



# Full wwPDB X-ray Structure Validation Report i

May 11, 2021 – 06:26 am BST

PDB ID : 6ZHH  
Title : Ca<sup>2+</sup>-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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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The following versions of software and data (see [references](#) i) 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

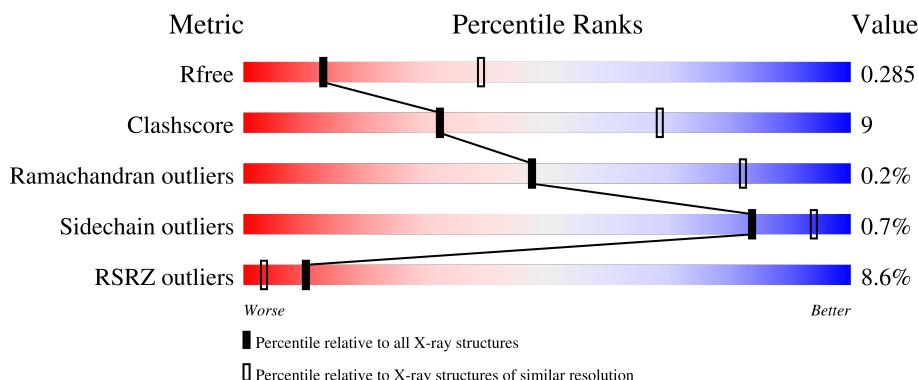
# 1 Overall quality at a glance

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.



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Mol	Chain	Length	Quality of chain		
1	F	911	8%	76%	20% .
1	G	911	9%	79%	17% .
1	H	911	18%	74%	21% ..

## 2 Entry composition (i)

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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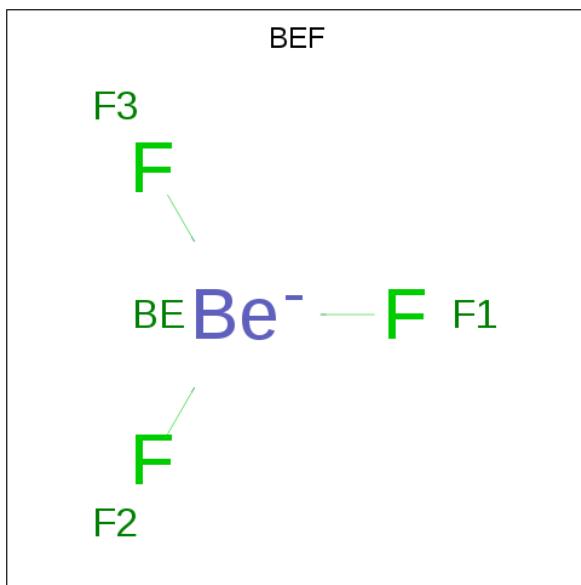
Chain	Residue	Modelled	Actual	Comment	Reference
F	896	GLU	-	expression tag	UNP A0A1C7PY84
F	897	HIS	-	expression tag	UNP A0A1C7PY84
F	898	HIS	-	expression tag	UNP A0A1C7PY84
F	899	HIS	-	expression tag	UNP A0A1C7PY84
F	900	HIS	-	expression tag	UNP A0A1C7PY84
F	901	HIS	-	expression tag	UNP A0A1C7PY84
F	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<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



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

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

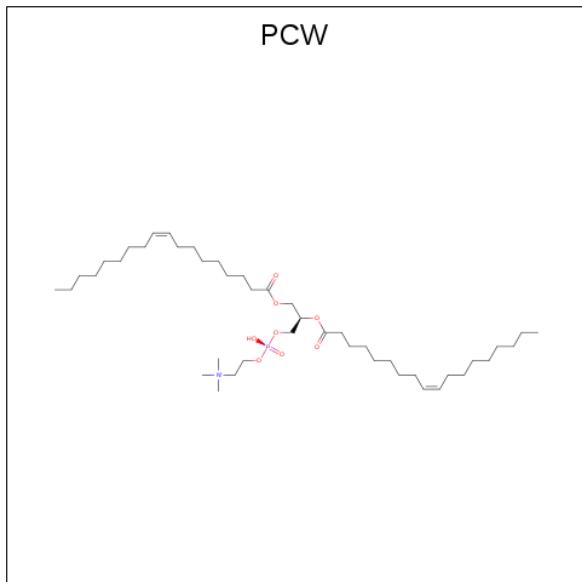
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

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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<sub>44</sub>H<sub>85</sub>NO<sub>8</sub>P).



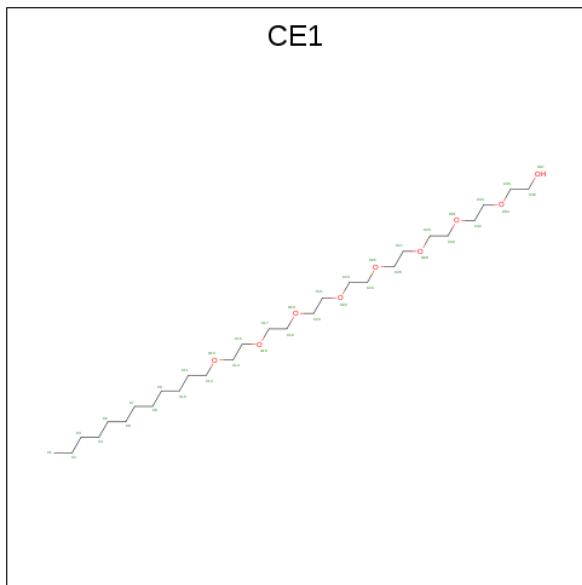
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	Total	C	N	O	P		
			54	44	1	8	1	0	0
4	A	1	Total	C	N	O	P		
			54	44	1	8	1	0	0
4	B	1	Total	C	N	O	P		
			54	44	1	8	1	0	0
4	B	1	Total	C	N	O	P		
			54	44	1	8	1	0	0
4	B	1	Total	C	N	O	P		
			54	44	1	8	1	0	0
4	B	1	Total	C	N	O	P		
			54	44	1	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<sub>28</sub>H<sub>58</sub>O<sub>9</sub>).



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

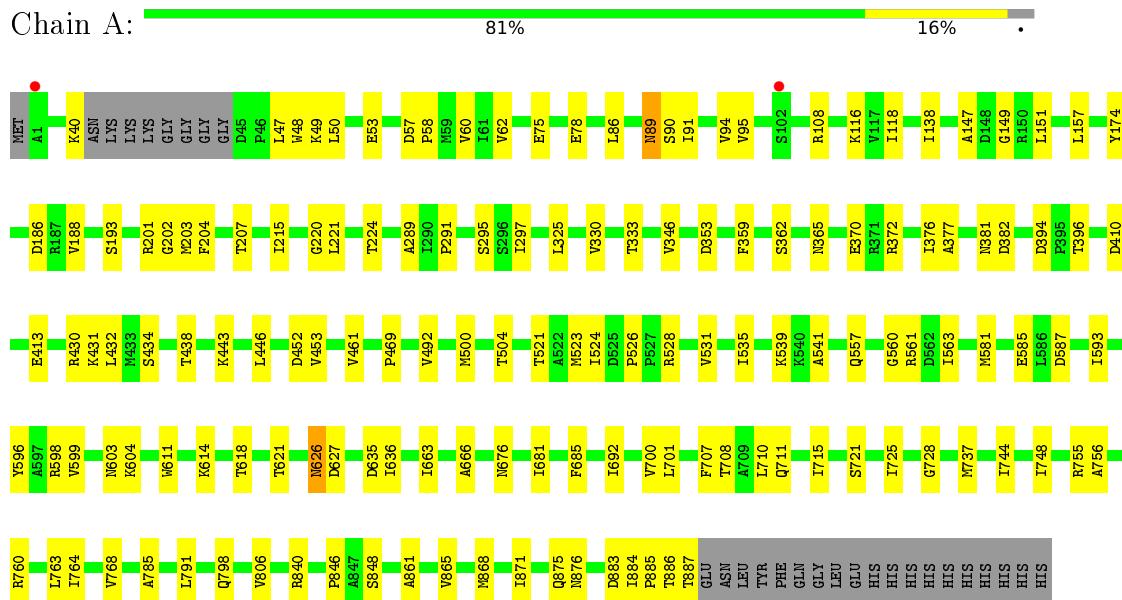
- Molecule 6 is water.

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

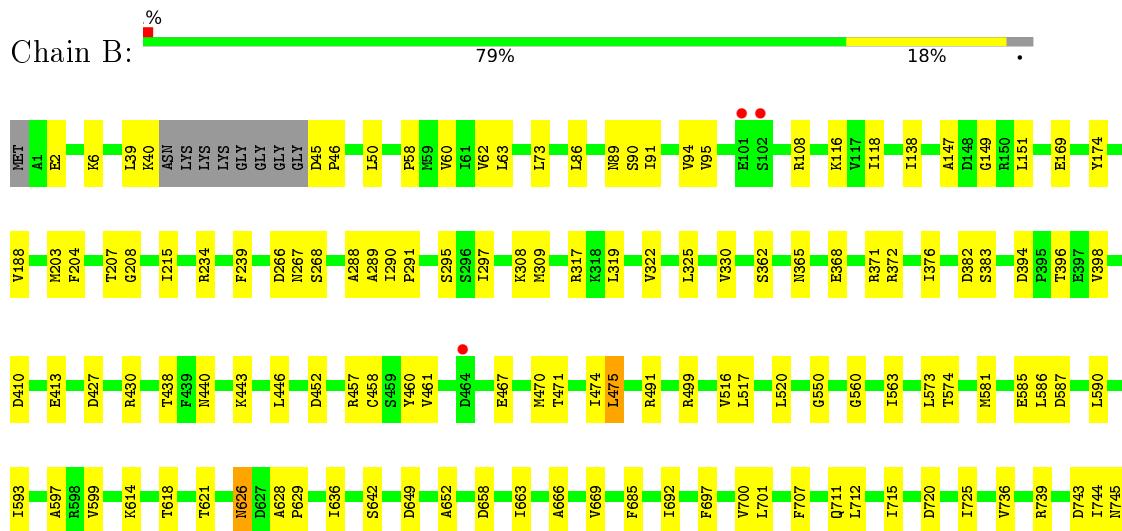
### 3 Residue-property plots [\(i\)](#)

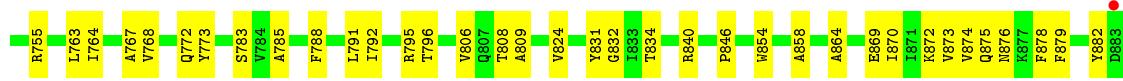
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

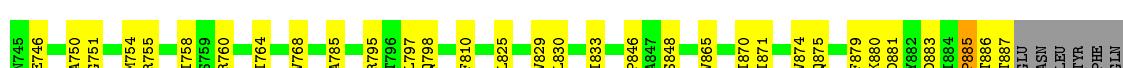
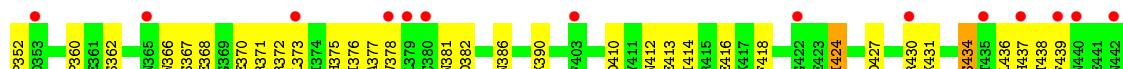
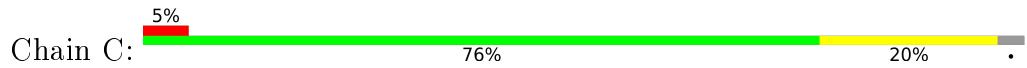


- Molecule 1: Calcium-transporting ATPase

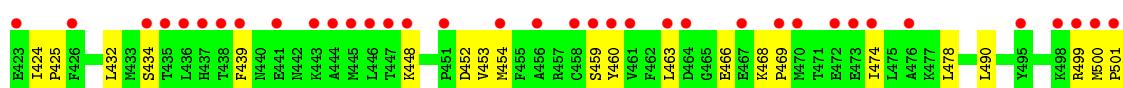
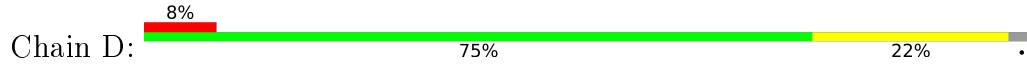


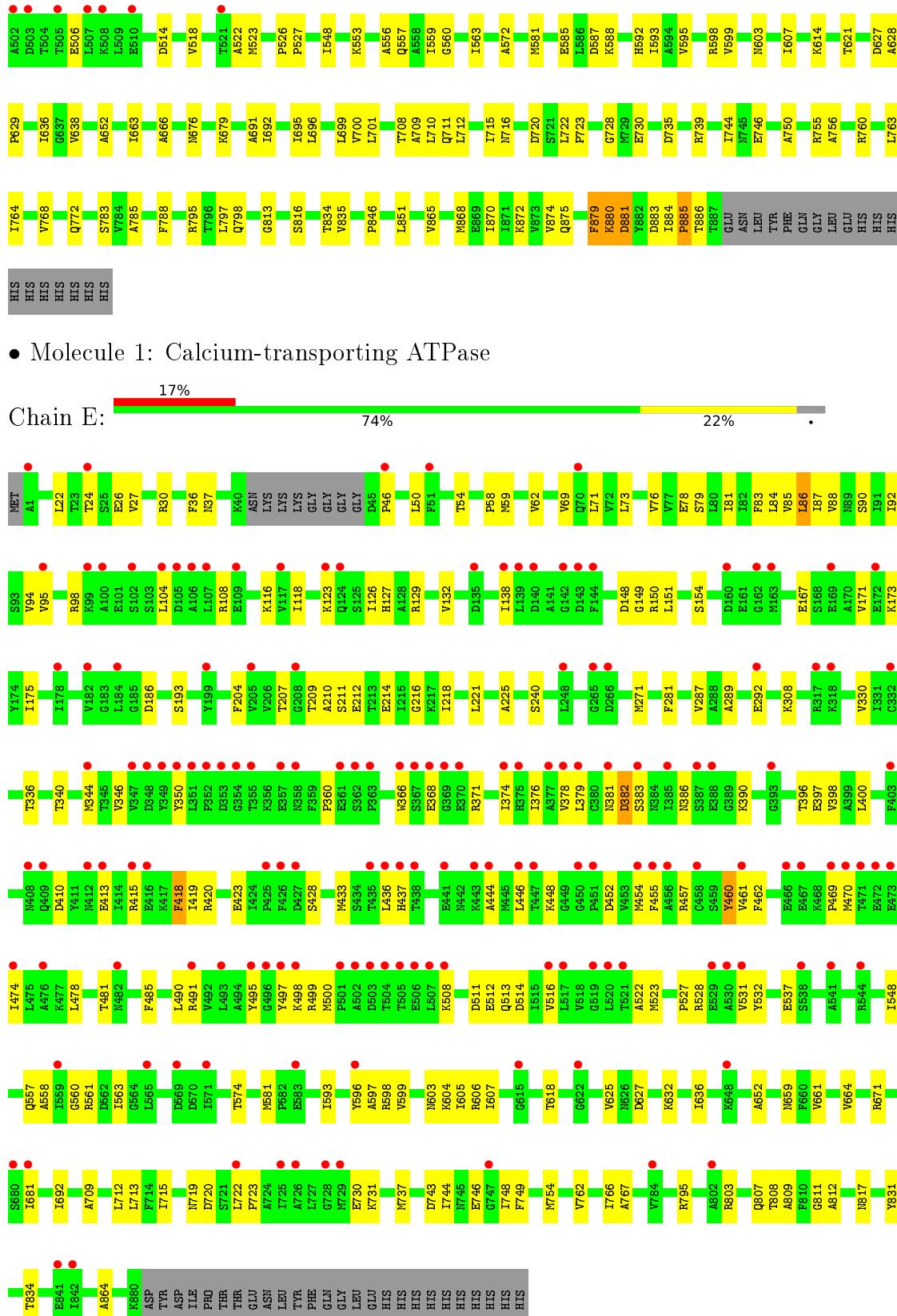


- Molecule 1: Calcium-transporting ATPase

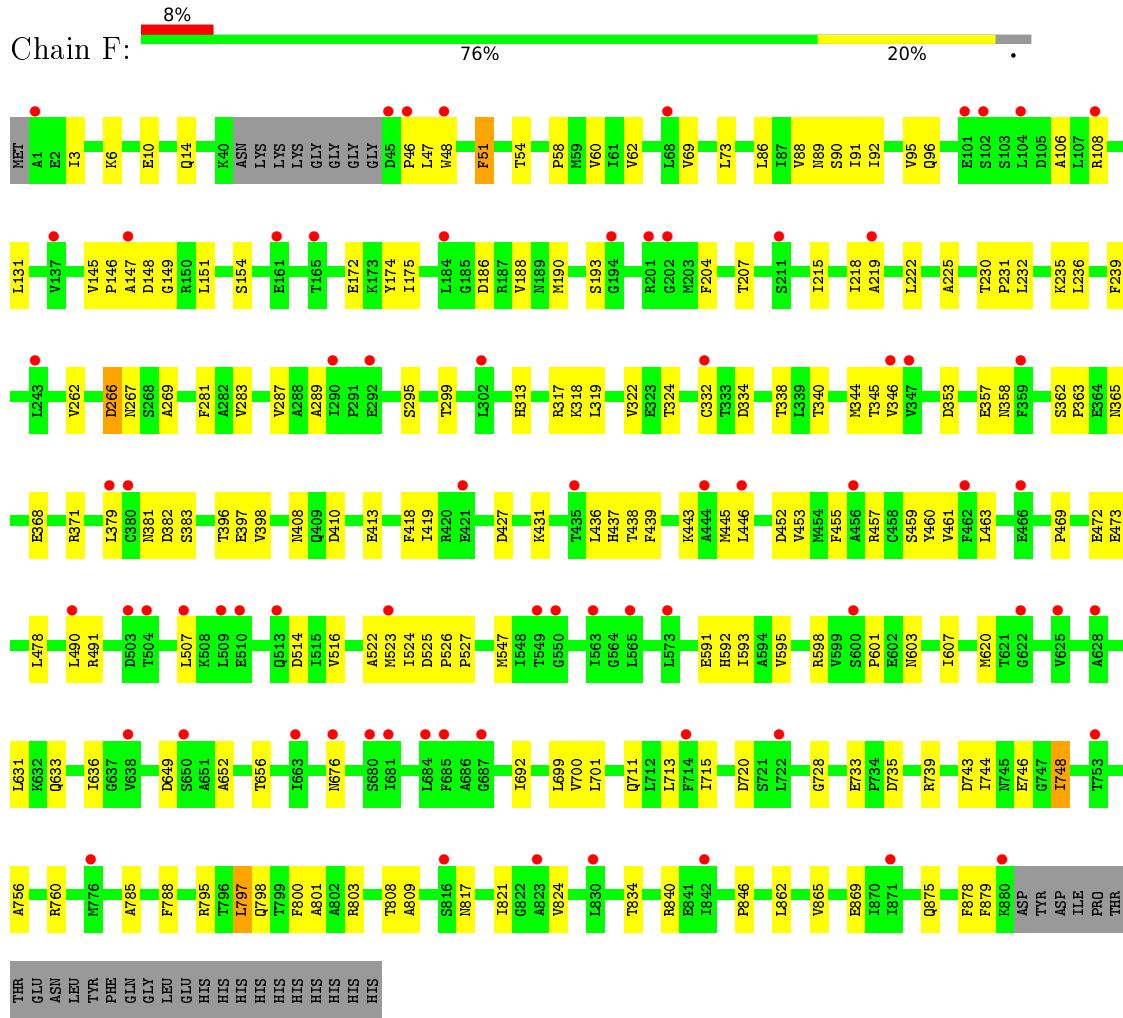


- Molecule 1: Calcium-transporting ATPase

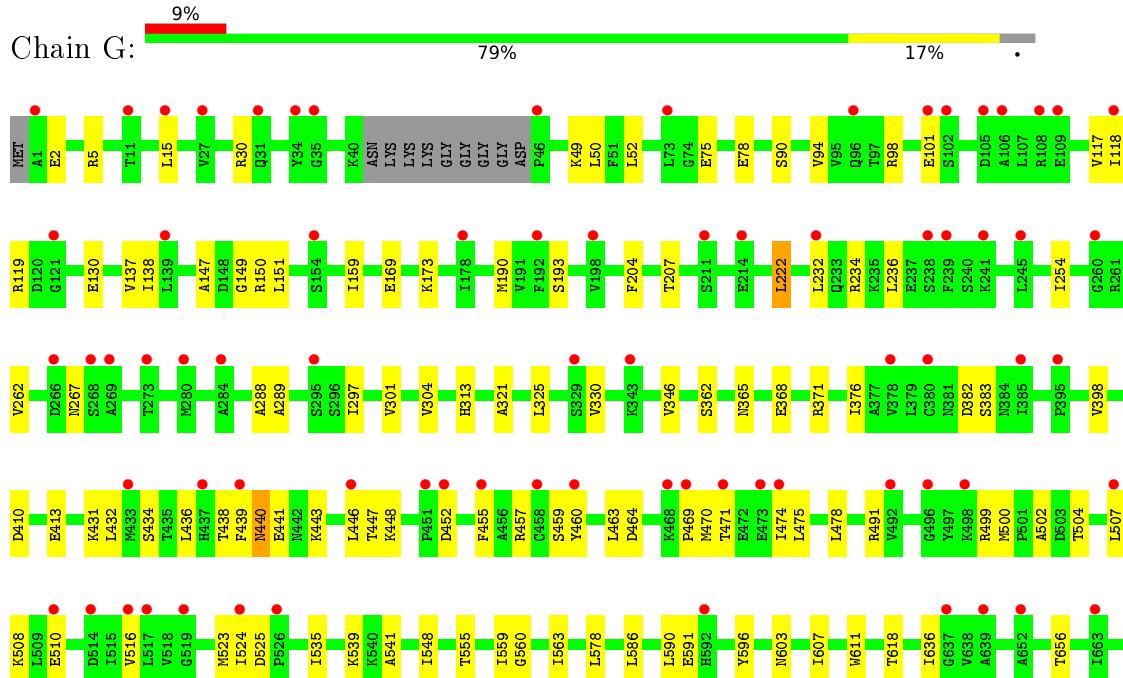


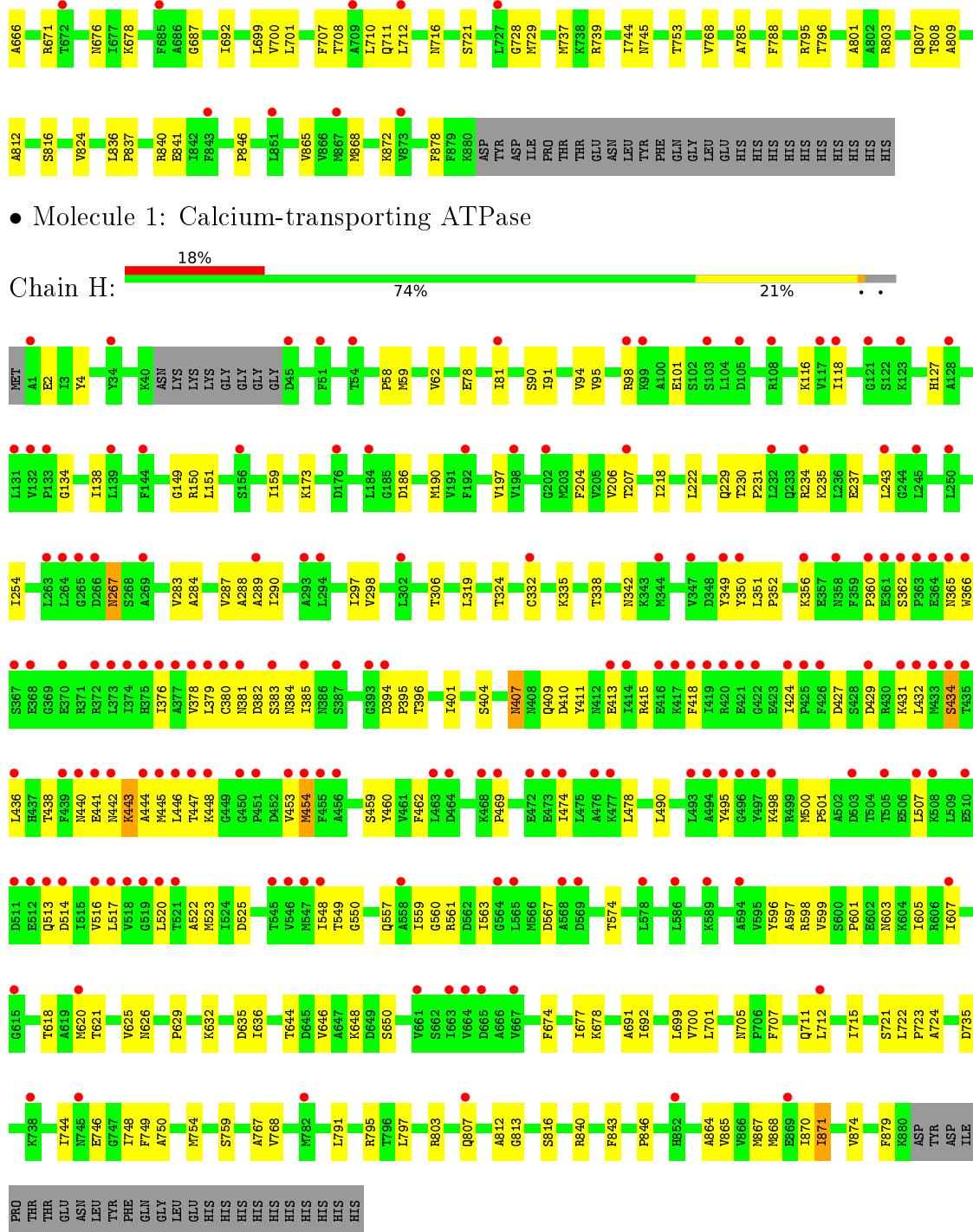


- Molecule 1: Calcium-transporting ATPase



- Molecule 1: Calcium-transporting ATPase





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.06 Å    188.50 Å    350.01 Å 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
$\langle I/\sigma(I) \rangle^1$	1.35 (at 3.01 Å)	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 <sup>2</sup> )	67.1	Xtriage
Anisotropy	0.274	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 60.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 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.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
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
1	G	222	LEU	CA-CB-CG	-5.35	102.99	115.30
1	C	222	LEU	CA-CB-CG	5.26	127.39	115.30
1	C	424	ILE	O-C-N	5.02	130.65	121.10

