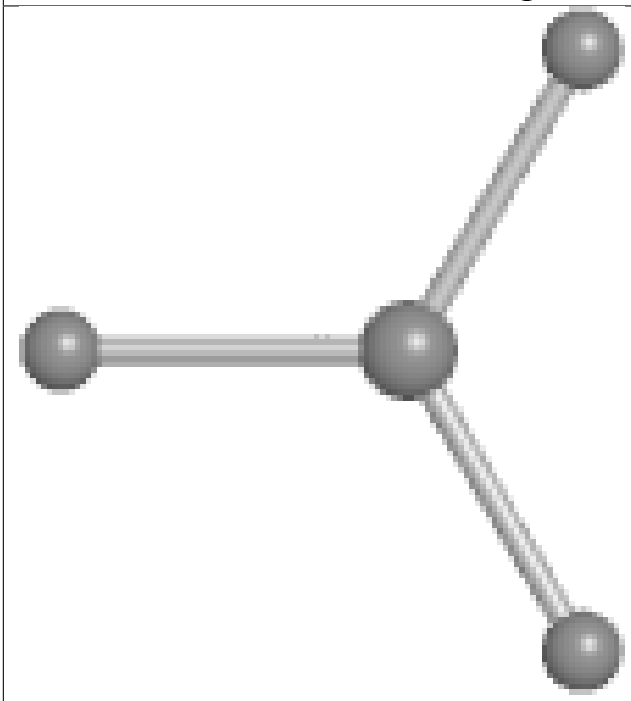
There are no ring outliers.

19 monomers are involved in 57 short contacts:

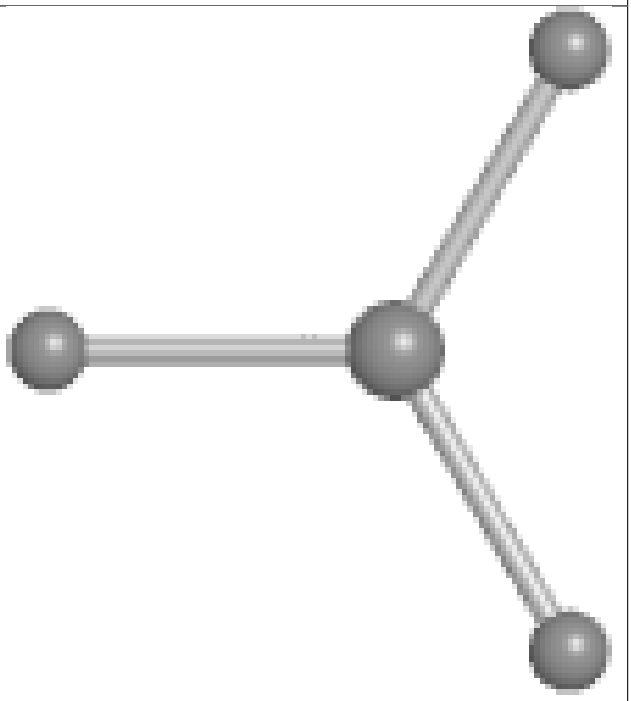
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1006	PCW	2	0
5	D	1009	CE1	1	0
4	C	1004	PCW	8	0
4	A	1004	PCW	1	0
4	C	1008	PCW	4	0
4	C	1006	PCW	2	0
4	B	1004	PCW	3	0
4	A	1003	PCW	2	0
4	B	1008	PCW	2	0
2	H	1001	BEF	1	0
4	B	1007	PCW	3	0
5	D	1005	CE1	3	0
4	D	1003	PCW	4	0
4	B	1009	PCW	4	0
5	D	1008	CE1	2	0
4	B	1003	PCW	5	0
4	C	1003	PCW	2	0
5	D	1006	CE1	4	0
4	C	1005	PCW	5	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.

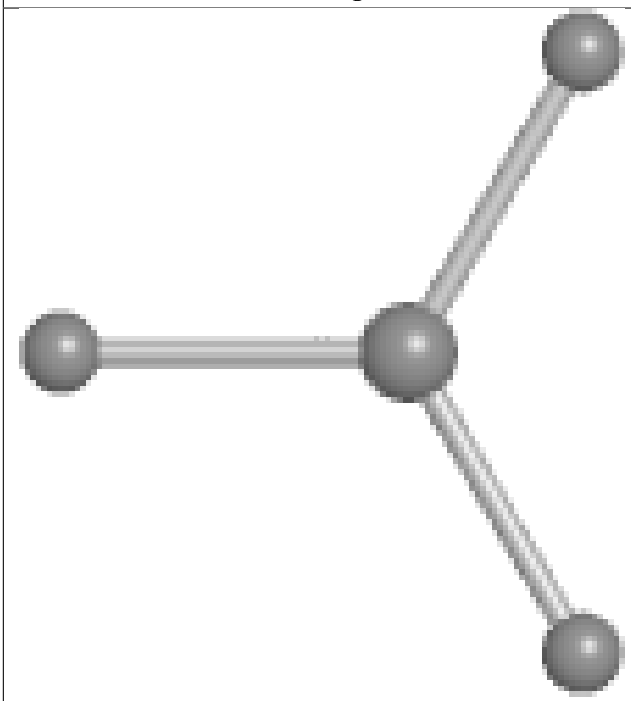
Ligand BEF E 1001



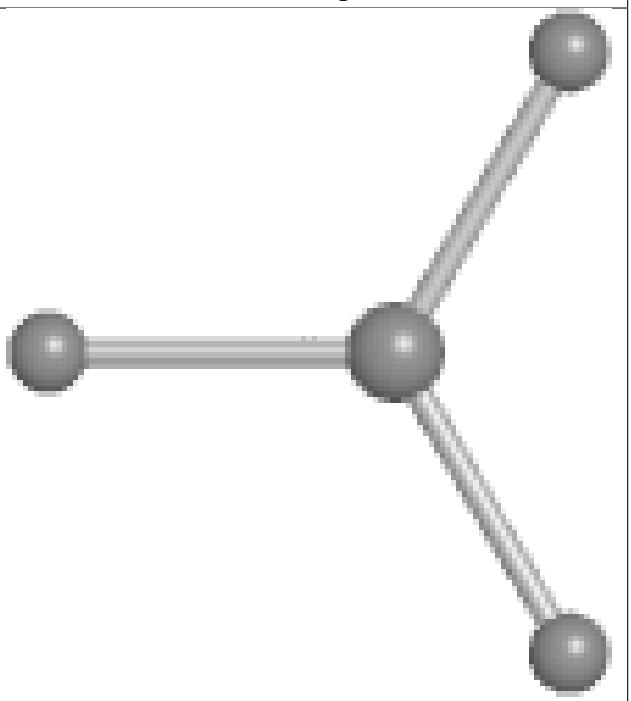
Bond lengths



Bond angles

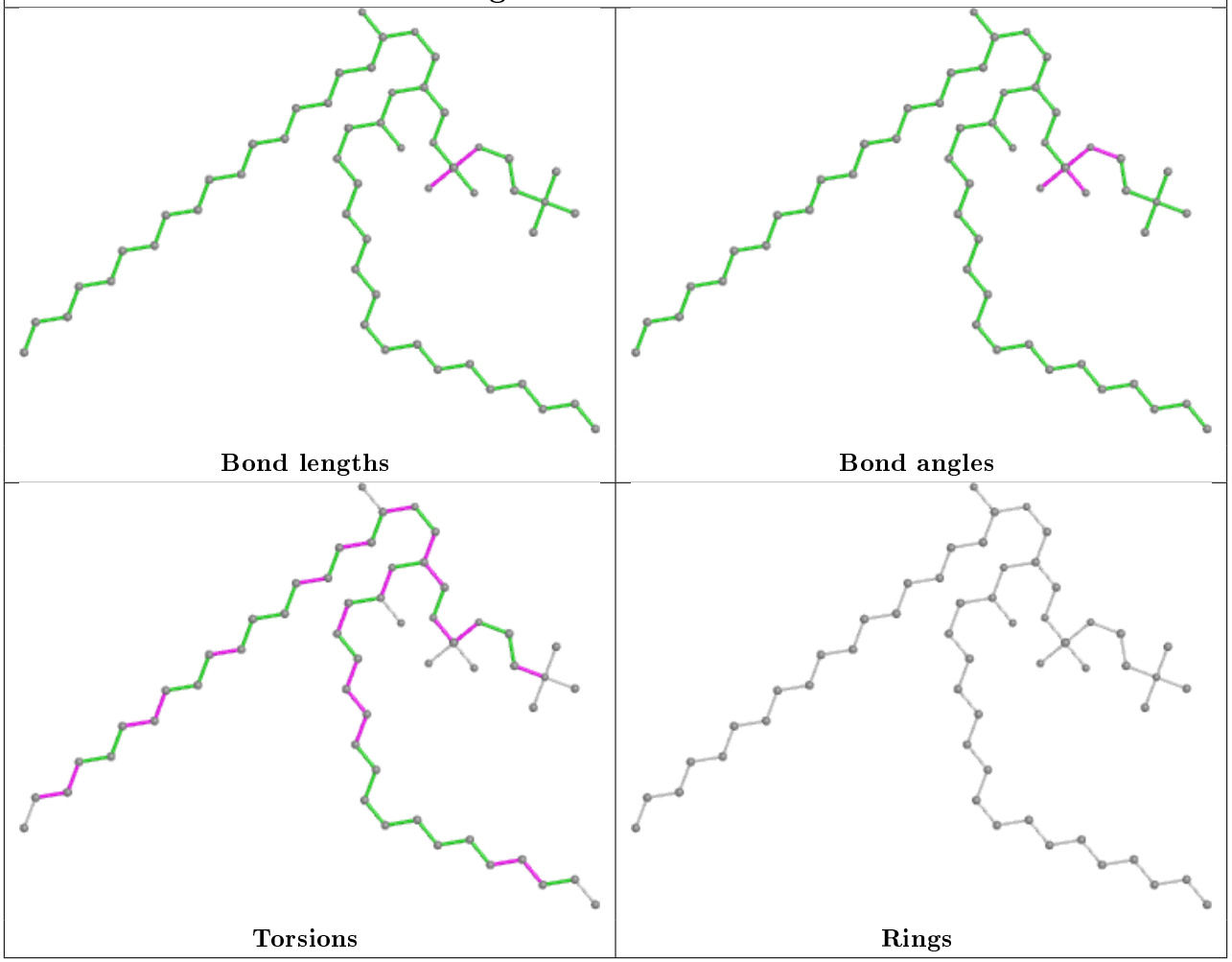


Torsions

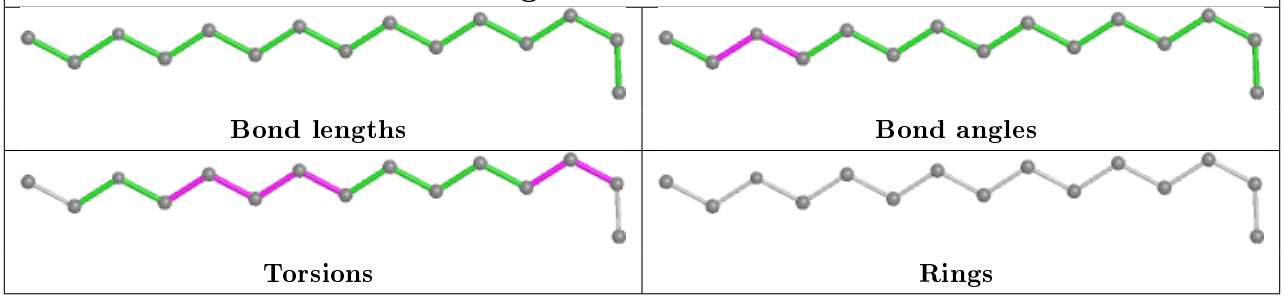


Rings

Ligand PCW B 1006



Ligand CE1 C 1007



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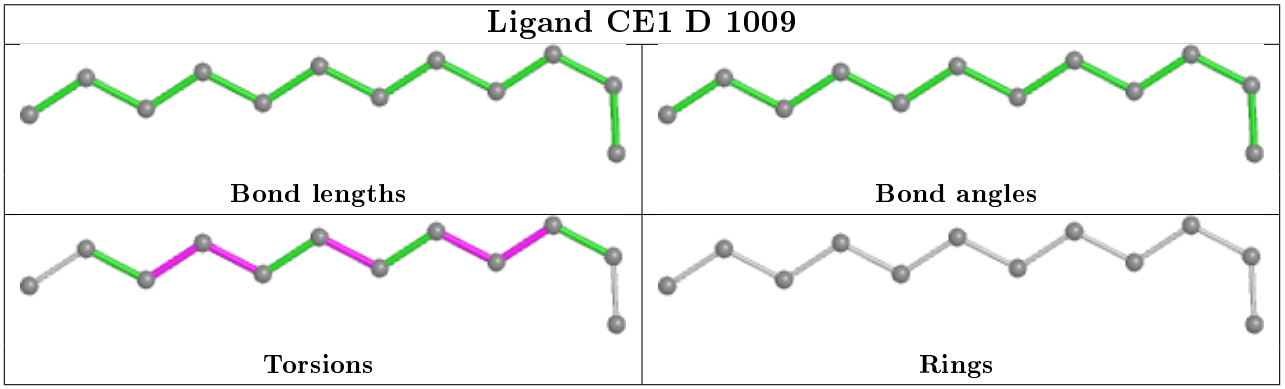
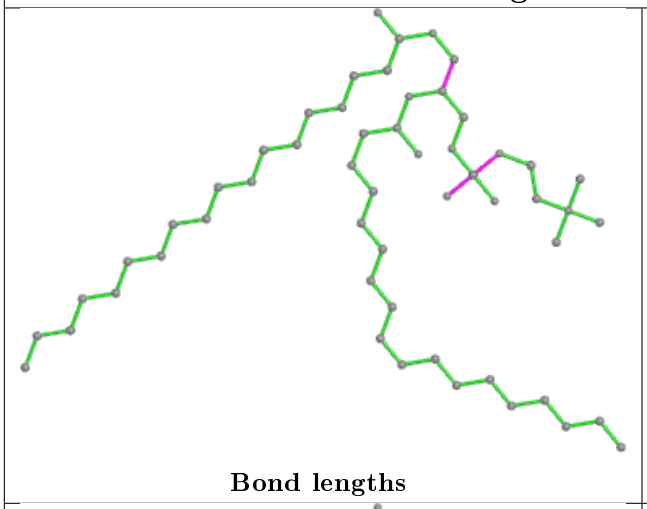
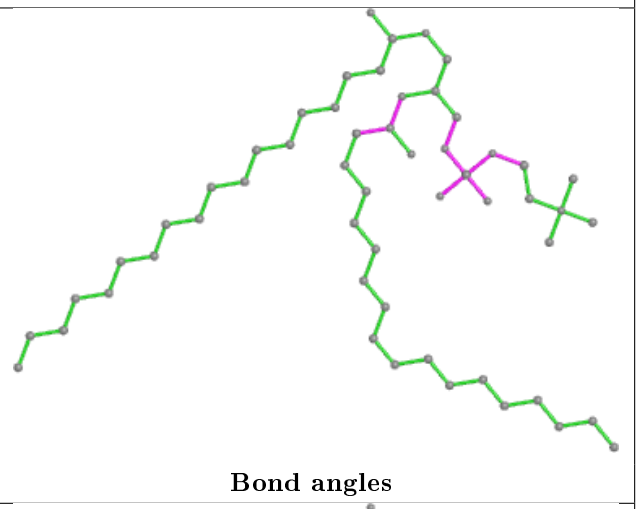


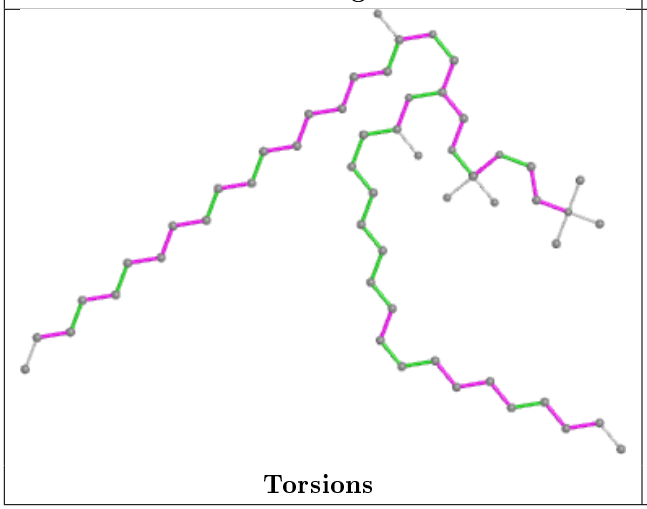
Ligand PCW C 1004



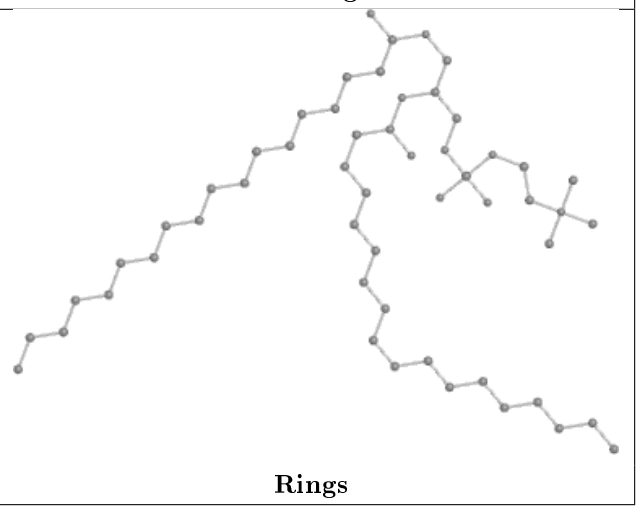
Bond lengths



Bond angles

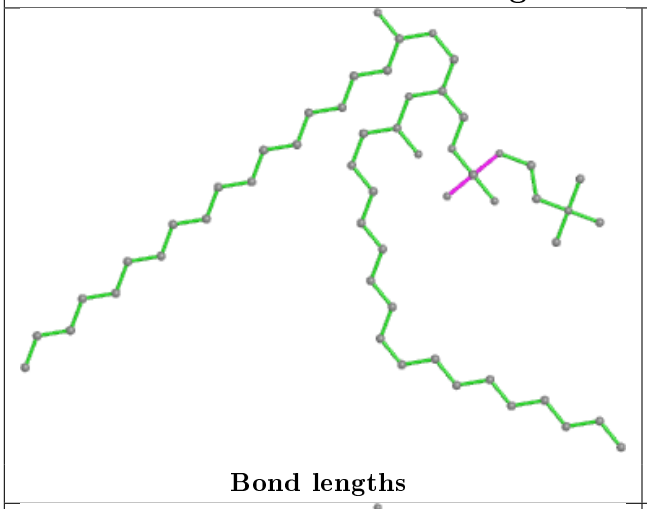


Torsions



Rings

Ligand PCW A 1004



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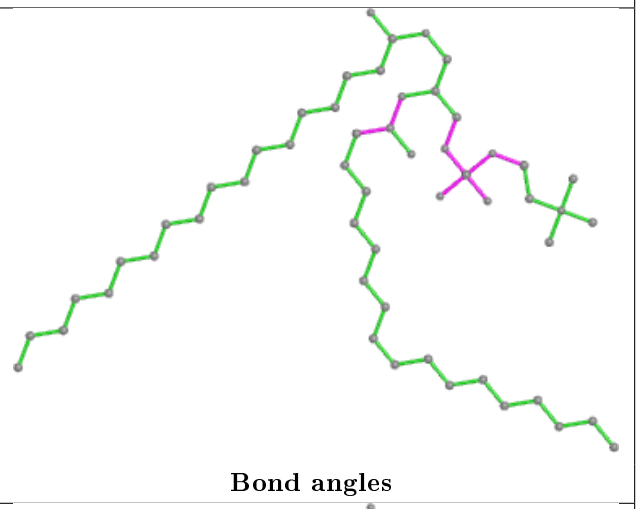
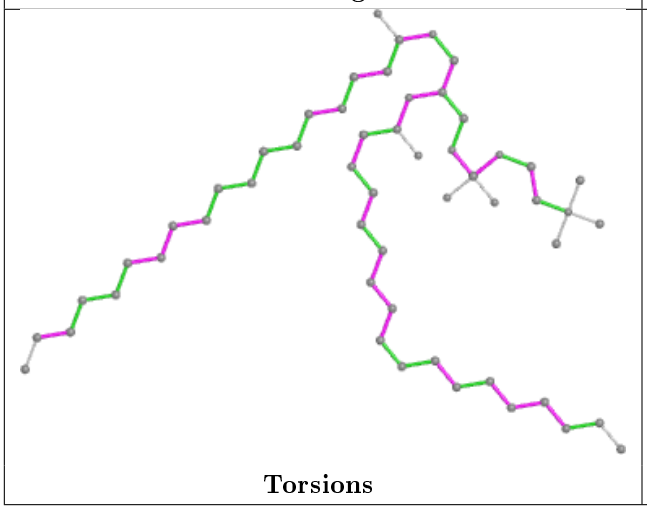
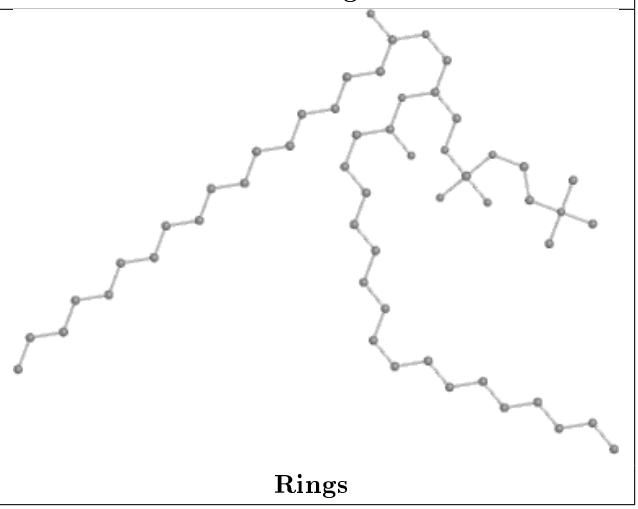


Bond angles

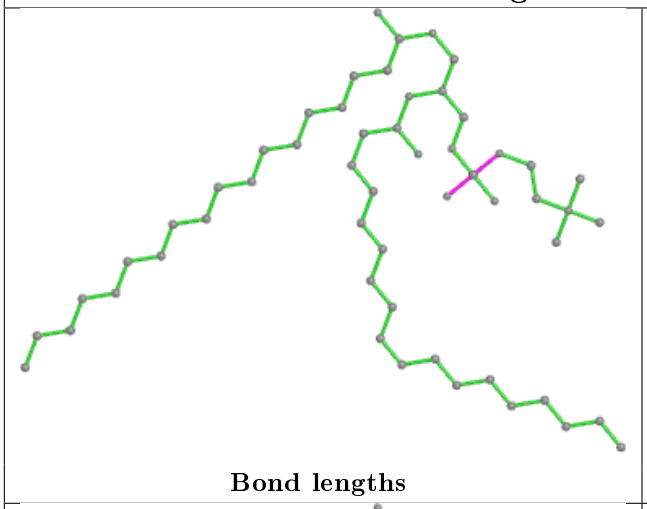


Torsions

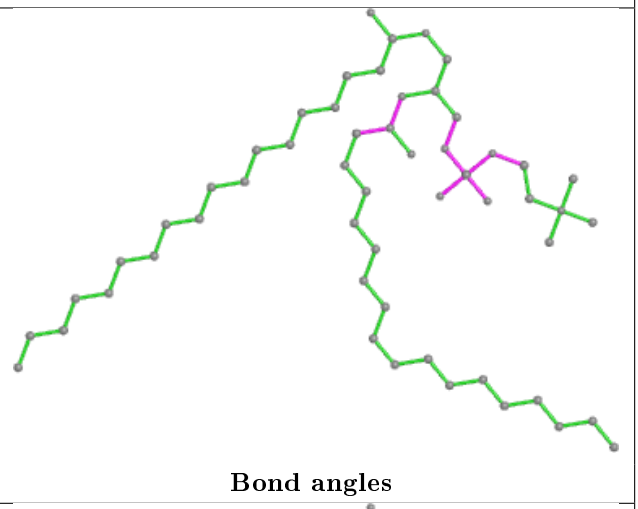


Rings

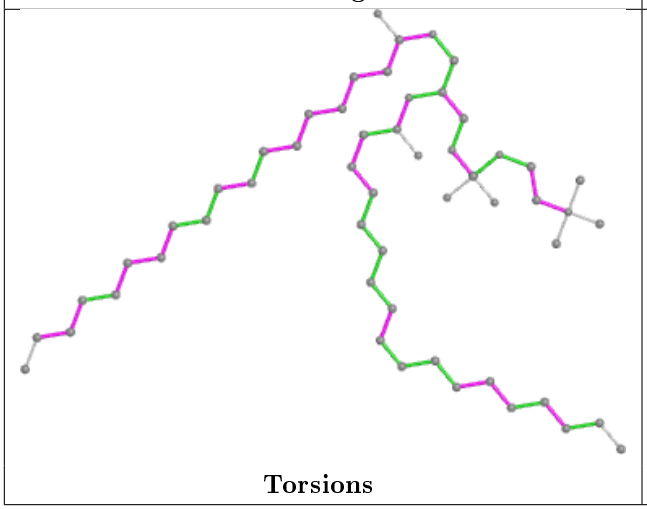
Ligand PCW C 1008



Bond lengths



Bond angles



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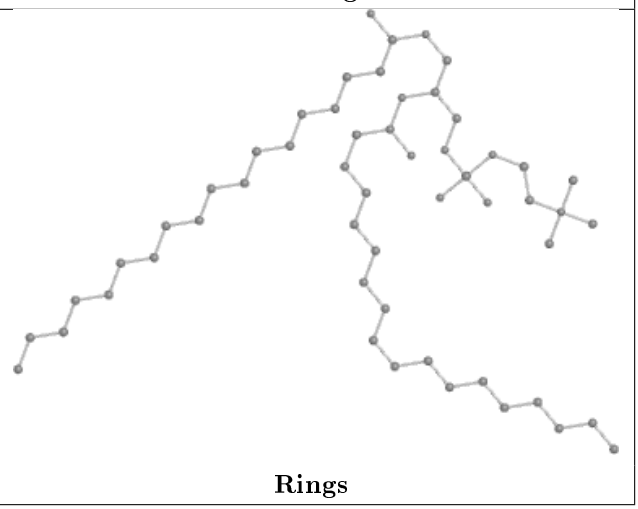
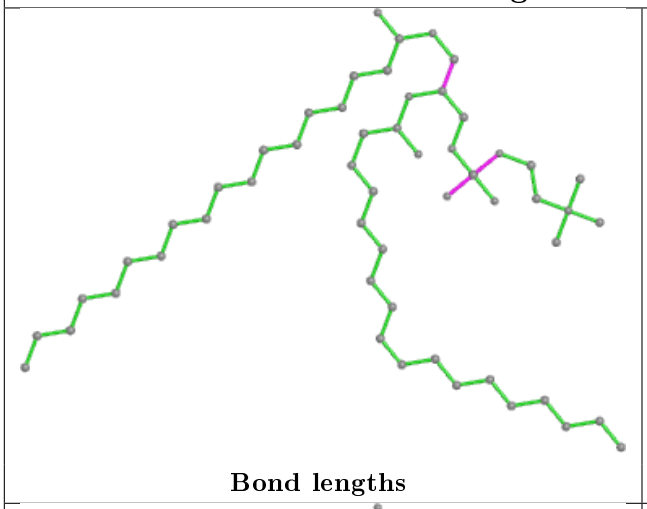


