



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:50 AM UTC

PDB ID : 6ZHH / pdb_00006zhh
Title : Ca²⁺-ATPase from *Listeria Monocytogenes* with G4 insertion.
Authors : Basse Hansen, S.; Dyla, M.; Neumann, C.; Quistgaard, E.M.H.; Lauwring Andersen, J.; Kjaergaard, M.; Nissen, P.
Deposited on : 2020-06-23
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

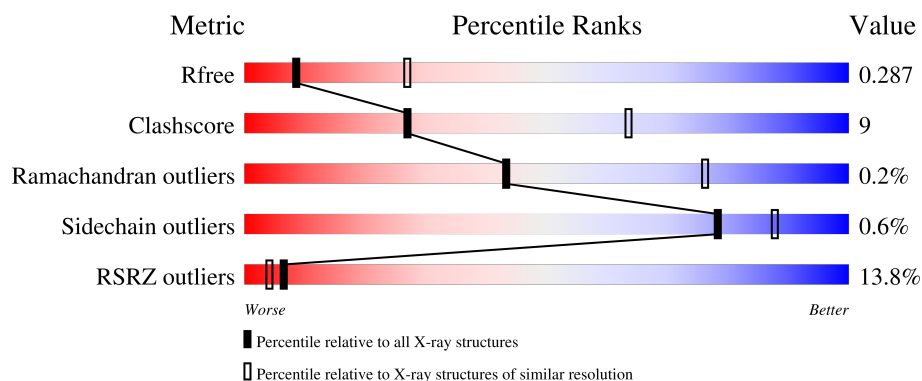
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	911	2% 79%17%.
1	B	911	% 77%20%.
1	C	911	5% 76%21%.
1	D	911	6% 75%21%..
1	E	911	24% 73%23%. .

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Mol	Chain	Length	Quality of chain
1	F	911	24% 75% 21% .
1	G	911	22% 78% 18% .
1	H	911	23% 73% 22% ..

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 54572 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Calcium-transporting ATPase.

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

There are 256 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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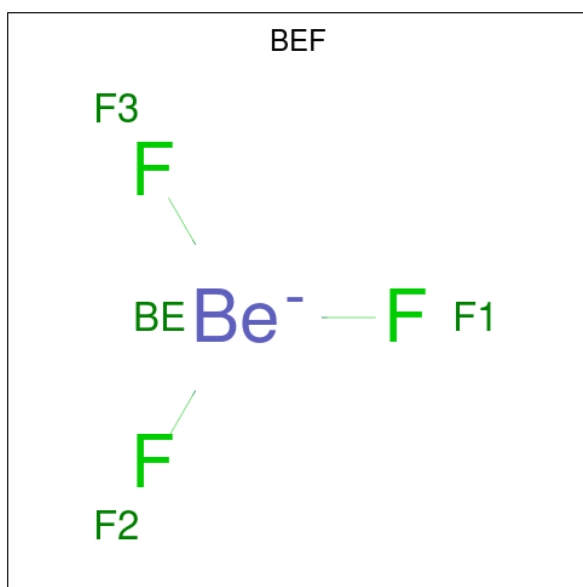
Chain	Residue	Modelled	Actual	Comment	Reference
F	896	GLU	-	expression tag	UNP A0A1C7PY84
F	897	HIS	-	expression tag	UNP A0A1C7PY84
F	898	HIS	-	expression tag	UNP A0A1C7PY84
F	899	HIS	-	expression tag	UNP A0A1C7PY84
F	900	HIS	-	expression tag	UNP A0A1C7PY84
F	901	HIS	-	expression tag	UNP A0A1C7PY84
F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

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

- Molecule 2 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF₃) (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 (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

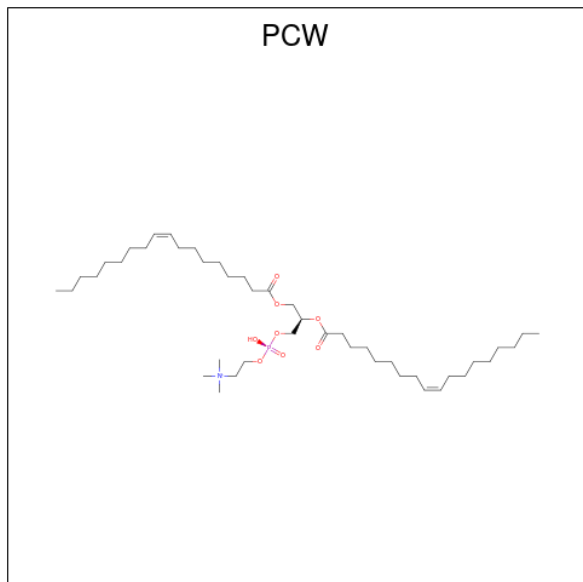
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

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

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



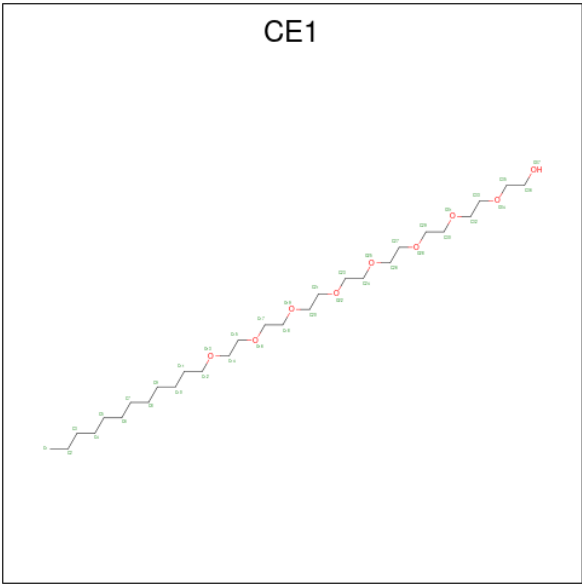
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
4	A	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
4	B	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
4	B	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
4	B	1	Total	C	N	O	P	0	0
			54	44	1	8	1		

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

- Molecule 5 is O-DODECANYL OCTAETHYLENE GLYCOL (CCD ID: CE1) (formula: C₂₈H₅₈O₉).



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

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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

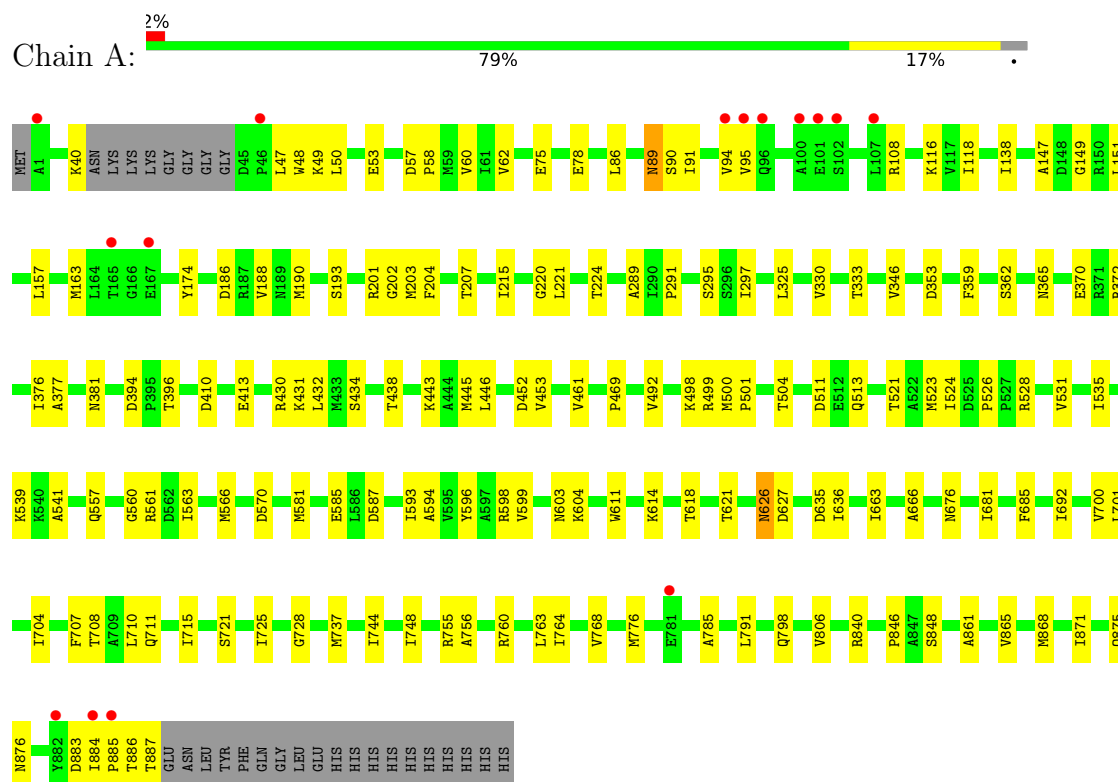
- Molecule 6 is water.

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

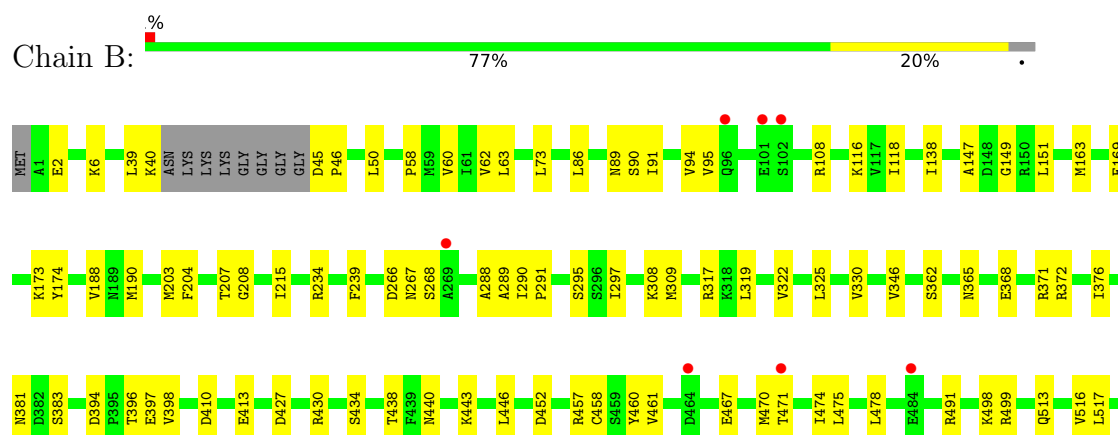
3 Residue-property plots

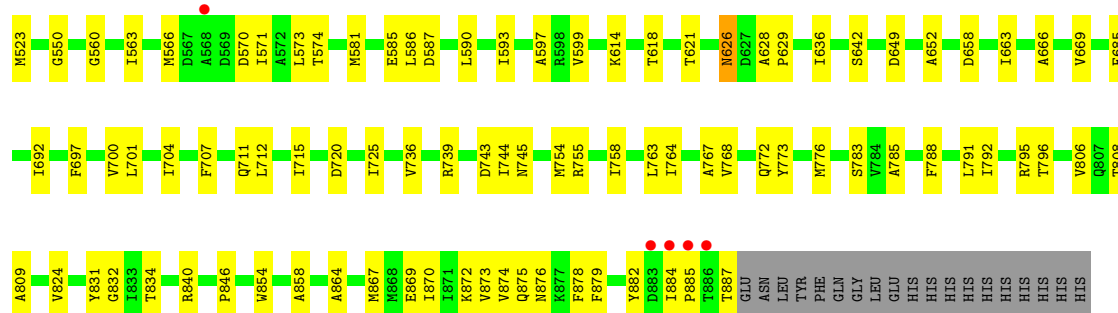
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

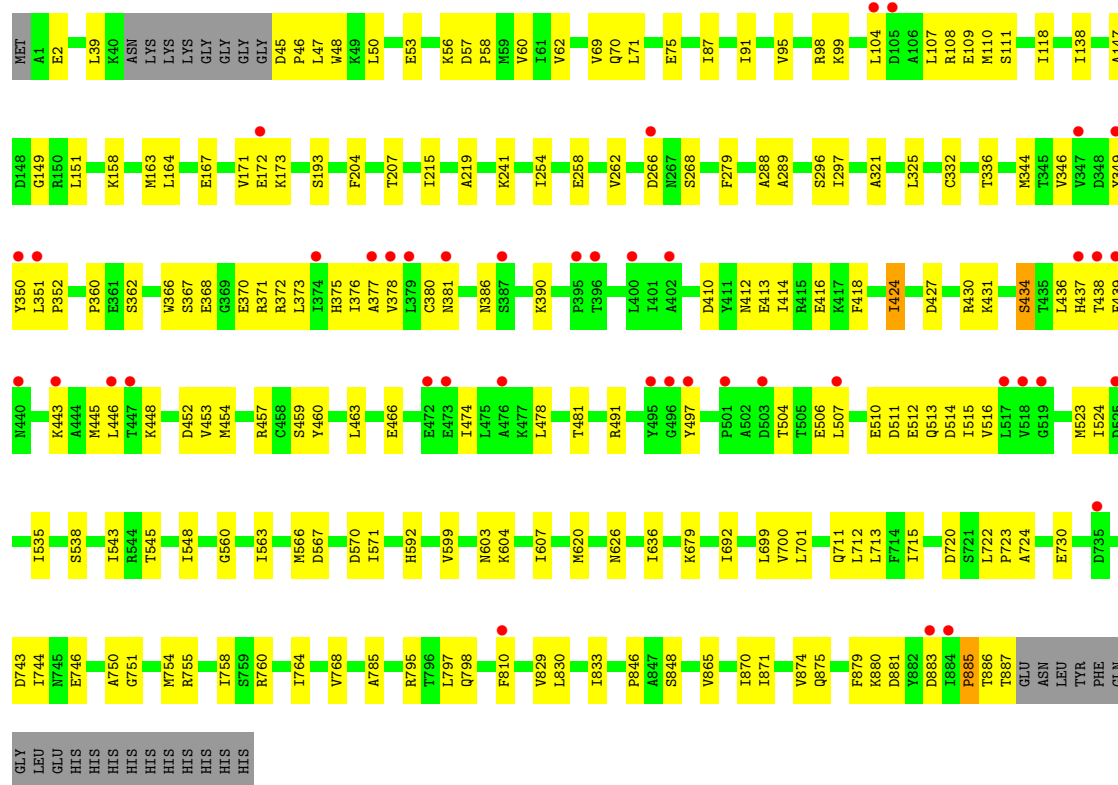
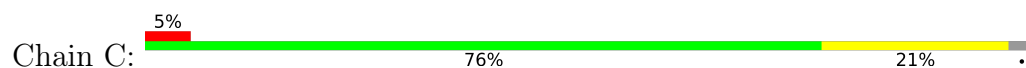


• Molecule 1: Calcium-transporting ATPase

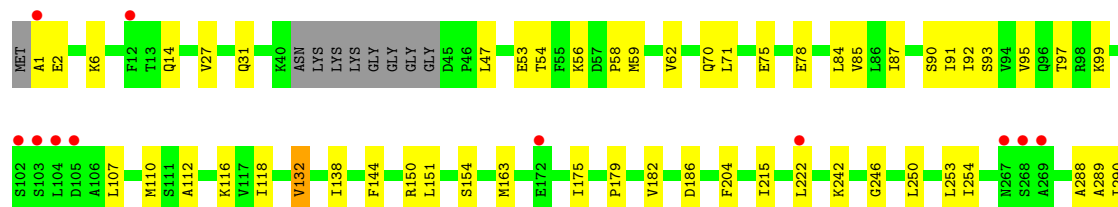
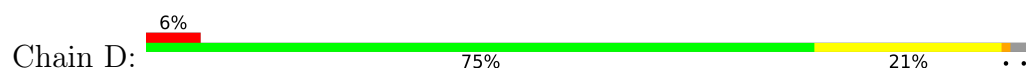


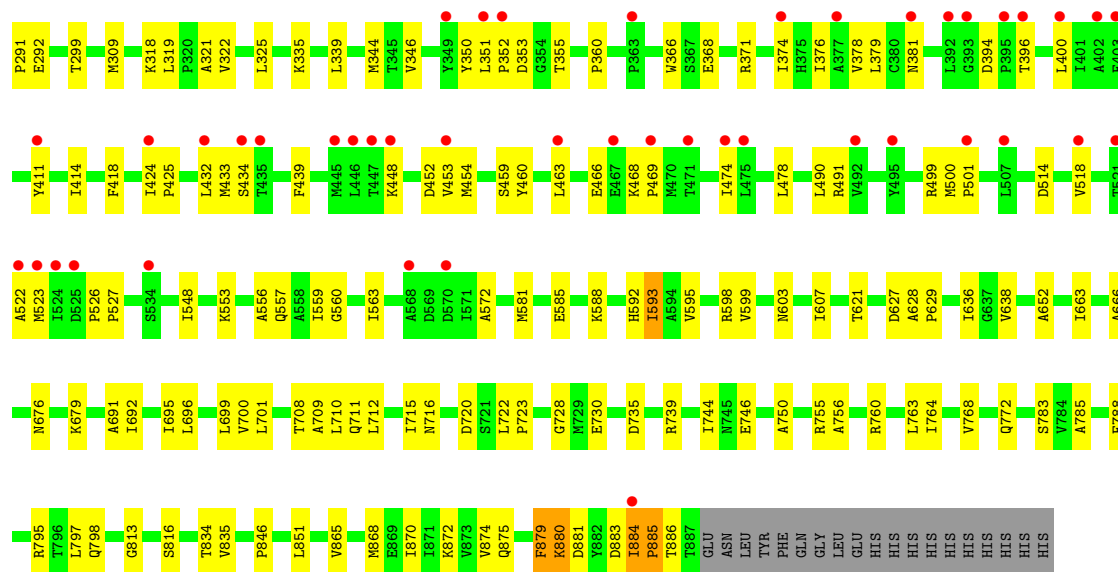


● Molecule 1: Calcium-transporting ATPase

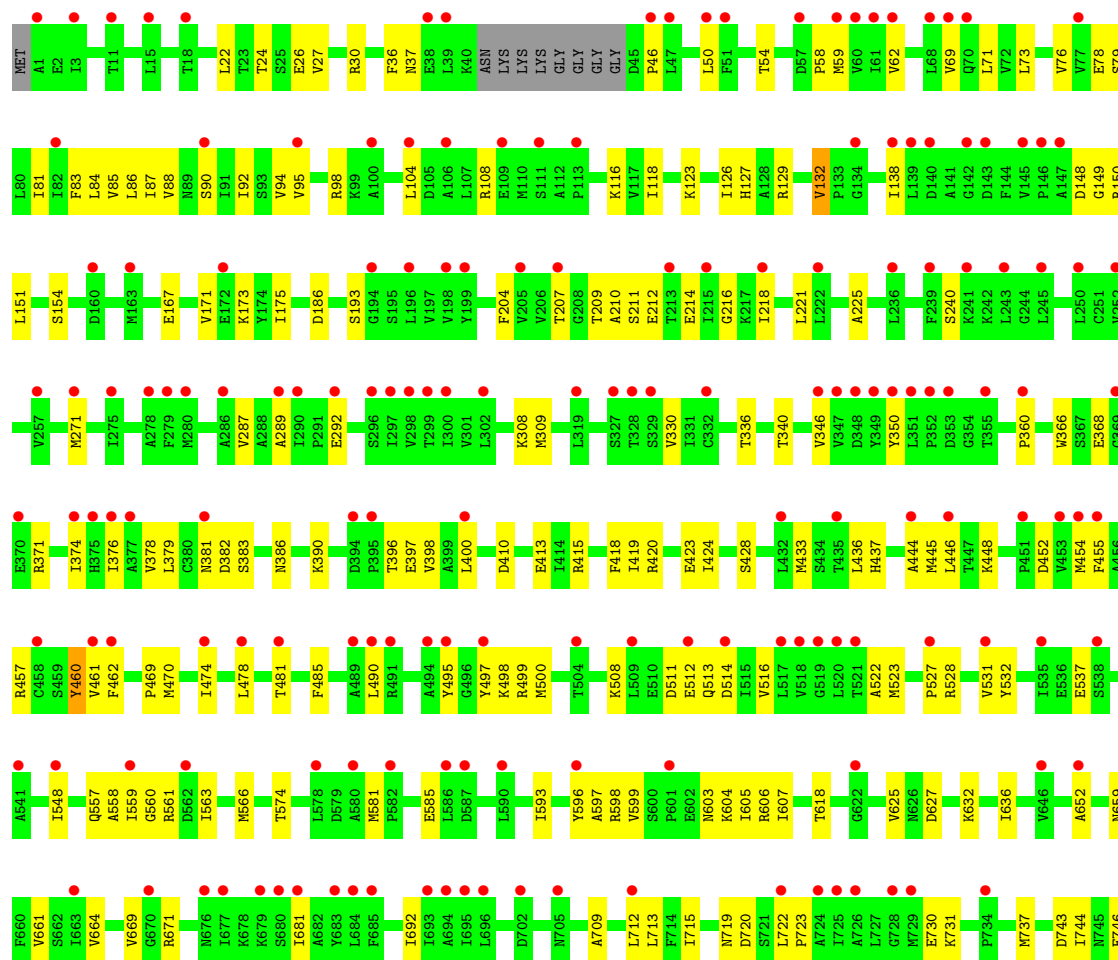
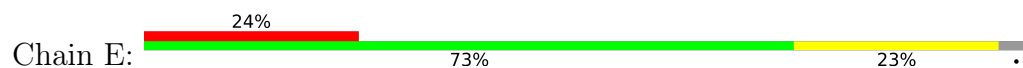


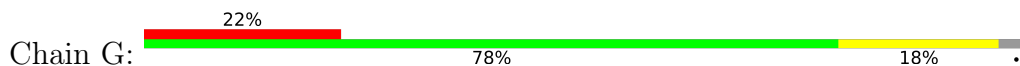
● Molecule 1: Calcium-transporting ATPase

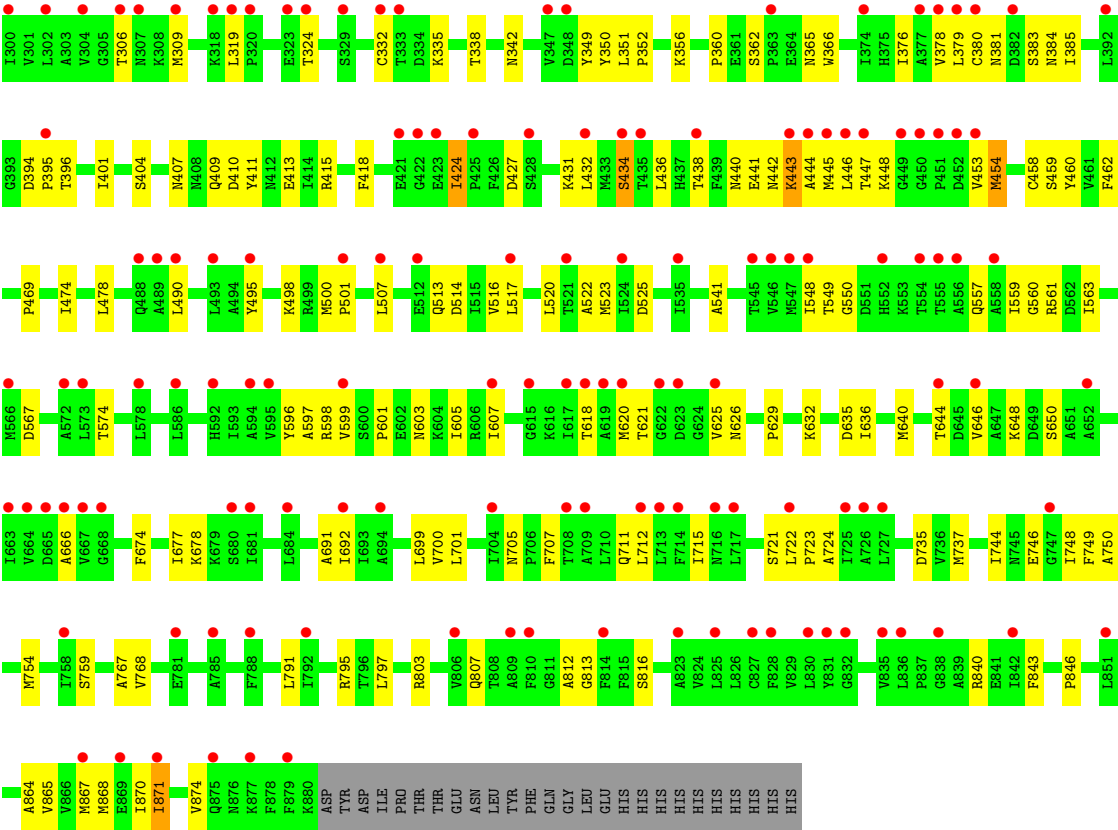




• Molecule 1: Calcium-transporting ATPase







4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.06Å 188.50Å 350.01Å 90.00° 91.94° 90.00°	Depositor
Resolution (Å)	49.58 – 3.00 49.58 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.1 (49.58-3.00) 96.0 (49.58-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.255 , 0.285 0.255 , 0.287	Depositor DCC
R_{free} test set	2000 reflections (1.04%)	wwPDB-VP
Wilson B-factor (Å ²)	67.1	Xtriage
Anisotropy	0.274	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 96.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	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 ²)	128.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.37	0/6832	0.67	3/9248 (0.0%)
1	B	0.38	0/6832	0.66	0/9248
1	C	0.39	1/6832 (0.0%)	0.65	3/9248 (0.0%)
1	D	0.36	1/6832 (0.0%)	0.64	0/9248
1	E	0.25	1/6773 (0.0%)	0.52	0/9165
1	F	0.25	1/6773 (0.0%)	0.51	0/9165
1	G	0.24	0/6765	0.51	0/9153
1	H	0.28	2/6773 (0.0%)	0.52	1/9165 (0.0%)
All	All	0.32	6/54412 (0.0%)	0.59	7/73640 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	424	ILE	CA-C	14.24	1.65	1.53
1	H	132	VAL	C-O	7.81	1.29	1.24
1	H	424	ILE	CA-C	-7.76	1.47	1.52
1	F	132	VAL	C-O	5.65	1.28	1.24
1	E	132	VAL	C-O	5.64	1.28	1.24
1	D	132	VAL	C-O	-5.36	1.20	1.24

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	424	ILE	O-C-N	10.24	130.65	121.12
1	A	594	ALA	N-CA-C	-7.64	105.91	114.62
1	A	499	ARG	CA-C-N	-6.05	112.28	123.65
1	A	499	ARG	C-N-CA	-6.05	112.28	123.65
1	C	424	ILE	CA-C-N	-5.62	114.18	119.85
1	C	424	ILE	C-N-CA	-5.62	114.18	119.85
1	H	132	VAL	O-C-N	-5.09	118.48	121.69