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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
1:H:149:GLY:HA2	1:H:207:THR:HG23	1.61	0.81
1:G:443:LYS:HG3	1:G:502:ALA:HA	1.64	0.80
1:G:149:GLY:HA2	1:G:207:THR:HG23	1.64	0.80
1:B:884:ILE:HD11	1:C:47:LEU:HB2	1.63	0.80
1:G:50:LEU:HD22	1:G:94:VAL:HG13	1.64	0.80
1:F:797:LEU:HD21	1:F:862:LEU:HA	1.64	0.80
1:F:149:GLY:HA2	1:F:207:THR:HG23	1.64	0.79
1:H:759:SER:HB3	1:H:871:ILE:HD13	1.63	0.79
1:F:368:GLU:OE2	1:F:371:ARG:NH1	2.14	0.78
1:F:410:ASP:HB3	1:F:413:GLU:HG3	1.66	0.78
1:E:743:ASP:HB3	1:E:746:GLU:HB2	1.64	0.78
1:F:108:ARG:HH22	1:F:219:ALA:HB2	1.48	0.78
1:B:875:GLN:HB3	1:B:885:PRO:HB3	1.66	0.77
1:A:755:ARG:HD3	1:A:885:PRO:HD3	1.63	0.77
1:C:424:ILE:HG13	1:C:507:LEU:HD11	1.66	0.77
1:E:382:ASP:OD1	1:E:420:ARG:NH1	2.16	0.77
1:A:47:LEU:HD23	1:A:49:LYS:H	1.51	0.76
1:E:54:THR:HG21	1:E:90:SER:HA	1.67	0.76
1:B:266:ASP:O	1:B:268:SER:N	2.18	0.75
1:D:851:LEU:HG	4:D:1003:PCW:H2	1.68	0.74
1:B:560:GLY:HA2	1:B:563:ILE:HG12	1.69	0.74
1:C:351:LEU:HD11	1:C:370:GLU:HG3	1.70	0.73
1:F:547:MET:HB3	1:F:595:VAL:HG12	1.70	0.73
1:F:266:ASP:OD1	1:F:266:ASP:N	2.21	0.73
1:E:330:VAL:HB	1:E:618:THR:HG22	1.70	0.73
1:D:6:LYS:NZ	1:D:14:GLN:OE1	2.22	0.73
1:H:803:ARG:NH1	1:H:813:GLY:O	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:471:THR:HA	1:G:475:LEU:HB3	1.70	0.72
1:F:733:GLU:OE2	1:F:739:ARG:NH1	2.21	0.72
1:E:149:GLY:HA2	1:E:207:THR:HG22	1.69	0.72
1:H:235:LYS:HB3	1:H:748:ILE:HG23	1.71	0.71
1:F:438:THR:HG22	1:F:443:LYS:HG3	1.71	0.71
1:C:163:MET:HE3	1:C:215:ILE:HD13	1.73	0.71
1:D:107:LEU:HD11	1:D:222:LEU:HD12	1.73	0.71
1:C:410:ASP:HB3	1:C:413:GLU:HG3	1.73	0.70
1:B:430:ARG:HD3	1:B:457:ARG:HH12	1.57	0.70
1:C:755:ARG:HD3	1:C:885:PRO:HG2	1.74	0.70
1:B:234:ARG:NH2	1:B:745:ASN:OD1	2.24	0.70
1:F:6:LYS:NZ	1:F:14:GLN:OE1	2.25	0.70
1:H:230:THR:O	1:H:234:ARG:HG3	1.92	0.70
1:C:47:LEU:HD21	1:C:98:ARG:HD2	1.74	0.69
1:H:711:GLN:NE2	1:H:843:PHE:O	2.24	0.69
1:D:151:LEU:HD23	1:D:204:PHE:HB3	1.74	0.69
1:H:490:LEU:HB3	1:H:522:ALA:HB1	1.73	0.69
1:D:70:GLN:NE2	1:D:75:GLU:OE2	2.23	0.69
1:D:360:PRO:HB2	1:D:366:TRP:CD1	2.27	0.69
1:B:317:ARG:HH22	1:B:649:ASP:HA	1.58	0.68
1:A:871:ILE:HG23	1:A:885:PRO:HB2	1.75	0.68
1:E:366:TRP:HZ3	1:E:374:ILE:HG13	1.59	0.68
1:C:880:LYS:H	1:C:885:PRO:HB3	1.58	0.68
1:D:711:GLN:O	1:D:715:ILE:HG13	1.94	0.68
1:H:498:LYS:HD3	1:H:514:ASP:O	1.94	0.68
1:B:587:ASP:O	1:B:614:LYS:NZ	2.28	0.67
1:H:91:ILE:HA	1:H:94:VAL:HG22	1.77	0.67
1:H:410:ASP:HB2	1:H:413:GLU:HG3	1.76	0.67
1:D:335:LYS:HD2	1:D:559:ILE:HD12	1.76	0.67
1:E:360:PRO:HB2	1:E:366:TRP:HE1	1.58	0.66
1:H:376:ILE:HA	1:H:446:LEU:HD23	1.78	0.66
1:B:151:LEU:HD23	1:B:204:PHE:HB3	1.77	0.66
1:D:557:GLN:HE21	1:D:572:ALA:H	1.43	0.66
1:C:459:SER:HB3	1:C:514:ASP:HA	1.77	0.66
1:F:427:ASP:HB2	1:F:431:LYS:HB2	1.76	0.66
1:A:151:LEU:HD23	1:A:204:PHE:HB3	1.78	0.66
1:C:241:LYS:HD3	4:C:1008:PCW:H61	1.78	0.66
1:E:604:LYS:NZ	1:E:627:ASP:OD1	2.29	0.65
1:D:490:LEU:HB3	1:D:522:ALA:HB1	1.76	0.65
1:C:58:PRO:O	1:C:62:VAL:HG23	1.95	0.65
1:D:879:PHE:O	1:D:885:PRO:HG2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:384:ASN:OD1	1:H:415:ARG:NH1	2.28	0.65
1:D:788:PHE:HE2	1:D:834:THR:HG21	1.60	0.65
1:E:88:VAL:O	1:E:92:ILE:HG13	1.97	0.65
1:G:700:VAL:HG23	1:G:701:LEU:HD12	1.79	0.65
1:C:70:GLN:HG3	1:C:75:GLU:HB2	1.80	0.64
1:E:95:VAL:HG11	1:F:878:PHE:HB3	1.79	0.64
1:C:879:PHE:HB3	1:C:885:PRO:HB3	1.79	0.64
1:D:865:VAL:HG22	1:D:868:MET:HE3	1.79	0.64
1:H:438:THR:HA	1:H:443:LYS:HA	1.78	0.64
1:B:149:GLY:HA2	1:B:207:THR:HG23	1.80	0.64
1:B:288:ALA:HB2	1:B:712:LEU:HD13	1.78	0.64
1:C:848:SER:HA	4:C:1003:PCW:H62	1.80	0.64
1:G:803:ARG:HH22	1:G:816:SER:HG	1.45	0.64
1:H:229:GLN:HG2	1:H:234:ARG:HG2	1.80	0.64
1:C:810:PHE:HE1	4:C:1006:PCW:H171	1.63	0.64
1:C:368:GLU:O	1:C:371:ARG:HG2	1.97	0.64
1:B:875:GLN:HB3	1:B:885:PRO:CB	2.28	0.64
1:E:218:ILE:HA	1:E:221:LEU:HD12	1.79	0.64
1:C:711:GLN:O	1:C:715:ILE:HG13	1.98	0.64
1:C:755:ARG:HH11	1:C:885:PRO:CG	2.10	0.64
1:D:746:GLU:HG2	1:D:750:ALA:HB3	1.80	0.64
4:C:1005:PCW:H172	1:D:253:LEU:HD21	1.79	0.63
1:E:457:ARG:HD3	1:E:512:GLU:O	1.99	0.63
1:C:360:PRO:HB2	1:C:366:TRP:HE3	1.63	0.63
1:B:755:ARG:NE	1:B:884:ILE:HG22	2.14	0.63
1:C:378:VAL:HG21	1:C:414:ILE:HD12	1.80	0.63
1:D:84:LEU:HD22	5:D:1005:CE1:H81	1.81	0.63
1:D:788:PHE:CE2	1:D:834:THR:HG21	2.33	0.63
1:F:219:ALA:HA	1:F:222:LEU:HD12	1.81	0.62
1:F:797:LEU:HG	1:F:865:VAL:HG21	1.80	0.62
1:B:460:TYR:HB2	1:B:516:VAL:HG22	1.79	0.62
1:B:773:TYR:HE1	4:B:1007:PCW:H42	1.63	0.62
1:D:368:GLU:OE2	1:D:371:ARG:NH1	2.32	0.62
1:E:548:ILE:HG22	1:E:599:VAL:HG21	1.81	0.62
1:G:169:GLU:OE1	1:G:491:ARG:NH2	2.32	0.62
1:D:352:PRO:HB2	1:D:463:LEU:HD12	1.81	0.62
1:E:581:MET:O	1:E:606:ARG:NH2	2.30	0.62
1:G:711:GLN:N	1:G:711:GLN:OE1	2.32	0.62
1:F:106:ALA:HB1	1:F:222:LEU:HD13	1.81	0.61
1:H:459:SER:HA	1:H:469:PRO:HG3	1.80	0.61
1:C:118:ILE:HG13	1:C:138:ILE:HD11	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:GLU:O	1:C:110:MET:HG2	2.01	0.61
1:H:432:LEU:HD11	1:H:453:VAL:HG13	1.82	0.61
4:C:1008:PCW:H262	1:D:870:ILE:HG21	1.82	0.61
1:A:410:ASP:HB3	1:A:413:GLU:HG3	1.82	0.61
1:E:410:ASP:HB3	1:E:413:GLU:HG2	1.82	0.61
4:C:1008:PCW:H322	4:C:1008:PCW:H121	1.81	0.61
1:D:91:ILE:O	1:D:95:VAL:HG23	2.00	0.61
1:D:379:LEU:HD13	1:D:439:PHE:HZ	1.66	0.61
1:B:89:ASN:OD1	1:B:295:SER:OG	2.18	0.60
1:C:158:LYS:HE2	1:C:172:GLU:HG2	1.83	0.60
1:H:284:ALA:HB2	1:H:705:ASN:HD21	1.66	0.60
1:H:380:CYS:O	1:H:448:LYS:NZ	2.34	0.60
1:H:711:GLN:O	1:H:715:ILE:HG13	2.01	0.60
1:C:875:GLN:HA	1:C:879:PHE:HD2	1.66	0.60
1:D:163:MET:HE3	1:D:215:ILE:HD13	1.82	0.60
1:H:383:SER:O	1:H:415:ARG:NH2	2.34	0.60
1:H:459:SER:HB2	1:H:514:ASP:HA	1.83	0.60
1:E:346:VAL:HA	1:E:523:MET:HA	1.83	0.60
1:H:222:LEU:HD11	1:H:629:PRO:HG3	1.83	0.60
1:E:83:PHE:HD1	1:E:86:LEU:HD12	1.66	0.60
1:E:460:TYR:CE2	1:E:516:VAL:HG22	2.37	0.60
1:B:309:MET:HE3	1:B:669:VAL:HG21	1.84	0.60
1:A:560:GLY:HA2	1:A:563:ILE:HG12	1.81	0.60
1:A:806:VAL:HG12	1:A:876:ASN:HD21	1.67	0.60
1:B:58:PRO:O	1:B:62:VAL:HG23	2.01	0.60
1:B:60:VAL:HG13	1:B:86:LEU:HD22	1.84	0.60
1:E:460:TYR:HA	1:E:469:PRO:HD3	1.82	0.60
1:E:537:GLU:HB3	1:E:664:VAL:HG11	1.84	0.60
1:G:460:TYR:HB2	1:G:516:VAL:HG22	1.84	0.60
1:C:349:TYR:HE1	1:C:351:LEU:HB3	1.67	0.60
1:G:118:ILE:HG13	1:G:138:ILE:HD11	1.83	0.60
1:H:118:ILE:HG13	1:H:138:ILE:HD11	1.83	0.60
1:B:736:VAL:HG23	1:B:739:ARG:NH2	2.17	0.60
1:F:743:ASP:HB3	1:F:746:GLU:HB2	1.83	0.59
1:D:755:ARG:NH1	1:D:875:GLN:HB3	2.17	0.59
1:B:289:ALA:HB2	1:B:692:ILE:HD11	1.82	0.59
1:D:879:PHE:HB3	1:D:885:PRO:HB2	1.83	0.59
1:A:604:LYS:NZ	1:A:627:ASP:OD1	2.30	0.59
1:F:788:PHE:HE2	1:F:834:THR:HG21	1.67	0.59
1:H:222:LEU:O	1:H:632:LYS:NZ	2.34	0.59
1:D:560:GLY:HA2	1:D:563:ILE:HG12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:593:ILE:HD11	1:E:596:TYR:CZ	2.36	0.59
1:H:427:ASP:HB3	1:H:431:LYS:HG2	1.84	0.59
1:B:878:PHE:HB3	1:C:95:VAL:HG11	1.84	0.59
1:C:720:ASP:OD2	1:C:795:ARG:HD3	2.03	0.59
1:E:58:PRO:O	1:E:62:VAL:HG23	2.03	0.59
1:F:262:VAL:HG23	1:F:269:ALA:HB3	1.84	0.59
1:G:151:LEU:HD23	1:G:204:PHE:HB3	1.85	0.59
1:C:460:TYR:HD2	1:C:466:GLU:HB3	1.66	0.58
1:B:626:ASN:OD1	1:B:626:ASN:N	2.34	0.58
1:B:755:ARG:CZ	1:B:884:ILE:HG22	2.33	0.58
1:B:840:ARG:NH2	4:B:1003:PCW:O31	2.36	0.58
1:C:438:THR:HB	1:C:443:LYS:HG2	1.85	0.58
1:C:880:LYS:HB3	1:C:885:PRO:HG3	1.85	0.58
1:D:886:THR:HA	5:D:1006:CE1:H51	1.84	0.58
1:C:151:LEU:HD23	1:C:204:PHE:HB3	1.86	0.58
1:F:340:THR:HA	1:F:527:PRO:HA	1.85	0.58
1:B:438:THR:HB	1:B:443:LYS:HD3	1.85	0.58
1:D:85:VAL:HG12	5:D:1005:CE1:H112	1.86	0.58
1:G:878:PHE:HB3	1:H:95:VAL:HG12	1.86	0.58
1:A:875:GLN:HB2	1:A:885:PRO:CB	2.32	0.58
1:B:581:MET:HE3	1:B:585:GLU:HG2	1.86	0.58
1:C:755:ARG:HH11	1:C:885:PRO:HG2	1.69	0.58
1:H:459:SER:O	1:H:469:PRO:HD3	2.04	0.58
1:H:360:PRO:O	1:H:407:ASN:ND2	2.34	0.58
1:H:289:ALA:HB2	1:H:692:ILE:HD11	1.86	0.57
1:C:879:PHE:HB3	1:C:885:PRO:CB	2.33	0.57
1:A:376:ILE:HG12	1:A:446:LEU:HG	1.86	0.57
1:A:848:SER:HA	4:A:1003:PCW:H61	1.86	0.57
1:B:884:ILE:HD11	1:C:47:LEU:CB	2.34	0.57
1:H:222:LEU:CD1	1:H:629:PRO:HG3	2.33	0.57
1:D:58:PRO:O	1:D:62:VAL:HG23	2.04	0.57
1:D:700:VAL:HG23	1:D:701:LEU:HD12	1.86	0.57
1:F:379:LEU:HD13	1:F:437:HIS:NE2	2.19	0.57
1:G:362:SER:HB3	1:G:365:ASN:HB2	1.86	0.57
1:C:53:GLU:HG2	1:C:56:LYS:HE3	1.87	0.57
1:D:708:THR:HG22	1:D:710:LEU:H	1.68	0.57
1:C:427:ASP:HB2	1:C:431:LYS:HB2	1.86	0.57
1:F:108:ARG:HH21	1:F:215:ILE:HG12	1.69	0.57
1:G:234:ARG:NH2	1:G:745:ASN:OD1	2.36	0.57
1:G:368:GLU:OE2	1:G:371:ARG:NH1	2.38	0.57
1:A:708:THR:HG22	1:A:710:LEU:H	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:186:ASP:OD1	1:E:598:ARG:NH2	2.37	0.57
1:F:875:GLN:HA	1:F:879:PHE:HD2	1.70	0.57
1:H:306:THR:HG21	1:H:319:LEU:HD12	1.87	0.57
1:E:366:TRP:CZ3	1:E:374:ILE:HG13	2.40	0.56
1:F:436:LEU:HD21	1:F:443:LYS:HE2	1.87	0.56
1:G:678:LYS:NZ	1:G:753:THR:OG1	2.38	0.56
1:B:108:ARG:HH21	1:B:215:ILE:HD11	1.69	0.56
1:G:807:GLN:HB3	1:G:812:ALA:HB2	1.86	0.56
1:A:330:VAL:HB	1:A:618:THR:HG22	1.87	0.56
1:E:498:LYS:HE3	1:E:500:MET:SD	2.44	0.56
1:E:560:GLY:HA2	1:E:563:ILE:HG12	1.86	0.56
1:F:151:LEU:HD23	1:F:204:PHE:HB3	1.87	0.56
1:H:797:LEU:HB2	1:H:865:VAL:HG21	1.87	0.56
1:D:581:MET:HE3	1:D:585:GLU:HG2	1.87	0.56
1:F:445:MET:SD	1:F:507:LEU:HD22	2.45	0.56
1:D:798:GLN:O	1:D:798:GLN:HG2	2.05	0.56
1:G:611:TRP:HB3	1:G:618:THR:HG21	1.86	0.56
1:H:298:VAL:HG13	1:H:677:ILE:HD13	1.87	0.56
1:A:461:VAL:HG23	1:A:469:PRO:HB3	1.87	0.56
1:D:466:GLU:OE1	1:D:499:ARG:NE	2.34	0.56
1:B:720:ASP:OD2	1:B:795:ARG:NE	2.37	0.56
1:H:218:ILE:O	1:H:222:LEU:HD13	2.06	0.56
1:H:438:THR:OG1	1:H:443:LYS:HG2	2.06	0.56
1:C:366:TRP:NE1	1:C:371:ARG:HB3	2.17	0.56
1:F:381:ASN:HB2	1:F:397:GLU:HB3	1.87	0.56
1:F:317:ARG:HH22	1:F:649:ASP:HA	1.71	0.55
1:A:362:SER:HB3	1:A:365:ASN:HB2	1.88	0.55
1:C:288:ALA:HB2	1:C:712:LEU:HD13	1.88	0.55
1:D:99:LYS:NZ	1:D:318:LYS:HB3	2.21	0.55
1:D:379:LEU:HD13	1:D:439:PHE:CZ	2.42	0.55
1:H:94:VAL:HB	1:H:98:ARG:HH11	1.71	0.55
4:B:1007:PCW:H241	4:B:1008:PCW:H421	1.89	0.55
1:F:295:SER:O	1:F:299:THR:OG1	2.25	0.55
1:B:832:GLY:HA3	4:B:1003:PCW:H162	1.88	0.55
1:E:360:PRO:HB2	1:E:366:TRP:NE1	2.21	0.55
1:G:840:ARG:HG3	1:G:841:GLU:H	1.71	0.55
1:H:871:ILE:HA	1:H:874:VAL:HG22	1.87	0.55
1:D:53:GLU:HG2	1:D:56:LYS:HE3	1.88	0.55
1:C:744:ILE:HD12	1:C:744:ILE:H	1.70	0.55
1:E:287:VAL:HG11	1:E:713:LEU:HD22	1.88	0.55
1:B:878:PHE:CZ	4:B:1009:PCW:H121	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:366:TRP:HD1	1:C:367:SER:O	1.89	0.55
1:A:174:TYR:HD2	1:A:188:VAL:HG11	1.71	0.55
1:D:182:VAL:HG12	1:D:186:ASP:HB2	1.88	0.55
1:D:254:ILE:HG12	1:D:699:LEU:HD22	1.89	0.55
1:G:383:SER:HB2	1:G:398:VAL:HG22	1.89	0.55
1:C:436:LEU:HD13	1:C:507:LEU:HD12	1.88	0.55
1:C:535:ILE:HD12	1:C:545:THR:HG21	1.89	0.55
1:F:490:LEU:HB3	1:F:522:ALA:HB1	1.89	0.55
1:A:557:GLN:O	1:A:561:ARG:HB2	2.07	0.54
1:B:884:ILE:CD1	1:C:47:LEU:HB2	2.37	0.54
1:E:730:GLU:OE2	1:E:731:LYS:NZ	2.40	0.54
1:C:453:VAL:HB	1:C:457:ARG:HH22	1.70	0.54
1:H:574:THR:HA	1:H:597:ALA:O	2.06	0.54
1:B:362:SER:HB3	1:B:365:ASN:HB2	1.90	0.54
1:C:149:GLY:HA2	1:C:207:THR:HG23	1.87	0.54
1:C:886:THR:HG22	1:C:887:THR:HG22	1.88	0.54
1:E:24:THR:O	1:E:27:VAL:HG12	2.08	0.54
1:A:581:MET:HE3	1:A:585:GLU:HG2	1.88	0.54
1:G:801:ALA:O	1:G:872:LYS:NZ	2.40	0.54
1:C:46:PRO:HB2	1:C:48:TRP:CD1	2.43	0.54
1:C:368:GLU:HG3	1:C:371:ARG:HD3	1.90	0.54
1:E:368:GLU:OE2	1:E:371:ARG:NH2	2.40	0.54
1:A:325:LEU:HG	1:A:636:ILE:HG12	1.90	0.54
1:D:118:ILE:HG13	1:D:138:ILE:HD11	1.90	0.54
1:E:346:VAL:HG22	1:E:523:MET:HB3	1.89	0.54
1:A:325:LEU:HD13	1:A:666:ALA:HB1	1.90	0.54
1:C:883:ASP:O	1:C:885:PRO:HD3	2.07	0.54
1:D:744:ILE:HD12	1:D:744:ILE:H	1.72	0.54
1:D:755:ARG:HB2	5:D:1006:CE1:HG2	1.90	0.54
1:D:772:GLN:HG2	1:D:783:SER:HB2	1.89	0.54
4:B:1009:PCW:HG1	1:C:296:SER:OG	2.08	0.54
1:B:621:THR:HG21	1:B:663:ILE:HD13	1.90	0.54
1:A:291:PRO:HG3	1:A:685:PHE:CE2	2.42	0.53
1:G:591:GLU:OE1	1:H:127:HIS:NE2	2.31	0.53
1:C:460:TYR:CD2	1:C:466:GLU:HB3	2.43	0.53
1:D:500:MET:HG3	1:D:501:PRO:HD2	1.89	0.53
1:G:78:GLU:HB3	1:G:710:LEU:HD13	1.90	0.53
1:H:707:PHE:HZ	1:H:768:VAL:HG11	1.72	0.53
1:A:587:ASP:O	1:A:614:LYS:NZ	2.40	0.53
1:G:463:LEU:HG	1:G:464:ASP:H	1.73	0.53
1:D:378:VAL:O	1:D:381:ASN:ND2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:147:ALA:HA	1:G:193:SER:HB2	1.91	0.53
1:E:433:MET:SD	1:E:448:LYS:NZ	2.66	0.53
1:A:700:VAL:HG23	1:A:701:LEU:HD12	1.91	0.53
1:B:831:TYR:O	1:B:834:THR:OG1	2.26	0.53
1:E:85:VAL:HG11	1:E:292:GLU:HB3	1.91	0.53
1:F:711:GLN:O	1:F:715:ILE:HG13	2.07	0.53
1:H:436:LEU:HD22	1:H:507:LEU:HD21	1.91	0.53
1:F:289:ALA:HB2	1:F:692:ILE:HD11	1.90	0.53
4:B:1008:PCW:H321	4:B:1008:PCW:O11	2.09	0.53
1:E:557:GLN:HB3	1:E:561:ARG:HH11	1.73	0.53
1:F:427:ASP:HB2	1:F:431:LYS:CB	2.38	0.53
1:G:288:ALA:HB2	1:G:712:LEU:HD13	1.91	0.53
1:B:430:ARG:CD	1:B:457:ARG:HH12	2.20	0.53
1:E:148:ASP:OD1	1:E:193:SER:N	2.37	0.53
1:E:470:MET:H	1:E:474:ILE:HD12	1.73	0.53
1:F:809:ALA:HB2	1:F:869:GLU:HB3	1.91	0.53
1:G:459:SER:O	1:G:469:PRO:HD3	2.09	0.53
1:B:467:GLU:OE2	1:B:499:ARG:NE	2.35	0.52
1:E:381:ASN:HB2	1:E:397:GLU:HB3	1.90	0.52
1:C:755:ARG:HH11	1:C:885:PRO:HG3	1.74	0.52
1:E:485:PHE:HB3	1:E:490:LEU:HB2	1.91	0.52
1:F:345:THR:HB	1:F:526:PRO:HG3	1.91	0.52
1:H:870:ILE:O	1:H:874:VAL:HG13	2.09	0.52
1:A:90:SER:O	1:A:94:VAL:HG23	2.09	0.52
1:B:430:ARG:HD3	1:B:457:ARG:HH22	1.75	0.52
1:C:754:MET:O	1:C:758:ILE:HG13	2.09	0.52
1:E:490:LEU:HD13	1:E:522:ALA:HB1	1.91	0.52
1:F:459:SER:HB2	1:F:514:ASP:HA	1.91	0.52
1:A:528:ARG:HB2	1:A:531:VAL:HG23	1.91	0.52
1:C:797:LEU:HB2	1:C:865:VAL:HG21	1.92	0.52
1:E:603:ASN:O	1:E:607:ILE:HG12	2.09	0.52
1:H:288:ALA:HB2	1:H:712:LEU:HD13	1.92	0.52
1:B:636:ILE:HD12	1:B:652:ALA:HB3	1.92	0.52
1:B:697:PHE:CE1	1:B:701:LEU:HD22	2.44	0.52
1:E:151:LEU:HD23	1:E:204:PHE:HB3	1.91	0.52
1:E:803:ARG:HD2	1:E:817:ASN:OD1	2.09	0.52
1:E:446:LEU:HA	1:E:497:TYR:HA	1.91	0.52
1:E:803:ARG:HH21	1:E:809:ALA:HA	1.75	0.52
1:D:75:GLU:HB3	1:D:78:GLU:CG	2.40	0.52
1:D:676:ASN:HB3	1:D:728:GLY:HA2	1.91	0.52
1:H:549:THR:OG1	2:H:1001:BEF:F2	2.04	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:438:THR:O	1:C:439:PHE:HD1	1.93	0.52
1:D:432:LEU:HD11	1:D:453:VAL:HG23	1.91	0.52
1:G:803:ARG:NH2	1:G:816:SER:OG	2.35	0.52
1:D:289:ALA:HB2	1:D:692:ILE:HD11	1.92	0.52
1:D:679:LYS:HE2	1:D:730:GLU:HG2	1.92	0.52
1:E:720:ASP:OD2	1:E:795:ARG:HD3	2.10	0.52
1:H:297:ILE:HD11	1:H:721:SER:HA	1.92	0.52
1:A:60:VAL:HG13	1:A:86:LEU:HD22	1.92	0.51
1:A:431:LYS:H	1:A:431:LYS:HD2	1.75	0.51
1:D:553:LYS:H	1:D:553:LYS:HD2	1.74	0.51
1:E:452:ASP:OD1	1:E:452:ASP:N	2.43	0.51
1:C:346:VAL:HA	1:C:523:MET:HA	1.92	0.51
1:F:362:SER:HB3	1:F:365:ASN:HB2	1.93	0.51
1:G:325:LEU:HD13	1:G:666:ALA:HB1	1.93	0.51
1:H:474:ILE:O	1:H:478:LEU:HD13	2.10	0.51
1:D:346:VAL:HG21	1:D:400:LEU:HD23	1.92	0.51
1:E:118:ILE:HG12	1:E:123:LYS:HG2	1.90	0.51
1:G:289:ALA:HB2	1:G:692:ILE:HD11	1.91	0.51
1:B:872:LYS:HA	1:B:875:GLN:HE21	1.76	0.51
1:C:321:ALA:HB1	1:C:636:ILE:HD12	1.93	0.51
1:H:767:ALA:HB2	1:H:864:ALA:HB2	1.91	0.51
1:D:246:GLY:HA3	5:D:1008:CE1:H21	1.92	0.51
1:E:383:SER:HB2	1:E:398:VAL:HG22	1.92	0.51
1:F:418:PHE:HB3	1:F:437:HIS:CE1	2.45	0.51
1:G:90:SER:O	1:G:94:VAL:HG23	2.11	0.51
1:A:755:ARG:HD3	1:A:884:ILE:HA	1.92	0.51
1:B:452:ASP:OD1	1:B:452:ASP:N	2.44	0.51
1:G:785:ALA:HB2	1:G:846:PRO:HD2	1.93	0.51
1:C:452:ASP:N	1:C:452:ASP:OD1	2.43	0.51
1:D:346:VAL:HA	1:D:523:MET:HA	1.92	0.51
1:F:379:LEU:HD13	1:F:437:HIS:HE2	1.74	0.51
1:G:2:GLU:HB3	1:G:5:ARG:HB2	1.93	0.51
1:A:58:PRO:O	1:A:62:VAL:HG23	2.11	0.51
1:B:711:GLN:O	1:B:715:ILE:HG13	2.10	0.51
1:D:182:VAL:CG1	1:D:186:ASP:HB2	2.41	0.51
1:G:470:MET:HB3	1:G:474:ILE:HB	1.93	0.51
1:H:700:VAL:HG23	1:H:701:LEU:HD12	1.92	0.51
1:F:154:SER:HB3	1:F:175:ILE:HG23	1.93	0.50
1:A:621:THR:HG21	1:A:663:ILE:HD13	1.92	0.50
1:B:45:ASP:N	1:B:46:PRO:HD2	2.27	0.50
1:F:344:MET:HE2	1:F:491:ARG:HD2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:58:PRO:O	1:H:62:VAL:HG23	2.11	0.50
1:A:452:ASP:N	1:A:452:ASP:OD1	2.44	0.50
1:C:147:ALA:HA	1:C:193:SER:HB2	1.92	0.50
1:C:755:ARG:CD	1:C:885:PRO:HG2	2.39	0.50
1:F:231:PRO:O	1:F:235:LYS:HG3	2.12	0.50
1:F:357:GLU:HG3	1:F:358:ASN:N	2.27	0.50
1:D:381:ASN:HB3	1:D:448:LYS:NZ	2.26	0.50
1:D:587:ASP:O	1:D:614:LYS:NZ	2.28	0.50
1:F:461:VAL:HG23	1:F:469:PRO:HG3	1.92	0.50
1:E:457:ARG:HH22	1:E:513:GLN:NE2	2.09	0.50
1:F:418:PHE:HB3	1:F:437:HIS:ND1	2.26	0.50
1:C:2:GLU:O	1:C:2:GLU:HG2	2.11	0.50
1:F:700:VAL:HG23	1:F:701:LEU:HD12	1.93	0.50
1:B:319:LEU:O	1:B:322:VAL:HG12	2.10	0.50
1:B:872:LYS:O	1:B:875:GLN:HG2	2.11	0.50
1:C:567:ASP:O	1:C:570:ASP:HB2	2.12	0.50
1:C:700:VAL:HG23	1:C:701:LEU:HD12	1.94	0.50
1:D:452:ASP:OD1	1:D:452:ASP:N	2.45	0.50
1:D:459:SER:HB2	1:D:514:ASP:CB	2.42	0.50
1:G:119:ARG:NH2	1:G:130:GLU:O	2.44	0.50
1:A:149:GLY:HA2	1:A:207:THR:HG23	1.94	0.50
1:A:785:ALA:HB2	1:A:846:PRO:HD2	1.94	0.50
1:B:169:GLU:OE1	1:B:491:ARG:NH2	2.45	0.50
1:B:870:ILE:O	1:B:873:VAL:HG12	2.12	0.50
1:D:593:ILE:HD12	1:D:593:ILE:O	2.11	0.50
1:F:603:ASN:O	1:F:607:ILE:HG12	2.12	0.50
1:H:865:VAL:HA	1:H:868:MET:HB2	1.94	0.50
1:B:325:LEU:HD13	1:B:666:ALA:HB1	1.94	0.49
1:D:186:ASP:OD1	1:D:598:ARG:NH2	2.41	0.49
1:E:27:VAL:HG23	1:E:132:VAL:HG21	1.94	0.49
1:E:436:LEU:HD12	1:E:444:ALA:O	2.11	0.49
1:F:60:VAL:HG13	1:F:86:LEU:HD22	1.94	0.49
1:G:98:ARG:O	1:G:101:GLU:HG2	2.12	0.49
1:H:151:LEU:HD23	1:H:204:PHE:HB3	1.94	0.49
1:H:436:LEU:HD12	1:H:444:ALA:O	2.12	0.49
1:C:289:ALA:HB2	1:C:692:ILE:HD11	1.94	0.49
1:C:372:ARG:O	1:C:375:HIS:HB2	2.12	0.49
1:D:424:ILE:HD12	1:D:425:PRO:HD2	1.93	0.49
1:A:535:ILE:HG22	1:A:539:LYS:HE2	1.94	0.49
1:C:679:LYS:HE2	1:C:730:GLU:HG2	1.94	0.49
1:C:797:LEU:CB	1:C:865:VAL:HG21	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:134:GLY:N	1:H:206:VAL:O	2.40	0.49
1:B:39:LEU:O	1:B:40:LYS:HG2	2.12	0.49
1:B:461:VAL:HG21	1:B:474:ILE:HG21	1.93	0.49
1:C:69:VAL:HG21	4:C:1004:PCW:HG21	1.94	0.49
1:F:88:VAL:O	1:F:92:ILE:HG13	2.12	0.49
1:A:626:ASN:N	1:A:626:ASN:HD22	2.10	0.49
1:H:379:LEU:HD11	1:H:418:PHE:HD2	1.77	0.49
1:A:438:THR:OG1	1:A:443:LYS:HD3	2.12	0.49
1:A:798:GLN:O	1:A:798:GLN:HG2	2.11	0.49
1:C:746:GLU:HG2	1:C:750:ALA:HB3	1.93	0.49
1:C:171:VAL:HG23	1:C:173:LYS:HE2	1.95	0.49
1:E:24:THR:HA	1:E:27:VAL:HG12	1.94	0.49
1:E:150:ARG:NH1	1:E:151:LEU:O	2.45	0.49
1:F:419:ILE:O	1:F:437:HIS:HB2	2.13	0.49
1:F:800:PHE:CZ	1:F:824:VAL:HG21	2.48	0.49
1:G:687:GLY:HA3	1:G:795:ARG:HD3	1.94	0.49
1:H:434:SER:HB3	1:H:447:THR:OG1	2.13	0.49
1:F:460:TYR:HB2	1:F:516:VAL:HG22	1.93	0.49
1:F:676:ASN:HB3	1:F:728:GLY:HA2	1.94	0.49
1:A:75:GLU:HB3	1:A:78:GLU:CG	2.43	0.49
1:C:418:PHE:CE1	1:C:437:HIS:HA	2.48	0.49
1:D:319:LEU:O	1:D:322:VAL:HG12	2.13	0.49
1:F:48:TRP:O	1:F:51:PHE:HB3	2.12	0.49
1:H:460:TYR:HB2	1:H:516:VAL:HG22	1.95	0.49
1:E:378:VAL:O	1:E:381:ASN:ND2	2.46	0.49
1:H:360:PRO:HB2	1:H:366:TRP:CD1	2.47	0.49
1:G:173:LYS:NZ	1:G:190:MET:O	2.46	0.48
1:H:90:SER:O	1:H:94:VAL:HG13	2.13	0.48
1:H:338:THR:HG21	1:H:621:THR:OG1	2.13	0.48
1:A:541:ALA:HB2	1:A:737:MET:HE3	1.95	0.48
1:A:707:PHE:CZ	1:A:791:LEU:HD22	2.48	0.48
1:B:297:ILE:HG23	1:B:725:ILE:HD13	1.94	0.48
1:C:47:LEU:CD2	1:C:50:LEU:HD12	2.43	0.48
1:D:886:THR:OG1	5:D:1006:CE1:H62	2.12	0.48
1:B:461:VAL:HG23	1:B:470:MET:SD	2.53	0.48
1:A:118:ILE:HG13	1:A:138:ILE:HD11	1.95	0.48
1:A:886:THR:O	1:A:887:THR:HB	2.13	0.48
1:C:104:LEU:HD23	1:C:104:LEU:H	1.79	0.48
1:D:376:ILE:HD12	1:D:518:VAL:HG21	1.95	0.48
1:D:474:ILE:O	1:D:478:LEU:HD13	2.12	0.48
1:E:340:THR:HA	1:E:527:PRO:HA	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:376:ILE:HG21	1:E:495:TYR:HB3	1.95	0.48
1:F:439:PHE:CZ	1:F:446:LEU:HD11	2.48	0.48
1:G:676:ASN:HB3	1:G:728:GLY:HA2	1.94	0.48
1:H:350:TYR:HB3	1:H:520:LEU:H	1.79	0.48
1:A:840:ARG:NH2	4:A:1003:PCW:O31	2.46	0.48
1:C:109:GLU:C	1:C:111:SER:H	2.16	0.48
1:C:798:GLN:O	1:C:798:GLN:HG2	2.14	0.48
1:E:83:PHE:O	1:E:87:ILE:HG12	2.13	0.48
1:E:171:VAL:HG23	1:E:173:LYS:HE2	1.96	0.48
1:G:603:ASN:O	1:G:607:ILE:HG12	2.13	0.48
1:H:557:GLN:HB3	1:H:561:ARG:NH1	2.29	0.48
1:A:524:ILE:O	1:A:526:PRO:HD3	2.13	0.48
1:B:325:LEU:HG	1:B:636:ILE:HG12	1.94	0.48
1:A:711:GLN:O	1:A:715:ILE:HG13	2.14	0.48
1:B:50:LEU:HD22	1:B:94:VAL:HG13	1.95	0.48
1:B:470:MET:O	1:B:471:THR:OG1	2.25	0.48
4:C:1006:PCW:H321	4:C:1006:PCW:H2	1.59	0.48
1:D:691:ALA:O	1:D:695:ILE:HG13	2.14	0.48
1:E:26:GLU:OE1	1:E:30:ARG:HD2	2.14	0.48
1:A:289:ALA:HB2	1:A:692:ILE:HD11	1.96	0.48
1:D:835:VAL:HG21	4:D:1003:PCW:H122	1.96	0.48
1:E:225:ALA:HB3	1:E:632:LYS:HE3	1.95	0.48
1:E:500:MET:HE3	1:E:511:ASP:HB3	1.96	0.48
1:E:807:GLN:HB3	1:E:812:ALA:HB2	1.95	0.48
1:F:148:ASP:OD1	1:F:193:SER:N	2.38	0.48
1:F:452:ASP:N	1:F:452:ASP:OD1	2.46	0.48
1:H:352:PRO:HB2	1:H:462:PHE:O	2.13	0.48
1:H:626:ASN:O	1:H:629:PRO:HD2	2.14	0.48
1:D:880:LYS:HD2	1:D:883:ASP:H	1.79	0.48
1:E:154:SER:HB3	1:E:175:ILE:HG23	1.95	0.48
1:G:321:ALA:HB1	1:G:636:ILE:HD13	1.95	0.48
1:G:452:ASP:OD1	1:G:452:ASP:N	2.46	0.48
1:H:548:ILE:HG12	1:H:596:TYR:HD2	1.78	0.48
1:D:813:GLY:HA3	1:D:816:SER:HB2	1.95	0.48
1:F:332:CYS:O	1:F:620:MET:HA	2.14	0.48
1:H:332:CYS:O	1:H:620:MET:HA	2.13	0.48
1:B:772:GLN:HG2	1:B:783:SER:HB2	1.96	0.47
1:G:535:ILE:HG22	1:G:539:LYS:HE2	1.94	0.47
1:A:333:THR:HG22	1:A:621:THR:OG1	2.14	0.47
1:A:431:LYS:O	1:A:453:VAL:HG21	2.14	0.47
1:A:593:ILE:HD13	1:A:596:TYR:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:627:ASP:OD2	6:D:1101:HOH:O	2.20	0.47
1:H:513:GLN:HG3	1:H:514:ASP:H	1.78	0.47
1:C:560:GLY:HA2	1:C:563:ILE:HG12	1.95	0.47
1:F:287:VAL:HG11	1:F:713:LEU:HG	1.96	0.47
1:F:383:SER:HB2	1:F:398:VAL:HG22	1.97	0.47
1:G:541:ALA:HB2	1:G:737:MET:HE3	1.97	0.47
1:H:404:SER:OG	1:H:409:GLN:O	2.25	0.47
1:D:254:ILE:HA	1:D:699:LEU:HD21	1.96	0.47
1:F:319:LEU:O	1:F:322:VAL:HG12	2.15	0.47
1:G:878:PHE:HB3	1:H:95:VAL:CG1	2.44	0.47
1:B:90:SER:O	1:B:94:VAL:HG23	2.14	0.47
1:D:325:LEU:HD13	1:D:666:ALA:HB1	1.96	0.47
1:E:386:ASN:HD21	1:E:390:LYS:HB3	1.78	0.47
1:F:636:ILE:HD12	1:F:652:ALA:HB3	1.95	0.47
1:H:498:LYS:HG3	1:H:500:MET:HG2	1.96	0.47
1:B:858:ALA:HB1	4:B:1003:PCW:H451	1.96	0.47
1:B:875:GLN:HA	1:B:879:PHE:HD2	1.77	0.47
1:C:592:HIS:CE1	1:D:588:LYS:O	2.68	0.47
1:D:720:ASP:OD2	1:D:795:ARG:NE	2.44	0.47
1:D:722:LEU:HB2	1:D:723:PRO:HD3	1.97	0.47
1:G:548:ILE:HG23	1:G:596:TYR:HB2	1.97	0.47
1:H:478:LEU:HD21	1:H:517:LEU:HD13	1.96	0.47
1:A:89:ASN:N	1:A:89:ASN:HD22	2.13	0.47
1:A:377:ALA:O	1:A:381:ASN:ND2	2.48	0.47
1:B:574:THR:HA	1:B:597:ALA:O	2.14	0.47
1:G:443:LYS:NZ	1:G:504:THR:O	2.46	0.47
1:C:62:VAL:HG13	4:C:1004:PCW:H181	1.96	0.47
1:E:744:ILE:HD12	1:E:744:ILE:H	1.80	0.47
1:E:803:ARG:HH22	1:E:812:ALA:HB3	1.79	0.47
1:F:174:TYR:HD2	1:F:188:VAL:HG11	1.80	0.47
1:G:117:VAL:HG23	1:G:137:VAL:HG22	1.97	0.47
1:B:118:ILE:HG13	1:B:138:ILE:HD11	1.97	0.47
1:D:351:LEU:O	1:D:355:THR:HG23	2.15	0.47
1:E:126:ILE:HA	1:F:592:HIS:CE1	2.50	0.47
1:E:396:THR:HG23	1:E:523:MET:SD	2.55	0.47
1:E:461:VAL:HG23	1:E:469:PRO:HB3	1.95	0.47
1:F:186:ASP:OD1	1:F:598:ARG:NH2	2.45	0.47
1:A:50:LEU:HA	1:A:53:GLU:OE1	2.15	0.47
1:B:785:ALA:HB2	1:B:846:PRO:HD2	1.97	0.47
1:C:254:ILE:HA	1:C:699:LEU:HD21	1.97	0.47
4:C:1004:PCW:H20	4:C:1004:PCW:H232	1.58	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:808:THR:HB	1:E:811:GLY:HA3	1.97	0.47
1:F:353:ASP:HB3	1:F:463:LEU:HD12	1.97	0.47
1:H:432:LEU:HD21	1:H:454:MET:HB2	1.96	0.47
1:H:605:ILE:HB	1:H:629:PRO:HB2	1.97	0.47
1:H:644:THR:O	1:H:648:LYS:HG3	2.15	0.47
1:A:116:LYS:HB2	1:A:116:LYS:HE3	1.67	0.46
1:B:854:TRP:HZ2	4:B:1003:PCW:H412	1.79	0.46
1:C:504:THR:HG22	1:C:506:GLU:H	1.79	0.46
1:D:756:ALA:O	1:D:760:ARG:HG3	2.15	0.46
1:F:313:HIS:HB3	1:F:656:THR:HB	1.96	0.46
1:G:431:LYS:HD3	1:G:457:ARG:HH12	1.78	0.46
1:H:335:LYS:HZ3	1:H:559:ILE:HD12	1.79	0.46
1:H:349:TYR:CE2	1:H:351:LEU:HG	2.50	0.46
1:B:470:MET:HE2	1:B:475:LEU:HB2	1.96	0.46
1:C:751:GLY:H	4:C:1005:PCW:H71	1.81	0.46
4:B:1006:PCW:HZ11	4:B:1006:PCW:HZ12	1.97	0.46
1:D:593:ILE:H	1:D:593:ILE:HG13	1.54	0.46
1:F:54:THR:HG21	1:F:90:SER:HA	1.98	0.46
4:C:1004:PCW:HZ83	4:C:1004:PCW:HZ21	1.64	0.46
1:H:98:ARG:O	1:H:101:GLU:HG2	2.15	0.46
1:H:378:VAL:O	1:H:381:ASN:ND2	2.48	0.46
1:H:744:ILE:HD12	1:H:744:ILE:H	1.81	0.46
1:C:445:MET:O	1:C:497:TYR:HA	2.15	0.46
1:G:190:MET:HB2	1:G:190:MET:HE3	1.86	0.46
1:G:837:PRO:O	1:G:840:ARG:HG2	2.16	0.46
1:C:548:ILE:O	1:C:604:LYS:NZ	2.44	0.46
1:F:108:ARG:NH2	1:F:219:ALA:HB2	2.25	0.46
1:F:760:ARG:HD2	1:F:798:GLN:NE2	2.30	0.46
1:H:567:ASP:OD1	1:H:567:ASP:N	2.47	0.46
1:C:474:ILE:O	1:C:478:LEU:HB2	2.16	0.46
1:E:78:GLU:HA	1:E:81:ILE:HB	1.98	0.46
1:E:118:ILE:HG13	1:E:138:ILE:HD11	1.97	0.46
1:A:147:ALA:HA	1:A:193:SER:HB2	1.98	0.46
1:H:159:ILE:HD12	1:H:173:LYS:HE3	1.98	0.46
1:H:632:LYS:HG3	1:H:650:SER:OG	2.16	0.46
1:H:722:LEU:HB2	1:H:723:PRO:HD3	1.97	0.46
1:A:186:ASP:OD1	1:A:598:ARG:NH2	2.42	0.46
1:C:592:HIS:HE1	1:D:588:LYS:O	1.99	0.46
1:E:596:TYR:HB3	1:E:599:VAL:HG11	1.98	0.46
1:E:831:TYR:O	1:E:834:THR:OG1	2.20	0.46
1:H:283:VAL:O	1:H:287:VAL:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:603:ASN:O	1:H:607:ILE:HG12	2.16	0.46
1:A:861:ALA:O	1:A:865:VAL:HG23	2.16	0.45
1:C:258:GLU:O	1:C:262:VAL:HG23	2.16	0.45
1:D:883:ASP:O	1:D:885:PRO:HD3	2.16	0.45
1:H:59:MET:SD	1:H:243:LEU:HD23	2.55	0.45
1:H:342:ASN:HA	1:H:525:ASP:OD2	2.16	0.45
4:C:1004:PCW:H73	4:C:1004:PCW:H42	1.56	0.45
1:D:116:LYS:HB2	1:D:116:LYS:HE3	1.73	0.45
1:D:880:LYS:HG3	1:D:881:ASP:N	2.30	0.45
1:E:346:VAL:HG21	1:E:400:LEU:HD23	1.98	0.45
1:F:283:VAL:O	1:F:287:VAL:HG23	2.15	0.45
1:G:49:LYS:HB3	1:G:52:LEU:CD2	2.46	0.45
1:G:254:ILE:HG12	1:G:699:LEU:HD22	1.99	0.45
1:G:313:HIS:HB3	1:G:656:THR:HB	1.98	0.45
1:G:432:LEU:HB2	1:G:448:LYS:O	2.16	0.45
1:H:150:ARG:NH1	1:H:151:LEU:O	2.49	0.45
1:H:424:ILE:HD12	1:H:434:SER:HB2	1.97	0.45
1:E:36:PHE:O	1:E:210:ALA:HB2	2.16	0.45
1:E:214:GLU:O	1:E:218:ILE:HG13	2.16	0.45
1:E:420:ARG:HG2	1:E:423:GLU:OE1	2.16	0.45
1:F:3:ILE:HG22	1:F:190:MET:HE1	1.99	0.45
1:H:267:ASN:OD1	1:H:267:ASN:N	2.49	0.45
1:C:457:ARG:HD3	1:C:512:GLU:O	2.17	0.45
1:D:1:ALA:O	1:D:2:GLU:HG2	2.16	0.45
1:D:154:SER:HB3	1:D:175:ILE:HG23	1.98	0.45
1:E:59:MET:HG3	1:E:240:SER:OG	2.17	0.45
1:E:104:LEU:HD23	1:E:104:LEU:O	2.17	0.45
1:E:498:LYS:HG3	1:E:514:ASP:O	2.17	0.45
1:G:432:LEU:H	1:G:432:LEU:HG	1.55	0.45
1:H:78:GLU:HA	1:H:81:ILE:HG22	1.98	0.45
1:A:744:ILE:H	1:A:744:ILE:HD12	1.82	0.45
1:B:586:LEU:HD11	1:B:590:LEU:HD13	1.98	0.45
1:B:806:VAL:HA	1:B:876:ASN:ND2	2.32	0.45
1:D:764:ILE:O	1:D:768:VAL:HG23	2.17	0.45
1:F:396:THR:HG23	1:F:523:MET:SD	2.56	0.45
1:F:720:ASP:OD2	1:F:795:ARG:NH2	2.49	0.45
1:G:15:LEU:O	1:G:30:ARG:NH1	2.49	0.45
1:A:297:ILE:HG23	1:A:725:ILE:HD13	1.99	0.45
1:A:593:ILE:H	1:A:593:ILE:HG13	1.50	0.45
1:A:618:THR:O	1:A:635:ASP:HB2	2.16	0.45
1:B:2:GLU:HG3	1:B:6:LYS:HE3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:700:VAL:HG23	1:B:701:LEU:HD12	1.99	0.45
1:B:763:LEU:HD23	1:B:763:LEU:HA	1.84	0.45
1:D:59:MET:CE	1:D:290:ILE:HG23	2.46	0.45
1:D:99:LYS:HZ1	1:D:318:LYS:HB3	1.81	0.45
1:E:83:PHE:HA	1:E:86:LEU:HD12	1.98	0.45
1:E:221:LEU:HD22	1:E:605:ILE:HG21	1.97	0.45
1:F:803:ARG:CZ	1:F:817:ASN:HD22	2.30	0.45
1:G:707:PHE:HZ	1:G:768:VAL:HG11	1.82	0.45
1:H:218:ILE:HD11	1:H:601:PRO:HG2	1.98	0.45
1:H:297:ILE:HD13	1:H:724:ALA:HB3	1.98	0.45
1:A:157:LEU:HD22	1:A:202:GLY:HA3	1.99	0.45
1:A:220:GLY:O	1:A:224:THR:HG23	2.17	0.45
1:B:383:SER:HB2	1:B:398:VAL:HG22	1.99	0.45
1:C:592:HIS:NE2	1:D:592:HIS:CE1	2.85	0.45
1:D:112:ALA:HB2	1:D:144:PHE:HB3	1.98	0.45
1:H:411:TYR:HE2	1:H:415:ARG:NH2	2.14	0.45
1:B:330:VAL:HB	1:B:618:THR:HG22	1.99	0.45
1:D:353:ASP:OD1	1:D:353:ASP:N	2.41	0.45
1:E:289:ALA:HB2	1:E:692:ILE:HD11	1.99	0.45
1:F:58:PRO:O	1:F:62:VAL:HG23	2.17	0.45
1:A:443:LYS:NZ	1:A:504:THR:O	2.50	0.45
1:C:418:PHE:HB2	1:C:439:PHE:CZ	2.51	0.45
1:E:381:ASN:OD1	1:E:415:ARG:NH2	2.50	0.45
1:E:749:PHE:O	1:E:754:MET:N	2.46	0.45
1:F:232:LEU:O	1:F:236:LEU:HG	2.17	0.45
1:F:472:GLU:O	1:F:473:GLU:HB2	2.16	0.45
1:H:254:ILE:HA	1:H:699:LEU:HD21	1.99	0.45
1:D:71:LEU:HA	1:D:71:LEU:HD12	1.67	0.44
1:E:116:LYS:HE3	1:E:116:LYS:HB2	1.70	0.44
1:F:131:LEU:HD12	1:F:146:PRO:HB2	1.98	0.44
1:H:362:SER:HB3	1:H:365:ASN:HB3	1.99	0.44
4:B:1004:PCW:O2P	4:B:1004:PCW:H32	2.18	0.44
1:C:460:TYR:HB2	1:C:516:VAL:HG22	1.99	0.44
1:D:870:ILE:O	1:D:874:VAL:HG23	2.17	0.44
1:F:427:ASP:H	1:F:431:LYS:HB3	1.82	0.44
1:H:550:GLY:HA2	1:H:599:VAL:H	1.82	0.44
1:H:618:THR:O	1:H:635:ASP:HB2	2.17	0.44
1:B:788:PHE:O	1:B:792:ILE:HG22	2.18	0.44
4:B:1004:PCW:H122	4:B:1004:PCW:H152	1.78	0.44
1:C:57:ASP:HB3	1:C:60:VAL:HG23	2.00	0.44
1:C:351:LEU:HD11	1:C:370:GLU:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:508:LYS:HG2	1:E:511:ASP:OD2	2.18	0.44
1:E:528:ARG:HB2	1:E:531:VAL:HG23	1.99	0.44
1:F:455:PHE:CZ	1:F:478:LEU:HD22	2.52	0.44
1:G:716:ASN:OD1	1:G:795:ARG:NH2	2.50	0.44
4:C:1003:PCW:H41	4:C:1003:PCW:H83	1.66	0.44
1:D:381:ASN:HB3	1:D:448:LYS:HZ3	1.82	0.44
1:F:281:PHE:HD2	1:F:699:LEU:HD12	1.82	0.44
1:G:708:THR:HB	1:G:711:GLN:OE1	2.16	0.44
1:H:840:ARG:NH1	1:H:846:PRO:O	2.51	0.44
1:A:221:LEU:HD23	1:A:221:LEU:HA	1.88	0.44
1:A:599:VAL:HB	1:A:603:ASN:HB2	1.98	0.44
1:B:394:ASP:OD2	1:B:396:THR:HB	2.17	0.44
1:C:603:ASN:O	1:C:607:ILE:HG12	2.17	0.44
4:D:1003:PCW:H221	4:D:1003:PCW:H251	1.68	0.44
1:F:106:ALA:CB	1:F:222:LEU:HD13	2.48	0.44
1:G:330:VAL:HG21	1:G:611:TRP:CE3	2.52	0.44
1:A:346:VAL:HG22	1:A:523:MET:HE2	2.00	0.44
1:A:611:TRP:HB3	1:A:618:THR:HG21	2.00	0.44
1:A:871:ILE:HG12	1:A:887:THR:HG22	2.00	0.44
4:B:1004:PCW:H371	4:B:1004:PCW:H40	1.58	0.44
1:C:885:PRO:HB2	1:C:886:THR:H	1.55	0.44
1:D:93:SER:O	1:D:97:THR:HB	2.18	0.44
1:F:69:VAL:O	1:F:73:LEU:HG	2.18	0.44
1:F:735:ASP:OD1	1:F:735:ASP:N	2.50	0.44
1:G:118:ILE:CG1	1:G:138:ILE:HD11	2.46	0.44
1:A:394:ASP:OD2	1:A:396:THR:HB	2.18	0.44
1:A:492:VAL:HA	1:A:521:THR:O	2.17	0.44
1:C:870:ILE:O	1:C:874:VAL:HG23	2.18	0.44
1:D:603:ASN:O	1:D:607:ILE:HG12	2.15	0.44
1:E:379:LEU:HD22	1:E:418:PHE:CE1	2.53	0.44
1:G:440:ASN:HB3	1:G:441:GLU:H	1.63	0.44
1:G:865:VAL:HG22	1:G:868:MET:HE3	1.99	0.44
1:H:159:ILE:HG12	1:H:197:VAL:HG22	1.99	0.44
1:B:808:THR:HG22	1:B:809:ALA:N	2.33	0.44
1:C:434:SER:HA	1:C:446:LEU:O	2.18	0.44
1:D:785:ALA:HB2	1:D:846:PRO:HD2	2.00	0.44
1:E:659:ASN:OD1	1:E:661:VAL:HG12	2.18	0.44
1:G:262:VAL:O	1:G:267:ASN:ND2	2.51	0.44
1:G:671:ARG:NH1	1:G:739:ARG:O	2.48	0.44
1:H:749:PHE:O	1:H:754:MET:N	2.51	0.44
1:D:460:TYR:HA	1:D:468:LYS:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:715:ILE:HA	1:E:719:ASN:HB3	2.00	0.44
1:G:297:ILE:O	1:G:301:VAL:HG23	2.17	0.44
1:H:441:GLU:O	1:H:443:LYS:N	2.50	0.44
1:H:867:MET:O	1:H:871:ILE:HB	2.17	0.44
1:B:430:ARG:HD3	1:B:457:ARG:NH1	2.29	0.43
1:B:764:ILE:O	1:B:768:VAL:HG23	2.17	0.43
1:C:538:SER:HB2	1:C:543:ILE:HB	2.00	0.43
1:D:54:THR:HG21	1:D:90:SER:HA	1.99	0.43
1:D:350:TYR:HE2	1:D:478:LEU:HD12	1.83	0.43
1:D:556:ALA:O	1:D:595:VAL:HG11	2.18	0.43
5:D:1009:CE1:H21	5:D:1009:CE1:H52	1.90	0.43
1:E:50:LEU:HB3	1:E:94:VAL:HG13	1.99	0.43
1:G:325:LEU:HG	1:G:636:ILE:HG12	2.00	0.43
1:B:550:GLY:HA2	1:B:599:VAL:H	1.83	0.43
1:C:332:CYS:O	1:C:620:MET:HA	2.18	0.43
1:G:578:LEU:HD21	1:G:607:ILE:HD11	2.00	0.43
1:H:548:ILE:HG23	1:H:596:TYR:HB2	1.99	0.43
1:B:427:ASP:OD1	1:B:430:ARG:N	2.50	0.43
1:D:288:ALA:HB2	1:D:712:LEU:HD13	2.00	0.43
1:E:532:TYR:CE1	1:E:563:ILE:HG22	2.54	0.43
1:E:709:ALA:O	1:E:713:LEU:HD23	2.18	0.43
1:G:150:ARG:NH1	1:G:151:LEU:O	2.51	0.43
1:G:410:ASP:HB3	1:G:413:GLU:HG3	2.00	0.43
1:H:356:LYS:HD2	1:H:356:LYS:HA	1.83	0.43
1:H:803:ARG:HH22	1:H:816:SER:HB3	1.83	0.43
1:A:89:ASN:OD1	1:A:295:SER:OG	2.36	0.43
1:A:681:ILE:HD12	1:A:748:ILE:HD11	2.00	0.43
1:B:628:ALA:HB3	1:B:629:PRO:HD3	2.00	0.43
1:E:84:LEU:O	1:E:88:VAL:HG23	2.19	0.43
1:E:209:THR:O	1:E:212:GLU:HG2	2.18	0.43
1:G:222:LEU:HD23	1:G:222:LEU:HA	1.82	0.43
1:C:87:ILE:O	1:C:91:ILE:HG13	2.18	0.43
1:D:710:LEU:HD11	5:D:1005:CE1:H13	2.01	0.43
1:D:720:ASP:OD2	1:D:795:ARG:NH2	2.47	0.43
1:E:76:VAL:O	1:E:79:SER:HB3	2.18	0.43
1:F:524:ILE:O	1:F:526:PRO:HD3	2.18	0.43
1:F:744:ILE:H	1:F:744:ILE:HD12	1.82	0.43
1:B:870:ILE:O	1:B:874:VAL:HG23	2.19	0.43
1:C:592:HIS:NE2	1:D:592:HIS:HE1	2.17	0.43
1:C:829:VAL:O	1:C:833:ILE:HG13	2.18	0.43
1:C:880:LYS:HB3	1:C:885:PRO:CG	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1003:PCW:H381	4:D:1003:PCW:H352	1.50	0.43
1:H:349:TYR:HE2	1:H:351:LEU:HG	1.83	0.43
1:D:772:GLN:CG	1:D:783:SER:HB2	2.48	0.43
1:E:69:VAL:O	1:E:73:LEU:HG	2.18	0.43
1:E:90:SER:O	1:E:94:VAL:HG23	2.18	0.43
1:F:700:VAL:HG23	1:F:701:LEU:CD1	2.48	0.43
1:G:439:PHE:CZ	1:G:446:LEU:HD11	2.53	0.43
1:G:508:LYS:HB3	1:G:510:GLU:OE1	2.18	0.43
1:G:808:THR:HG22	1:G:809:ALA:N	2.33	0.43
1:A:91:ILE:O	1:A:95:VAL:HG22	2.19	0.43
1:G:304:VAL:HG21	1:G:729:MET:SD	2.58	0.43
1:H:865:VAL:HA	1:H:868:MET:HE3	2.00	0.43
1:B:707:PHE:CZ	1:B:791:LEU:HD22	2.52	0.43
1:F:756:ALA:O	1:F:760:ARG:HG3	2.19	0.43
1:B:308:LYS:HE3	1:B:308:LYS:HB2	1.82	0.43
4:B:1003:PCW:H82	4:B:1003:PCW:H42	1.72	0.43
4:B:1007:PCW:H83	4:B:1007:PCW:H41	1.62	0.43
1:C:713:LEU:HD23	1:C:713:LEU:HA	1.94	0.43
1:C:785:ALA:HB2	1:C:846:PRO:HD2	2.01	0.43
4:C:1004:PCW:H442	4:C:1004:PCW:H281	2.00	0.43
1:D:87:ILE:O	1:D:91:ILE:HG13	2.19	0.43
1:B:869:GLU:OE2	1:B:872:LYS:NZ	2.40	0.42
1:D:379:LEU:HD22	1:D:418:PHE:HB2	2.01	0.42
1:D:763:LEU:HD23	1:D:763:LEU:HA	1.82	0.42
1:E:767:ALA:HB2	1:E:864:ALA:HB2	2.00	0.42
1:G:455:PHE:CZ	1:G:478:LEU:HB3	2.54	0.42
1:G:560:GLY:HA2	1:G:563:ILE:HG12	2.01	0.42
1:H:2:GLU:O	1:H:2:GLU:HG2	2.18	0.42
1:H:396:THR:HA	1:H:523:MET:CE	2.49	0.42
1:B:63:LEU:HA	1:B:63:LEU:HD23	1.73	0.42
1:B:91:ILE:O	1:B:95:VAL:HG22	2.19	0.42
1:B:239:PHE:HE2	1:B:685:PHE:CE2	2.37	0.42
1:C:289:ALA:CB	1:C:692:ILE:HD11	2.49	0.42
1:F:620:MET:HG3	1:F:631:LEU:HD23	2.01	0.42
1:G:744:ILE:HD12	1:G:744:ILE:H	1.83	0.42
1:H:691:ALA:HB2	1:H:795:ARG:HH21	1.83	0.42
1:A:40:LYS:HA	1:A:40:LYS:HD2	1.81	0.42
1:C:349:TYR:OH	1:C:373:LEU:HB3	2.19	0.42
1:C:412:ASN:O	1:C:416:GLU:HG3	2.18	0.42
1:D:70:GLN:HE22	1:D:709:ALA:CB	2.32	0.42
1:G:75:GLU:HB3	1:G:78:GLU:CG	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:872:LYS:HE3	1:B:872:LYS:HB2	1.67	0.42
1:C:45:ASP:N	1:C:46:PRO:CD	2.83	0.42
1:C:418:PHE:HZ	1:C:436:LEU:O	2.03	0.42
1:D:150:ARG:NH1	1:D:151:LEU:O	2.52	0.42
1:D:797:LEU:HB2	1:D:865:VAL:HG21	2.01	0.42
1:F:172:GLU:O	1:F:188:VAL:HG13	2.19	0.42
1:G:555:THR:O	1:G:559:ILE:HD12	2.20	0.42
1:H:495:TYR:O	1:H:517:LEU:HG	2.19	0.42
1:A:763:LEU:HD23	1:A:763:LEU:HA	1.84	0.42
1:B:368:GLU:OE2	1:B:371:ARG:HD3	2.20	0.42
1:B:372:ARG:O	1:B:376:ILE:HG13	2.20	0.42
1:B:560:GLY:CA	1:B:563:ILE:HG12	2.46	0.42
1:B:796:THR:HG22	1:B:824:VAL:HG13	2.01	0.42
1:B:875:GLN:OE1	1:B:885:PRO:HD3	2.19	0.42
1:B:882:TYR:HB2	1:C:98:ARG:HH11	1.85	0.42
1:C:297:ILE:HD13	1:C:724:ALA:HB3	2.02	0.42
1:C:350:TYR:HE2	1:C:481:THR:HG1	1.62	0.42
1:C:377:ALA:O	1:C:381:ASN:ND2	2.52	0.42
1:C:880:LYS:HG3	1:C:881:ASP:N	2.34	0.42
1:E:211:SER:HA	1:E:216:GLY:HA3	2.02	0.42
1:E:762:VAL:O	1:E:766:ILE:HG13	2.19	0.42
1:G:297:ILE:HD11	1:G:721:SER:HA	2.01	0.42
1:G:840:ARG:HG3	1:G:841:GLU:N	2.33	0.42
1:H:59:MET:HE3	1:H:290:ILE:HG23	2.01	0.42
1:A:430:ARG:NH2	1:A:432:LEU:HB3	2.34	0.42
4:B:1009:PCW:H63	4:B:1009:PCW:H42	1.83	0.42
1:H:807:GLN:HB3	1:H:812:ALA:HB2	2.02	0.42
1:H:229:GLN:NE2	1:H:237:GLU:OE1	2.52	0.42
1:H:324:THR:HB	1:H:636:ILE:HD11	2.02	0.42
1:H:560:GLY:HA2	1:H:563:ILE:HG12	2.01	0.42
1:H:735:ASP:OD1	1:H:735:ASP:N	2.53	0.42
1:A:108:ARG:HD2	1:A:215:ILE:HD11	2.02	0.42
1:A:359:PHE:CE1	1:A:370:GLU:HG2	2.54	0.42
1:C:167:GLU:OE2	1:C:336:THR:OG1	2.21	0.42
4:C:1008:PCW:H42	4:C:1008:PCW:H63	1.58	0.42
1:G:711:GLN:HB3	1:G:788:PHE:CE1	2.54	0.42
1:H:460:TYR:HB2	1:H:516:VAL:HA	2.02	0.42
1:C:266:ASP:O	1:C:268:SER:N	2.48	0.42
1:C:760:ARG:O	1:C:764:ILE:HG13	2.20	0.42
1:D:292:GLU:OE1	1:D:716:ASN:ND2	2.51	0.42
1:E:167:GLU:OE2	1:E:336:THR:OG1	2.21	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:6:LYS:HB3	1:F:10:GLU:HB2	2.02	0.42
1:F:147:ALA:HA	1:F:193:SER:HB2	2.01	0.42
1:A:721:SER:O	1:A:725:ILE:HG12	2.20	0.42
1:A:865:VAL:HA	1:A:868:MET:CE	2.50	0.42
1:C:98:ARG:O	1:C:99:LYS:HB2	2.20	0.42
1:C:107:LEU:HD11	1:C:219:ALA:HB2	2.02	0.42
1:C:548:ILE:HG22	1:C:599:VAL:HG21	2.01	0.42
1:D:321:ALA:HB1	1:D:636:ILE:CD1	2.50	0.42
1:D:335:LYS:HA	1:D:339:LEU:HB2	2.01	0.42
1:D:621:THR:HA	1:D:638:VAL:O	2.19	0.42
1:E:558:ALA:O	1:E:561:ARG:HG2	2.20	0.42
1:F:346:VAL:HA	1:F:523:MET:HA	2.02	0.42
1:F:439:PHE:HZ	1:F:446:LEU:HD11	1.85	0.42
1:F:840:ARG:NH1	1:F:846:PRO:O	2.52	0.42
1:H:335:LYS:HB2	1:H:549:THR:HB	2.02	0.42
1:H:460:TYR:CB	1:H:516:VAL:HG22	2.50	0.42
1:E:37:ASN:HB3	1:E:129:ARG:HA	2.01	0.41
1:G:432:LEU:CD1	1:G:447:THR:HG23	2.50	0.41
1:G:586:LEU:O	1:G:590:LEU:HB2	2.20	0.41
1:A:875:GLN:NE2	1:A:883:ASP:HB2	2.34	0.41
1:B:291:PRO:HG3	1:B:685:PHE:CE2	2.55	0.41
1:C:871:ILE:CD1	4:C:1005:PCW:HG371	2.50	0.41
1:D:242:LYS:HD2	5:D:1008:CE1:HG2	2.01	0.41
1:D:289:ALA:CB	1:D:692:ILE:HD11	2.50	0.41
1:E:108:ARG:HH12	1:E:625:VAL:HG13	1.85	0.41
1:F:357:GLU:HG3	1:F:358:ASN:H	1.84	0.41
1:F:593:ILE:H	1:F:593:ILE:HG13	1.58	0.41
1:H:746:GLU:HG2	1:H:750:ALA:HB3	2.02	0.41
1:A:353:ASP:OD1	1:A:353:ASP:N	2.48	0.41
1:B:147:ALA:HB1	1:B:208:GLY:O	2.20	0.41
1:E:108:ARG:HA	1:E:108:ARG:HD3	1.76	0.41
1:E:127:HIS:NE2	1:F:591:GLU:OE2	2.53	0.41
1:F:91:ILE:O	1:F:95:VAL:HG22	2.20	0.41
1:G:796:THR:HG22	1:G:824:VAL:HG13	2.02	0.41
1:H:868:MET:O	1:H:871:ILE:HG22	2.20	0.41
1:B:138:ILE:HG13	1:B:203:MET:HG3	2.02	0.41
1:C:279:PHE:CE1	4:C:1004:PCW:HG242	2.54	0.41
1:C:460:TYR:CB	1:C:516:VAL:HG22	2.51	0.41
1:D:886:THR:HG23	5:D:1006:CE1:HG42	2.02	0.41
1:E:636:ILE:HD12	1:E:652:ALA:HB3	2.02	0.41
1:F:145:VAL:HA	1:F:146:PRO:HD3	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:230:THR:HG23	1:F:324:THR:OG1	2.20	0.41
1:F:524:ILE:HG12	1:F:525:ASP:H	1.85	0.41
1:F:801:ALA:HA	1:F:808:THR:CG2	2.50	0.41
1:H:186:ASP:OD1	1:H:598:ARG:NH2	2.48	0.41
1:H:632:LYS:HB3	1:H:632:LYS:HE2	1.82	0.41
1:H:707:PHE:CZ	1:H:791:LEU:HD22	2.56	0.41
1:A:48:TRP:HB2	4:A:1004:PCW:H152	2.01	0.41
1:B:174:TYR:HD2	1:B:188:VAL:HG11	1.85	0.41
1:B:878:PHE:HE1	4:B:1009:PCW:H2	1.85	0.41
1:C:722:LEU:HB2	1:C:723:PRO:HD3	2.02	0.41
1:C:830:LEU:HD23	1:C:833:ILE:HD12	2.01	0.41
1:D:318:LYS:HE2	1:D:652:ALA:CB	2.51	0.41
1:D:360:PRO:HB2	1:D:366:TRP:NE1	2.35	0.41
1:F:47:LEU:HD13	1:F:47:LEU:HA	1.92	0.41
1:F:96:GLN:OE1	1:F:318:LYS:HD2	2.21	0.41
1:F:218:ILE:HD11	1:F:601:PRO:HG2	2.03	0.41
1:F:436:LEU:HB2	1:F:445:MET:HG3	2.02	0.41
1:H:548:ILE:HA	1:H:596:TYR:HB2	2.02	0.41
1:C:39:LEU:O	1:C:108:ARG:NH1	2.53	0.41
1:C:386:ASN:OD1	1:C:390:LYS:N	2.51	0.41
1:C:743:ASP:HB3	1:C:746:GLU:HB2	2.03	0.41
1:D:31:GLN:HG3	1:D:132:VAL:HG11	2.01	0.41
1:F:363:PRO:HD3	1:F:408:ASN:HB2	2.03	0.41
1:F:524:ILE:HG12	1:F:525:ASP:N	2.36	0.41
1:F:800:PHE:HE1	1:F:821:ILE:HD13	1.86	0.41
1:A:57:ASP:HB3	1:A:60:VAL:HG23	2.02	0.41
1:A:764:ILE:O	1:A:768:VAL:HG23	2.21	0.41
1:B:63:LEU:HD11	1:B:290:ILE:HG21	2.03	0.41
1:C:352:PRO:HB2	1:C:463:LEU:HD23	2.02	0.41
1:C:511:ASP:C	1:C:513:GLN:H	2.24	0.41
1:E:574:THR:HA	1:E:597:ALA:O	2.20	0.41
1:G:232:LEU:O	1:G:236:LEU:HG	2.21	0.41
1:H:674:PHE:CE2	1:H:678:LYS:HD2	2.56	0.41
1:B:376:ILE:HG12	1:B:446:LEU:HG	2.02	0.41
1:C:430:ARG:O	1:C:453:VAL:HG11	2.20	0.41
1:D:250:LEU:HD22	1:D:696:LEU:HD11	2.02	0.41
1:E:376:ILE:CG2	1:E:495:TYR:HB3	2.50	0.41
1:F:225:ALA:HA	1:F:633:GLN:OE1	2.19	0.41
1:G:346:VAL:HA	1:G:523:MET:HA	2.02	0.41
1:A:756:ALA:O	1:A:760:ARG:HG3	2.20	0.41
1:B:73:LEU:HD23	1:B:73:LEU:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:743:ASP:OD1	1:B:744:ILE:N	2.54	0.41
1:B:744:ILE:HD12	1:B:744:ILE:H	1.84	0.41
1:C:887:THR:O	1:C:887:THR:OG1	2.33	0.41
4:C:1005:PCW:H482	4:C:1005:PCW:H451	1.64	0.41
1:D:59:MET:HE1	1:D:290:ILE:HG23	2.02	0.41
1:D:366:TRP:CZ3	1:D:374:ILE:HG13	2.56	0.41
1:D:548:ILE:HG22	1:D:599:VAL:HG21	2.03	0.41
1:E:346:VAL:HG13	1:E:522:ALA:O	2.21	0.41
1:E:419:ILE:HD12	1:E:419:ILE:HA	1.95	0.41
1:E:455:PHE:CE1	1:E:478:LEU:HD13	2.56	0.41
1:E:599:VAL:HB	1:E:603:ASN:HB2	2.03	0.41
1:E:681:ILE:HD12	1:E:748:ILE:HD11	2.03	0.41
1:E:722:LEU:HB2	1:E:723:PRO:HD3	2.03	0.41
1:F:218:ILE:O	1:F:222:LEU:HG	2.21	0.41
1:F:334:ASP:O	1:F:338:THR:HB	2.20	0.41
1:G:330:VAL:HB	1:G:618:THR:HG22	2.03	0.41
1:G:499:ARG:O	1:G:500:MET:HB2	2.21	0.41
1:H:116:LYS:HE3	1:H:116:LYS:HB2	1.78	0.41
1:H:445:MET:O	1:H:446:LEU:HD12	2.21	0.41
1:C:376:ILE:HG12	1:C:446:LEU:HD22	2.03	0.41
1:C:510:GLU:CD	1:C:510:GLU:H	2.24	0.41
4:C:1005:PCW:H73	4:C:1005:PCW:H41	1.74	0.41
1:D:318:LYS:HE2	1:D:652:ALA:HB1	2.02	0.41
1:D:460:TYR:HA	1:D:469:PRO:HD3	2.03	0.41
1:D:872:LYS:HB2	1:D:872:LYS:HE3	1.69	0.41
1:E:379:LEU:HD21	1:E:437:HIS:CD2	2.56	0.41
1:H:4:TYR:HB3	1:H:190:MET:HE3	2.02	0.41
1:H:235:LYS:HE2	1:H:674:PHE:CZ	2.55	0.41
1:A:755:ARG:HD3	1:A:885:PRO:CD	2.42	0.40
1:B:642:SER:OG	1:B:658:ASP:OD2	2.19	0.40
1:D:526:PRO:HA	1:D:527:PRO:HD3	1.98	0.40
1:E:22:LEU:HD13	1:E:27:VAL:HB	2.03	0.40
1:E:71:LEU:HD12	1:E:76:VAL:HG22	2.03	0.40
1:E:308:LYS:HE3	1:E:308:LYS:HB2	1.87	0.40
1:E:344:MET:HE2	1:E:491:ARG:HE	1.86	0.40
1:E:461:VAL:HG12	1:E:462:PHE:N	2.35	0.40
1:G:524:ILE:HG12	1:G:525:ASP:H	1.85	0.40
1:H:396:THR:HA	1:H:523:MET:HE1	2.03	0.40
4:B:1006:PCW:H122	4:B:1006:PCW:H362	2.02	0.40
1:E:498:LYS:CD	1:E:500:MET:HG2	2.52	0.40
1:E:712:LEU:HA	1:E:715:ILE:HG12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:453:VAL:O	1:F:457:ARG:HG3	2.20	0.40
1:G:376:ILE:HG12	1:G:446:LEU:HG	2.03	0.40
1:H:385:ILE:HG13	1:H:401:ILE:HD12	2.03	0.40
1:A:500:MET:HE2	1:A:500:MET:HB3	1.94	0.40
1:B:108:ARG:NH2	1:B:215:ILE:HD11	2.36	0.40
1:B:116:LYS:HE3	1:B:116:LYS:HB2	1.61	0.40
1:B:573:LEU:HD22	1:B:593:ILE:HD13	2.02	0.40
1:C:764:ILE:O	1:C:768:VAL:HG23	2.21	0.40
1:D:628:ALA:HB3	1:D:629:PRO:HD3	2.03	0.40
1:F:785:ALA:HB2	1:F:846:PRO:HD2	2.03	0.40
1:G:346:VAL:HG22	1:G:523:MET:HB3	2.04	0.40
1:G:436:LEU:HB2	1:G:507:LEU:HD21	2.03	0.40
1:H:231:PRO:O	1:H:235:LYS:HG3	2.21	0.40
1:H:440:ASN:OD1	1:H:441:GLU:N	2.55	0.40
1:B:884:ILE:HG21	1:B:884:ILE:HD13	1.65	0.40
1:C:71:LEU:HD23	1:C:71:LEU:HA	1.86	0.40
1:D:411:TYR:O	1:D:414:ILE:HG13	2.22	0.40
1:D:621:THR:HG21	1:D:663:ILE:HD13	2.04	0.40
1:D:735:ASP:O	1:D:739:ARG:HG3	2.21	0.40
1:F:239:PHE:CG	1:F:748:ILE:HD11	2.57	0.40
1:G:159:ILE:HD12	1:G:173:LYS:HE3	2.02	0.40
1:G:478:LEU:HD23	1:G:478:LEU:HA	1.89	0.40
1:H:394:ASP:OD1	1:H:395:PRO:HD2	2.20	0.40
1:H:625:VAL:HG22	1:H:646:VAL:HG21	2.03	0.40
1:A:201:ARG:HH21	1:A:203:MET:HE2	1.87	0.40
1:A:372:ARG:O	1:A:376:ILE:HG13	2.21	0.40
1:A:676:ASN:HB3	1:A:728:GLY:HA2	2.02	0.40
1:A:865:VAL:HA	1:A:868:MET:HE3	2.03	0.40
1:B:410:ASP:HB3	1:B:413:GLU:HG3	2.03	0.40
1:B:458:CYS:SG	1:B:517:LEU:HD12	2.62	0.40
1:B:767:ALA:HB2	1:B:864:ALA:HB2	2.03	0.40
1:D:92:ILE:CG2	1:D:299:THR:HG21	2.51	0.40
1:D:394:ASP:OD2	1:D:396:THR:HB	2.22	0.40
1:D:883:ASP:OD1	1:D:884:ILE:HG13	2.22	0.40
1:E:350:TYR:CD2	1:E:481:THR:HG21	2.57	0.40
1:E:498:LYS:NZ	1:E:499:ARG:O	2.41	0.40
1:E:671:ARG:HD2	1:E:737:MET:CE	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	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