Rings

Ligand PCW C 1006



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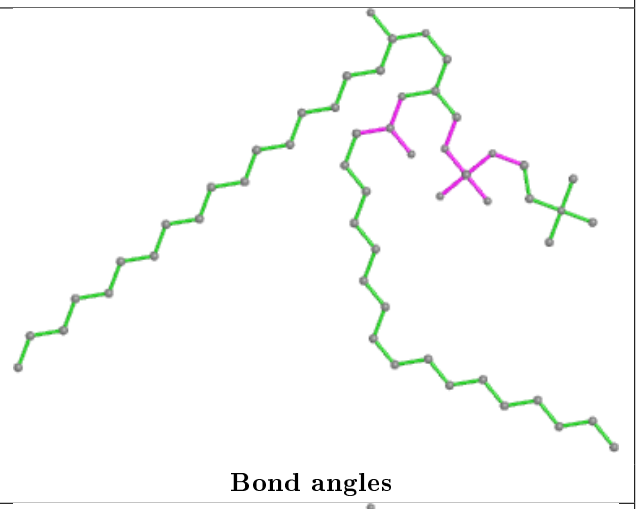
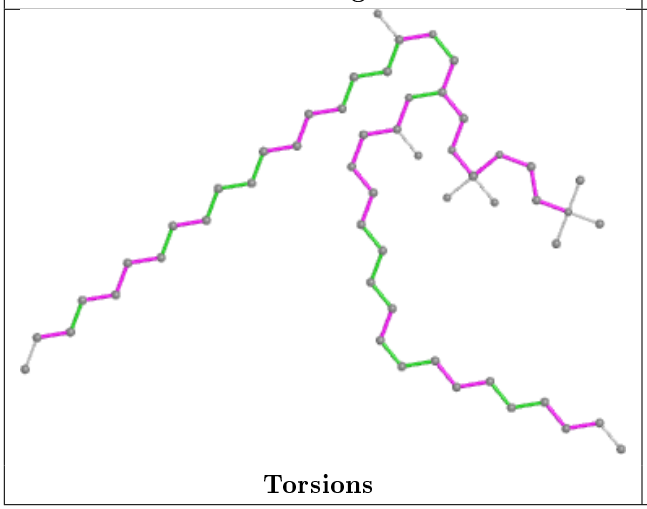


Bond angles



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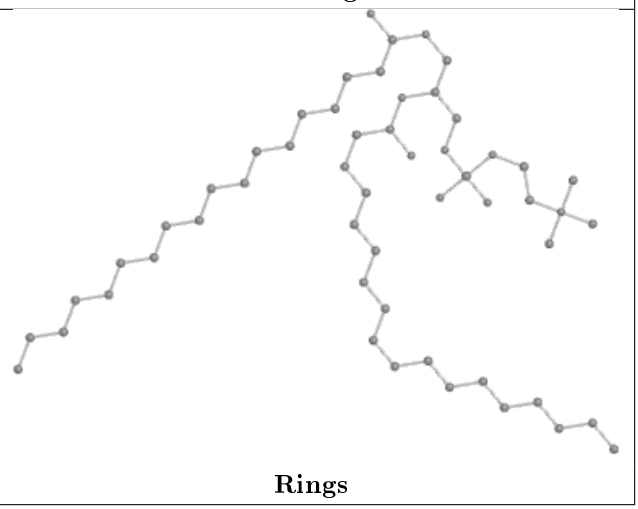
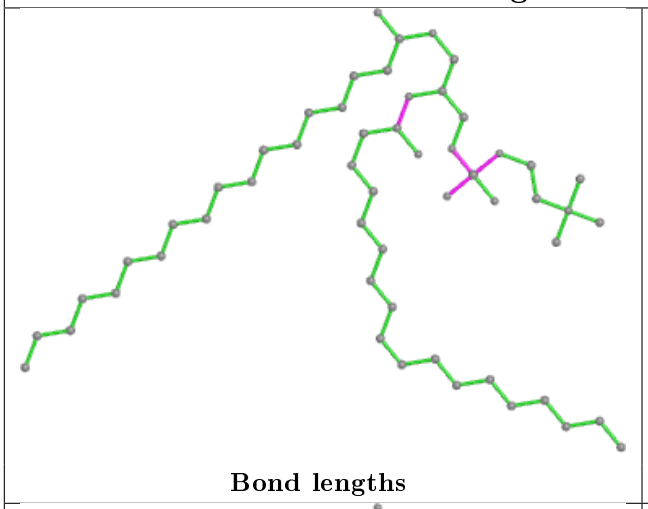


Rings

Ligand PCW B 1004



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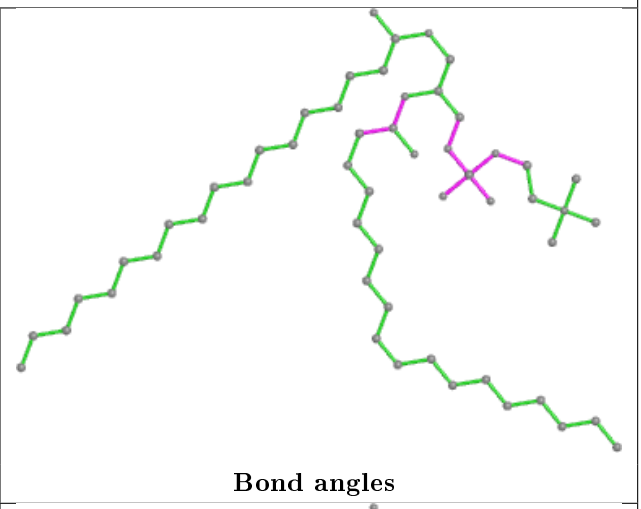
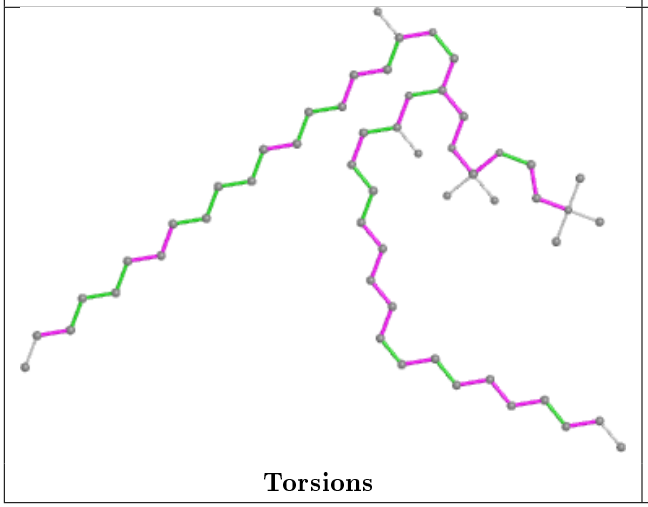


Bond angles



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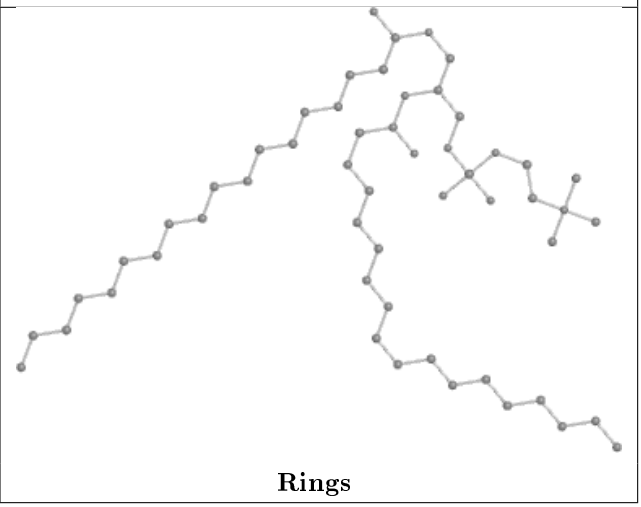
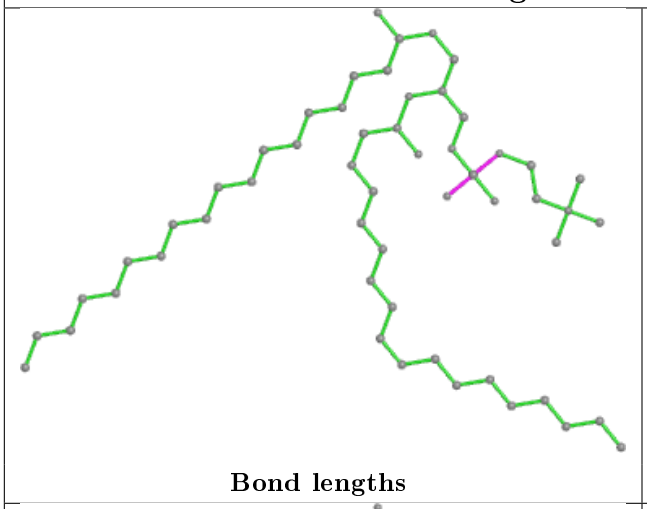
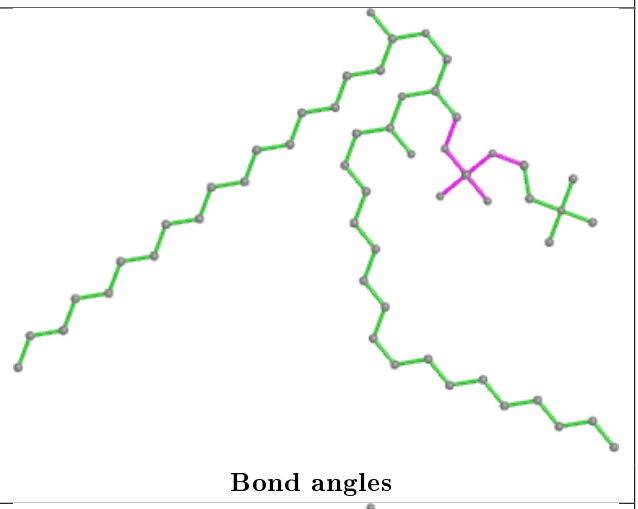


Rings

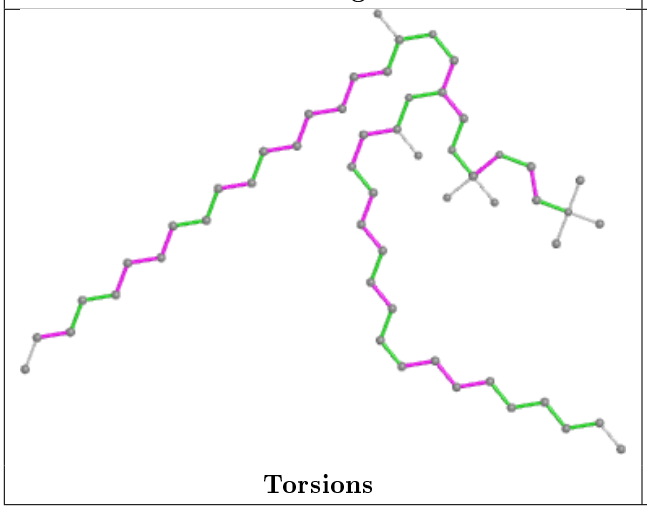
Ligand PCW A 1003



Bond lengths



Bond angles



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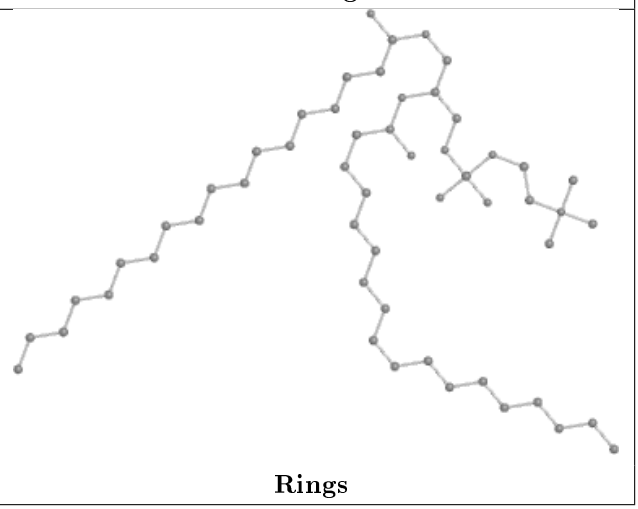
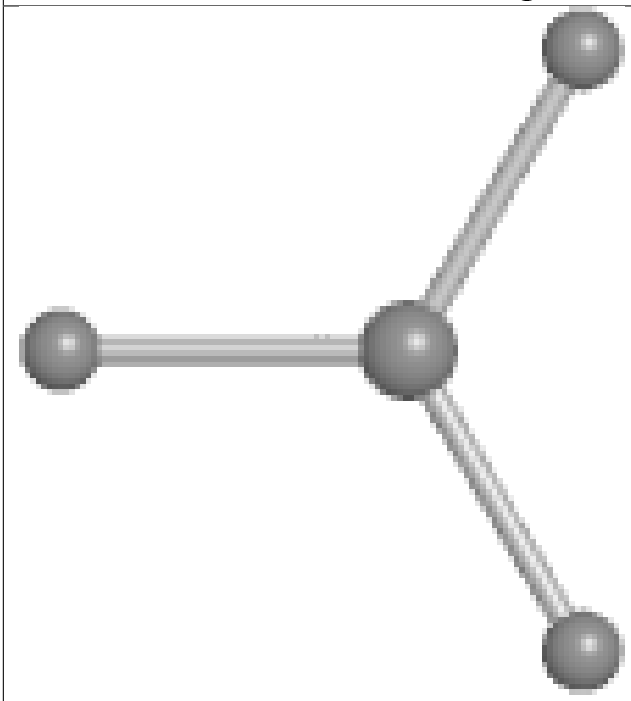
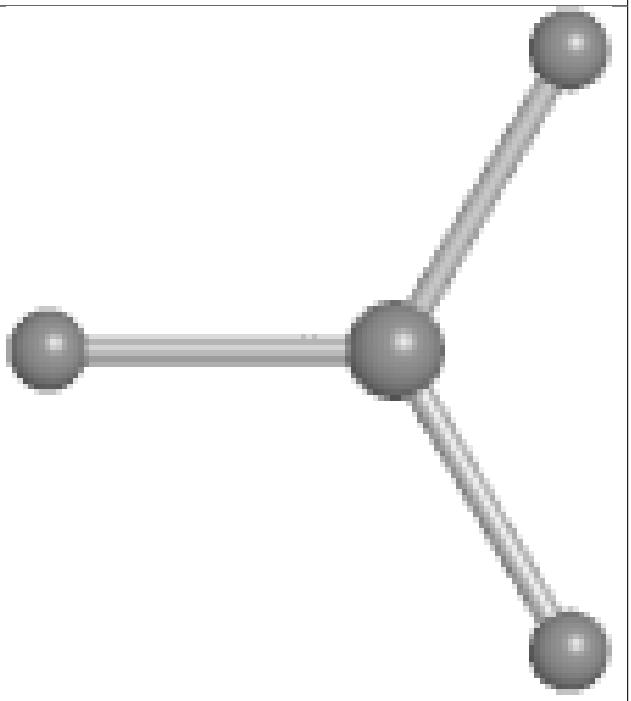


Rings

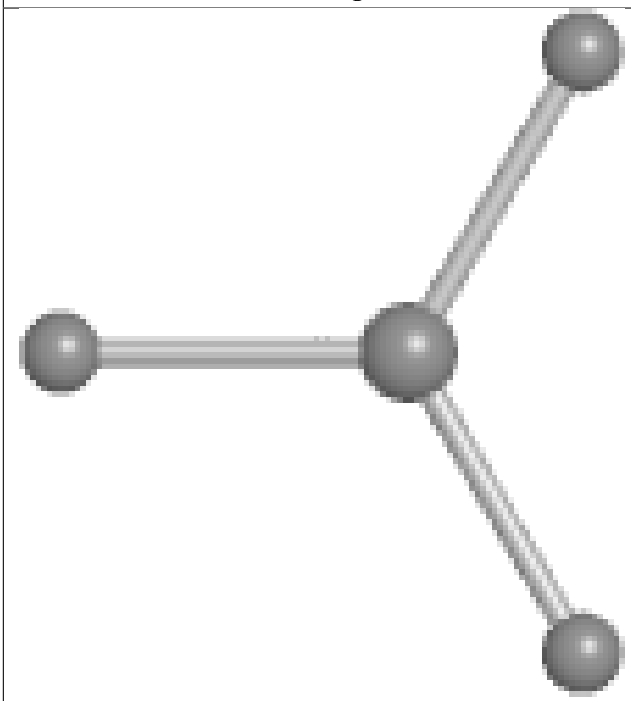
Ligand BEF F 1001



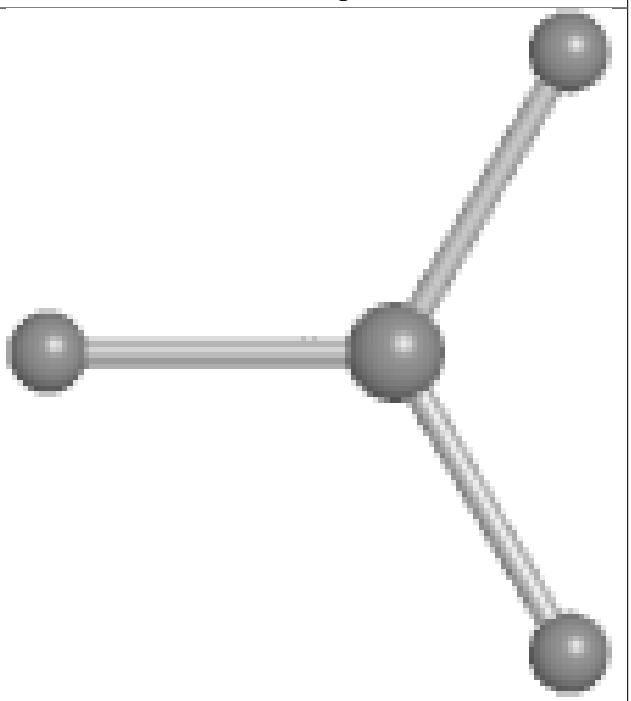
Bond lengths



Bond angles

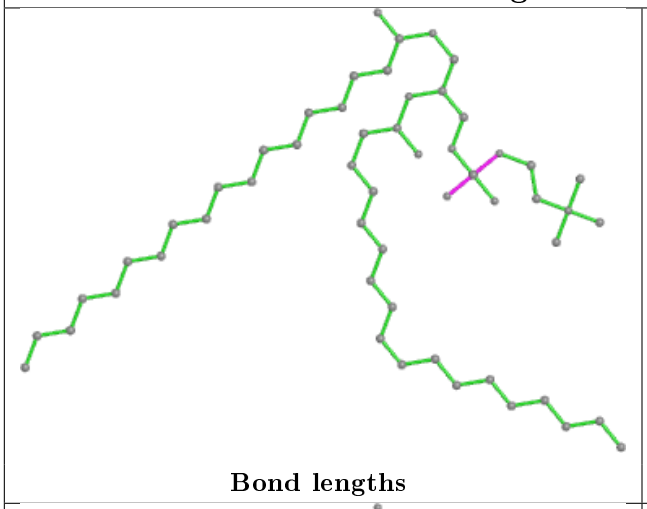


Torsions

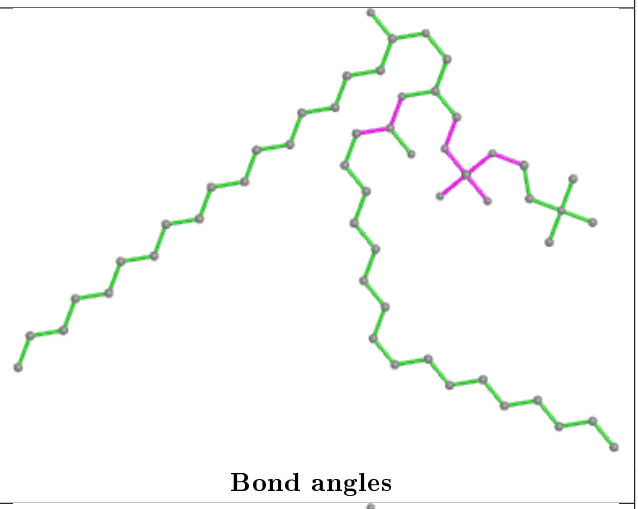


Rings

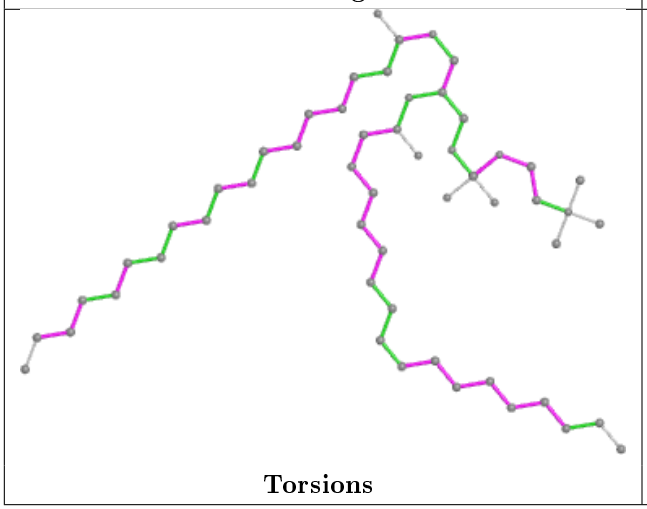
Ligand PCW B 1005



Bond lengths



Bond angles



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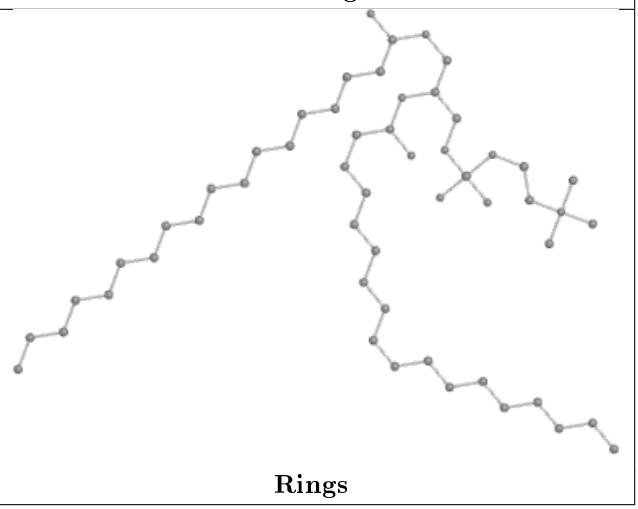
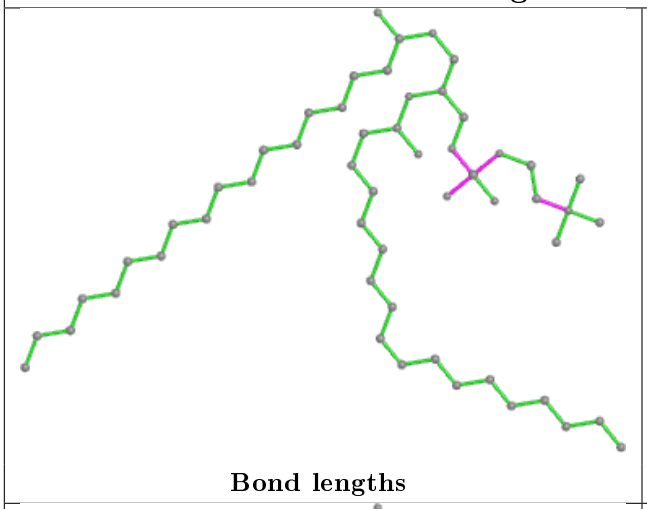
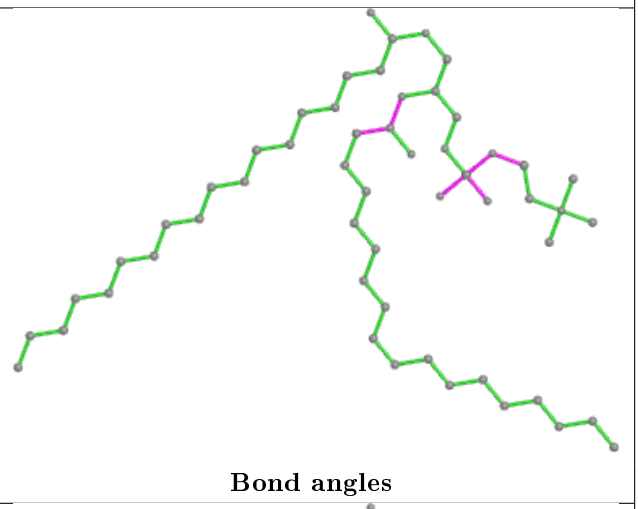