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6732	0	6905	99	0
1	B	6732	0	6905	128	0
1	C	6732	0	6905	145	0
1	D	6732	0	6905	142	0
1	E	6675	0	6856	137	0
1	F	6675	0	6856	120	0
1	G	6667	0	6853	104	0
1	H	6675	0	6856	142	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	19	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	2	0	0	1	0
6	E	2	0	0	0	0
6	F	2	0	0	0	0
6	G	2	0	0	0	0
6	H	2	0	0	0	0
All	All	54572	0	56461	1025	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 (1025) 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:A:865:VAL:HA	1:A:868:MET:HE3	1.60	0.82
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:581:MET:HE3	1:A:585:GLU:HG2	1.71	0.72
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:335:LYS:HZ3	1:H:559:ILE:HD12	1.54	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:H:396:THR:HA	1:H:523:MET:HE1	1.72	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:E:865:VAL:HA	1:E:868:MET:HE2	1.72	0.70
1:B:234:ARG:NH2	1:B:745:ASN:OD1	2.24	0.70
1:D:865:VAL:HA	1:D:868:MET:HE3	1.74	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:B:581:MET:HE3	1:B:585:GLU:HG2	1.74	0.69
1:C:47:LEU:HD21	1:C:98:ARG:HD2	1.74	0.69
1:E:557:GLN:HG2	1:E:566:MET:HE1	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:G:865:VAL:HA	1:G:868:MET:HE3	1.75	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:867:MET:HE2	4:B:1008:PCW:H131	1.74	0.68
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:F:566:MET:HE2	1:F:570:ASP:HB3	1.76	0.67
1:H:91:ILE:HA	1:H:94:VAL:HG22	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:803:ARG:HH22	1:G:816:SER:HG	1.42	0.66
1:F:427:ASP:HB2	1:F:431:LYS:HB2	1.76	0.66
1:A:163:MET:HE1	1:A:215:ILE:HB	1.77	0.66
1:A:151:LEU:HD23	1:A:204:PHE:HB3	1.78	0.66
1:B:704:ILE:HG22	1:B:776:MET:HE1	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
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:344:MET:HE2	1:C:491:ARG:HD2	1.78	0.64
1:C:879:PHE:HB3	1:C:885:PRO:HB3	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: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:D:581:MET:HE3	1:D:585:GLU:HG2	1.80	0.63
1:E:457:ARG:HD3	1:E:512:GLU:O	1.99	0.63
1:H:59:MET:HE1	1:H:291:PRO:HD2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:549:THR:OG1	2:H:1001:BEF:F2	2.04	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:E:433:MET:SD	1:E:448:LYS:NZ	2.66	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:B:566:MET:HE2	1:B:570:ASP:HB3	1.81	0.61
1:C:118:ILE:HG13	1:C:138:ILE:HD11	1.82	0.61
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:H:222:LEU:O	1:H:632:LYS:NZ	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:460:TYR:CE2	1:E:516:VAL:HG22	2.37	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:F:788:PHE:HE2	1:F:834:THR:HG21	1.67	0.59
1:D:560:GLY:HA2	1:D:563:ILE:HG12	1.84	0.59
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:163:MET:HE1	1:C:215:ILE:HB	1.84	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:B:309:MET:HE2	1:B:309:MET:HA	1.83	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:C:755:ARG:HH11	1:C:885:PRO:HG2	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:163:MET:HE1	1:D:215:ILE:HB	1.84	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
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:B:470:MET:HE1	1:B:478:LEU:HD12	1.88	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:F:443:LYS:NZ	1:F:504:THR:O	2.32	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:G:566:MET:HE2	1:G:570:ASP:HB3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:831:TYR:O	1:E:834:THR:OG1	2.20	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:346:VAL:HG22	1:A:523:MET:HE2	1.87	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:59:MET:HE3	1:D:290:ILE:HG23	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
1:C:344:MET:HE3	1:C:524:ILE:HA	1.89	0.55
1:C:366:TRP:HD1	1:C:367:SER:O	1.89	0.55
1:H:309:MET:HE2	1:H:666:ALA:HB2	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:A:201:ARG:HH21	1:A:203:MET:HE2	1.72	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:H72	1.90	0.54
1:D:772:GLN:HG2	1:D:783:SER:HB2	1.89	0.54
4:B:1009:PCW:H261	1:C:296:SER:OG	2.08	0.54
1:B:163:MET:HE1	1:B:215:ILE:HD13	1.89	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
1:G:147:ALA:HA	1:G:193:SER:HB2	1.91	0.53
1:A:566:MET:HE2	1:A:570:ASP:HB3	1.91	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:C:109:GLU:C	1:C:111:SER:H	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:430:ARG:CD	1:B:457:ARG:HH12	2.20	0.53
1:D:344:MET:HE2	1:D:491:ARG:HD2	1.90	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:H:338:THR:HG23	1:H:640:MET:HE2	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: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:B:867:MET:HE1	1:B:887:THR:HG23	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:309:MET:HE3	1:B:669:VAL:HG21	1.92	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:E:452:ASP:OD1	1:E:452:ASP:N	2.43	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:F:640:MET:HE1	1:F:655:LEU:HD12	1.93	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:309:MET:HE2	1:D:666:ALA:HB2	1.93	0.51
1:D:346:VAL:HA	1:D:523:MET:HA	1.92	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: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:F:461:VAL:HG23	1:F:469:PRO:HG3	1.92	0.50
1:A:498:LYS:NZ	1:A:513:GLN:O	2.32	0.50
1:E:457:ARG:HH22	1:E:513:GLN:NE2	2.09	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:418:PHE:HB3	1:F:437:HIS:ND1	2.26	0.50
1:B:173:LYS:NZ	1:B:190:MET:O	2.41	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:G:447:THR:HG22	1:G:454:MET:HE1	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
1:H:134:GLY:N	1:H:206:VAL:O	2.40	0.49
1:B:39:LEU:O	1:B:40:LYS:HB2	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:H241	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:754:MET:HE2	1:B:758:ILE:HG13	1.94	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:B:470:MET:O	1:B:471:THR:OG1	2.25	0.49
1:E:309:MET:HE3	1:E:669:VAL:HG21	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: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:C:454:MET:HE3	1:C:515:ILE:HG21	1.96	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:642:SER:OG	1:B:658:ASP:OD2	2.19	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
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: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:G:703:TRP:CG	1:G:776:MET:HE3	2.48	0.48
1:H:332:CYS:O	1:H:620:MET:HA	2.13	0.48
1:A:604:LYS:NZ	1:A:627:ASP:OD1	2.30	0.47
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:H:541:ALA:HB2	1:H:737:MET:HE3	1.96	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
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:A:500:MET:HE3	1:A:501:PRO:HD2	1.96	0.47
1:B:452:ASP:OD1	1:B:452:ASP:N	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:190:MET:HE3	1:A:190:MET:HB3	1.75	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:344:MET:HE2	1:G:491:ARG:HD2	1.95	0.47
1:G:443:LYS:NZ	1:G:504:THR:O	2.46	0.47
1:A:445:MET:HE1	1:A:511:ASP:O	2.14	0.47
1:C:62:VAL:HG13	4:C:1004:PCW:H181	1.96	0.47
1:E:396:THR:HG23	1:E:523:MET:HE1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:1004:PCW:H20	4:C:1004:PCW:H232	1.58	0.47
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:349:TYR:CE2	1:H:351:LEU:HG	2.50	0.46
1:C:751:GLY:H	4:C:1005:PCW:H71	1.81	0.46
1:D:381:ASN:HB3	1:D:448:LYS:HZ1	1.80	0.46
4:B:1006:PCW:H411	4:B:1006:PCW:H182	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:H283	4:C:1004:PCW:H251	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:837:PRO:O	1:G:840:ARG:HG2	2.16	0.46
1:B:190:MET:HE2	1:B:190:MET:HB3	1.79	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:F:498:LYS:HE3	1:F:500:MET:HE2	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:511:ASP:C	1:C:513:GLN:H	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:283:VAL:O	1:H:287:VAL:HG23	2.15	0.46
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: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:C:510:GLU:CD	1:C:510:GLU:H	2.24	0.45
1:E:36:PHE:O	1:E:210:ALA:HB2	2.16	0.45
1:H:865:VAL:HA	1:H:868:MET:HE3	1.98	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: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:346:VAL:HG22	1:B:523:MET:HE2	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:GLU:HG3	1:B:6:LYS:HE3	1.98	0.45
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:E:500:MET:HE3	1:E:511:ASP:HB3	1.99	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:H:266:ASP:C	1:H:268:SER:H	2.25	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:4:TYR:HB3	1:H:190:MET:HE3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:267:ASN:OD1	1:H:267:ASN:N	2.49	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: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
1:A:875:GLN:HG3	1:A:884:ILE:C	2.43	0.44
4:B:1004:PCW:H371	4:B:1004:PCW:H40	1.58	0.44
1:C:163:MET:HE2	1:C:164:LEU:HD21	1.99	0.44
1:C:885:PRO:HB2	1:C:886:THR:H	1.55	0.44
1:D:75:GLU:HB3	1:D:78:GLU:CD	2.42	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:F:620:MET:HE2	1:F:630:ALA:HB3	2.01	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:190:MET:HE3	1:G:190:MET:HB2	1.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:75:GLU:HB3	1:G:78:GLU:CD	2.44	0.43
1:B:754:MET:HE3	1:B:754:MET:HA	1.99	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
4:D:1003:PCW:H381	4:D:1003:PCW:H352	1.50	0.43
1:E:581:MET:HE3	1:E:585:GLU:HG2	2.01	0.43
1:H:349:TYR:HE2	1:H:351:LEU:HG	1.83	0.43
1:A:704:ILE:HG22	1:A:776:MET:HE1	2.01	0.43
1:C:350:TYR:HE2	1:C:481:THR:HG1	1.61	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:D:110:MET:HE2	1:D:110:MET:HB3	1.83	0.43
1:G:304:VAL:HG21	1:G:729:MET:SD	2.58	0.43
1:G:510:GLU:H	1:G:510:GLU:CD	2.25	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
1:B:470:MET:HE3	1:B:475:LEU:HB2	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:2:GLU:O	1:H:2:GLU:HG2	2.18	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:B:381:ASN:HB2	1:B:397:GLU:CD	2.44	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
1:B:566:MET:HE1	1:B:571:ILE:C	2.44	0.42
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:541:ALA:HB2	1:G:737:MET:HE3	2.02	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: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:D:59:MET:HE1	1:D:291:PRO:HD2	2.02	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:E:786:MET:HE2	1:E:786:MET:HB3	1.86	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:445:MET:HE1	1:H:507:LEU:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:445:MET:HE1	1:E:511:ASP:HB3	2.02	0.42
1:H:807:GLN:HB3	1:H:812:ALA:HB2	2.02	0.42
1:F:865:VAL:HA	1:F:868:MET:HE3	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:D:883:ASP:C	1:D:885:PRO:HD3	2.45	0.42
1:E:167:GLU:OE2	1:E:336:THR:OG1	2.21	0.42
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:H:454:MET:HE3	1:H:458:CYS:SG	2.59	0.42
1:A:721:SER:O	1:A:725:ILE:HG12	2.20	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:346:VAL:HG22	1:G:523:MET:HE2	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:PRO:HG3	1:B:685:PHE:CE2	2.55	0.41
1:C:871:ILE:CD1	4:C:1005:PCW:H371	2.50	0.41
1:D:242:LYS:HD2	5:D:1008:CE1:H82	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:H242	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:H42	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
1:F:190:MET:HE2	1:F:190:MET:HB2	1.81	0.41
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:B:498:LYS:NZ	1:B:513:GLN:O	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:541:ALA:HB2	1:A:737:MET:HE3	2.03	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
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:380:CYS:O	1:C:448:LYS:NZ	2.49	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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: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
4:B:1006:PCW:H122	4:B:1006:PCW:H362	2.02	0.40
1:C:566:MET:HE1	1:C:571:ILE:O	2.21	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:625:VAL:HG22	1:H:646:VAL:HG21	2.03	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: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:433:MET:HE2	1:D:433:MET:HB3	1.82	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%)	43	76
1	C	879/911 (96%)	836 (95%)	41 (5%)	2 (0%)	43	76
1	D	879/911 (96%)	838 (95%)	38 (4%)	3 (0%)	36	70
1	E	872/911 (96%)	843 (97%)	28 (3%)	1 (0%)	48	80
1	F	872/911 (96%)	830 (95%)	40 (5%)	2 (0%)	43	76
1	G	871/911 (96%)	838 (96%)	32 (4%)	1 (0%)	48	80
1	H	872/911 (96%)	830 (95%)	38 (4%)	4 (0%)	24	60
All	All	7003/7288 (96%)	6701 (96%)	287 (4%)	15 (0%)	43	76

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 ⓘ

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%)	724 (100%)	3 (0%)	84	90
1	B	727/750 (97%)	725 (100%)	2 (0%)	86	91
1	C	727/750 (97%)	725 (100%)	2 (0%)	86	91
1	D	727/750 (97%)	719 (99%)	8 (1%)	65	83
1	E	720/750 (96%)	715 (99%)	5 (1%)	76	86
1	F	720/750 (96%)	714 (99%)	6 (1%)	73	86
1	G	719/750 (96%)	714 (99%)	5 (1%)	76	86
1	H	720/750 (96%)	716 (99%)	4 (1%)	78	88
All	All	5787/6000 (96%)	5752 (99%)	35 (1%)	78	88

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	ASN
1	A	434	SER
1	A	626	ASN
1	B	434	SER
1	B	626	ASN
1	C	434	SER
1	C	626	ASN
1	D	27	VAL
1	D	47	LEU
1	D	434	SER
1	D	454	MET
1	D	593	ILE
1	D	880	LYS
1	D	881	ASP
1	D	884	ILE
1	E	271	MET
1	E	424	ILE
1	E	454	MET
1	E	460	TYR
1	E	559	ILE
1	F	27	VAL
1	F	89	ASN
1	F	266	ASP
1	F	454	MET
1	F	593	ILE
1	F	748	ILE
1	G	27	VAL
1	G	434	SER
1	G	438	THR
1	G	454	MET
1	G	836	LEU
1	H	27	VAL
1	H	434	SER
1	H	454	MET
1	H	871	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	552	HIS
1	A	626	ASN
1	B	229	GLN
1	B	375	HIS

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Mol	Chain	Res	Type
1	B	384	ASN
1	B	442	ASN
1	B	552	HIS
1	B	633	GLN
1	B	688	ASN
1	B	777	GLN
1	B	875	GLN
1	C	375	HIS
1	C	482	ASN
1	C	552	HIS
1	C	745	ASN
1	D	384	ASN
1	D	552	HIS
1	D	557	GLN
1	D	592	HIS
1	D	633	GLN
1	D	772	GLN
1	D	807	GLN
1	D	876	ASN
1	E	233	GLN
1	E	552	HIS
1	E	876	ASN
1	F	277	ASN
1	F	307	ASN
1	F	342	ASN
1	F	482	ASN
1	F	745	ASN
1	F	777	GLN
1	G	70	GLN
1	G	124	GLN
1	G	407	ASN
1	G	552	HIS
1	G	576	GLN
1	G	876	ASN
1	H	70	GLN
1	H	552	HIS
1	H	705	ASN
1	H	777	GLN

5.3.3 RNA ⓘ

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 oligosaccharides 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$
4	PCW	A	1004	-	53,53,53	0.95	2 (3%)	59,61,61	1.08	5 (8%)
4	PCW	C	1003	-	53,53,53	0.86	2 (3%)	59,61,61	1.08	6 (10%)
4	PCW	B	1003	-	53,53,53	1.09	5 (9%)	59,61,61	1.06	6 (10%)
4	PCW	C	1006	-	53,53,53	1.02	3 (5%)	59,61,61	1.10	6 (10%)
4	PCW	C	1008	-	53,53,53	1.02	2 (3%)	59,61,61	1.12	5 (8%)
4	PCW	B	1009	-	53,53,53	1.01	4 (7%)	59,61,61	1.02	4 (6%)
2	BEF	C	1001	1	0,3,3	-	-	-	-	-
4	PCW	D	1003	-	53,53,53	1.06	4 (7%)	59,61,61	1.03	5 (8%)
4	PCW	B	1006	-	53,53,53	1.01	3 (5%)	59,61,61	1.00	3 (5%)
2	BEF	E	1001	1	0,3,3	-	-	-	-	-
4	PCW	B	1005	-	53,53,53	0.87	2 (3%)	59,61,61	1.12	6 (10%)
5	CE1	D	1009	-	11,11,36	0.45	0	10,10,35	0.77	0
2	BEF	G	1001	1	0,3,3	-	-	-	-	-
5	CE1	D	1008	-	10,10,36	0.70	0	9,9,35	0.63	0
2	BEF	B	1001	1	0,3,3	-	-	-	-	-
5	CE1	D	1004	-	11,11,36	0.58	0	10,10,35	0.74	0
5	CE1	D	1005	-	11,11,36	0.31	0	10,10,35	0.92	0
2	BEF	F	1001	1	0,3,3	-	-	-	-	-
2	BEF	H	1001	1	0,3,3	-	-	-	-	-
4	PCW	B	1008	-	53,53,53	1.13	4 (7%)	59,61,61	1.07	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PCW	A	1003	-	53,53,53	0.84	2 (3%)	59,61,61	1.02	5 (8%)
2	BEF	D	1001	1	0,3,3	-	-	-	-	-
5	CE1	D	1006	-	11,11,36	0.91	0	10,10,35	0.85	0
4	PCW	B	1007	-	53,53,53	1.09	4 (7%)	59,61,61	1.07	4 (6%)
5	CE1	D	1007	-	11,11,36	0.42	0	10,10,35	0.91	0
4	PCW	B	1004	-	53,53,53	1.00	4 (7%)	59,61,61	1.00	5 (8%)
4	PCW	C	1005	-	53,53,53	1.12	5 (9%)	59,61,61	1.06	5 (8%)
5	CE1	C	1007	-	14,14,36	0.57	0	13,13,35	0.96	1 (7%)
4	PCW	C	1004	-	53,53,53	0.97	3 (5%)	59,61,61	1.06	5 (8%)
2	BEF	A	1001	1	0,3,3	-	-	-	-	-

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	A	1004	-	-	28/57/57/57	-
4	PCW	C	1003	-	-	22/57/57/57	-
4	PCW	C	1006	-	-	36/57/57/57	-
4	PCW	B	1003	-	-	25/57/57/57	-
4	PCW	C	1008	-	-	31/57/57/57	-
4	PCW	B	1009	-	-	29/57/57/57	-
4	PCW	D	1003	-	-	25/57/57/57	-
4	PCW	B	1006	-	-	30/57/57/57	-
4	PCW	B	1005	-	-	30/57/57/57	-
5	CE1	D	1009	-	-	5/9/9/34	-
5	CE1	D	1008	-	-	5/8/8/34	-
5	CE1	D	1004	-	-	5/9/9/34	-
5	CE1	D	1005	-	-	3/9/9/34	-
4	PCW	B	1008	-	-	31/57/57/57	-
4	PCW	A	1003	-	-	26/57/57/57	-
5	CE1	D	1006	-	-	4/9/9/34	-
4	PCW	B	1007	-	-	30/57/57/57	-
5	CE1	D	1007	-	-	1/9/9/34	-
4	PCW	B	1004	-	-	32/57/57/57	-
4	PCW	C	1005	-	-	27/57/57/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CE1	C	1007	-	-	6/12/12/34	-
4	PCW	C	1004	-	-	32/57/57/57	-

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1005	PCW	P-O4P	4.56	1.77	1.59
4	B	1008	PCW	P-O4P	4.56	1.77	1.59
4	B	1007	PCW	P-O4P	4.48	1.76	1.59
4	C	1008	PCW	P-O4P	4.41	1.76	1.59
4	C	1006	PCW	P-O4P	4.40	1.76	1.59
4	B	1006	PCW	P-O4P	4.39	1.76	1.59
4	A	1004	PCW	P-O4P	4.23	1.75	1.59
4	B	1004	PCW	P-O4P	4.20	1.75	1.59
4	B	1005	PCW	P-O4P	4.09	1.75	1.59
4	C	1004	PCW	P-O4P	3.95	1.74	1.59
4	B	1009	PCW	P-O4P	3.90	1.74	1.59
4	D	1003	PCW	P-O4P	3.89	1.74	1.59
4	C	1003	PCW	P-O4P	3.61	1.73	1.59
4	A	1003	PCW	P-O4P	3.55	1.73	1.59
4	B	1003	PCW	P-O4P	3.45	1.72	1.59
4	B	1008	PCW	C5-N	3.10	1.60	1.51
4	B	1007	PCW	C3-C2	2.96	1.60	1.50
4	C	1006	PCW	C3-C2	2.90	1.59	1.50
4	B	1003	PCW	C3-C2	2.88	1.59	1.50
4	C	1005	PCW	C5-N	2.46	1.59	1.51
4	D	1003	PCW	C8-N	2.42	1.57	1.50
4	B	1009	PCW	P-O3P	2.34	1.68	1.59
4	C	1005	PCW	C3-C2	2.33	1.58	1.50
4	B	1003	PCW	P-O3P	2.30	1.68	1.59
4	B	1007	PCW	P-O3P	2.27	1.68	1.59
4	B	1003	PCW	O3-C11	2.19	1.39	1.33
4	A	1003	PCW	P-O1P	-2.15	1.45	1.55
4	B	1008	PCW	P-O1P	-2.15	1.45	1.55
4	B	1008	PCW	P-O3P	2.15	1.67	1.59
4	B	1003	PCW	P-O1P	-2.14	1.45	1.55
4	C	1005	PCW	P-O3P	2.13	1.67	1.59
4	C	1003	PCW	P-O1P	-2.13	1.45	1.55
4	B	1007	PCW	P-O1P	-2.13	1.45	1.55
4	B	1004	PCW	P-O1P	-2.13	1.45	1.55
4	D	1003	PCW	P-O1P	-2.12	1.45	1.55
4	C	1006	PCW	P-O1P	-2.12	1.45	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1004	PCW	P-O3P	2.12	1.67	1.59
4	A	1004	PCW	P-O1P	-2.11	1.45	1.55
4	C	1008	PCW	P-O1P	-2.11	1.45	1.55
4	B	1005	PCW	P-O1P	-2.11	1.45	1.55
4	C	1005	PCW	P-O1P	-2.10	1.45	1.55
4	B	1006	PCW	P-O1P	-2.10	1.45	1.55
4	B	1009	PCW	P-O1P	-2.10	1.45	1.55
4	B	1009	PCW	O2-C31	2.10	1.40	1.34
4	C	1004	PCW	P-O1P	-2.09	1.45	1.55
4	C	1004	PCW	C3-C2	2.06	1.57	1.50
4	D	1003	PCW	O2-C31	2.05	1.40	1.34
4	B	1004	PCW	O2-C31	2.05	1.40	1.34
4	B	1006	PCW	C5-N	2.01	1.57	1.51

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1003	PCW	O1P-P-O2P	3.38	128.19	112.44
4	B	1006	PCW	O1P-P-O2P	3.27	127.67	112.44
4	B	1003	PCW	O1P-P-O2P	3.25	127.55	112.44
4	B	1008	PCW	O1P-P-O2P	3.22	127.43	112.44
4	C	1008	PCW	O1P-P-O2P	3.17	127.18	112.44
4	D	1003	PCW	O1P-P-O2P	3.14	127.03	112.44
4	B	1009	PCW	O1P-P-O2P	3.13	126.98	112.44
4	C	1006	PCW	O1P-P-O2P	3.11	126.92	112.44
4	B	1004	PCW	O1P-P-O2P	3.11	126.89	112.44
4	B	1005	PCW	O1P-P-O2P	3.09	126.81	112.44
4	A	1004	PCW	O1P-P-O2P	3.08	126.78	112.44
4	C	1005	PCW	O1P-P-O2P	3.05	126.65	112.44
4	D	1003	PCW	O4P-P-O2P	-3.04	96.89	108.94
4	C	1004	PCW	O1P-P-O2P	3.03	126.56	112.44
4	C	1008	PCW	O2-C31-C32	3.01	117.98	111.48
4	B	1005	PCW	O2-C31-C32	2.98	117.93	111.48
4	B	1007	PCW	O1P-P-O2P	2.97	126.28	112.44
4	C	1008	PCW	O4P-P-O2P	-2.96	97.19	108.94
4	B	1003	PCW	O4P-P-O2P	-2.95	97.25	108.94
4	B	1003	PCW	P-O4P-C4	-2.95	107.24	121.26
4	A	1003	PCW	O1P-P-O2P	2.93	126.06	112.44
4	B	1008	PCW	O4P-P-O2P	-2.91	97.39	108.94
4	C	1006	PCW	O2-C31-C32	2.90	117.75	111.48
4	C	1006	PCW	O4P-P-O2P	-2.89	97.49	108.94
4	B	1007	PCW	O4P-P-O2P	-2.88	97.51	108.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1004	PCW	O4P-P-O2P	-2.87	97.55	108.94
4	B	1009	PCW	O4P-P-O2P	-2.85	97.64	108.94
4	B	1004	PCW	O2-C31-C32	2.80	117.55	111.48
4	A	1003	PCW	O4P-P-O2P	-2.80	97.83	108.94
4	C	1003	PCW	C4-C5-N	-2.79	106.86	115.82
4	A	1004	PCW	O4P-P-O2P	-2.76	97.98	108.94
4	B	1007	PCW	P-O4P-C4	-2.75	108.17	121.26
4	B	1005	PCW	P-O4P-C4	-2.74	108.22	121.26
4	B	1006	PCW	O4P-P-O2P	-2.72	98.16	108.94
4	C	1005	PCW	O4P-P-O2P	-2.72	98.16	108.94
4	C	1003	PCW	O4P-P-O2P	-2.71	98.19	108.94
4	C	1004	PCW	O4P-P-O2P	-2.69	98.28	108.94
4	C	1003	PCW	P-O4P-C4	-2.68	108.50	121.26
4	B	1009	PCW	O2-C31-C32	2.66	117.25	111.48
4	B	1007	PCW	O2-C31-C32	2.66	117.24	111.48
4	C	1004	PCW	O2-C31-C32	2.65	117.22	111.48
4	B	1005	PCW	O4P-P-O2P	-2.64	98.47	108.94
4	C	1008	PCW	P-O4P-C4	-2.63	108.74	121.26
4	A	1003	PCW	P-O4P-C4	-2.62	108.78	121.26
4	B	1009	PCW	P-O4P-C4	-2.61	108.83	121.26
4	B	1008	PCW	O2-C31-C32	2.60	117.10	111.48
4	B	1005	PCW	P-O3P-C1	-2.57	106.59	121.35
4	C	1004	PCW	P-O4P-C4	-2.57	109.03	121.26
4	D	1003	PCW	P-O4P-C4	-2.56	109.06	121.26
4	C	1005	PCW	O2-C31-C32	2.56	117.02	111.48
4	D	1003	PCW	P-O3P-C1	-2.56	106.69	121.35
4	B	1006	PCW	P-O4P-C4	-2.55	109.12	121.26
4	B	1008	PCW	P-O4P-C4	-2.52	109.27	121.26
4	C	1006	PCW	P-O3P-C1	-2.45	107.29	121.35
4	B	1004	PCW	P-O4P-C4	-2.45	109.60	121.26
4	A	1004	PCW	O2-C31-C32	2.44	116.75	111.48
4	C	1005	PCW	P-O4P-C4	-2.39	109.86	121.26
4	D	1003	PCW	C4-C5-N	-2.39	108.16	115.82
4	A	1004	PCW	P-O3P-C1	-2.38	107.72	121.35
4	A	1004	PCW	P-O4P-C4	-2.35	110.08	121.26
4	C	1003	PCW	P-O3P-C1	-2.34	107.97	121.35
4	B	1003	PCW	P-O3P-C1	-2.33	108.02	121.35
4	C	1006	PCW	P-O4P-C4	-2.22	110.68	121.26
4	C	1004	PCW	P-O3P-C1	-2.20	108.72	121.35
4	C	1008	PCW	P-O3P-C1	-2.18	108.84	121.35
4	A	1003	PCW	P-O3P-C1	-2.18	108.88	121.35
4	C	1006	PCW	O2-C31-O31	-2.13	118.72	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1004	PCW	P-O3P-C1	-2.13	109.13	121.35
4	C	1005	PCW	P-O3P-C1	-2.12	109.22	121.35
4	B	1003	PCW	C4-C5-N	-2.12	109.03	115.82
5	C	1007	CE1	C14-O13-C12	-2.11	105.67	113.06
4	C	1003	PCW	O2-C31-C32	2.10	116.03	111.48
4	A	1003	PCW	C4-C5-N	-2.09	109.12	115.82
4	B	1005	PCW	C4-C5-N	-2.08	109.14	115.82
4	B	1003	PCW	O2-C31-C32	2.03	115.87	111.48

There are no chirality outliers.

All (463) 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	C1-O3P-P-O4P
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	1003	PCW	C4-O4P-P-O3P
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	1004	PCW	C4-O4P-P-O3P
4	B	1005	PCW	O4P-C4-C5-N
4	B	1005	PCW	C4-O4P-P-O2P
4	B	1005	PCW	C4-O4P-P-O3P
4	B	1006	PCW	C1-O3P-P-O2P
4	B	1006	PCW	C1-O3P-P-O4P
4	B	1006	PCW	C4-O4P-P-O1P
4	B	1006	PCW	C4-O4P-P-O2P
4	B	1006	PCW	C4-O4P-P-O3P
4	B	1007	PCW	C1-O3P-P-O1P
4	B	1007	PCW	C1-O3P-P-O4P
4	B	1007	PCW	C4-O4P-P-O1P
4	B	1007	PCW	C4-O4P-P-O2P

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Mol	Chain	Res	Type	Atoms
4	B	1007	PCW	C4-O4P-P-O3P
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	C1-O3P-P-O4P
4	B	1008	PCW	C4-O4P-P-O1P
4	B	1008	PCW	C4-O4P-P-O3P
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	B	1009	PCW	C4-O4P-P-O3P
4	C	1003	PCW	C1-O3P-P-O4P
4	C	1003	PCW	C4-O4P-P-O1P
4	C	1003	PCW	C4-O4P-P-O2P
4	C	1003	PCW	C4-O4P-P-O3P
4	C	1004	PCW	O4P-C4-C5-N
4	C	1004	PCW	C4-O4P-P-O1P
4	C	1004	PCW	C4-O4P-P-O3P
4	C	1005	PCW	O4P-C4-C5-N
4	C	1005	PCW	C32-C31-O2-C2
4	C	1005	PCW	C4-O4P-P-O1P
4	C	1005	PCW	C4-O4P-P-O3P
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	1006	PCW	C1-O3P-P-O4P
4	C	1006	PCW	C4-O4P-P-O3P
4	C	1008	PCW	O4P-C4-C5-N
4	C	1008	PCW	C1-O3P-P-O1P
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

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Mol	Chain	Res	Type	Atoms
4	B	1008	PCW	O11-C11-O3-C3
5	C	1007	CE1	C10-C11-C12-O13
4	A	1004	PCW	C12-C11-O3-C3
4	A	1004	PCW	O11-C11-O3-C3
4	C	1006	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	B	1006	PCW	C4-C5-N-C6
4	D	1003	PCW	C42-C43-C44-C45
4	B	1004	PCW	C12-C11-O3-C3
4	C	1005	PCW	C31-C32-C33-C34
4	B	1004	PCW	C35-C36-C37-C38
4	B	1004	PCW	C11-C12-C13-C14
4	A	1003	PCW	C31-C32-C33-C34
4	C	1005	PCW	C11-C12-C13-C14
4	D	1003	PCW	C31-C32-C33-C34
4	A	1004	PCW	C31-C32-C33-C34
4	B	1006	PCW	C31-C32-C33-C34
4	C	1008	PCW	C31-C32-C33-C34
4	D	1003	PCW	C11-C12-C13-C14
4	C	1006	PCW	O11-C11-O3-C3
4	B	1009	PCW	C31-C32-C33-C34
4	D	1003	PCW	C40-C41-C42-C43
4	B	1004	PCW	O11-C11-O3-C3
5	D	1005	CE1	C11-C10-C9-C8
4	B	1004	PCW	C4-C5-N-C8
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	C	1004	PCW	C20-C21-C22-C23
4	C	1005	PCW	C42-C43-C44-C45
4	C	1005	PCW	C3-C2-O2-C31
4	B	1006	PCW	C32-C31-O2-C2

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

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

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Mol	Chain	Res	Type	Atoms
5	D	1004	CE1	C3-C4-C5-C6
4	C	1008	PCW	C24-C25-C26-C27
4	B	1003	PCW	C22-C23-C24-C25
4	C	1005	PCW	C32-C33-C34-C35
4	A	1003	PCW	C14-C15-C16-C17
4	C	1004	PCW	C4-C5-N-C7
5	D	1006	CE1	C6-C7-C8-C9
4	A	1003	PCW	C36-C37-C38-C39
4	A	1004	PCW	C36-C37-C38-C39
4	B	1006	PCW	C20-C21-C22-C23
4	B	1008	PCW	C16-C17-C18-C19
4	C	1005	PCW	C20-C21-C22-C23
4	B	1003	PCW	C35-C36-C37-C38
4	B	1006	PCW	C34-C35-C36-C37
4	B	1008	PCW	C43-C44-C45-C46
4	D	1003	PCW	C33-C34-C35-C36
5	D	1009	CE1	C2-C3-C4-C5
4	B	1007	PCW	C41-C42-C43-C44
4	B	1009	PCW	C12-C13-C14-C15
4	C	1005	PCW	C34-C35-C36-C37
4	B	1004	PCW	C21-C22-C23-C24
4	B	1004	PCW	C20-C21-C22-C23
4	B	1004	PCW	C36-C37-C38-C39
4	D	1003	PCW	C36-C37-C38-C39
4	B	1006	PCW	C44-C45-C46-C47
4	B	1006	PCW	C12-C11-O3-C3
4	B	1005	PCW	C43-C44-C45-C46
4	C	1003	PCW	C21-C22-C23-C24
4	B	1009	PCW	C13-C14-C15-C16
4	C	1006	PCW	C41-C42-C43-C44
4	B	1003	PCW	C41-C42-C43-C44
4	B	1003	PCW	C15-C16-C17-C18
4	A	1003	PCW	C20-C21-C22-C23
4	A	1003	PCW	C40-C41-C42-C43
4	B	1003	PCW	C16-C17-C18-C19
4	C	1005	PCW	C40-C41-C42-C43
4	B	1005	PCW	C22-C23-C24-C25
4	A	1004	PCW	C13-C14-C15-C16
4	B	1005	PCW	C12-C13-C14-C15
4	B	1008	PCW	C32-C33-C34-C35
4	B	1003	PCW	C25-C26-C27-C28
4	B	1005	PCW	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	B	1004	PCW	C45-C46-C47-C48
4	A	1003	PCW	C12-C13-C14-C15
4	C	1006	PCW	C33-C34-C35-C36
5	C	1007	CE1	C2-C3-C4-C5
4	B	1009	PCW	C19-C20-C21-C22
4	B	1007	PCW	C25-C26-C27-C28
4	B	1004	PCW	C39-C40-C41-C42
4	B	1009	PCW	C37-C38-C39-C40
4	B	1008	PCW	C2-C1-O3P-P
4	C	1006	PCW	C2-C1-O3P-P
4	B	1006	PCW	C25-C26-C27-C28
5	D	1008	CE1	C4-C5-C6-C7
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	B	1004	PCW	C25-C26-C27-C28
4	C	1004	PCW	C45-C46-C47-C48
4	A	1003	PCW	C41-C42-C43-C44
4	B	1008	PCW	C31-C32-C33-C34
4	B	1006	PCW	O11-C11-O3-C3
4	B	1004	PCW	C41-C42-C43-C44
4	C	1008	PCW	C21-C22-C23-C24
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	1005	PCW	C24-C25-C26-C27
4	B	1005	PCW	C14-C15-C16-C17
4	C	1004	PCW	C4-C5-N-C8
4	B	1009	PCW	C33-C34-C35-C36
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	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
4	C	1004	PCW	O31-C31-O2-C2
4	C	1006	PCW	C23-C24-C25-C26

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

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Mol	Chain	Res	Type	Atoms
4	B	1008	PCW	C41-C42-C43-C44
4	B	1007	PCW	C33-C34-C35-C36
4	C	1008	PCW	C25-C26-C27-C28
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	B	1007	PCW	O2-C2-C3-O3
4	C	1006	PCW	O2-C2-C3-O3
4	C	1008	PCW	C41-C42-C43-C44
4	A	1003	PCW	C1-C2-C3-O3
4	B	1005	PCW	C1-C2-C3-O3
5	C	1007	CE1	C11-C10-C9-C8
5	D	1006	CE1	C11-C10-C9-C8
4	C	1008	PCW	O11-C11-O3-C3
4	B	1005	PCW	C34-C35-C36-C37
4	A	1004	PCW	C4-O4P-P-O1P
4	A	1004	PCW	C4-O4P-P-O3P
4	B	1004	PCW	C1-O3P-P-O2P
4	B	1005	PCW	C4-O4P-P-O1P
4	B	1006	PCW	C1-O3P-P-O1P
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	C1-O3P-P-O4P
4	B	1009	PCW	C4-O4P-P-O2P
4	C	1003	PCW	C1-O3P-P-O1P
4	C	1003	PCW	C1-O3P-P-O2P
4	C	1006	PCW	C4-O4P-P-O2P
4	D	1003	PCW	C1-O3P-P-O2P
4	C	1004	PCW	C41-C42-C43-C44
4	C	1004	PCW	C40-C41-C42-C43
4	B	1009	PCW	C23-C24-C25-C26
4	C	1003	PCW	C24-C25-C26-C27
4	C	1004	PCW	C25-C26-C27-C28
4	A	1003	PCW	C17-C18-C19-C20
4	B	1003	PCW	C19-C20-C21-C22
4	A	1004	PCW	C11-C12-C13-C14
4	C	1006	PCW	C31-C32-C33-C34
5	C	1007	CE1	C1-C2-C3-C4
4	A	1004	PCW	C1-C2-O2-C31
5	D	1008	CE1	C11-C10-C9-C8
4	B	1007	PCW	C4-C5-N-C6