All (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
1	H	442	ASN
1	F	46	PRO
1	H	267	ASN
1	B	440	ASN
1	F	267	ASN
1	D	179	PRO
1	E	428	SER
1	G	440	ASN
1	H	443	LYS
1	H	501	PRO
1	C	362	SER

### 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	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

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	ASN
1	A	382	ASP
1	A	434	SER
1	A	626	ASN
1	B	382	ASP
1	B	626	ASN
1	C	382	ASP
1	C	434	SER
1	C	514	ASP
1	C	536	GLU
1	C	626	ASN
1	D	47	LEU
1	D	98	ARG
1	D	140	ASP
1	D	382	ASP
1	D	434	SER
1	D	454	MET
1	D	506	GLU
1	D	880	LYS

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Mol	Chain	Res	Type
1	D	881	ASP
1	E	271	MET
1	E	281	PHE
1	E	382	ASP
1	E	418	PHE
1	E	454	MET
1	E	460	TYR
1	F	51	PHE
1	F	89	ASN
1	F	266	ASP
1	F	382	ASP
1	F	748	ILE
1	G	382	ASP
1	G	434	SER
1	G	438	THR
1	G	836	LEU
1	H	382	ASP
1	H	407	ASN
1	H	429	ASP
1	H	434	SER
1	H	454	MET
1	H	871	ILE
1	H	879	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	603	ASN
1	A	626	ASN
1	B	229	GLN
1	D	437	HIS
1	D	557	GLN
1	D	592	HIS
1	F	233	GLN

### 5.3.3 RNA [\(i\)](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [\(i\)](#)

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	-	-		
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	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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	-
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CE1	D	1006	-	-	4/9/9/34	-
4	PCW	C	1005	-	-	29/57/57/57	-

All (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
4	B	1006	PCW	P-O4P	4.27	1.76	1.59
4	A	1004	PCW	P-O4P	4.11	1.75	1.59
4	B	1004	PCW	P-O4P	4.08	1.75	1.59
4	B	1005	PCW	P-O4P	3.98	1.75	1.59
4	C	1004	PCW	P-O4P	3.85	1.74	1.59
4	B	1009	PCW	P-O4P	3.79	1.74	1.59
4	D	1003	PCW	P-O4P	3.78	1.74	1.59
4	C	1003	PCW	P-O4P	3.52	1.73	1.59
4	A	1003	PCW	P-O4P	3.46	1.73	1.59
4	B	1003	PCW	P-O4P	3.36	1.72	1.59
4	B	1007	PCW	C3-C2	3.06	1.60	1.50
4	C	1006	PCW	C3-C2	2.99	1.59	1.50
4	B	1003	PCW	C3-C2	2.97	1.59	1.50
4	B	1008	PCW	C5-N	2.90	1.60	1.51
4	C	1005	PCW	C3-C2	2.41	1.58	1.50
4	D	1003	PCW	C8-N	2.40	1.57	1.50
4	C	1005	PCW	C5-N	2.31	1.59	1.51
4	B	1009	PCW	P-O3P	2.28	1.68	1.59
4	B	1003	PCW	P-O3P	2.25	1.68	1.59
4	B	1007	PCW	P-O3P	2.21	1.68	1.59
4	B	1003	PCW	O3-C11	2.19	1.39	1.33
4	C	1004	PCW	C3-C2	2.14	1.57	1.50
4	A	1003	PCW	P-O1P	-2.12	1.45	1.55
4	B	1008	PCW	P-O1P	-2.11	1.45	1.55
4	B	1003	PCW	P-O1P	-2.10	1.45	1.55
4	C	1003	PCW	P-O1P	-2.10	1.45	1.55
4	B	1008	PCW	P-O3P	2.10	1.67	1.59
4	B	1007	PCW	P-O1P	-2.10	1.45	1.55
4	B	1004	PCW	P-O1P	-2.09	1.45	1.55
4	D	1003	PCW	P-O1P	-2.09	1.45	1.55
4	C	1006	PCW	P-O1P	-2.09	1.45	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1009	PCW	O2-C31	2.09	1.40	1.34
4	C	1005	PCW	P-O3P	2.08	1.67	1.59
4	A	1004	PCW	P-O1P	-2.08	1.45	1.55
4	C	1008	PCW	P-O1P	-2.08	1.45	1.55
4	B	1005	PCW	P-O1P	-2.08	1.45	1.55
4	B	1004	PCW	P-O3P	2.07	1.67	1.59
4	C	1005	PCW	P-O1P	-2.07	1.45	1.55
4	B	1006	PCW	P-O1P	-2.07	1.45	1.55
4	B	1009	PCW	P-O1P	-2.06	1.45	1.55
4	C	1004	PCW	P-O1P	-2.06	1.45	1.55
4	D	1003	PCW	O2-C31	2.04	1.40	1.34
4	B	1009	PCW	C3-C2	2.04	1.57	1.50
4	B	1004	PCW	O2-C31	2.04	1.40	1.34

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
4	C	1008	PCW	O4P-P-O2P	-3.04	97.19	109.07
4	B	1003	PCW	O4P-P-O2P	-3.02	97.25	109.07
4	C	1008	PCW	O1P-P-O2P	3.02	127.18	112.24
4	C	1008	PCW	O2-C31-C32	3.01	117.98	111.50
4	D	1003	PCW	O1P-P-O2P	2.99	127.03	112.24
4	B	1008	PCW	O4P-P-O2P	-2.99	97.39	109.07
4	B	1005	PCW	O2-C31-C32	2.99	117.93	111.50
4	B	1009	PCW	O1P-P-O2P	2.98	126.98	112.24
4	C	1006	PCW	O1P-P-O2P	2.97	126.92	112.24
4	B	1004	PCW	O1P-P-O2P	2.96	126.89	112.24
4	C	1006	PCW	O4P-P-O2P	-2.96	97.49	109.07
4	B	1007	PCW	O4P-P-O2P	-2.96	97.51	109.07
4	B	1004	PCW	O4P-P-O2P	-2.95	97.55	109.07
4	B	1005	PCW	O1P-P-O2P	2.95	126.81	112.24
4	A	1004	PCW	O1P-P-O2P	2.94	126.78	112.24
4	B	1009	PCW	O4P-P-O2P	-2.92	97.64	109.07
4	B	1003	PCW	P-O4P-C4	-2.91	107.24	121.59
4	C	1005	PCW	O1P-P-O2P	2.91	126.65	112.24
4	C	1006	PCW	O2-C31-C32	2.90	117.75	111.50
4	C	1004	PCW	O1P-P-O2P	2.90	126.56	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1003	PCW	O4P-P-O2P	-2.88	97.83	109.07
4	B	1007	PCW	O1P-P-O2P	2.84	126.28	112.24
4	A	1004	PCW	O4P-P-O2P	-2.84	97.98	109.07
4	B	1004	PCW	O2-C31-C32	2.81	117.55	111.50
4	A	1003	PCW	O1P-P-O2P	2.79	126.06	112.24
4	B	1006	PCW	O4P-P-O2P	-2.79	98.16	109.07
4	C	1005	PCW	O4P-P-O2P	-2.79	98.16	109.07
4	C	1003	PCW	O4P-P-O2P	-2.78	98.19	109.07
4	C	1004	PCW	O4P-P-O2P	-2.76	98.28	109.07
4	B	1007	PCW	P-O4P-C4	-2.73	108.17	121.59
4	B	1005	PCW	P-O4P-C4	-2.71	108.22	121.59
4	B	1005	PCW	O4P-P-O2P	-2.71	98.47	109.07
4	C	1003	PCW	C4-C5-N	-2.67	106.86	115.78
4	B	1009	PCW	O2-C31-C32	2.67	117.25	111.50
4	B	1007	PCW	O2-C31-C32	2.66	117.24	111.50
4	C	1003	PCW	P-O4P-C4	-2.66	108.50	121.59
4	C	1004	PCW	O2-C31-C32	2.65	117.22	111.50
4	C	1008	PCW	P-O4P-C4	-2.61	108.74	121.59
4	A	1003	PCW	P-O4P-C4	-2.60	108.78	121.59
4	B	1008	PCW	O2-C31-C32	2.60	117.10	111.50
4	B	1009	PCW	P-O4P-C4	-2.59	108.83	121.59
4	B	1005	PCW	P-O3P-C1	-2.57	106.59	121.68
4	C	1005	PCW	O2-C31-C32	2.56	117.02	111.50
4	D	1003	PCW	P-O3P-C1	-2.56	106.69	121.68
4	C	1004	PCW	P-O4P-C4	-2.55	109.03	121.59
4	D	1003	PCW	P-O4P-C4	-2.55	109.06	121.59
4	B	1006	PCW	P-O4P-C4	-2.53	109.12	121.59
4	B	1008	PCW	P-O4P-C4	-2.50	109.27	121.59
4	C	1006	PCW	P-O3P-C1	-2.45	107.29	121.68
4	A	1004	PCW	O2-C31-C32	2.44	116.75	111.50
4	B	1004	PCW	P-O4P-C4	-2.43	109.60	121.59
4	C	1005	PCW	P-O4P-C4	-2.38	109.86	121.59
4	A	1004	PCW	P-O3P-C1	-2.38	107.72	121.68
4	C	1003	PCW	P-O3P-C1	-2.34	107.97	121.68
4	A	1004	PCW	P-O4P-C4	-2.34	110.08	121.59
4	B	1003	PCW	P-O3P-C1	-2.33	108.02	121.68
4	D	1003	PCW	C4-C5-N	-2.28	108.16	115.78
4	C	1006	PCW	P-O4P-C4	-2.22	110.68	121.59
4	C	1004	PCW	P-O3P-C1	-2.21	108.72	121.68
4	C	1008	PCW	P-O3P-C1	-2.19	108.84	121.68
4	A	1003	PCW	P-O3P-C1	-2.18	108.88	121.68
4	B	1004	PCW	P-O3P-C1	-2.14	109.13	121.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1005	PCW	P-O3P-C1	-2.13	109.22	121.68
4	C	1003	PCW	O2-C31-C32	2.10	116.03	111.50
4	C	1006	PCW	O2-C31-O31	-2.06	118.72	123.70
4	B	1003	PCW	O2-C31-C32	2.03	115.87	111.50
4	B	1003	PCW	C4-C5-N	-2.02	109.03	115.78
5	C	1007	CE1	C14-O13-C12	-2.02	105.67	112.90

There are no chirality outliers.

All (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
4	A	1004	PCW	C32-C31-O2-C2
4	A	1004	PCW	C1-O3P-P-O1P
4	A	1004	PCW	C4-O4P-P-O2P
4	B	1003	PCW	O4P-C4-C5-N
4	B	1003	PCW	C4-O4P-P-O1P
4	B	1003	PCW	C4-O4P-P-O2P
4	B	1004	PCW	C32-C31-O2-C2
4	B	1004	PCW	O31-C31-O2-C2
4	B	1004	PCW	C4-O4P-P-O1P
4	B	1005	PCW	O4P-C4-C5-N
4	B	1005	PCW	C4-O4P-P-O2P
4	B	1006	PCW	C1-O3P-P-O2P
4	B	1006	PCW	C4-O4P-P-O1P
4	B	1006	PCW	C4-O4P-P-O2P
4	B	1007	PCW	C1-O3P-P-O1P
4	B	1007	PCW	C4-O4P-P-O1P
4	B	1007	PCW	C4-O4P-P-O2P
4	B	1008	PCW	O4P-C4-C5-N
4	B	1008	PCW	C32-C31-O2-C2
4	B	1008	PCW	C1-O3P-P-O1P
4	B	1008	PCW	C4-O4P-P-O1P
4	B	1009	PCW	C40-C41-C42-C43
4	B	1009	PCW	C1-O3P-P-O1P
4	B	1009	PCW	C1-O3P-P-O2P
4	B	1009	PCW	C4-O4P-P-O1P
4	C	1003	PCW	C4-O4P-P-O1P

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Mol	Chain	Res	Type	Atoms
4	C	1003	PCW	C4-O4P-P-O2P
4	C	1004	PCW	O4P-C4-C5-N
4	C	1004	PCW	C4-O4P-P-O1P
4	C	1005	PCW	O4P-C4-C5-N
4	C	1005	PCW	C32-C31-O2-C2
4	C	1006	PCW	O4P-C4-C5-N
4	C	1006	PCW	C5-C4-O4P-P
4	C	1006	PCW	C32-C31-O2-C2
4	C	1006	PCW	O31-C31-O2-C2
4	C	1006	PCW	C1-O3P-P-O2P
4	C	1008	PCW	O4P-C4-C5-N
4	C	1008	PCW	C1-O3P-P-O4P
4	D	1003	PCW	O4P-C4-C5-N
4	B	1005	PCW	O11-C11-O3-C3
4	B	1005	PCW	C12-C11-O3-C3
4	A	1004	PCW	O31-C31-O2-C2
4	B	1008	PCW	O31-C31-O2-C2
4	C	1005	PCW	O31-C31-O2-C2
4	B	1007	PCW	C12-C11-O3-C3
4	B	1007	PCW	O11-C11-O3-C3
4	B	1008	PCW	C12-C11-O3-C3
4	C	1003	PCW	C15-C16-C17-C18
4	D	1003	PCW	C22-C23-C24-C25
5	D	1004	CE1	C7-C8-C9-C10
4	D	1003	PCW	C42-C43-C44-C45
5	C	1007	CE1	C10-C11-C12-O13
4	B	1008	PCW	O11-C11-O3-C3
4	A	1004	PCW	C12-C11-O3-C3
4	A	1004	PCW	O11-C11-O3-C3
4	B	1004	PCW	C35-C36-C37-C38
4	B	1006	PCW	C4-C5-N-C6
4	C	1006	PCW	C12-C11-O3-C3
4	C	1005	PCW	C31-C32-C33-C34
4	B	1004	PCW	C12-C11-O3-C3
4	B	1004	PCW	C11-C12-C13-C14
4	B	1009	PCW	C31-C32-C33-C34
4	A	1003	PCW	C31-C32-C33-C34
4	A	1004	PCW	C31-C32-C33-C34
4	C	1005	PCW	C11-C12-C13-C14
4	C	1008	PCW	C31-C32-C33-C34
4	D	1003	PCW	C11-C12-C13-C14
4	D	1003	PCW	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
5	D	1005	CE1	C11-C10-C9-C8
4	B	1004	PCW	C4-C5-N-C8
4	B	1006	PCW	C31-C32-C33-C34
4	C	1005	PCW	C42-C43-C44-C45
4	C	1006	PCW	O11-C11-O3-C3
4	B	1004	PCW	O11-C11-O3-C3
4	C	1004	PCW	C20-C21-C22-C23
4	D	1003	PCW	C40-C41-C42-C43
4	A	1004	PCW	C4-O4P-P-O3P
4	B	1003	PCW	C4-O4P-P-O3P
4	B	1004	PCW	C4-O4P-P-O3P
4	B	1005	PCW	C4-O4P-P-O3P
4	B	1006	PCW	C1-O3P-P-O4P
4	B	1006	PCW	C4-O4P-P-O3P
4	B	1007	PCW	C1-O3P-P-O4P
4	B	1007	PCW	C4-O4P-P-O3P
4	B	1008	PCW	C1-O3P-P-O4P
4	B	1008	PCW	C4-O4P-P-O3P
4	B	1009	PCW	C1-O3P-P-O4P
4	B	1009	PCW	C4-O4P-P-O3P
4	C	1003	PCW	C1-O3P-P-O4P
4	C	1003	PCW	C4-O4P-P-O3P
4	C	1004	PCW	C4-O4P-P-O3P
4	C	1005	PCW	C4-O4P-P-O3P
4	C	1006	PCW	C1-O3P-P-O4P
4	C	1006	PCW	C4-O4P-P-O3P
4	B	1006	PCW	C4-C5-N-C7
4	B	1006	PCW	C4-C5-N-C8
4	B	1009	PCW	C4-C5-N-C6
4	B	1009	PCW	C4-C5-N-C7
4	B	1009	PCW	C4-C5-N-C8
4	C	1005	PCW	C4-C5-N-C6
4	C	1005	PCW	C4-C5-N-C7
4	C	1005	PCW	C4-C5-N-C8
4	C	1006	PCW	C4-C5-N-C6
4	C	1006	PCW	C4-C5-N-C7
4	C	1006	PCW	C4-C5-N-C8
4	B	1004	PCW	C12-C13-C14-C15
4	B	1008	PCW	C34-C35-C36-C37
4	C	1003	PCW	C44-C45-C46-C47
4	C	1005	PCW	C44-C45-C46-C47
4	D	1003	PCW	C43-C44-C45-C46

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Mol	Chain	Res	Type	Atoms
4	B	1009	PCW	C15-C16-C17-C18
4	C	1008	PCW	C14-C15-C16-C17
4	C	1008	PCW	C22-C23-C24-C25
4	A	1004	PCW	C21-C22-C23-C24
4	D	1003	PCW	C13-C14-C15-C16
4	C	1005	PCW	C3-C2-O2-C31
4	A	1003	PCW	C15-C16-C17-C18
4	A	1004	PCW	C44-C45-C46-C47
4	B	1005	PCW	C24-C25-C26-C27
4	B	1009	PCW	C32-C33-C34-C35
4	B	1009	PCW	C43-C44-C45-C46
4	C	1004	PCW	C21-C22-C23-C24
4	A	1004	PCW	C35-C36-C37-C38
4	B	1004	PCW	C43-C44-C45-C46
4	B	1006	PCW	C13-C14-C15-C16
4	A	1004	PCW	C43-C44-C45-C46
4	B	1007	PCW	C22-C23-C24-C25
4	C	1006	PCW	C21-C22-C23-C24
4	A	1003	PCW	C11-C12-C13-C14
4	C	1008	PCW	C11-C12-C13-C14
4	B	1003	PCW	O2-C2-C3-O3
5	D	1004	CE1	C4-C5-C6-C7
4	A	1004	PCW	C33-C34-C35-C36
4	B	1004	PCW	C15-C16-C17-C18
4	B	1004	PCW	C34-C35-C36-C37
4	C	1003	PCW	C22-C23-C24-C25
4	C	1008	PCW	C32-C33-C34-C35
4	C	1004	PCW	C11-C12-C13-C14
4	B	1008	PCW	C42-C43-C44-C45
4	C	1004	PCW	C12-C13-C14-C15
4	C	1008	PCW	C15-C16-C17-C18
4	D	1003	PCW	C15-C16-C17-C18
4	D	1003	PCW	C35-C36-C37-C38
5	D	1007	CE1	C4-C5-C6-C7
5	D	1009	CE1	C3-C4-C5-C6
4	B	1006	PCW	O31-C31-O2-C2
4	B	1006	PCW	C32-C31-O2-C2
4	B	1006	PCW	C33-C34-C35-C36
4	D	1003	PCW	C12-C13-C14-C15
4	B	1007	PCW	C12-C13-C14-C15
4	C	1006	PCW	C14-C15-C16-C17
4	B	1006	PCW	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
4	C	1005	PCW	C43-C44-C45-C46
4	C	1003	PCW	C31-C32-C33-C34
4	B	1005	PCW	C44-C45-C46-C47
5	D	1008	CE1	C6-C7-C8-C9
4	B	1005	PCW	C32-C33-C34-C35
4	C	1003	PCW	C41-C42-C43-C44
4	C	1006	PCW	C13-C14-C15-C16
4	B	1007	PCW	C32-C33-C34-C35
4	B	1008	PCW	C24-C25-C26-C27
4	D	1003	PCW	C14-C15-C16-C17
4	B	1006	PCW	C35-C36-C37-C38
5	C	1007	CE1	C7-C8-C9-C10
5	D	1009	CE1	C11-C10-C9-C8
4	B	1009	PCW	C32-C31-O2-C2
4	B	1004	PCW	C42-C43-C44-C45
4	B	1008	PCW	C13-C14-C15-C16
5	D	1008	CE1	C5-C6-C7-C8
4	B	1007	PCW	C40-C41-C42-C43
4	C	1006	PCW	C40-C41-C42-C43
4	B	1003	PCW	C21-C22-C23-C24
4	B	1005	PCW	C41-C42-C43-C44
5	D	1004	CE1	C3-C4-C5-C6
4	B	1003	PCW	C22-C23-C24-C25
4	C	1005	PCW	C32-C33-C34-C35
5	D	1006	CE1	C6-C7-C8-C9
4	B	1005	PCW	C31-C32-C33-C34
4	A	1003	PCW	C14-C15-C16-C17
4	C	1005	PCW	C45-C46-C47-C48
4	B	1003	PCW	C35-C36-C37-C38
4	B	1008	PCW	C43-C44-C45-C46
4	B	1008	PCW	C16-C17-C18-C19
4	B	1008	PCW	C36-C37-C38-C39
4	B	1009	PCW	C20-C21-C22-C23
4	C	1008	PCW	C20-C21-C22-C23
4	B	1009	PCW	O31-C31-O2-C2
4	C	1008	PCW	O31-C31-O2-C2
4	B	1006	PCW	C11-C12-C13-C14
4	B	1009	PCW	C11-C12-C13-C14
4	C	1004	PCW	C13-C14-C15-C16
4	B	1004	PCW	C31-C32-C33-C34
4	B	1004	PCW	C21-C22-C23-C24
4	B	1007	PCW	C41-C42-C43-C44

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Mol	Chain	Res	Type	Atoms
4	B	1009	PCW	C12-C13-C14-C15
5	D	1006	CE1	C9-C10-C11-C12
4	C	1005	PCW	C34-C35-C36-C37
4	C	1008	PCW	C24-C25-C26-C27
4	C	1008	PCW	C32-C31-O2-C2
4	C	1003	PCW	C21-C22-C23-C24
4	B	1009	PCW	C13-C14-C15-C16
4	B	1003	PCW	C41-C42-C43-C44
4	C	1006	PCW	C41-C42-C43-C44
4	B	1004	PCW	C4-C5-N-C6
4	B	1004	PCW	C4-C5-N-C7
4	C	1004	PCW	C4-C5-N-C7
4	A	1003	PCW	C36-C37-C38-C39
4	A	1003	PCW	C40-C41-C42-C43
4	A	1004	PCW	C36-C37-C38-C39
4	B	1006	PCW	C20-C21-C22-C23
4	C	1005	PCW	C20-C21-C22-C23
4	D	1003	PCW	C36-C37-C38-C39
4	D	1003	PCW	C33-C34-C35-C36
5	D	1009	CE1	C2-C3-C4-C5
5	C	1007	CE1	C9-C10-C11-C12
4	B	1006	PCW	C34-C35-C36-C37
4	C	1004	PCW	C32-C31-O2-C2
4	B	1003	PCW	C15-C16-C17-C18
4	B	1005	PCW	C19-C20-C21-C22
4	A	1004	PCW	C1-O3P-P-O4P
4	B	1005	PCW	C22-C23-C24-C25
4	A	1004	PCW	C13-C14-C15-C16
4	A	1003	PCW	C20-C21-C22-C23
4	B	1004	PCW	C20-C21-C22-C23
4	B	1004	PCW	C36-C37-C38-C39
4	B	1006	PCW	C44-C45-C46-C47
4	B	1008	PCW	C32-C33-C34-C35
4	B	1005	PCW	C43-C44-C45-C46
4	B	1003	PCW	C25-C26-C27-C28
4	B	1004	PCW	C45-C46-C47-C48
5	C	1007	CE1	C2-C3-C4-C5
4	B	1007	PCW	C25-C26-C27-C28
4	B	1003	PCW	C16-C17-C18-C19
4	C	1005	PCW	C40-C41-C42-C43
4	B	1005	PCW	C12-C13-C14-C15
4	B	1004	PCW	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
4	A	1003	PCW	C12-C13-C14-C15
4	C	1006	PCW	C33-C34-C35-C36
5	D	1008	CE1	C4-C5-C6-C7
4	B	1006	PCW	C12-C11-O3-C3
4	C	1004	PCW	C45-C46-C47-C48
4	B	1005	PCW	O2-C2-C3-O3
4	B	1004	PCW	C25-C26-C27-C28
4	A	1003	PCW	C41-C42-C43-C44
4	B	1008	PCW	C31-C32-C33-C34
4	B	1009	PCW	C19-C20-C21-C22
4	B	1004	PCW	C41-C42-C43-C44
4	B	1006	PCW	C25-C26-C27-C28
4	C	1008	PCW	C21-C22-C23-C24
4	B	1009	PCW	C37-C38-C39-C40
4	B	1003	PCW	O3P-C1-C2-C3
4	B	1007	PCW	O3P-C1-C2-C3
4	C	1004	PCW	O3P-C1-C2-C3
4	C	1005	PCW	O3P-C1-C2-C3
4	C	1005	PCW	C24-C25-C26-C27
4	B	1007	PCW	C11-C12-C13-C14
4	B	1005	PCW	C14-C15-C16-C17
4	B	1009	PCW	C33-C34-C35-C36
4	B	1008	PCW	C2-C1-O3P-P
4	C	1006	PCW	C2-C1-O3P-P
4	B	1003	PCW	C1-C2-C3-O3
4	B	1004	PCW	C1-C2-C3-O3
4	B	1006	PCW	C1-C2-C3-O3
4	B	1007	PCW	C1-C2-C3-O3
4	B	1008	PCW	C1-C2-C3-O3
4	C	1004	PCW	C1-C2-C3-O3
4	C	1004	PCW	O31-C31-O2-C2
4	C	1006	PCW	C23-C24-C25-C26
4	C	1004	PCW	C15-C16-C17-C18
4	B	1003	PCW	C14-C15-C16-C17
4	B	1006	PCW	O3P-C1-C2-O2
4	B	1009	PCW	O3P-C1-C2-O2
4	C	1004	PCW	O3P-C1-C2-O2
4	B	1006	PCW	O11-C11-O3-C3
4	A	1003	PCW	O2-C2-C3-O3
4	B	1006	PCW	O2-C2-C3-O3
4	B	1008	PCW	O2-C2-C3-O3
4	C	1004	PCW	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	B	1006	PCW	C17-C18-C19-C20
4	A	1003	PCW	C22-C23-C24-C25
4	B	1003	PCW	C34-C35-C36-C37
4	B	1005	PCW	C40-C41-C42-C43
4	C	1003	PCW	C45-C46-C47-C48
4	C	1005	PCW	C13-C14-C15-C16
4	C	1004	PCW	C4-C5-N-C8
4	B	1007	PCW	C35-C36-C37-C38
5	D	1009	CE1	C7-C8-C9-C10
4	C	1005	PCW	C15-C16-C17-C18
4	C	1008	PCW	C42-C43-C44-C45
4	A	1003	PCW	O3P-C1-C2-C3
4	D	1003	PCW	O3P-C1-C2-C3
4	C	1005	PCW	C12-C13-C14-C15
4	D	1003	PCW	C23-C24-C25-C26
4	B	1006	PCW	C24-C25-C26-C27
4	B	1007	PCW	O31-C31-O2-C2
4	B	1009	PCW	C12-C11-O3-C3
4	B	1003	PCW	C33-C34-C35-C36
4	A	1004	PCW	C25-C26-C27-C28
5	D	1004	CE1	C5-C6-C7-C8
4	A	1003	PCW	C1-C2-C3-O3
4	B	1007	PCW	C32-C31-O2-C2
4	A	1003	PCW	O3P-C1-C2-O2
4	C	1008	PCW	O3P-C1-C2-O2
4	A	1003	PCW	C21-C22-C23-C24
4	C	1004	PCW	C44-C45-C46-C47
4	B	1009	PCW	C14-C15-C16-C17
4	A	1004	PCW	O2-C2-C3-O3
4	B	1004	PCW	O2-C2-C3-O3
4	D	1003	PCW	O2-C2-C3-O3
4	B	1008	PCW	C15-C16-C17-C18
4	B	1009	PCW	O11-C11-O3-C3
4	C	1006	PCW	C32-C33-C34-C35
4	B	1005	PCW	C13-C14-C15-C16
4	C	1008	PCW	C25-C26-C27-C28
4	B	1008	PCW	C41-C42-C43-C44
4	B	1003	PCW	C1-O3P-P-O4P
4	C	1005	PCW	C1-O3P-P-O4P
4	D	1003	PCW	C1-O3P-P-O4P
4	B	1007	PCW	C33-C34-C35-C36
4	A	1004	PCW	C4-O4P-P-O1P