Rings

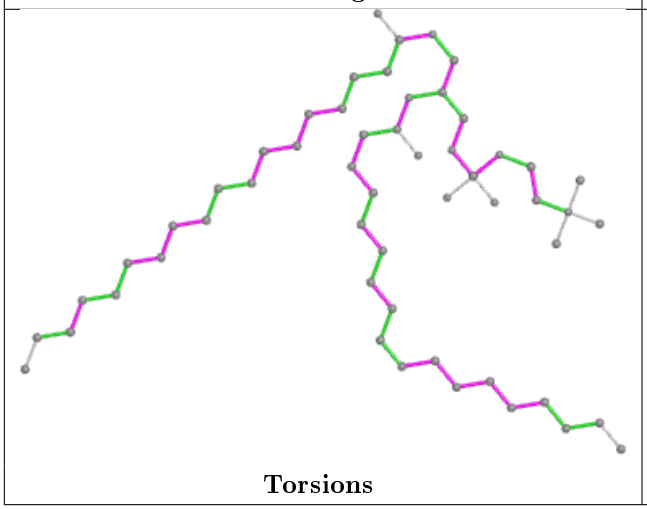
Ligand PCW B 1008



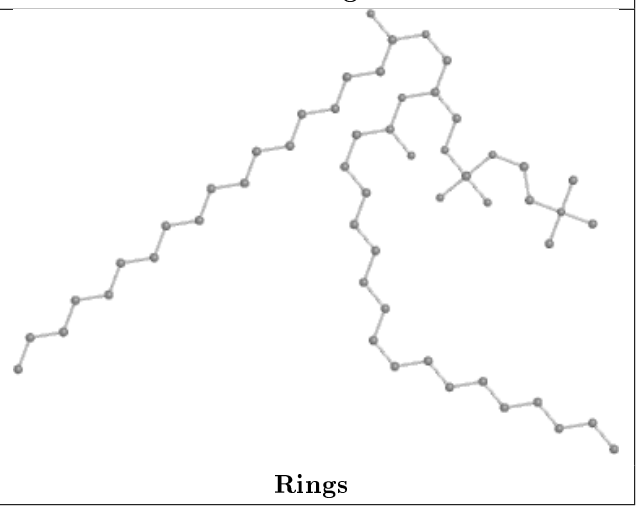
Bond lengths



Bond angles

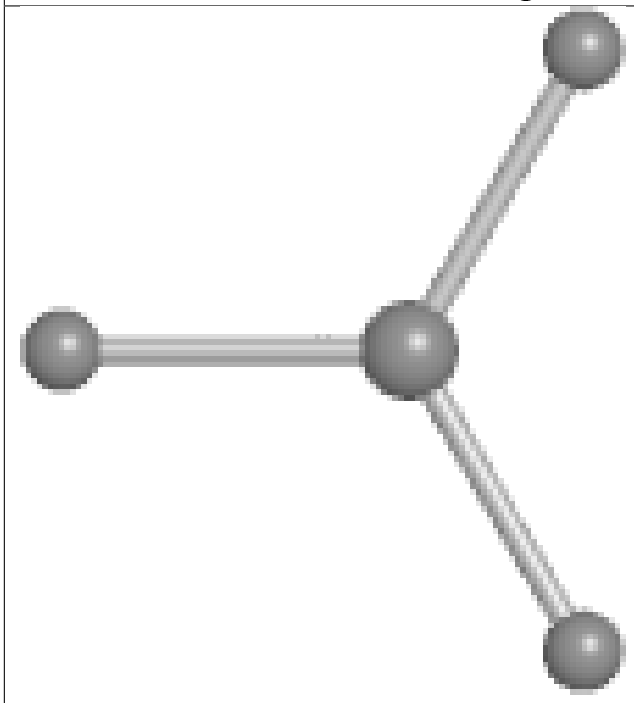


Torsions

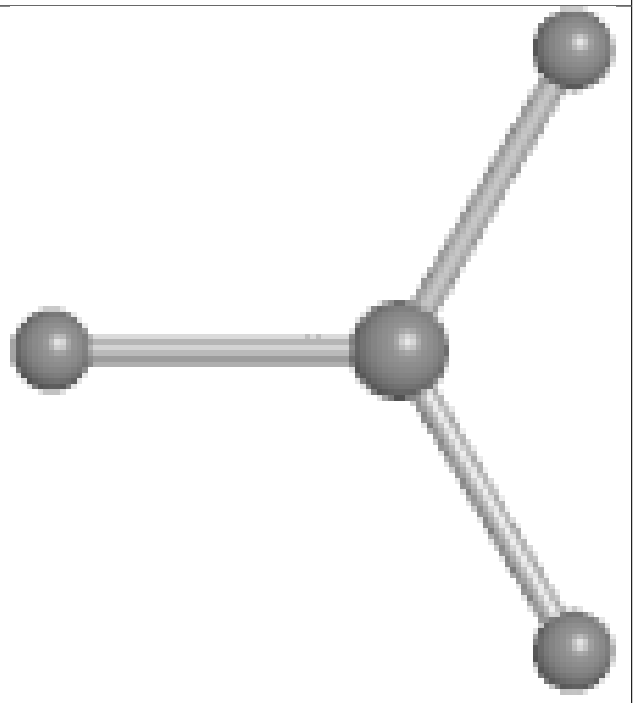


Rings

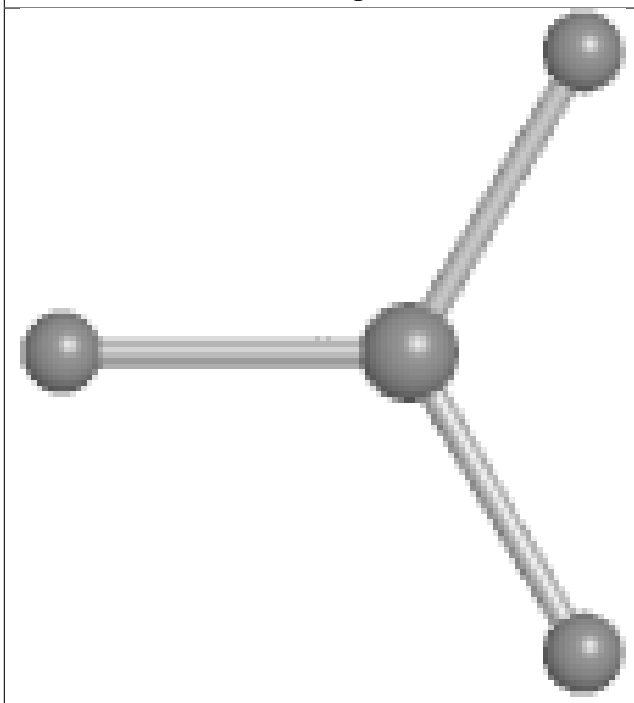
Ligand BEF H 1001



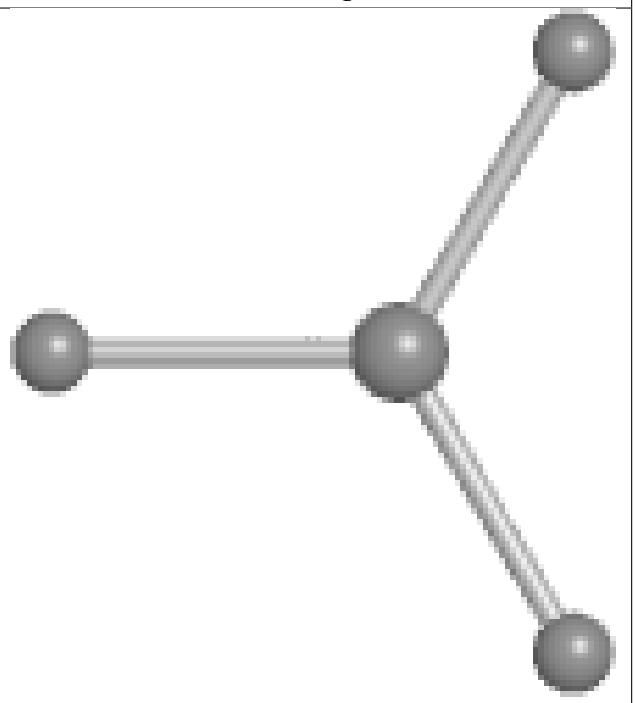
Bond lengths



Bond angles

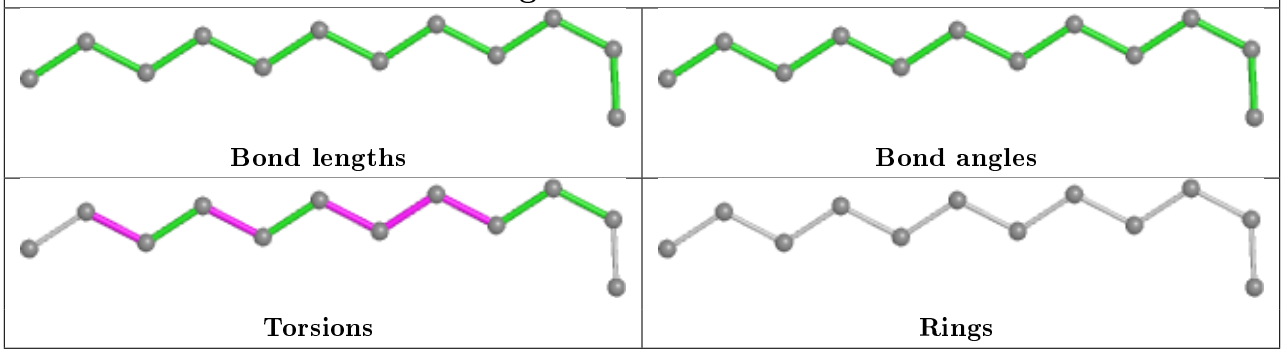


Torsions

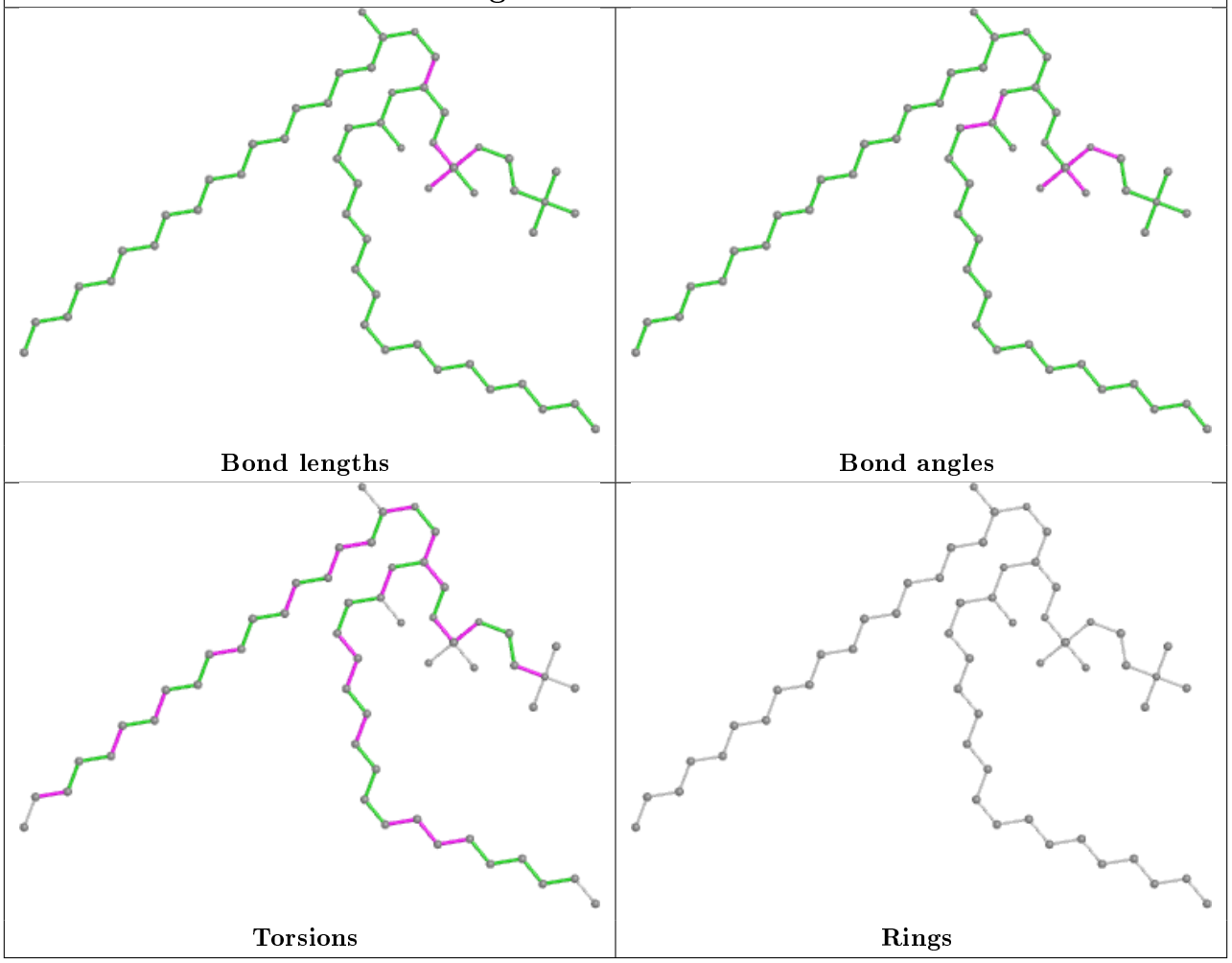


Rings

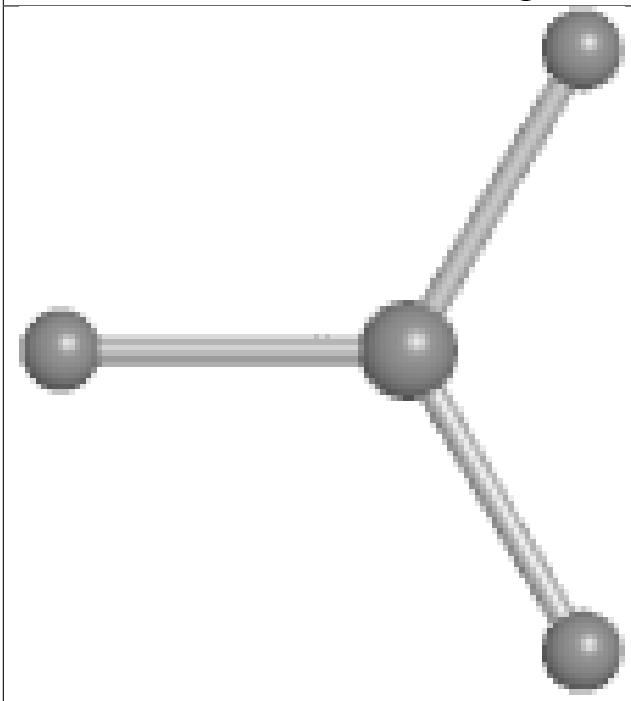
Ligand CE1 D 1004



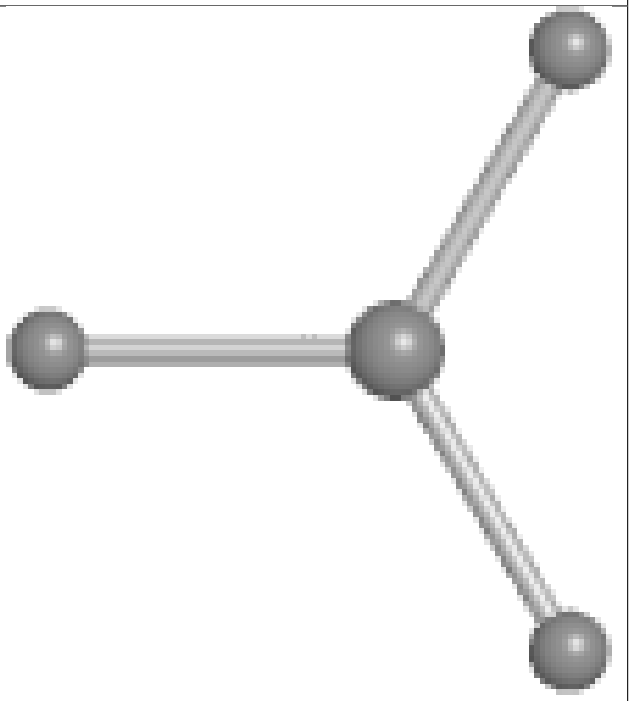
Ligand PCW B 1007



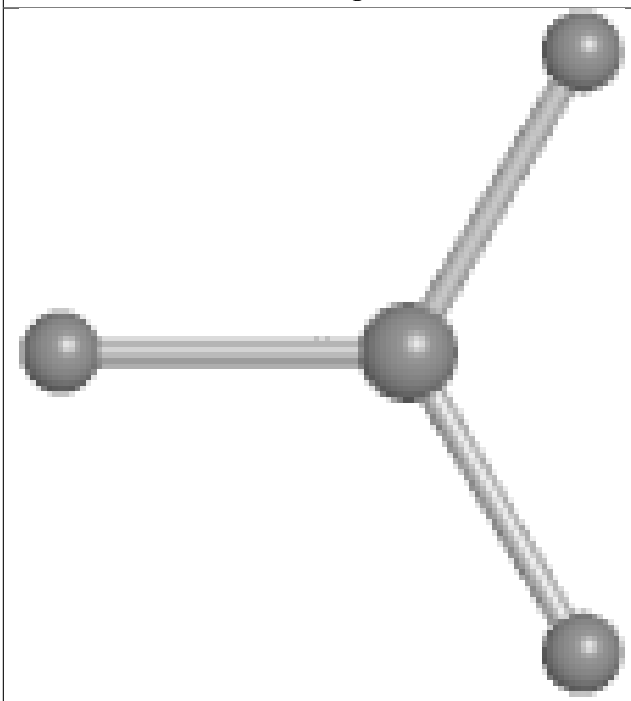
Ligand BEF B 1001



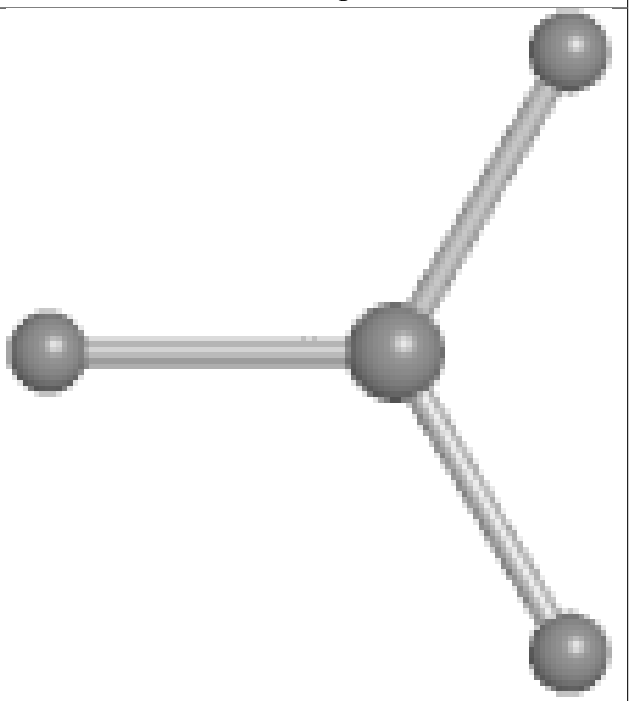
Bond lengths



Bond angles

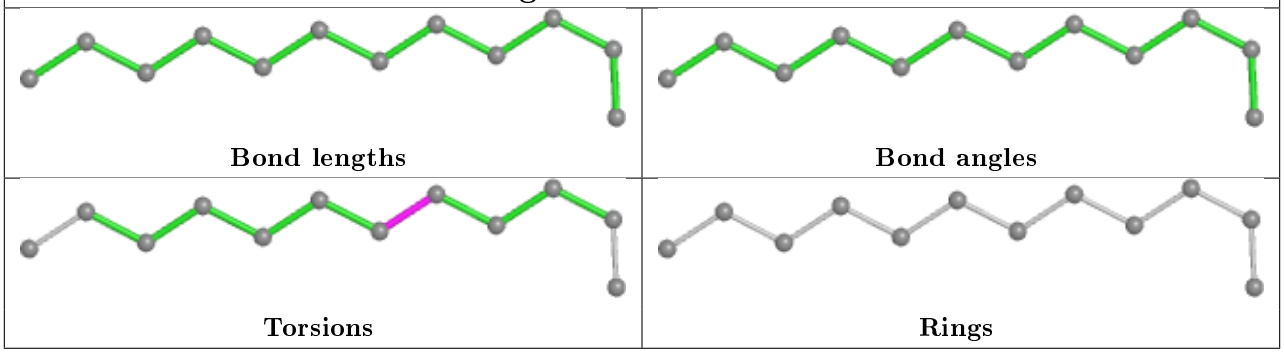


Torsions

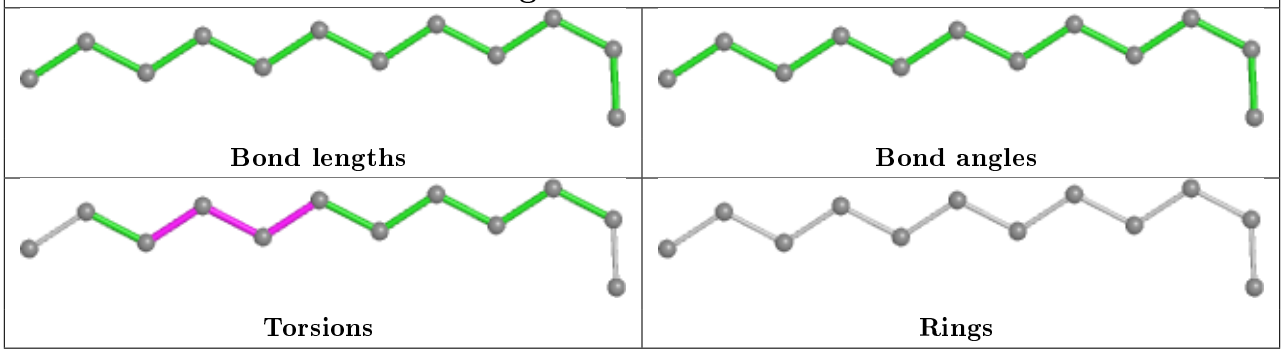


Rings

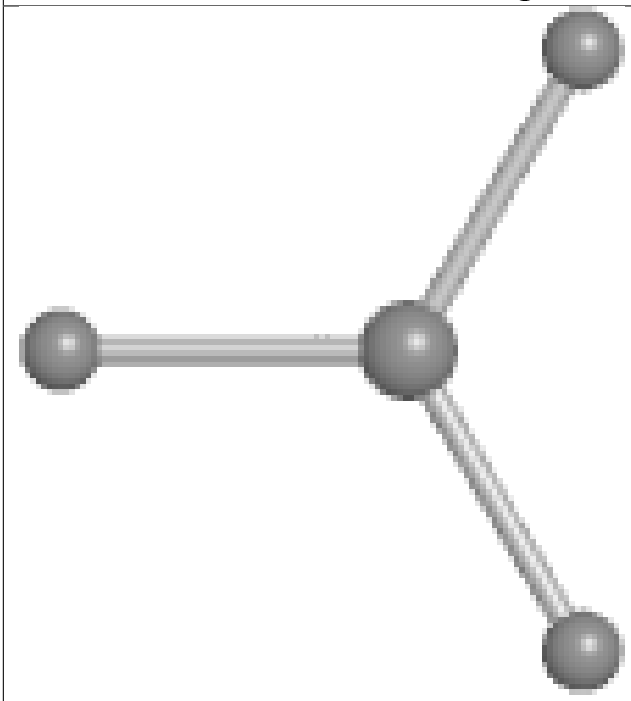
Ligand CE1 D 1007



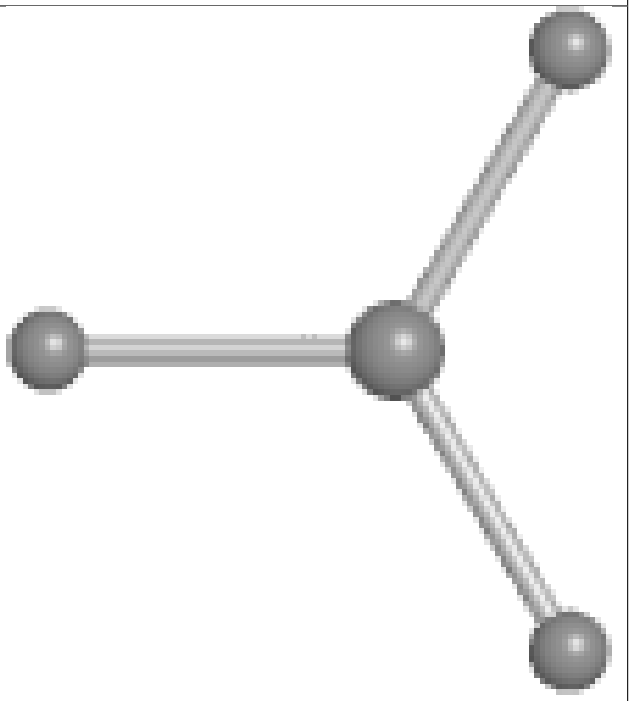
Ligand CE1 D 1005



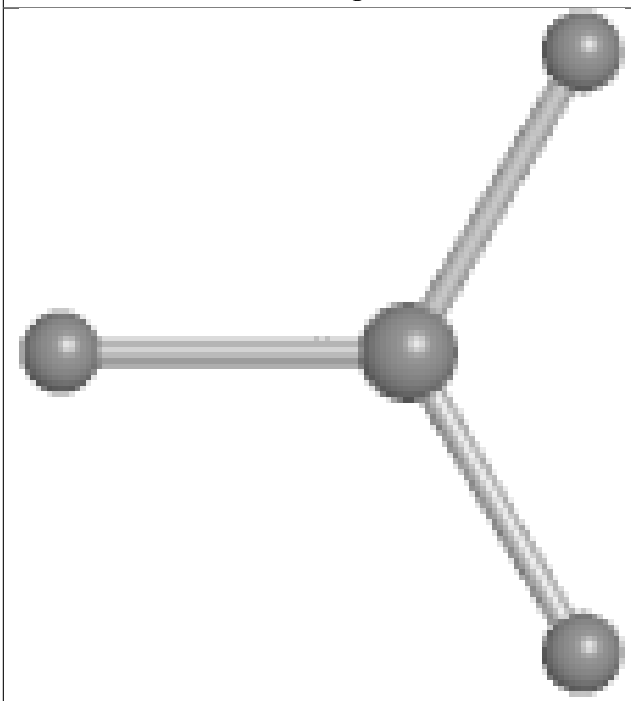
Ligand BEF A 1001



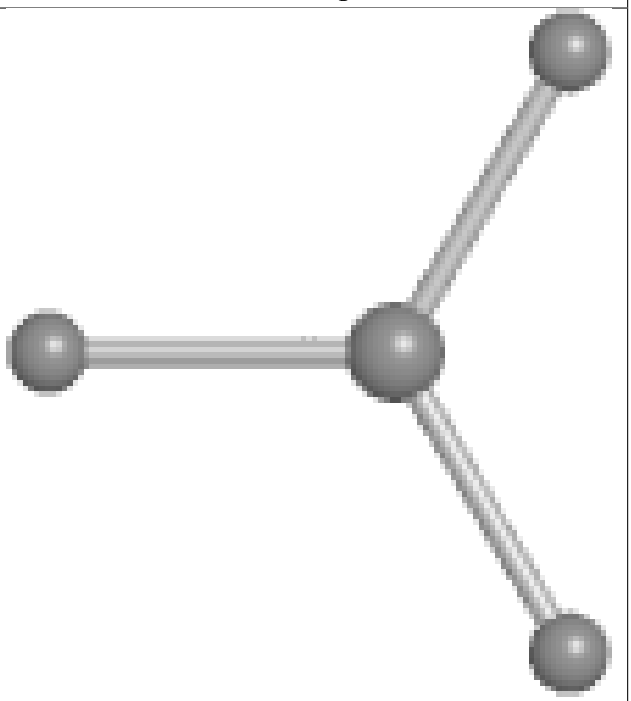
Bond lengths



Bond angles

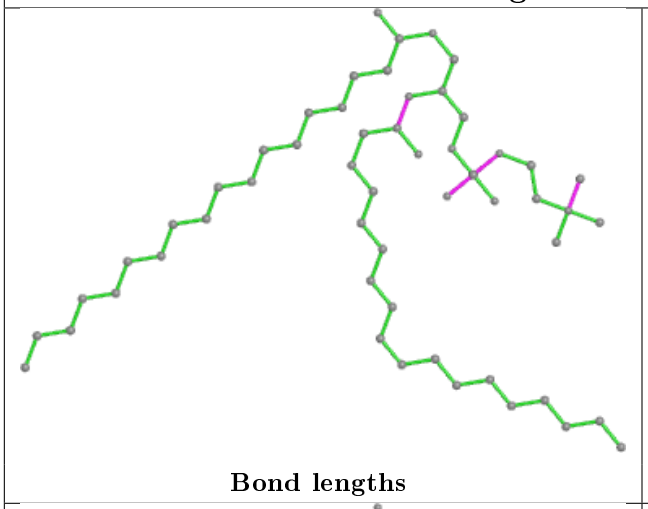


Torsions

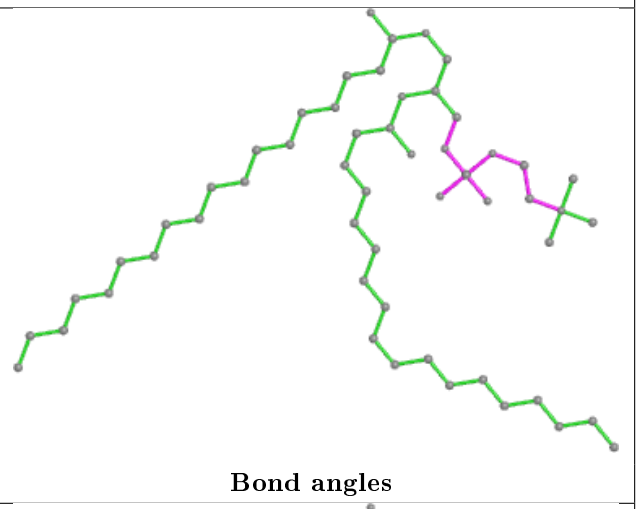


Rings

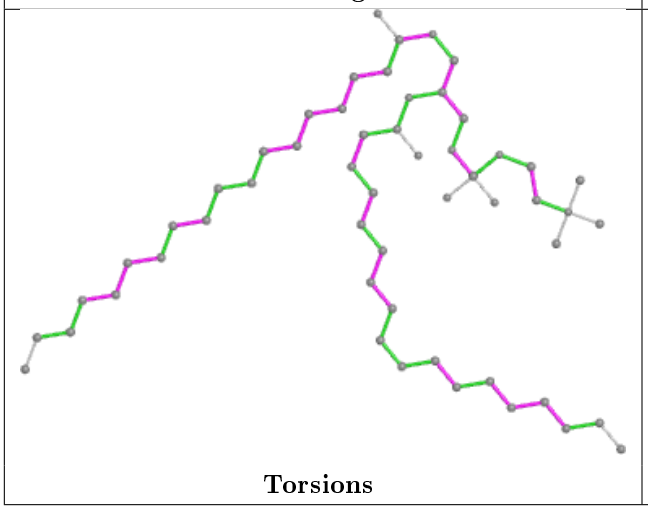
Ligand PCW D 1003



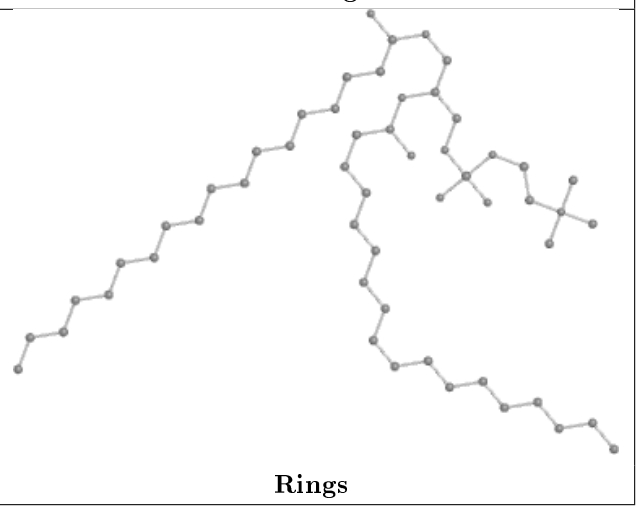
Bond lengths



Bond angles

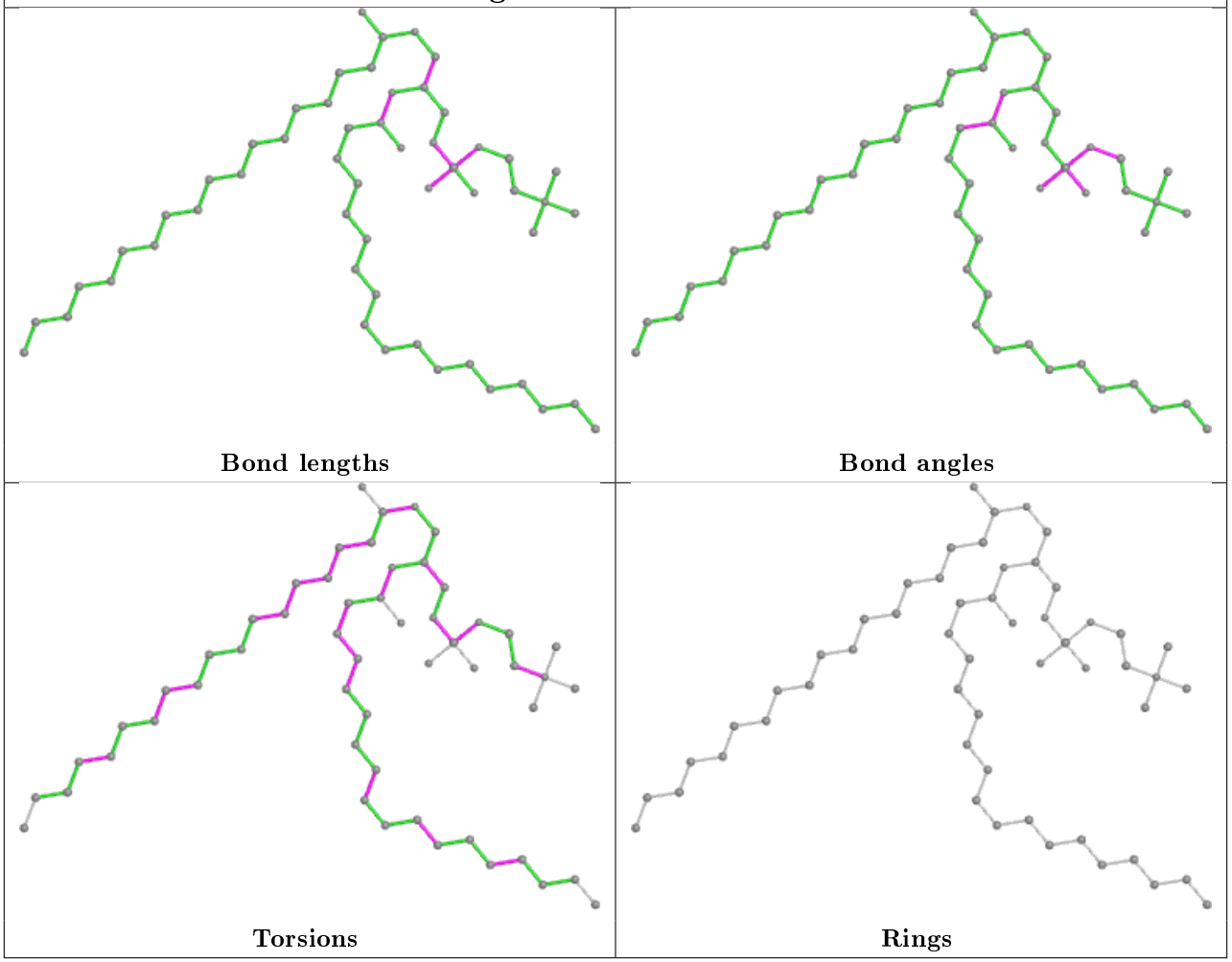


Torsions

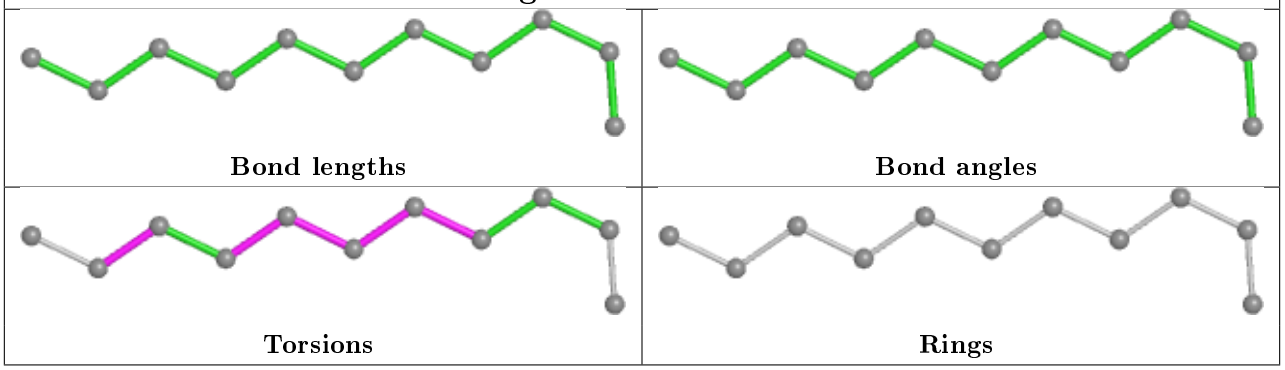


Rings

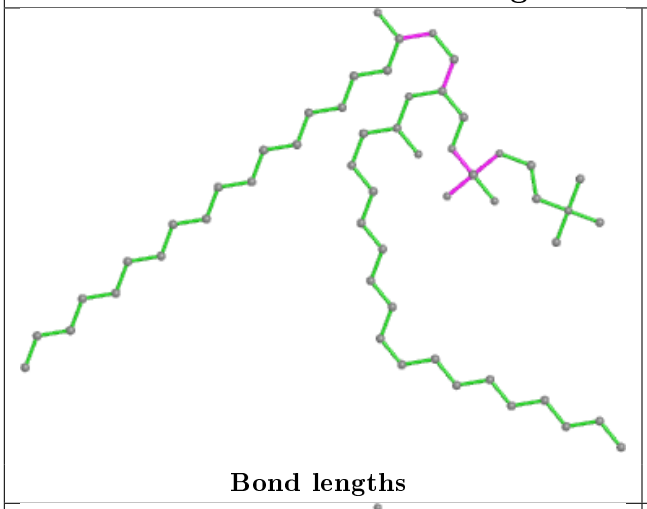
Ligand PCW B 1009



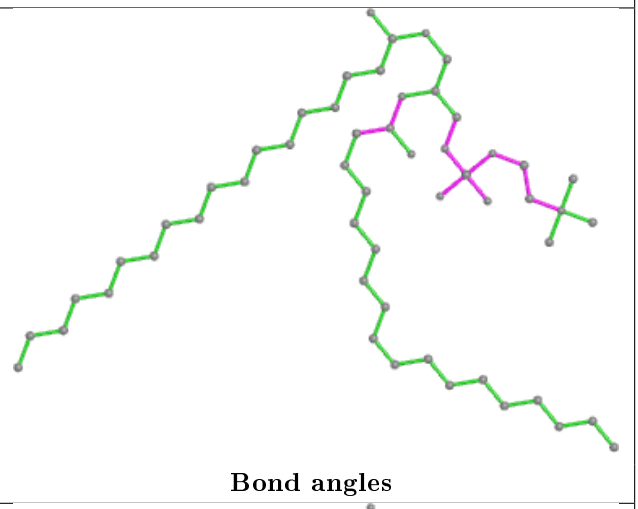
Ligand CE1 D 1008



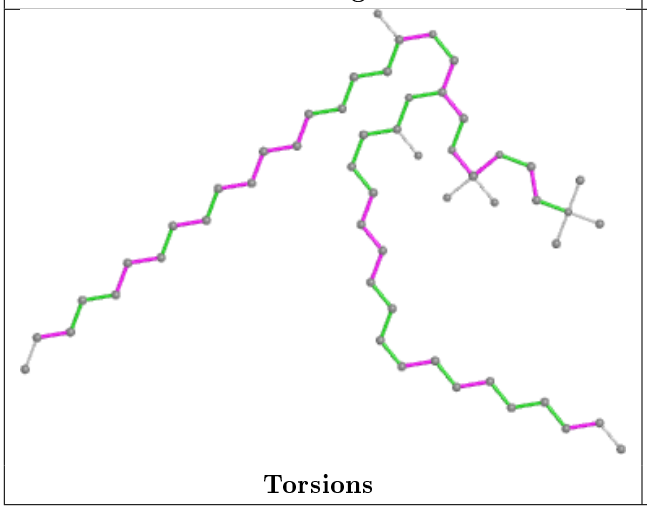
Ligand PCW B 1003



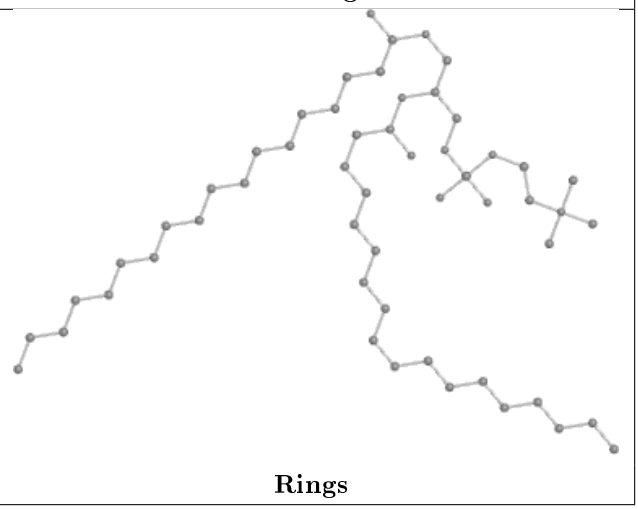
Bond lengths



Bond angles

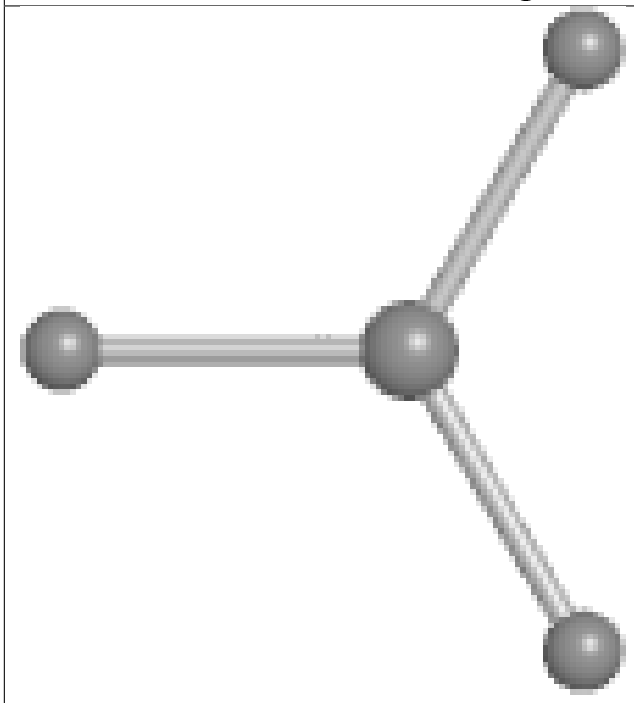


Torsions

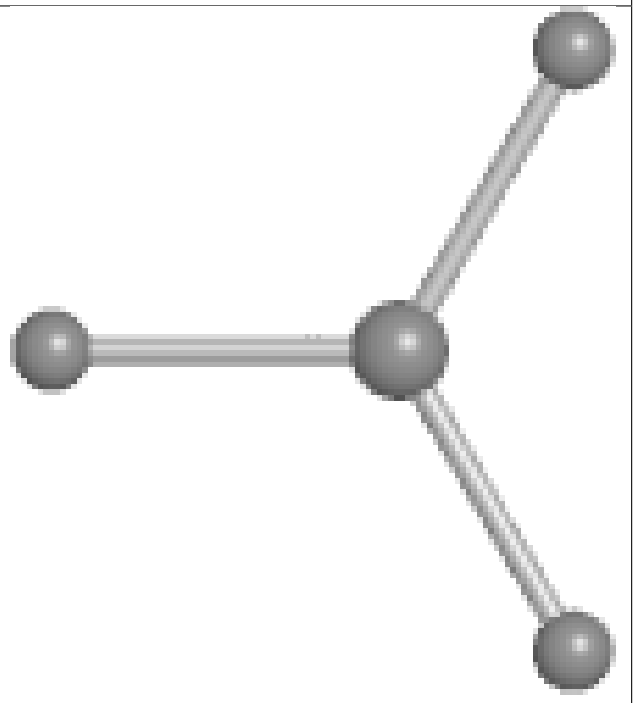


Rings

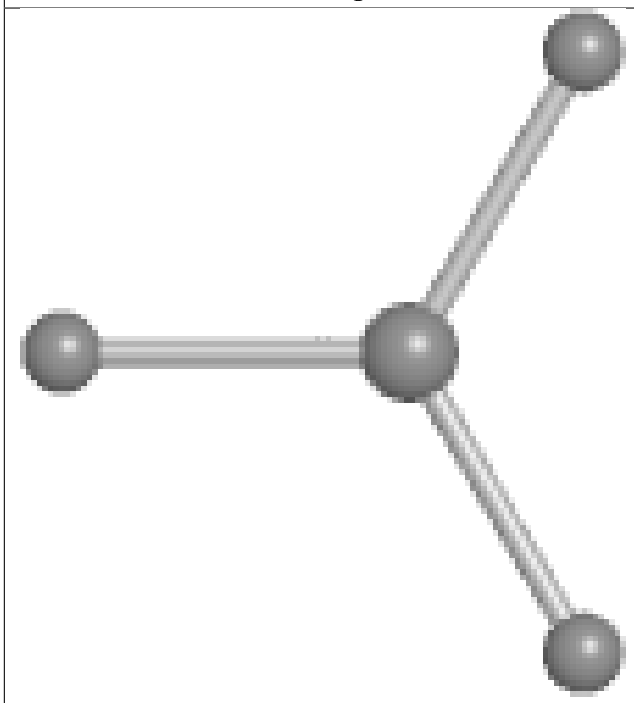
Ligand BEF D 1001