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Mol	Chain	Res	Type	Atoms
4	C	1004	PCW	C4-C5-N-C6
4	B	1009	PCW	O3P-C1-C2-C3
4	D	1003	PCW	O3P-C1-C2-O2
4	B	1005	PCW	C42-C43-C44-C45
4	B	1008	PCW	C20-C21-C22-C23
4	C	1008	PCW	C12-C11-O3-C3
4	C	1006	PCW	C25-C26-C27-C28
4	B	1005	PCW	C33-C34-C35-C36
4	A	1004	PCW	C20-C21-C22-C23
4	C	1006	PCW	C22-C23-C24-C25
4	C	1005	PCW	C33-C34-C35-C36
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	C	1004	PCW	C17-C18-C19-C20
4	D	1003	PCW	C19-C20-C21-C22
4	C	1003	PCW	C32-C33-C34-C35
4	D	1003	PCW	C44-C45-C46-C47
4	B	1004	PCW	C2-C1-O3P-P
4	C	1008	PCW	C44-C45-C46-C47
4	B	1007	PCW	C4-C5-N-C7
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	C	1006	PCW	O3P-C1-C2-O2
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
5	D	1009	CE1	C5-C6-C7-C8
4	C	1008	PCW	C12-C13-C14-C15
4	C	1004	PCW	O11-C11-O3-C3
4	D	1003	PCW	C1-C2-C3-O3
4	B	1003	PCW	O3P-C1-C2-O2
4	C	1004	PCW	C37-C38-C39-C40
4	A	1004	PCW	C40-C41-C42-C43
4	A	1004	PCW	C42-C43-C44-C45
4	D	1003	PCW	C21-C22-C23-C24
4	B	1006	PCW	O3P-C1-C2-C3
4	A	1004	PCW	C37-C38-C39-C40
4	B	1005	PCW	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
4	C	1006	PCW	C44-C45-C46-C47
5	D	1005	CE1	C7-C8-C9-C10
5	D	1004	CE1	C9-C10-C11-C12
4	A	1004	PCW	C19-C20-C21-C22
4	B	1003	PCW	C39-C40-C41-C42
4	C	1006	PCW	C37-C38-C39-C40
4	B	1003	PCW	C17-C18-C19-C20
4	B	1005	PCW	C39-C40-C41-C42
4	B	1007	PCW	C17-C18-C19-C20
4	C	1006	PCW	C19-C20-C21-C22
4	C	1008	PCW	C17-C18-C19-C20
4	C	1008	PCW	C37-C38-C39-C40
4	B	1008	PCW	C19-C20-C21-C22
4	C	1004	PCW	C42-C43-C44-C45
4	C	1004	PCW	C2-C1-O3P-P
4	A	1003	PCW	C25-C26-C27-C28
4	B	1003	PCW	C45-C46-C47-C48
4	C	1008	PCW	C4-C5-N-C6
4	A	1004	PCW	C1-C2-C3-O3
4	C	1008	PCW	C13-C14-C15-C16
4	A	1003	PCW	C39-C40-C41-C42
4	B	1005	PCW	C17-C18-C19-C20
4	C	1004	PCW	C19-C20-C21-C22
4	B	1005	PCW	O2-C31-C32-C33
4	B	1004	PCW	C37-C38-C39-C40
4	C	1003	PCW	O3-C11-C12-C13
4	C	1003	PCW	O2-C31-C32-C33
4	B	1008	PCW	C39-C40-C41-C42
4	C	1003	PCW	C17-C18-C19-C20
4	C	1006	PCW	C45-C46-C47-C48
4	C	1004	PCW	C14-C15-C16-C17
4	B	1007	PCW	C39-C40-C41-C42
4	C	1003	PCW	C23-C24-C25-C26
4	C	1008	PCW	O3-C11-C12-C13
4	B	1005	PCW	C25-C26-C27-C28
4	C	1004	PCW	C23-C24-C25-C26
4	C	1006	PCW	C1-C2-C3-O3
4	C	1008	PCW	C4-C5-N-C7
4	A	1003	PCW	O2-C31-C32-C33
4	D	1003	PCW	O11-C11-O3-C3
4	C	1005	PCW	C37-C38-C39-C40
4	C	1006	PCW	O2-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
4	B	1005	PCW	C35-C36-C37-C38
4	C	1006	PCW	O3P-C1-C2-C3
4	A	1003	PCW	C34-C35-C36-C37
4	B	1005	PCW	O31-C31-C32-C33
4	C	1003	PCW	O31-C31-C32-C33
4	C	1008	PCW	O11-C11-C12-C13
4	A	1003	PCW	C33-C34-C35-C36
4	C	1003	PCW	O11-C11-C12-C13
5	D	1005	CE1	C6-C7-C8-C9
4	C	1008	PCW	C4-C5-N-C8
4	C	1006	PCW	O31-C31-C32-C33
4	B	1006	PCW	C43-C44-C45-C46
4	B	1003	PCW	O2-C31-C32-C33
4	D	1003	PCW	C12-C11-O3-C3

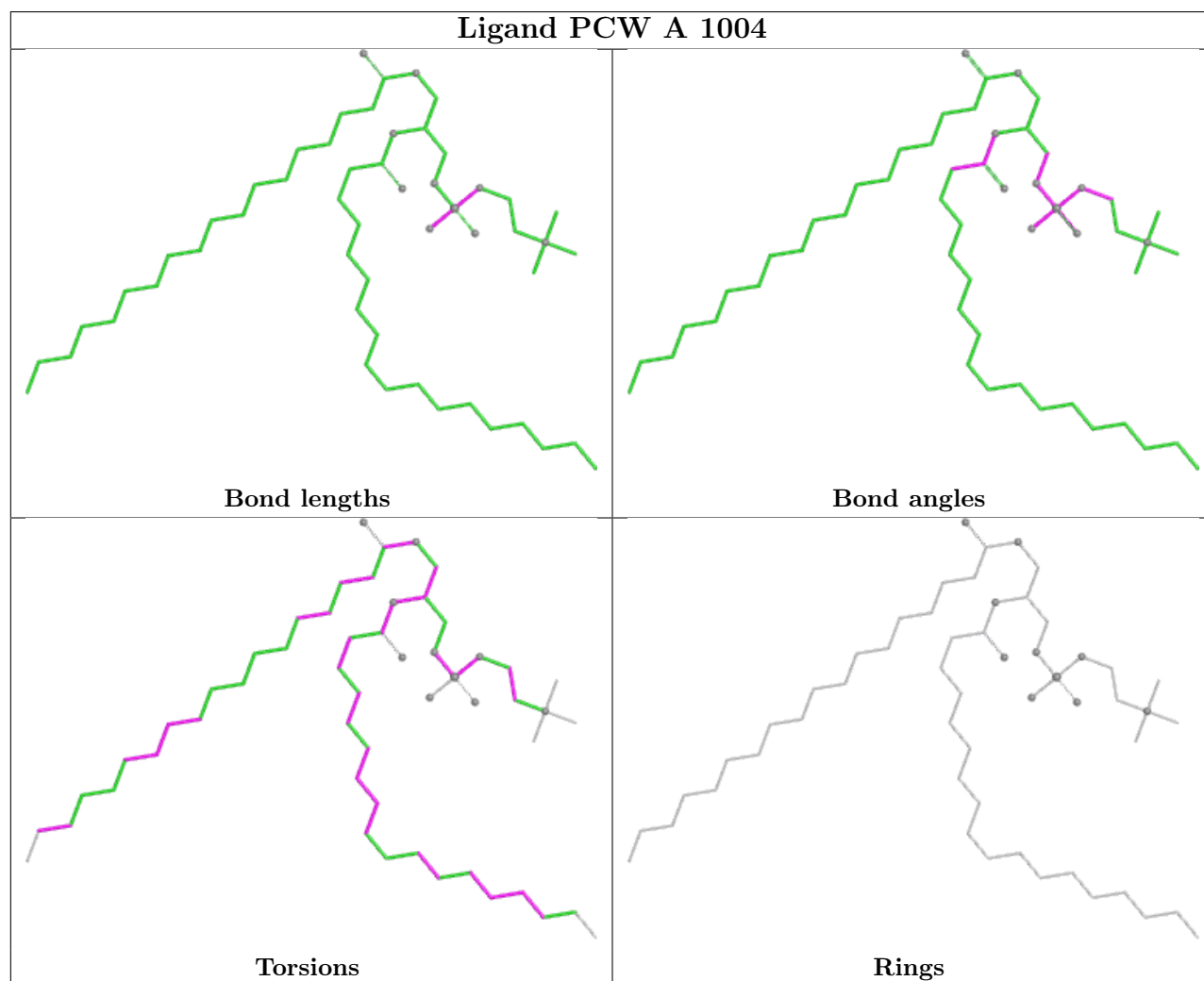
There are no ring outliers.

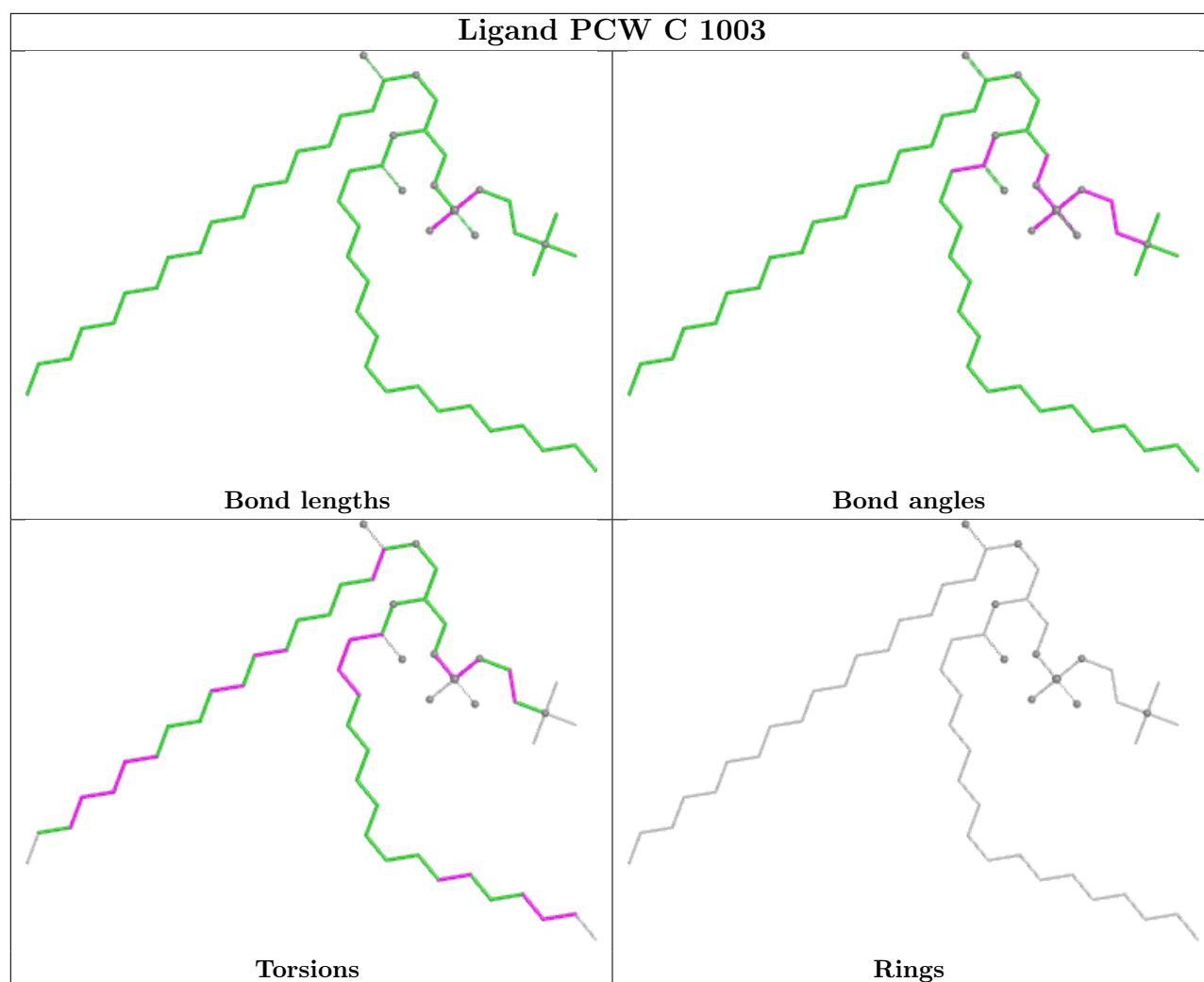
19 monomers are involved in 58 short contacts:

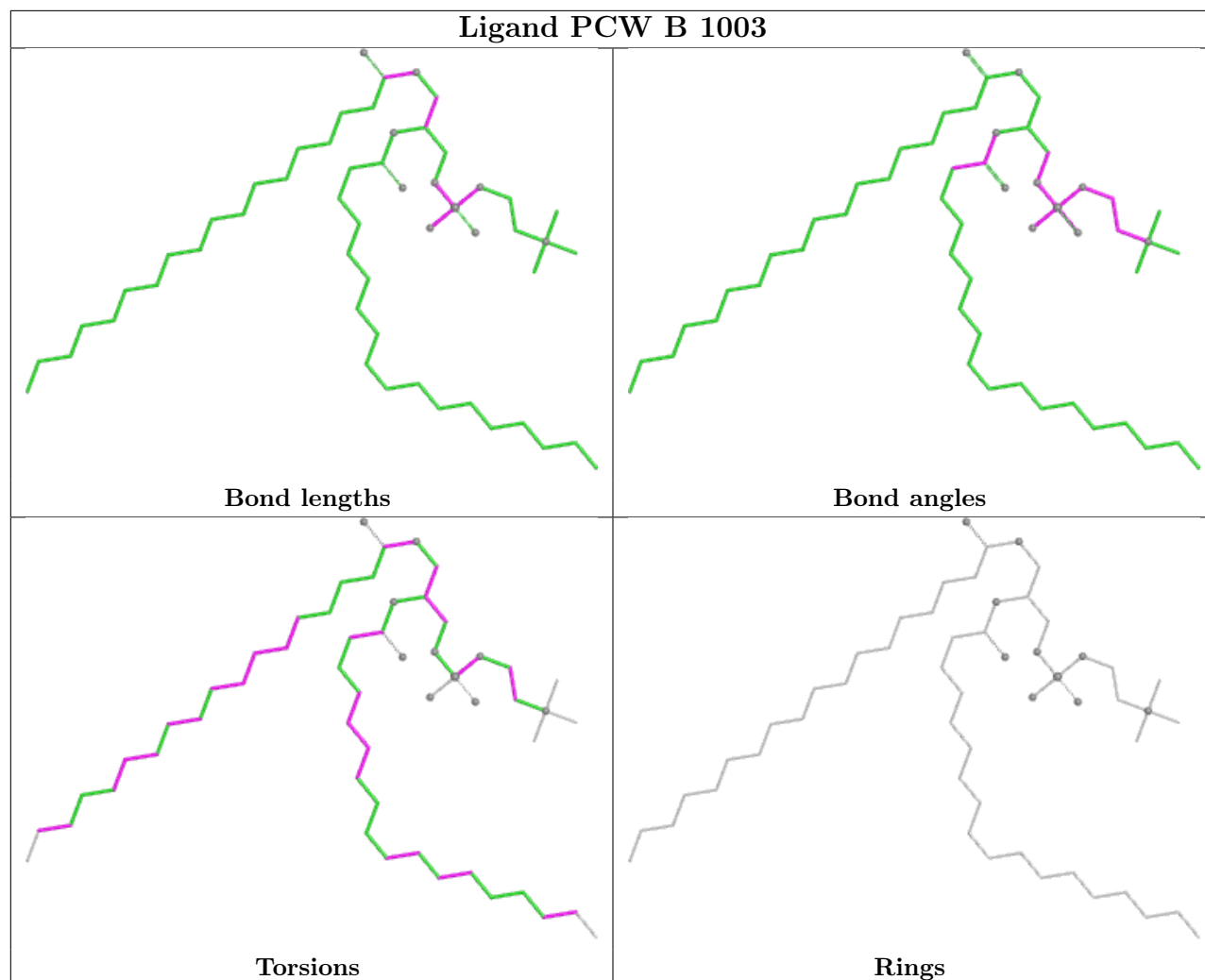
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1004	PCW	1	0
4	C	1003	PCW	2	0
4	B	1003	PCW	5	0
4	C	1006	PCW	2	0
4	C	1008	PCW	4	0
4	B	1009	PCW	4	0
4	D	1003	PCW	4	0
4	B	1006	PCW	2	0
5	D	1009	CE1	1	0
5	D	1008	CE1	2	0
5	D	1005	CE1	3	0
2	H	1001	BEF	1	0
4	B	1008	PCW	3	0
4	A	1003	PCW	2	0
5	D	1006	CE1	4	0
4	B	1007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

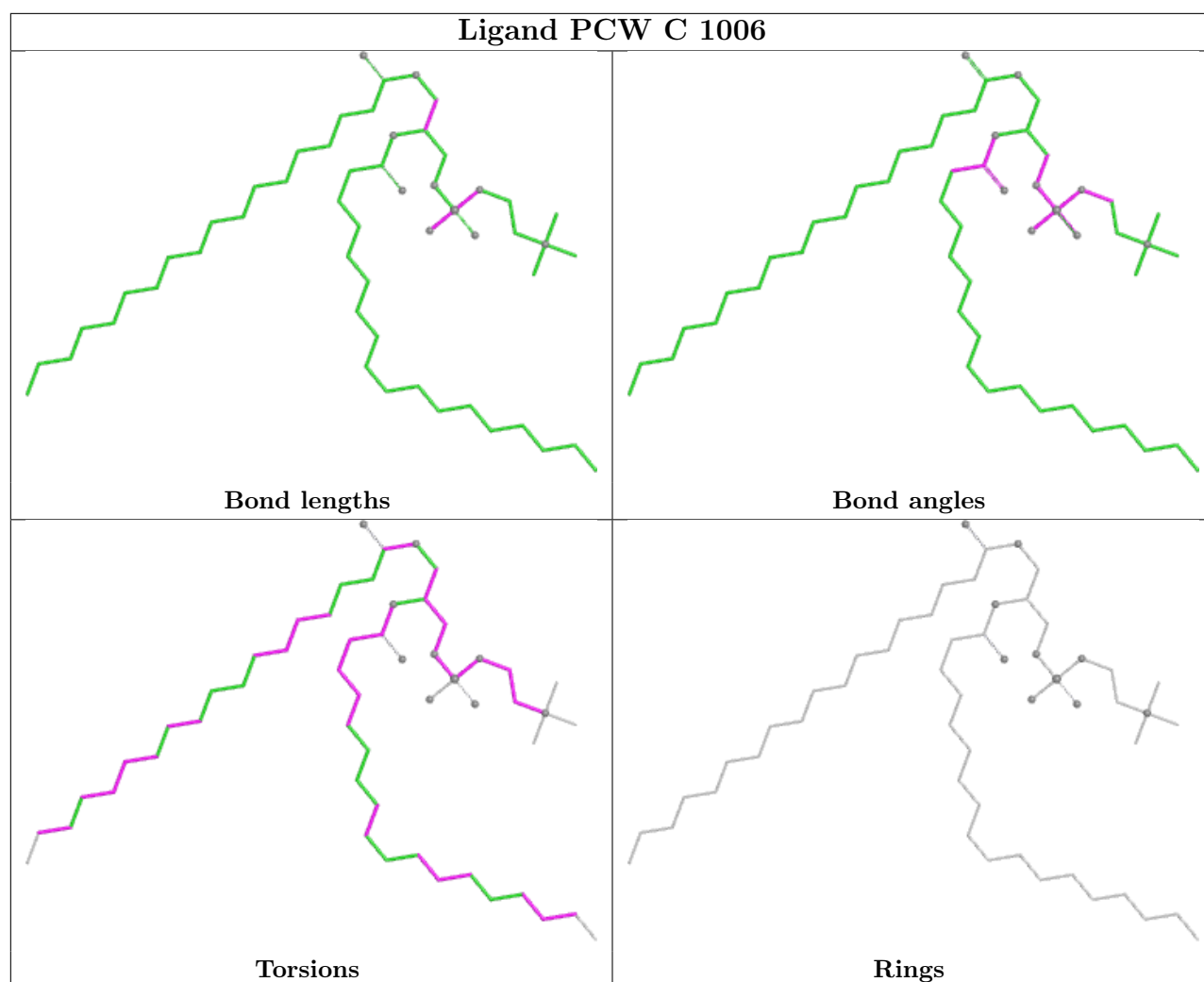
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

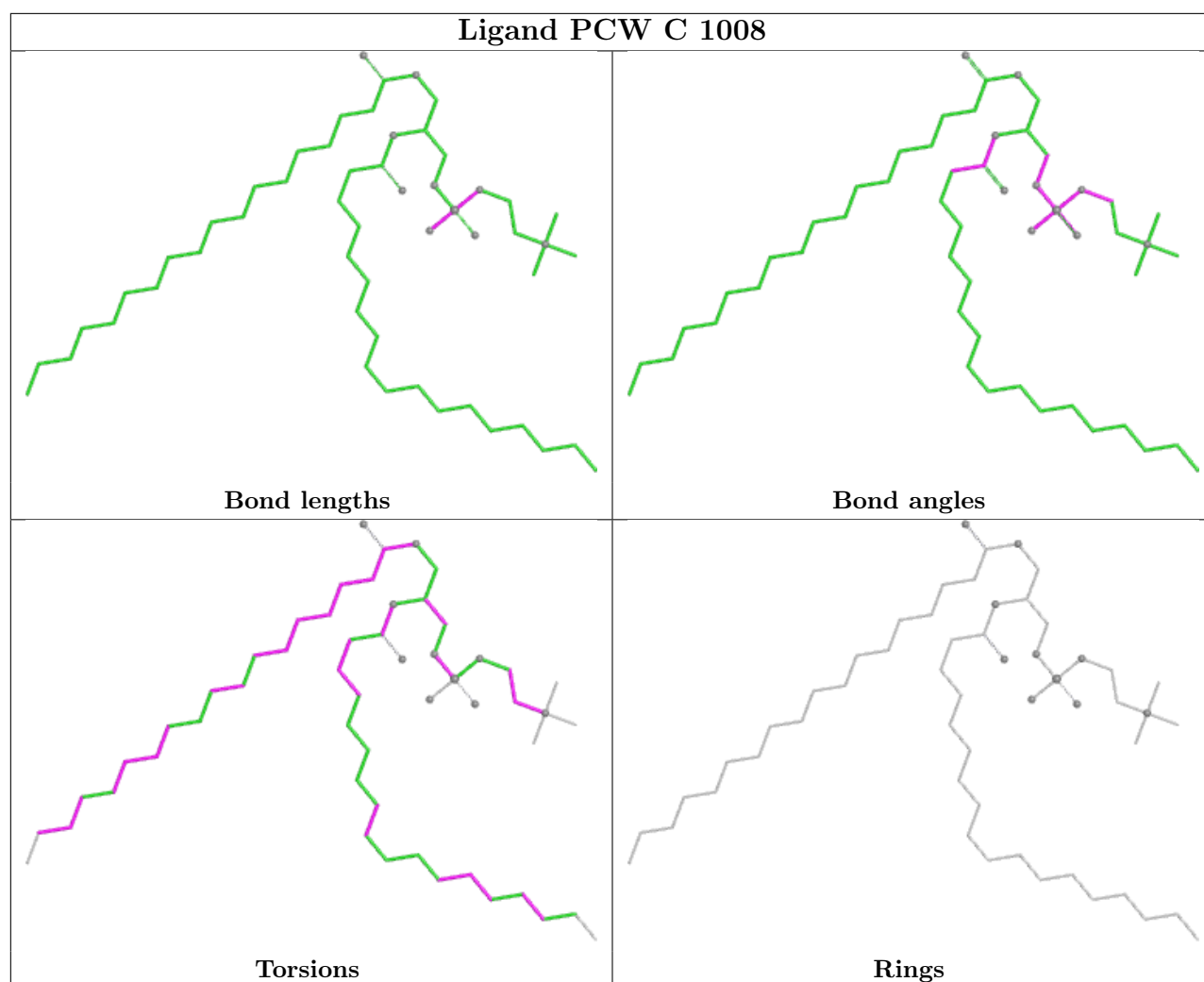
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.