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Mol	Chain	Res	Type	Atoms
4	B	1005	PCW	C4-O4P-P-O1P
4	B	1006	PCW	C1-O3P-P-O1P
4	B	1007	PCW	C4-C5-N-C8
4	B	1007	PCW	C1-O3P-P-O2P
4	B	1008	PCW	C1-O3P-P-O2P
4	B	1008	PCW	C4-O4P-P-O2P
4	B	1009	PCW	C4-O4P-P-O2P
4	C	1003	PCW	C1-O3P-P-O1P
4	C	1005	PCW	C4-O4P-P-O1P
4	C	1006	PCW	C4-O4P-P-O2P
4	C	1008	PCW	C1-O3P-P-O1P
4	B	1004	PCW	O3P-C1-C2-C3
4	C	1008	PCW	O3P-C1-C2-C3
4	B	1008	PCW	C40-C41-C42-C43
4	C	1008	PCW	C41-C42-C43-C44
5	C	1007	CE1	C11-C10-C9-C8
4	B	1004	PCW	O3P-C1-C2-O2
4	B	1007	PCW	O3P-C1-C2-O2
4	C	1005	PCW	O3P-C1-C2-O2
4	C	1006	PCW	C31-C32-C33-C34
5	D	1006	CE1	C11-C10-C9-C8
4	A	1004	PCW	C11-C12-C13-C14
4	B	1005	PCW	C34-C35-C36-C37
4	B	1004	PCW	O4P-C4-C5-N
4	B	1005	PCW	C1-C2-C3-O3
4	C	1003	PCW	O4P-C4-C5-N
4	B	1007	PCW	O2-C2-C3-O3
4	C	1006	PCW	O2-C2-C3-O3
4	C	1004	PCW	C41-C42-C43-C44
4	B	1009	PCW	C23-C24-C25-C26
5	C	1007	CE1	C1-C2-C3-C4
4	C	1008	PCW	O11-C11-O3-C3
5	D	1008	CE1	C11-C10-C9-C8
4	C	1003	PCW	C24-C25-C26-C27
4	C	1004	PCW	C25-C26-C27-C28
4	C	1004	PCW	C40-C41-C42-C43
4	B	1005	PCW	C42-C43-C44-C45
4	B	1005	PCW	C33-C34-C35-C36
4	A	1004	PCW	C1-C2-O2-C31
4	B	1009	PCW	O3P-C1-C2-C3
4	C	1006	PCW	C22-C23-C24-C25
4	C	1005	PCW	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
4	C	1006	PCW	C25-C26-C27-C28
4	D	1003	PCW	O3P-C1-C2-O2
4	B	1007	PCW	C4-C5-N-C6
4	C	1004	PCW	C4-C5-N-C6
4	C	1008	PCW	C12-C11-O3-C3
4	B	1004	PCW	C1-O3P-P-O4P
4	A	1003	PCW	C17-C18-C19-C20
4	B	1003	PCW	C19-C20-C21-C22
4	B	1008	PCW	C20-C21-C22-C23
4	B	1003	PCW	C12-C11-O3-C3
4	B	1003	PCW	O11-C11-O3-C3
4	B	1007	PCW	C14-C15-C16-C17
4	B	1004	PCW	C2-C1-O3P-P
4	C	1004	PCW	C17-C18-C19-C20
4	A	1004	PCW	C20-C21-C22-C23
4	C	1003	PCW	C32-C33-C34-C35
4	D	1003	PCW	C44-C45-C46-C47
4	C	1008	PCW	C44-C45-C46-C47
4	B	1008	PCW	C14-C15-C16-C17
4	C	1006	PCW	C15-C16-C17-C18
5	D	1008	CE1	C3-C4-C5-C6
4	A	1003	PCW	C13-C14-C15-C16
4	D	1003	PCW	C1-C2-C3-O3
4	C	1004	PCW	C12-C11-O3-C3
5	D	1006	CE1	C5-C6-C7-C8
4	B	1007	PCW	C20-C21-C22-C23
4	B	1008	PCW	C21-C22-C23-C24
4	B	1007	PCW	C4-C5-N-C7
4	D	1003	PCW	C19-C20-C21-C22
4	C	1008	PCW	C12-C13-C14-C15
4	C	1006	PCW	O3P-C1-C2-O2
5	D	1009	CE1	C5-C6-C7-C8
4	C	1004	PCW	O11-C11-O3-C3
4	A	1004	PCW	C42-C43-C44-C45
4	D	1003	PCW	C21-C22-C23-C24
4	B	1005	PCW	C15-C16-C17-C18
4	C	1006	PCW	C44-C45-C46-C47
5	D	1004	CE1	C9-C10-C11-C12
5	D	1005	CE1	C7-C8-C9-C10
4	A	1004	PCW	C37-C38-C39-C40
4	B	1004	PCW	C37-C38-C39-C40
4	B	1003	PCW	O3P-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	B	1006	PCW	O3P-C1-C2-C3
4	C	1006	PCW	C37-C38-C39-C40
4	C	1004	PCW	C2-C1-O3P-P
4	B	1005	PCW	O2-C31-C32-C33
4	C	1003	PCW	O3-C11-C12-C13
4	B	1003	PCW	C45-C46-C47-C48
4	C	1004	PCW	C42-C43-C44-C45
4	B	1003	PCW	C17-C18-C19-C20
4	B	1003	PCW	C39-C40-C41-C42
4	C	1008	PCW	C17-C18-C19-C20
4	C	1008	PCW	C4-C5-N-C6
4	C	1003	PCW	O2-C31-C32-C33
4	A	1003	PCW	C25-C26-C27-C28
4	C	1008	PCW	C13-C14-C15-C16
4	B	1005	PCW	C39-C40-C41-C42
4	B	1007	PCW	C17-C18-C19-C20
4	B	1008	PCW	C19-C20-C21-C22
4	C	1004	PCW	C37-C38-C39-C40
4	C	1008	PCW	O3-C11-C12-C13
4	A	1004	PCW	C19-C20-C21-C22
4	C	1004	PCW	C19-C20-C21-C22
4	C	1006	PCW	C19-C20-C21-C22
4	C	1008	PCW	C37-C38-C39-C40
4	A	1004	PCW	C40-C41-C42-C43
4	A	1004	PCW	C1-C2-C3-O3
4	C	1006	PCW	C45-C46-C47-C48
4	C	1004	PCW	C14-C15-C16-C17
4	C	1006	PCW	O2-C31-C32-C33
4	C	1003	PCW	C23-C24-C25-C26
4	C	1003	PCW	C17-C18-C19-C20
4	A	1003	PCW	O2-C31-C32-C33
4	B	1005	PCW	C25-C26-C27-C28
4	A	1003	PCW	C39-C40-C41-C42
4	B	1005	PCW	C17-C18-C19-C20
4	C	1004	PCW	C23-C24-C25-C26
4	B	1005	PCW	O31-C31-C32-C33
4	B	1008	PCW	C39-C40-C41-C42
4	C	1005	PCW	C37-C38-C39-C40
4	B	1005	PCW	C35-C36-C37-C38
4	D	1003	PCW	O11-C11-O3-C3
4	C	1003	PCW	O31-C31-C32-C33
4	A	1003	PCW	C34-C35-C36-C37

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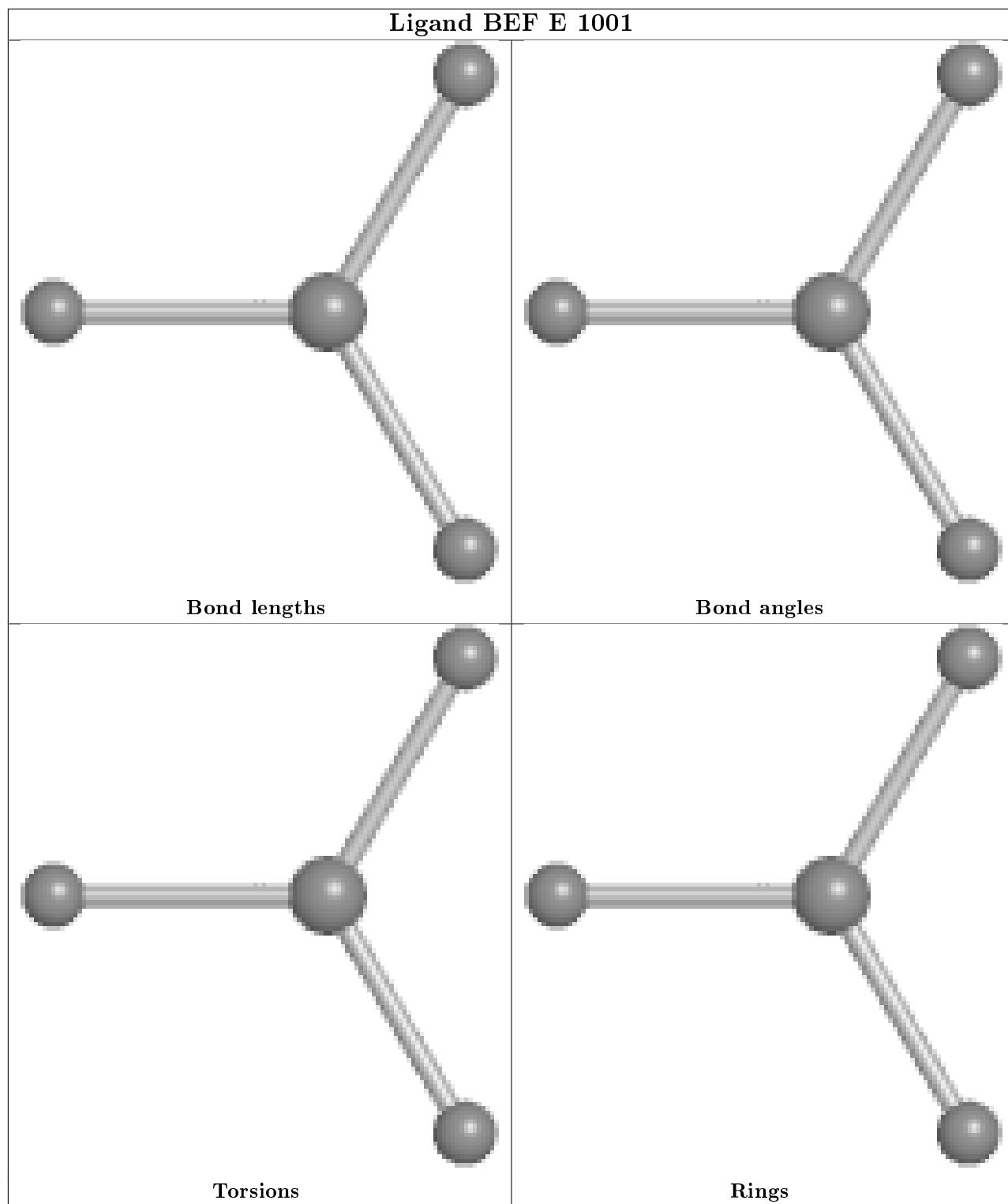
Mol	Chain	Res	Type	Atoms
4	B	1007	PCW	C39-C40-C41-C42
4	C	1003	PCW	O11-C11-C12-C13
4	C	1006	PCW	C1-C2-C3-O3
4	C	1008	PCW	O11-C11-C12-C13
4	B	1004	PCW	C1-O3P-P-O2P
4	C	1003	PCW	C1-O3P-P-O2P
4	D	1003	PCW	C1-O3P-P-O2P
4	C	1006	PCW	O3P-C1-C2-C3
4	C	1006	PCW	O31-C31-C32-C33
4	B	1005	PCW	C5-C4-O4P-P
4	A	1003	PCW	C33-C34-C35-C36
4	D	1003	PCW	C12-C11-O3-C3
4	C	1008	PCW	C4-C5-N-C7
4	C	1008	PCW	C4-C5-N-C8
4	B	1006	PCW	C43-C44-C45-C46
4	A	1003	PCW	O31-C31-C32-C33
5	D	1005	CE1	C6-C7-C8-C9
4	C	1005	PCW	C19-C20-C21-C22

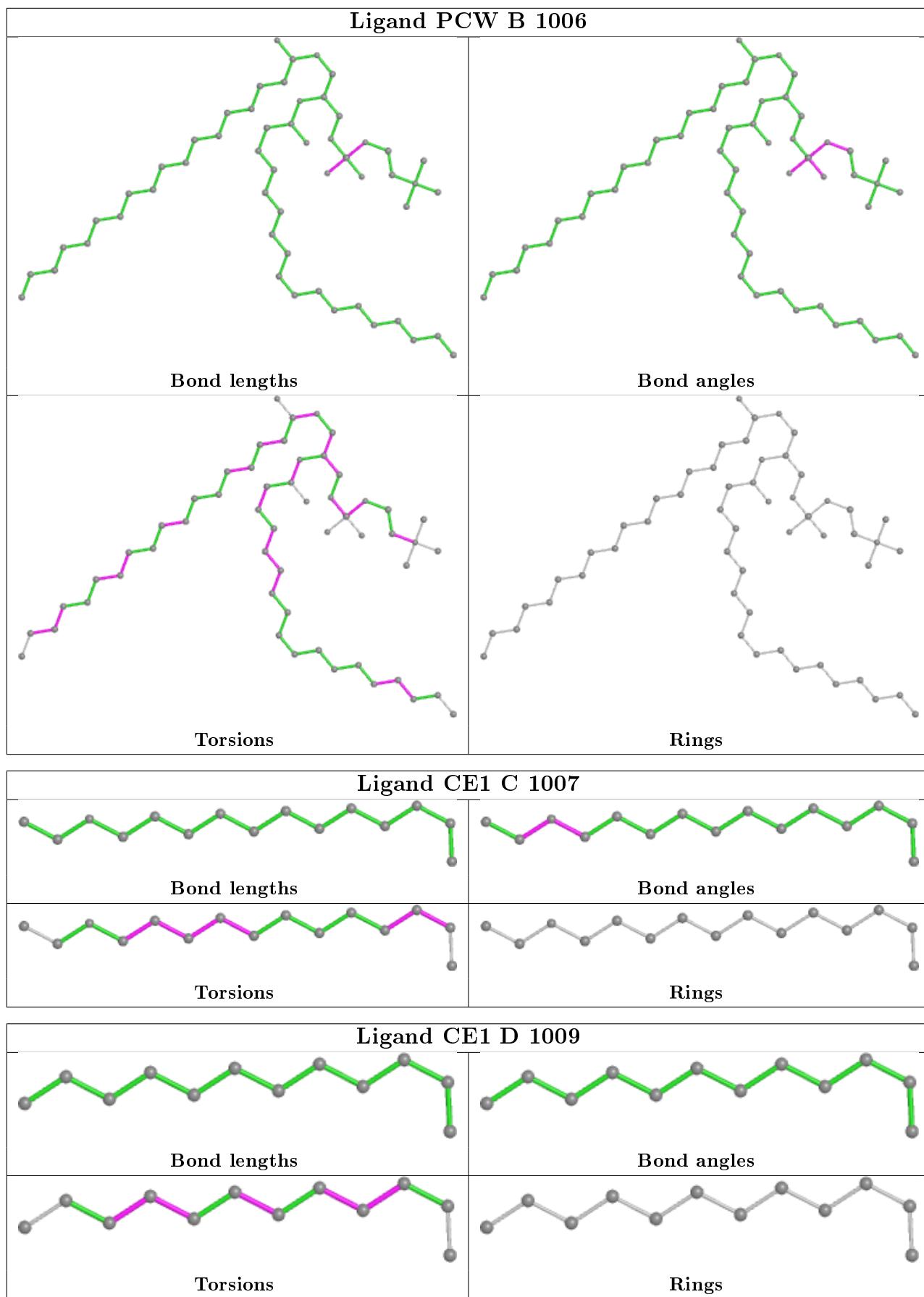
There are no ring outliers.

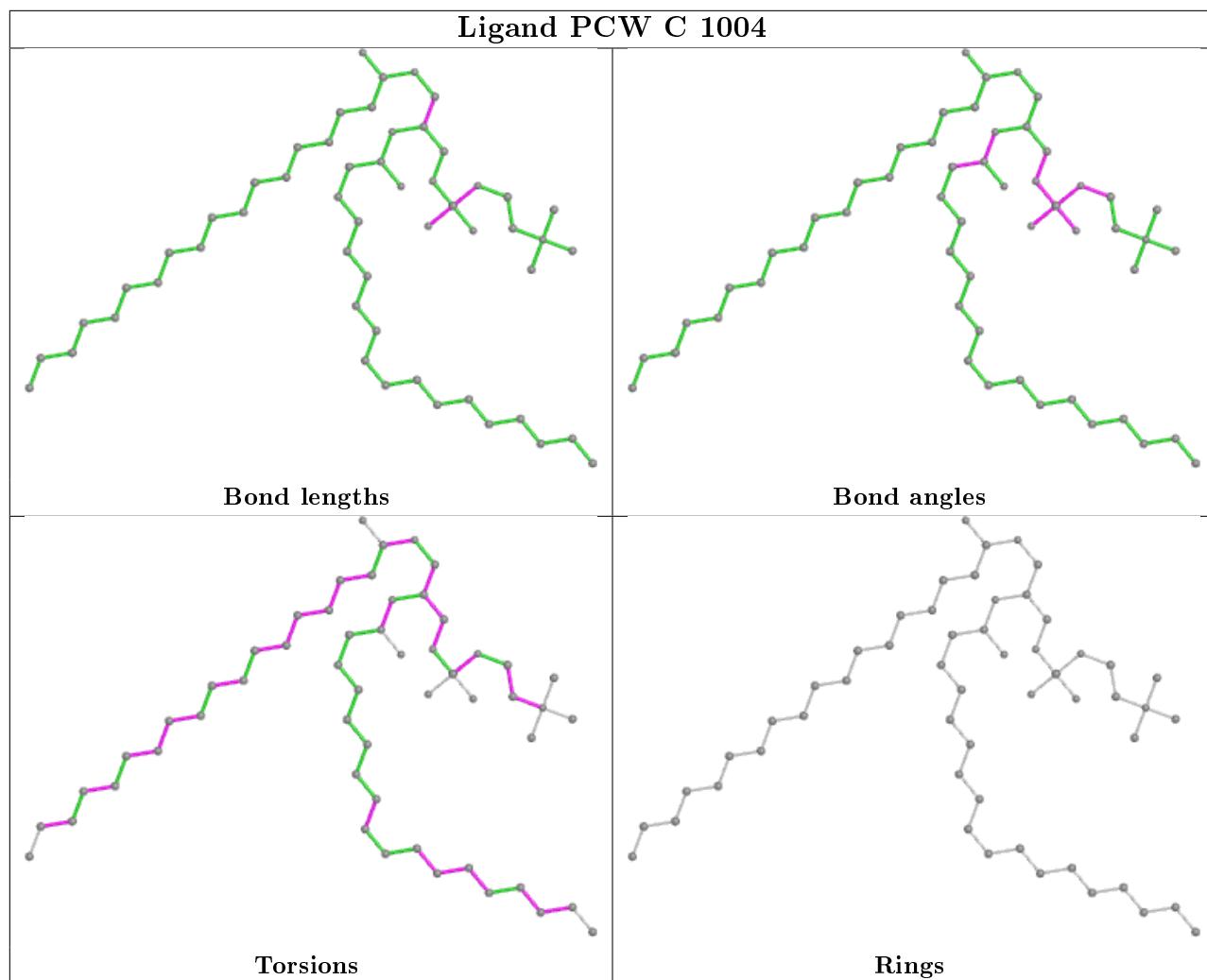
19 monomers are involved in 57 short contacts:

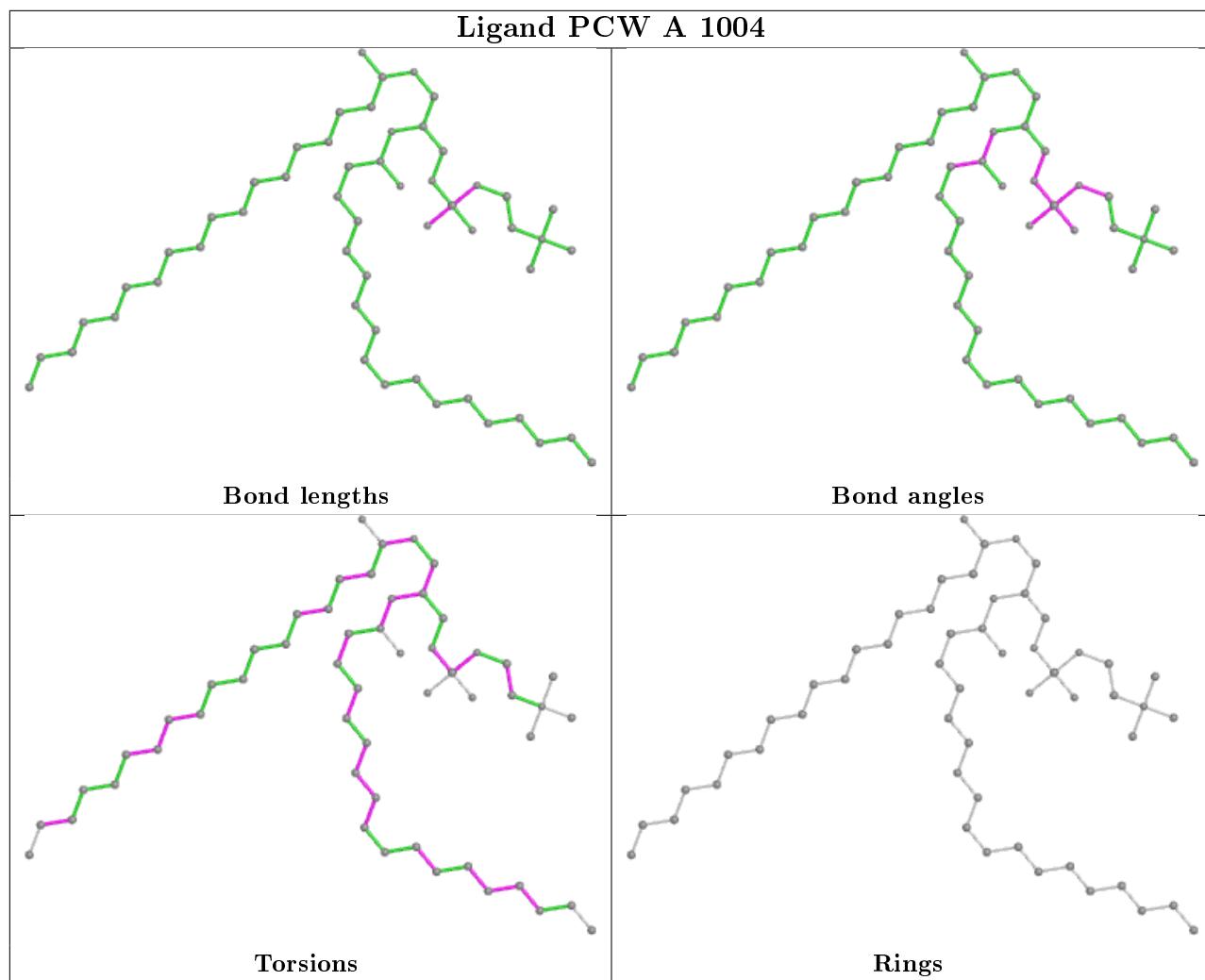
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1006	PCW	2	0
5	D	1009	CE1	1	0
4	C	1004	PCW	8	0
4	A	1004	PCW	1	0
4	C	1008	PCW	4	0
4	C	1006	PCW	2	0
4	B	1004	PCW	3	0
4	A	1003	PCW	2	0
4	B	1008	PCW	2	0
2	H	1001	BEF	1	0
4	B	1007	PCW	3	0
5	D	1005	CE1	3	0
4	D	1003	PCW	4	0
4	B	1009	PCW	4	0
5	D	1008	CE1	2	0
4	B	1003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

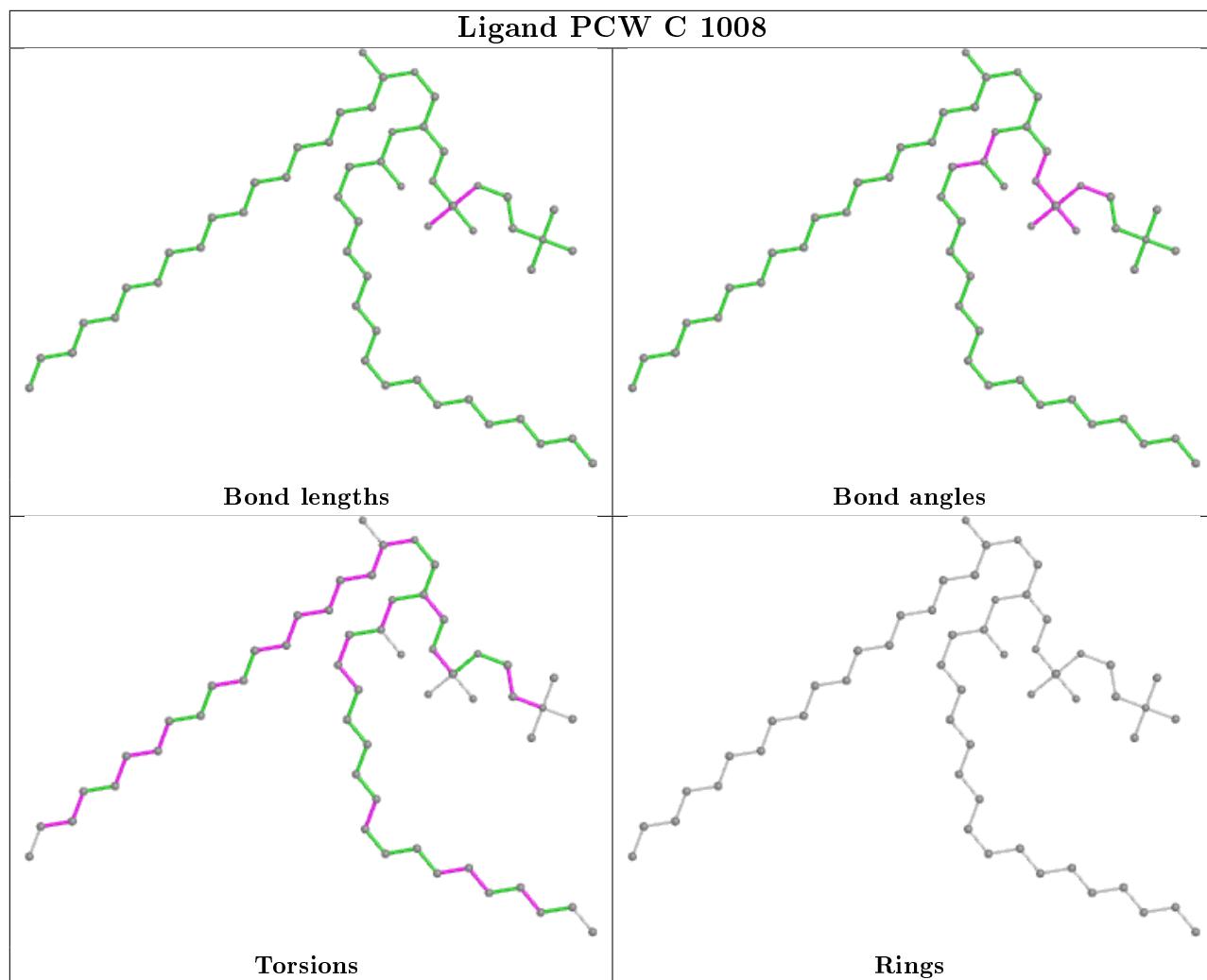
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