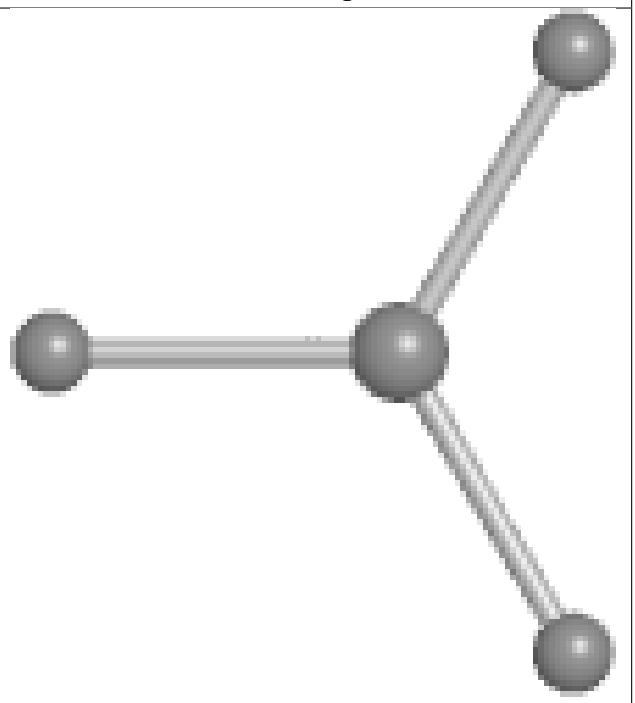
Bond lengths



Bond angles

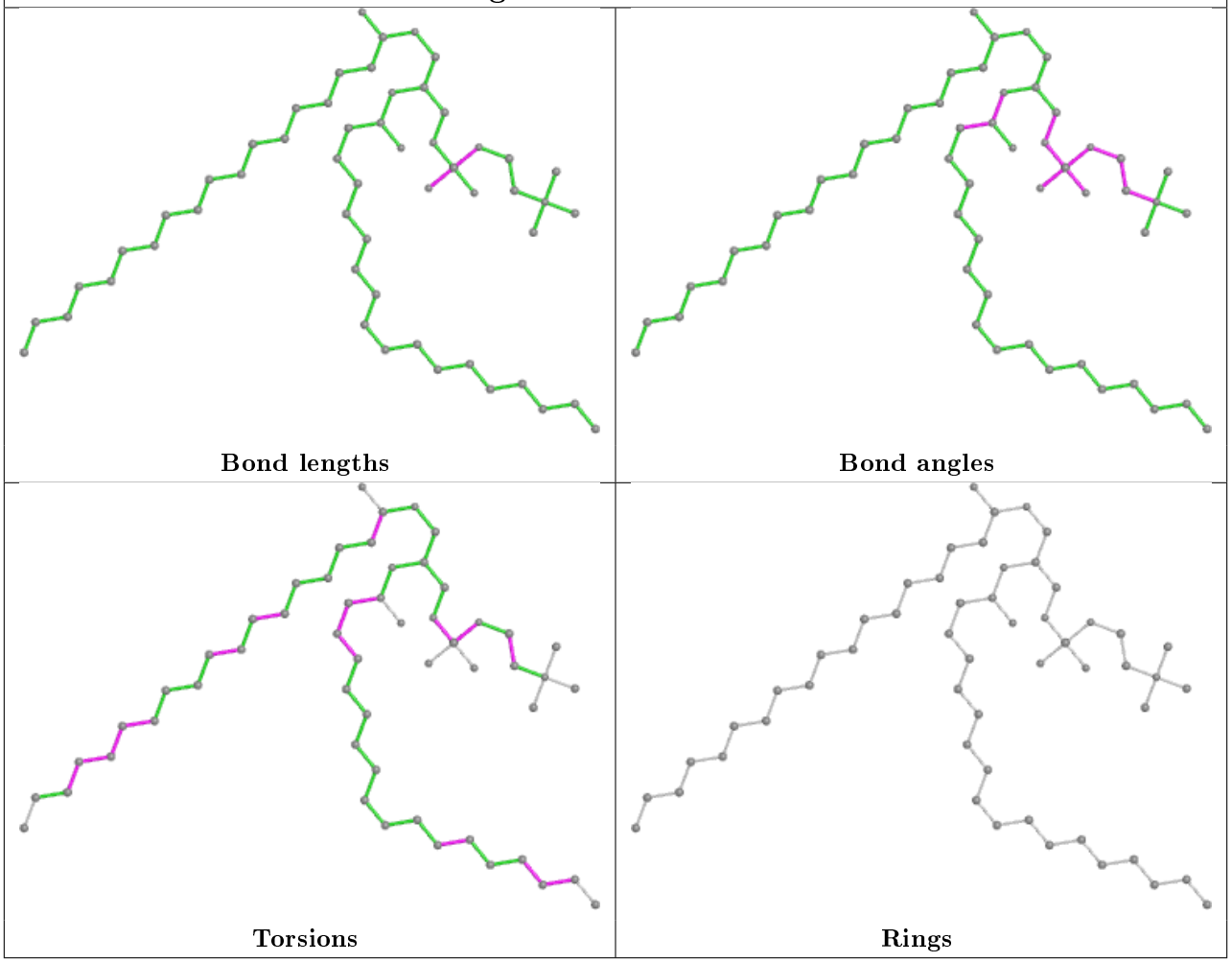


Torsions

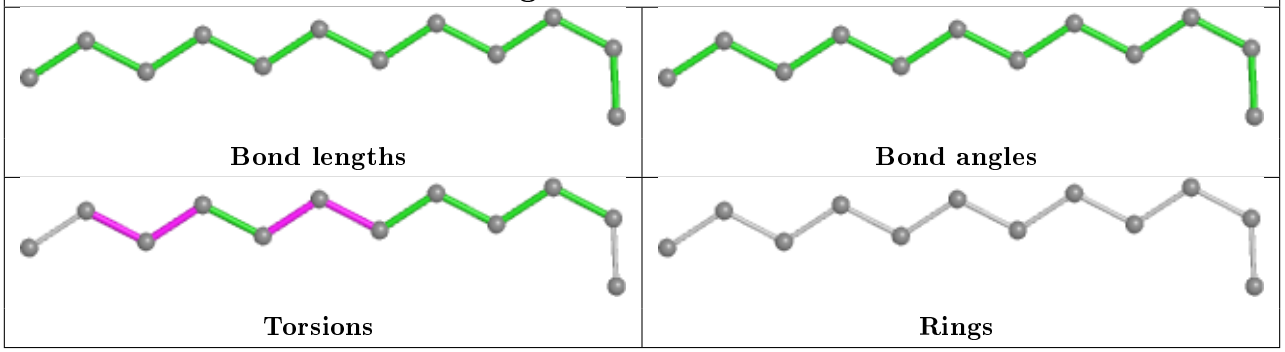


Rings

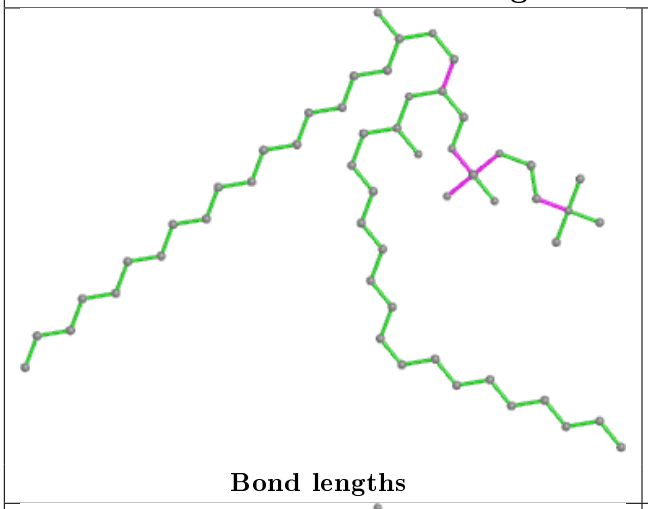
Ligand PCW C 1003



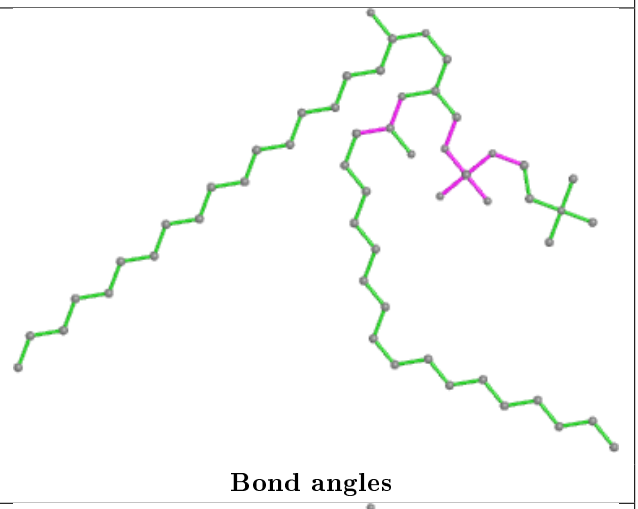
Ligand CE1 D 1006



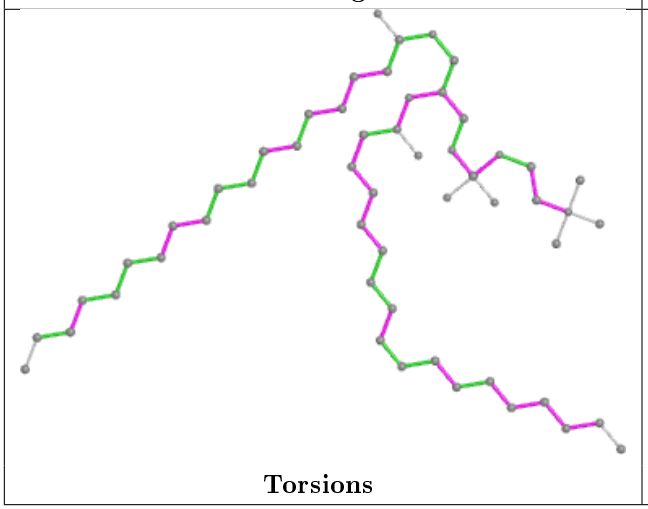
Ligand PCW C 1005



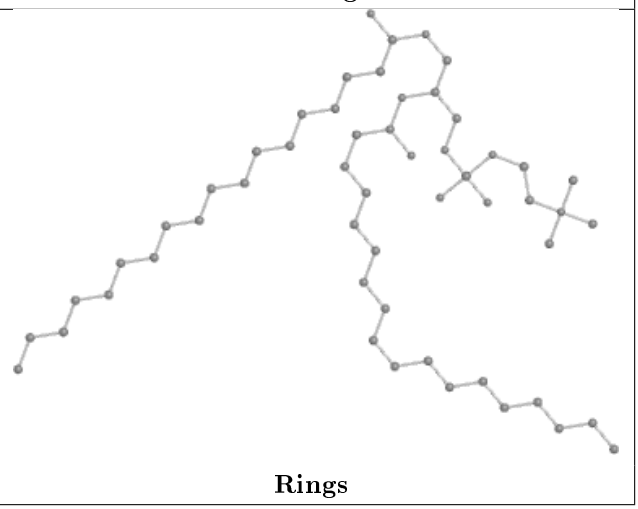
Bond lengths



Bond angles

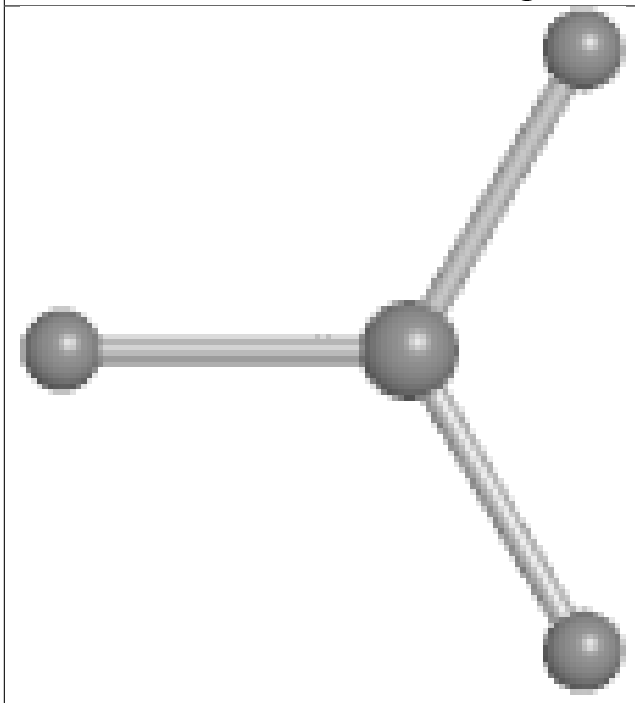


Torsions

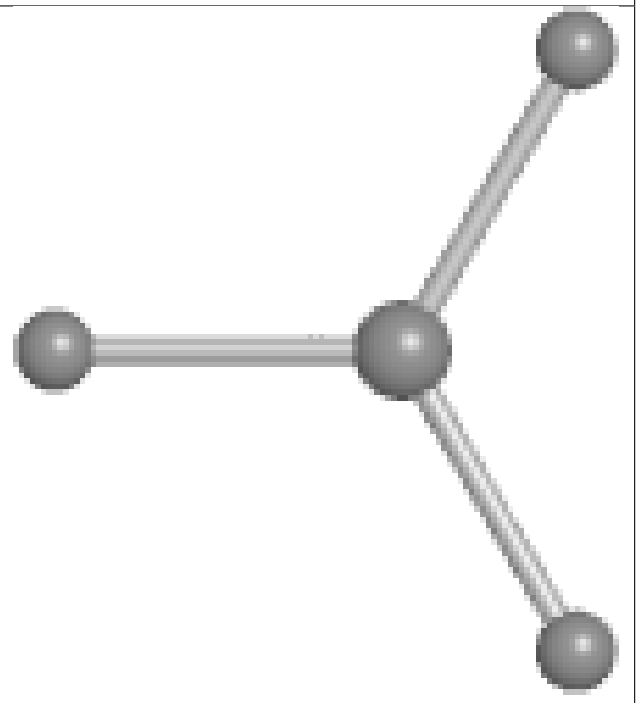


Rings

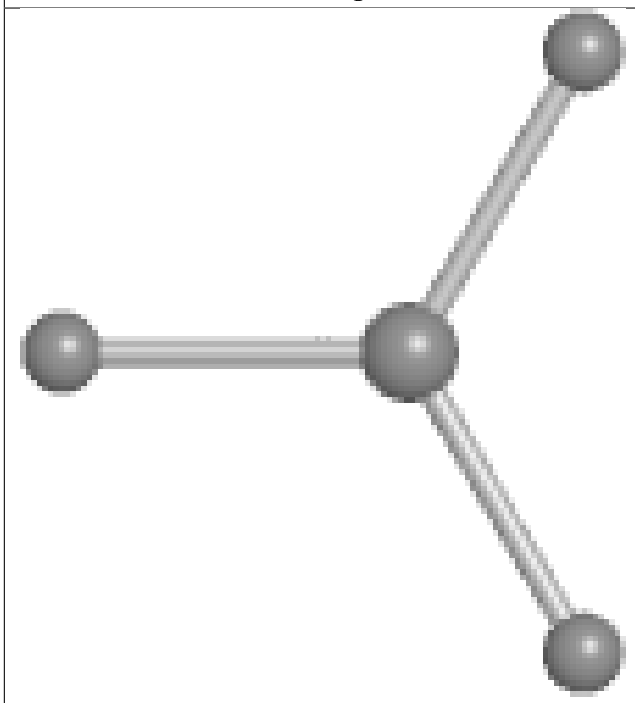
Ligand BEF C 1001



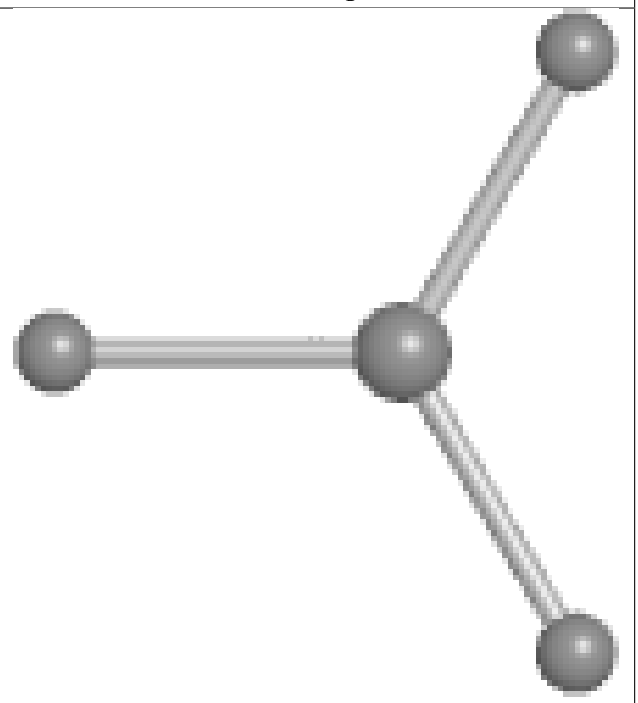
Bond lengths



Bond angles

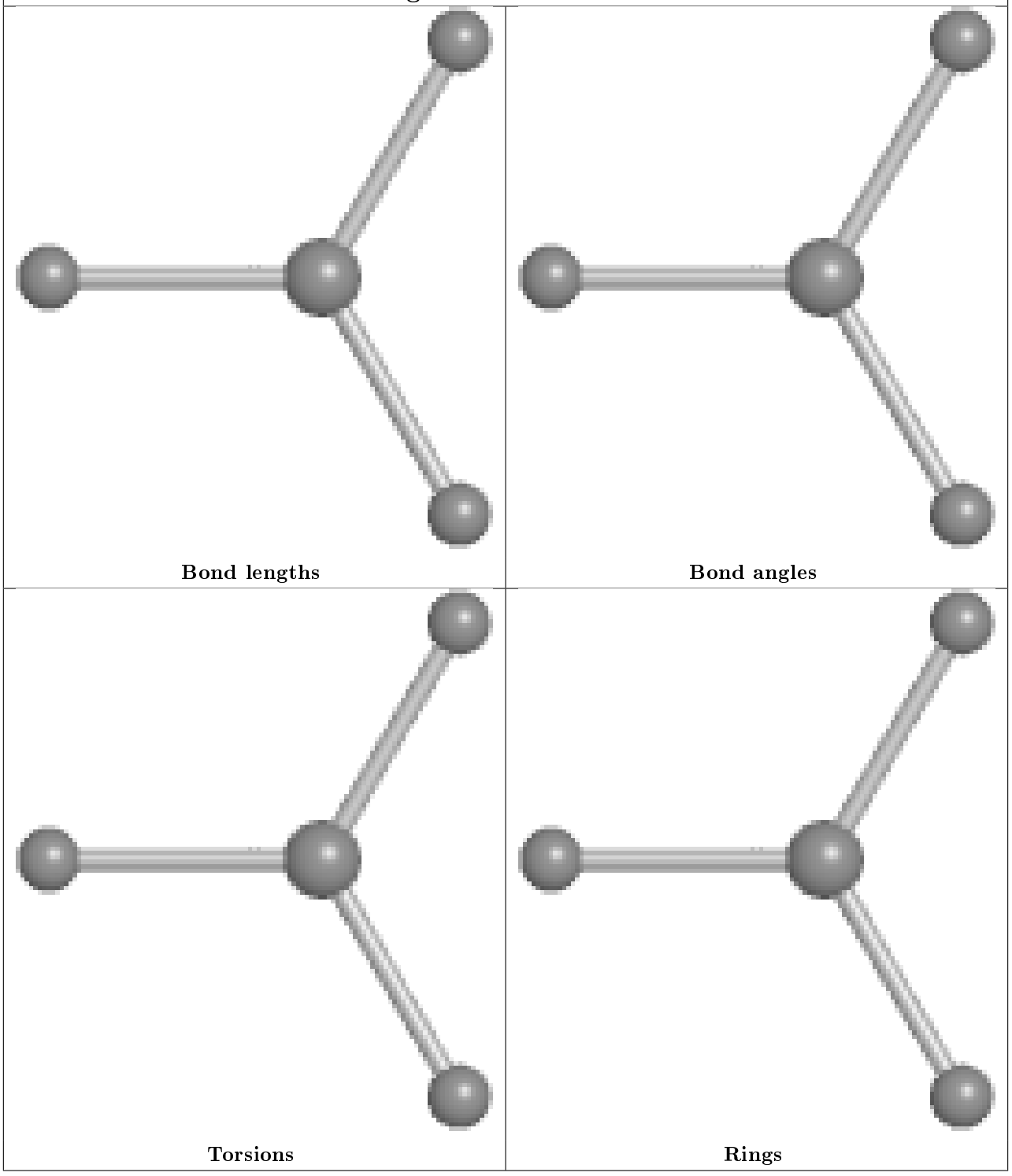


Torsions



Rings

Ligand BEF G 1001



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	A	883/911 (96%)	-0.46	2 (0%) 95 87	25, 51, 97, 128	0
1	B	883/911 (96%)	-0.43	6 (0%) 87 69	26, 51, 98, 130	0
1	C	883/911 (96%)	-0.04	47 (5%) 26 10	26, 68, 215, 259	0
1	D	883/911 (96%)	0.04	73 (8%) 11 3	25, 68, 231, 279	0
1	E	876/911 (96%)	0.99	155 (17%) 1 0	159, 182, 261, 273	0
1	F	876/911 (96%)	0.50	72 (8%) 11 3	155, 174, 199, 221	0
1	G	875/911 (96%)	0.61	83 (9%) 8 3	153, 173, 198, 226	0
1	H	876/911 (96%)	1.01	166 (18%) 1 0	144, 179, 265, 300	0
All	All	7035/7288 (96%)	0.27	604 (8%) 10 3	25, 162, 234, 300	0

The worst 5 of 604 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	495	TYR	9.5
1	H	362	SER	9.5
1	H	507	LEU	9.5
1	G	458	CYS	9.3
1	E	471	THR	9.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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
3	MG	H	1002	1/1	0.07	0.12	225,225,225,225	0
2	BEF	F	1001	4/4	0.59	0.18	206,207,209,213	0
3	MG	G	1002	1/1	0.61	0.09	213,213,213,213	0
2	BEF	H	1001	4/4	0.67	0.38	228,228,229,232	0
3	MG	E	1002	1/1	0.75	0.16	218,218,218,218	0
4	PCW	B	1006	54/54	0.81	0.25	48,78,119,132	0