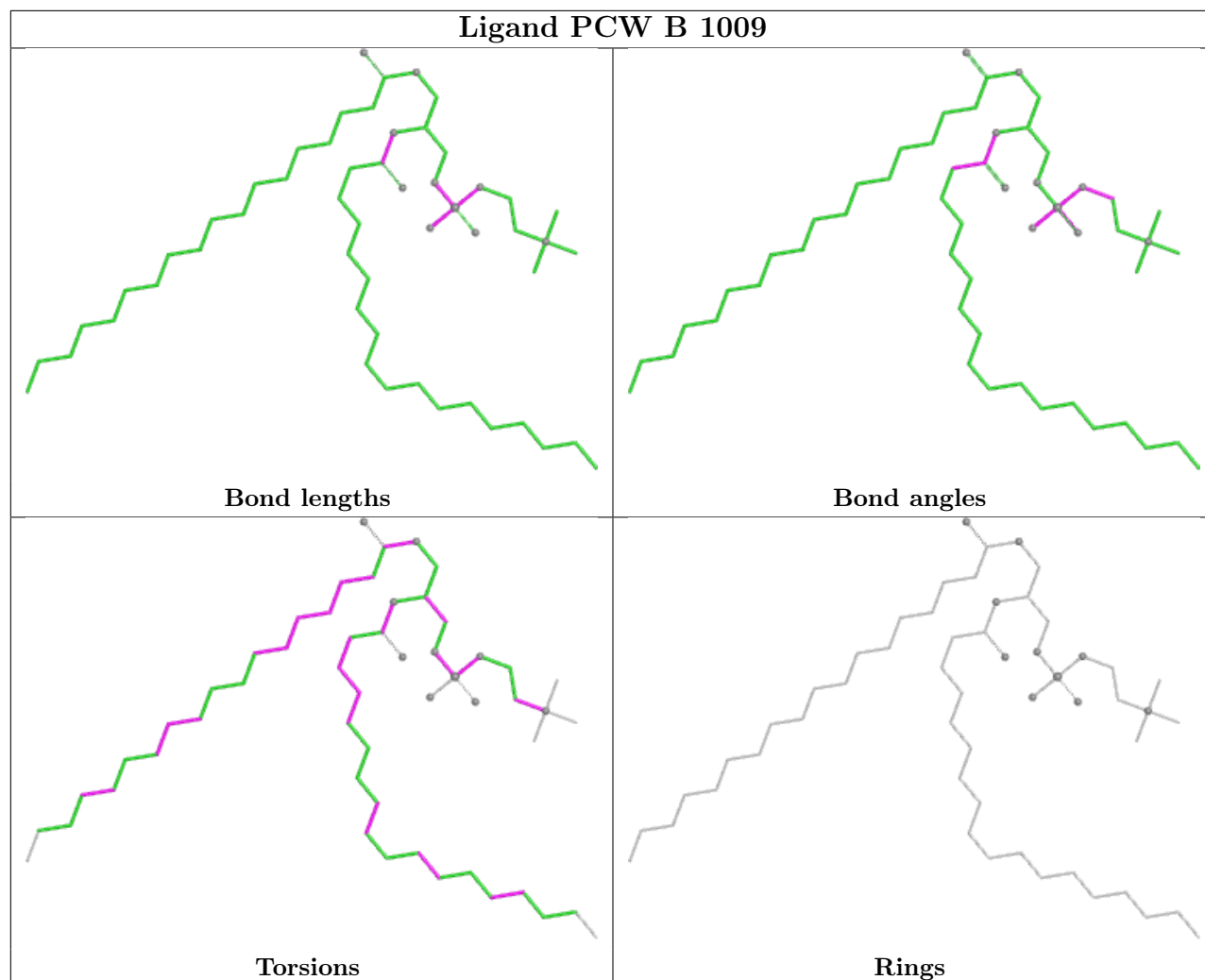


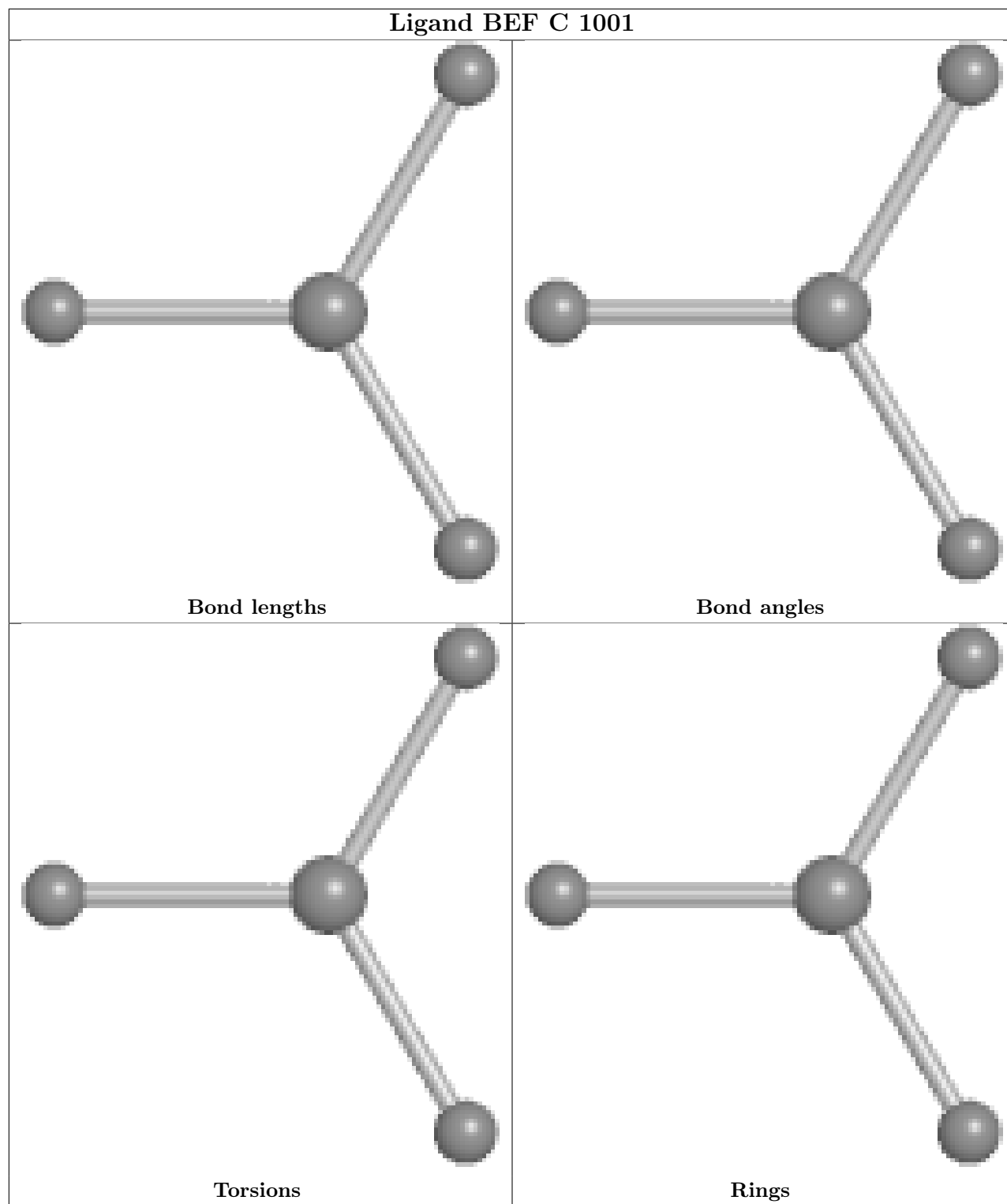


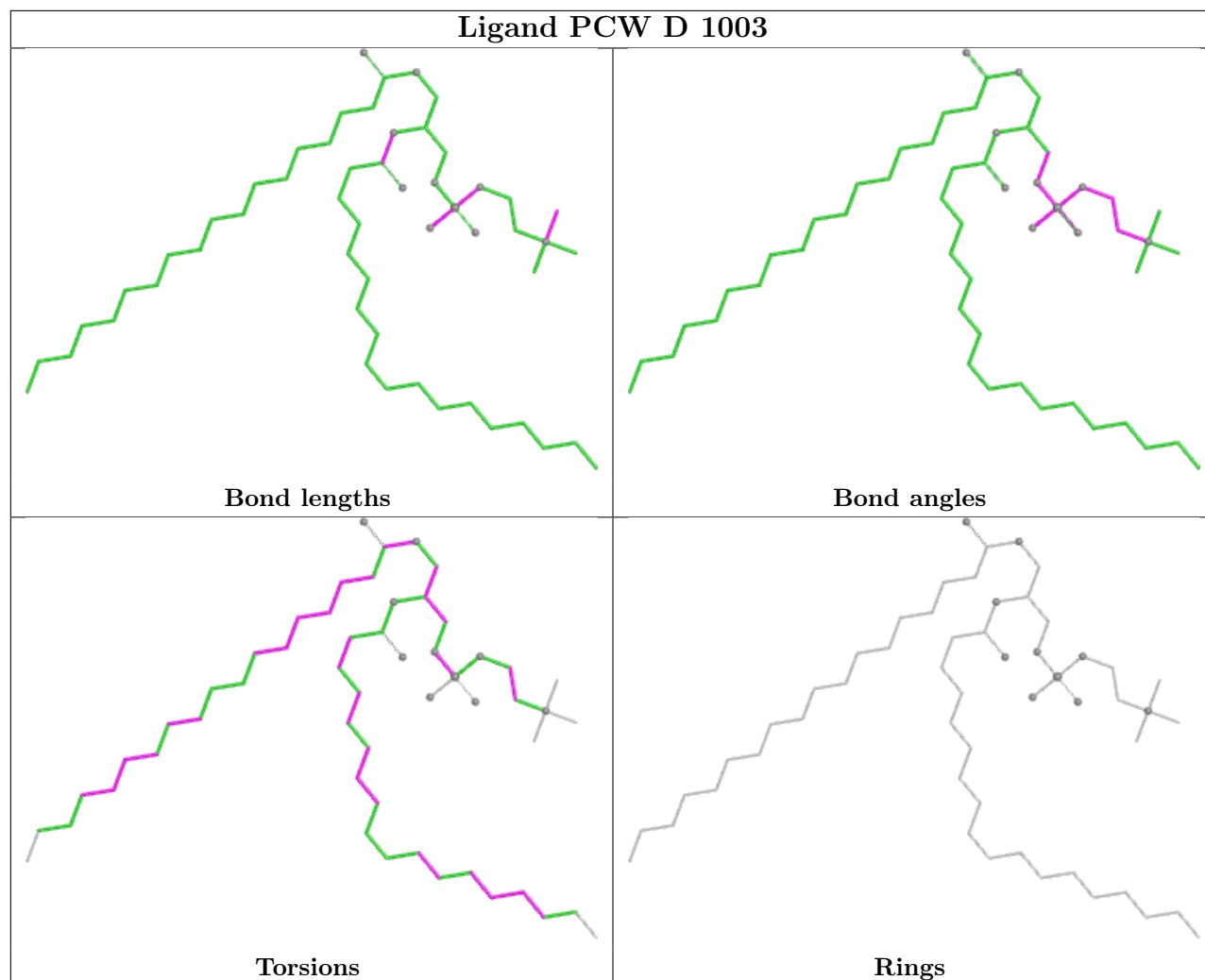


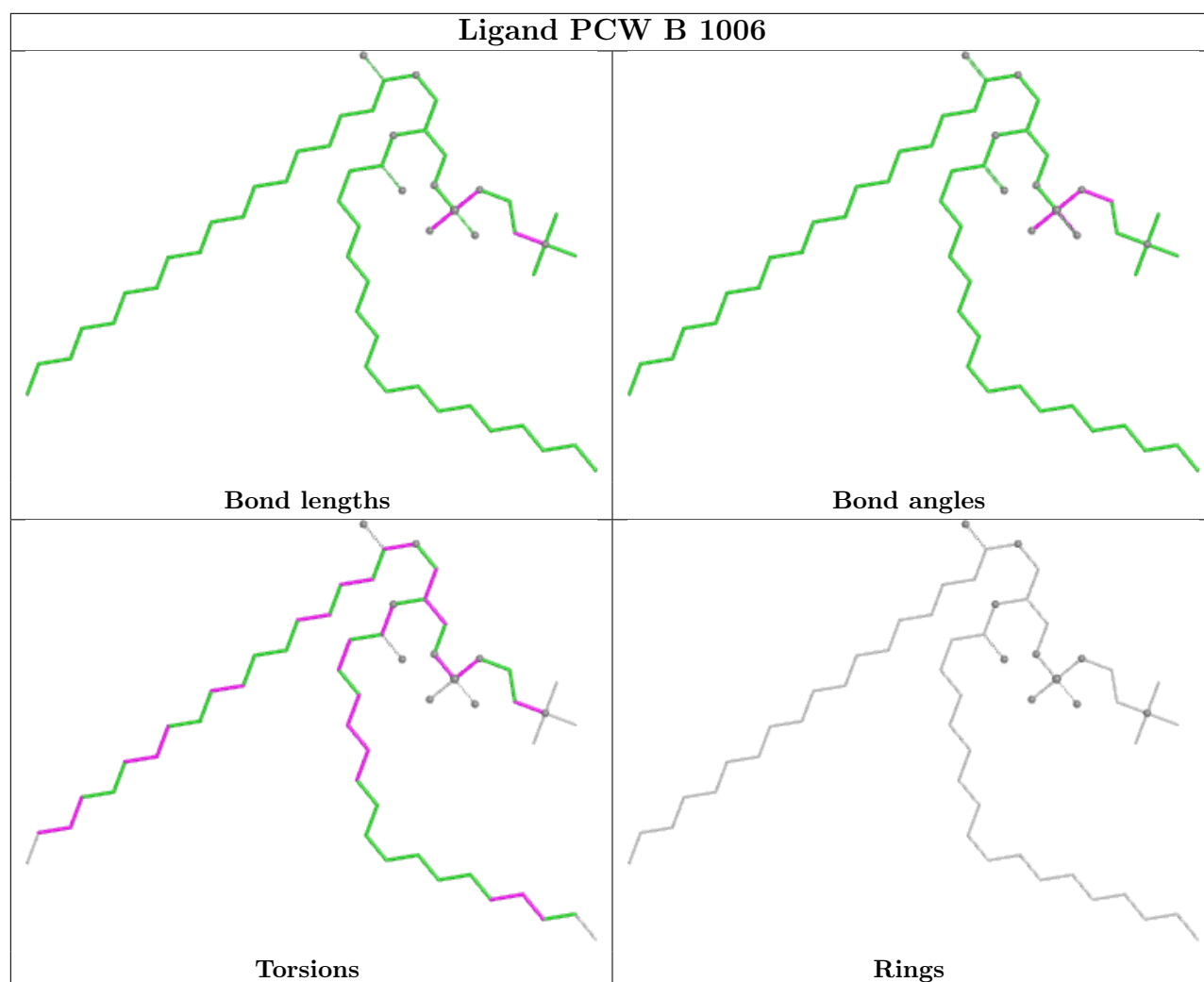


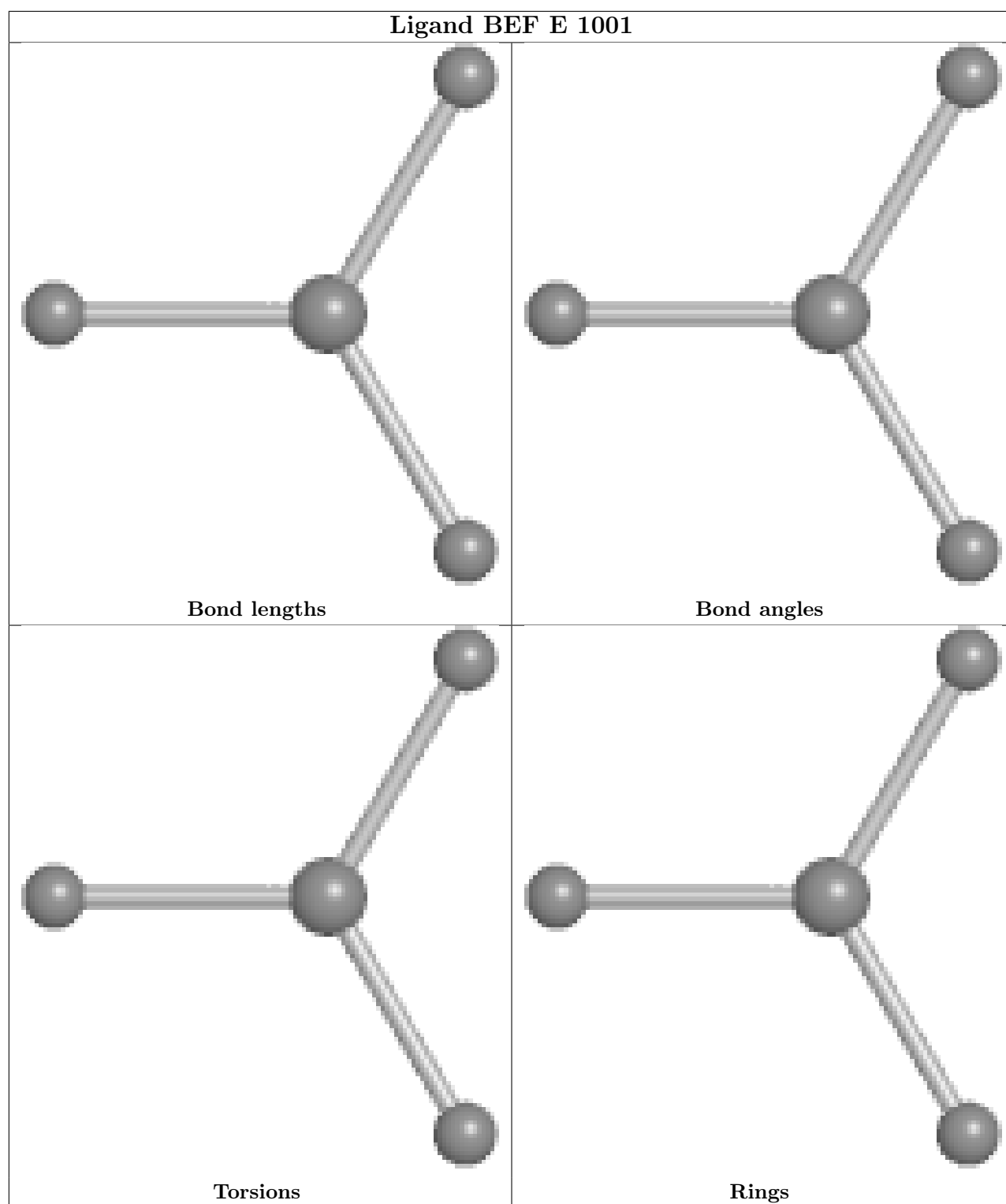


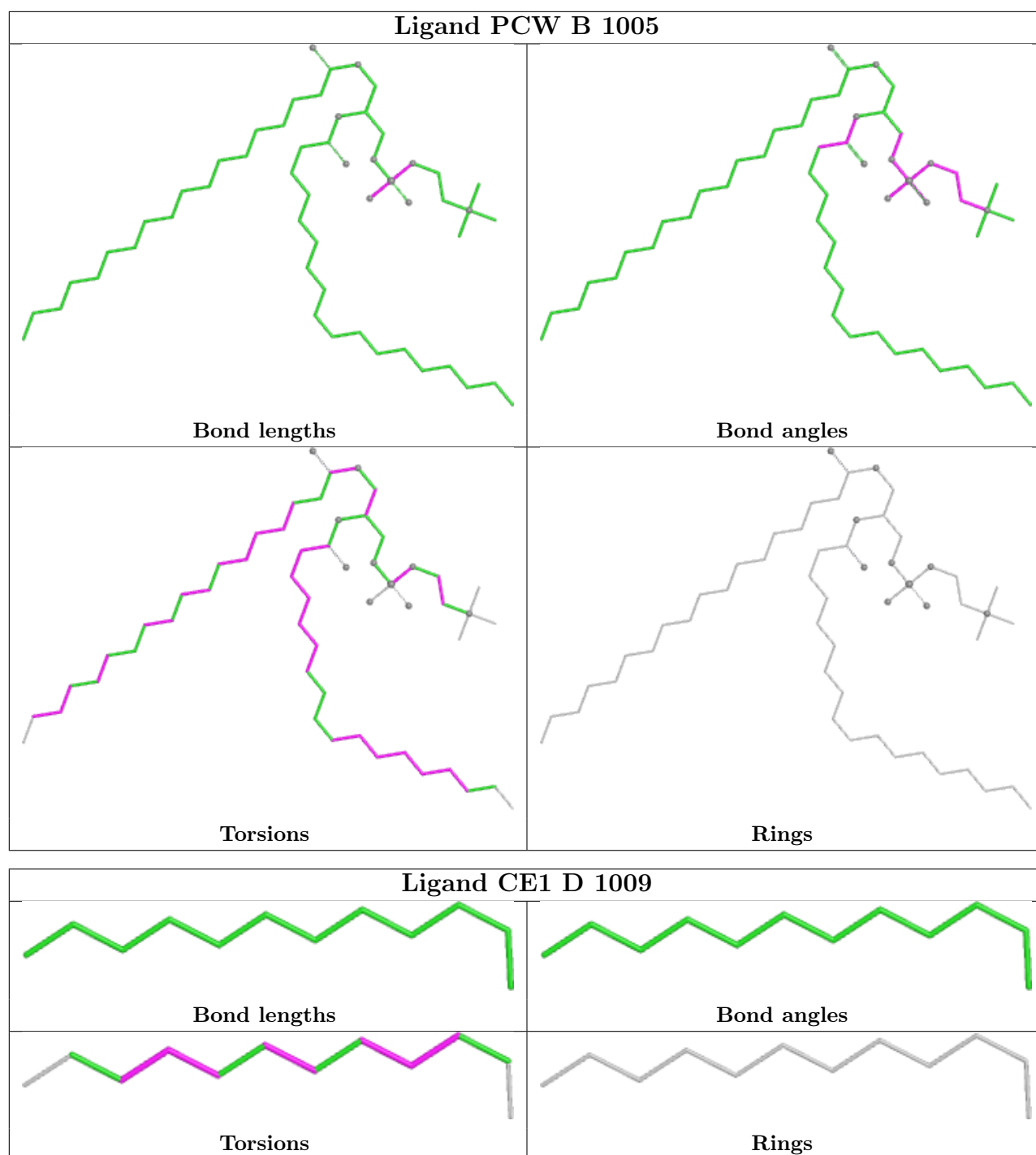


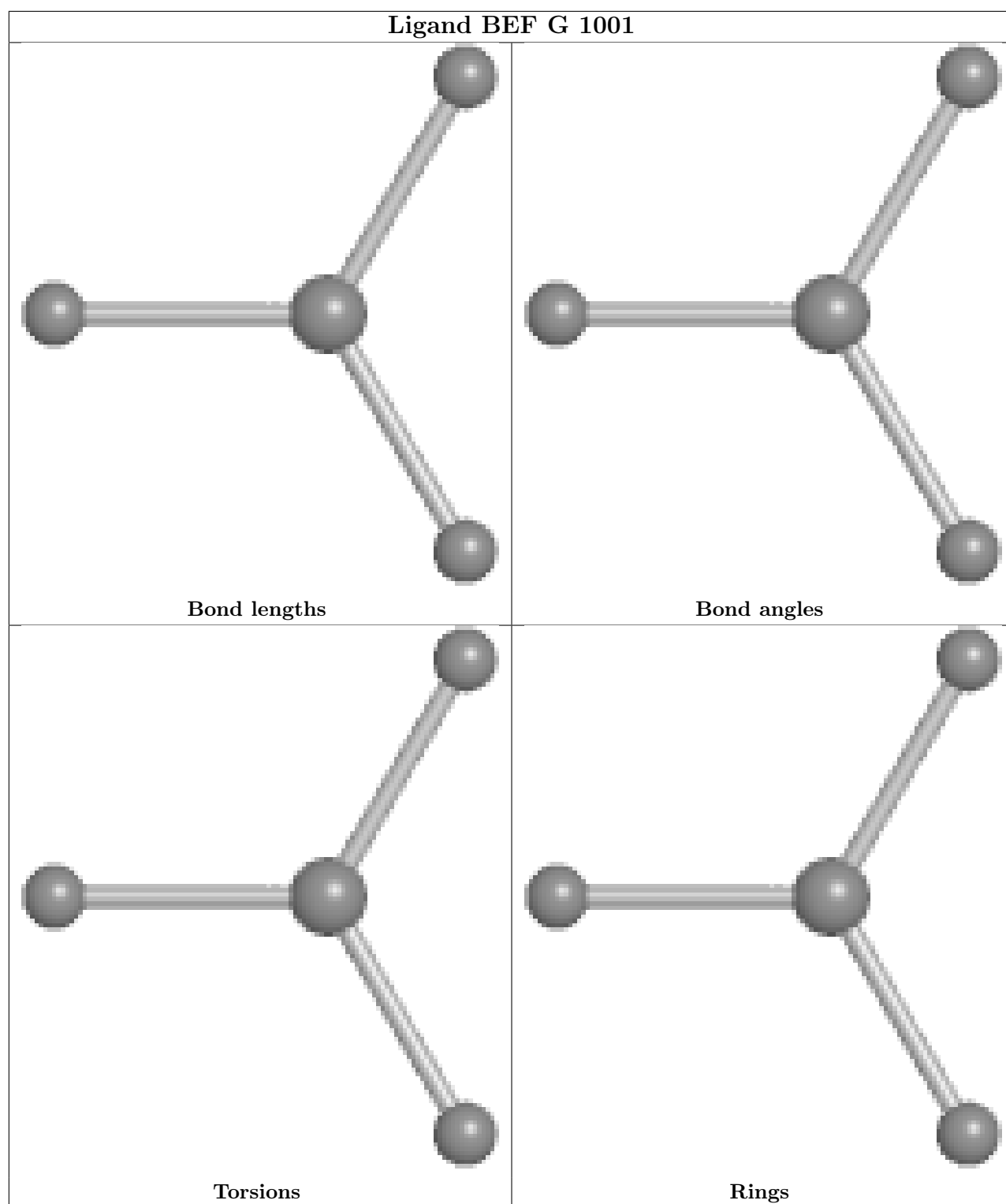


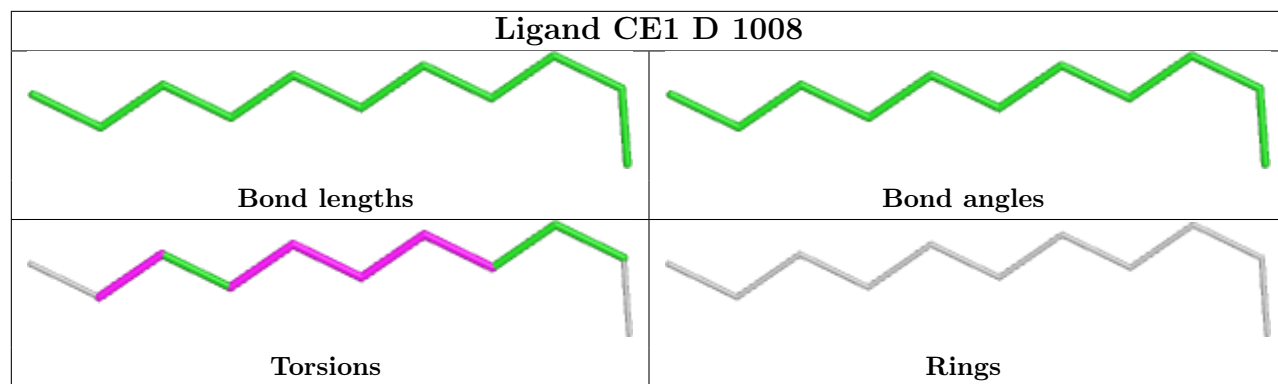


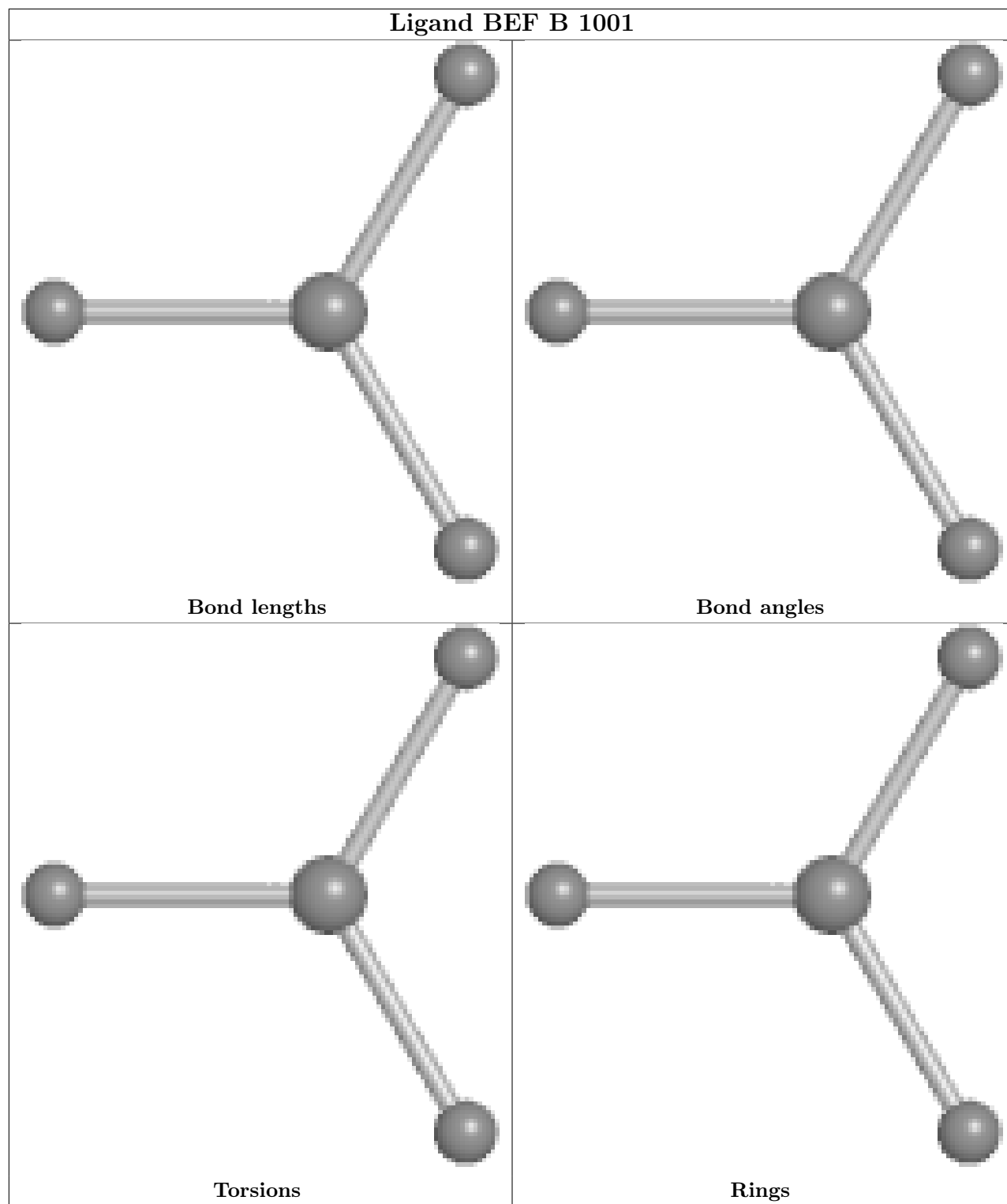


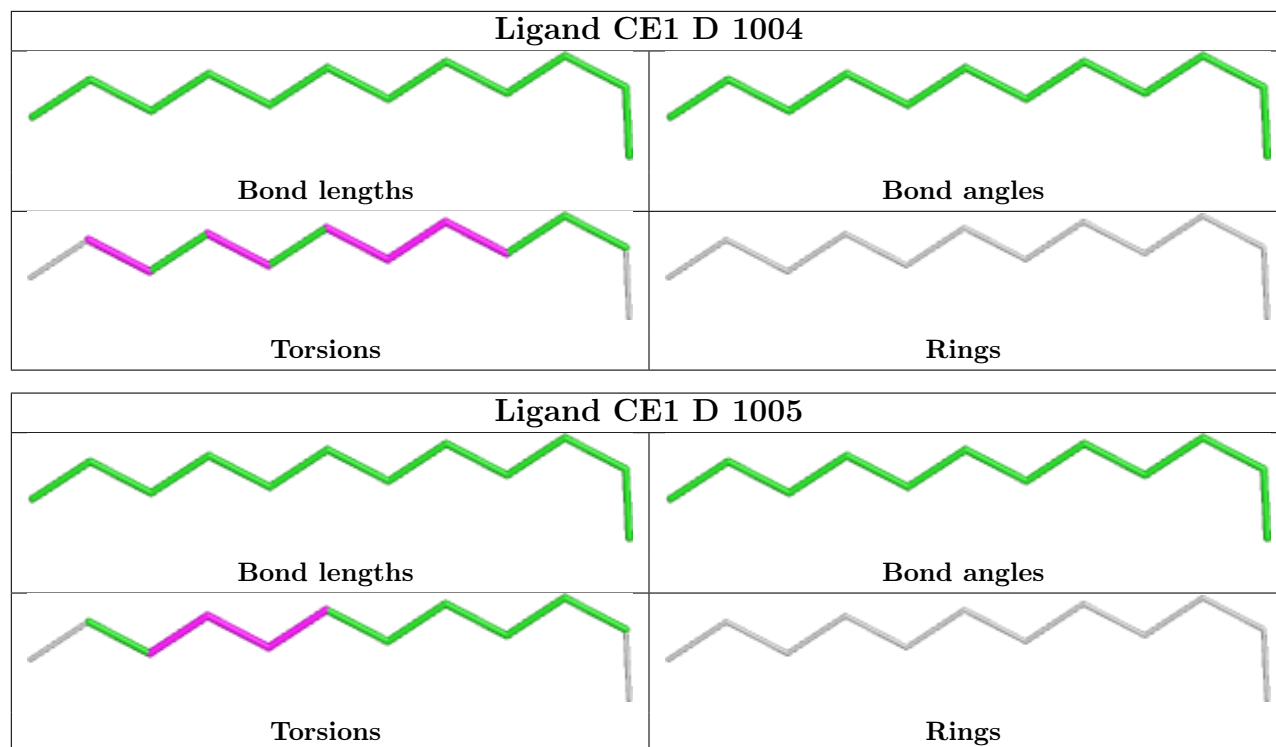


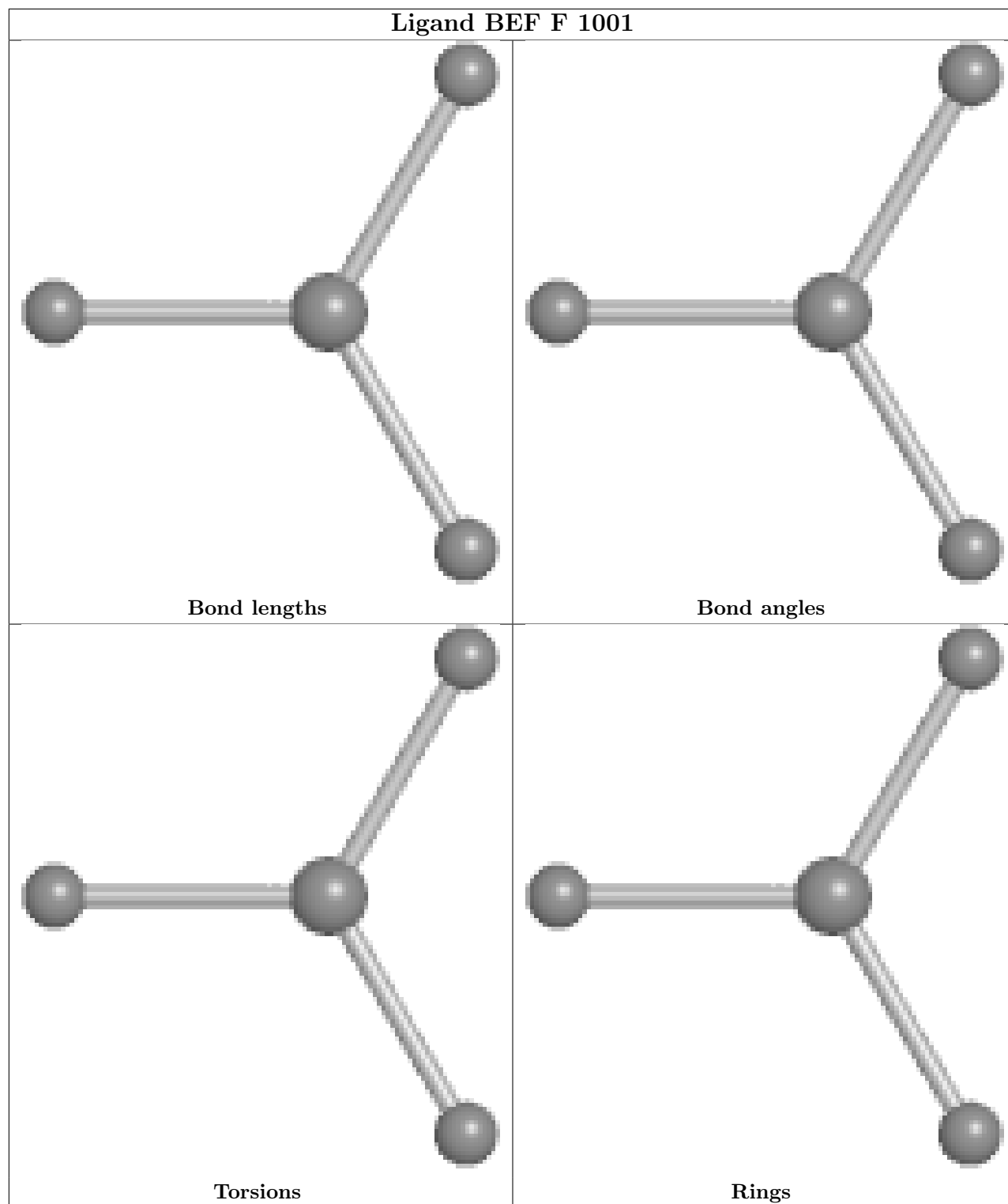


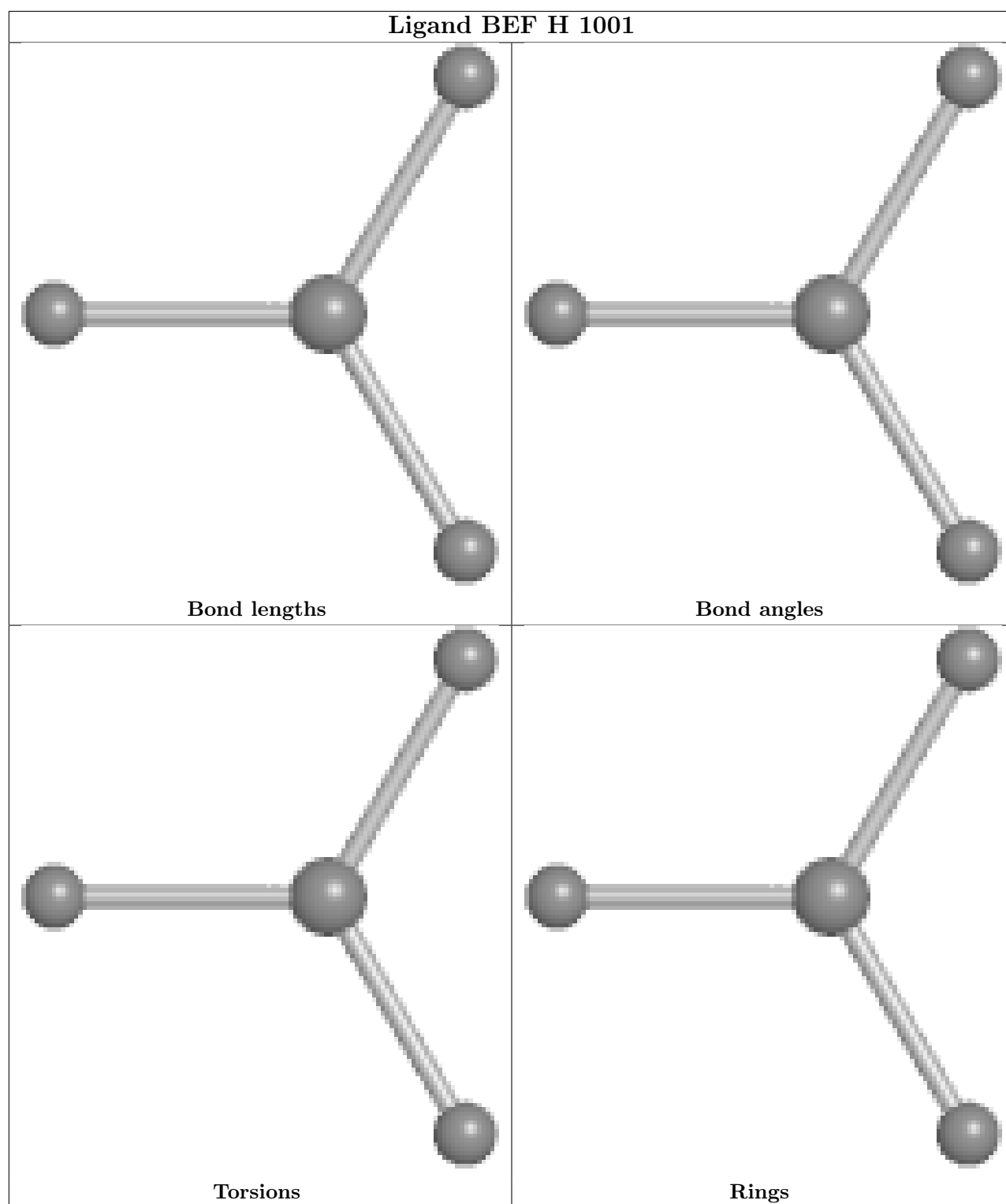


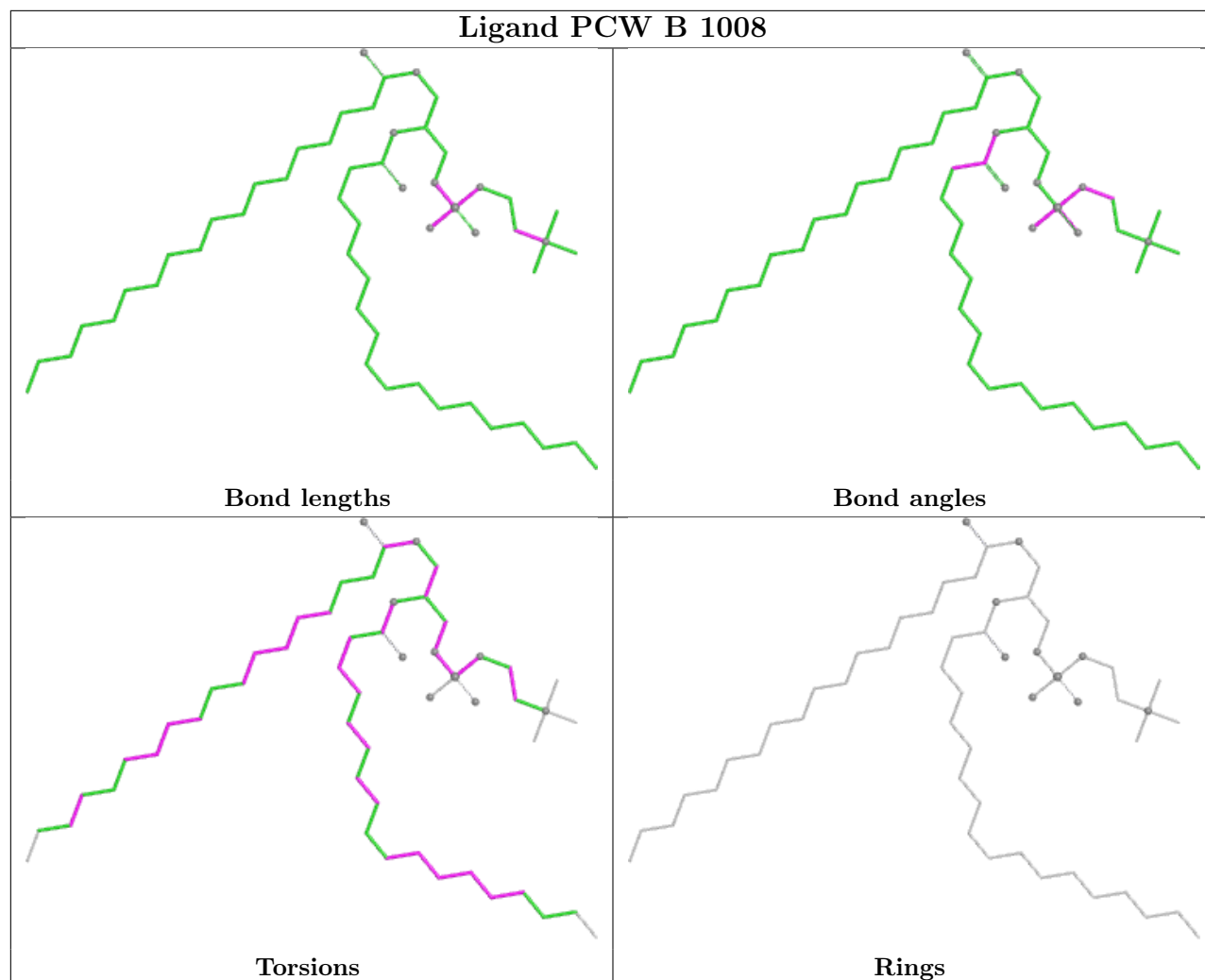


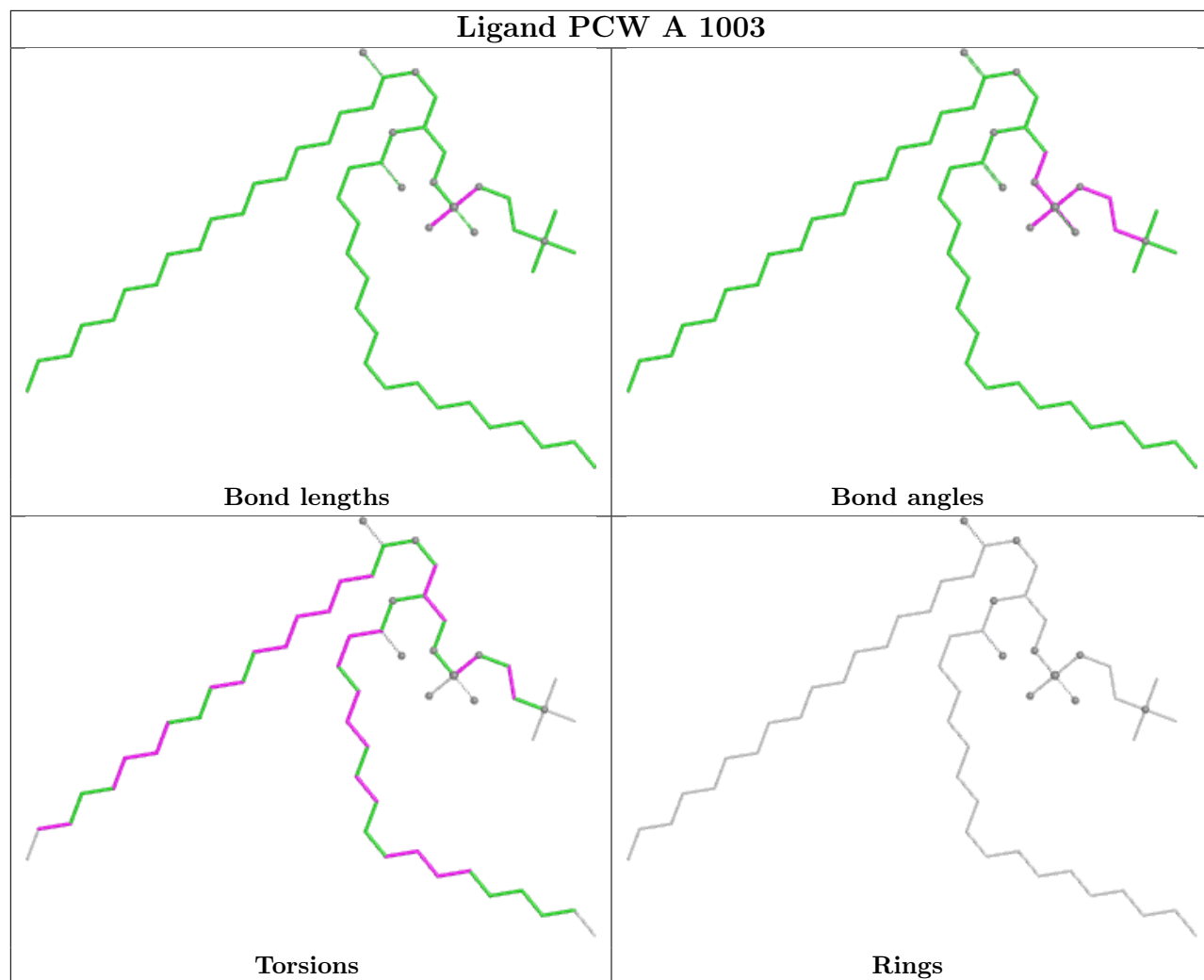


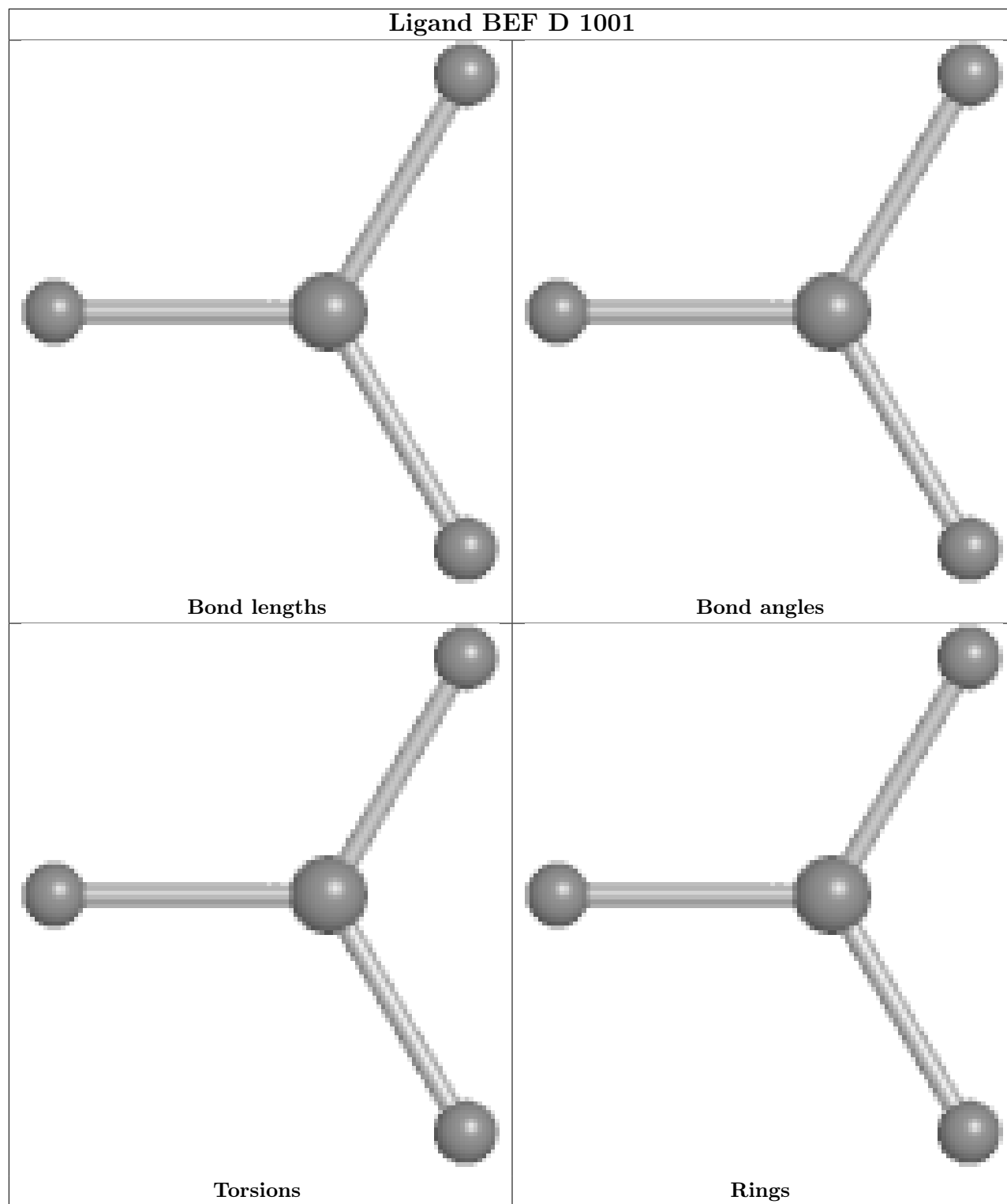


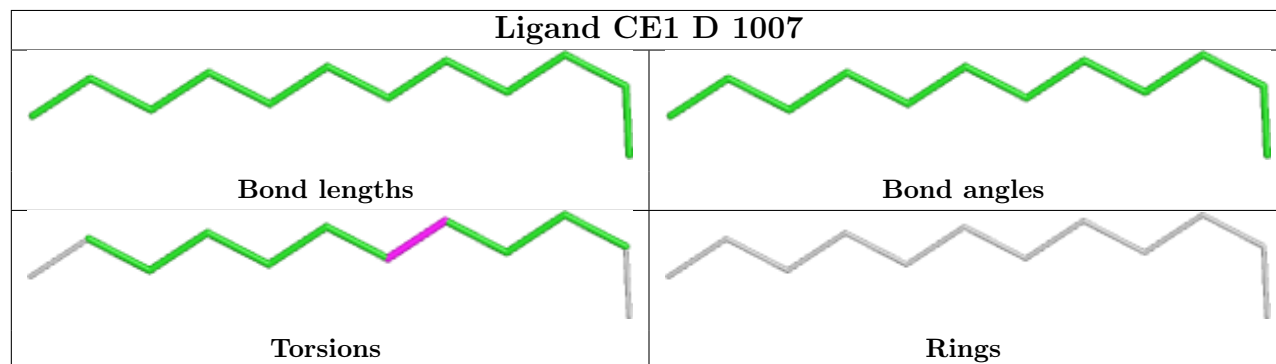
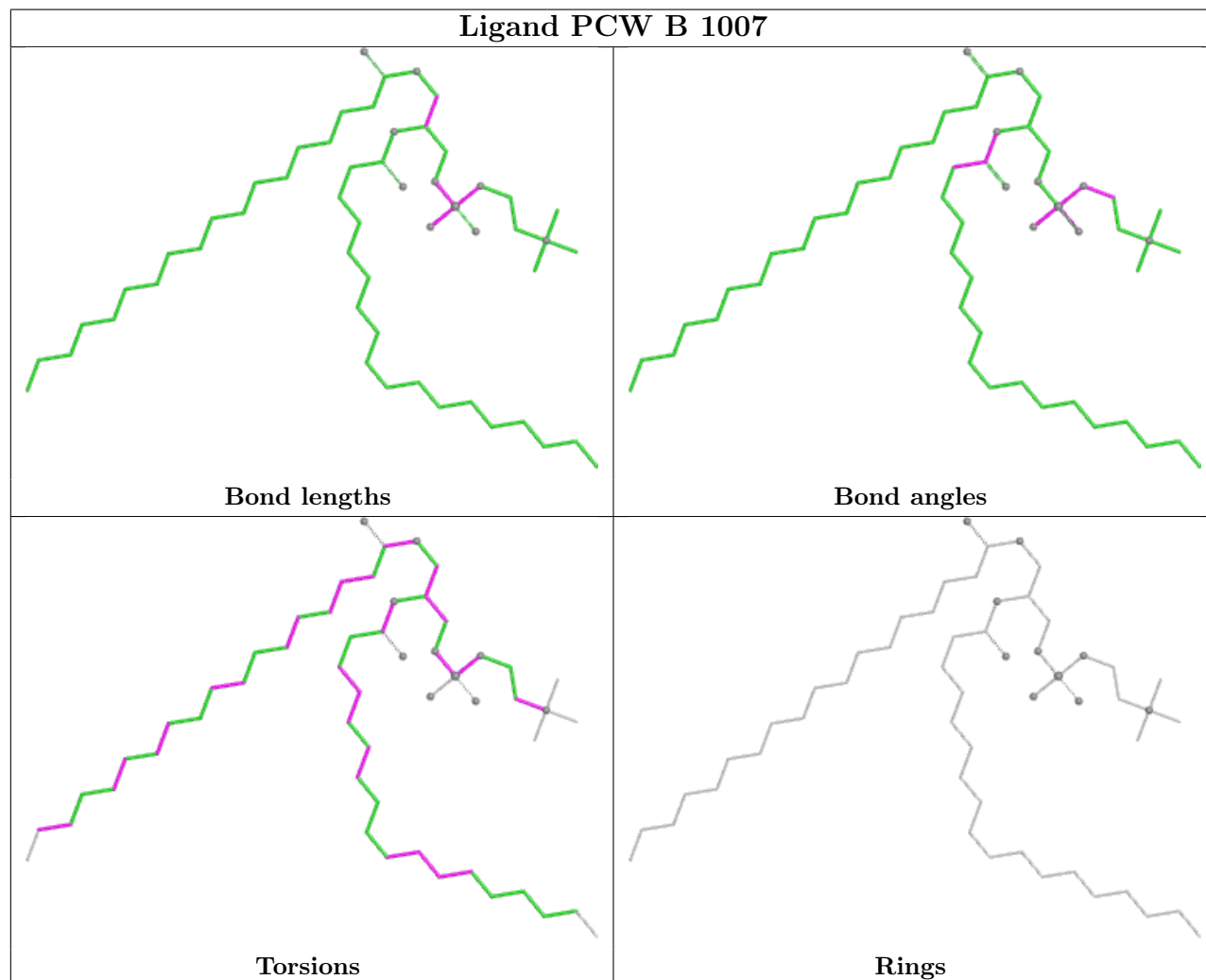
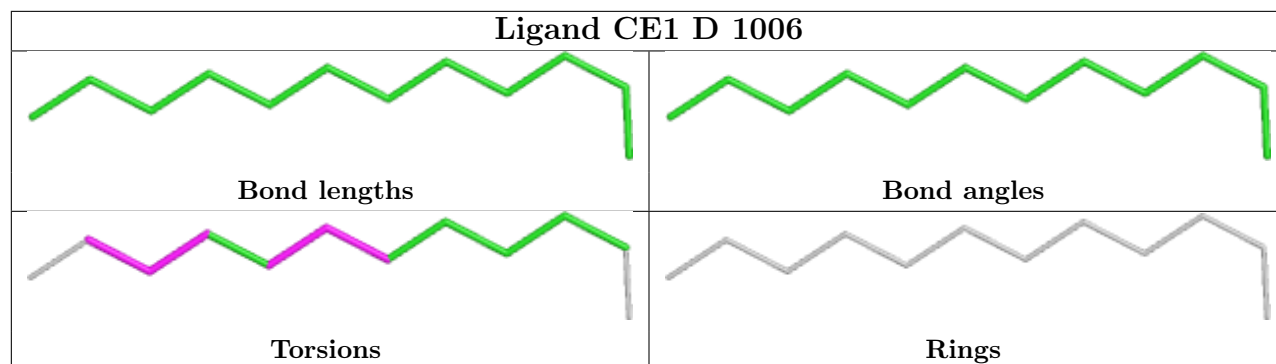