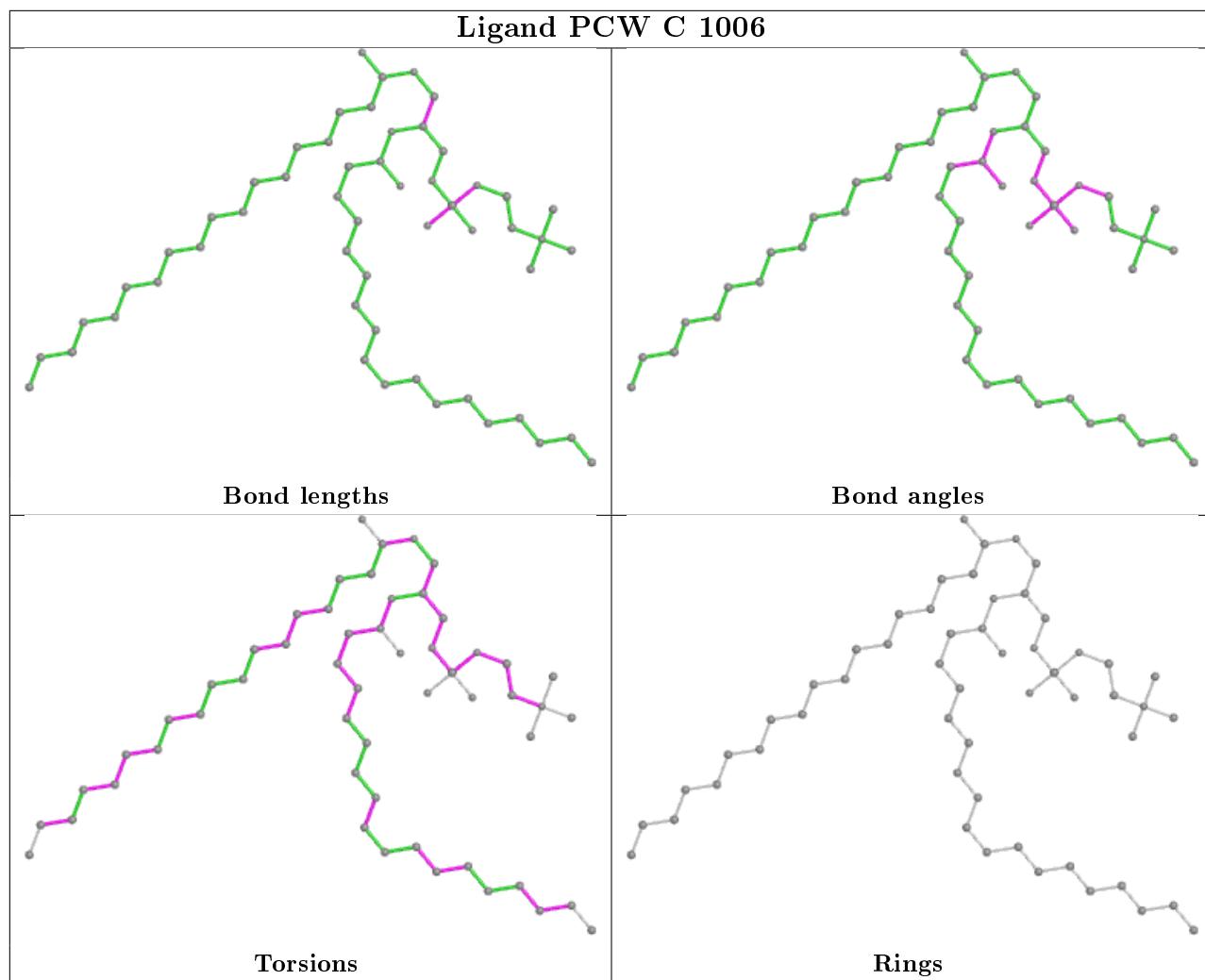


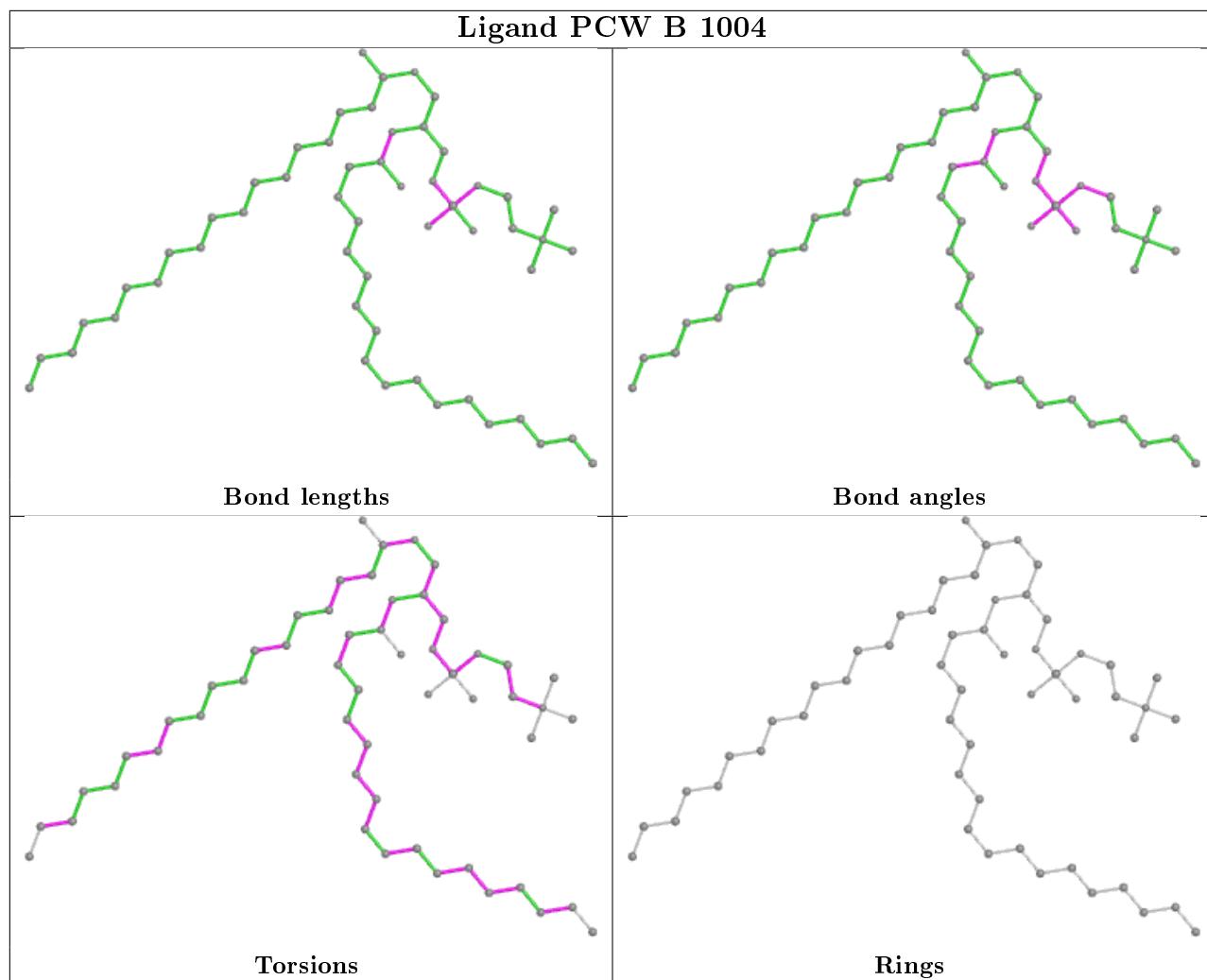


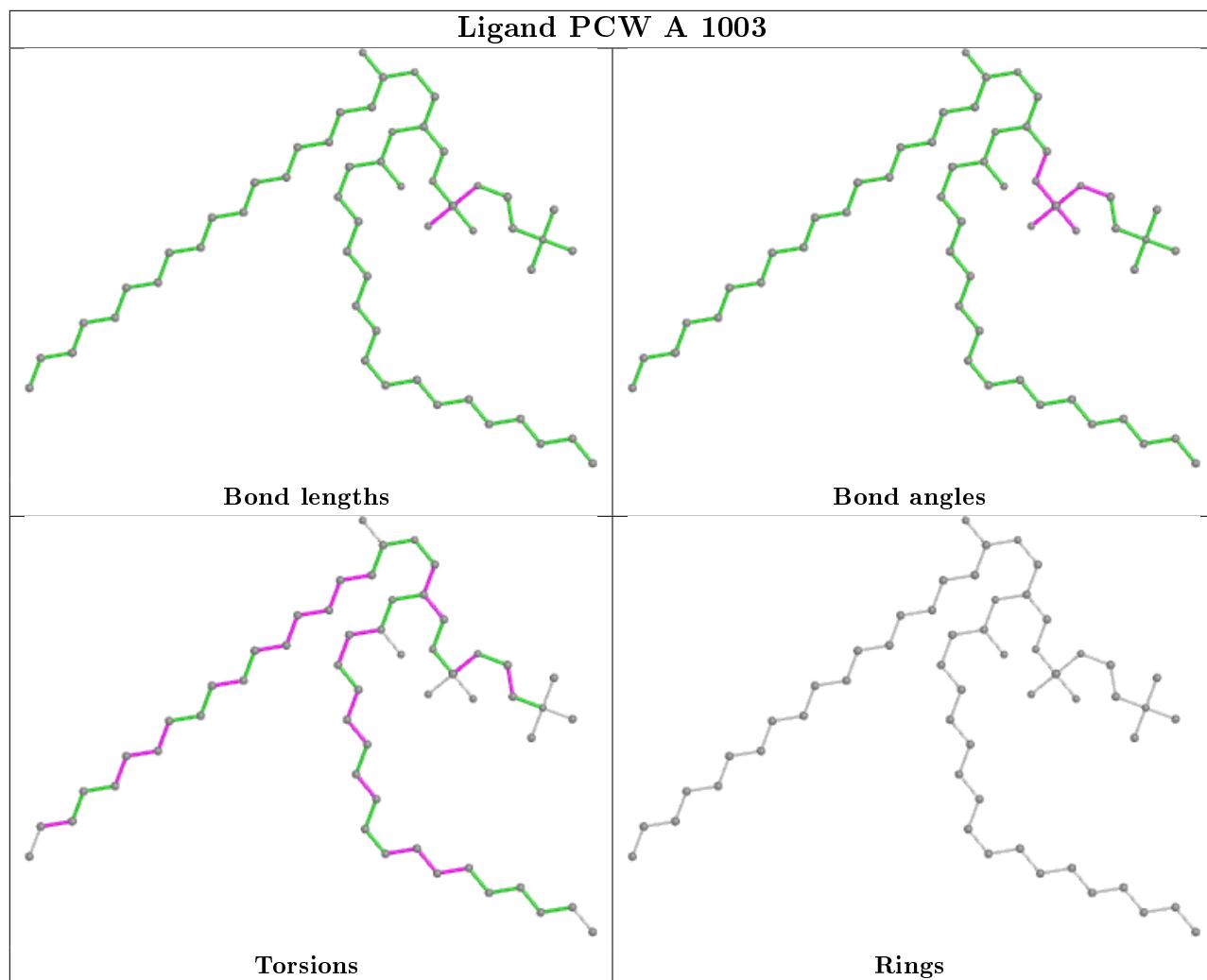


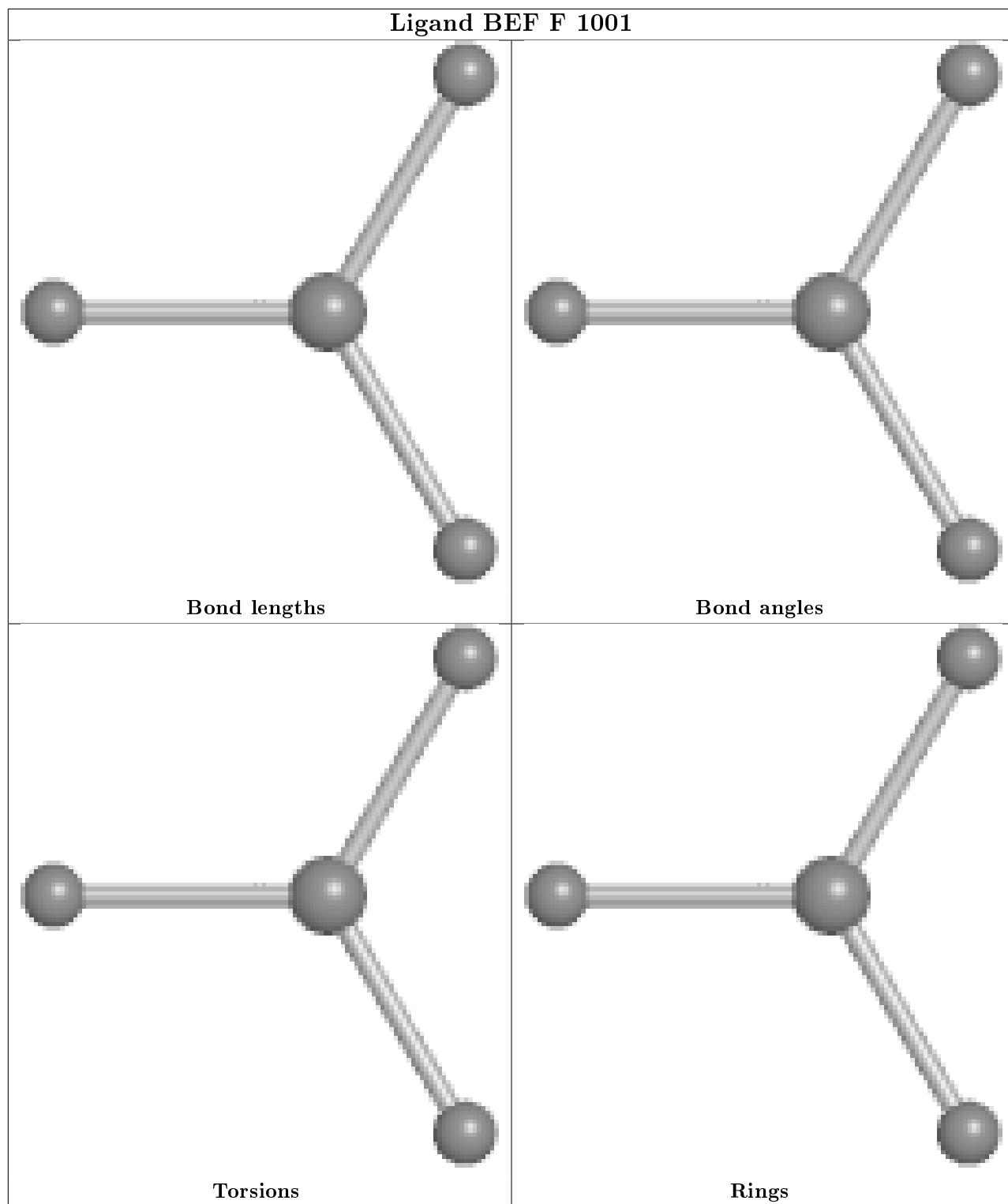


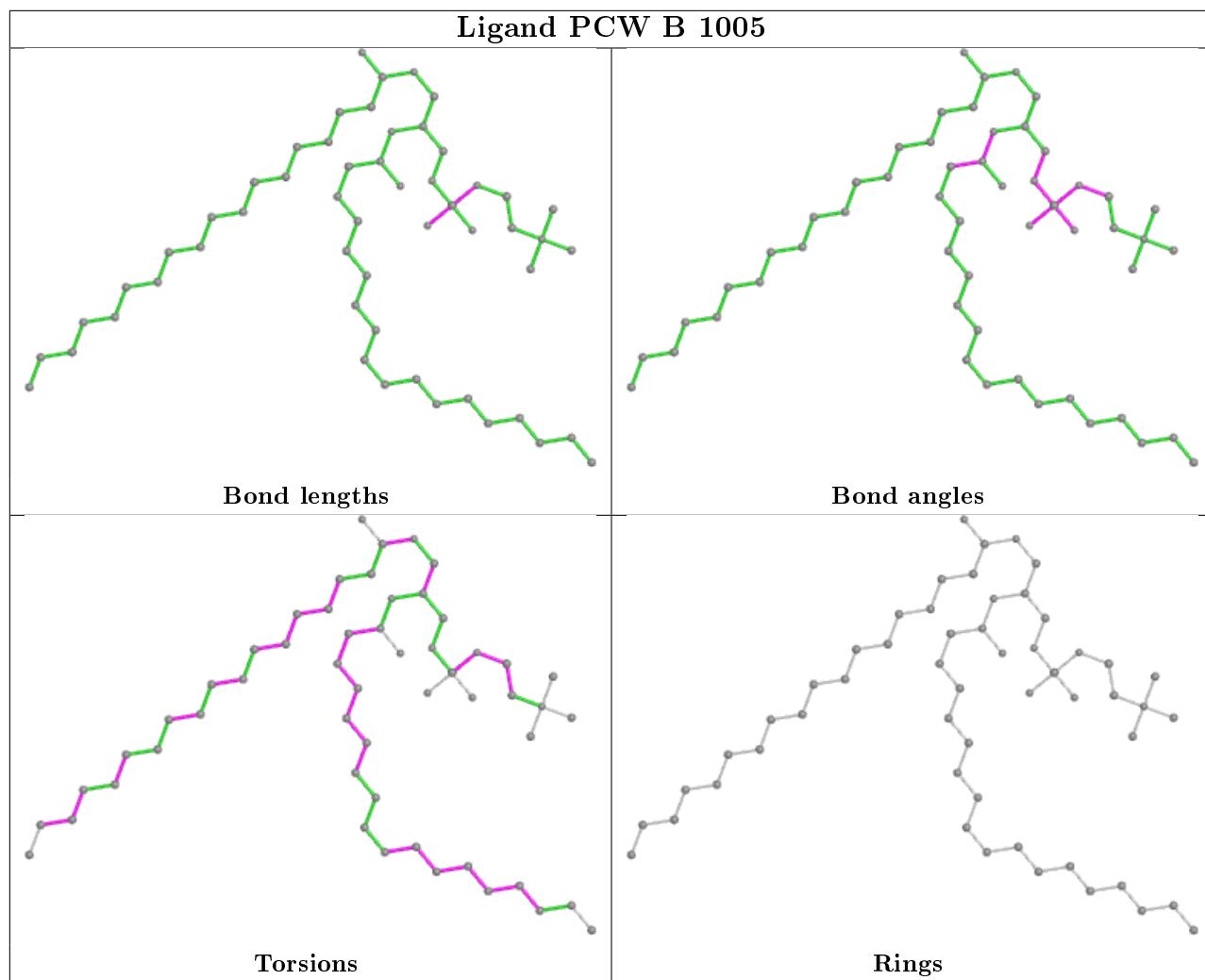


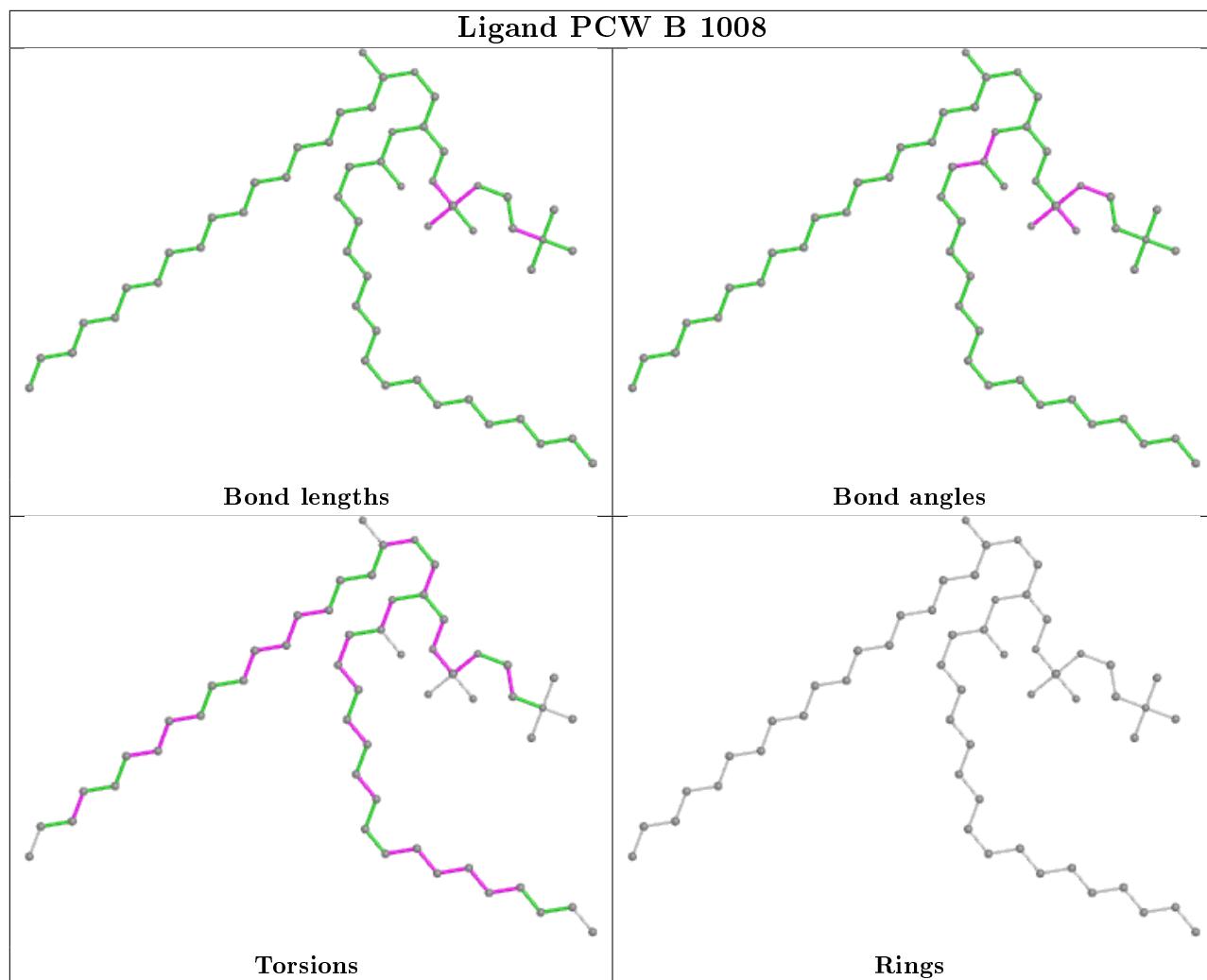


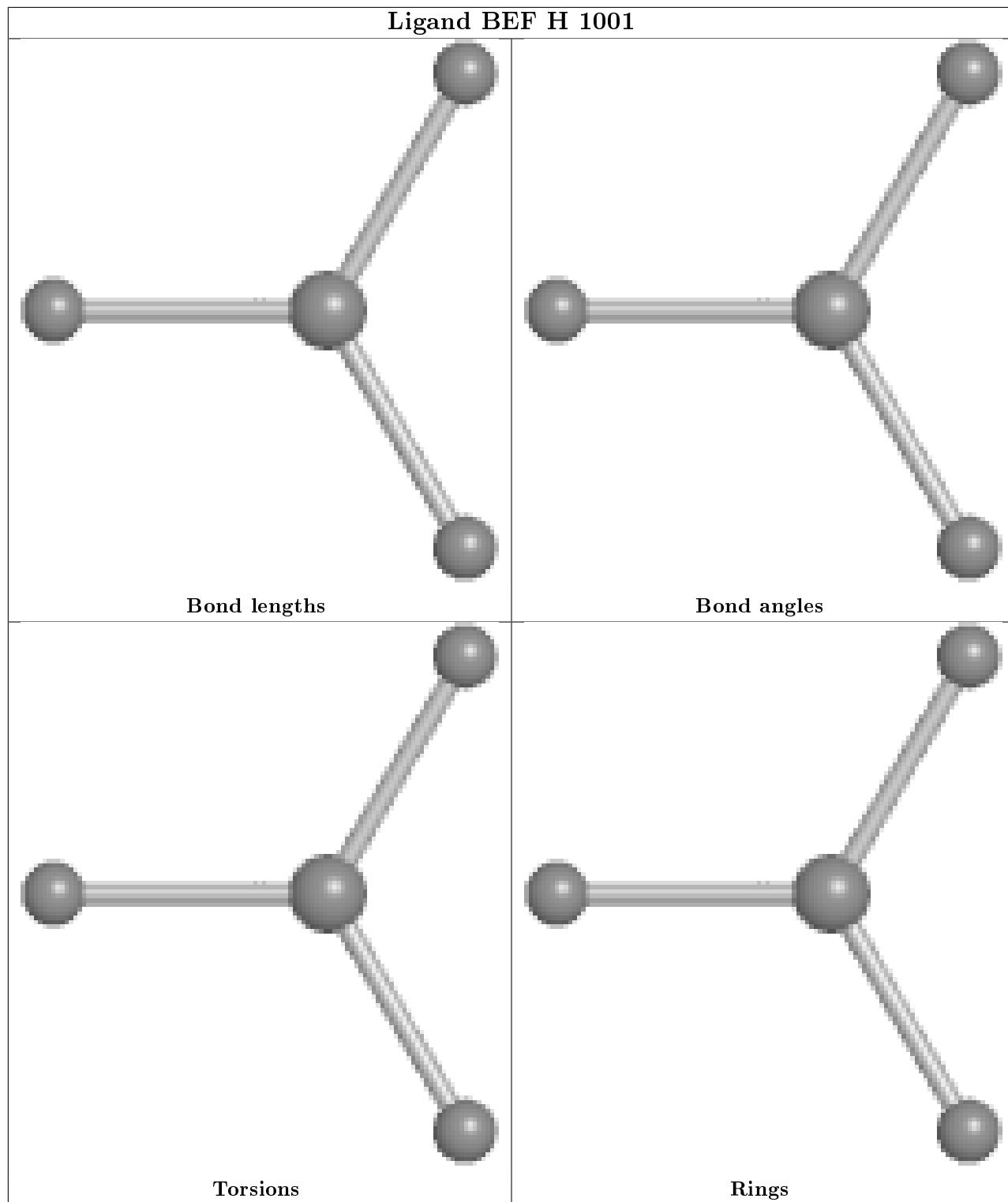


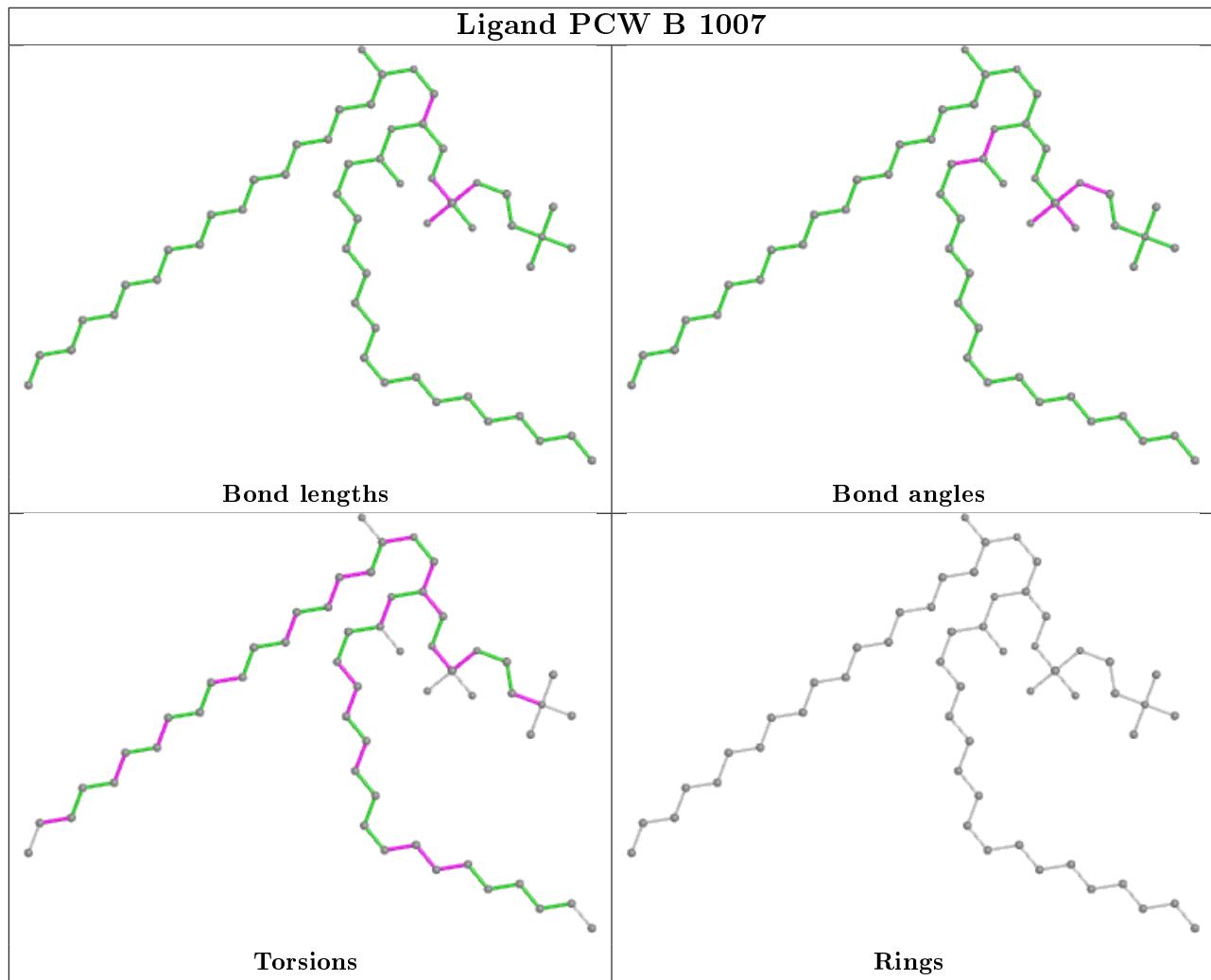
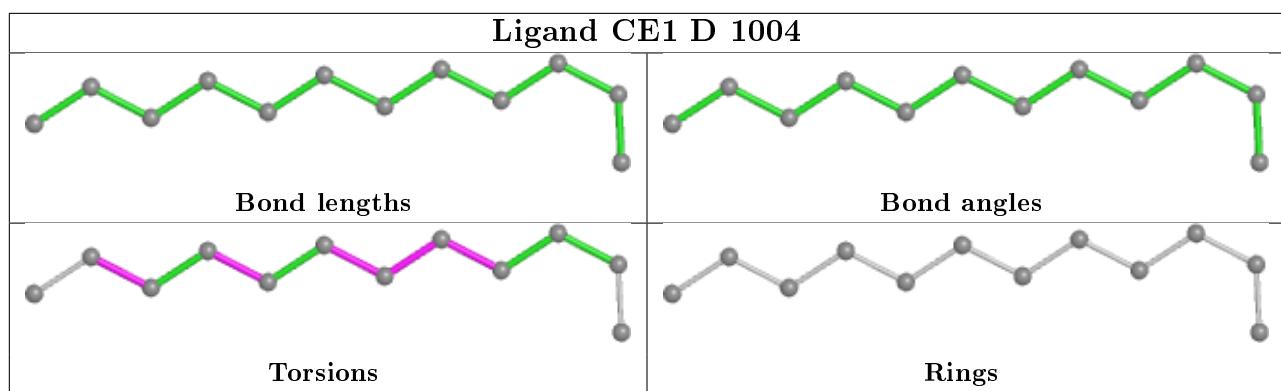


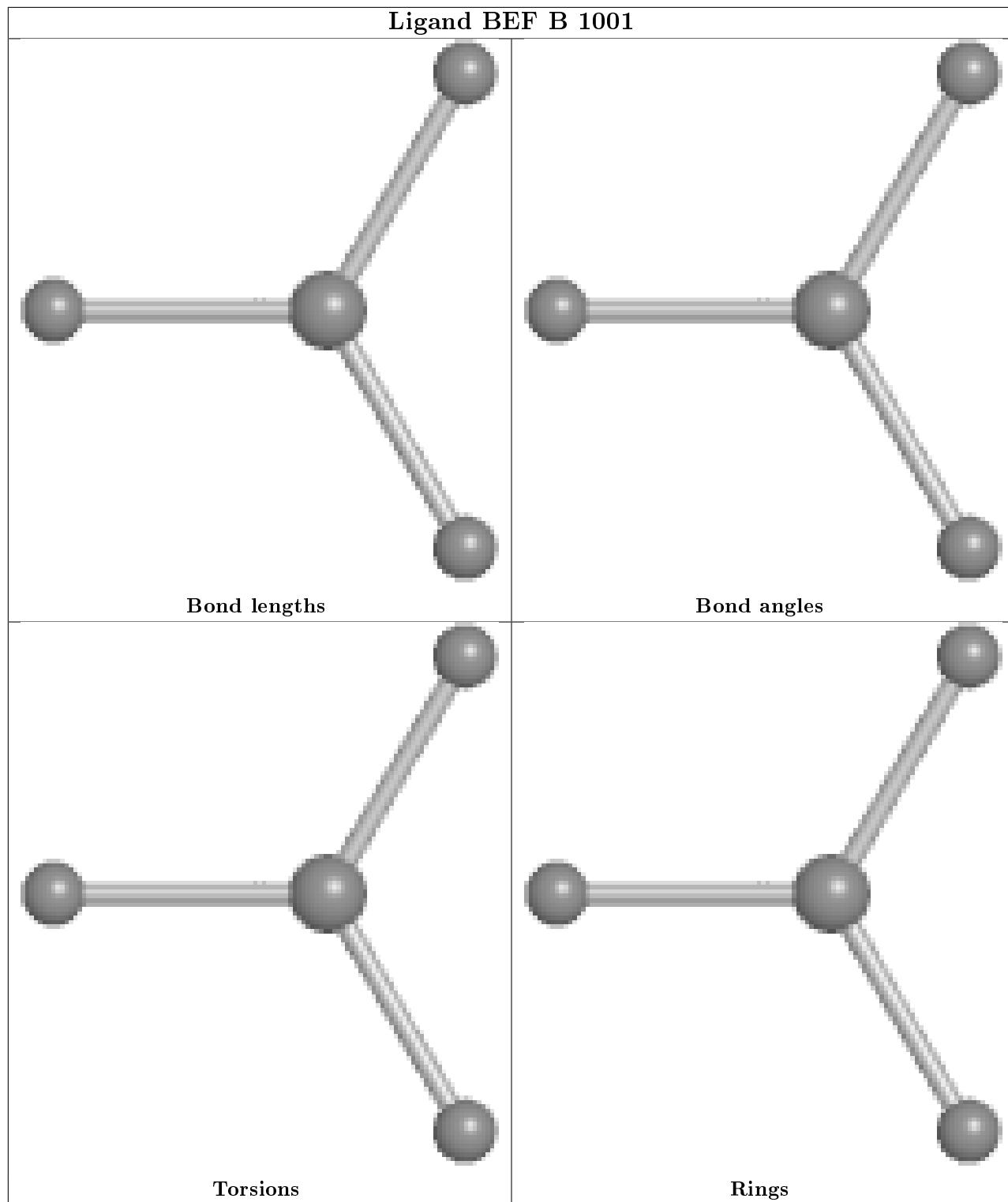


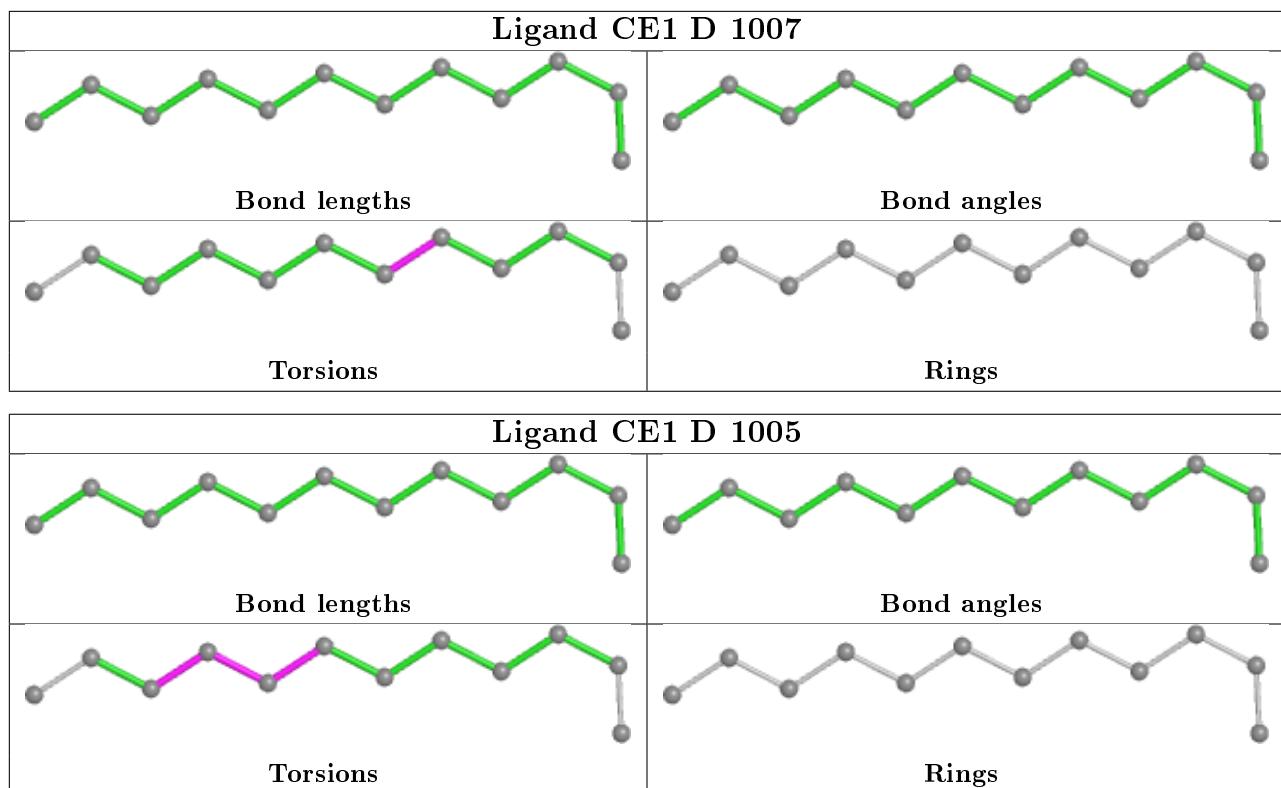


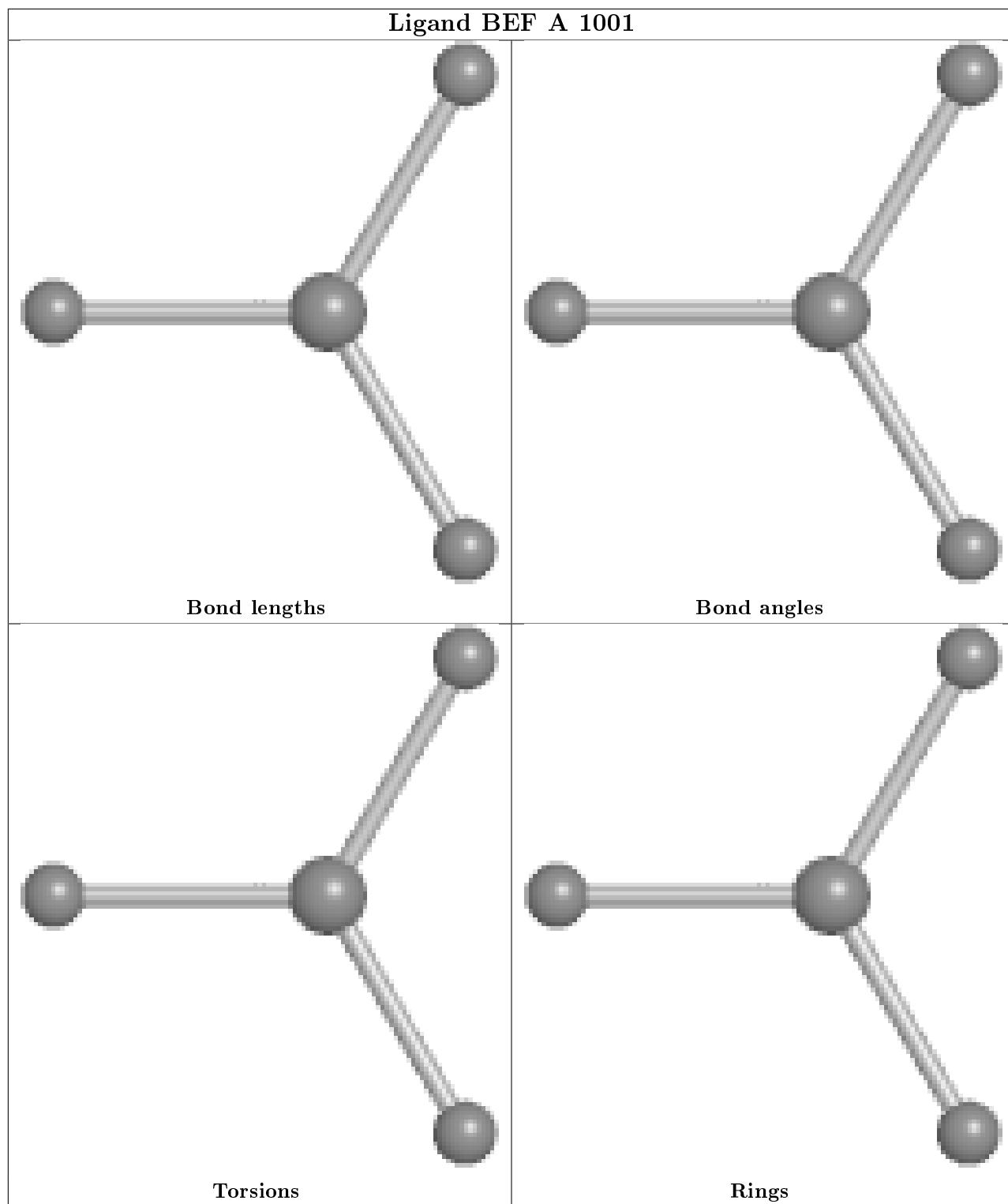


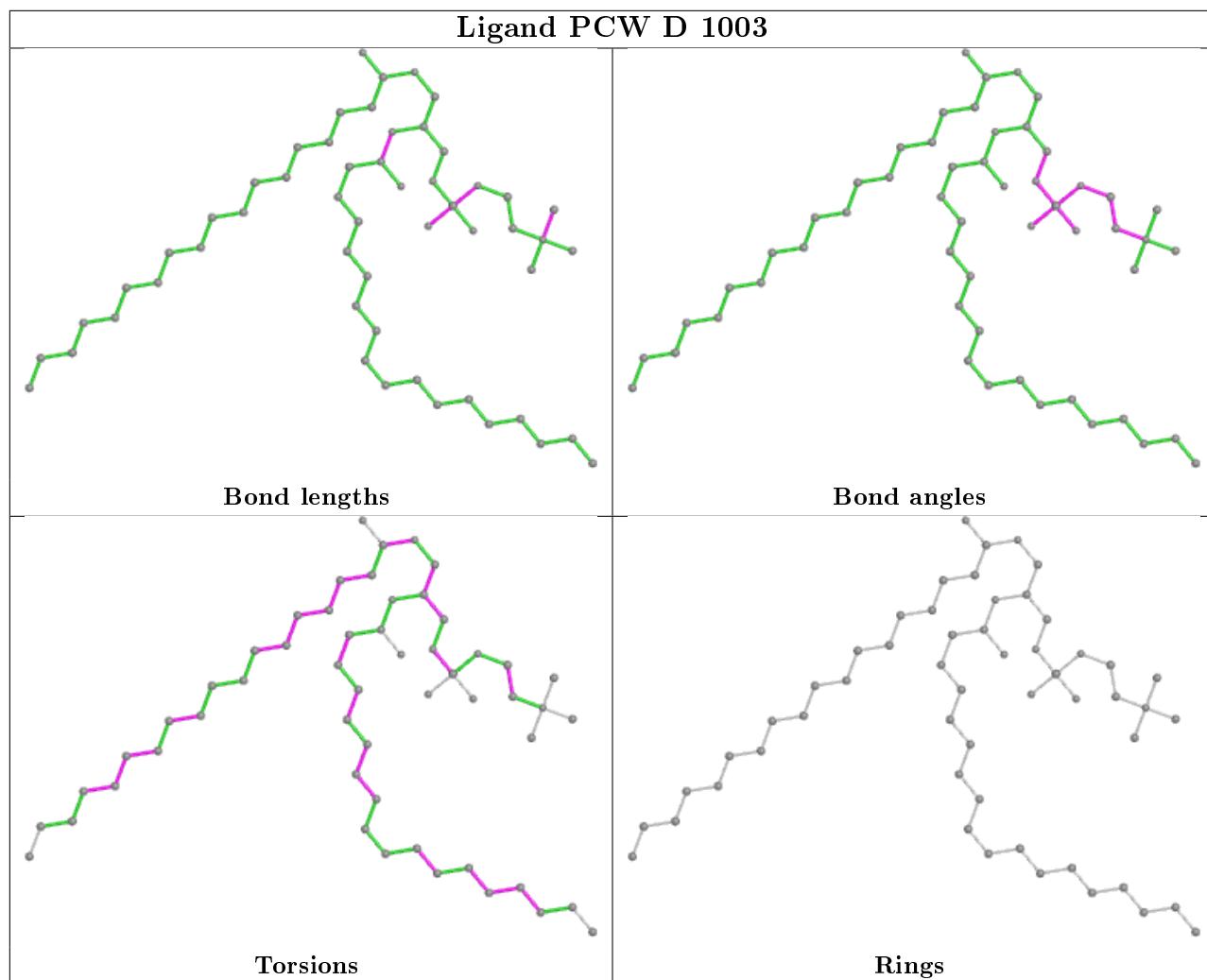


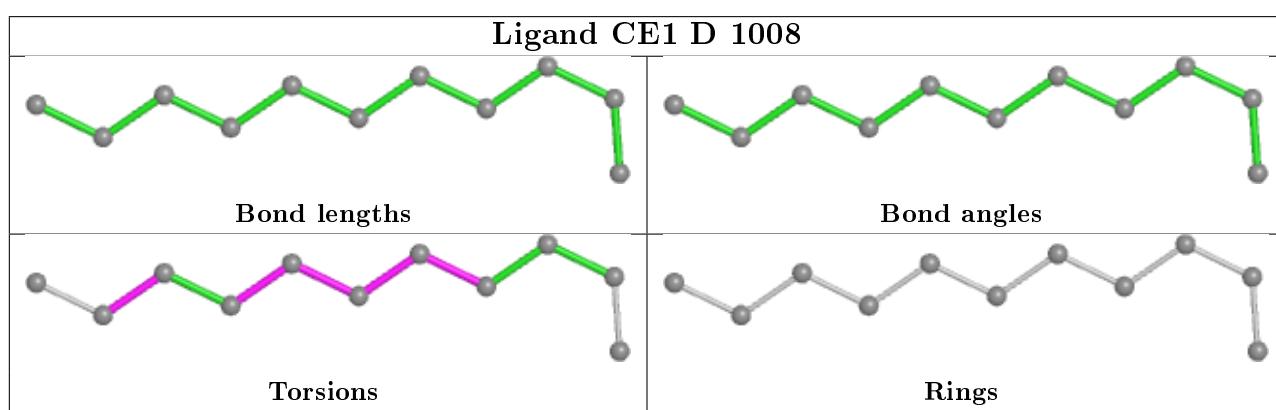
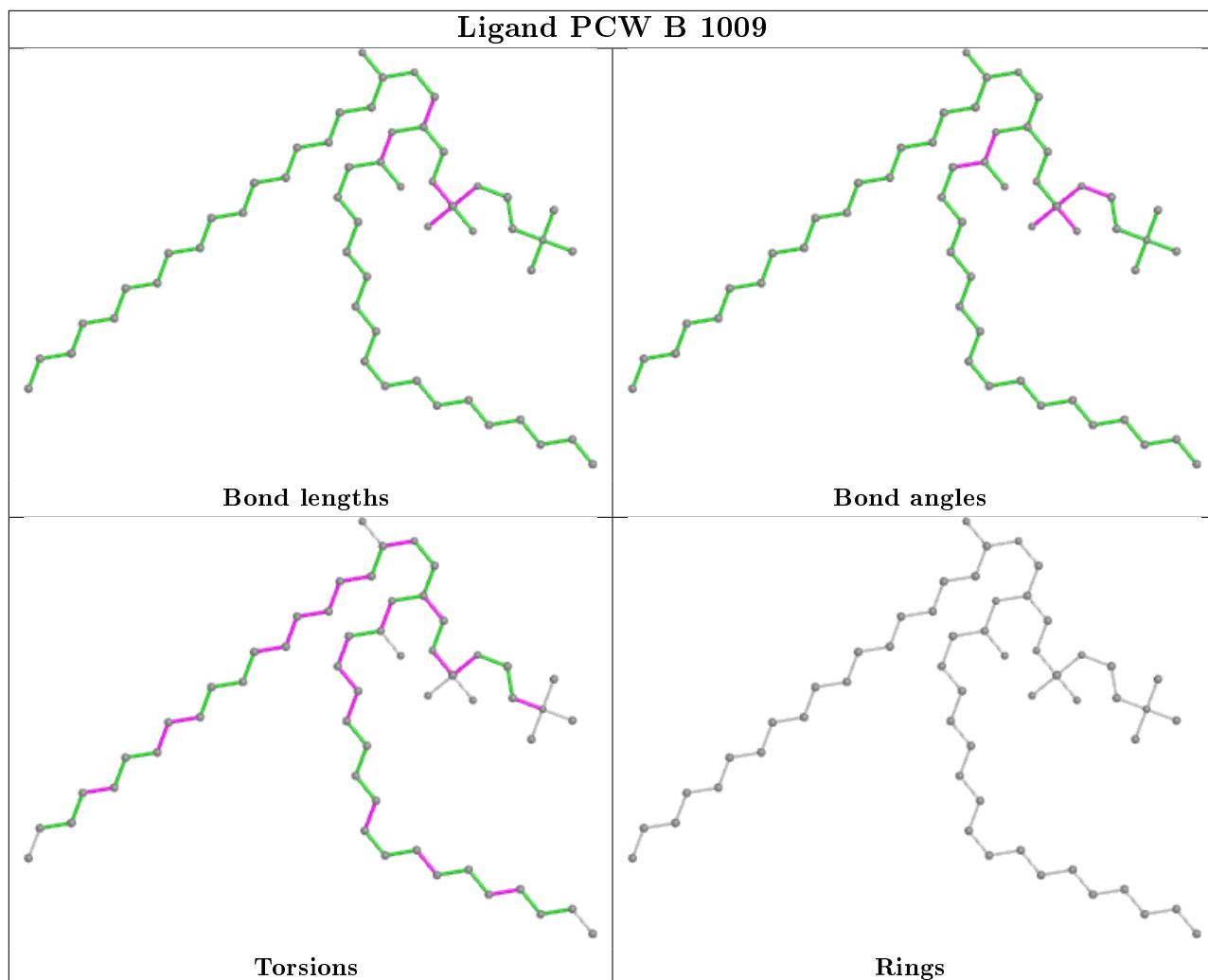


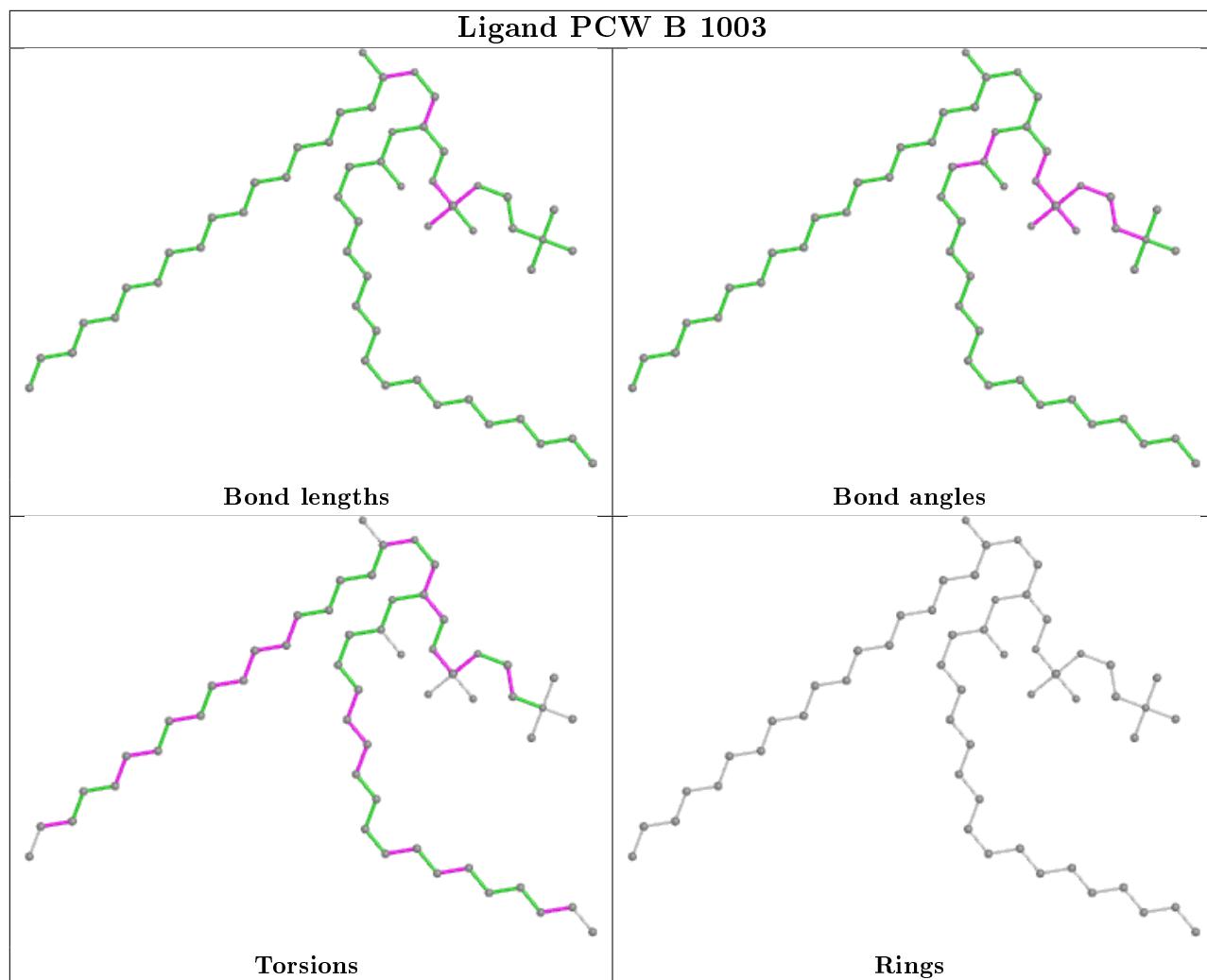


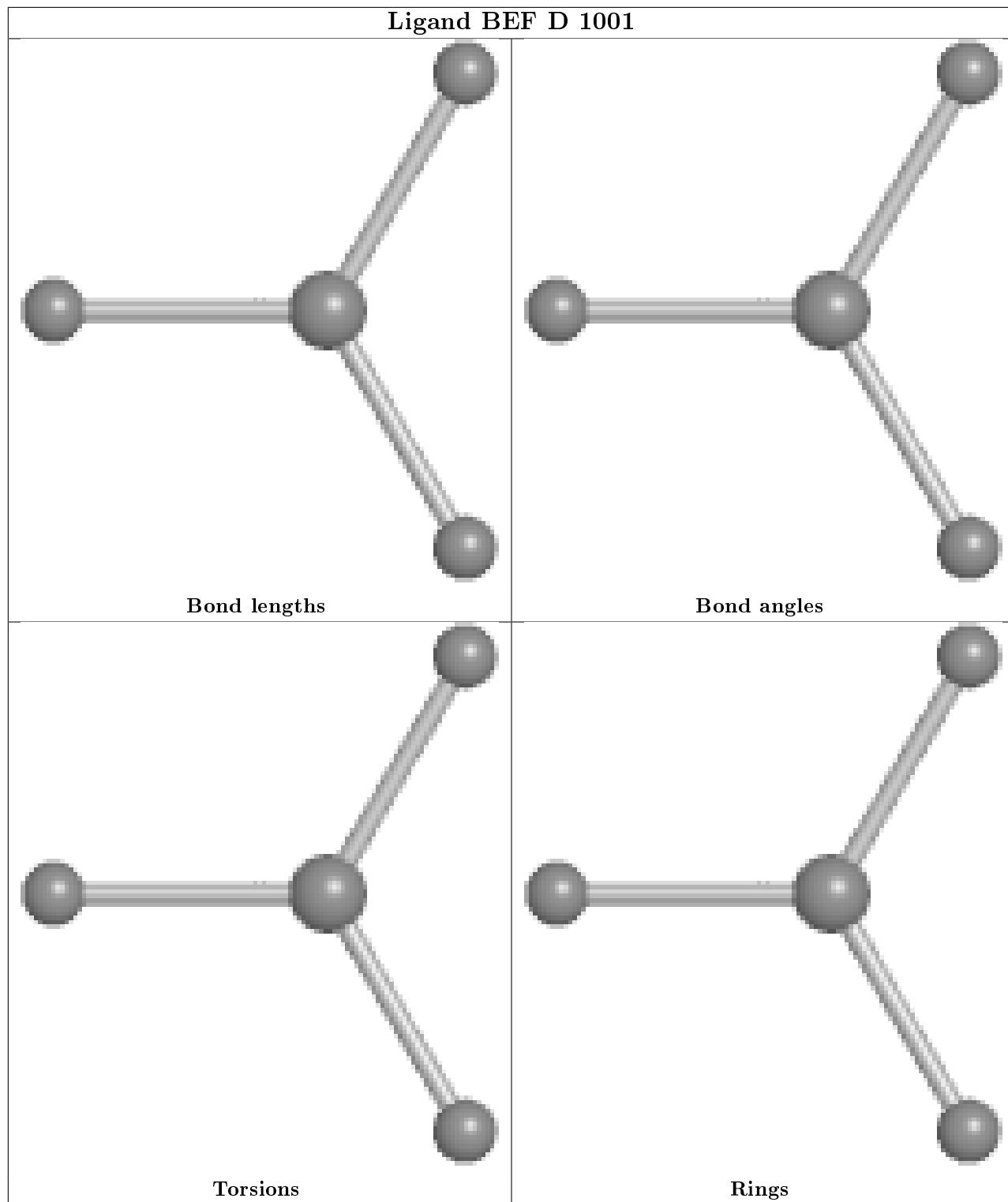


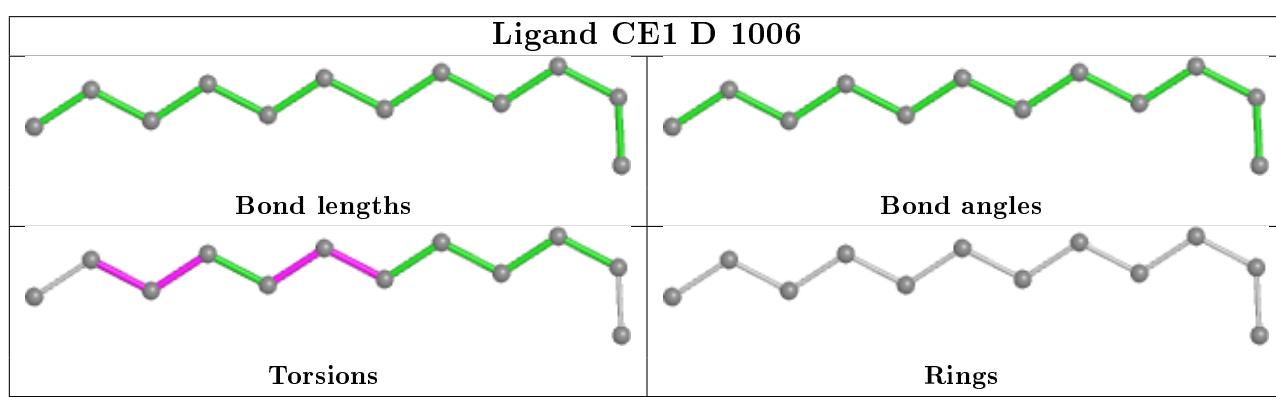
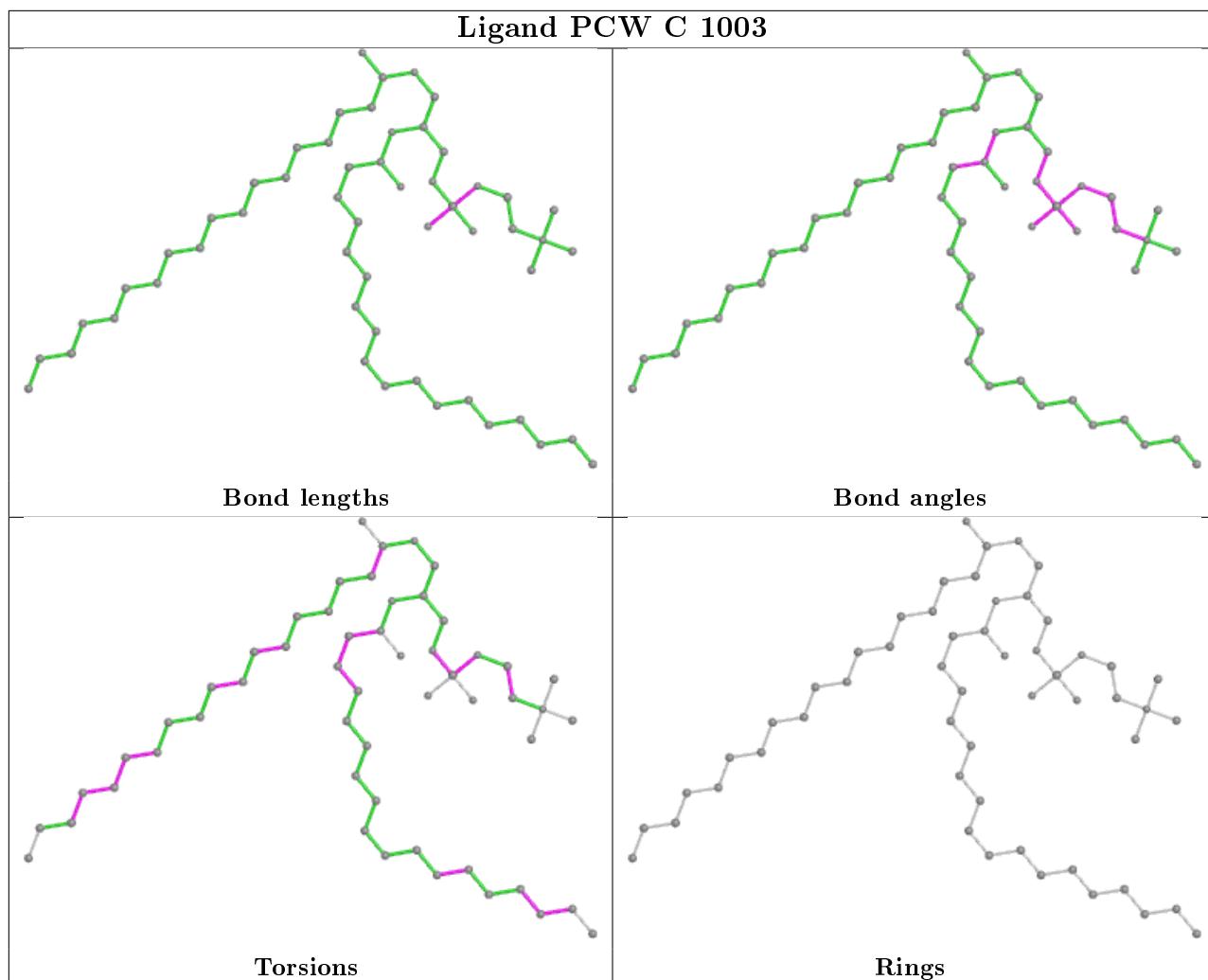