2	BEF	E	1001	4/4	0.82	0.18	224,224,225,227	0
3	MG	F	1002	1/1	0.83	0.06	182,182,182,182	0
2	BEF	G	1001	4/4	0.84	0.24	198,200,202,203	0
4	PCW	B	1004	54/54	0.86	0.26	52,87,129,138	0
4	PCW	B	1008	54/54	0.87	0.24	48,72,103,130	0
4	PCW	C	1004	54/54	0.87	0.27	28,80,119,130	0
4	PCW	C	1006	54/54	0.87	0.20	31,82,108,121	0
5	CE1	D	1006	12/37	0.87	0.21	48,61,76,81	0
4	PCW	C	1008	54/54	0.88	0.29	15,71,117,129	0
4	PCW	A	1004	54/54	0.88	0.28	40,77,124,128	0
4	PCW	B	1007	54/54	0.89	0.25	38,70,111,132	0
5	CE1	D	1009	12/37	0.89	0.20	49,54,73,77	0
4	PCW	B	1005	54/54	0.90	0.31	78,98,128,137	0
4	PCW	A	1003	54/54	0.91	0.28	53,93,127,137	0
5	CE1	D	1005	12/37	0.91	0.27	26,46,60,65	0
4	PCW	C	1005	54/54	0.91	0.26	26,67,108,120	0
4	PCW	C	1003	54/54	0.91	0.30	19,82,111,128	0
4	PCW	D	1003	54/54	0.92	0.26	25,70,100,109	0
4	PCW	B	1003	54/54	0.93	0.23	17,67,82,100	0
2	BEF	D	1001	4/4	0.94	0.15	70,71,75,87	0
4	PCW	B	1009	54/54	0.94	0.20	25,56,104,111	0
5	CE1	C	1007	15/37	0.94	0.22	21,37,49,50	0
5	CE1	D	1008	11/37	0.95	0.21	23,41,49,52	0
3	MG	C	1002	1/1	0.96	0.12	64,64,64,64	0
5	CE1	D	1004	12/37	0.96	0.19	19,33,37,44	0
5	CE1	D	1007	12/37	0.97	0.17	12,17,36,44	0
2	BEF	C	1001	4/4	0.97	0.19	84,84,86,86	0
2	BEF	B	1001	4/4	0.97	0.18	47,48,48,57	0
3	MG	D	1002	1/1	0.98	0.08	53,53,53,53	0
3	MG	B	1002	1/1	0.98	0.12	44,44,44,44	0
2	BEF	A	1001	4/4	0.98	0.15	46,46,46,63	0

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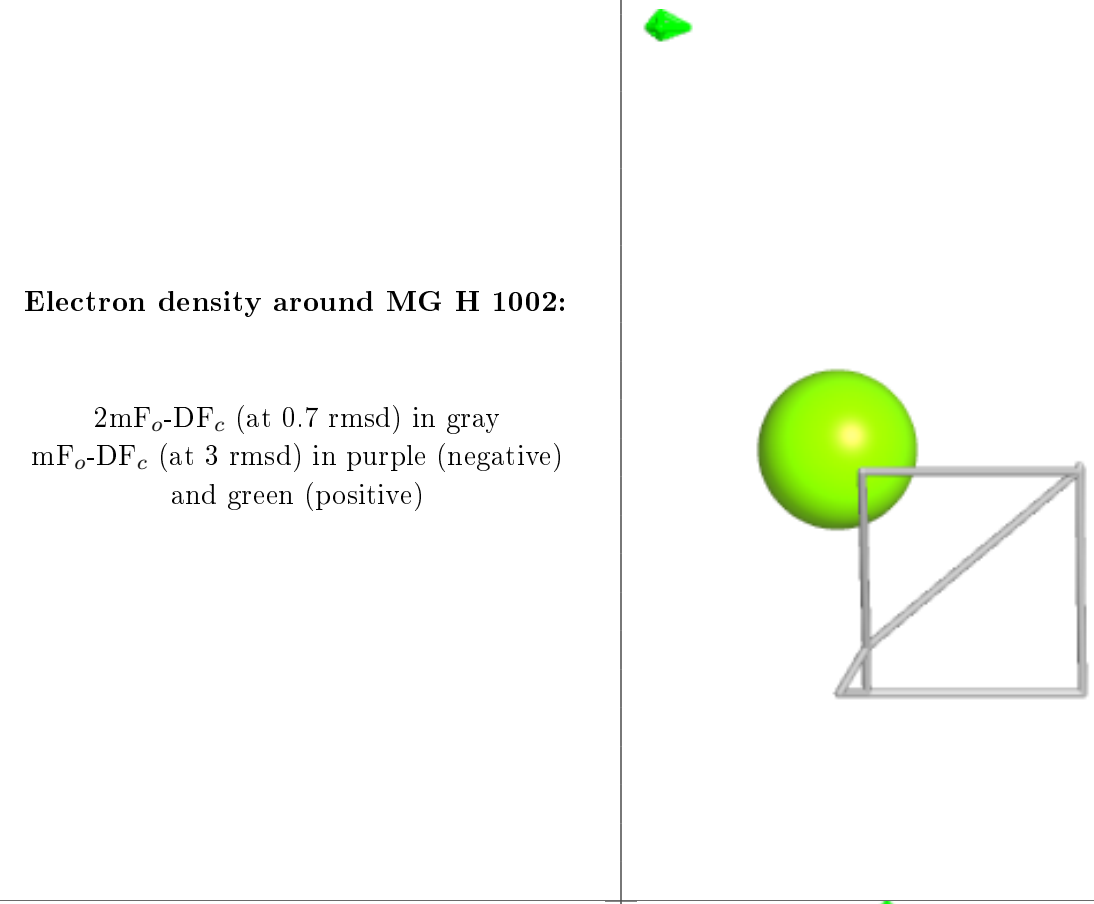
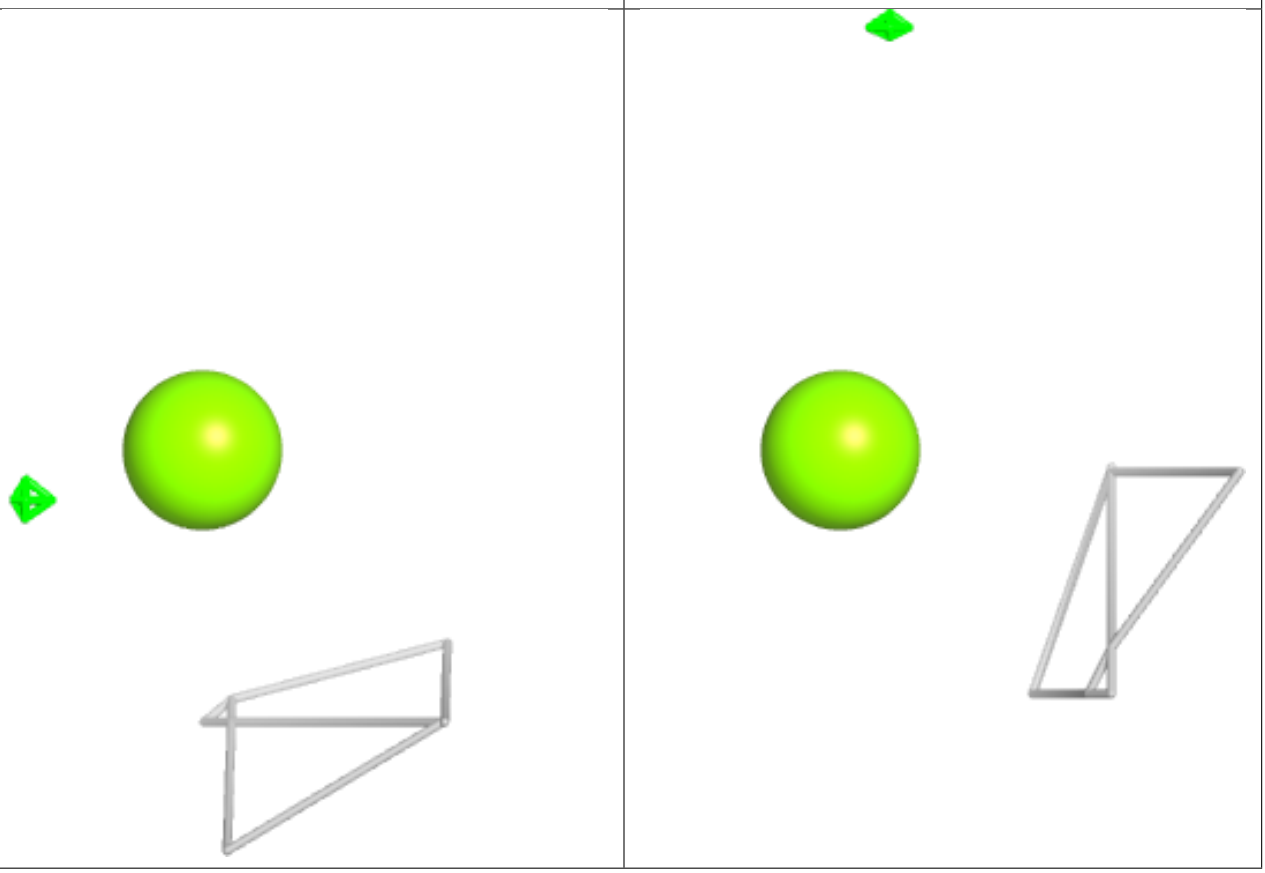
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	A	1002	1/1	0.99	0.16	44,44,44,44	0

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 MG H 1002:

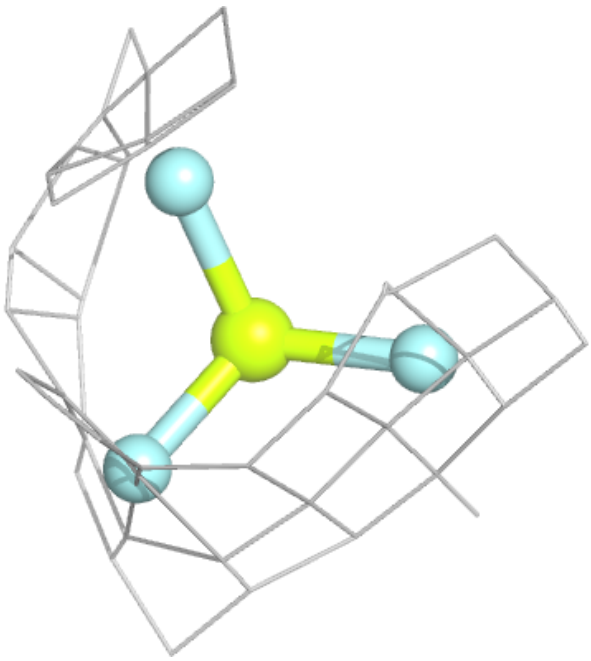
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

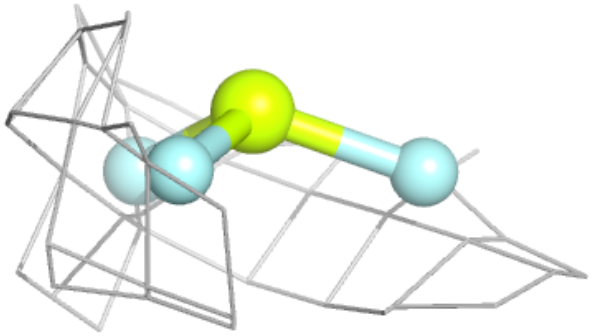


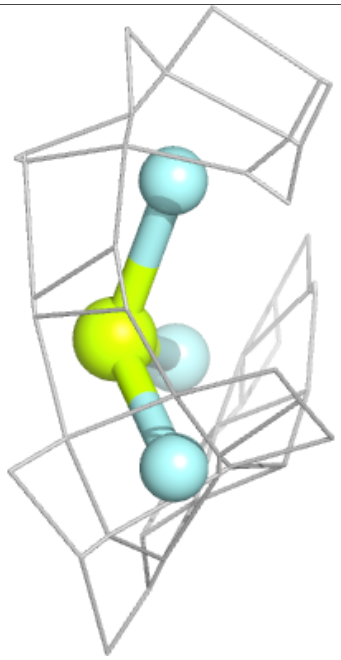


Electron density around BEF F 1001:

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

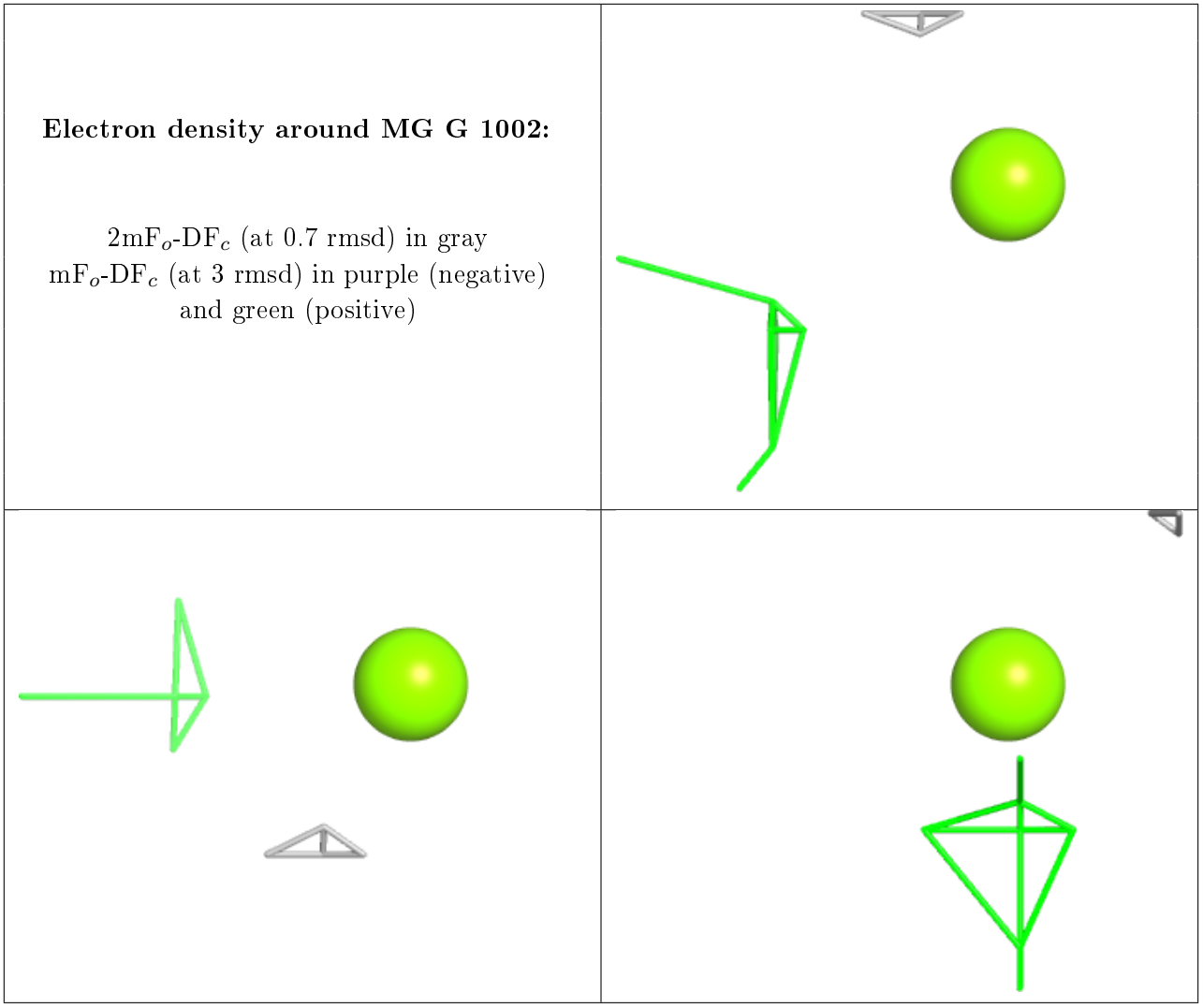






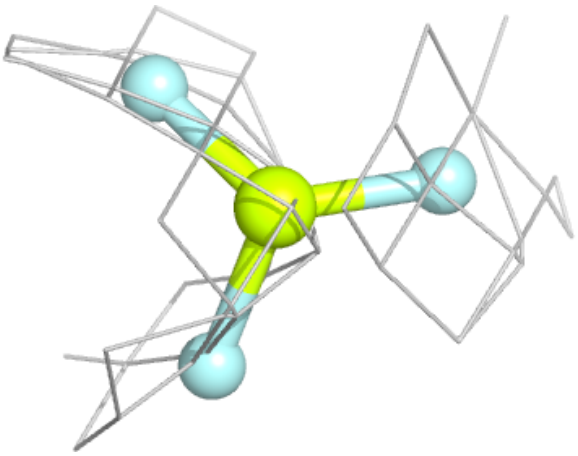
Electron density around MG G 1002:

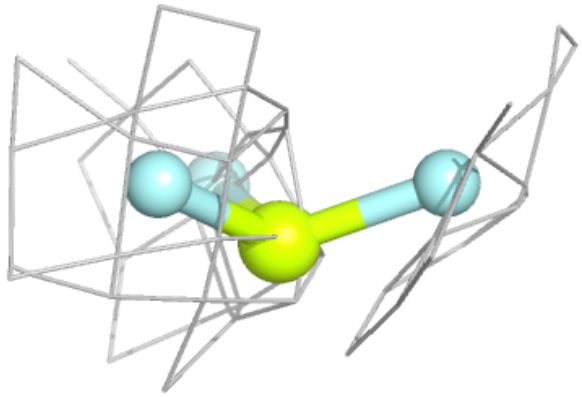
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

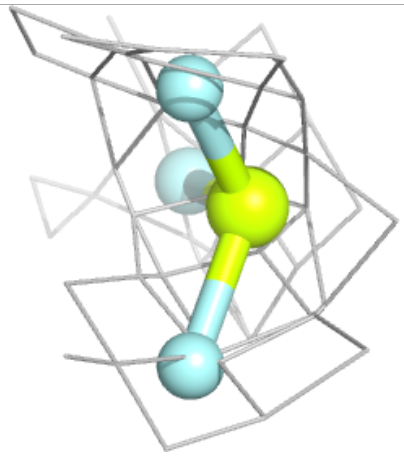


Electron density around BEF H 1001:

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

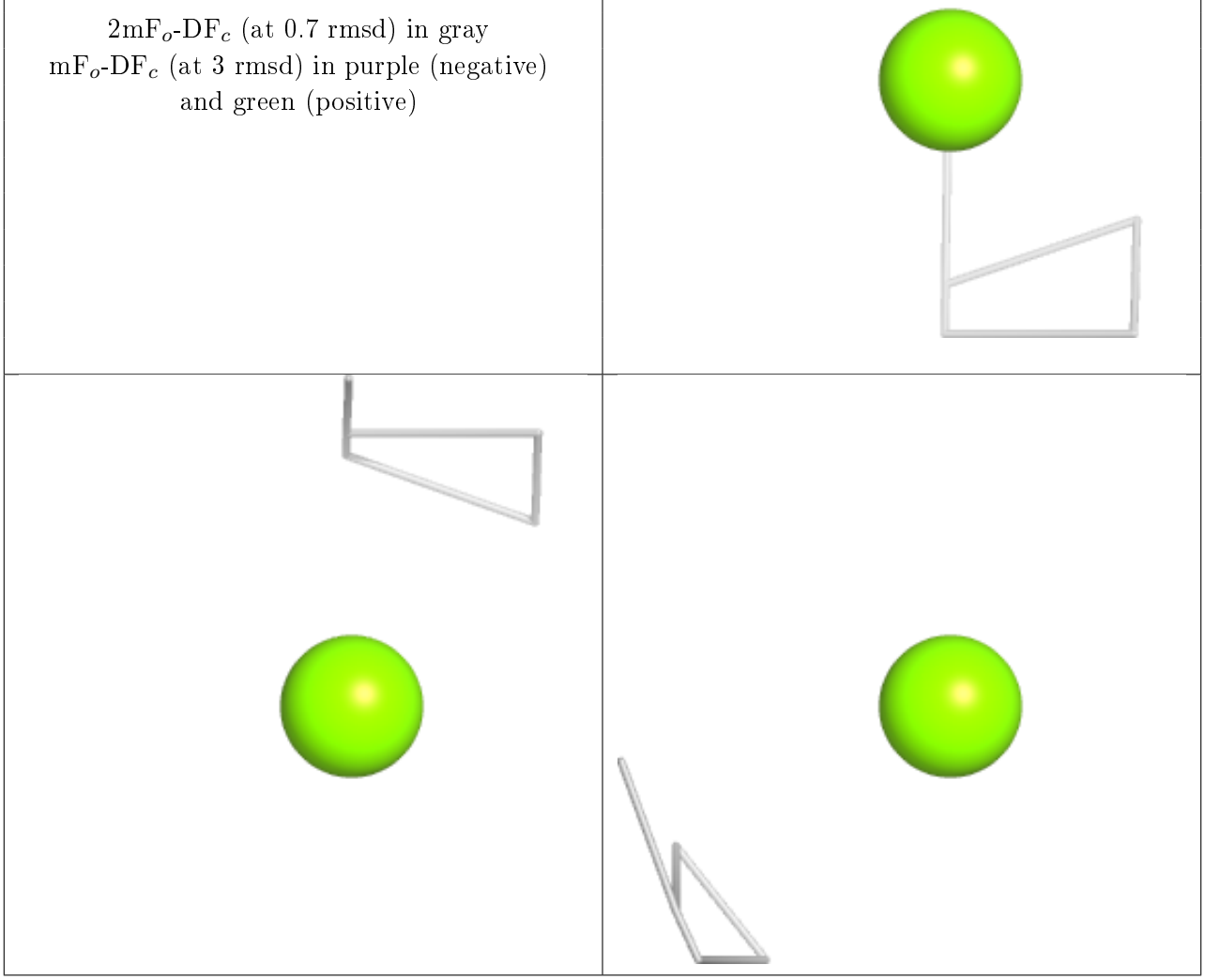






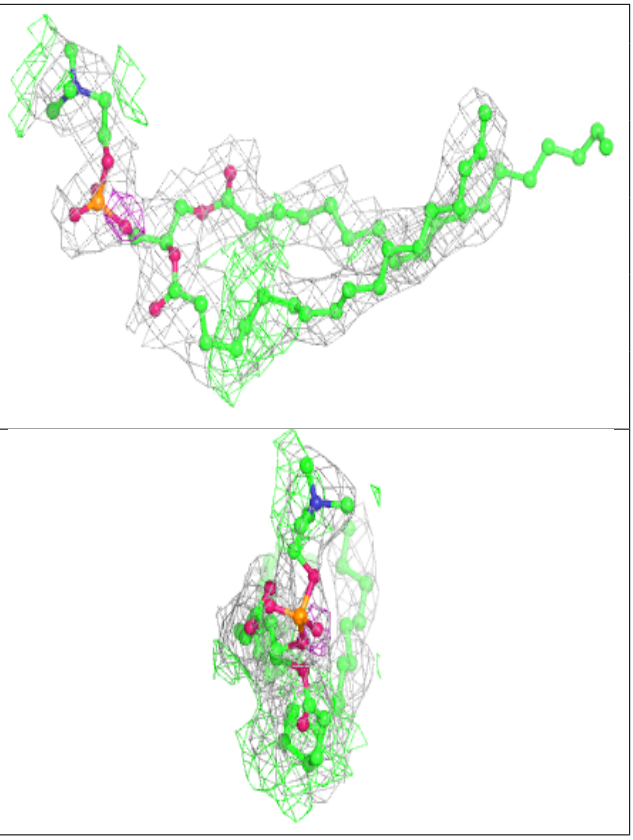
Electron density around MG E 1002:

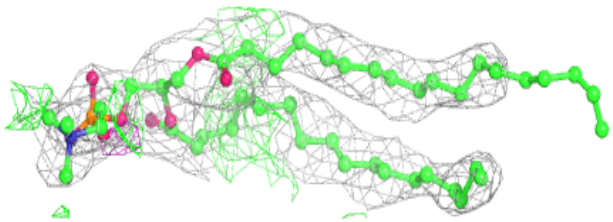
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around PCW B 1006:

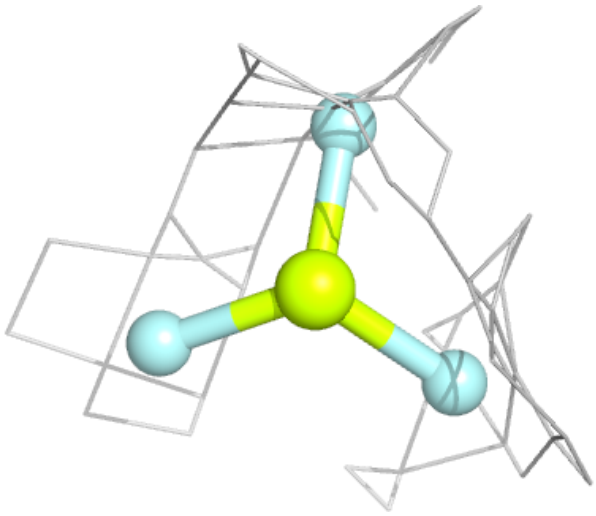
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

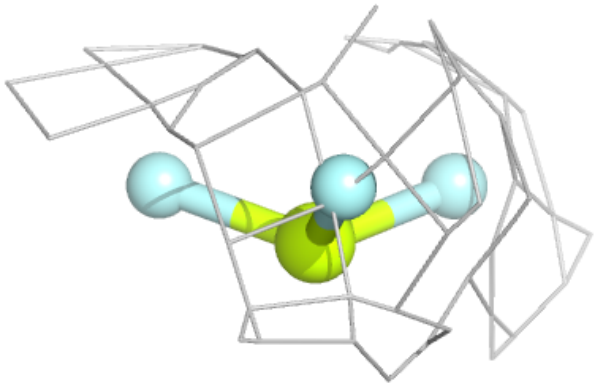


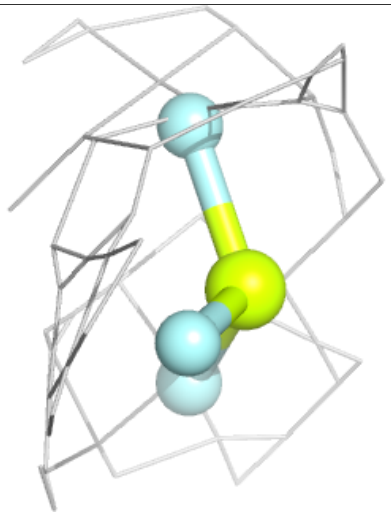


Electron density around BEF E 1001:

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





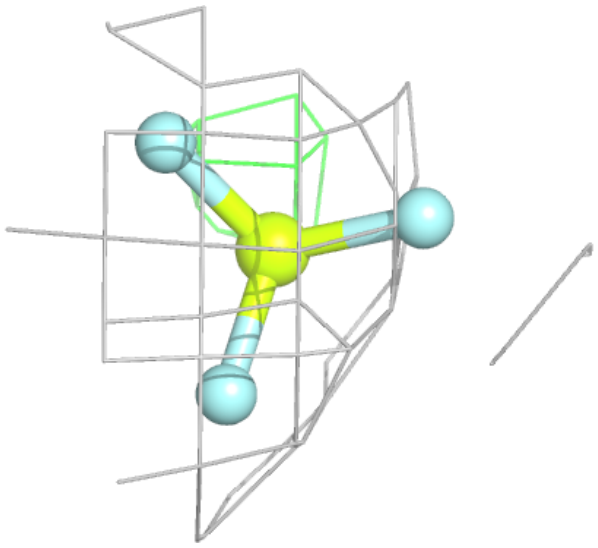


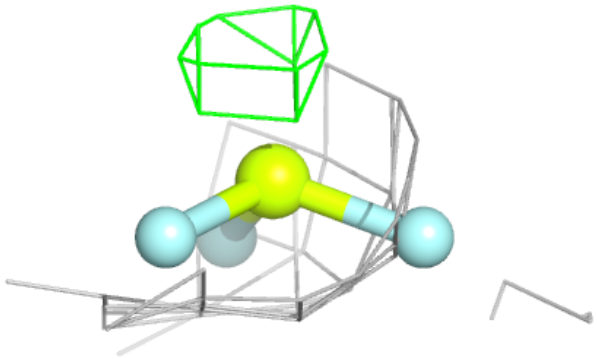
Electron density around MG F 1002:

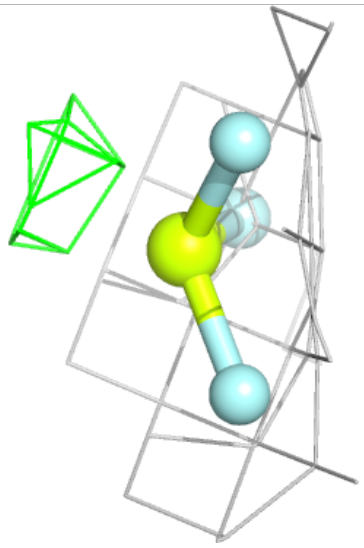
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

Electron density around BEF G 1001:

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

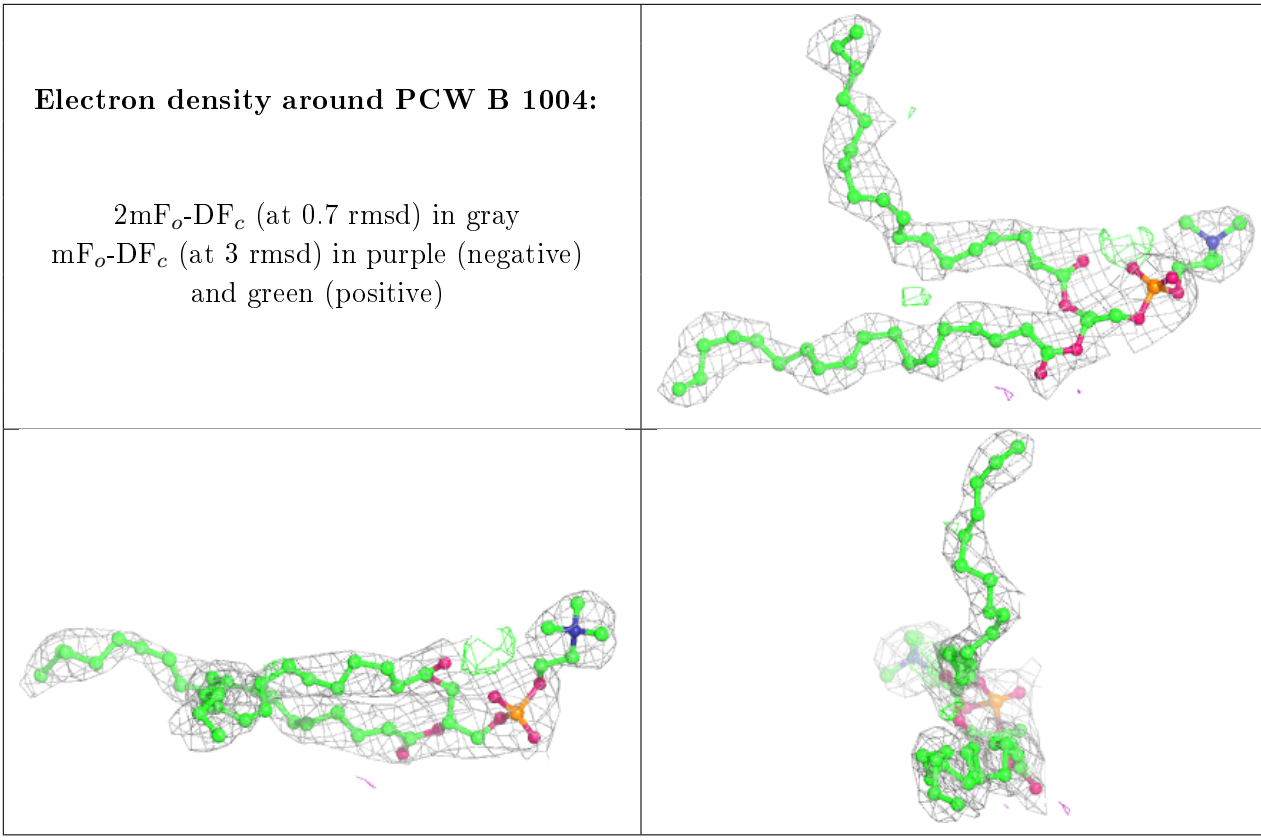






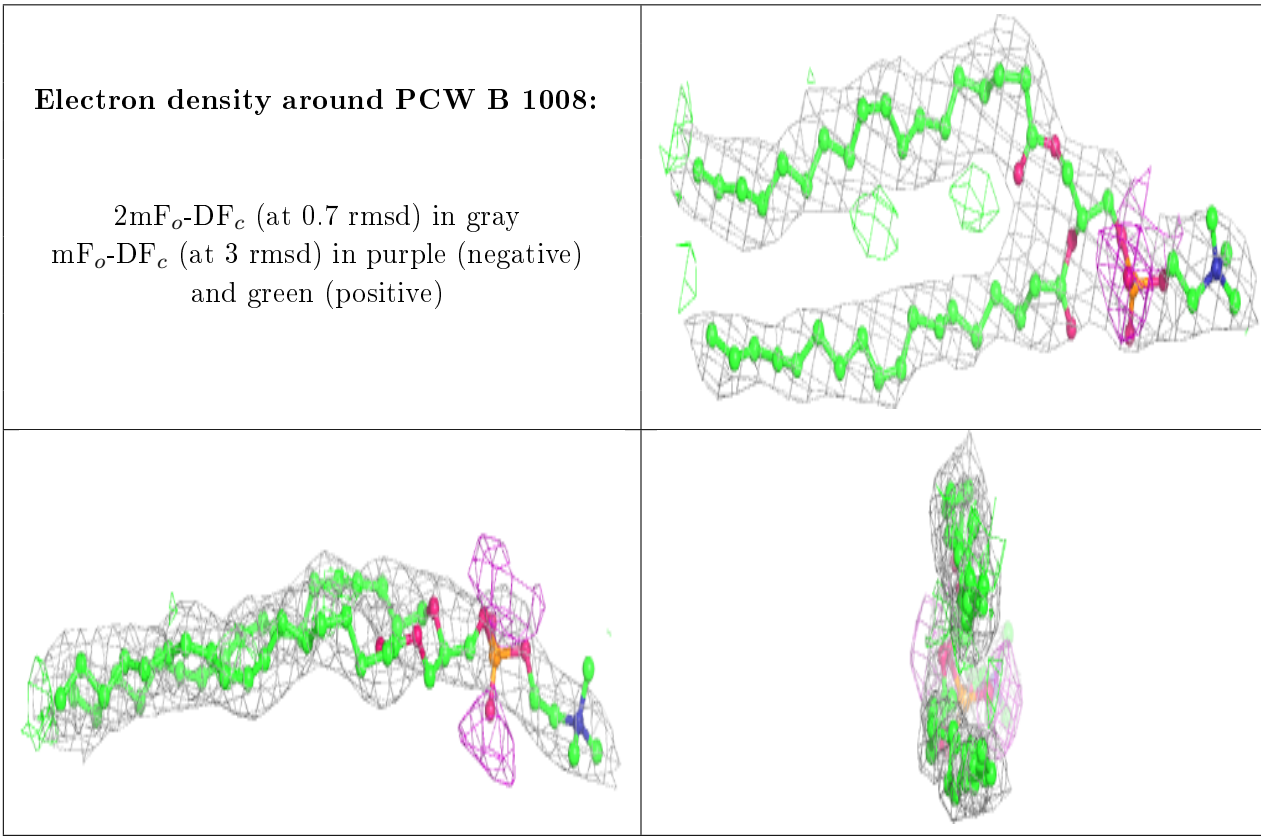
Electron density around PCW B 1004:

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



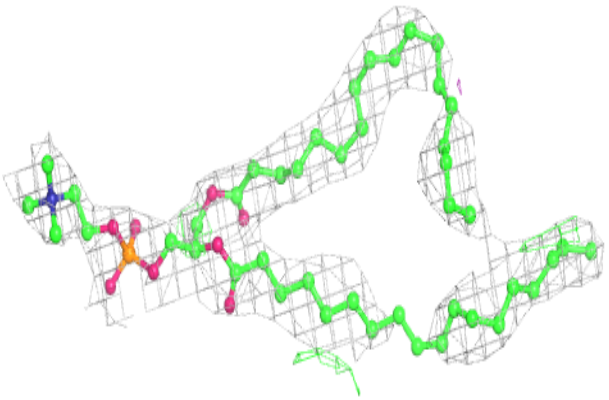
Electron density around PCW B 1008:

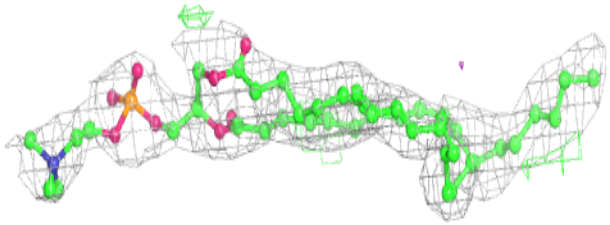
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

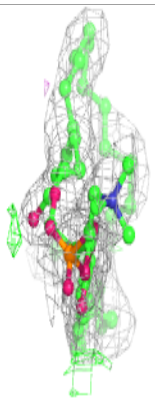


Electron density around PCW C 1004:

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

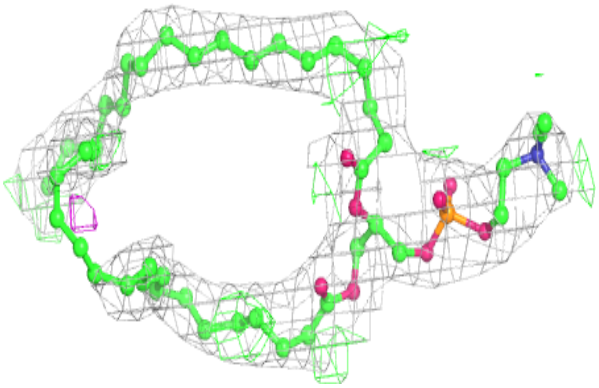


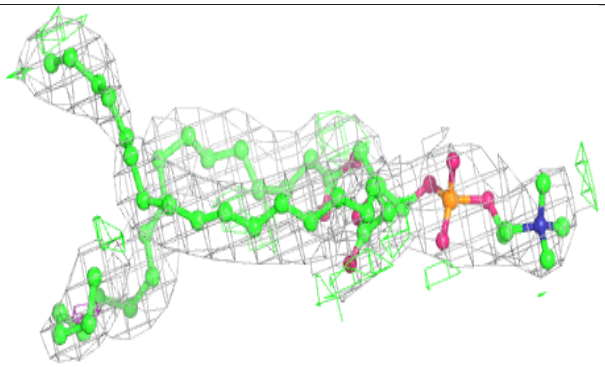




Electron density around PCW C 1006:

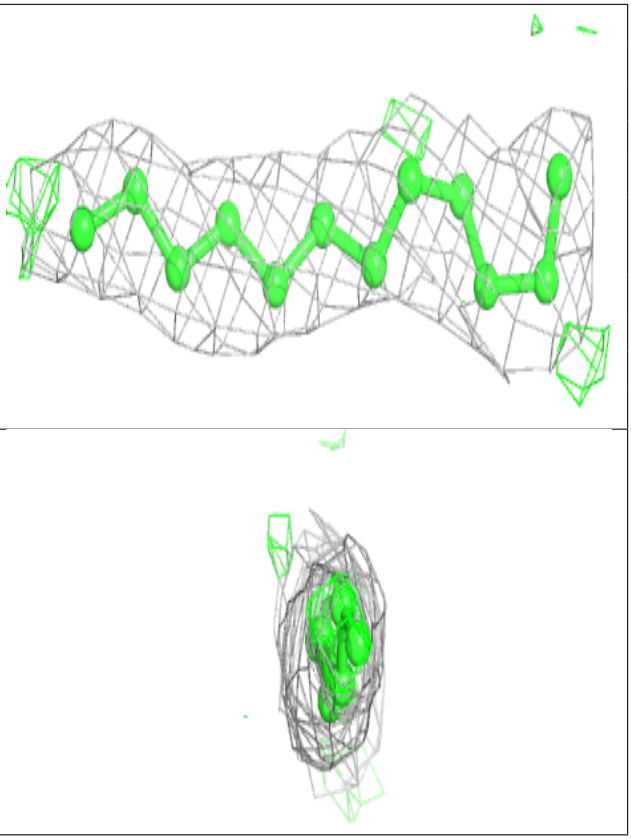
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