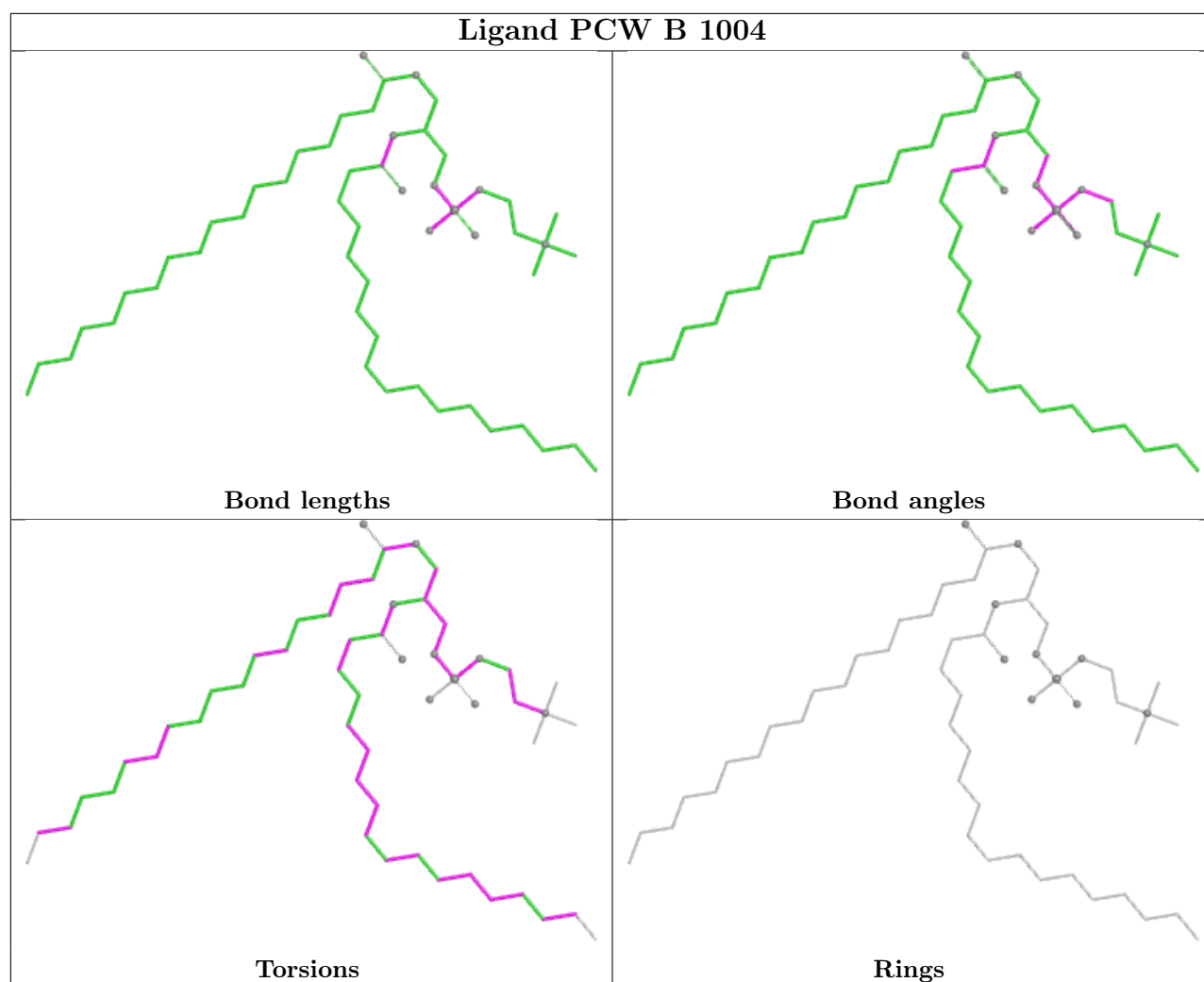


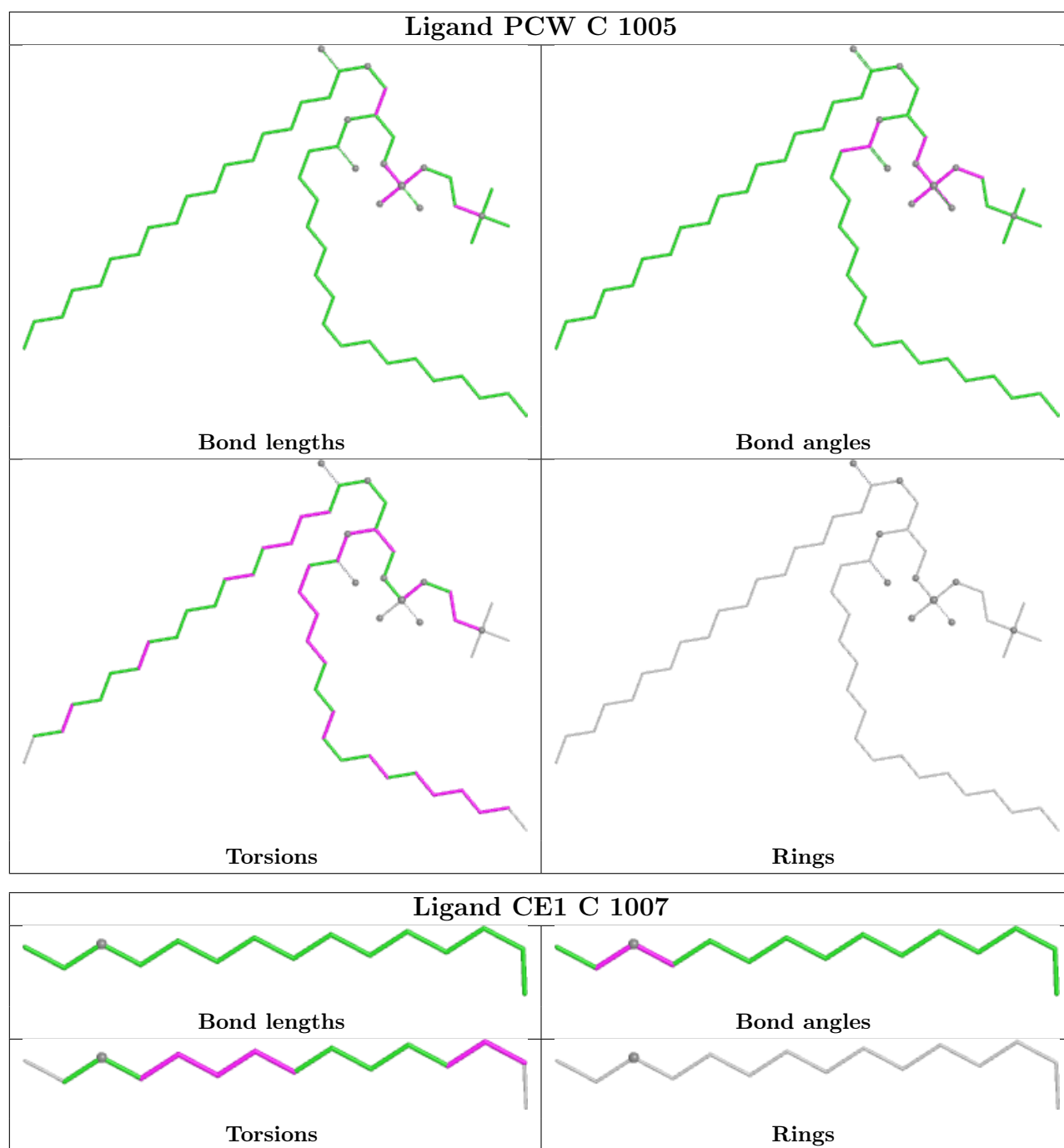


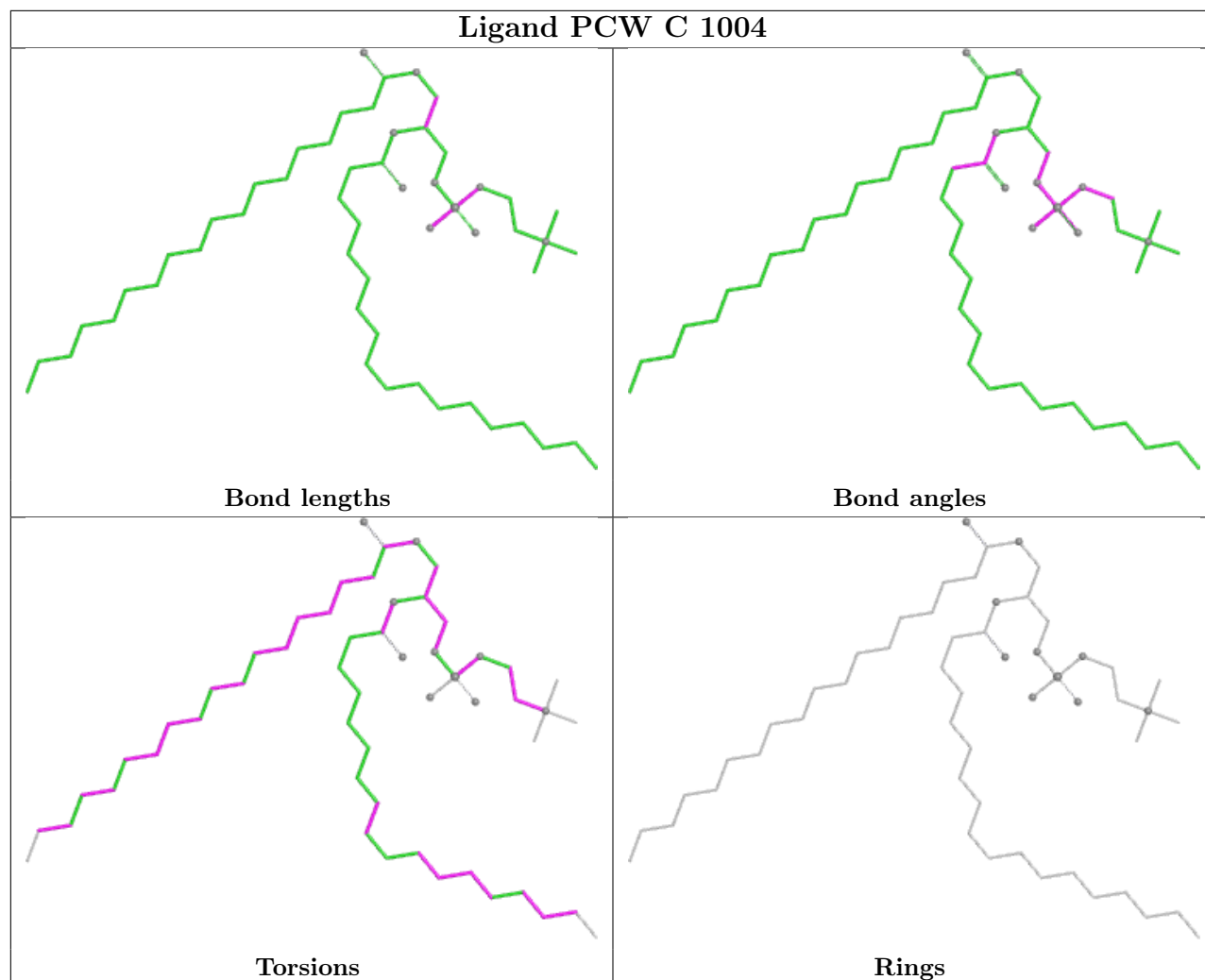


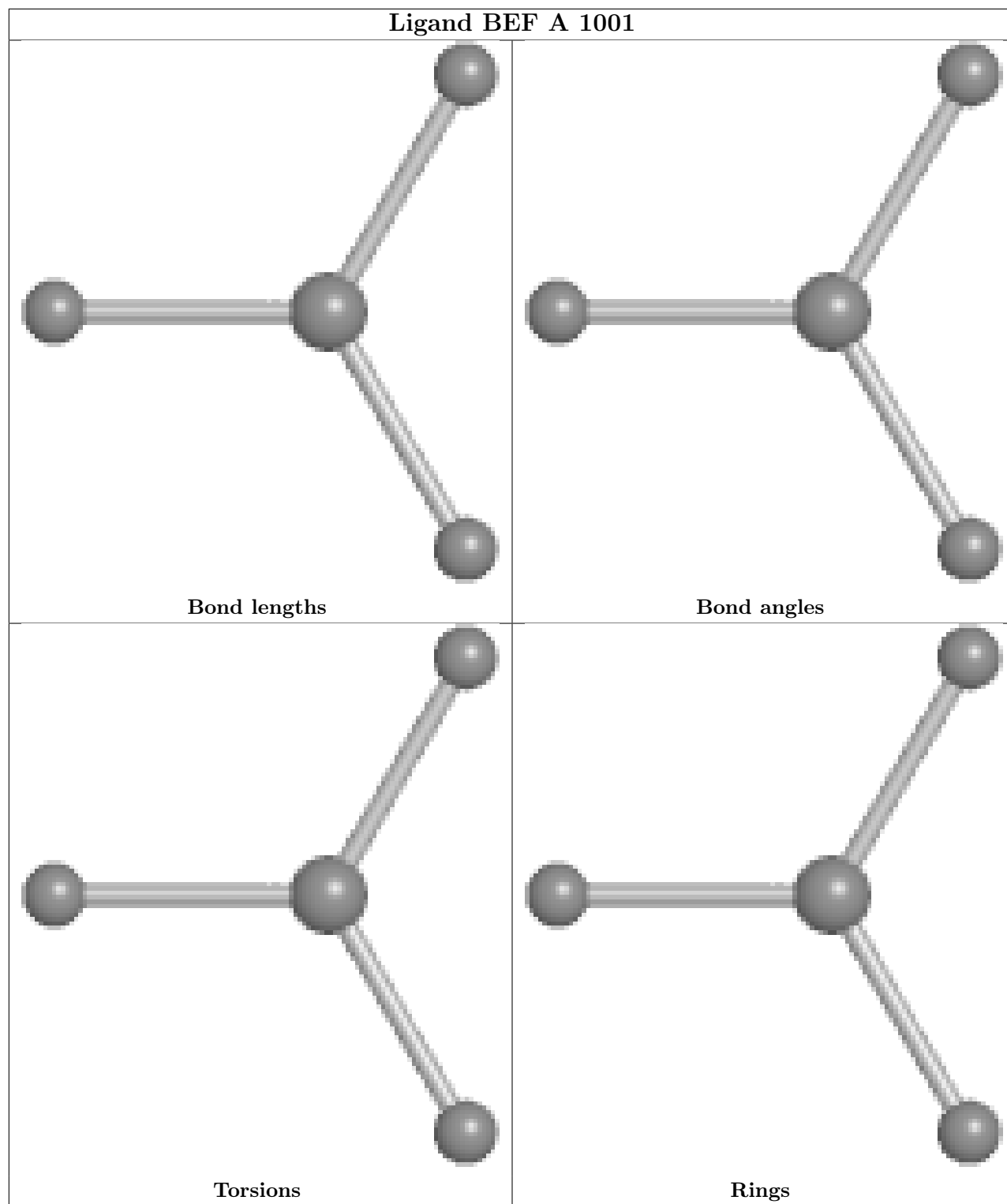












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	883/911 (96%)	-0.12	15 (1%)	69 45	25, 51, 97, 128	0
1	B	883/911 (96%)	-0.11	12 (1%)	73 51	26, 51, 98, 130	0
1	C	883/911 (96%)	0.27	42 (4%)	35 19	26, 68, 215, 259	0
1	D	883/911 (96%)	0.29	55 (6%)	26 14	25, 68, 231, 279	0
1	E	876/911 (96%)	1.50	216 (24%)	2 1	159, 182, 261, 273	0
1	F	876/911 (96%)	1.50	221 (25%)	1 1	155, 174, 199, 221	0
1	G	875/911 (96%)	1.47	198 (22%)	2 1	153, 173, 198, 226	0
1	H	876/911 (96%)	1.46	209 (23%)	2 1	144, 179, 265, 300	0
All	All	7035/7288 (96%)	0.78	968 (13%)	6 4	25, 162, 234, 300	0