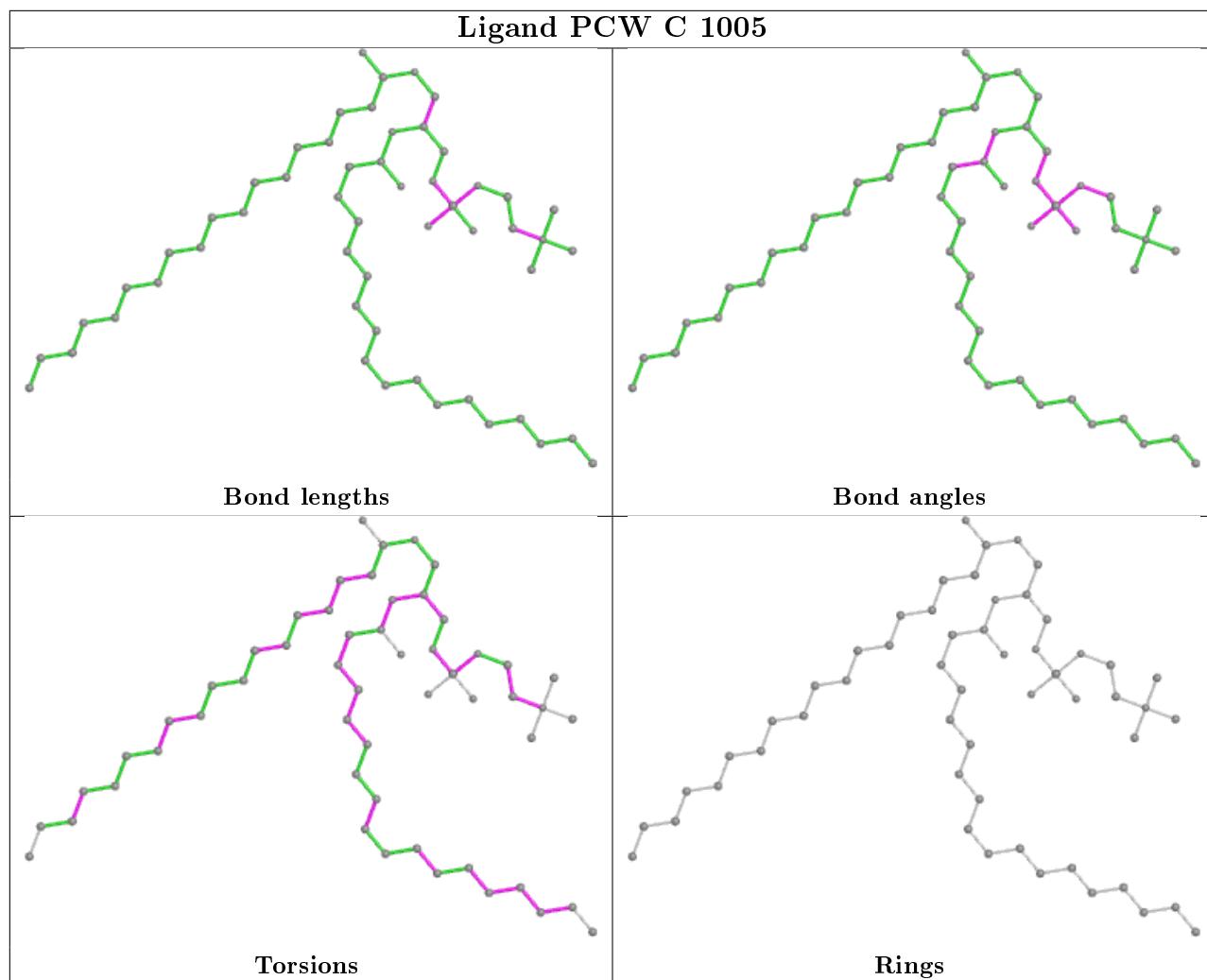


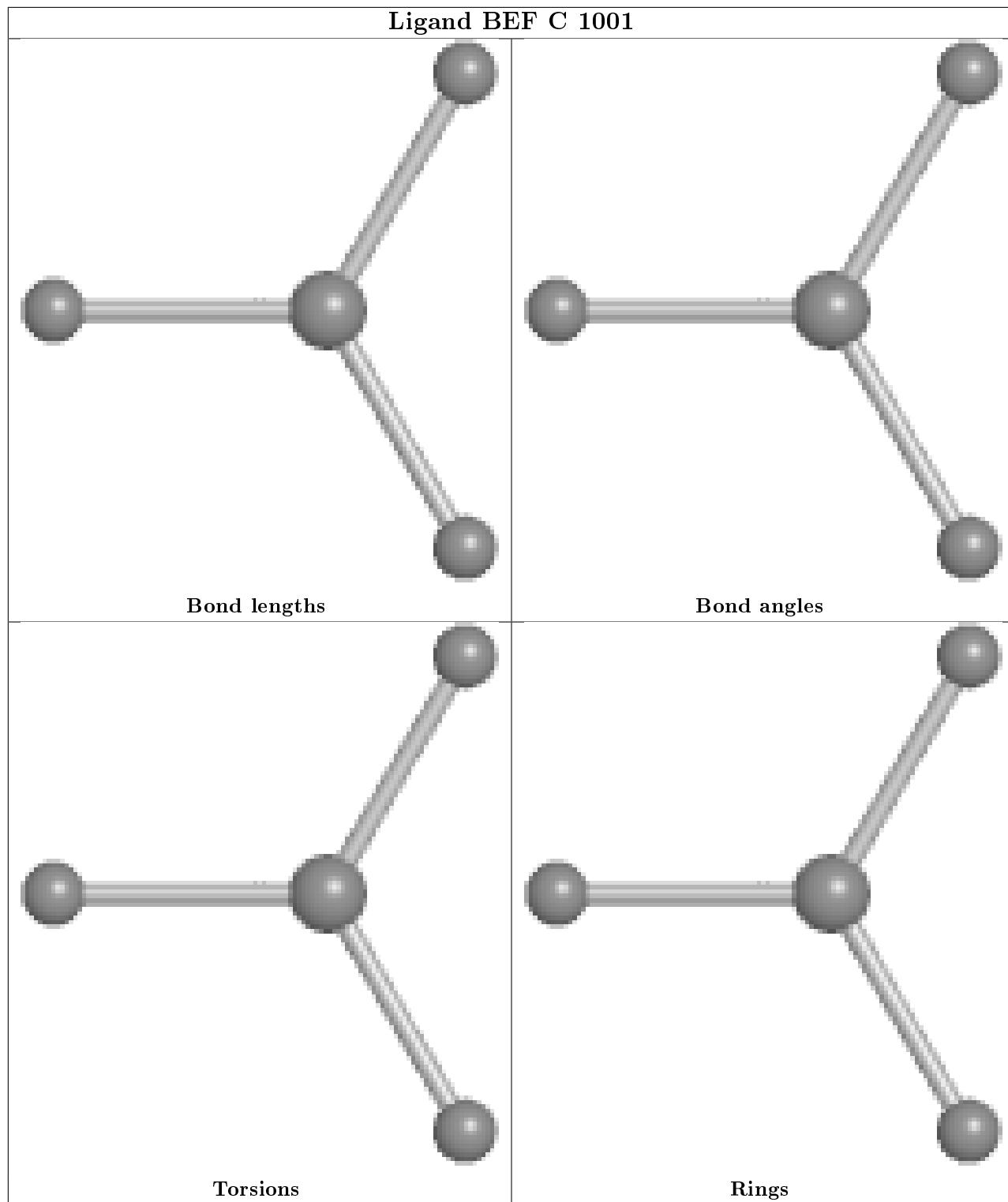


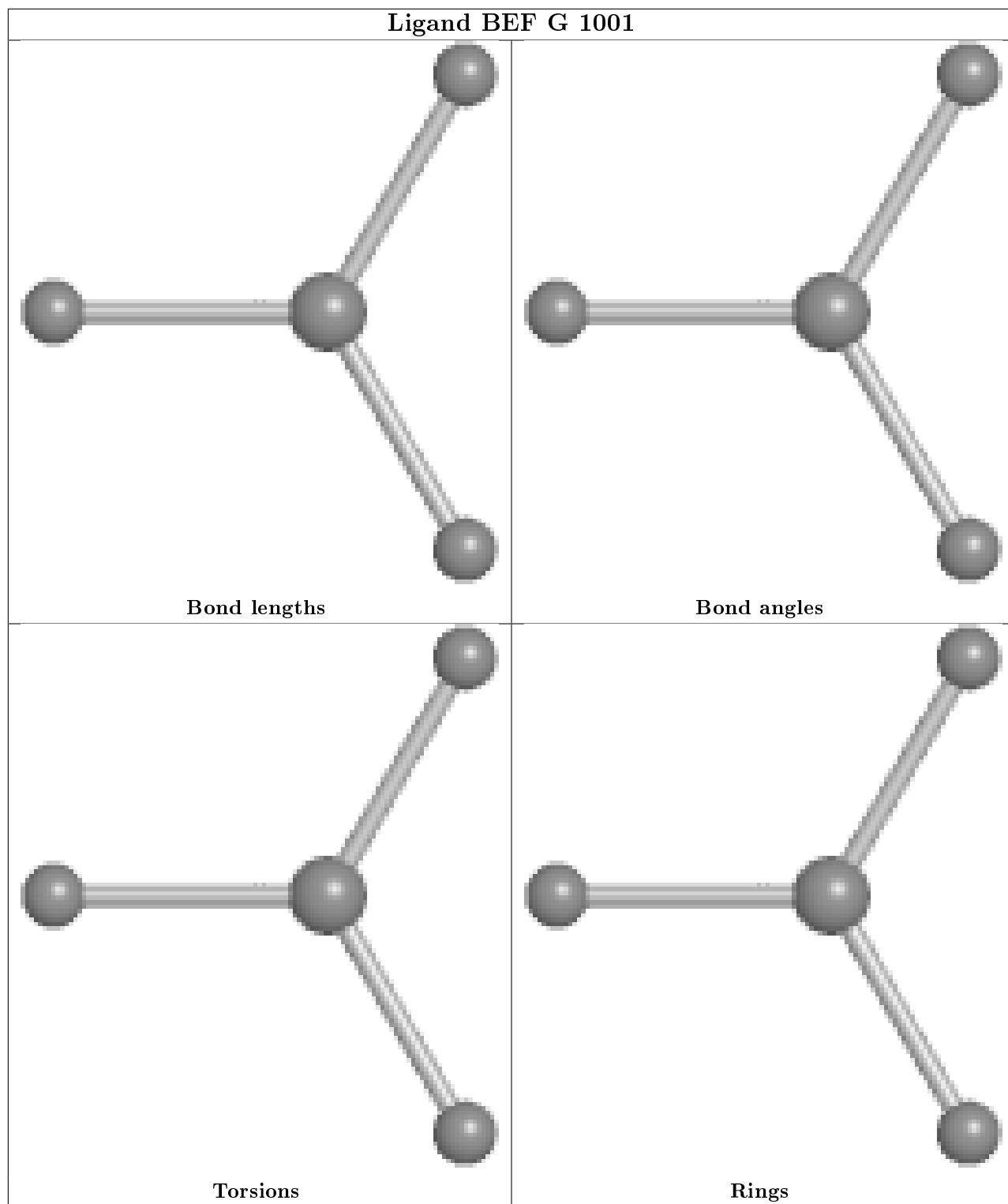












## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

## 6 Fit of model and data (i)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	883/911 (96%)	-0.46	2 (0%)	95	87	25, 51, 97, 128
1	B	883/911 (96%)	-0.43	6 (0%)	87	69	26, 51, 98, 130
1	C	883/911 (96%)	-0.04	47 (5%)	26	10	26, 68, 215, 259
1	D	883/911 (96%)	0.04	73 (8%)	11	3	25, 68, 231, 279
1	E	876/911 (96%)	0.99	155 (17%)	1	0	159, 182, 261, 273
1	F	876/911 (96%)	0.50	72 (8%)	11	3	155, 174, 199, 221
1	G	875/911 (96%)	0.61	83 (9%)	8	3	153, 173, 198, 226
1	H	876/911 (96%)	1.01	166 (18%)	1	0	144, 179, 265, 300
All	All	7035/7288 (96%)	0.27	604 (8%)	10	3	25, 162, 234, 300

All (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
1	H	379	LEU	9.0
1	E	517	LEU	9.0
1	E	438	THR	8.8
1	H	380	CYS	8.7
1	C	497	TYR	8.6
1	E	444	ALA	8.5
1	H	510	GLU	8.0
1	E	507	LEU	7.7
1	C	379	LEU	7.5
1	E	505	THR	7.5
1	H	414	ILE	7.5

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Mol	Chain	Res	Type	RSRZ
1	D	438	THR	7.5
1	E	109	GLU	7.4
1	H	517	LEU	7.4
1	E	497	TYR	7.3
1	H	503	ASP	7.2
1	H	444	ALA	7.2
1	H	374	ILE	7.1
1	E	1	ALA	7.1
1	C	349	TYR	7.1
1	H	456	ALA	7.0
1	D	437	HIS	6.9
1	D	498	LYS	6.8
1	E	355	THR	6.7
1	C	501	PRO	6.7
1	H	435	THR	6.7
1	E	521	THR	6.7
1	D	444	ALA	6.5
1	E	266	ASP	6.5
1	E	369	GLY	6.4
1	E	347	VAL	6.3
1	H	377	ALA	6.3
1	D	464	ASP	6.3
1	C	447	THR	6.2
1	E	435	THR	6.2
1	H	416	GLU	6.1
1	F	202	GLY	6.1
1	H	375	HIS	6.1
1	D	505	THR	6.0
1	E	503	ASP	6.0
1	C	437	HIS	6.0
1	F	509	LEU	6.0
1	E	496	GLY	5.9
1	D	507	LEU	5.9
1	H	448	LYS	5.9
1	E	381	ASN	5.8
1	H	361	GLU	5.8
1	H	464	ASP	5.7
1	E	370	GLU	5.7
1	H	378	VAL	5.7
1	H	121	GLY	5.6
1	H	293	ALA	5.6
1	D	470	MET	5.6

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Mol	Chain	Res	Type	RSRZ
1	H	455	PHE	5.6
1	C	517	LEU	5.6
1	H	446	LEU	5.6
1	E	172	GLU	5.5
1	E	504	THR	5.5
1	H	473	GLU	5.4
1	E	728	GLY	5.4
1	D	472	GLU	5.4
1	D	447	THR	5.4
1	D	473	GLU	5.4
1	H	497	TYR	5.4
1	E	454	MET	5.3
1	G	639	ALA	5.3
1	E	99	LYS	5.3
1	H	98	ARG	5.3
1	G	106	ALA	5.3
1	D	445	MET	5.2
1	E	353	ASP	5.2
1	G	102	SER	5.2
1	H	365	ASN	5.2
1	H	373	LEU	5.1
1	C	456	ALA	5.1
1	C	496	GLY	5.1
1	E	375	HIS	5.1
1	H	367	SER	5.1
1	C	463	LEU	5.0
1	E	506	GLU	5.0
1	D	474	ILE	5.0
1	F	102	SER	5.0
1	H	264	LEU	5.0
1	C	350	TYR	5.0
1	H	445	MET	4.9
1	C	446	LEU	4.9
1	E	362	SER	4.9
1	E	377	ALA	4.9
1	H	519	GLY	4.9
1	H	439	PHE	4.9
1	H	368	GLU	4.9
1	E	446	LEU	4.8
1	H	511	ASP	4.8
1	H	495	TYR	4.8
1	D	495	TYR	4.8

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Mol	Chain	Res	Type	RSRZ
1	D	362	SER	4.8
1	E	368	GLU	4.8
1	H	421	GLU	4.7
1	D	439	PHE	4.7
1	H	442	ASN	4.7
1	E	501	PRO	4.7
1	E	456	ALA	4.7
1	G	380	CYS	4.6
1	C	448	LYS	4.6
1	E	469	PRO	4.6
1	E	450	GLY	4.6
1	H	472	GLU	4.6
1	C	472	GLU	4.6
1	C	440	ASN	4.5
1	E	680	SER	4.5
1	H	463	LEU	4.5
1	E	102	SER	4.5
1	E	352	PRO	4.5
1	E	458	CYS	4.5
1	E	199	TYR	4.5
1	E	451	PRO	4.5
1	G	192	PHE	4.4
1	H	432	LEU	4.4
1	C	505	THR	4.4
1	E	143	ASP	4.4
1	E	385	ILE	4.4
1	B	101	GLU	4.4
1	E	472	GLU	4.4
1	E	139	LEU	4.3
1	E	516	VAL	4.3
1	H	450	GLY	4.3
1	C	521	THR	4.3
1	E	455	PHE	4.3
1	E	357	GLU	4.3
1	H	370	GLU	4.3
1	D	393	GLY	4.3
1	D	441	GLU	4.2
1	D	501	PRO	4.2
1	H	594	ALA	4.2
1	H	476	ALA	4.2
1	E	350	TYR	4.2
1	C	500	MET	4.1

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Mol	Chain	Res	Type	RSRZ
1	H	99	LYS	4.1
1	H	508	LYS	4.1
1	H	454	MET	4.1
1	G	460	TYR	4.1
1	E	441	GLU	4.1
1	H	512	GLU	4.1
1	D	446	LEU	4.1
1	F	194	GLY	4.1
1	F	622	GLY	4.0
1	E	508	LYS	4.0
1	F	1	ALA	4.0
1	F	681	ILE	4.0
1	H	417	LYS	4.0
1	E	107	LEU	4.0
1	H	505	THR	4.0
1	C	473	GLU	4.0
1	D	350	TYR	4.0
1	G	385	ILE	4.0
1	D	454	MET	4.0
1	F	444	ALA	4.0
1	E	378	VAL	4.0
1	G	517	LEU	4.0
1	H	332	CYS	3.9
1	H	45	ASP	3.9
1	F	510	GLU	3.9
1	D	416	GLU	3.9
1	C	454	MET	3.9
1	E	358	ASN	3.9
1	E	124	GLN	3.9
1	H	103	SER	3.9
1	C	507	LEU	3.9
1	D	385	ILE	3.9
1	D	347	VAL	3.8
1	C	520	LEU	3.8
1	G	46	PRO	3.8
1	E	502	ALA	3.8
1	E	498	LYS	3.8
1	H	202	GLY	3.8
1	E	681	ILE	3.8
1	H	358	ASN	3.8
1	E	436	LEU	3.8
1	H	518	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	G	672	THR	3.8
1	E	443	LYS	3.7
1	D	458	CYS	3.7
1	E	482	ASN	3.7
1	D	351	LEU	3.7
1	H	34	TYR	3.7
1	G	266	ASP	3.7
1	H	266	ASP	3.7
1	H	496	GLY	3.7
1	E	426	PHE	3.7
1	H	364	GLU	3.7
1	F	45	ASP	3.7
1	E	292	GLU	3.7
1	H	520	LEU	3.6
1	H	426	PHE	3.6
1	C	353	ASP	3.6
1	H	387	SER	3.6
1	D	354	GLY	3.6
1	D	403	PHE	3.6
1	E	379	LEU	3.6
1	E	138	ILE	3.6
1	H	498	LYS	3.6
1	H	516	VAL	3.6
1	G	519	GLY	3.6
1	H	589	LYS	3.6
1	F	421	GLU	3.6
1	E	351	LEU	3.6
1	E	354	GLY	3.6
1	G	34	TYR	3.6
1	H	302	LEU	3.6
1	E	437	HIS	3.6
1	F	523	MET	3.6
1	C	378	VAL	3.5
1	B	883	ASP	3.5
1	G	452	ASP	3.5
1	E	100	ALA	3.5
1	D	434	SER	3.5
1	E	802	ALA	3.5
1	D	463	LEU	3.5
1	E	24	THR	3.5
1	D	521	THR	3.5
1	H	663	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	H	569	ASP	3.5
1	H	468	LYS	3.5
1	H	477	LYS	3.5
1	G	178	ILE	3.5
1	A	1	ALA	3.5
1	E	51	PHE	3.5
1	F	211	SER	3.4
1	H	422	GLY	3.4
1	F	161	GLU	3.4
1	H	869	GLU	3.4
1	D	476	ALA	3.4
1	G	273	THR	3.4
1	E	447	THR	3.4
1	G	851	LEU	3.4
1	E	408	ASN	3.4
1	D	436	LEU	3.4
1	F	676	ASN	3.3
1	H	207	THR	3.3
1	E	184	LEU	3.3
1	H	493	LEU	3.3
1	E	403	PHE	3.3
1	D	352	PRO	3.3
1	F	507	LEU	3.3
1	H	245	LEU	3.3
1	D	469	PRO	3.2
1	G	269	ALA	3.2
1	F	462	PHE	3.2
1	H	1	ALA	3.2
1	H	441	GLU	3.2
1	G	105	ASP	3.2
1	C	442	ASN	3.2
1	G	685	PHE	3.2
1	C	365	ASN	3.2
1	H	366	TRP	3.2
1	G	471	THR	3.2
1	G	121	GLY	3.2
1	E	387	SER	3.2
1	H	413	GLU	3.2
1	H	232	LEU	3.2
1	E	144	PHE	3.2
1	H	568	ALA	3.2
1	C	512	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	427	ASP	3.2
1	G	11	THR	3.2
1	D	467	GLU	3.1
1	C	348	ASP	3.1
1	G	232	LEU	3.1
1	E	367	SER	3.1
1	F	549	THR	3.1
1	G	592	HIS	3.1
1	D	423	GLU	3.1
1	F	184	LEU	3.1
1	H	436	LEU	3.1
1	D	369	GLY	3.1
1	G	211	SER	3.1
1	H	745	ASN	3.1
1	G	101	GLU	3.1
1	H	198	VAL	3.1
1	E	725	ILE	3.1
1	H	418	PHE	3.1
1	G	473	GLU	3.1
1	D	443	LYS	3.1
1	E	491	ARG	3.1
1	H	615	GLY	3.1
1	E	344	MET	3.1
1	E	363	PRO	3.1
1	H	667	VAL	3.0
1	H	419	ILE	3.0
1	G	198	VAL	3.0
1	E	470	MET	3.0
1	F	108	ARG	3.0
1	D	508	LYS	3.0
1	E	519	GLY	3.0
1	H	513	GLN	3.0
1	G	439	PHE	3.0
1	E	178	ILE	3.0
1	E	374	ILE	3.0
1	C	451	PRO	3.0
1	C	476	ALA	3.0
1	G	469	PRO	3.0
1	C	519	GLY	3.0
1	G	514	ASP	3.0
1	H	451	PRO	3.0
1	E	123	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	383	SER	2.9
1	F	290	ILE	2.9
1	H	132	VAL	2.9
1	F	48	TRP	2.9
1	H	440	ASN	2.9
1	D	402	ALA	2.9
1	D	460	TYR	2.9
1	H	360	PRO	2.9
1	E	569	ASP	2.9
1	C	430	ARG	2.9
1	E	140	ASP	2.9
1	G	498	LYS	2.9
1	D	435	THR	2.9
1	H	434	SER	2.9
1	E	265	GLY	2.9
1	F	663	ILE	2.9
1	F	147	ALA	2.9
1	H	269	ALA	2.9
1	H	372	ARG	2.9
1	H	578	LEU	2.9
1	H	665	ASP	2.9
1	F	550	GLY	2.9
1	H	156	SER	2.8
1	D	502	ALA	2.8
1	E	361	GLU	2.8
1	E	415	ARG	2.8
1	F	201	ARG	2.8
1	F	684	LEU	2.8
1	H	381	ASN	2.8
1	B	102	SER	2.8
1	G	238	SER	2.8
1	H	547	MET	2.8
1	D	383	SER	2.8
1	H	494	ALA	2.8
1	C	468	LYS	2.8
1	H	424	ILE	2.8
1	F	104	LEU	2.8
1	H	363	PRO	2.8
1	G	241	LYS	2.8
1	D	375	HIS	2.7
1	F	68	LEU	2.7
1	G	139	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	H	712	LEU	2.7
1	E	476	ALA	2.7
1	G	712	LEU	2.7
1	E	388	GLU	2.7
1	E	466	GLU	2.7
1	H	349	TYR	2.7
1	F	714	PHE	2.7
1	F	871	ILE	2.7
1	G	507	LEU	2.7
1	D	268	SER	2.7
1	G	343	LYS	2.7
1	E	348	ASP	2.7
1	F	292	GLU	2.7
1	D	426	PHE	2.7
1	D	413	GLU	2.7
1	E	416	GLU	2.7
1	G	652	ALA	2.7
1	H	429	ASP	2.7
1	E	70	GLN	2.7
1	E	622	GLY	2.7
1	E	349	TYR	2.7
1	C	504	THR	2.7
1	E	520	LEU	2.7
1	H	433	MET	2.7
1	F	101	GLU	2.7
1	H	139	LEU	2.6
1	G	637	GLY	2.6
1	H	385	ILE	2.6
1	H	144	PHE	2.6
1	C	498	LYS	2.6
1	E	160	ASP	2.6
1	G	73	LEU	2.6
1	A	102	SER	2.6
1	E	248	LEU	2.6
1	F	563	ILE	2.6
1	E	105	ASP	2.6
1	H	514	ASP	2.6
1	B	884	ILE	2.6
1	E	318	LYS	2.6
1	G	108	ARG	2.6
1	C	347	VAL	2.6
1	E	722	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	295	SER	2.6
1	E	596	TYR	2.6
1	E	841	GLU	2.6
1	H	393	GLY	2.6
1	E	104	LEU	2.6
1	H	383	SER	2.6
1	F	466	GLU	2.6
1	F	504	THR	2.6
1	F	347	VAL	2.6
1	F	842	ILE	2.6
1	F	565	LEU	2.6
1	H	184	LEU	2.6
1	C	511	ASP	2.5
1	H	782	MET	2.5
1	F	243	LEU	2.5
1	H	105	ASP	2.5
1	E	46	PRO	2.5
1	H	545	THR	2.5
1	E	182	VAL	2.5
1	H	738	LYS	2.5
1	H	474	ILE	2.5
1	F	638	VAL	2.5
1	H	548	ILE	2.5
1	C	380	CYS	2.5
1	H	51	PHE	2.5
1	H	133	PRO	2.5
1	F	219	ALA	2.5
1	G	260	GLY	2.5
1	G	284	ALA	2.5
1	D	461	VAL	2.5
1	H	664	VAL	2.5
1	E	784	VAL	2.5
1	H	263	LEU	2.5
1	C	455	PHE	2.5
1	H	176	ASP	2.5
1	D	374	ILE	2.5
1	H	431	LYS	2.5
1	H	565	LEU	2.5
1	G	239	PHE	2.5
1	E	529	GLU	2.5
1	G	154	SER	2.5
1	E	142	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	377	ALA	2.4
1	E	106	ALA	2.4
1	E	726	ALA	2.4
1	D	414	ILE	2.4
1	D	503	ASP	2.4
1	H	265	GLY	2.4
1	F	573	LEU	2.4
1	G	727	LEU	2.4
1	H	546	VAL	2.4
1	G	455	PHE	2.4
1	H	350	TYR	2.4
1	F	880	LYS	2.4
1	G	451	PRO	2.4
1	B	464	ASP	2.4
1	E	366	TRP	2.4
1	E	648	LYS	2.4
1	G	245	LEU	2.4
1	G	492	VAL	2.4
1	F	685	PHE	2.4
1	E	473	GLU	2.4
1	F	753	THR	2.4
1	H	469	PRO	2.4
1	C	444	ALA	2.4
1	E	317	ARG	2.4
1	G	474	ILE	2.4
1	E	409	GLN	2.4
1	C	439	PHE	2.4
1	E	559	ILE	2.4
1	G	663	ILE	2.4
1	H	376	ILE	2.4
1	E	538	SER	2.4
1	H	118	ILE	2.4
1	G	446	LEU	2.4
1	B	885	PRO	2.4
1	D	412	ASN	2.4
1	E	530	ALA	2.4
1	F	490	LEU	2.4
1	C	495	TYR	2.4
1	D	451	PRO	2.4
1	C	435	THR	2.4
1	E	571	ILE	2.3
1	H	607	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	807	GLN	2.3
1	E	615	GLY	2.3
1	G	280	MET	2.3
1	D	381	ASN	2.3
1	C	403	PHE	2.3
1	D	355	THR	2.3
1	G	524	ILE	2.3
1	F	46	PRO	2.3
1	D	415	ARG	2.3
1	F	379	LEU	2.3
1	F	435	THR	2.3
1	F	380	CYS	2.3
1	G	378	VAL	2.3
1	D	389	GLY	2.3
1	D	384	ASN	2.3
1	H	289	ALA	2.3
1	H	447	THR	2.3
1	F	816	SER	2.3
1	C	373	LEU	2.3
1	E	842	ILE	2.3
1	H	54	THR	2.3
1	G	468	LYS	2.3
1	H	661	VAL	2.3
1	D	448	LYS	2.3
1	F	165	THR	2.3
1	E	493	LEU	2.3
1	H	586	LEU	2.3
1	E	474	ILE	2.3
1	D	500	MET	2.3
1	F	302	LEU	2.3
1	E	135	ASP	2.2
1	F	823	ALA	2.2
1	E	565	LEU	2.2
1	G	433	MET	2.2
1	C	422	GLY	2.2
1	F	776	MET	2.2
1	F	650	SER	2.2
1	D	456	ALA	2.2
1	E	583	GLU	2.2
1	F	513	GLN	2.2
1	G	1	ALA	2.2
1	H	558	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	15	LEU	2.2
1	G	329	SER	2.2
1	G	867	MET	2.2
1	E	117	VAL	2.2
1	D	417	LYS	2.2
1	G	526	PRO	2.2
1	F	687	GLY	2.2
1	H	564	GLY	2.2
1	E	163	MET	2.2
1	E	531	VAL	2.2
1	G	118	ILE	2.2
1	G	709	ALA	2.2
1	H	521	THR	2.2
1	H	453	VAL	2.2
1	G	35	GLY	2.2
1	H	108	ARG	2.2
1	D	459	SER	2.2
1	E	544	ARG	2.2
1	F	600	SER	2.2
1	F	680	SER	2.2
1	H	234	ARG	2.2
1	G	516	VAL	2.2
1	D	373	LEU	2.2
1	H	131	LEU	2.2
1	E	425	PRO	2.2
1	E	169	GLU	2.2
1	F	346	VAL	2.2
1	G	510	GLU	2.2
1	H	620	MET	2.2
1	D	499	ARG	2.2
1	F	830	LEU	2.1
1	G	214	GLU	2.1
1	H	394	ASP	2.1
1	H	243	LEU	2.1
1	H	250	LEU	2.1
1	H	425	PRO	2.1
1	E	541	ALA	2.1
1	H	852	HIS	2.1
1	D	366	TRP	2.1
1	E	208	GLY	2.1
1	G	109	GLU	2.1
1	F	332	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	503	ASP	2.1
1	F	628	ALA	2.1
1	C	518	VAL	2.1
1	E	412	ASN	2.1
1	H	81	ILE	2.1
1	E	747	GLY	2.1
1	F	722	LEU	2.1
1	G	843	PHE	2.1
1	D	510	GLU	2.1
1	H	128	ALA	2.1
1	F	456	ALA	2.1
1	F	137	VAL	2.1
1	E	393	GLY	2.1
1	D	368	GLU	2.1
1	G	873	VAL	2.1
1	H	117	VAL	2.1
1	G	437	HIS	2.1
1	E	95	VAL	2.1
1	G	27	VAL	2.1
1	F	446	LEU	2.1
1	G	268	SER	2.1
1	H	123	LYS	2.0
1	H	356	LYS	2.0
1	E	332	CYS	2.0
1	D	353	ASP	2.0
1	E	729	MET	2.0
1	H	192	PHE	2.0
1	E	461	VAL	2.0
1	H	347	VAL	2.0
1	G	496	GLY	2.0
1	E	413	GLU	2.0
1	G	96	GLN	2.0
1	E	162	GLY	2.0
1	G	395	PRO	2.0
1	E	467	GLU	2.0
1	F	625	VAL	2.0
1	H	294	LEU	2.0
1	G	31	GLN	2.0
1	H	420	ARG	2.0
1	F	359	PHE	2.0
1	H	344	MET	2.0
1	E	205	VAL	2.0

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

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

## 6.3 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [\(i\)](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.

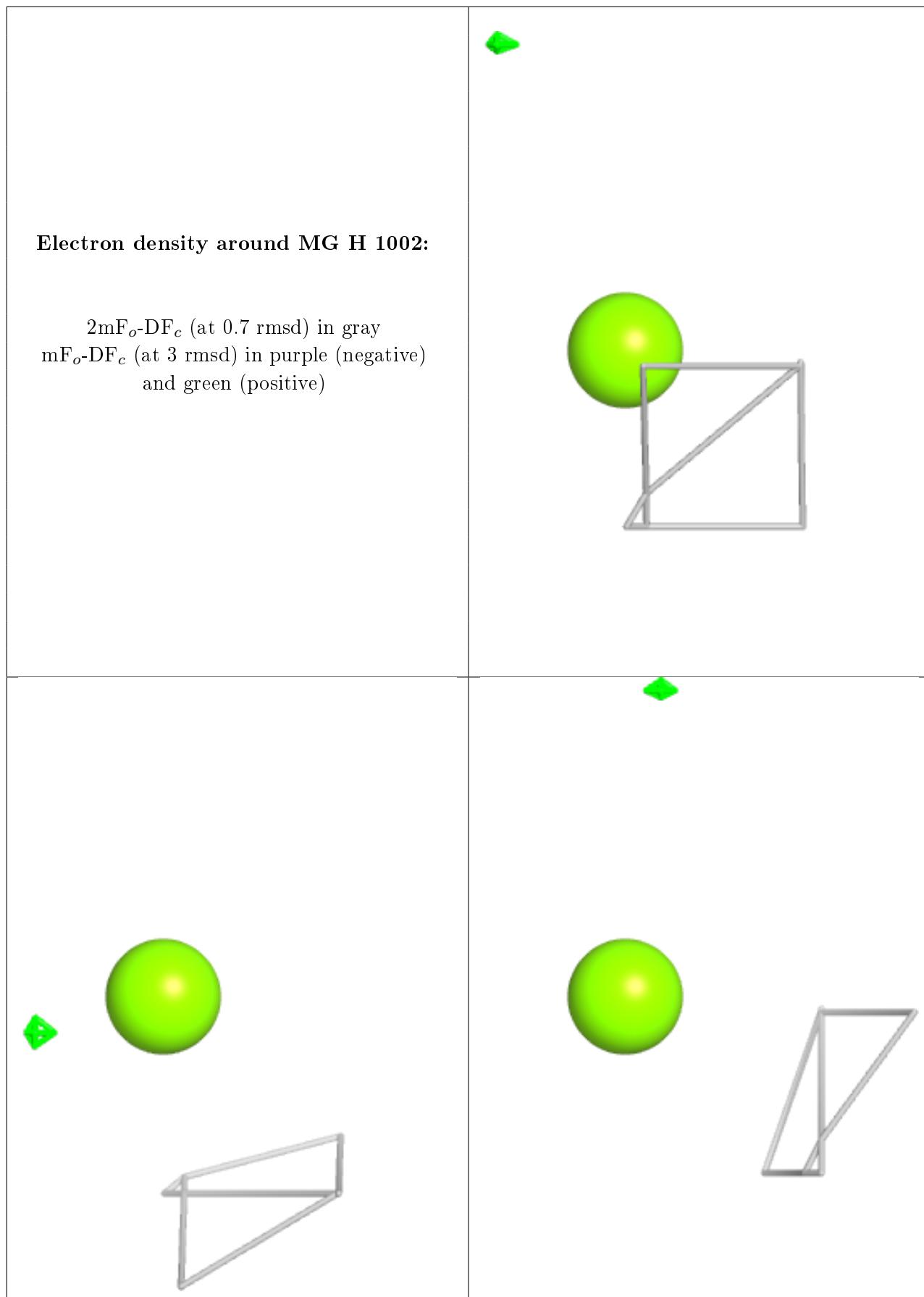
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	MG	H	1002	1/1	0.07	0.12	225,225,225,225	0
2	BEF	F	1001	4/4	0.59	0.18	206,207,209,213	0
3	MG	G	1002	1/1	0.61	0.09	213,213,213,213	0
2	BEF	H	1001	4/4	0.67	0.38	228,228,229,232	0
3	MG	E	1002	1/1	0.75	0.16	218,218,218,218	0
4	PCW	B	1006	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

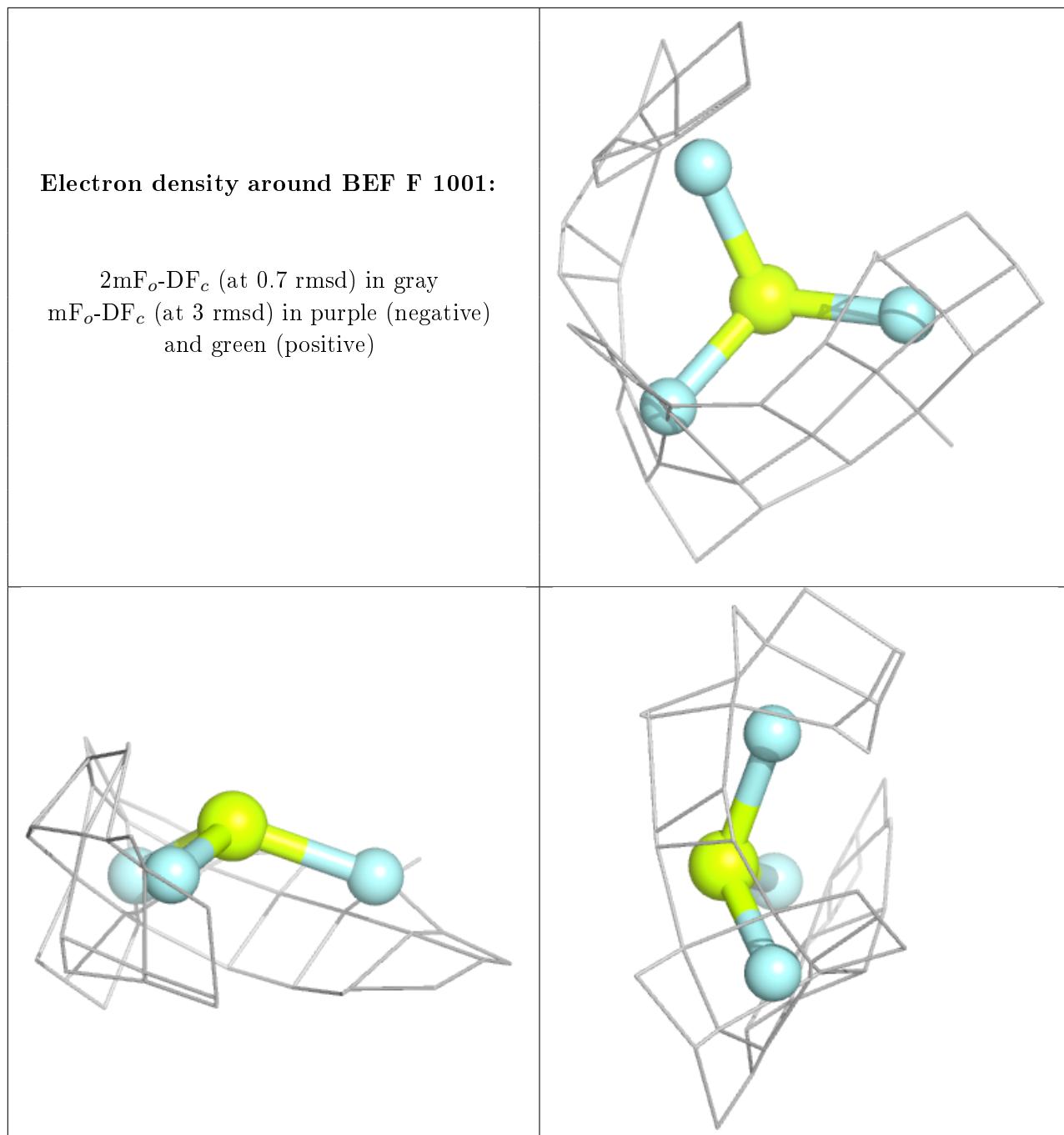
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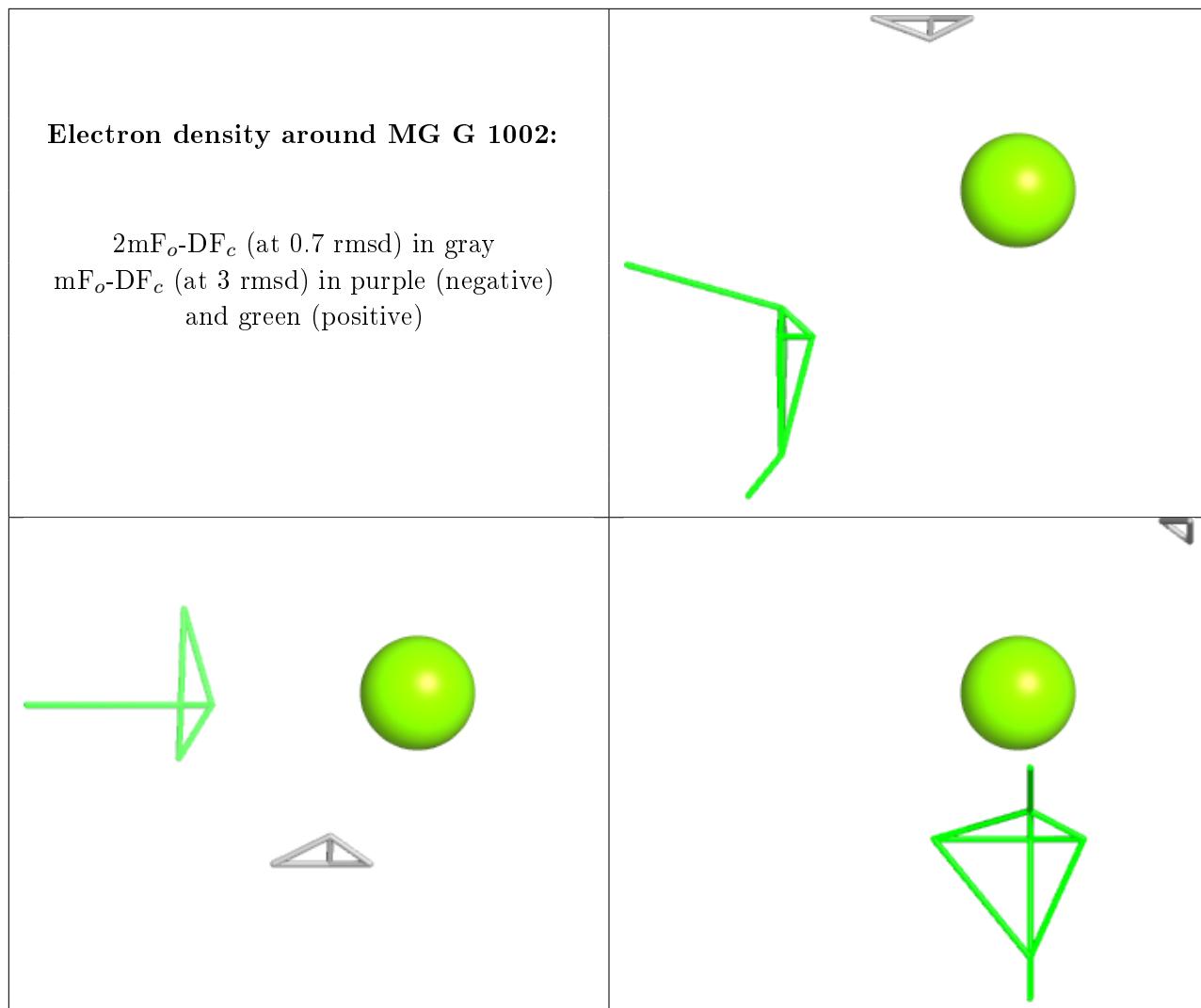
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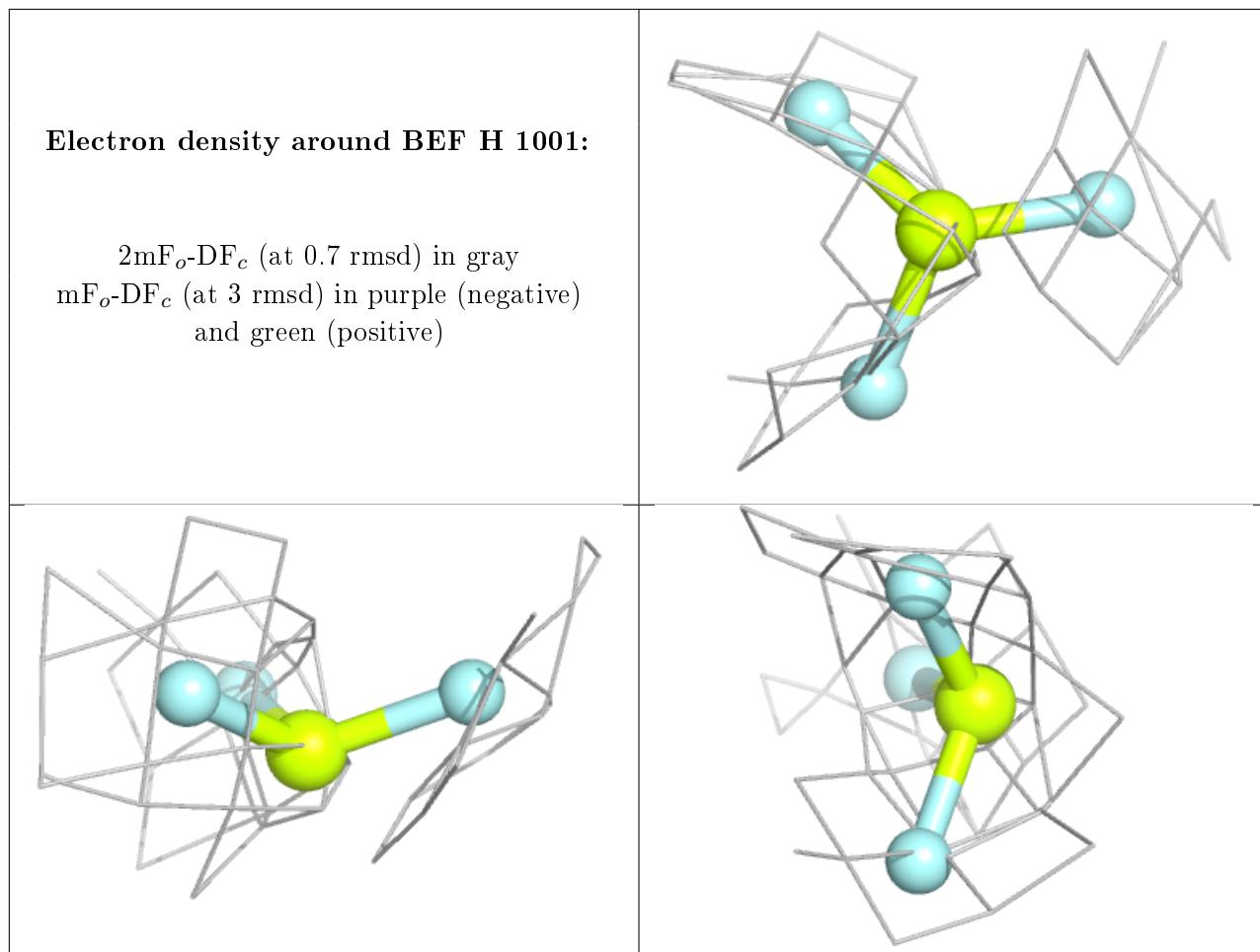
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	CE1	C	1007	15/37	0.94	0.22	21,37,49,50	0
5	CE1	D	1008	11/37	0.95	0.21	23,41,49,52	0
3	MG	C	1002	1/1	0.96	0.12	64,64,64,64	0
5	CE1	D	1004	12/37	0.96	0.19	19,33,37,44	0
5	CE1	D	1007	12/37	0.97	0.17	12,17,36,44	0
2	BEF	C	1001	4/4	0.97	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
3	MG	A	1002	1/1	0.99	0.16	44,44,44,44	0