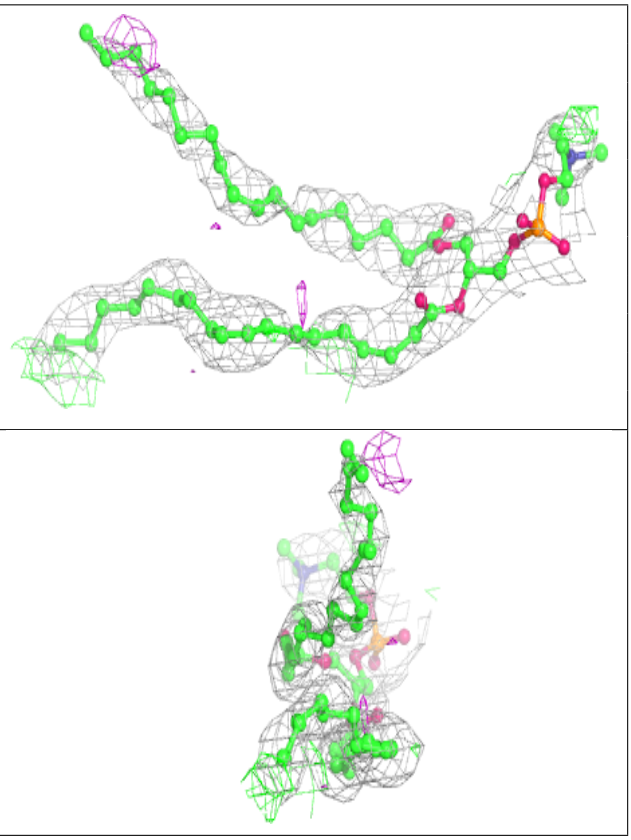
Electron density around CE1 D 1006:

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



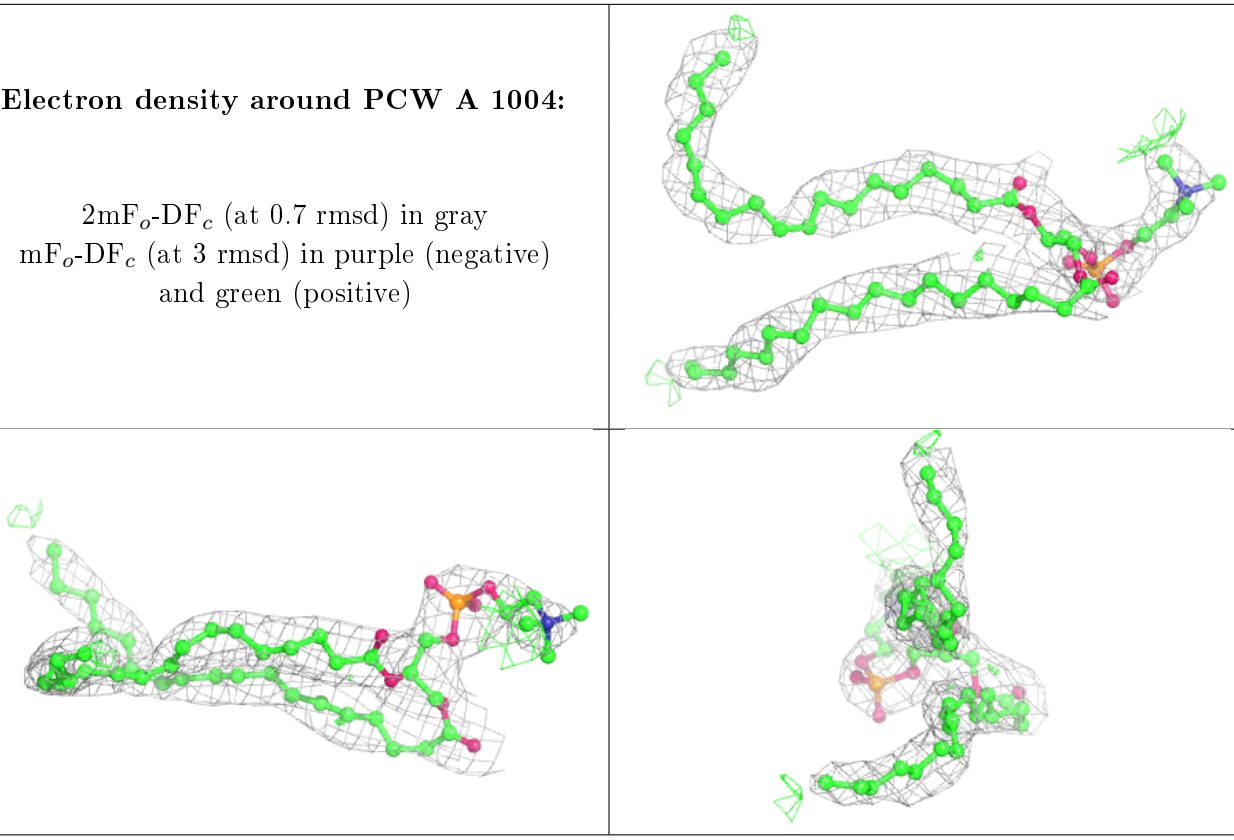
Electron density around PCW C 1008:

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



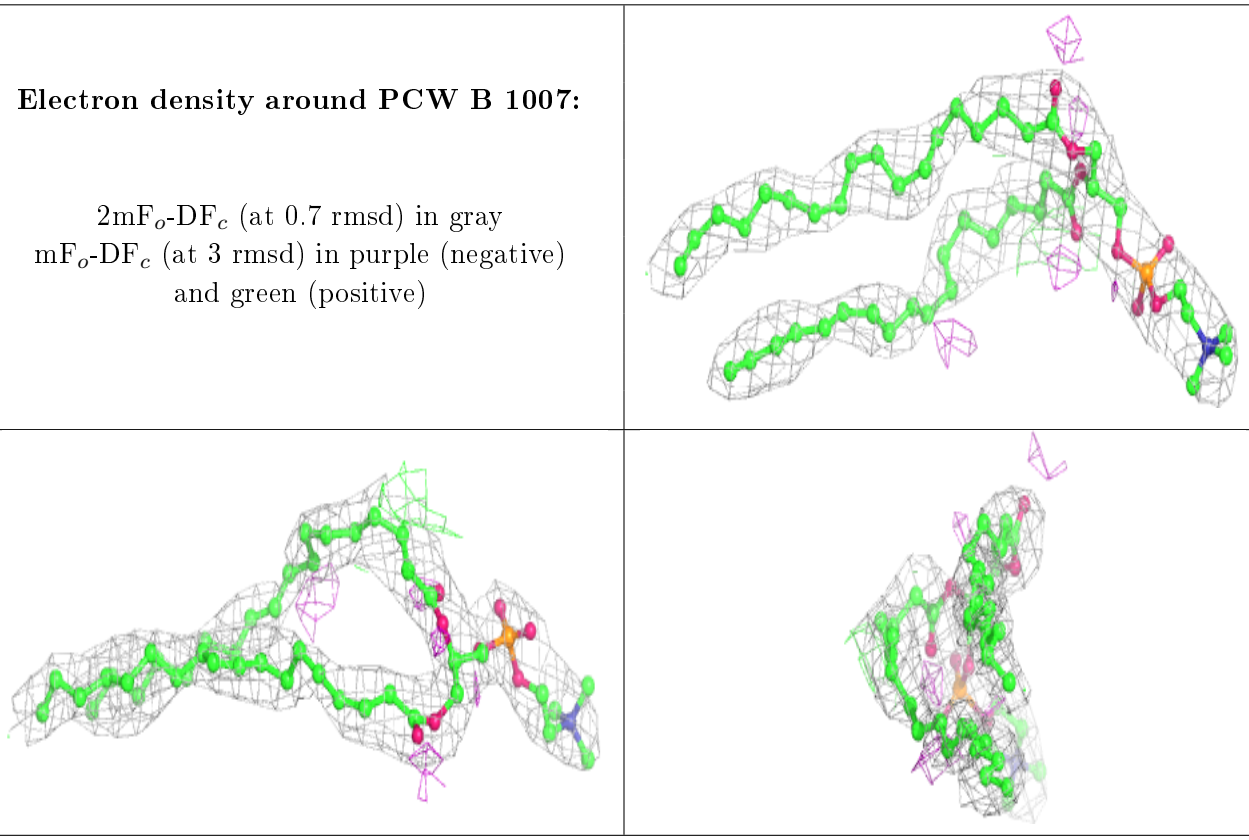
Electron density around PCW A 1004:

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



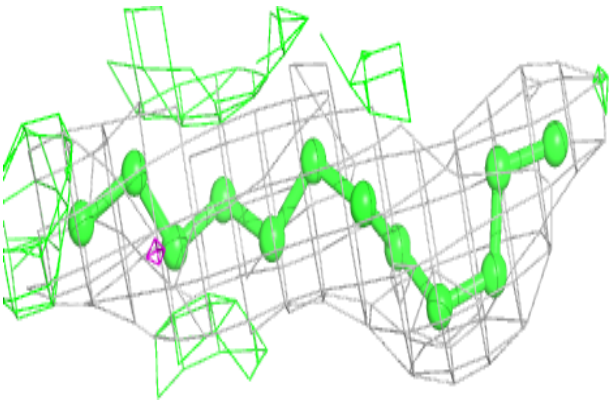
Electron density around PCW B 1007:

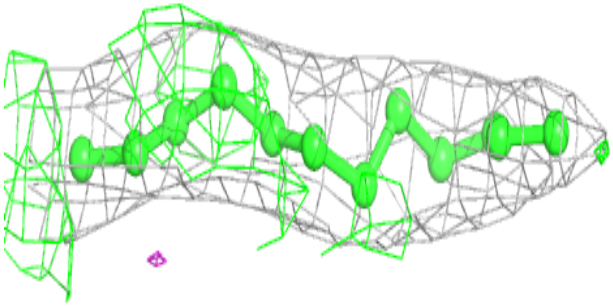
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

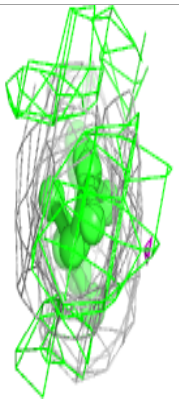


Electron density around CE1 D 1009:

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

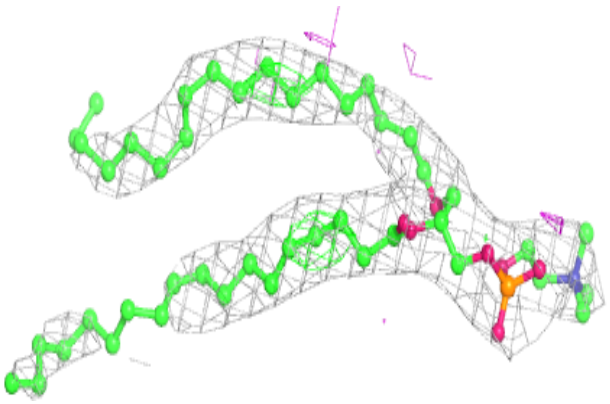


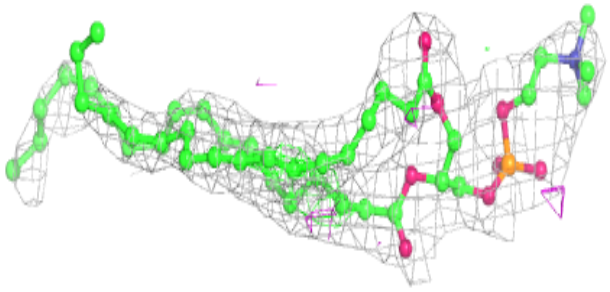




Electron density around PCW B 1005:

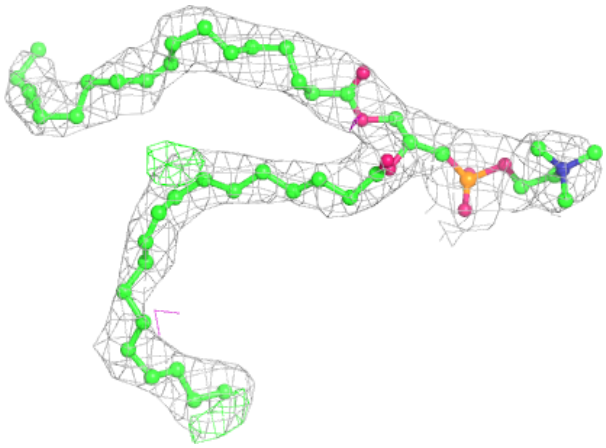
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

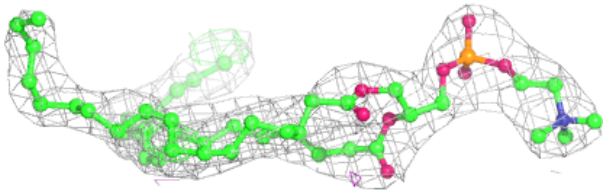


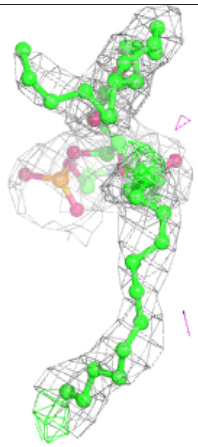


Electron density around PCW A 1003:

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

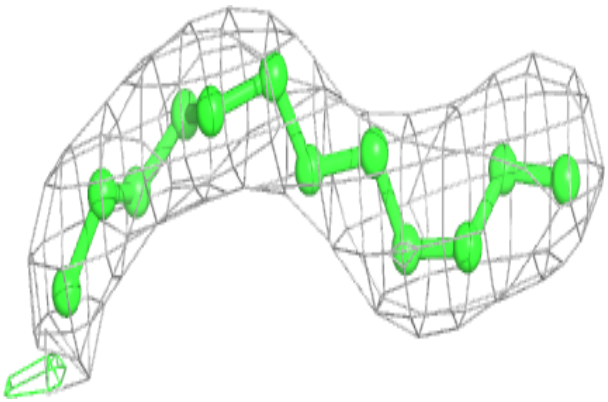


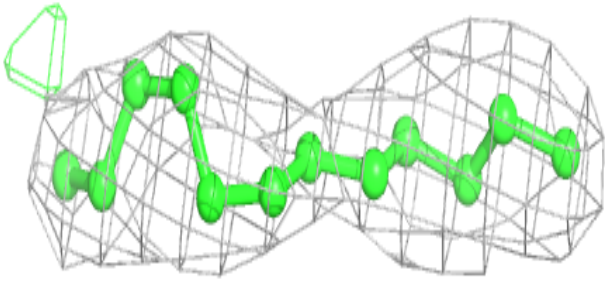


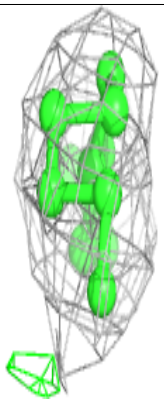


Electron density around CE1 D 1005:

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

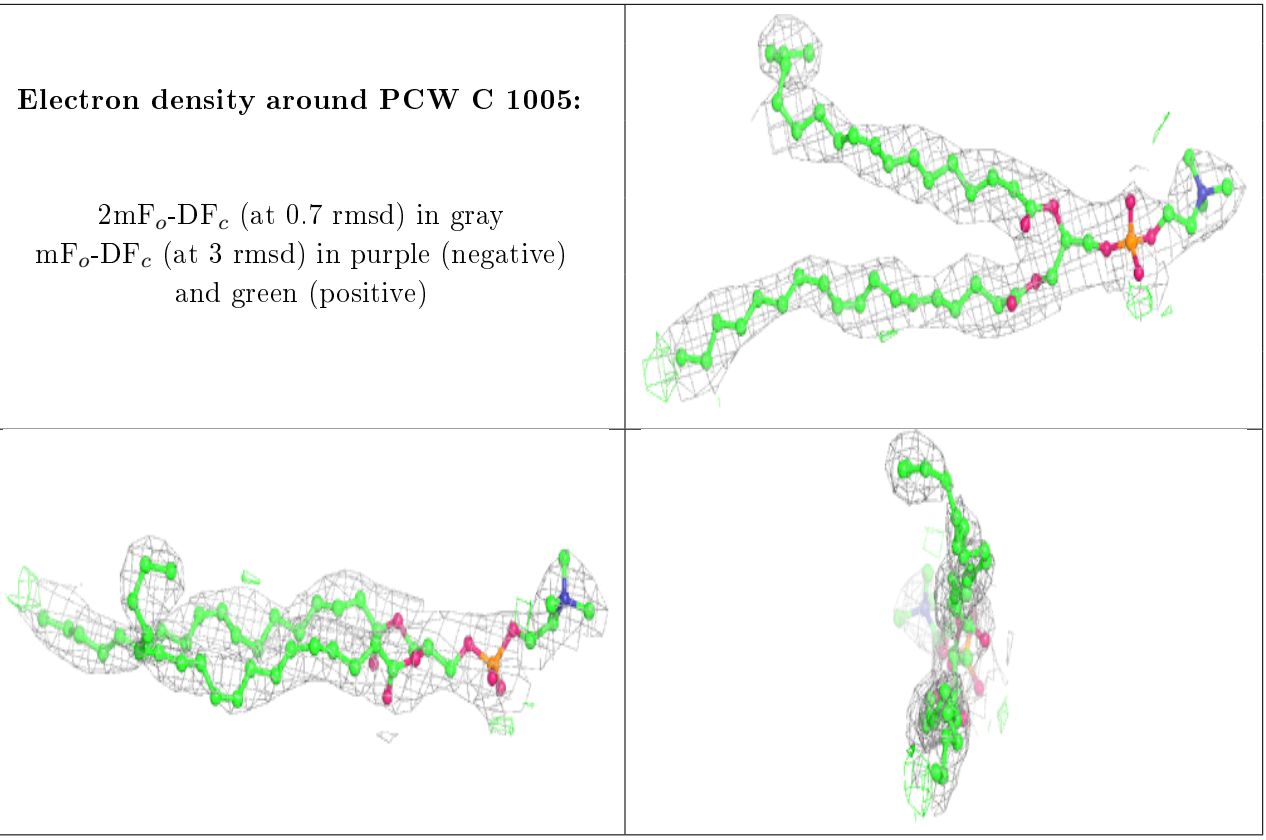






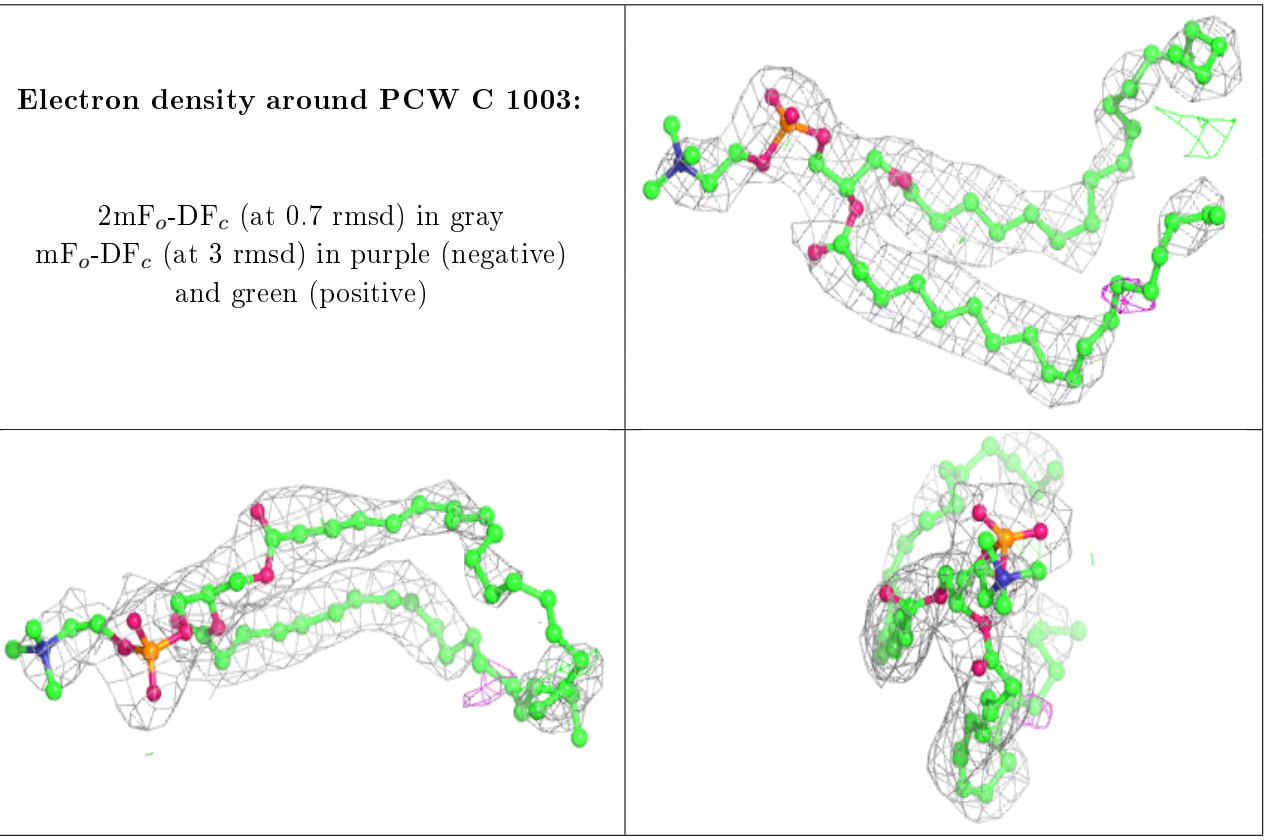
Electron density around PCW C 1005:

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



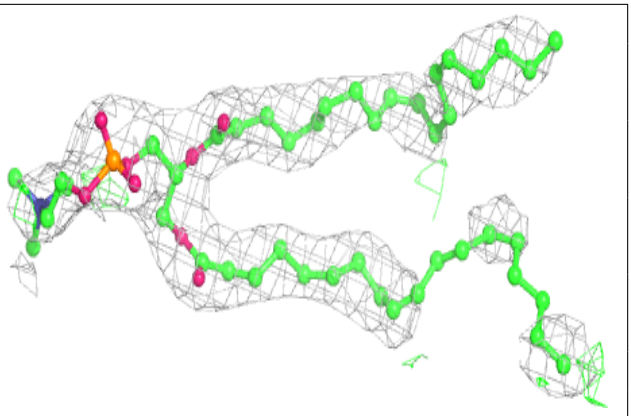
Electron density around PCW C 1003:

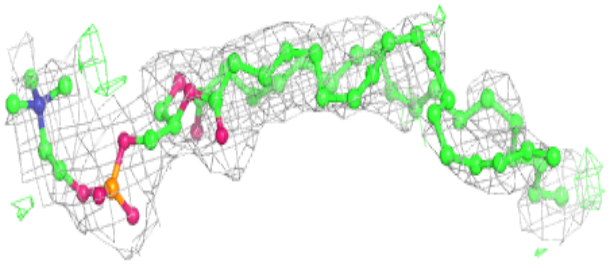
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around PCW D 1003:

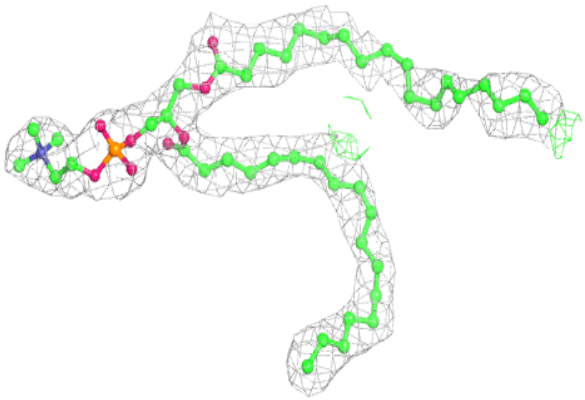
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

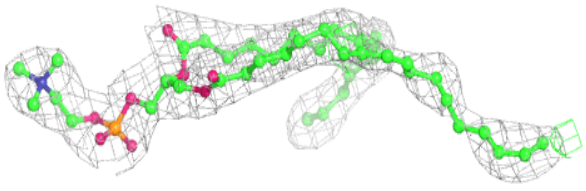


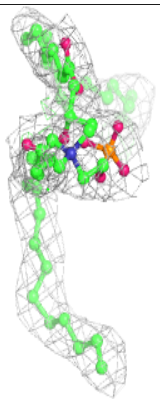


Electron density around PCW B 1003:

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

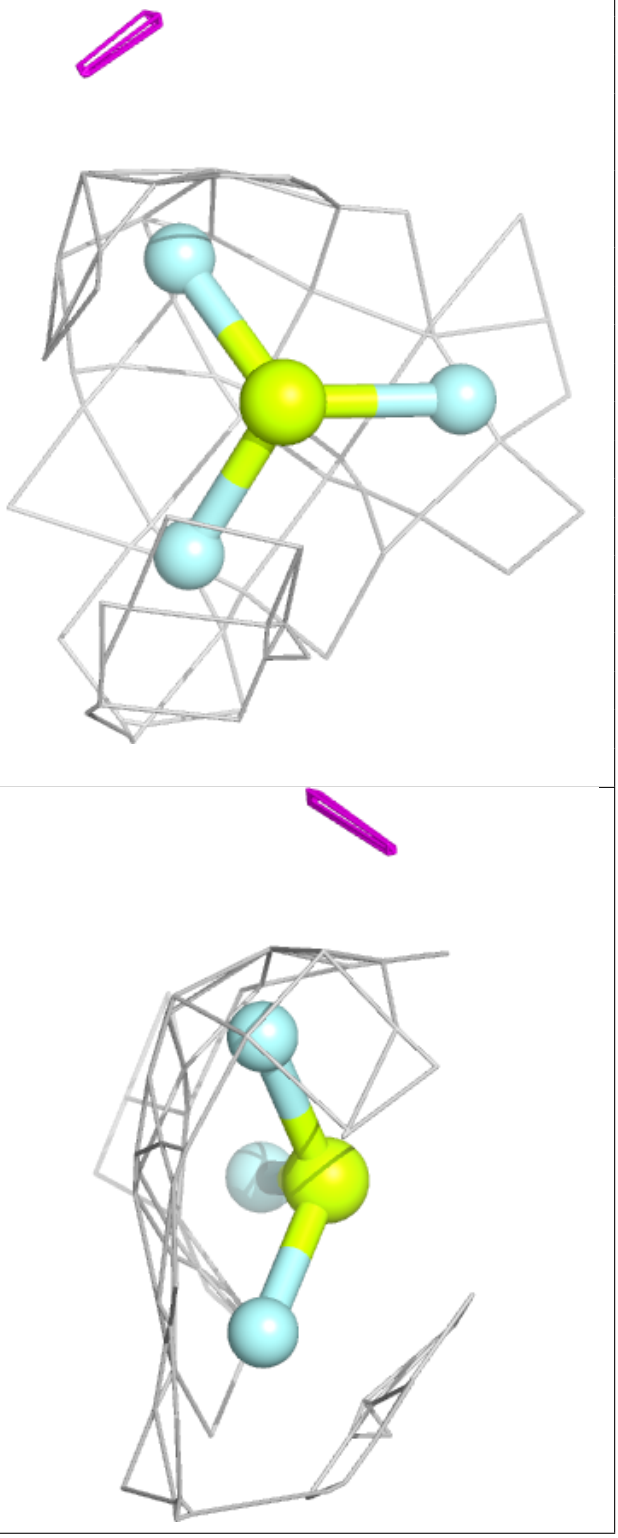


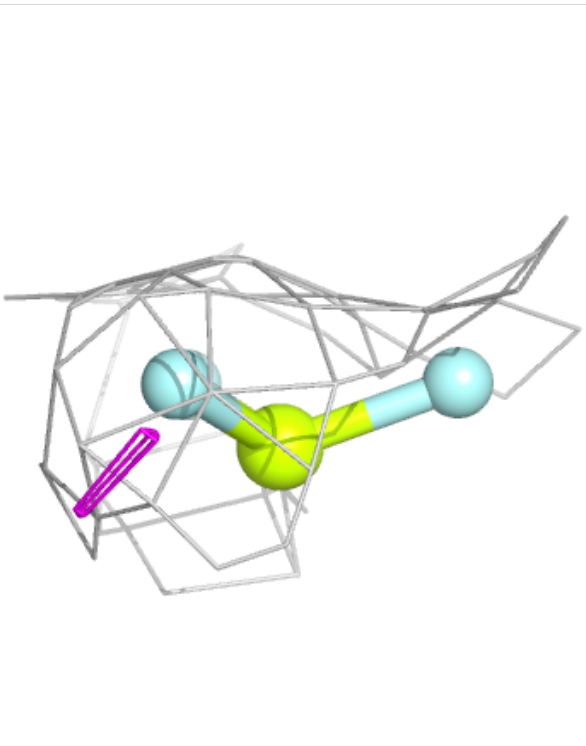




Electron density around BEF D 1001:

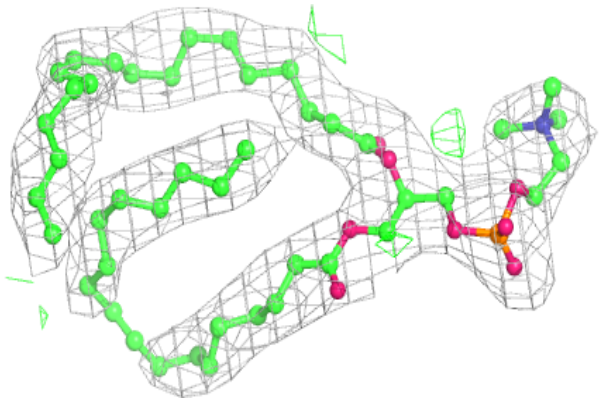
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

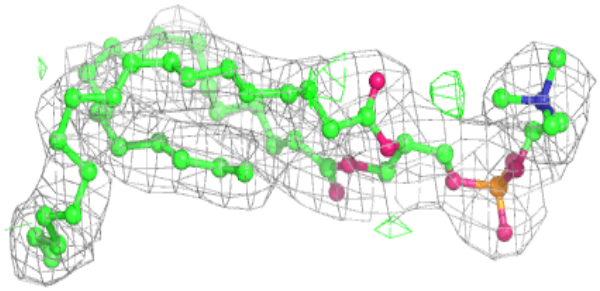


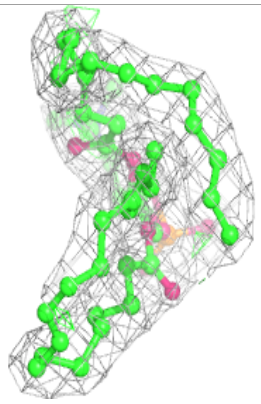


Electron density around PCW B 1009:

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

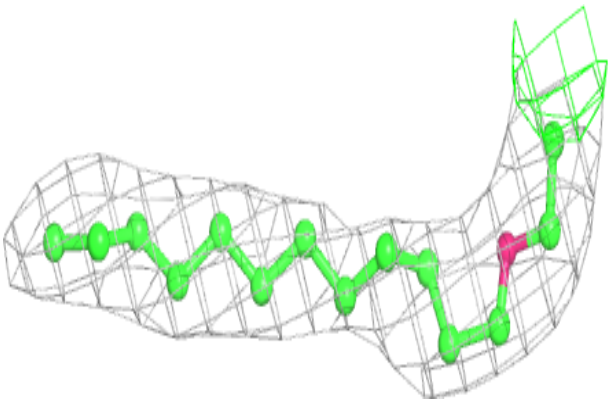


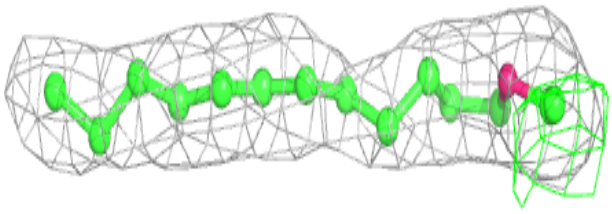


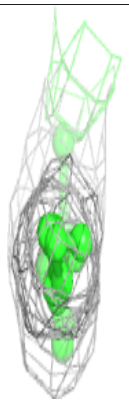


Electron density around CE1 C 1007:

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

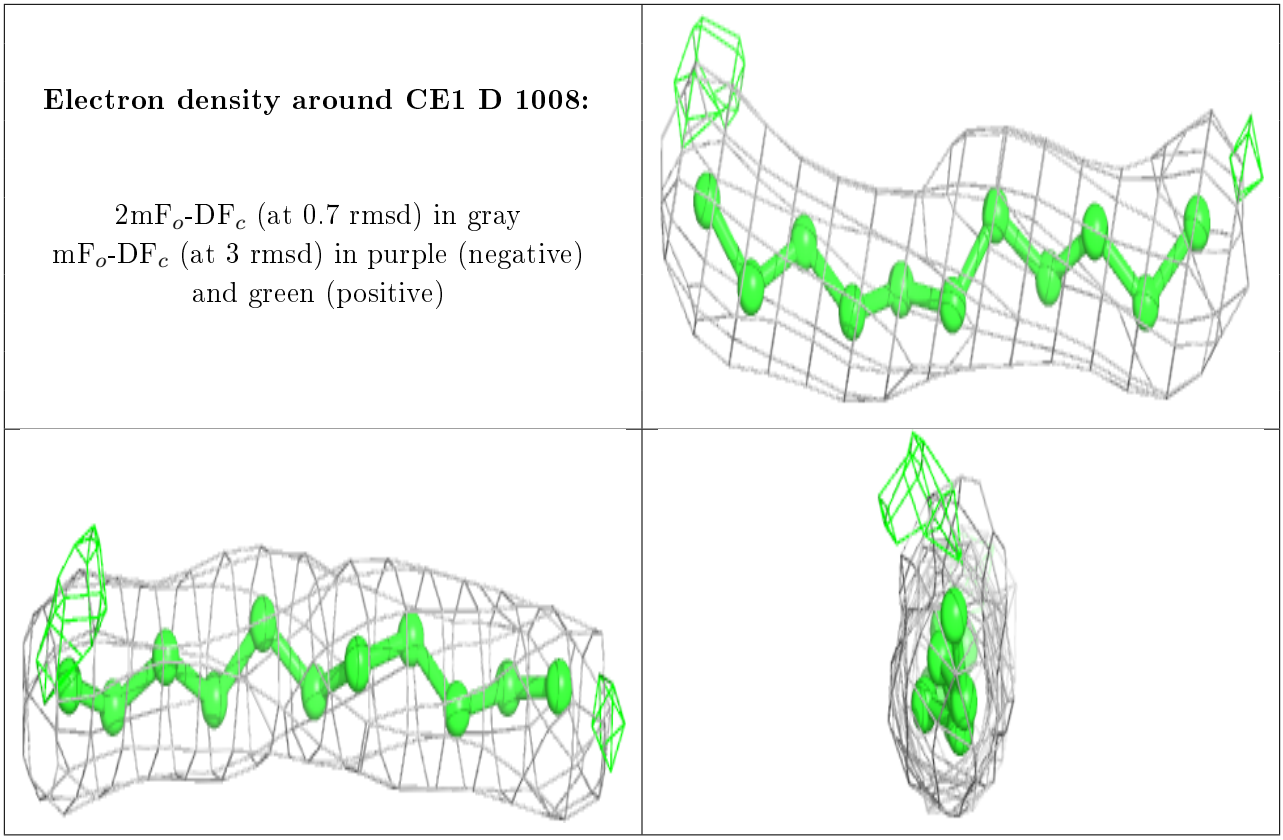






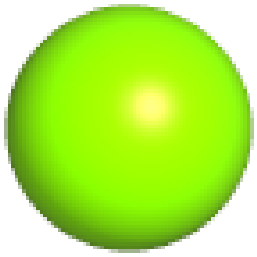
Electron density around CE1 D 1008:

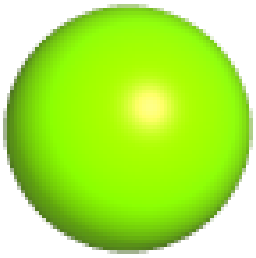
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

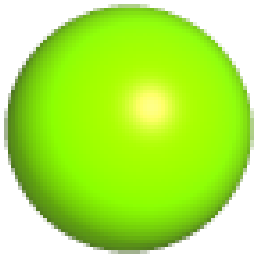


Electron density around MG C 1002:

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

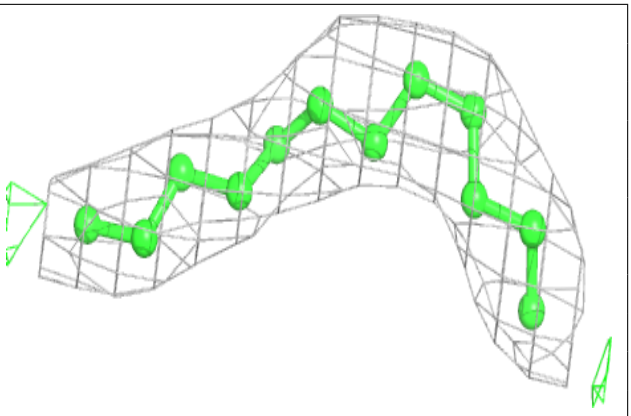


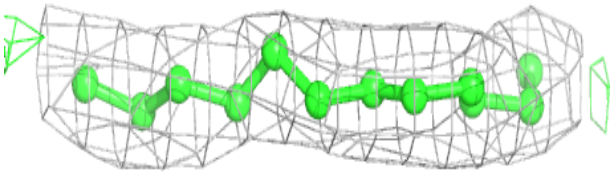


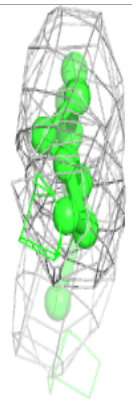


Electron density around CE1 D 1004:

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

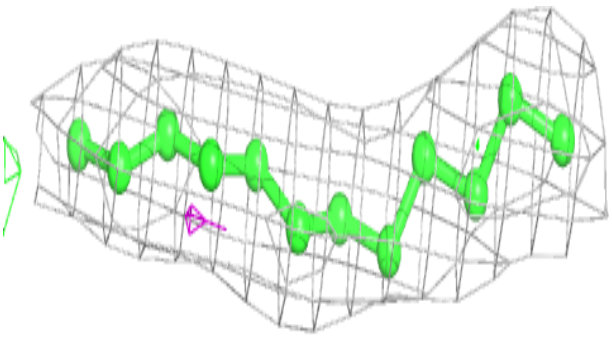


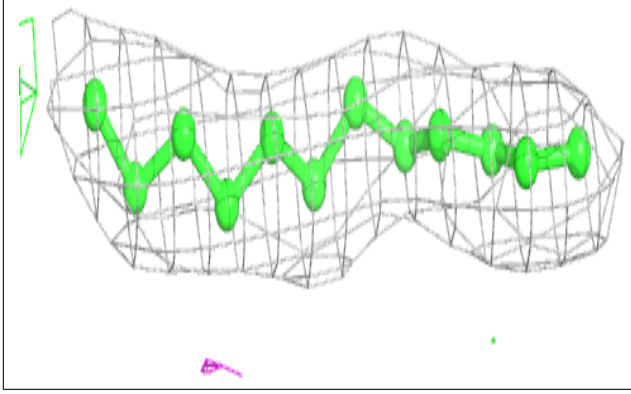


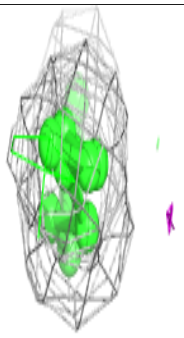


Electron density around CE1 D 1007:

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

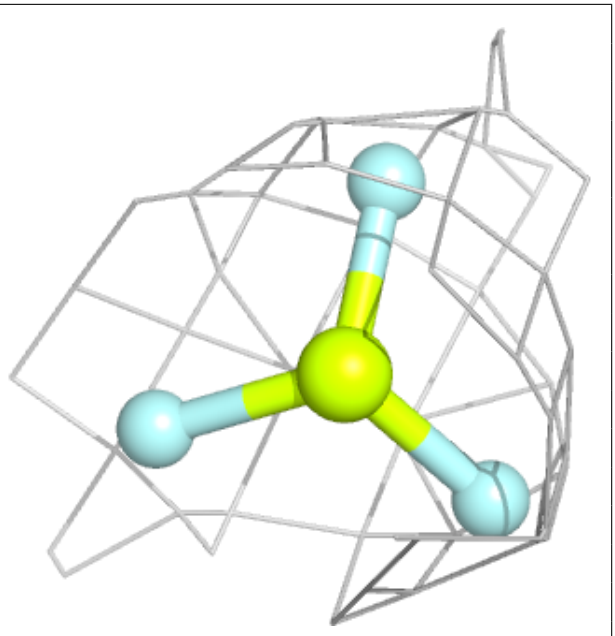


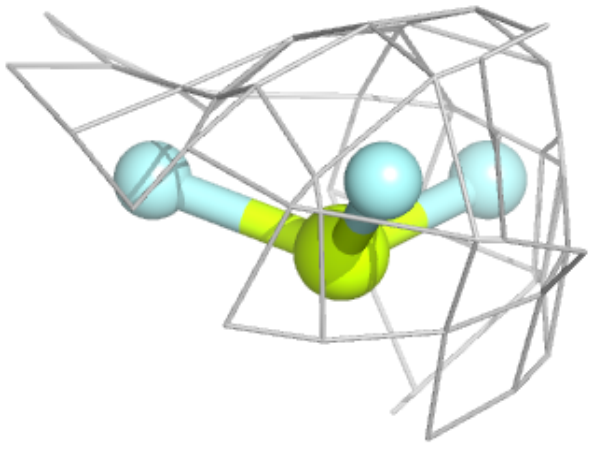


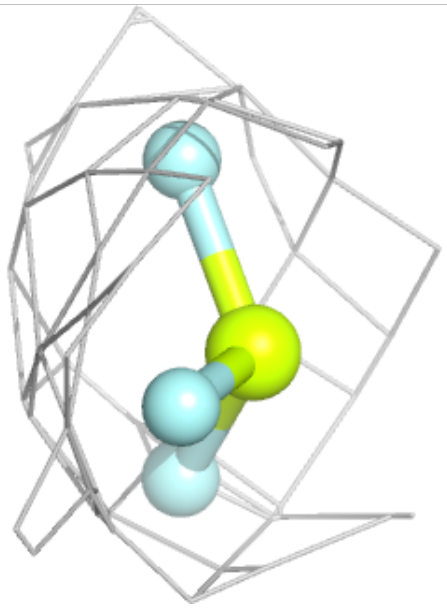


Electron density around BEF C 1001:

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

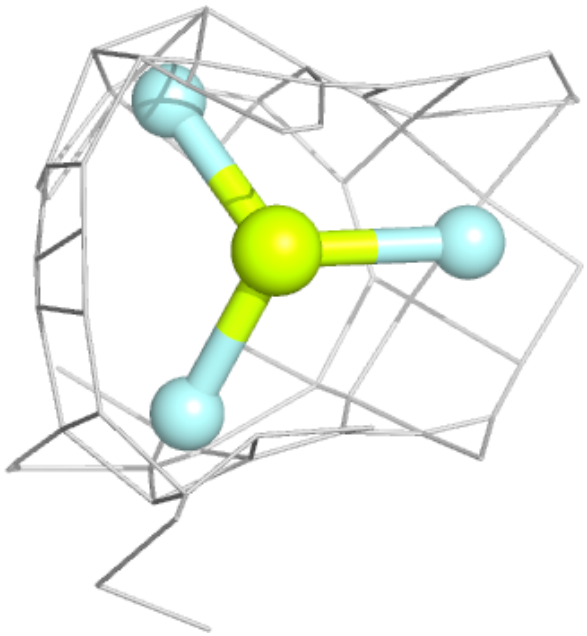


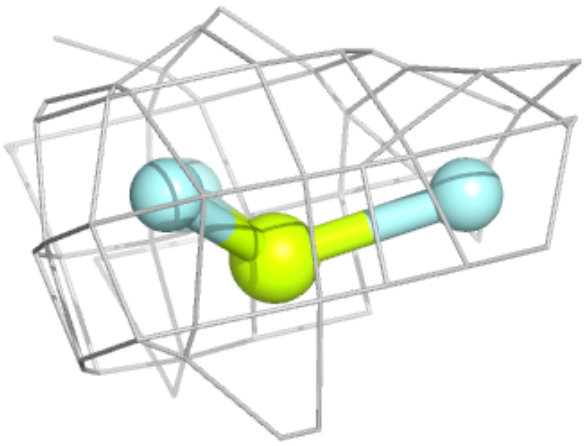


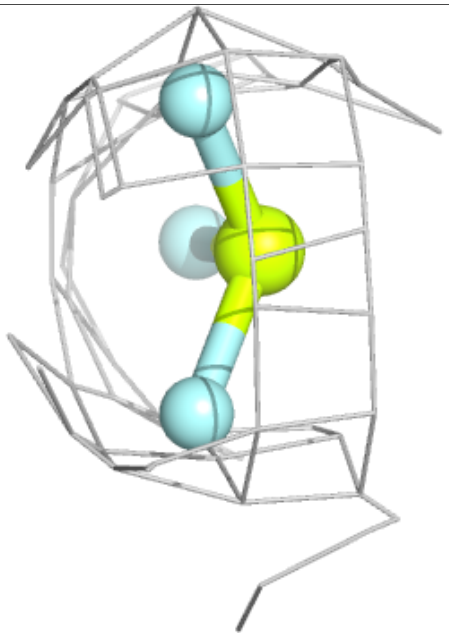


Electron density around BEF B 1001:

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

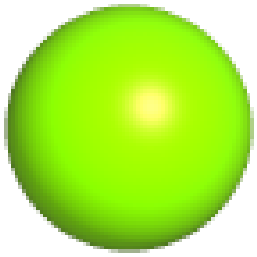


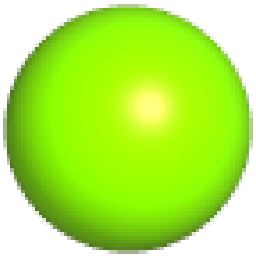


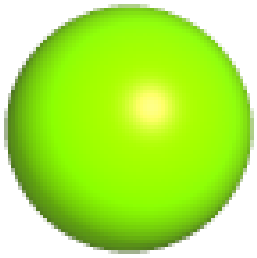


Electron density around MG D 1002:

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

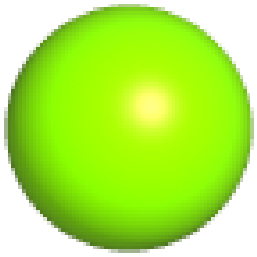


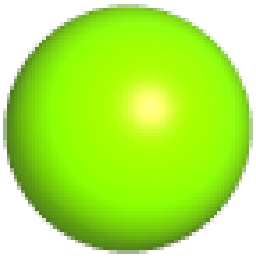


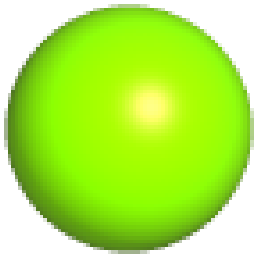


Electron density around MG B 1002:

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

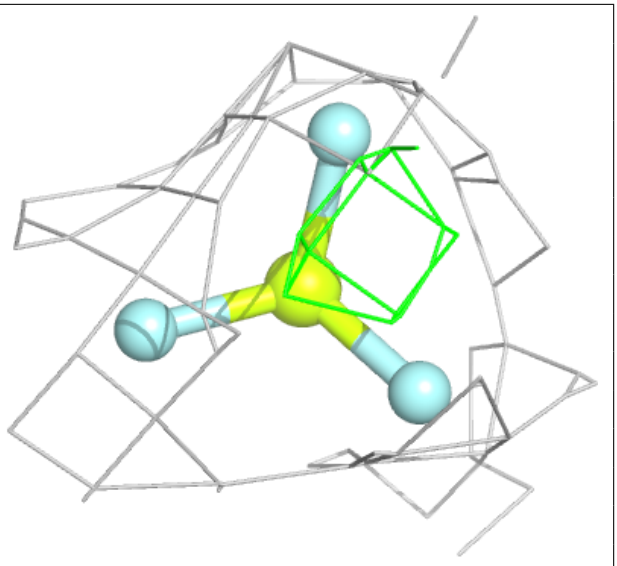


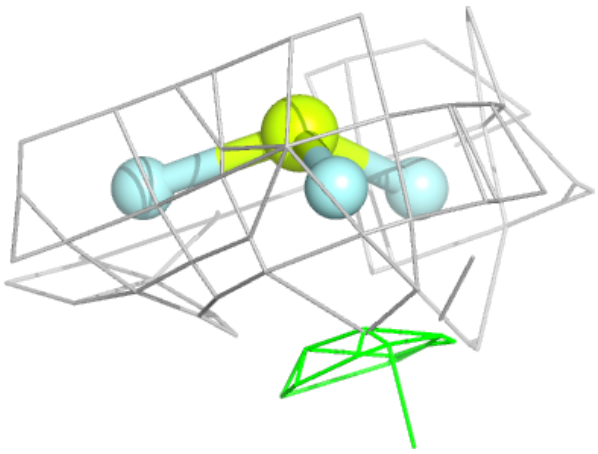


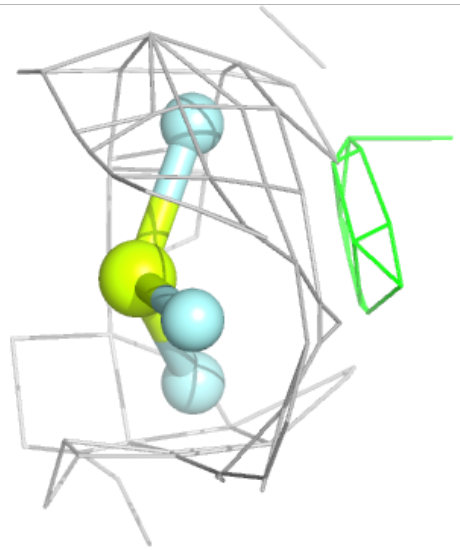


Electron density around BEF A 1001:

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

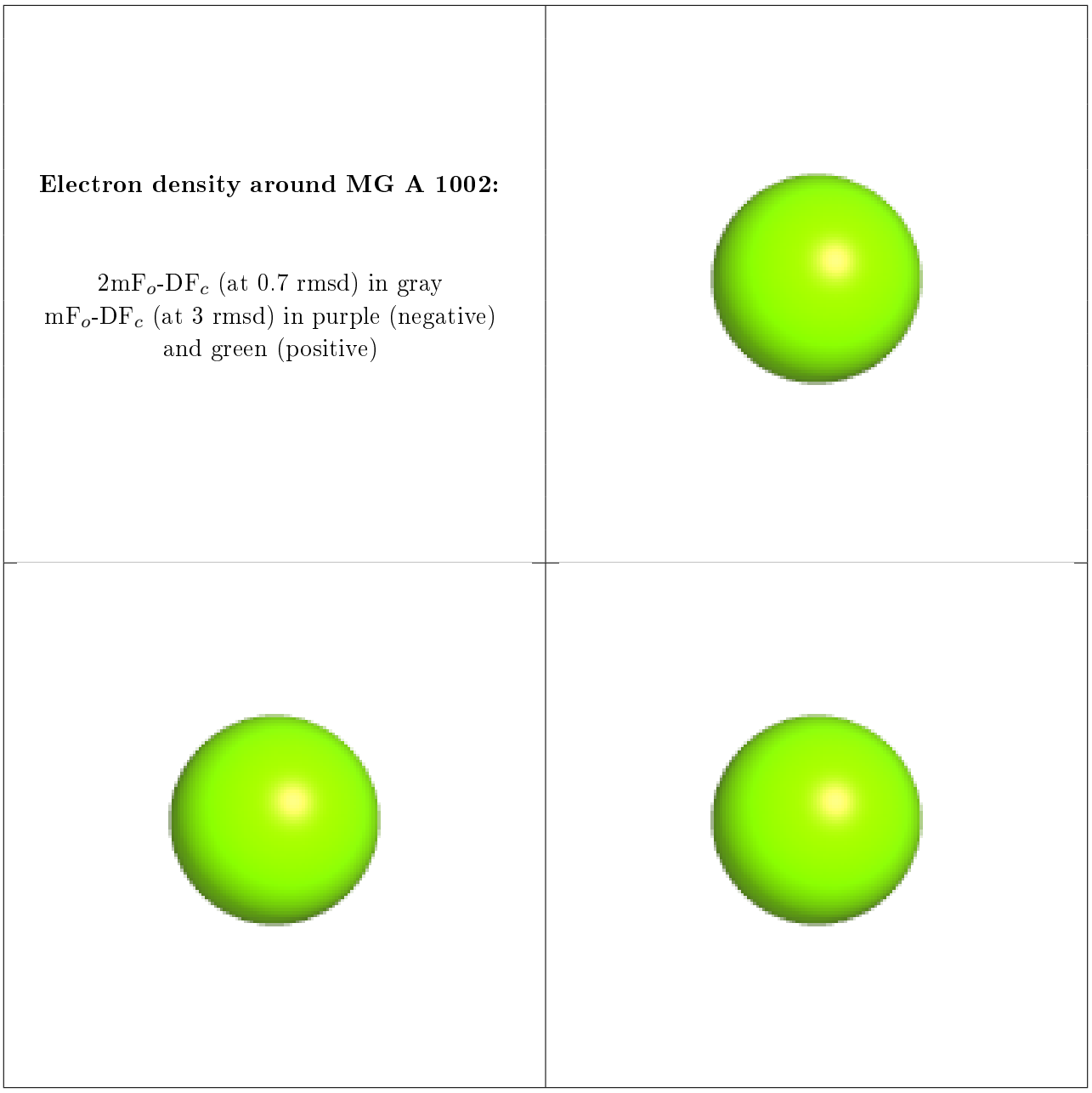






Electron density around MG A 1002:

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



6.5 Other polymers

There are no such residues in this entry.