All (968) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	458	CYS	7.7
1	E	728	GLY	7.2
1	E	725	ILE	6.7
1	E	377	ALA	6.3
1	E	680	SER	6.2
1	E	802	ALA	5.8
1	F	523	MET	5.5
1	G	396	THR	5.1
1	F	108	ARG	5.1
1	E	77	VAL	5.0
1	E	292	GLU	4.9
1	F	689	LEU	4.9
1	B	884	ILE	4.9
1	H	377	ALA	4.9
1	F	573	LEU	4.9
1	E	142	GLY	4.8

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Mol	Chain	Res	Type	RSRZ
1	H	869	GLU	4.8
1	E	681	ILE	4.8
1	H	302	LEU	4.8
1	F	725	ILE	4.7
1	H	594	ALA	4.7
1	G	461	VAL	4.6
1	B	883	ASP	4.6
1	G	517	LEU	4.5
1	E	495	TYR	4.5
1	E	347	VAL	4.5
1	F	275	ILE	4.4
1	H	95	VAL	4.4
1	H	548	ILE	4.4
1	F	332	CYS	4.4
1	F	248	LEU	4.3
1	G	830	LEU	4.3
1	E	138	ILE	4.3
1	H	304	VAL	4.3
1	H	332	CYS	4.2
1	H	722	LEU	4.2
1	F	830	LEU	4.1
1	E	275	ILE	4.1
1	G	446	LEU	4.1
1	F	255	PHE	4.1
1	G	11	THR	4.1
1	F	161	GLU	4.1
1	H	264	LEU	4.1
1	F	271	MET	4.0
1	H	298	VAL	4.0
1	H	300	ILE	4.0
1	E	518	VAL	4.0
1	G	455	PHE	4.0
1	B	885	PRO	3.9
1	H	293	ALA	3.9
1	E	815	PHE	3.9
1	G	639	ALA	3.9
1	F	676	ASN	3.9
1	F	757	VAL	3.9
1	E	729	MET	3.9
1	F	267	ASN	3.9
1	G	833	ILE	3.9
1	E	519	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	446	LEU	3.8
1	F	263	LEU	3.8
1	H	202	GLY	3.8
1	H	814	PHE	3.8
1	G	198	VAL	3.8
1	D	395	PRO	3.8
1	E	451	PRO	3.8
1	F	184	LEU	3.8
1	E	298	VAL	3.8
1	G	72	VAL	3.8
1	E	856	ILE	3.8
1	D	475	LEU	3.8
1	G	710	LEU	3.8
1	E	784	VAL	3.8
1	G	452	ASP	3.8
1	F	292	GLU	3.8
1	E	748	ILE	3.7
1	G	34	TYR	3.7
1	E	851	LEU	3.7
1	C	377	ALA	3.7
1	D	377	ALA	3.7
1	E	726	ALA	3.7
1	F	684	LEU	3.7
1	H	447	THR	3.6
1	F	252	VAL	3.6
1	H	435	THR	3.6
1	F	68	LEU	3.6
1	G	380	CYS	3.6
1	E	801	ALA	3.6
1	F	579	ASP	3.6
1	F	681	ILE	3.6
1	H	712	LEU	3.6
1	E	370	GLU	3.6
1	E	497	TYR	3.6
1	F	165	THR	3.6
1	G	280	MET	3.5
1	G	573	LEU	3.5
1	F	513	GLN	3.5
1	F	802	ALA	3.5
1	G	300	ILE	3.5
1	G	842	ILE	3.5
1	E	814	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	143	ASP	3.5
1	F	622	GLY	3.5
1	F	829	VAL	3.5
1	D	172	GLU	3.5
1	E	538	SER	3.5
1	F	625	VAL	3.5
1	G	680	SER	3.5
1	B	269	ALA	3.5
1	E	160	ASP	3.5
1	G	73	LEU	3.5
1	G	853	GLU	3.5
1	F	40	LYS	3.5
1	F	749	PHE	3.5
1	F	549	THR	3.5
1	E	394	ASP	3.5
1	H	34	TYR	3.4
1	F	35	GLY	3.4
1	H	493	LEU	3.4
1	F	748	ILE	3.4
1	G	630	ALA	3.4
1	H	726	ALA	3.4
1	E	381	ASN	3.4
1	F	600	SER	3.4
1	H	714	PHE	3.4
1	C	497	TYR	3.4
1	G	724	ALA	3.4
1	A	884	ILE	3.4
1	E	677	ILE	3.4
1	F	663	ILE	3.4
1	G	378	VAL	3.4
1	G	793	LEU	3.3
1	H	98	ARG	3.3
1	H	378	VAL	3.3
1	F	45	ASP	3.3
1	F	202	GLY	3.3
1	G	333	THR	3.3
1	G	61	ILE	3.3
1	G	542	GLY	3.3
1	E	352	PRO	3.3
1	C	447	THR	3.3
1	E	104	LEU	3.3
1	G	722	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	61	ILE	3.3
1	F	796	THR	3.3
1	G	59	MET	3.3
1	F	801	ALA	3.3
1	E	332	CYS	3.3
1	G	815	PHE	3.3
1	F	758	ILE	3.3
1	E	810	PHE	3.2
1	F	346	VAL	3.2
1	G	284	ALA	3.2
1	G	683	TYR	3.2
1	E	360	PRO	3.2
1	E	198	VAL	3.2
1	H	96	GLN	3.2
1	E	400	LEU	3.2
1	F	595	VAL	3.2
1	H	69	VAL	3.2
1	C	437	HIS	3.2
1	D	435	THR	3.2
1	E	827	CYS	3.2
1	F	753	THR	3.2
1	G	579	ASP	3.2
1	H	867	MET	3.2
1	E	747	GLY	3.2
1	F	825	LEU	3.2
1	G	727	LEU	3.2
1	G	69	VAL	3.2
1	C	374	ILE	3.2
1	D	374	ILE	3.2
1	H	535	ILE	3.2
1	E	694	ALA	3.2
1	G	580	ALA	3.2
1	E	245	LEU	3.2
1	C	347	VAL	3.2
1	G	395	PRO	3.2
1	F	766	ILE	3.2
1	H	709	ALA	3.2
1	H	382	ASP	3.1
1	H	747	GLY	3.1
1	C	379	LEU	3.1
1	F	696	LEU	3.1
1	G	276	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	816	SER	3.1
1	G	682	ALA	3.1
1	F	722	LEU	3.1
1	G	832	GLY	3.1
1	H	507	LEU	3.1
1	G	192	PHE	3.1
1	F	596	TYR	3.1
1	E	18	THR	3.1
1	H	207	THR	3.1
1	F	638	VAL	3.1
1	H	667	VAL	3.1
1	G	108	ARG	3.1
1	F	245	LEU	3.1
1	G	851	LEU	3.1
1	F	545	THR	3.1
1	B	464	ASP	3.1
1	F	810	PHE	3.1
1	G	843	PHE	3.1
1	G	178	ILE	3.1
1	F	628	ALA	3.1
1	D	507	LEU	3.1
1	F	680	SER	3.1
1	G	762	VAL	3.1
1	F	583	GLU	3.1
1	H	45	ASP	3.1
1	G	118	ILE	3.1
1	E	517	LEU	3.0
1	F	812	ALA	3.0
1	G	475	LEU	3.0
1	H	104	LEU	3.0
1	H	578	LEU	3.0
1	F	203	MET	3.0
1	H	107	LEU	3.0
1	F	813	GLY	3.0
1	E	207	THR	3.0
1	H	72	VAL	3.0
1	D	434	SER	3.0
1	F	293	ALA	3.0
1	G	709	ALA	3.0
1	C	496	GLY	3.0
1	E	817	ASN	3.0
1	G	700	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	H	835	VAL	3.0
1	D	523	MET	3.0
1	F	215	ILE	3.0
1	H	421	GLU	3.0
1	F	360	PRO	3.0
1	H	133	PRO	3.0
1	F	793	LEU	3.0
1	A	1	ALA	3.0
1	E	213	THR	3.0
1	E	280	MET	3.0
1	F	754	MET	3.0
1	H	830	LEU	3.0
1	F	102	SER	3.0
1	F	823	ALA	3.0
1	C	518	VAL	3.0
1	F	687	GLY	3.0
1	G	784	VAL	3.0
1	H	198	VAL	3.0
1	E	548	ILE	3.0
1	A	101	GLU	2.9
1	F	869	GLU	2.9
1	F	284	ALA	2.9
1	G	343	LYS	2.9
1	G	460	TYR	2.9
1	C	378	VAL	2.9
1	F	347	VAL	2.9
1	F	685	PHE	2.9
1	F	714	PHE	2.9
1	F	798	GLN	2.9
1	E	870	ILE	2.9
1	G	433	MET	2.9
1	H	65	ILE	2.9
1	H	374	ILE	2.9
1	C	443	LYS	2.9
1	E	880	LYS	2.9
1	E	444	ALA	2.9
1	H	66	ALA	2.9
1	G	429	ASP	2.9
1	H	348	ASP	2.9
1	H	445	MET	2.9
1	G	365	ASN	2.9
1	H	716	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	46	PRO	2.9
1	C	387	SER	2.9
1	G	275	ILE	2.9
1	C	517	LEU	2.9
1	F	463	LEU	2.9
1	G	711	GLN	2.9
1	H	432	LEU	2.9
1	H	684	LEU	2.9
1	F	808	THR	2.9
1	E	286	ALA	2.9
1	H	284	ALA	2.9
1	H	453	VAL	2.9
1	C	884	ILE	2.9
1	D	102	SER	2.9
1	E	693	ILE	2.9
1	H	488	GLN	2.9
1	G	469	PRO	2.9
1	B	484	GLU	2.9
1	F	48	TRP	2.9
1	C	495	TYR	2.9
1	F	84	LEU	2.9
1	F	565	LEU	2.9
1	H	297	ILE	2.9
1	A	885	PRO	2.8
1	D	521	THR	2.8
1	H	423	GLU	2.8
1	F	94	VAL	2.8
1	E	51	PHE	2.8
1	H	615	GLY	2.8
1	G	581	MET	2.8
1	H	296	SER	2.8
1	G	548	ILE	2.8
1	H	91	ILE	2.8
1	H	828	PHE	2.8
1	H	286	ALA	2.8
1	G	164	LEU	2.8
1	H	48	TRP	2.8
1	F	842	ILE	2.8
1	G	239	PHE	2.8
1	H	232	LEU	2.8
1	E	300	ILE	2.8
1	H	704	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	H	289	ALA	2.8
1	D	104	LEU	2.8
1	F	104	LEU	2.8
1	G	161	GLU	2.8
1	G	831	TYR	2.8
1	G	592	HIS	2.8
1	E	106	ALA	2.8
1	D	351	LEU	2.8
1	E	791	LEU	2.8
1	F	90	SER	2.8
1	H	93	SER	2.8
1	F	704	ILE	2.8
1	F	799	THR	2.8
1	F	821	ILE	2.8
1	G	163	MET	2.7
1	C	105	ASP	2.7
1	C	525	ASP	2.7
1	F	756	ALA	2.7
1	H	517	LEU	2.7
1	E	769	ILE	2.7
1	G	471	THR	2.7
1	F	550	GLY	2.7
1	C	440	ASN	2.7
1	F	866	VAL	2.7
1	F	873	VAL	2.7
1	F	601	PRO	2.7
1	F	851	LEU	2.7
1	H	363	PRO	2.7
1	H	663	ILE	2.7
1	H	438	THR	2.7
1	H	832	GLY	2.7
1	E	818	LYS	2.7
1	G	319	LEU	2.7
1	G	701	LEU	2.7
1	E	146	PRO	2.7
1	D	884	ILE	2.7
1	F	290	ILE	2.7
1	E	751	GLY	2.7
1	F	166	GLY	2.7
1	C	396	THR	2.7
1	E	328	THR	2.7
1	D	269	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	785	ALA	2.7
1	A	94	VAL	2.7
1	E	222	LEU	2.7
1	F	298	VAL	2.7
1	F	446	LEU	2.7
1	F	700	VAL	2.7
1	G	463	LEU	2.7
1	H	46	PRO	2.7
1	H	681	ILE	2.7
1	E	163	MET	2.7
1	H	547	MET	2.7
1	C	172	GLU	2.7
1	F	747	GLY	2.7
1	H	554	THR	2.7
1	E	100	ALA	2.7
1	H	489	ALA	2.7
1	C	349	TYR	2.7
1	C	350	TYR	2.7
1	D	392	LEU	2.7
1	E	60	VAL	2.7
1	E	346	VAL	2.7
1	G	137	VAL	2.7
1	G	232	LEU	2.7
1	H	717	LEU	2.7
1	E	780	PRO	2.6
1	E	842	ILE	2.6
1	G	65	ILE	2.6
1	H	451	PRO	2.6
1	E	462	PHE	2.6
1	E	369	GLY	2.6
1	G	183	GLY	2.6
1	H	134	GLY	2.6
1	E	521	THR	2.6
1	G	245	LEU	2.6
1	H	77	VAL	2.6
1	H	785	ALA	2.6
1	H	831	TYR	2.6
1	E	663	ILE	2.6
1	G	607	ILE	2.6
1	H	81	ILE	2.6
1	F	512	GLU	2.6
1	D	447	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	18	THR	2.6
1	G	621	THR	2.6
1	E	15	LEU	2.6
1	H	444	ALA	2.6
1	H	646	VAL	2.6
1	E	349	TYR	2.6
1	E	683	TYR	2.6
1	D	403	PHE	2.6
1	G	204	PHE	2.6
1	E	676	ASN	2.6
1	E	805	ASN	2.6
1	F	14	GLN	2.6
1	E	139	LEU	2.6
1	E	481	THR	2.6
1	E	520	LEU	2.6
1	H	54	THR	2.6
1	H	294	LEU	2.6
1	E	820	VAL	2.6
1	F	599	VAL	2.6
1	F	726	ALA	2.6
1	H	380	CYS	2.6
1	E	374	ILE	2.6
1	F	34	TYR	2.6
1	D	363	PRO	2.6
1	F	239	PHE	2.6
1	F	814	PHE	2.6
1	G	601	PRO	2.6
1	D	525	ASP	2.6
1	G	496	GLY	2.6
1	C	473	GLU	2.6
1	E	172	GLU	2.6
1	E	684	LEU	2.6
1	F	39	LEU	2.6
1	F	222	LEU	2.6
1	F	379	LEU	2.6
1	G	436	LEU	2.6
1	H	379	LEU	2.6
1	D	402	ALA	2.6
1	F	115	ALA	2.6
1	G	809	ALA	2.6
1	H	521	THR	2.6
1	D	424	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	215	ILE	2.6
1	H	215	ILE	2.6
1	H	275	ILE	2.6
1	G	523	MET	2.6
1	H	320	PRO	2.6
1	G	208	GLY	2.6
1	H	450	GLY	2.6
1	E	696	LEU	2.6
1	F	196	LEU	2.6
1	H	47	LEU	2.6
1	F	724	ALA	2.6
1	H	572	ALA	2.6
1	E	535	ILE	2.5
1	E	695	ILE	2.5
1	F	563	ILE	2.5
1	F	692	ILE	2.5
1	F	827	CYS	2.5
1	F	96	GLN	2.5
1	G	519	GLY	2.5
1	H	70	GLN	2.5
1	E	39	LEU	2.5
1	F	47	LEU	2.5
1	C	503	ASP	2.5
1	C	735	ASP	2.5
1	F	257	VAL	2.5
1	G	718	VAL	2.5
1	A	165	THR	2.5
1	G	685	PHE	2.5
1	E	722	LEU	2.5
1	E	860	LEU	2.5
1	F	728	GLY	2.5
1	G	35	GLY	2.5
1	G	84	LEU	2.5
1	H	586	LEU	2.5
1	F	98	ARG	2.5
1	F	160	ASP	2.5
1	F	805	ASN	2.5
1	G	716	ASN	2.5
1	H	323	GLU	2.5
1	H	558	ALA	2.5
1	E	766	ILE	2.5
1	F	218	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	144	PHE	2.5
1	C	395	PRO	2.5
1	D	352	PRO	2.5
1	H	425	PRO	2.5
1	H	827	CYS	2.5
1	E	869	GLU	2.5
1	F	421	GLU	2.5
1	G	331	ILE	2.5
1	G	748	ILE	2.5
1	F	59	MET	2.5
1	G	754	MET	2.5
1	C	810	PHE	2.5
1	F	815	PHE	2.5
1	E	446	LEU	2.5
1	F	763	LEU	2.5
1	G	104	LEU	2.5
1	G	184	LEU	2.5
1	H	392	LEU	2.5
1	D	393	GLY	2.5
1	E	70	GLN	2.5
1	E	806	VAL	2.5
1	H	599	VAL	2.5
1	E	90	SER	2.5
1	F	650	SER	2.5
1	F	759	SER	2.5
1	H	680	SER	2.5
1	G	758	ILE	2.5
1	D	445	MET	2.5
1	E	878	PHE	2.5
1	E	299	THR	2.5
1	D	469	PRO	2.5
1	G	596	TYR	2.5
1	G	171	VAL	2.5
1	E	494	ALA	2.4
1	F	809	ALA	2.4
1	E	474	ILE	2.4
1	G	297	ILE	2.4
1	H	725	ILE	2.4
1	F	101	GLU	2.4
1	F	853	GLU	2.4
1	G	781	GLU	2.4
1	F	490	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	825	LEU	2.4
1	F	819	TYR	2.4
1	C	519	GLY	2.4
1	F	262	VAL	2.4
1	H	422	GLY	2.4
1	H	449	GLY	2.4
1	A	100	ALA	2.4
1	F	444	ALA	2.4
1	G	847	ALA	2.4
1	F	833	ILE	2.4
1	E	432	LEU	2.4
1	F	107	LEU	2.4
1	F	797	LEU	2.4
1	G	294	LEU	2.4
1	G	836	LEU	2.4
1	E	11	THR	2.4
1	E	57	ASP	2.4
1	E	140	ASP	2.4
1	E	562	ASP	2.4
1	F	353	ASP	2.4
1	F	789	THR	2.4
1	H	97	THR	2.4
1	H	120	ASP	2.4
1	F	352	PRO	2.4
1	E	453	VAL	2.4
1	H	171	VAL	2.4
1	H	206	VAL	2.4
1	E	1	ALA	2.4
1	G	293	ALA	2.4
1	H	92	ILE	2.4
1	H	524	ILE	2.4
1	H	556	ALA	2.4
1	H	318	LYS	2.4
1	D	222	LEU	2.4
1	E	490	LEU	2.4
1	H	139	LEU	2.4
1	H	836	LEU	2.4
1	F	876	ASN	2.4
1	H	306	THR	2.4
1	H	324	THR	2.4
1	C	883	ASP	2.4
1	E	702	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	720	ASP	2.4
1	E	134	GLY	2.4
1	F	194	GLY	2.4
1	D	524	ILE	2.4
1	F	559	ILE	2.4
1	G	456	ALA	2.4
1	G	474	ILE	2.4
1	H	617	ILE	2.4
1	E	454	MET	2.4
1	H	877	LYS	2.4
1	E	800	PHE	2.4
1	H	55	PHE	2.4
1	C	472	GLU	2.4
1	H	68	LEU	2.4
1	A	102	SER	2.4
1	H	434	SER	2.4
1	E	461	VAL	2.4
1	E	874	VAL	2.4
1	F	137	VAL	2.4
1	G	599	VAL	2.4
1	A	882	TYR	2.4
1	D	411	TYR	2.4
1	F	695	ILE	2.4
1	G	541	ALA	2.4
1	G	556	ALA	2.4
1	F	280	MET	2.4
1	G	344	MET	2.4
1	F	800	PHE	2.4
1	E	351	LEU	2.4
1	E	590	LEU	2.4
1	H	84	LEU	2.4
1	H	713	LEU	2.4
1	H	727	LEU	2.4
1	D	103	SER	2.4
1	E	111	SER	2.4
1	A	95	VAL	2.4
1	C	501	PRO	2.4
1	E	458	CYS	2.4
1	E	622	GLY	2.3
1	G	505	THR	2.3
1	G	622	GLY	2.3
1	H	23	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	35	GLY	2.3
1	F	219	ALA	2.3
1	F	767	ALA	2.3
1	G	3	ILE	2.3
1	G	769	ILE	2.3
1	H	652	ALA	2.3
1	H	842	ILE	2.3
1	D	570	ASP	2.3
1	C	351	LEU	2.3
1	E	685	PHE	2.3
1	G	520	LEU	2.3
1	H	573	LEU	2.3
1	E	252	VAL	2.3
1	E	296	SER	2.3
1	G	162	GLY	2.3
1	E	289	ALA	2.3
1	E	724	ALA	2.3
1	G	445	MET	2.3
1	G	705	ASN	2.3
1	D	105	ASP	2.3
1	A	107	LEU	2.3
1	G	578	LEU	2.3
1	G	814	PHE	2.3
1	H	52	LEU	2.3
1	H	131	LEU	2.3
1	F	807	GLN	2.3
1	D	467	GLU	2.3
1	G	182	VAL	2.3
1	H	132	VAL	2.3
1	H	546	VAL	2.3
1	E	113	PRO	2.3
1	E	527	PRO	2.3
1	G	527	PRO	2.3
1	E	758	ILE	2.3
1	F	794	ALA	2.3
1	H	195	SER	2.3
1	H	545	THR	2.3
1	E	271	MET	2.3
1	H	199	TYR	2.3
1	D	381	ASN	2.3
1	F	164	LEU	2.3
1	G	264	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	426	PHE	2.3
1	E	353	ASP	2.3
1	G	427	ASP	2.3
1	E	257	VAL	2.3
1	G	820	VAL	2.3
1	H	347	VAL	2.3
1	E	803	ARG	2.3
1	E	582	PRO	2.3
1	H	290	ILE	2.3
1	H	395	PRO	2.3
1	H	501	PRO	2.3
1	E	580	ALA	2.3
1	F	568	ALA	2.3
1	H	619	ALA	2.3
1	D	268	SER	2.3
1	E	504	THR	2.3
1	F	24	THR	2.3
1	G	295	SER	2.3
1	H	333	THR	2.3
1	E	47	LEU	2.3
1	E	239	PHE	2.3
1	F	192	PHE	2.3
1	G	439	PHE	2.3
1	G	714	PHE	2.3
1	H	192	PHE	2.3
1	B	96	GLN	2.3
1	H	875	GLN	2.3
1	E	241	LYS	2.3
1	E	679	LYS	2.3
1	D	453	VAL	2.3
1	F	76	VAL	2.3
1	G	625	VAL	2.3
1	D	501	PRO	2.3
1	H	692	ILE	2.3
1	E	765	GLY	2.3
1	F	597	ALA	2.3
1	G	190	MET	2.3
1	G	533	ALA	2.3
1	F	392	LEU	2.3
1	G	107	LEU	2.3
1	G	263	LEU	2.3
1	G	834	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	359	PHE	2.3
1	F	843	PHE	2.3
1	G	56	LYS	2.3
1	F	865	VAL	2.3
1	G	873	VAL	2.3
1	E	734	PRO	2.2
1	F	179	PRO	2.2
1	F	566	MET	2.2
1	F	619	ALA	2.2
1	G	260	GLY	2.2
1	D	400	LEU	2.2
1	E	478	LEU	2.2
1	E	509	LEU	2.2
1	E	586	LEU	2.2
1	F	250	LEU	2.2
1	H	248	LEU	2.2
1	C	438	THR	2.2
1	E	355	THR	2.2
1	G	338	THR	2.2
1	D	534	SER	2.2
1	F	195	SER	2.2
1	F	211	SER	2.2
1	H	25	SER	2.2
1	E	531	VAL	2.2
1	G	301	VAL	2.2
1	H	595	VAL	2.2
1	B	101	GLU	2.2
1	F	78	GLU	2.2
1	F	258	GLU	2.2
1	H	623	ASP	2.2
1	E	871	ILE	2.2
1	F	543	ILE	2.2
1	F	677	ILE	2.2
1	C	104	LEU	2.2
1	D	522	ALA	2.2
1	E	196	LEU	2.2
1	E	541	ALA	2.2
1	F	100	ALA	2.2
1	G	422	GLY	2.2
1	H	245	LEU	2.2
1	H	622	GLY	2.2
1	H	838	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	279	PHE	2.2
1	G	796	THR	2.2
1	H	99	LYS	2.2
1	D	349	TYR	2.2
1	E	327	SER	2.2
1	E	329	SER	2.2
1	G	721	SER	2.2
1	E	646	VAL	2.2
1	C	381	ASN	2.2
1	H	307	ASN	2.2
1	E	3	ILE	2.2
1	E	109	GLU	2.2
1	G	258	GLU	2.2
1	H	607	ILE	2.2
1	A	46	PRO	2.2
1	E	250	LEU	2.2
1	E	489	ALA	2.2
1	E	797	LEU	2.2
1	E	836	LEU	2.2
1	F	71	LEU	2.2
1	H	151	LEU	2.2
1	G	123	LYS	2.2
1	E	435	THR	2.2
1	F	77	VAL	2.2
1	B	102	SER	2.2
1	H	428	SER	2.2
1	E	82	ILE	2.2
1	E	559	ILE	2.2
1	G	82	ILE	2.2
1	G	704	ILE	2.2
1	F	712	LEU	2.2
1	F	860	LEU	2.2
1	G	214	GLU	2.2
1	H	78	GLU	2.2
1	H	309	MET	2.2
1	H	620	MET	2.2
1	G	266	ASP	2.2
1	G	627	ASP	2.2
1	G	462	PHE	2.2
1	G	878	PHE	2.2
1	D	396	THR	2.2
1	F	273	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	618	THR	2.2
1	E	243	LEU	2.2
1	E	319	LEU	2.2
1	E	862	LEU	2.2
1	G	379	LEU	2.2
1	G	712	LEU	2.2
1	F	867	MET	2.2
1	G	577	GLU	2.2
1	G	583	GLU	2.2
1	G	526	PRO	2.2
1	G	604	LYS	2.2
1	G	619	ALA	2.2
1	H	781	GLU	2.2
1	D	448	LYS	2.2
1	F	152	PHE	2.2
1	H	452	ASP	2.2
1	H	665	ASP	2.2
1	H	810	PHE	2.2
1	H	592	HIS	2.2
1	D	471	THR	2.1
1	E	762	VAL	2.1
1	F	72	VAL	2.1
1	F	136	VAL	2.1
1	F	355	THR	2.1
1	D	495	TYR	2.1
1	F	350	TYR	2.1
1	F	683	TYR	2.1
1	G	636	ILE	2.1
1	G	821	ILE	2.1
1	F	264	LEU	2.1
1	F	578	LEU	2.1
1	E	59	MET	2.1
1	F	547	MET	2.1
1	E	147	ALA	2.1
1	E	652	ALA	2.1
1	G	8	ALA	2.1
1	H	103	SER	2.1
1	G	352	PRO	2.1
1	H	668	GLY	2.1
1	C	439	PHE	2.1
1	E	279	PHE	2.1
1	G	382	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	145	VAL	2.1
1	F	820	VAL	2.1
1	F	854	TRP	2.1
1	G	608	VAL	2.1
1	E	218	ILE	2.1
1	H	87	ILE	2.1
1	D	432	LEU	2.1
1	H	319	LEU	2.1
1	F	70	GLN	2.1
1	F	620	MET	2.1
1	G	141	ALA	2.1
1	A	167	GLU	2.1
1	F	79	SER	2.1
1	F	111	SER	2.1
1	E	705	ASN	2.1
1	F	403	PHE	2.1
1	F	660	PHE	2.1
1	H	788	PHE	2.1
1	E	348	ASP	2.1
1	E	514	ASP	2.1
1	F	283	VAL	2.1
1	F	736	VAL	2.1
1	C	507	LEU	2.1
1	E	199	TYR	2.1
1	E	596	TYR	2.1
1	E	712	LEU	2.1
1	E	763	LEU	2.1
1	F	253	LEU	2.1
1	F	769	ILE	2.1
1	F	871	ILE	2.1
1	H	11	THR	2.1
1	H	443	LYS	2.1
1	H	644	THR	2.1
1	H	708	THR	2.1
1	H	792	ILE	2.1
1	H	871	ILE	2.1
1	B	568	ALA	2.1
1	F	249	ALA	2.1
1	H	100	ALA	2.1
1	H	823	ALA	2.1
1	A	781	GLU	2.1
1	G	74	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	154	SER	2.1
1	D	518	VAL	2.1
1	E	829	VAL	2.1
1	F	301	VAL	2.1
1	F	835	VAL	2.1
1	F	382	ASP	2.1
1	G	356	LYS	2.1
1	G	431	LYS	2.1
1	G	196	LEU	2.1
1	G	215	ILE	2.1
1	G	376	ILE	2.1
1	G	424	ILE	2.1
1	G	543	ILE	2.1
1	H	552	HIS	2.1
1	B	471	THR	2.1
1	F	544	ARG	2.1
1	F	554	THR	2.1
1	F	831	TYR	2.1
1	H	299	THR	2.1
1	D	568	ALA	2.1
1	E	756	ALA	2.1
1	G	286	ALA	2.1
1	H	512	GLU	2.1
1	H	879	PHE	2.1
1	F	721	SER	2.1
1	H	329	SER	2.1
1	E	205	VAL	2.1
1	D	267	ASN	2.1
1	E	290	ILE	2.1
1	E	297	ILE	2.1
1	E	376	ILE	2.1
1	E	375	HIS	2.1
1	E	491	ARG	2.1
1	G	81	ILE	2.1
1	G	695	ILE	2.1
1	H	222	LEU	2.1
1	E	587	ASP	2.1
1	H	224	THR	2.1
1	E	278	ALA	2.1
1	F	639	ALA	2.1
1	H	666	ALA	2.1
1	H	694	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	813	GLY	2.1
1	G	747	GLY	2.1
1	E	38	GLU	2.1
1	E	395	PRO	2.1
1	E	455	PHE	2.1
1	E	512	GLU	2.1
1	F	462	PHE	2.1
1	G	585	GLU	2.1
1	H	144	PHE	2.1
1	E	62	VAL	2.0
1	G	76	VAL	2.0
1	H	625	VAL	2.0
1	H	664	VAL	2.0
1	H	806	VAL	2.0
1	G	862	LEU	2.0
1	H	758	ILE	2.0
1	C	266	ASP	2.0
1	D	1	ALA	2.0
1	F	328	THR	2.0
1	F	735	ASP	2.0
1	H	555	THR	2.0
1	H	809	ALA	2.0
1	A	96	GLN	2.0
1	D	12	PHE	2.0
1	E	194	GLY	2.0
1	E	670	GLY	2.0
1	G	641	GLY	2.0
1	E	601	PRO	2.0
1	F	46	PRO	2.0
1	E	69	VAL	2.0
1	E	95	VAL	2.0
1	F	198	VAL	2.0
1	D	446	LEU	2.0
1	E	50	LEU	2.0
1	E	68	LEU	2.0
1	E	302	LEU	2.0
1	E	578	LEU	2.0
1	H	263	LEU	2.0
1	H	446	LEU	2.0
1	H	851	LEU	2.0
1	D	474	ILE	2.0
1	E	759	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	774	ILE	2.0
1	G	102	SER	2.0
1	G	650	SER	2.0
1	G	744	ILE	2.0
1	G	626	ASN	2.0
1	H	566	MET	2.0
1	B	886	THR	2.0
1	C	402	ALA	2.0
1	C	476	ALA	2.0
1	E	350	TYR	2.0
1	E	808	THR	2.0
1	F	522	ALA	2.0
1	F	864	ALA	2.0
1	G	545	THR	2.0
1	G	823	ALA	2.0
1	H	495	TYR	2.0
1	F	449	GLY	2.0
1	G	46	PRO	2.0
1	H	29	LYS	2.0
1	D	492	VAL	2.0
1	G	62	VAL	2.0
1	G	531	VAL	2.0
1	C	400	LEU	2.0
1	D	463	LEU	2.0
1	E	236	LEU	2.0
1	F	701	LEU	2.0
1	F	717	LEU	2.0
1	H	490	LEU	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