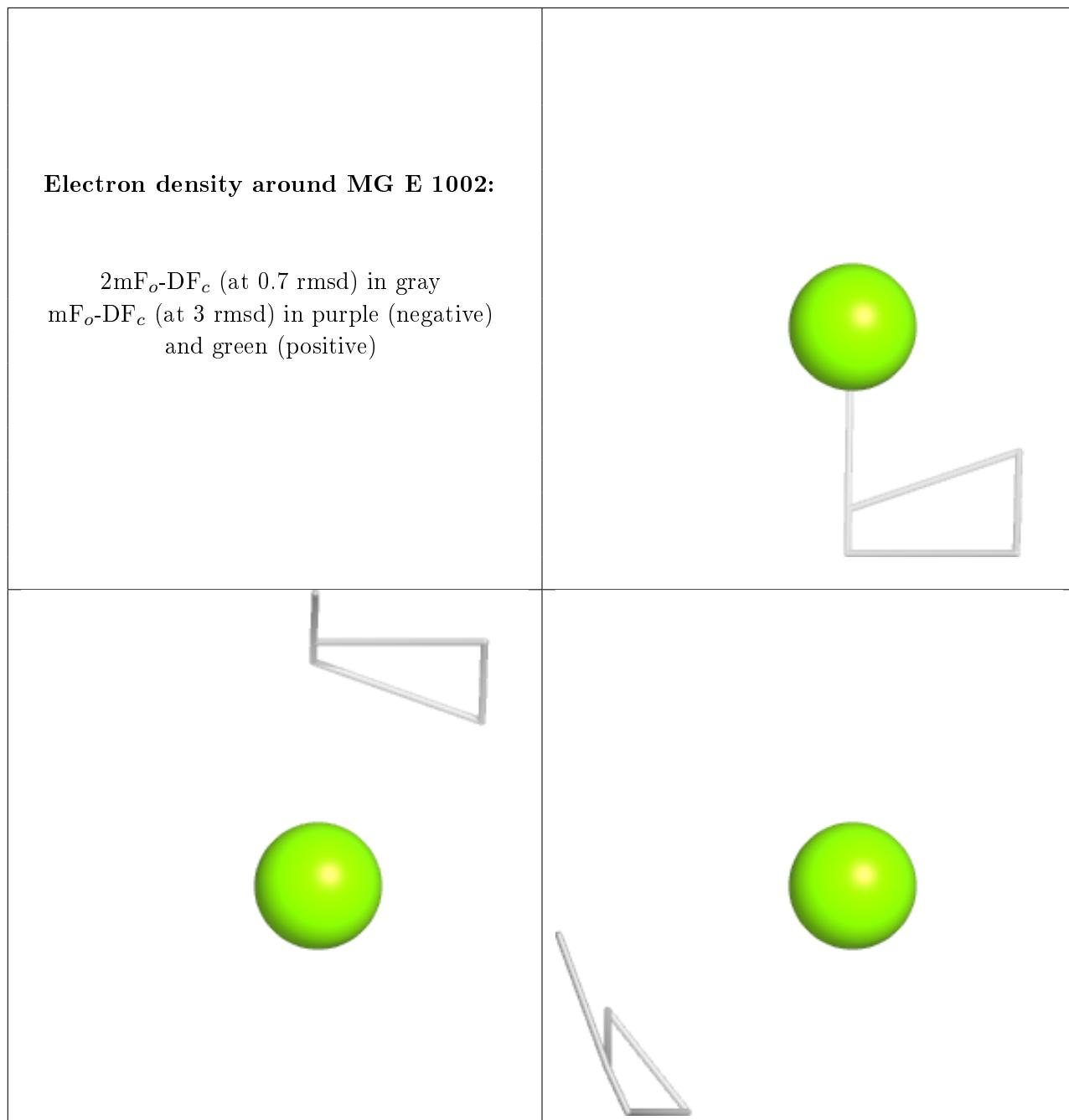
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

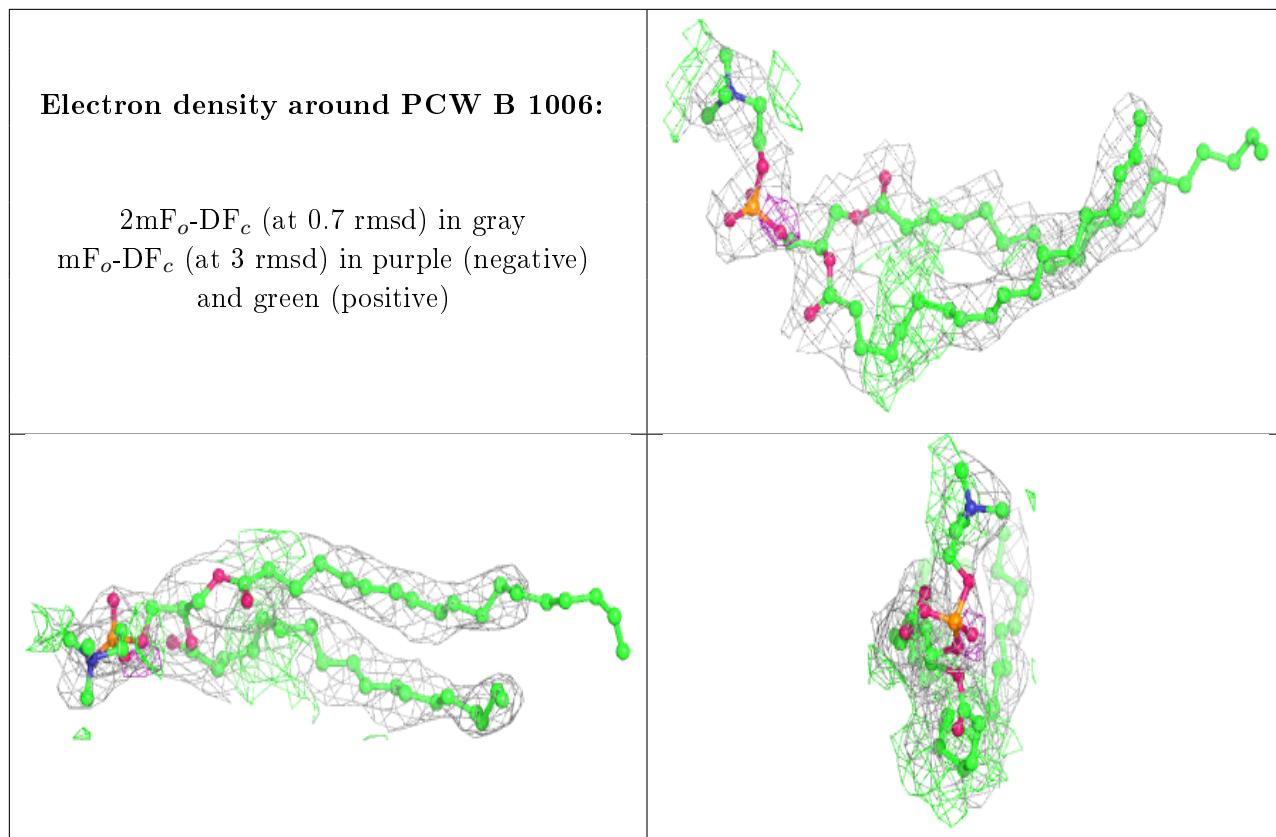


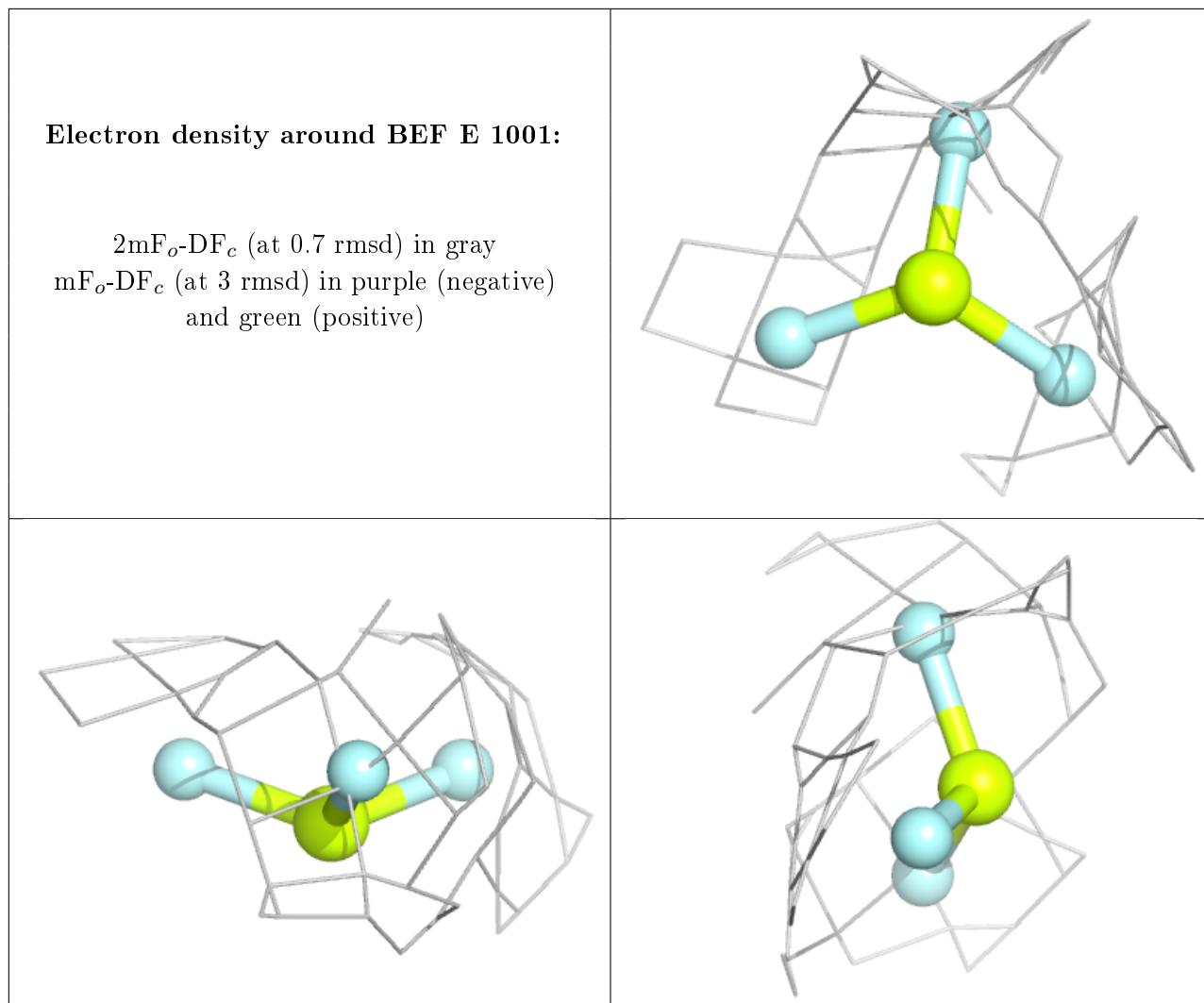




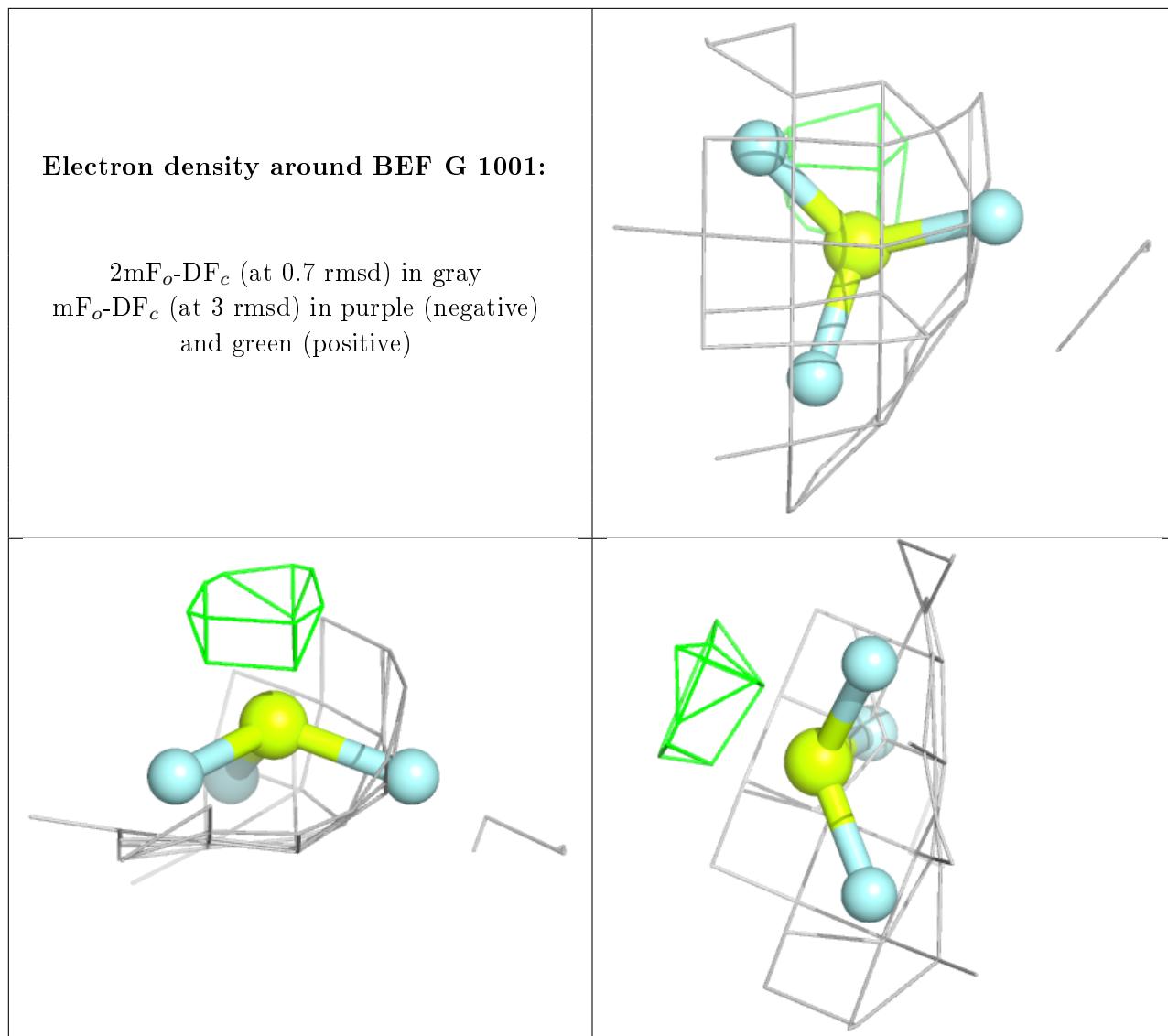


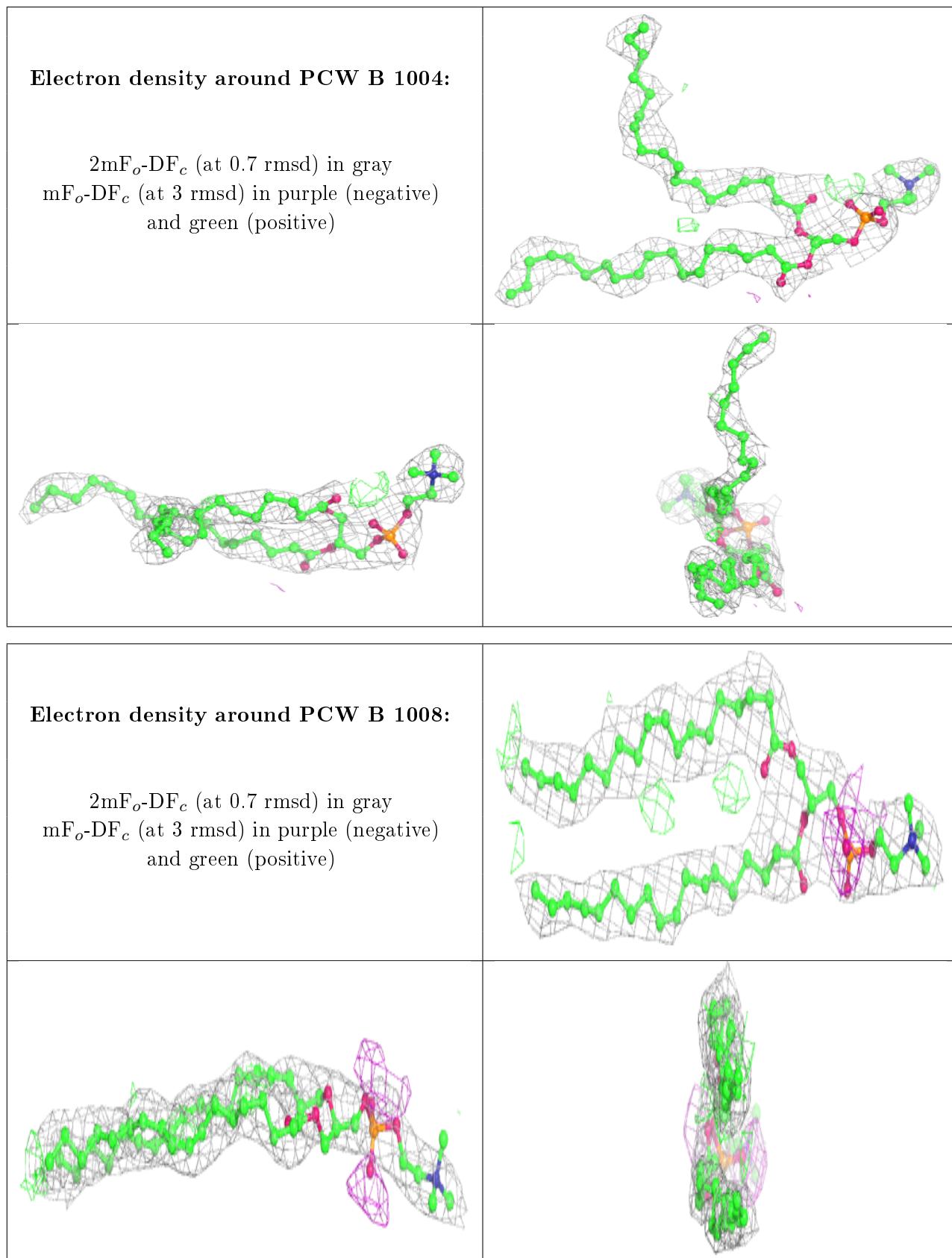


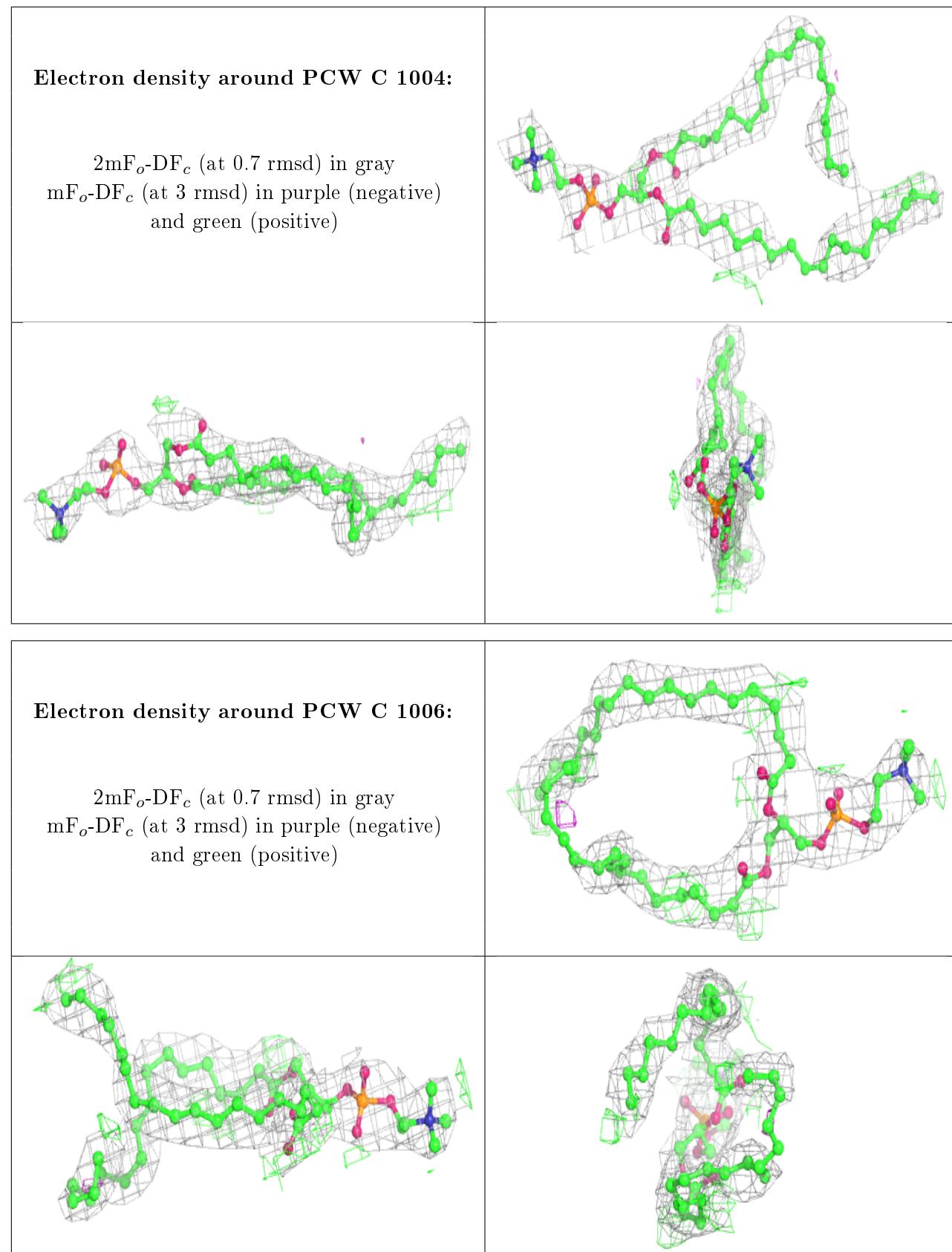


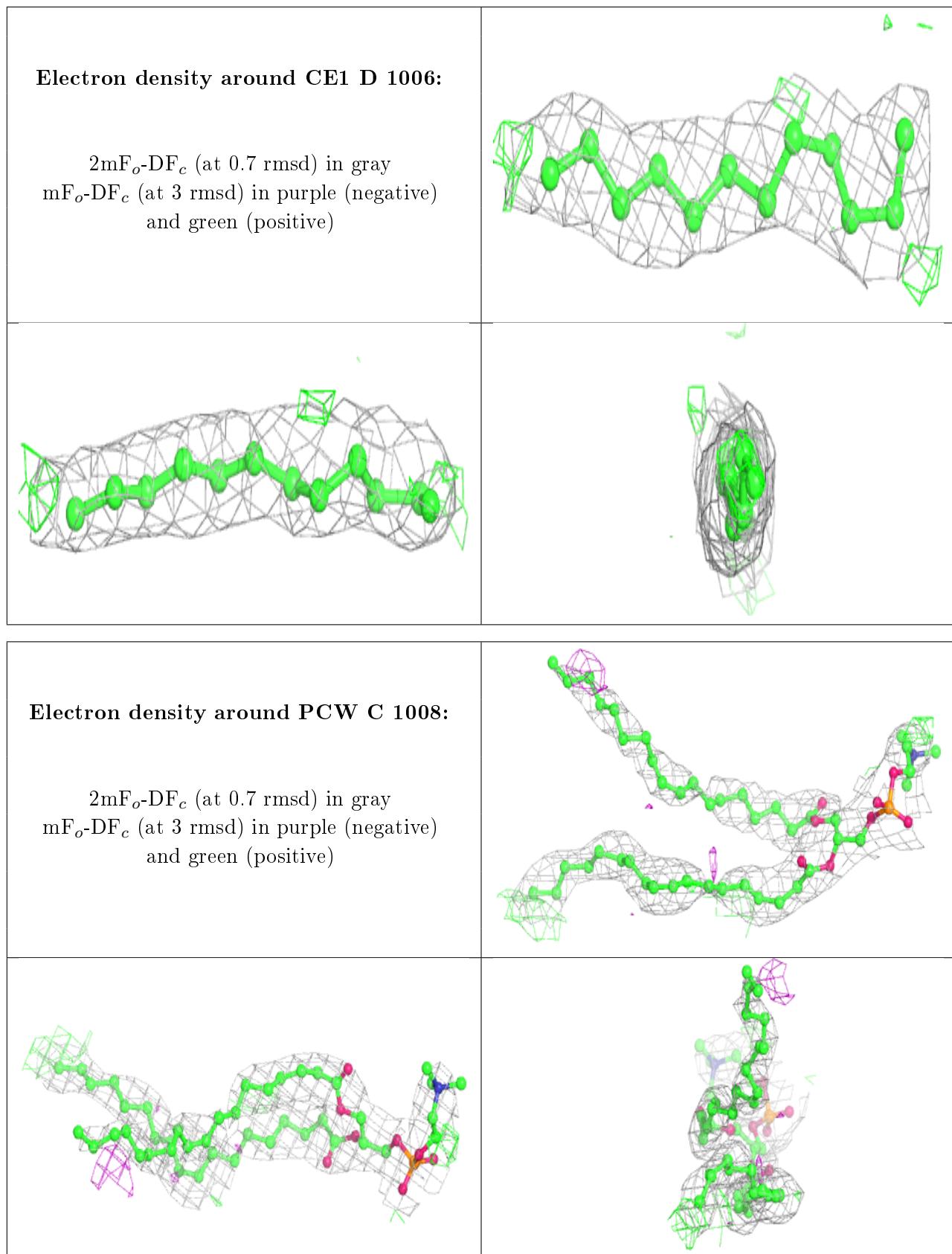


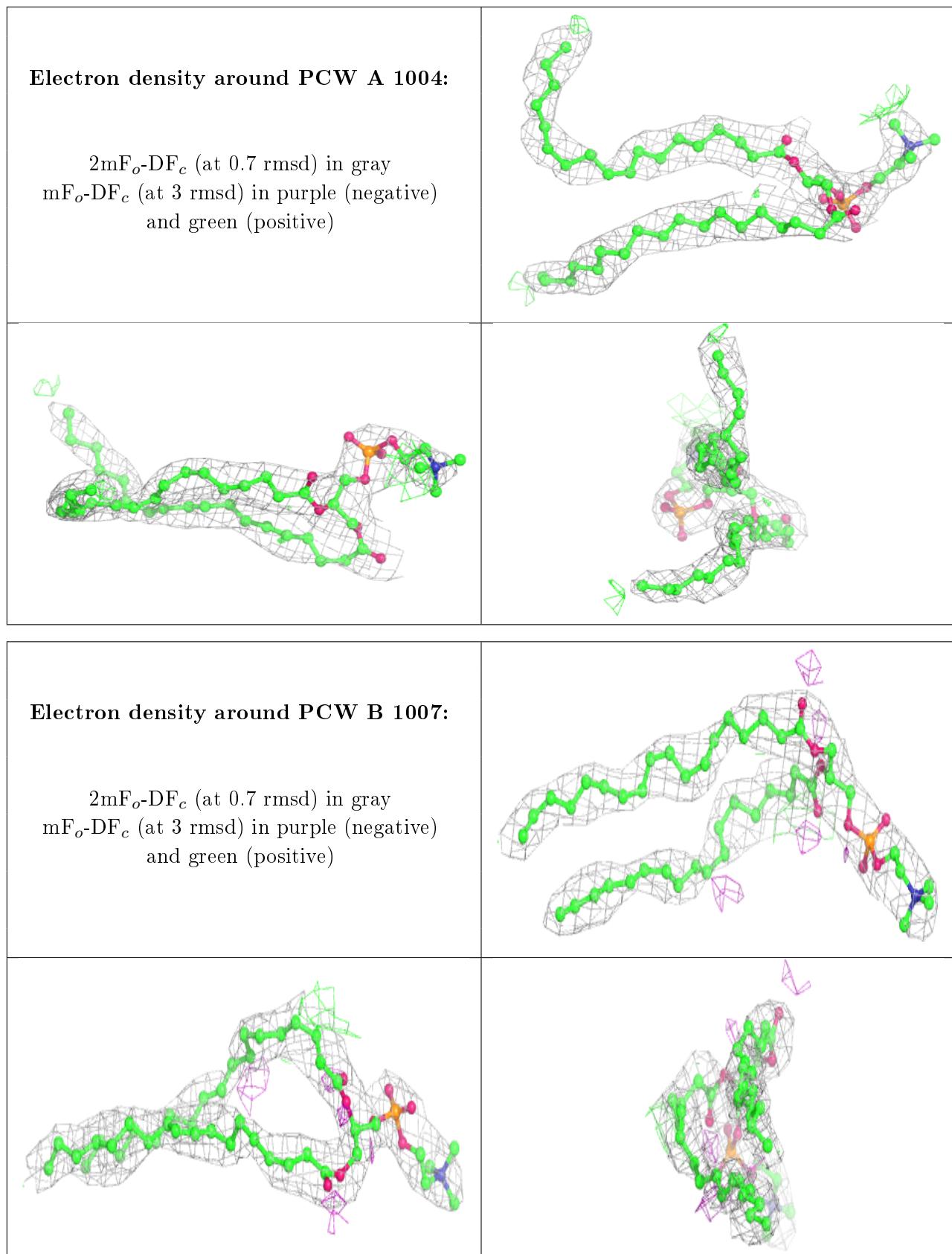


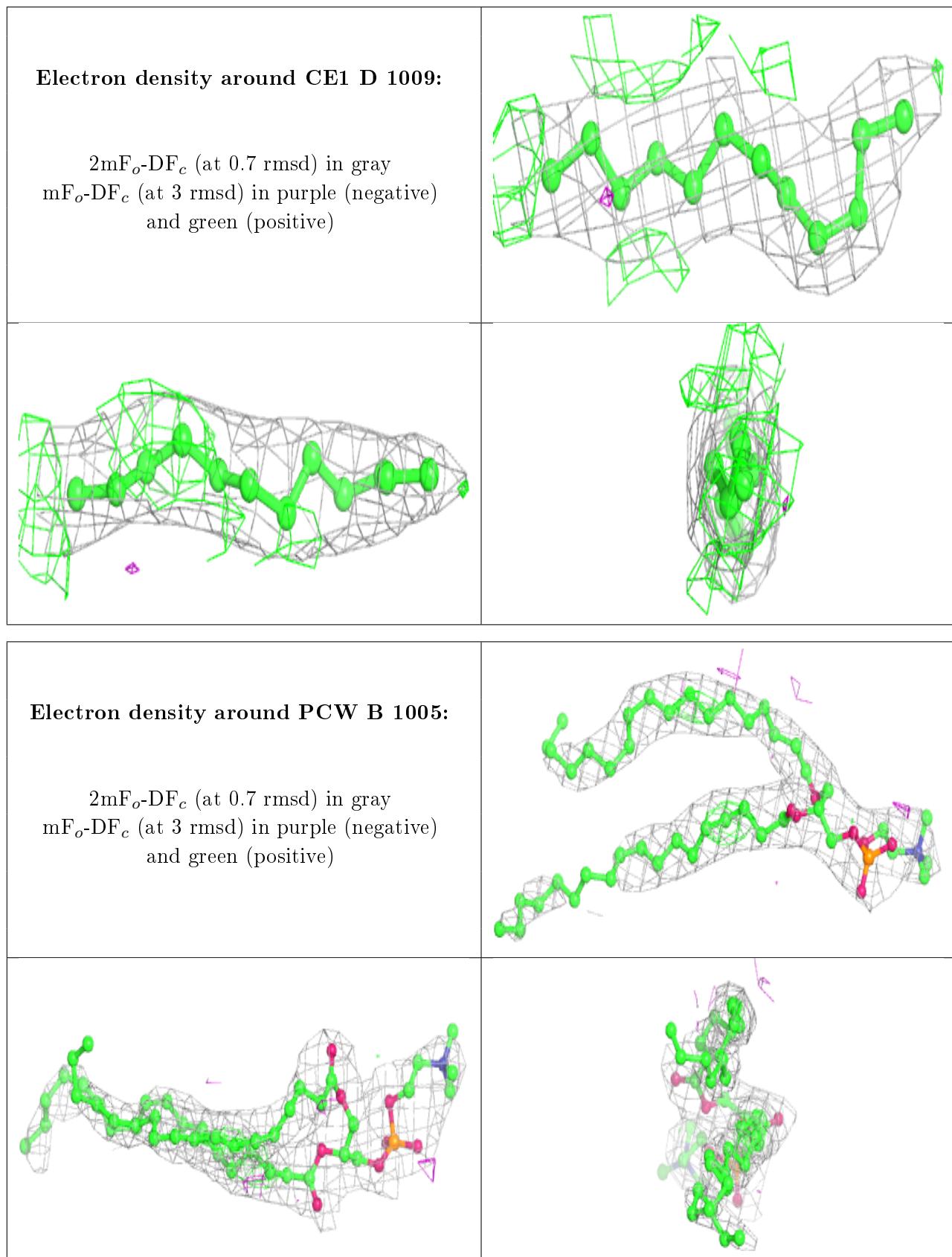


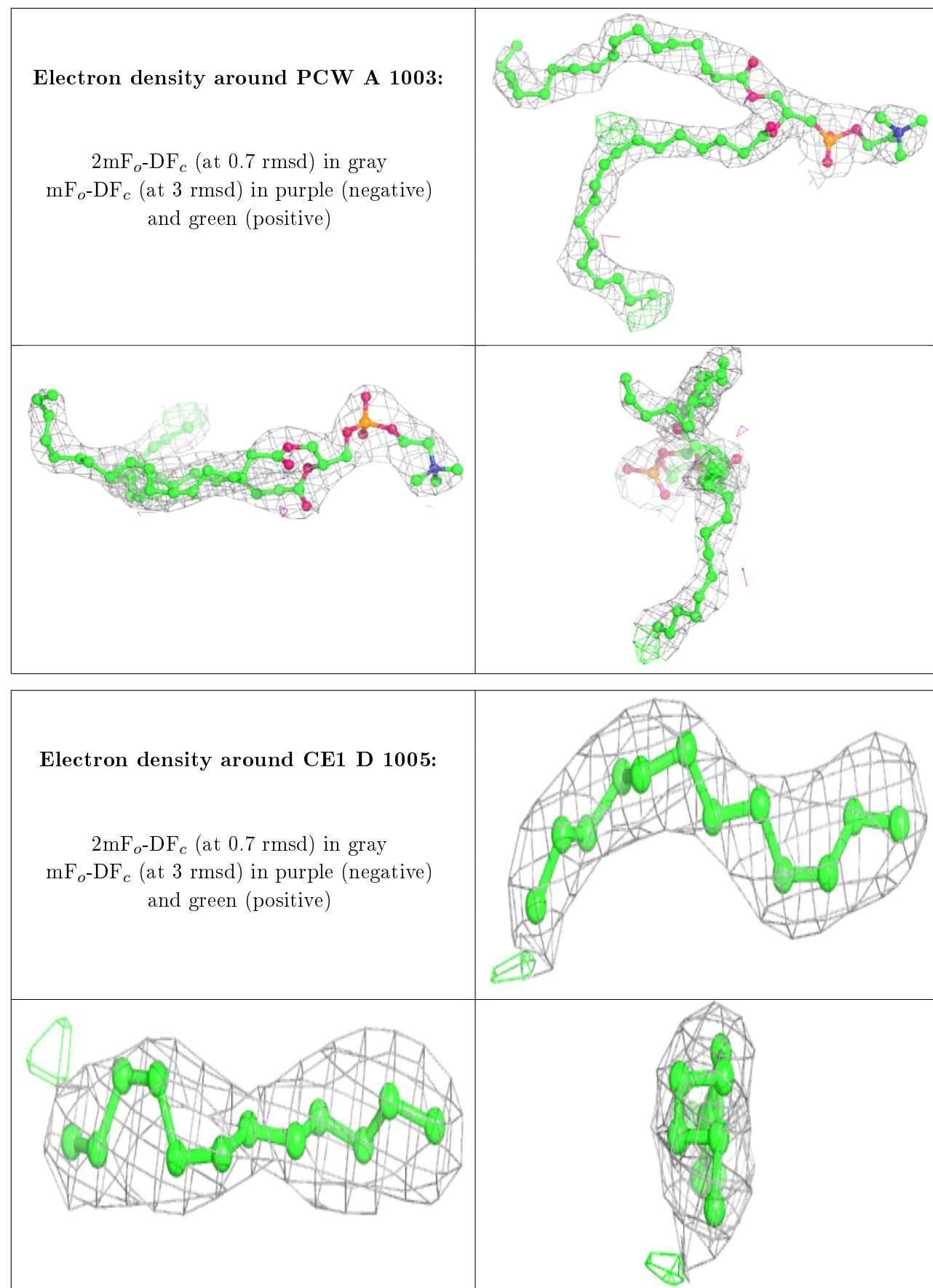


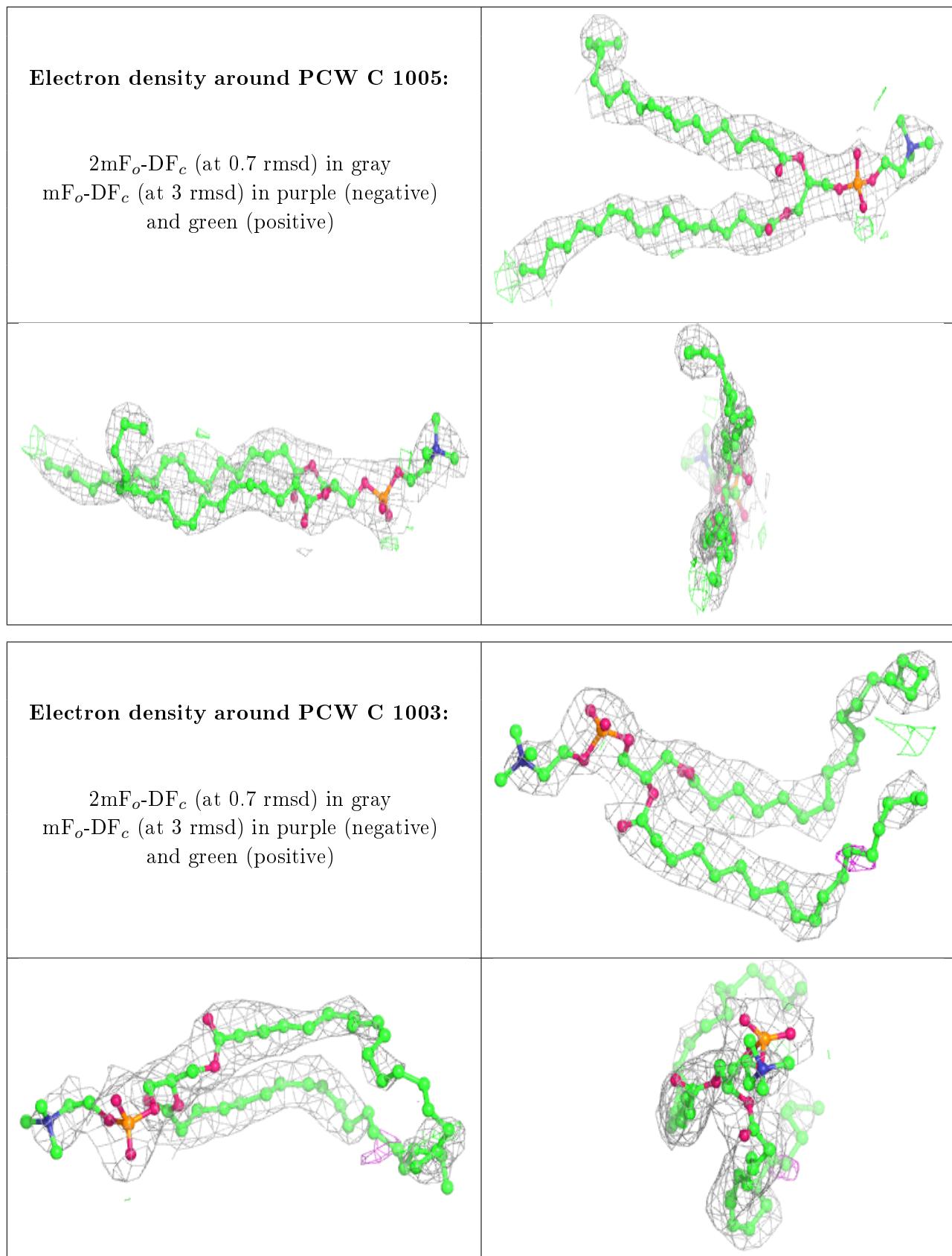


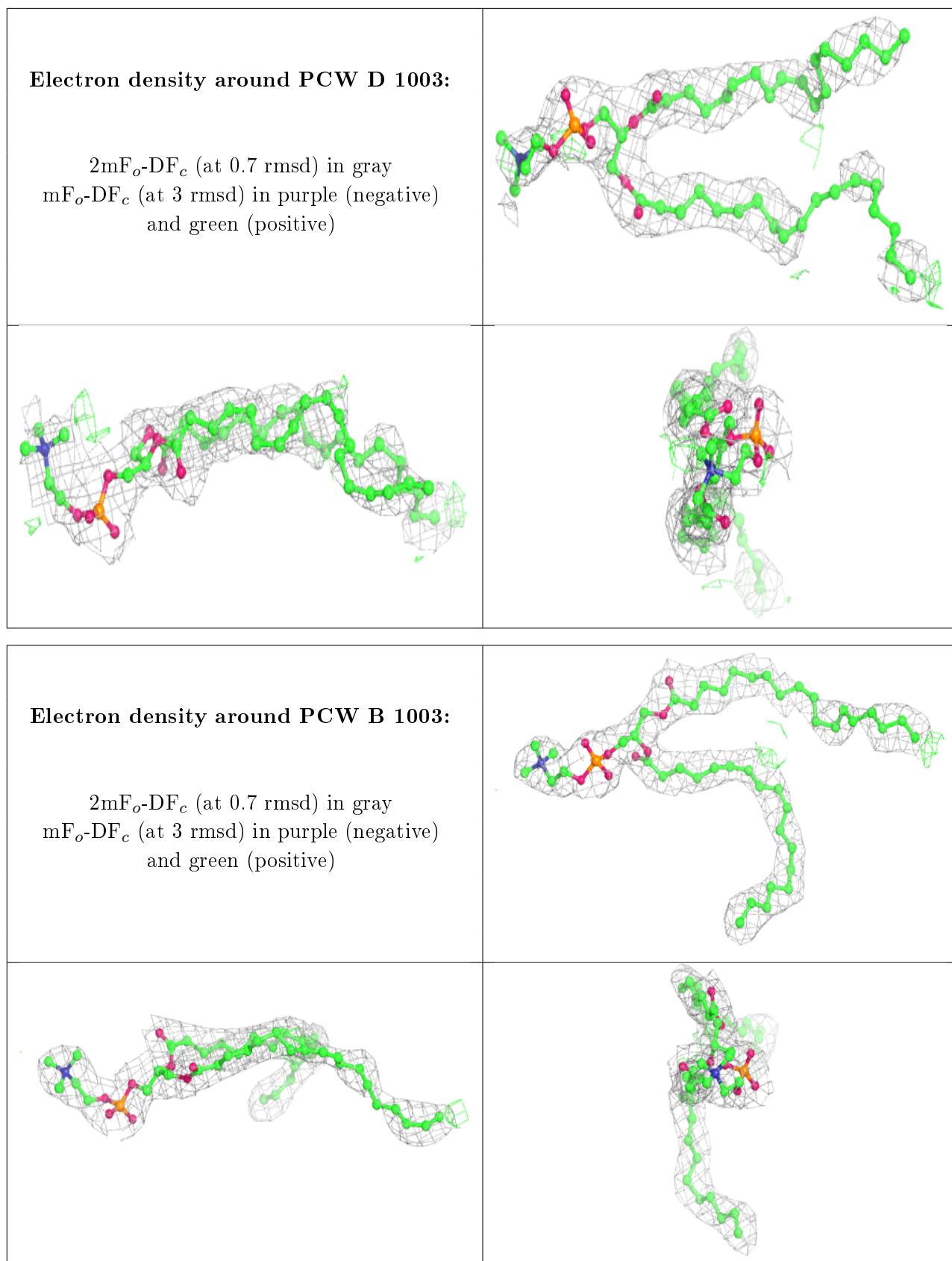


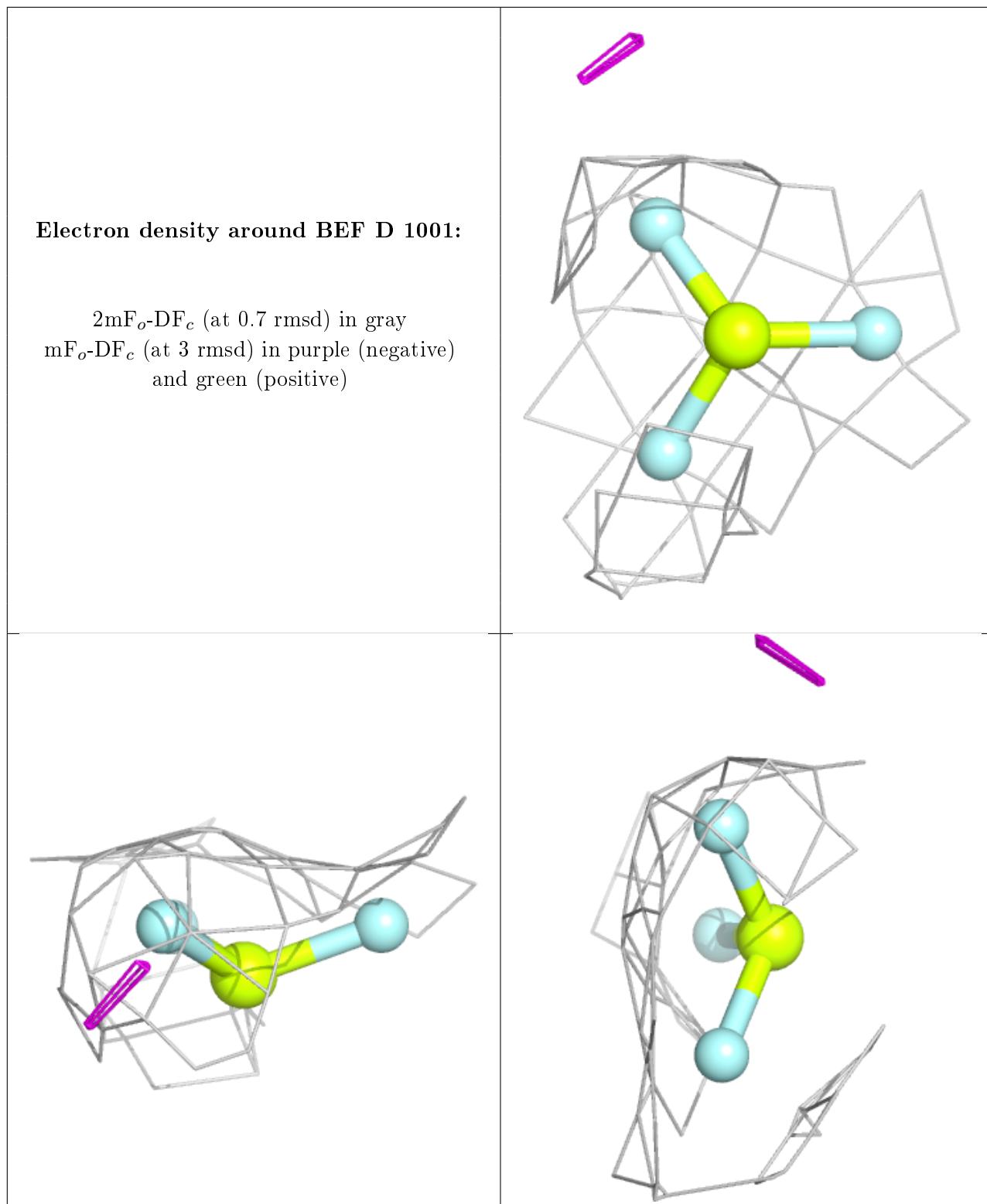


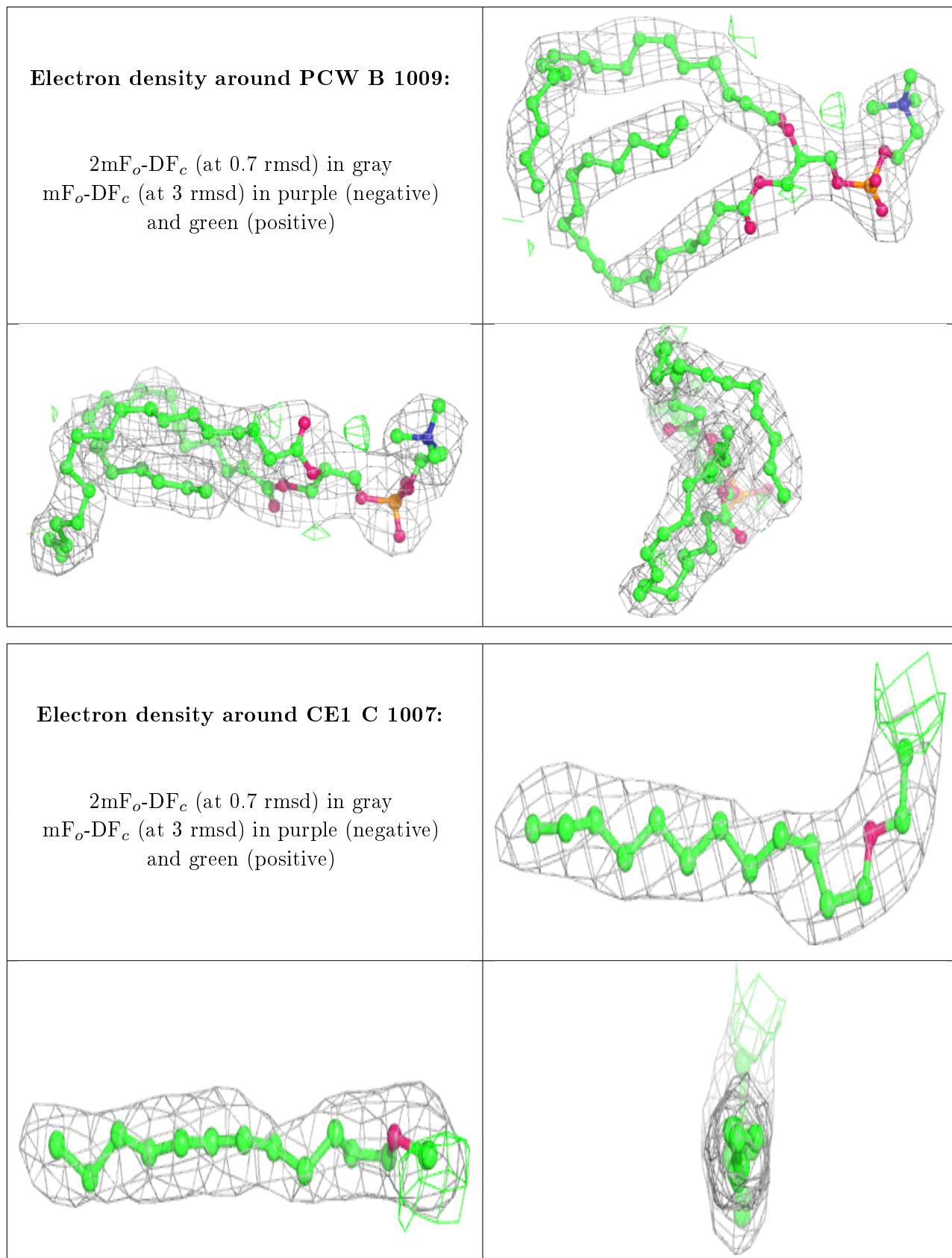


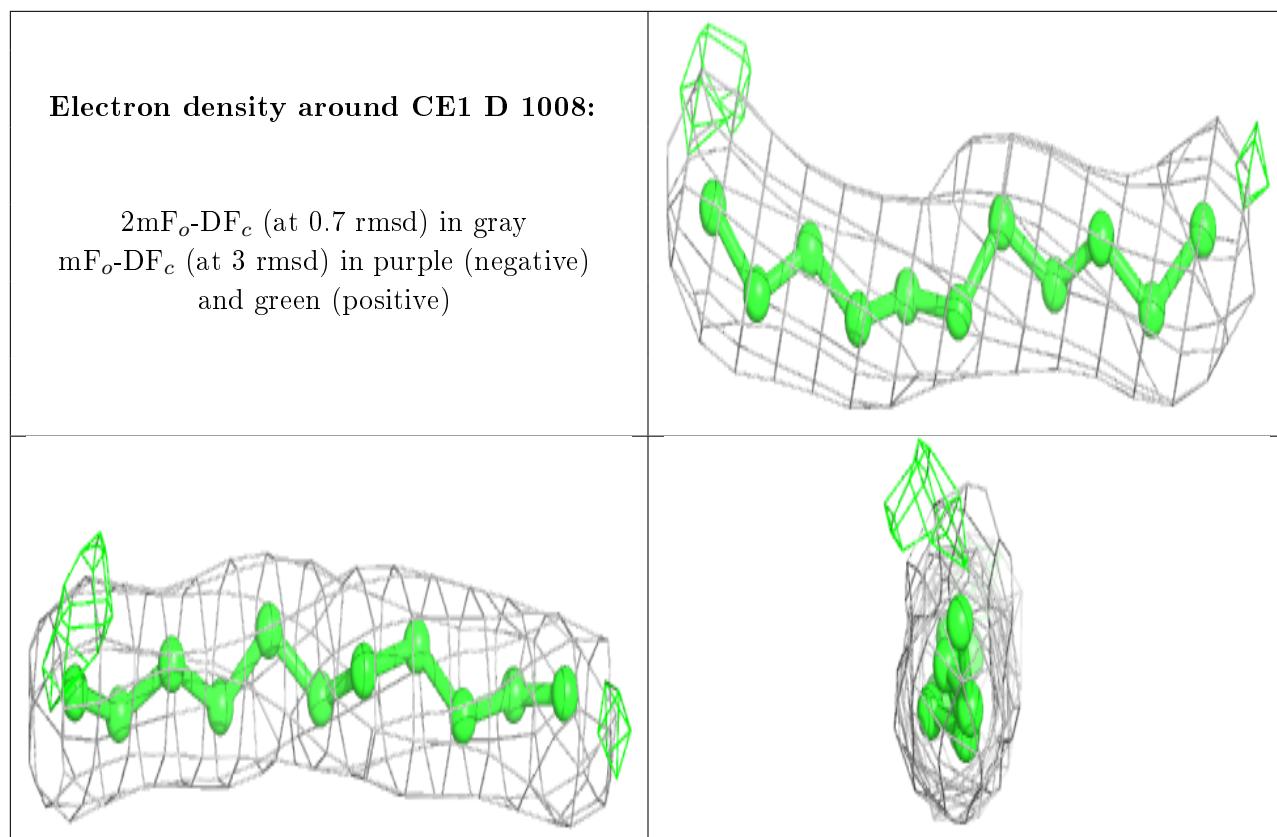


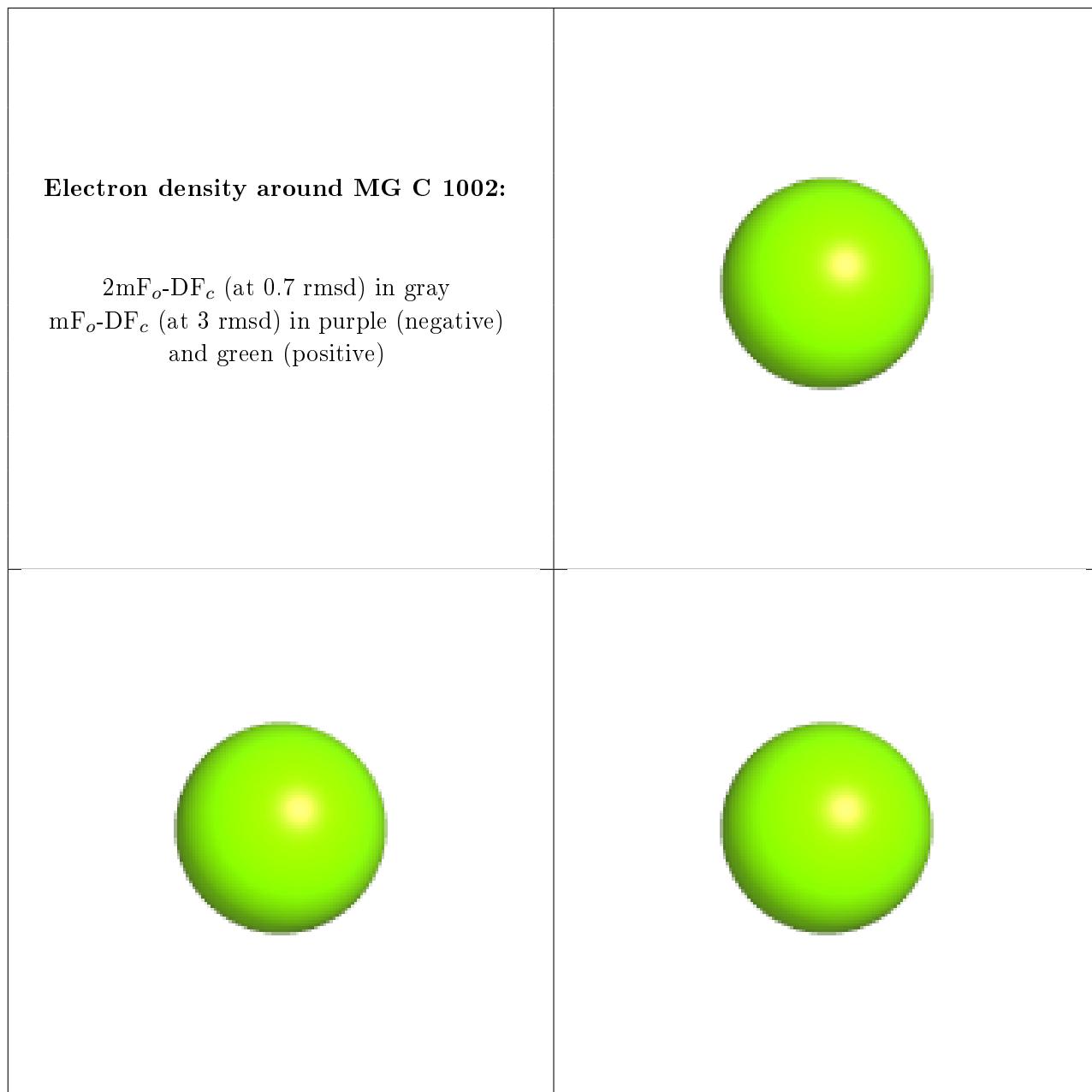


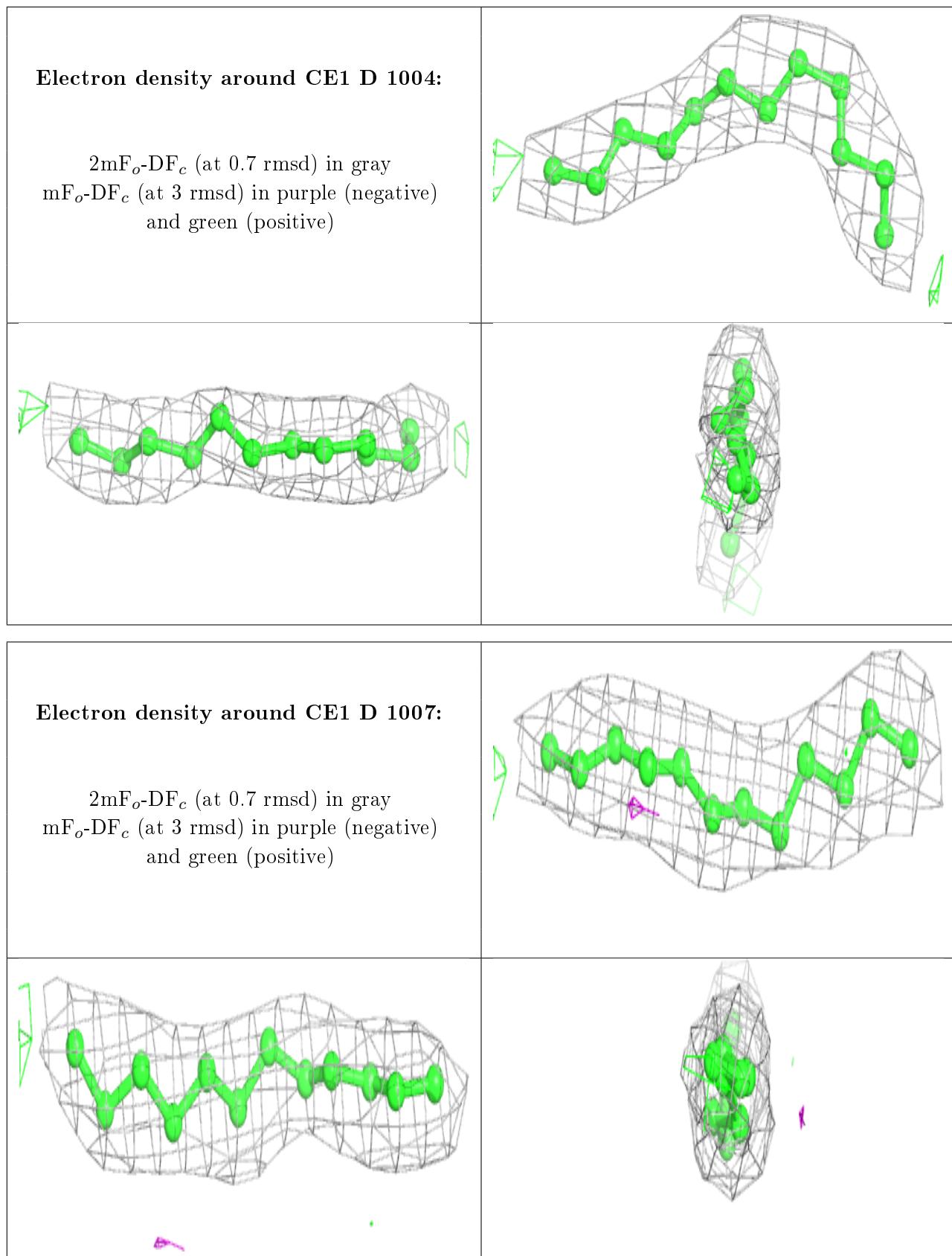


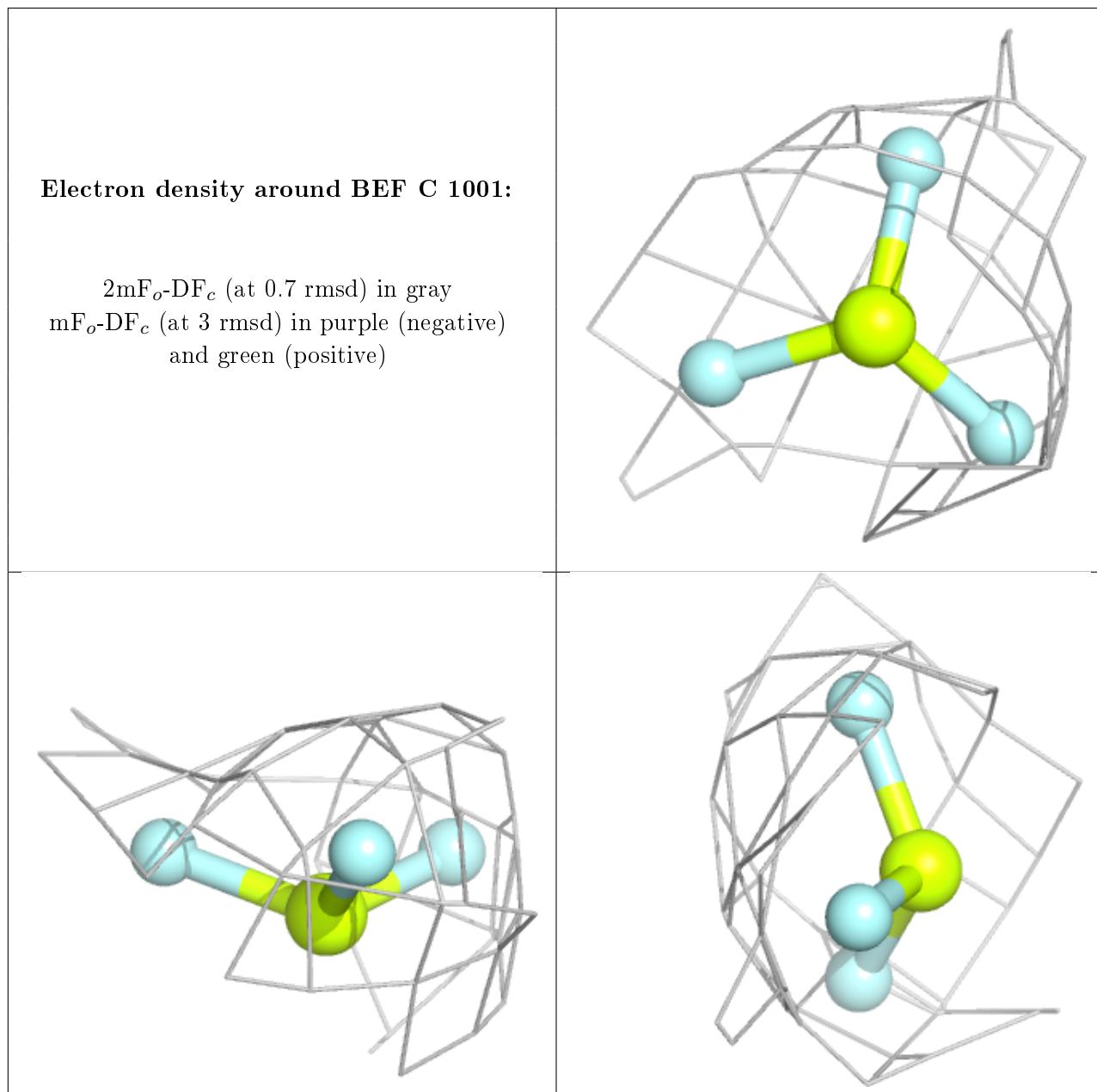


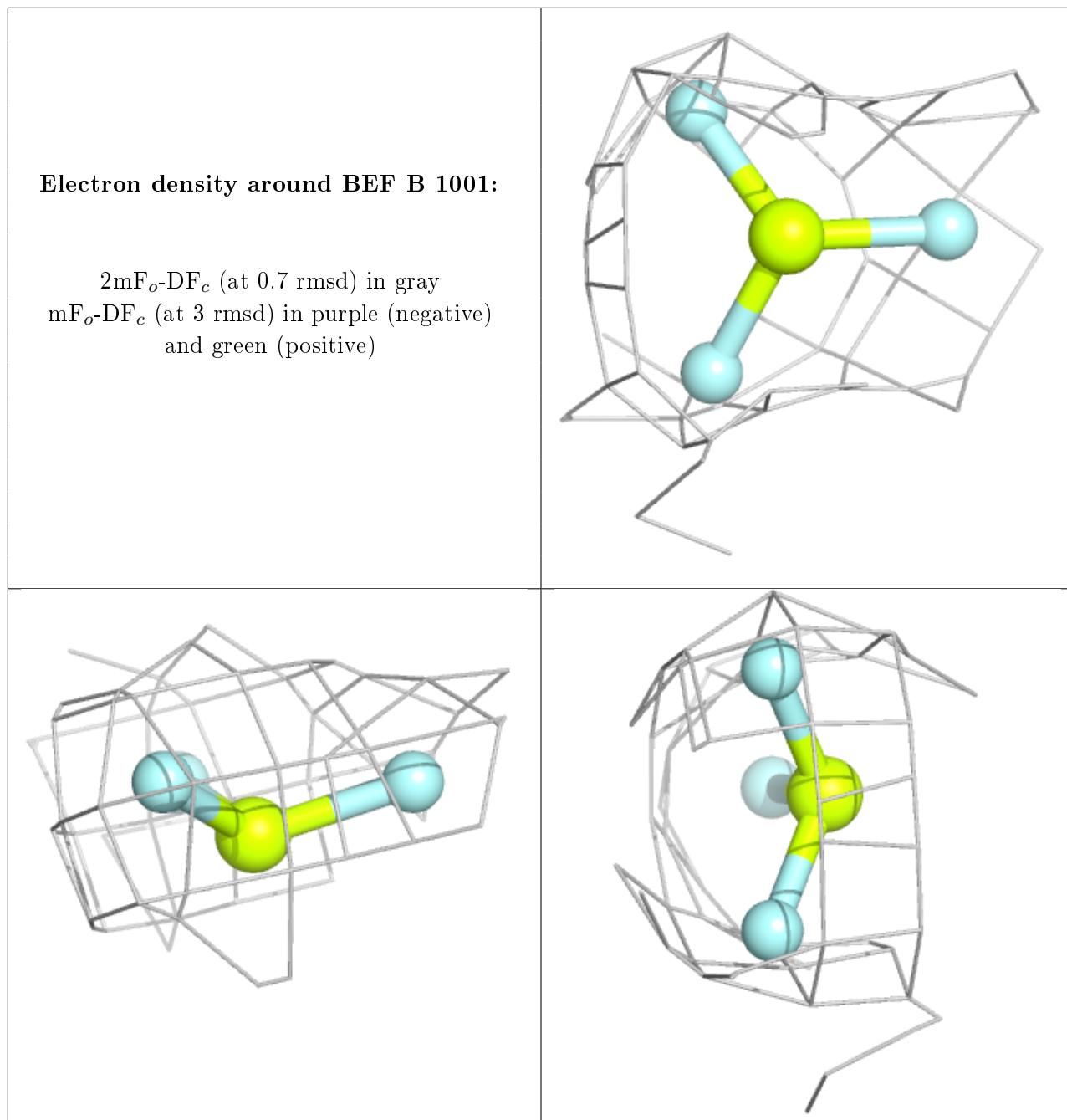


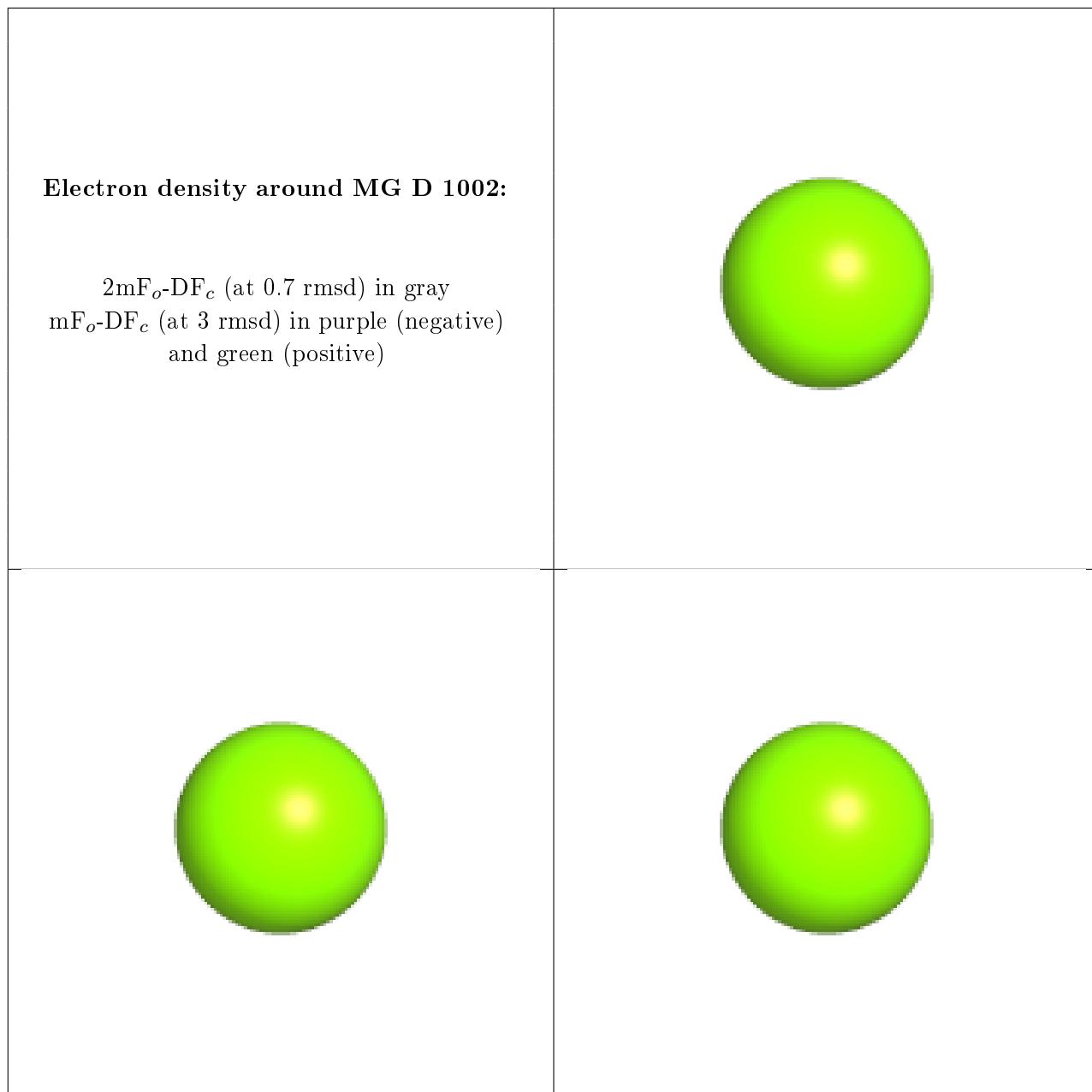


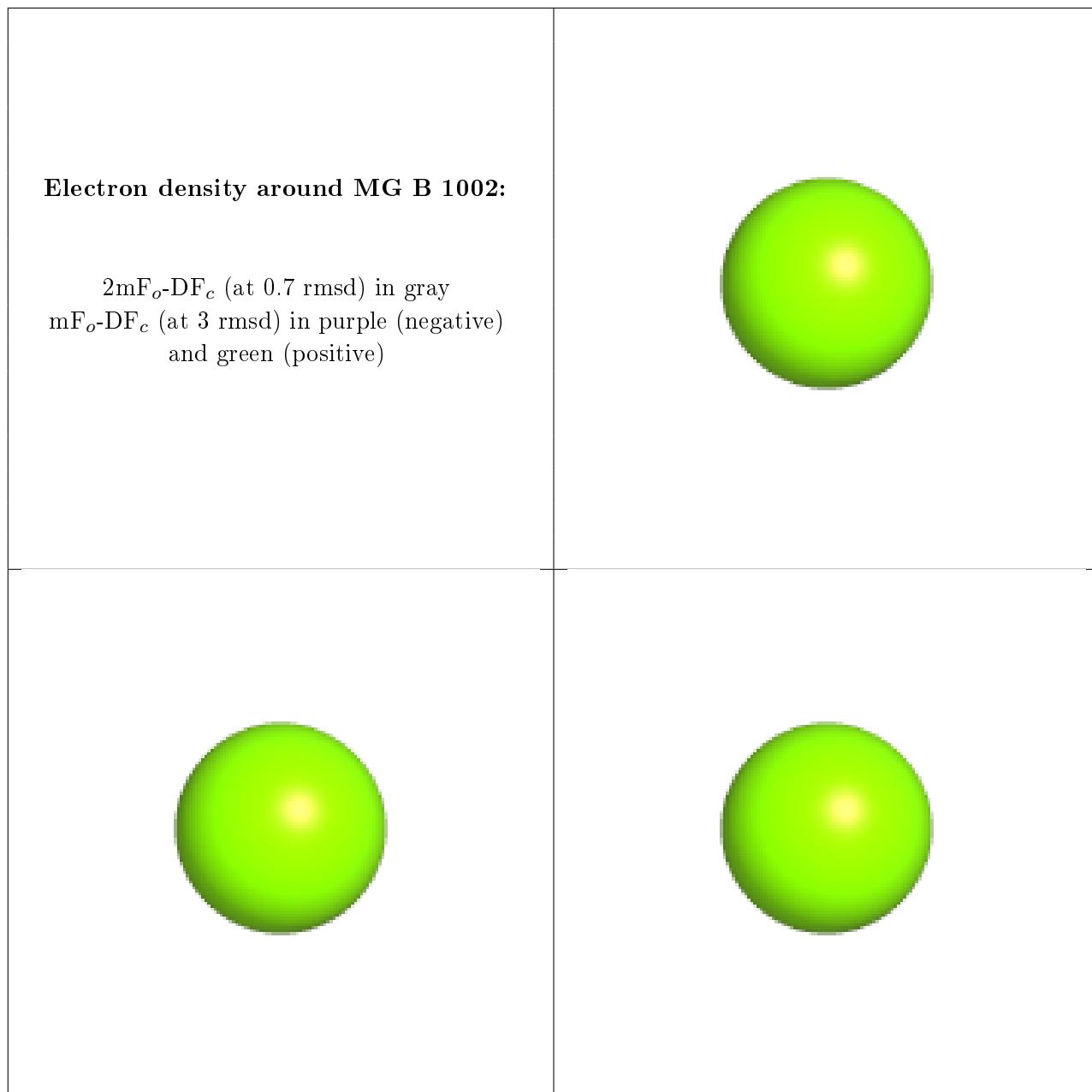


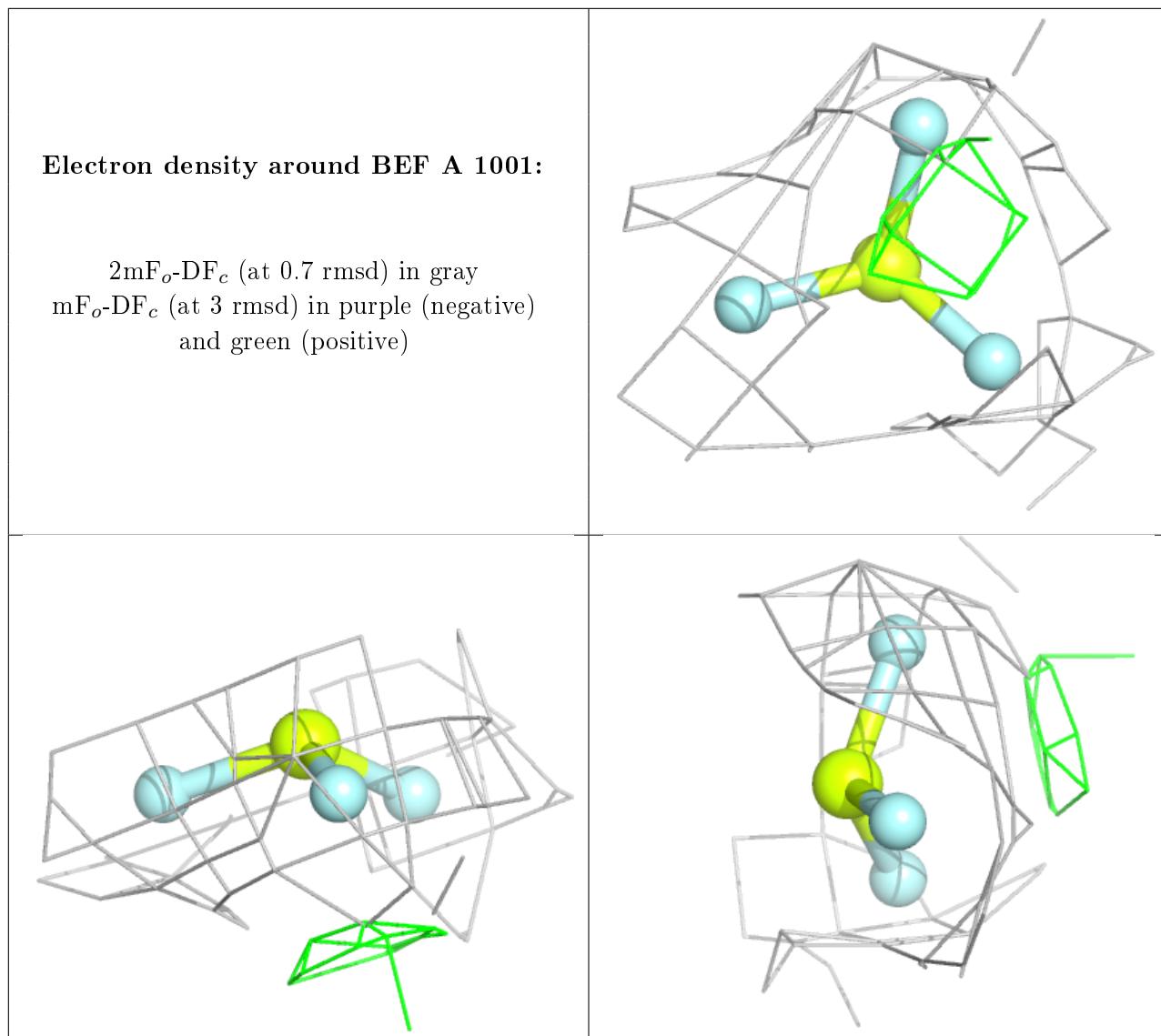


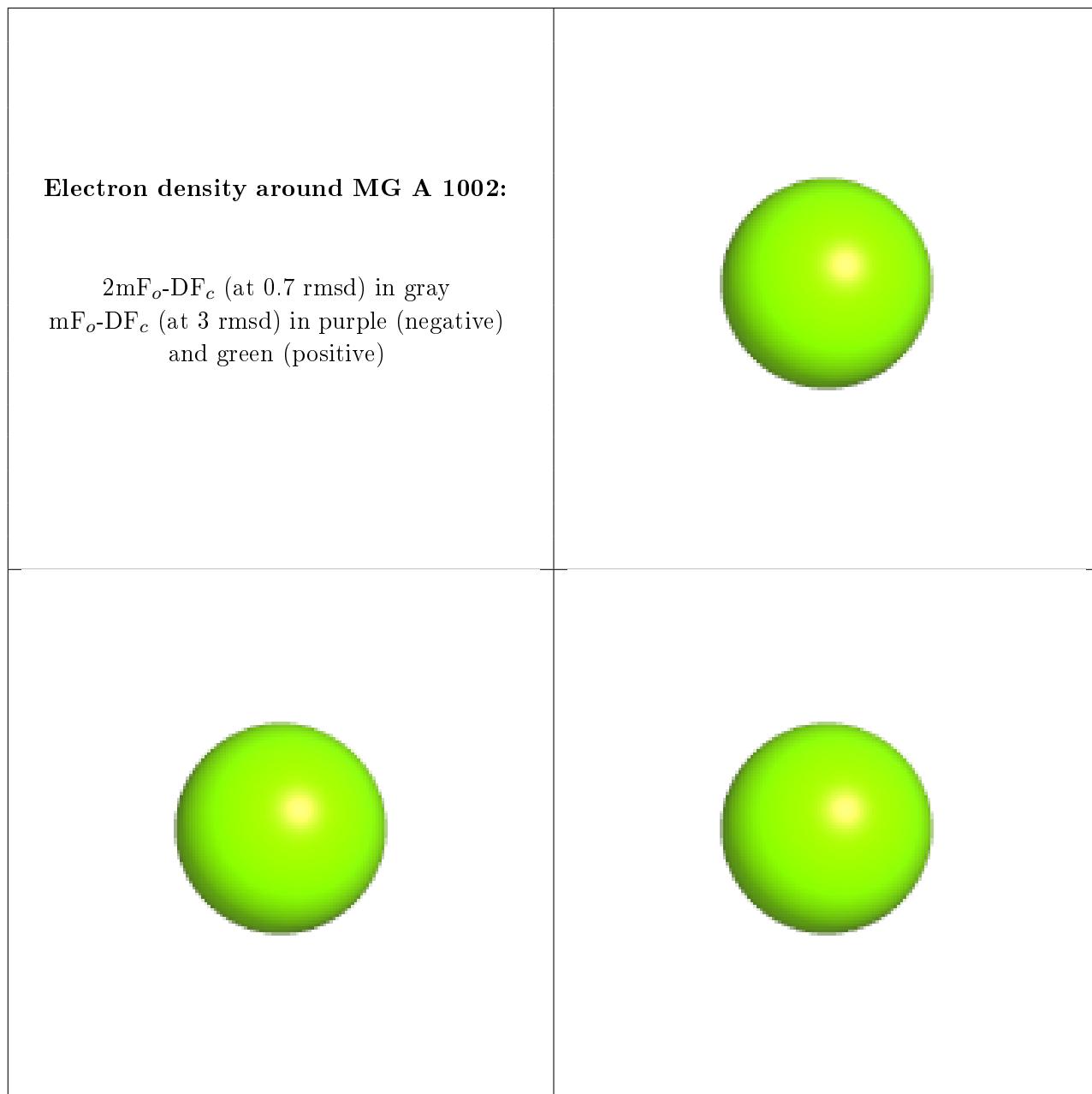












## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.