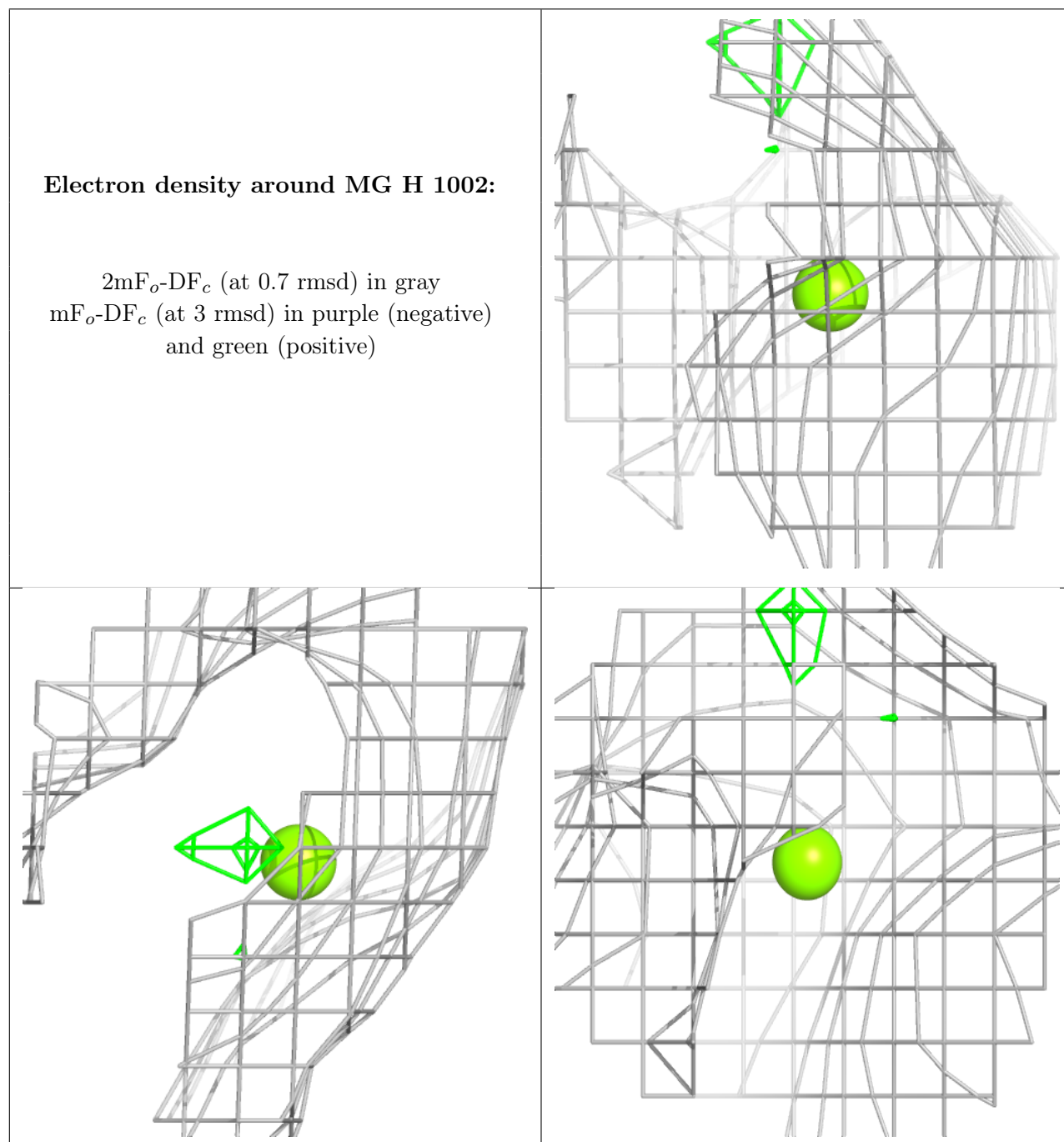
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MG	H	1002	1/1	0.56	0.16	225,225,225,225	0
2	BEF	G	1001	4/4	0.67	0.17	198,200,202,203	0
2	BEF	F	1001	4/4	0.67	0.16	206,207,209,213	0
2	BEF	H	1001	4/4	0.71	0.15	228,228,229,232	0
4	PCW	B	1008	54/54	0.74	0.18	48,72,103,130	0
4	PCW	B	1006	54/54	0.75	0.20	48,78,119,132	0
3	MG	G	1002	1/1	0.75	0.14	213,213,213,213	0
4	PCW	C	1006	54/54	0.79	0.16	31,82,108,121	0
4	PCW	B	1007	54/54	0.80	0.17	38,70,111,132	0
2	BEF	E	1001	4/4	0.81	0.12	224,224,225,227	0
4	PCW	B	1004	54/54	0.81	0.17	52,87,129,138	0
4	PCW	A	1004	54/54	0.82	0.17	40,77,124,128	0
4	PCW	C	1004	54/54	0.82	0.18	28,80,119,130	0
4	PCW	C	1005	54/54	0.82	0.15	26,67,108,120	0
3	MG	F	1002	1/1	0.82	0.10	182,182,182,182	0
5	CE1	C	1007	15/37	0.83	0.12	21,37,49,50	0
5	CE1	D	1009	12/37	0.84	0.16	49,54,73,77	0
4	PCW	C	1008	54/54	0.85	0.18	15,71,117,129	0
5	CE1	D	1006	12/37	0.85	0.19	48,61,76,81	0
4	PCW	D	1003	54/54	0.85	0.15	25,70,100,109	0
4	PCW	C	1003	54/54	0.86	0.16	19,82,111,128	0
5	CE1	D	1008	11/37	0.87	0.13	23,41,49,52	0
3	MG	E	1002	1/1	0.88	0.12	218,218,218,218	0
4	PCW	B	1003	54/54	0.88	0.14	17,67,82,100	0
5	CE1	D	1005	12/37	0.89	0.14	26,46,60,65	0
5	CE1	D	1004	12/37	0.89	0.10	19,33,37,44	0
4	PCW	B	1005	54/54	0.90	0.21	78,98,128,137	0
2	BEF	C	1001	4/4	0.90	0.12	84,84,86,86	0
2	BEF	D	1001	4/4	0.90	0.10	70,71,75,87	0
4	PCW	A	1003	54/54	0.90	0.19	53,93,127,137	0
4	PCW	B	1009	54/54	0.91	0.13	25,56,104,111	0
2	BEF	B	1001	4/4	0.93	0.12	47,48,48,57	0
2	BEF	A	1001	4/4	0.94	0.07	46,46,46,63	0
5	CE1	D	1007	12/37	0.96	0.07	12,17,36,44	0
3	MG	C	1002	1/1	0.98	0.04	64,64,64,64	0
3	MG	D	1002	1/1	0.99	0.06	53,53,53,53	0
3	MG	A	1002	1/1	1.00	0.01	44,44,44,44	0
3	MG	B	1002	1/1	1.00	0.04	44,44,44,44	0

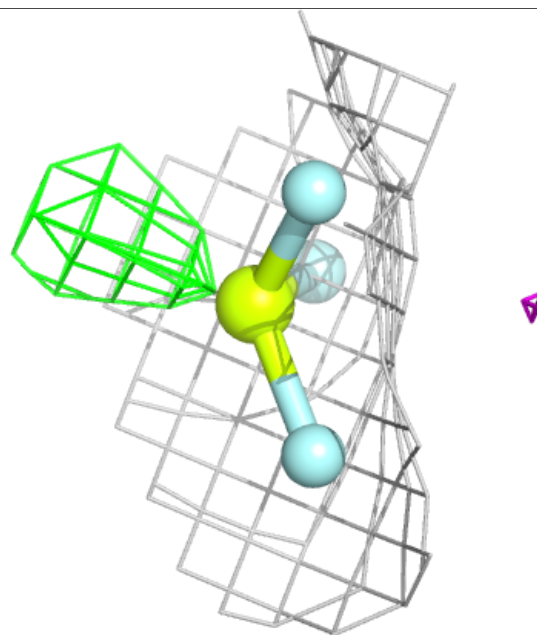
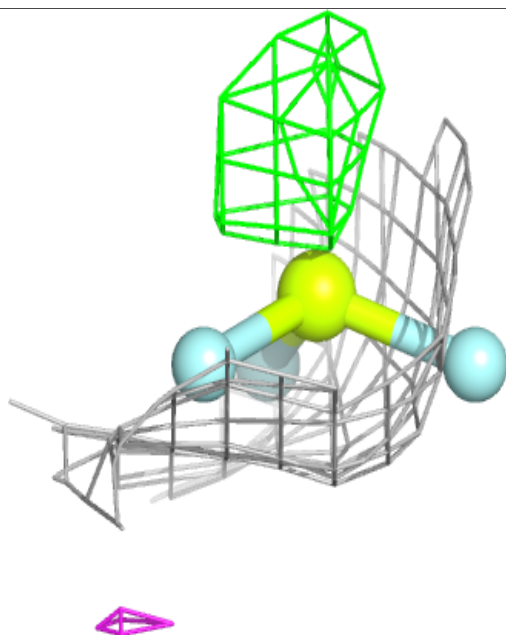
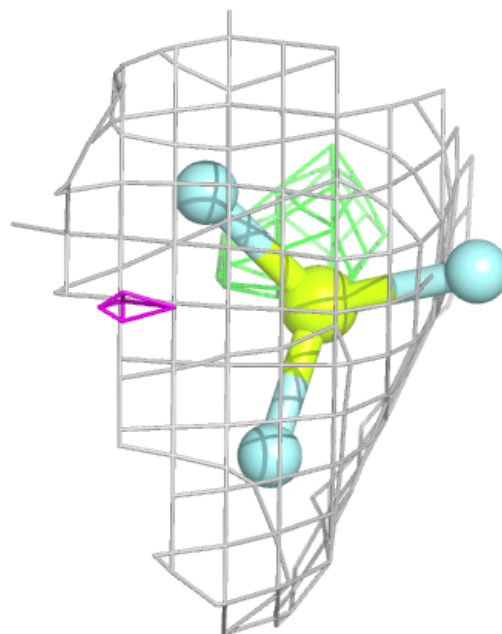
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



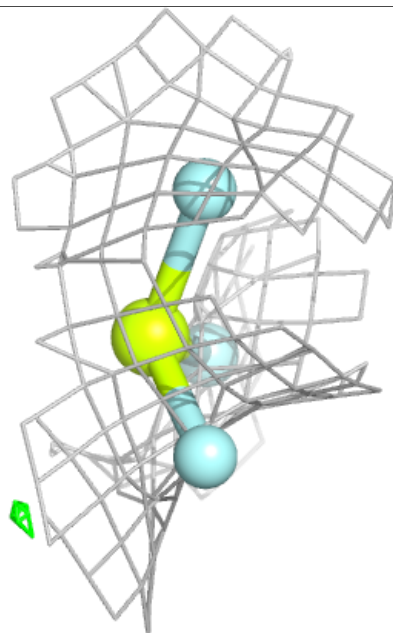
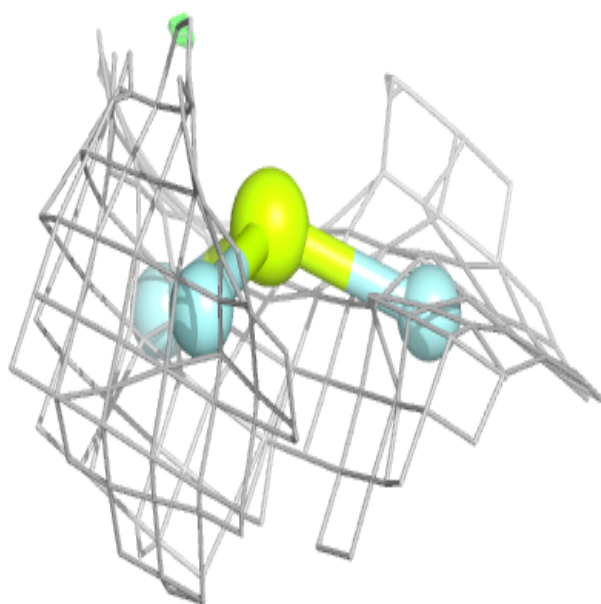
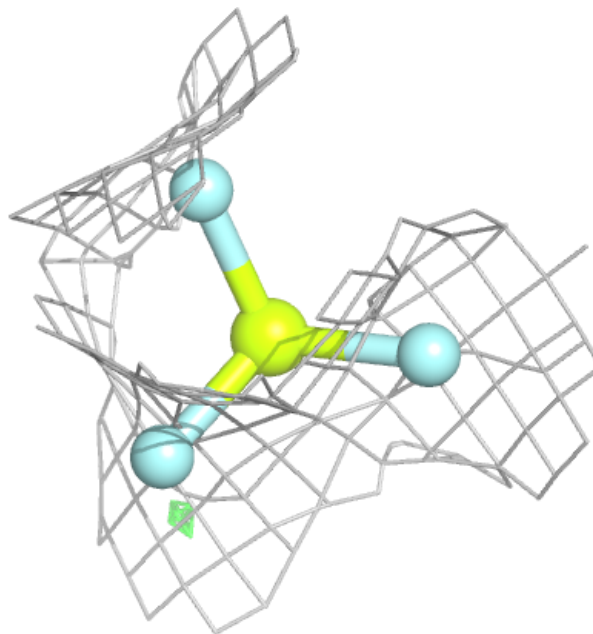
Electron density around BEF G 1001:

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



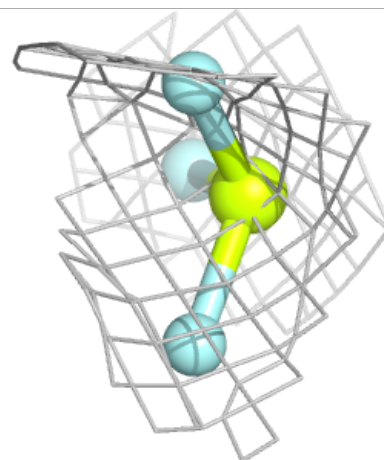
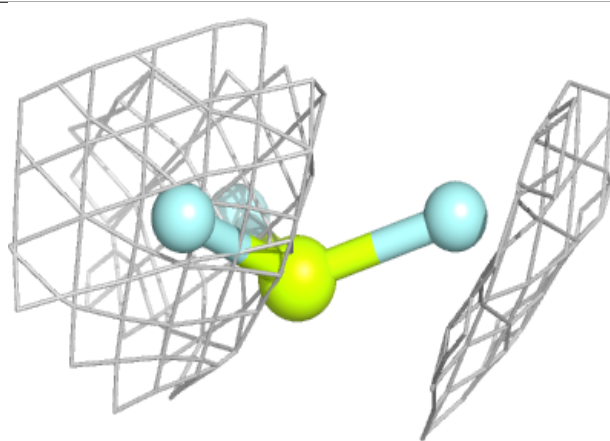
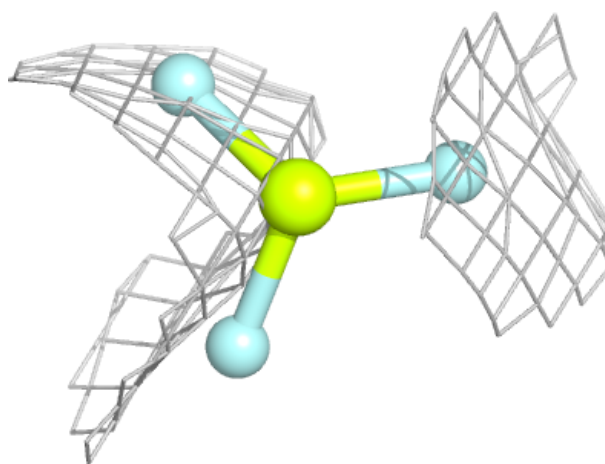
Electron density around BEF F 1001:

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



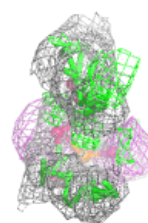
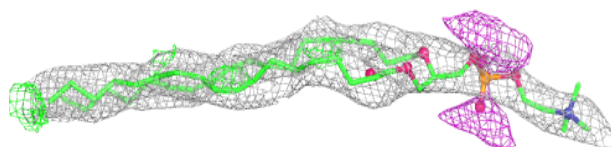
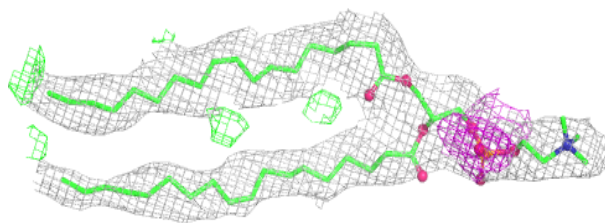
Electron density around BEF H 1001:

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

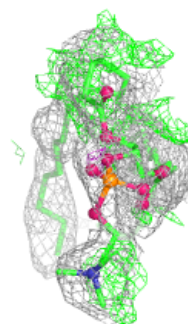
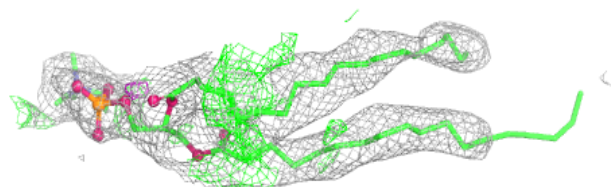
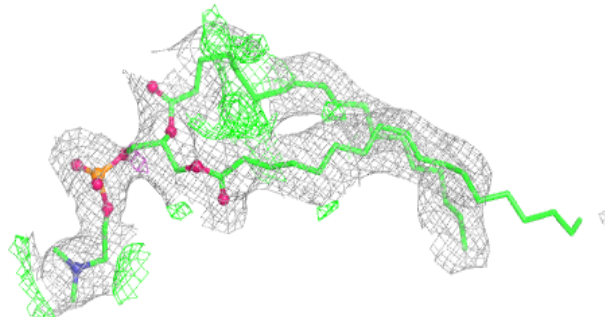


Electron density around PCW B 1008:

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

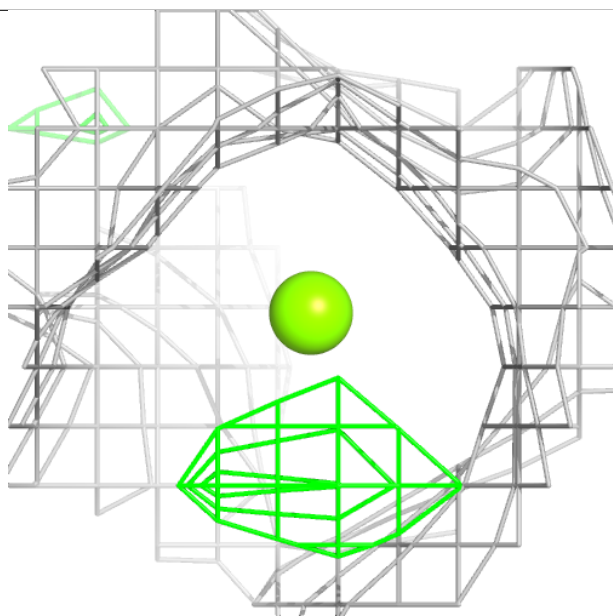
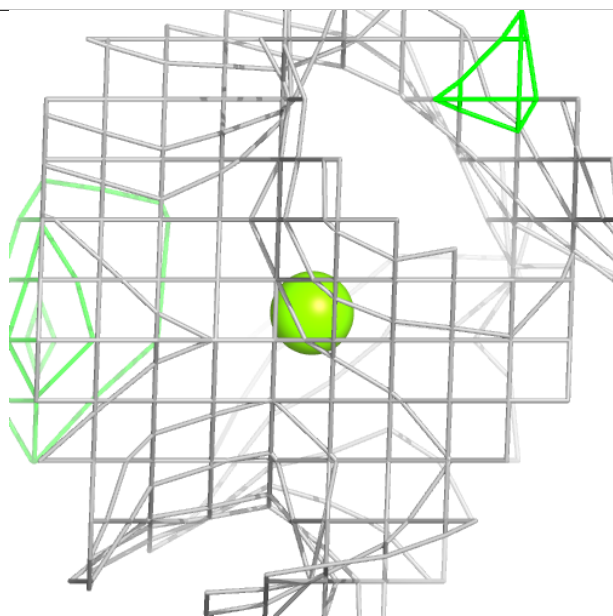
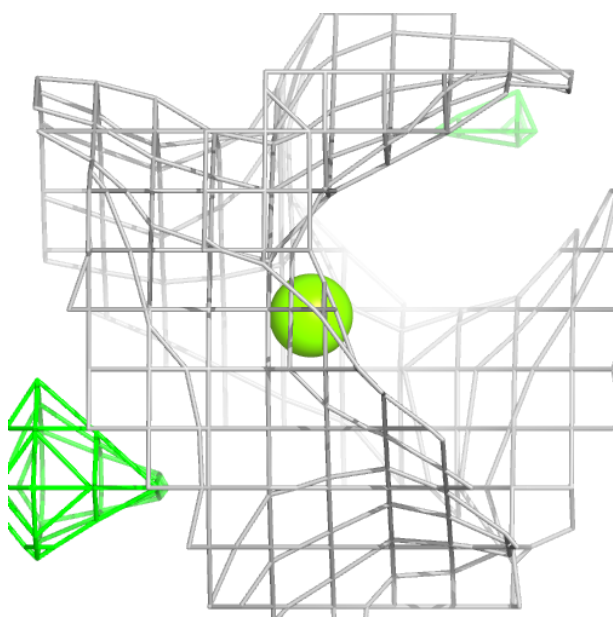
**Electron density around PCW B 1006:**

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



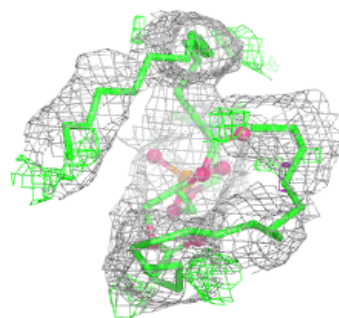
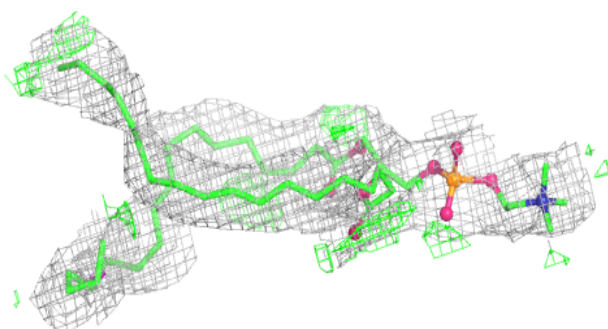
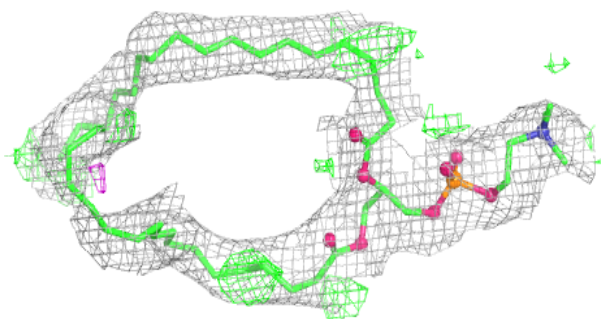
Electron density around MG G 1002:

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

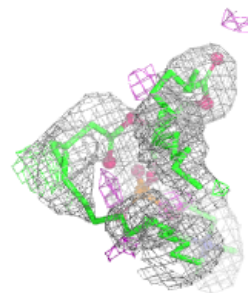
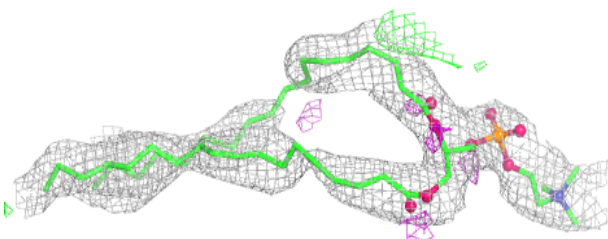
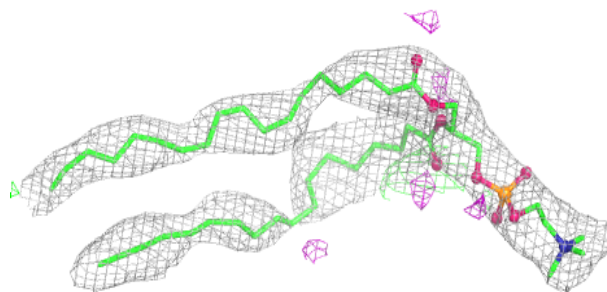


Electron density around PCW C 1006:

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

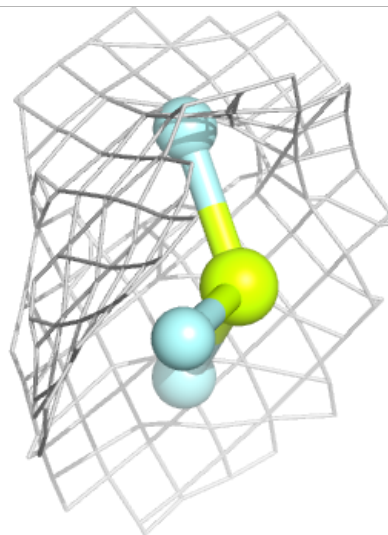
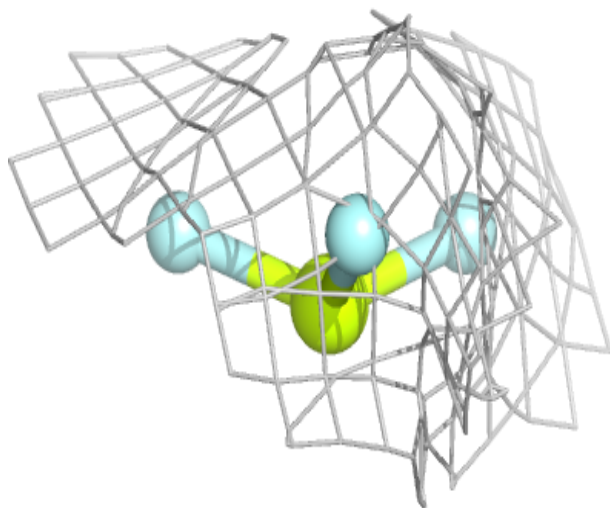
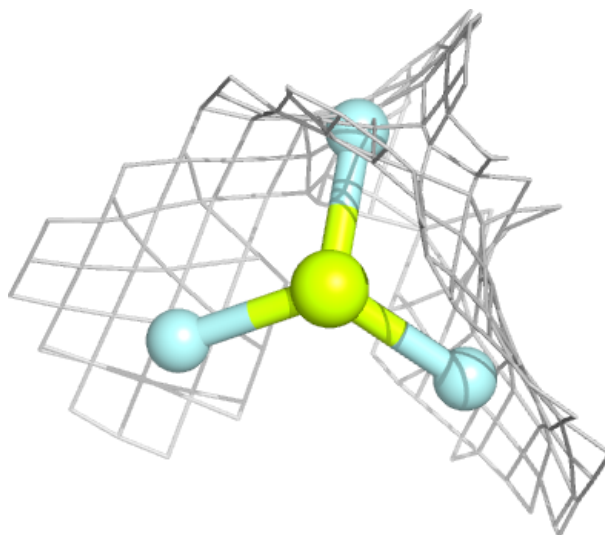
**Electron density around PCW B 1007:**

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



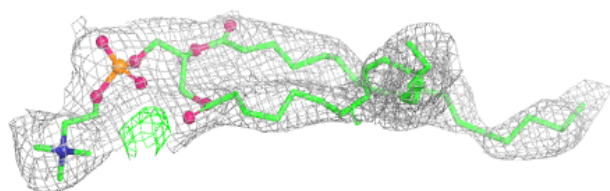
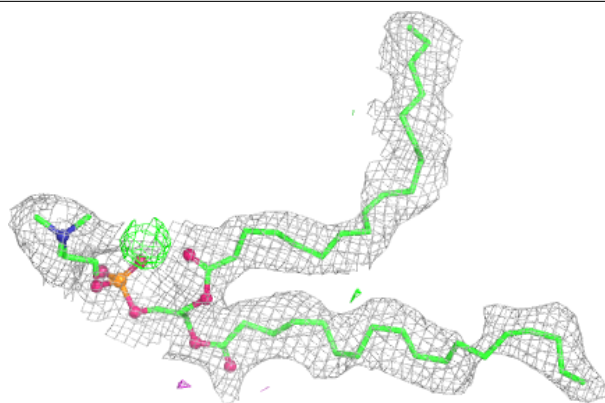
Electron density around BEF E 1001:

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

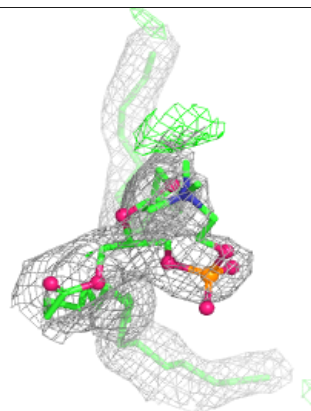
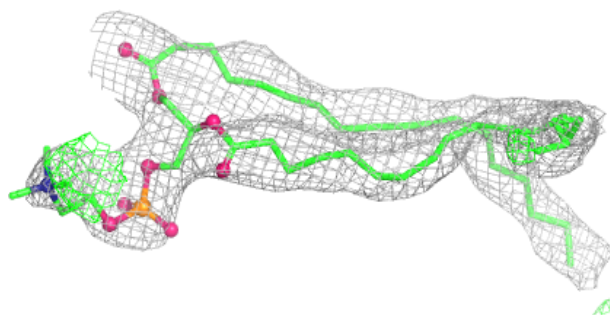
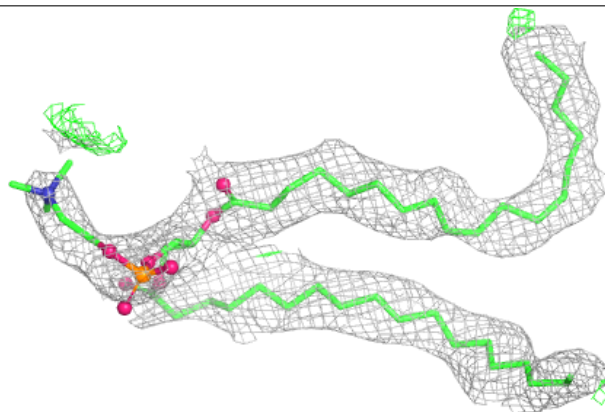


Electron density around PCW B 1004:

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and green (positive)

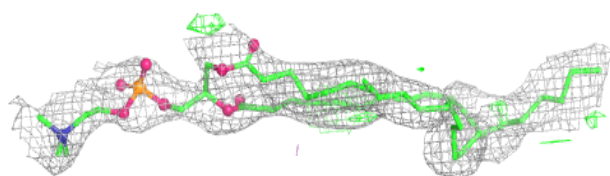
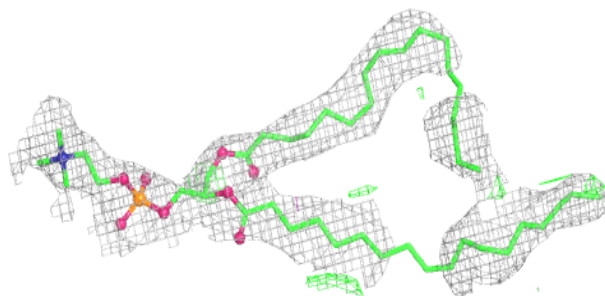
**Electron density around PCW A 1004:**

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and green (positive)

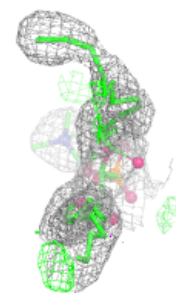
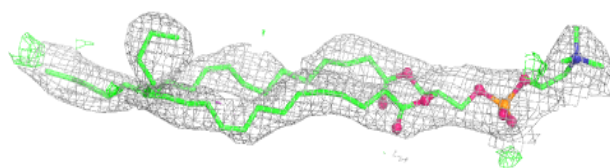
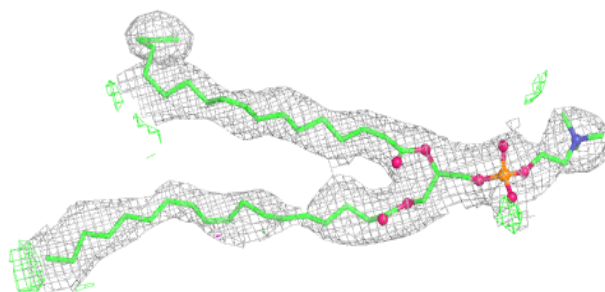


Electron density around PCW C 1004:

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

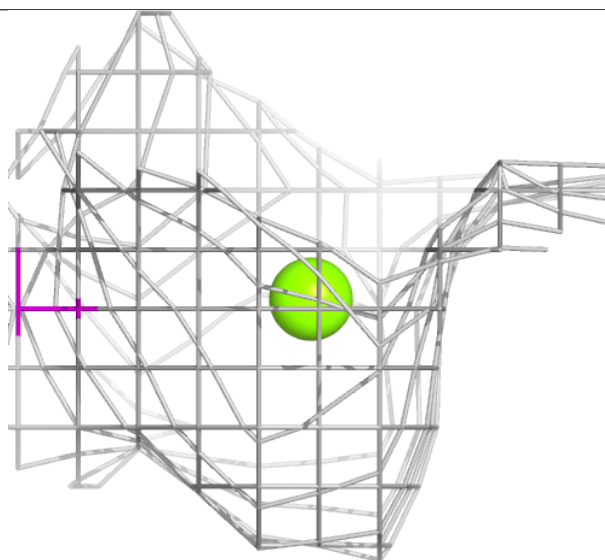
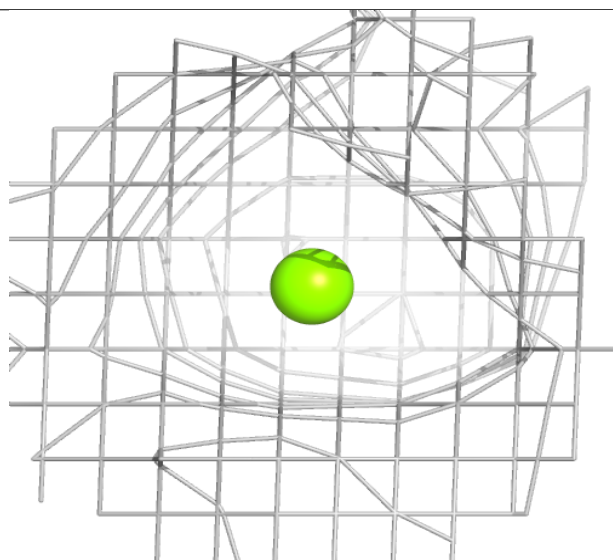
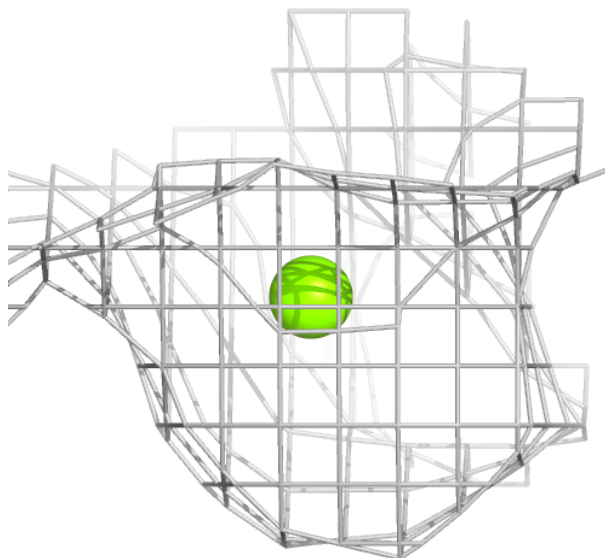
**Electron density around PCW C 1005:**

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



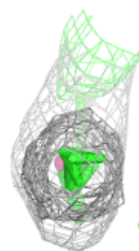
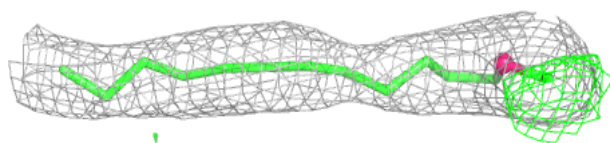
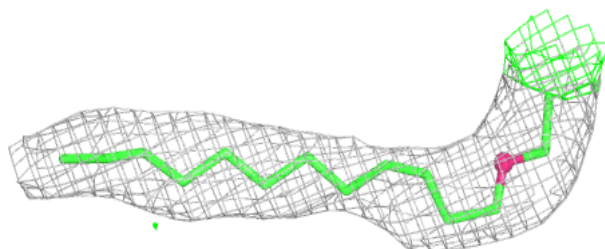
Electron density around MG F 1002:

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

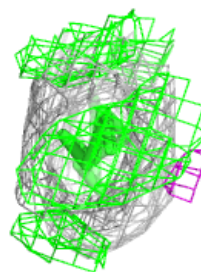
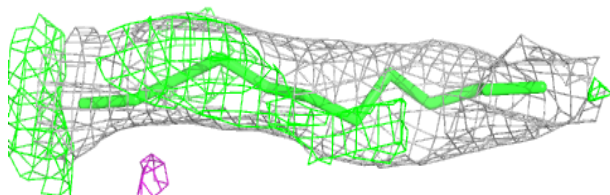
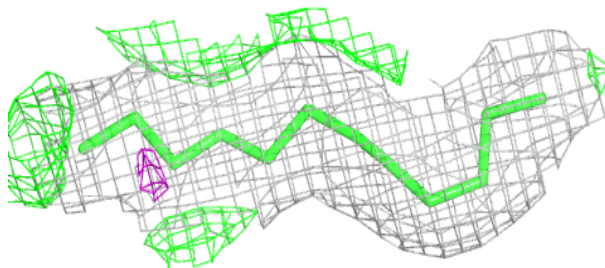


Electron density around CE1 C 1007:

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

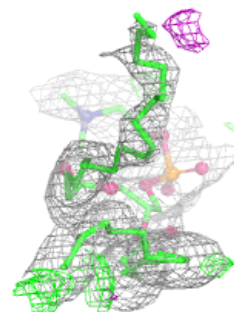
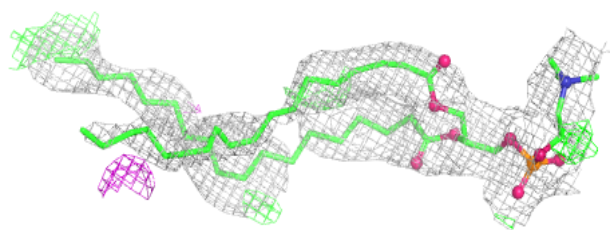
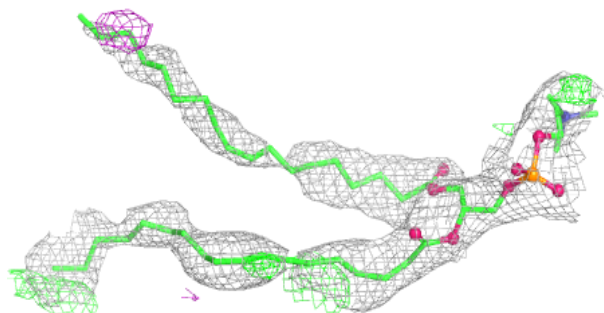
**Electron density around CE1 D 1009:**

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

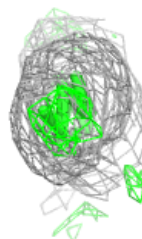
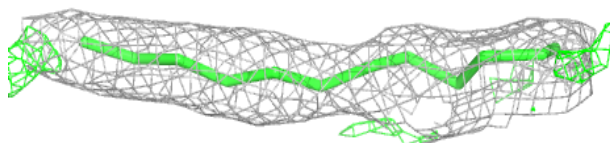
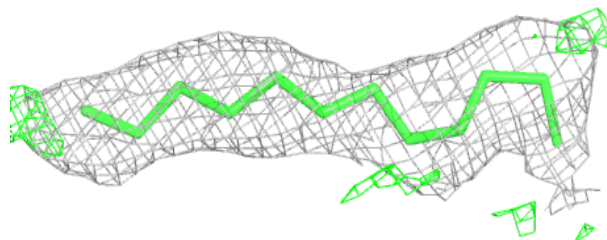


Electron density around PCW C 1008:

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

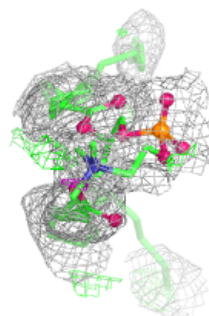
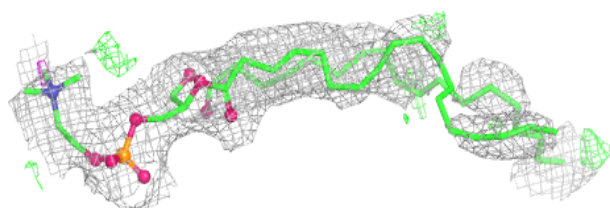
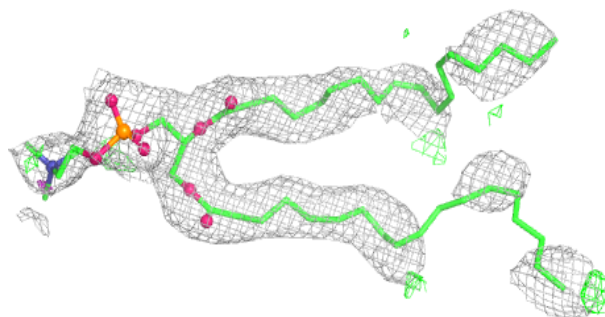
**Electron density around CE1 D 1006:**

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

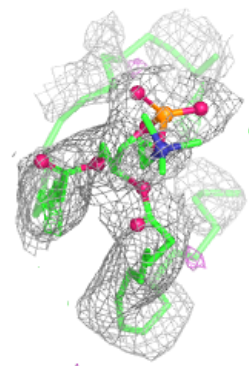
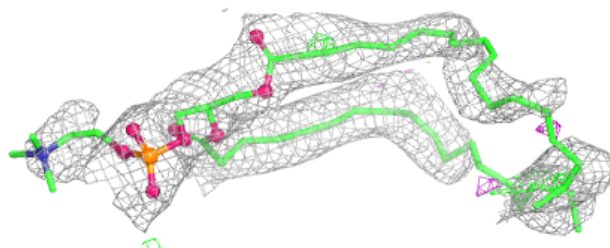
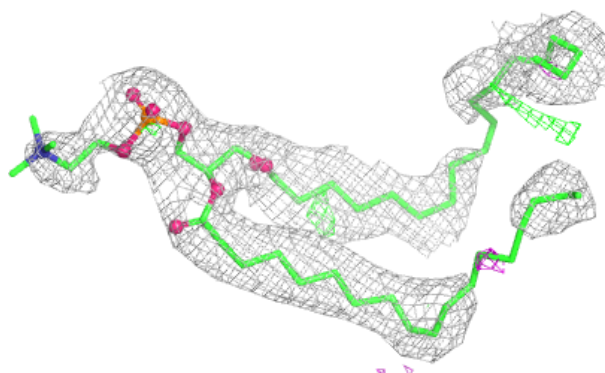


Electron density around PCW D 1003:

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

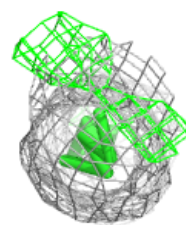
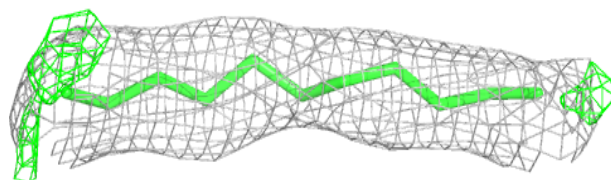
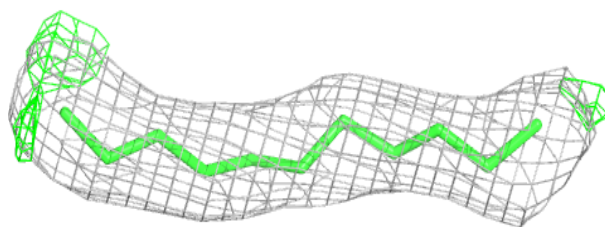
**Electron density around PCW C 1003:**

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



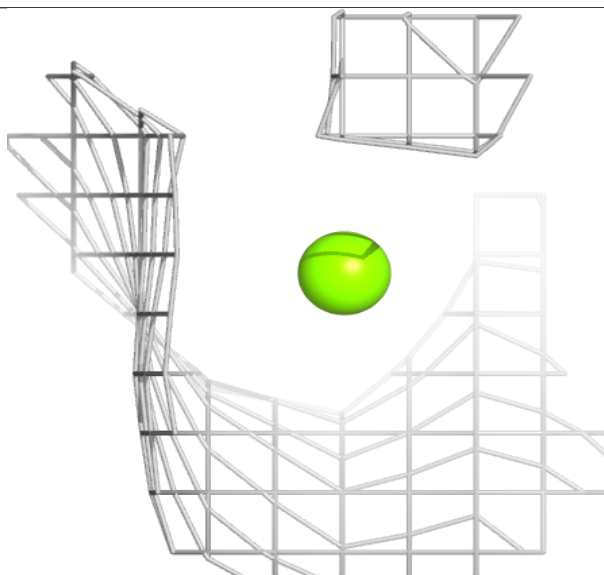
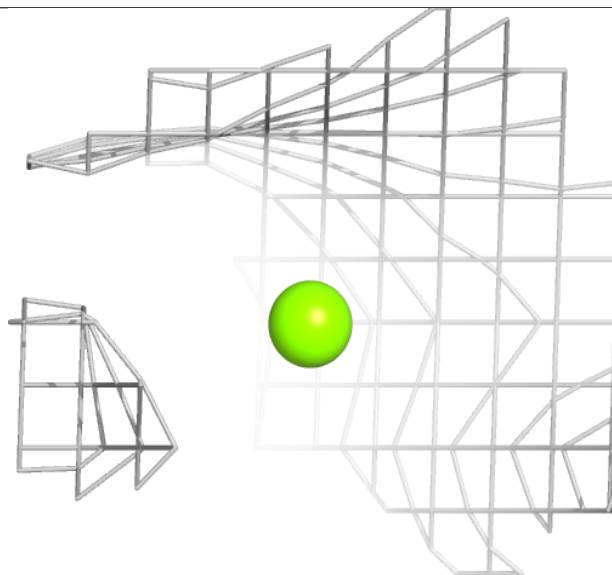
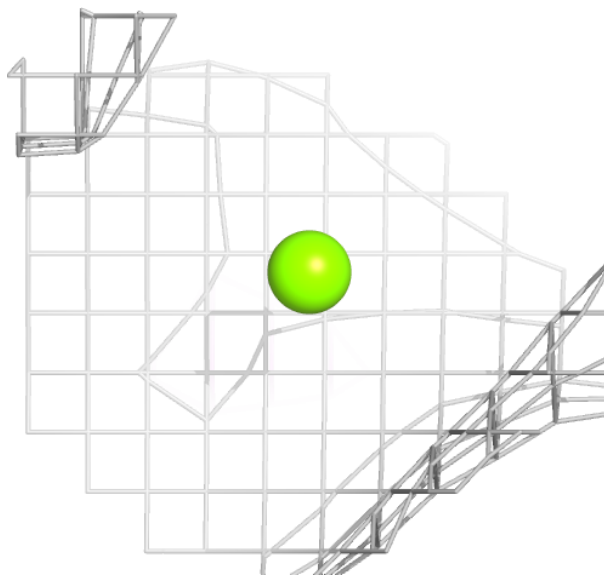
Electron density around CE1 D 1008:

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



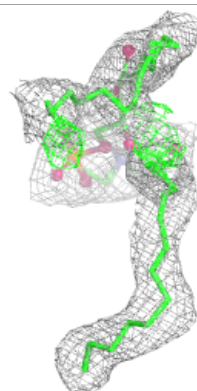
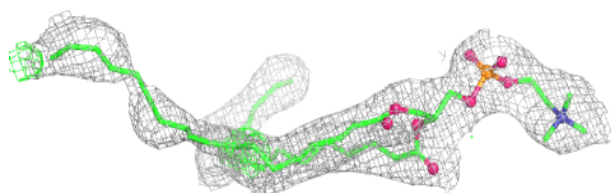
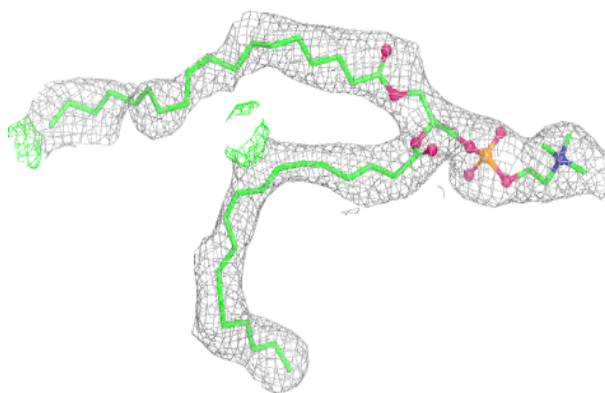
Electron density around MG E 1002:

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

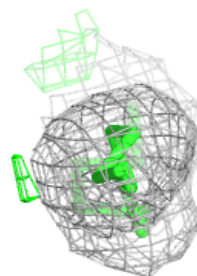
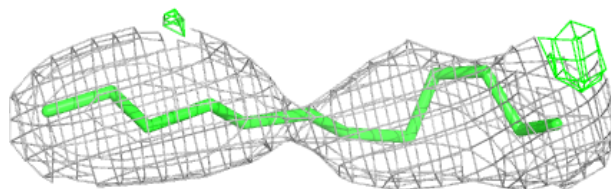
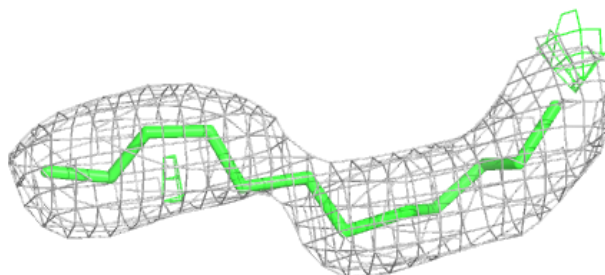


Electron density around PCW B 1003:

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

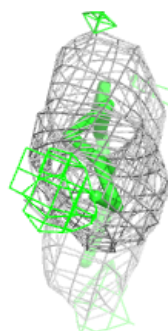
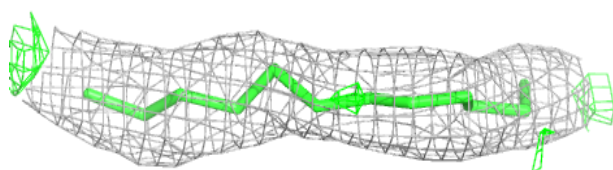
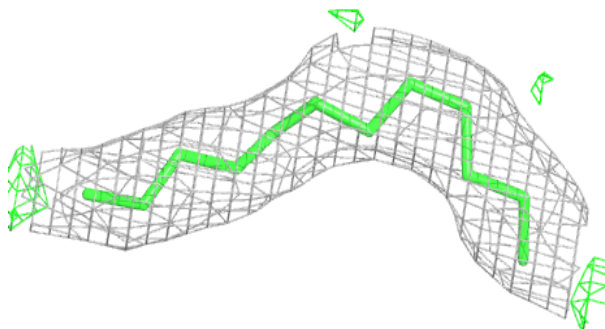
**Electron density around CE1 D 1005:**

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

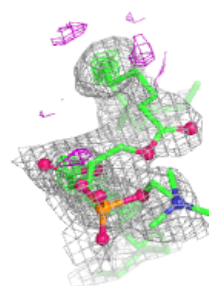
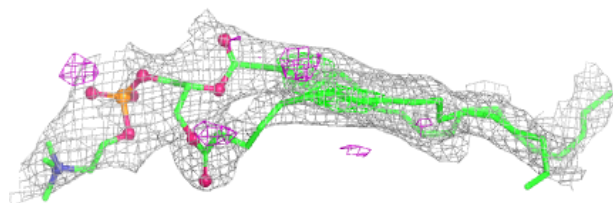
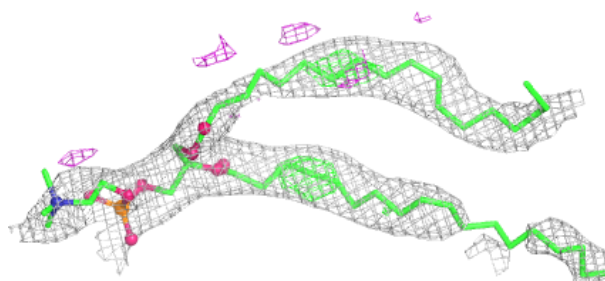


Electron density around CE1 D 1004:

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

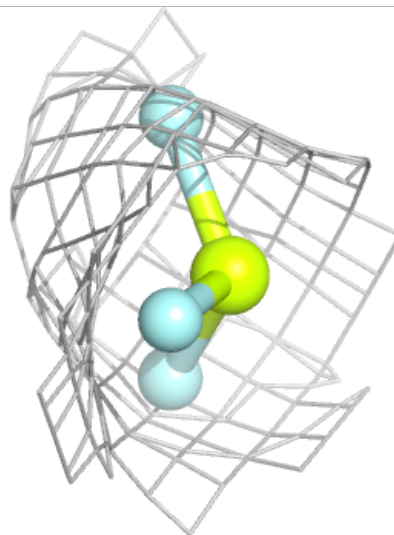
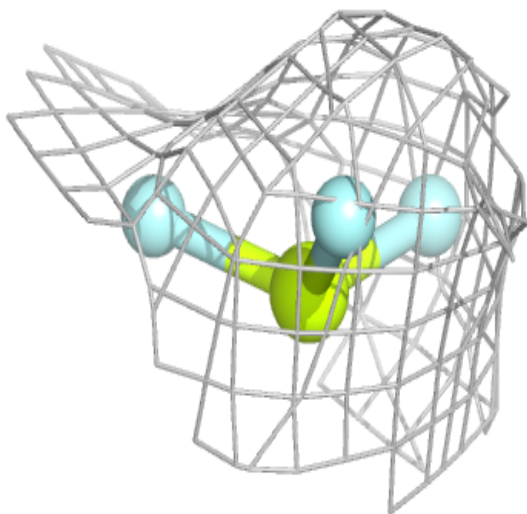
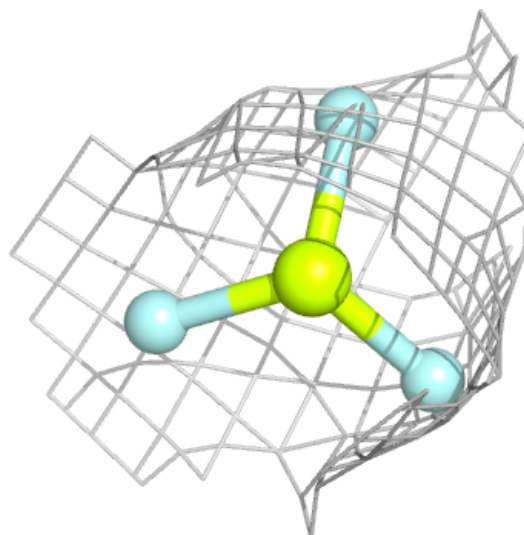
**Electron density around PCW B 1005:**

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



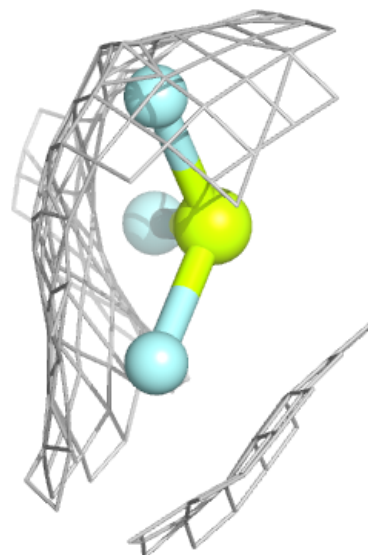
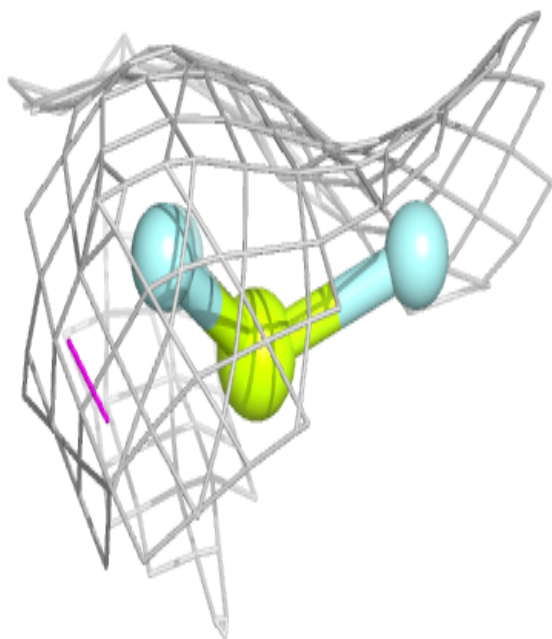
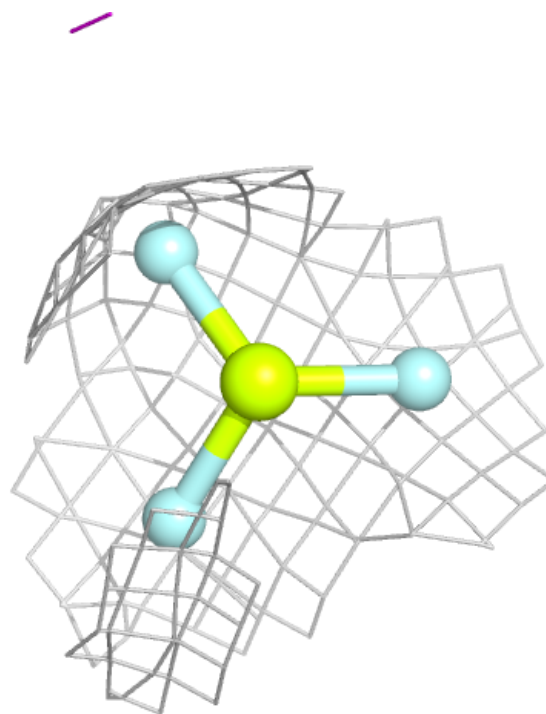
Electron density around BEF C 1001:

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



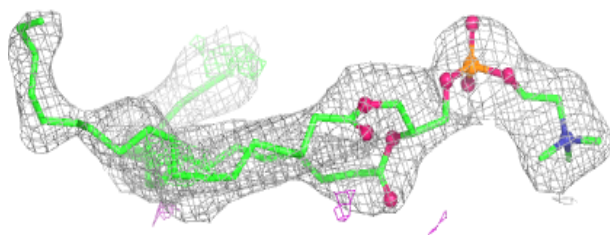
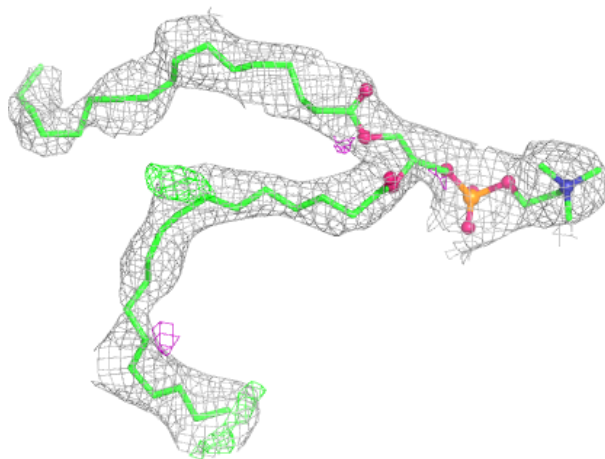
Electron density around BEF D 1001:

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



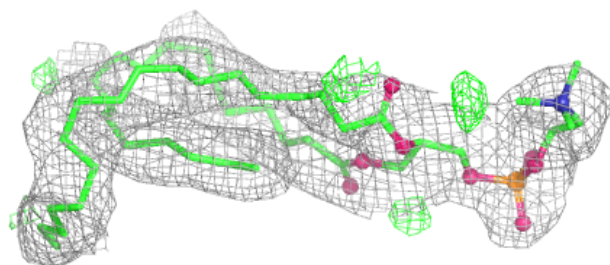
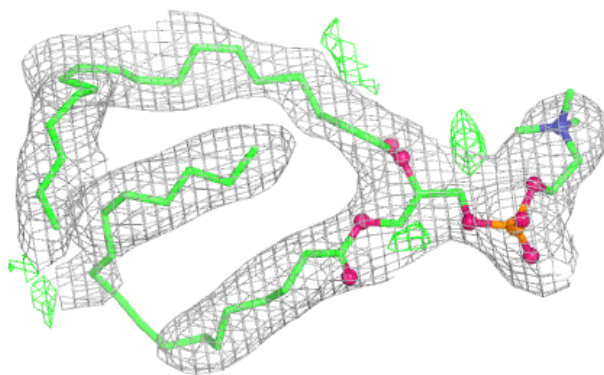
Electron density around PCW A 1003:

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



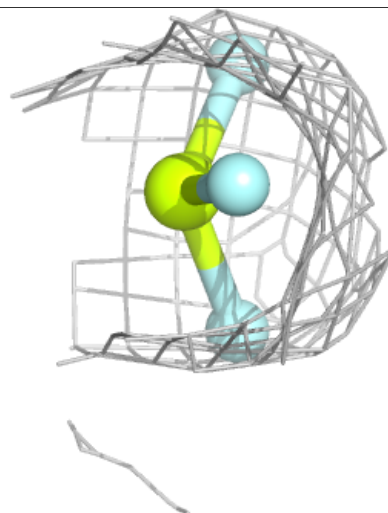
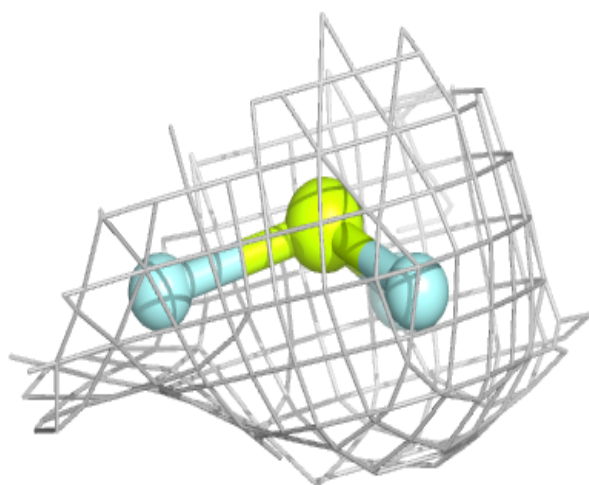
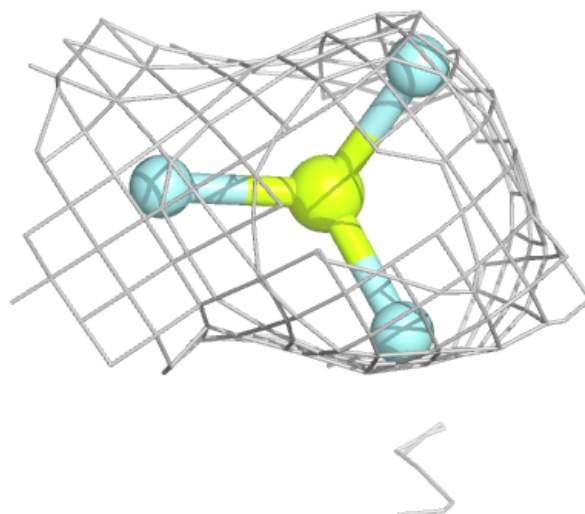
Electron density around PCW B 1009:

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



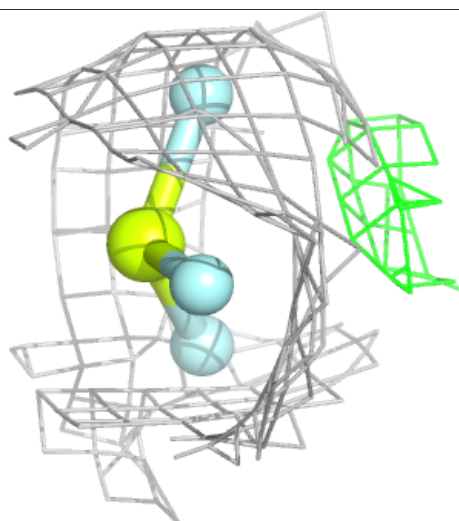
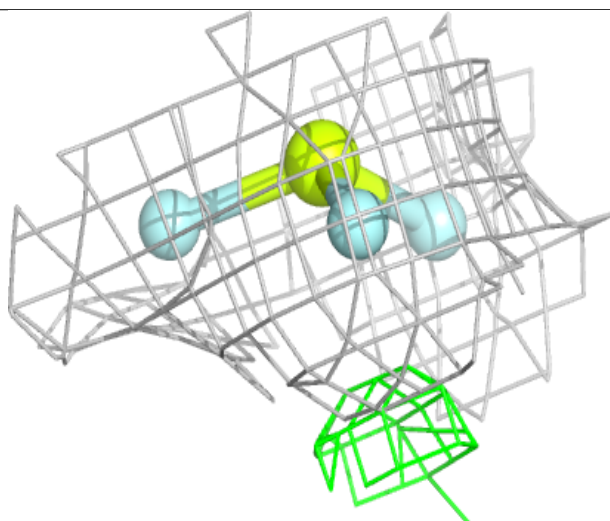
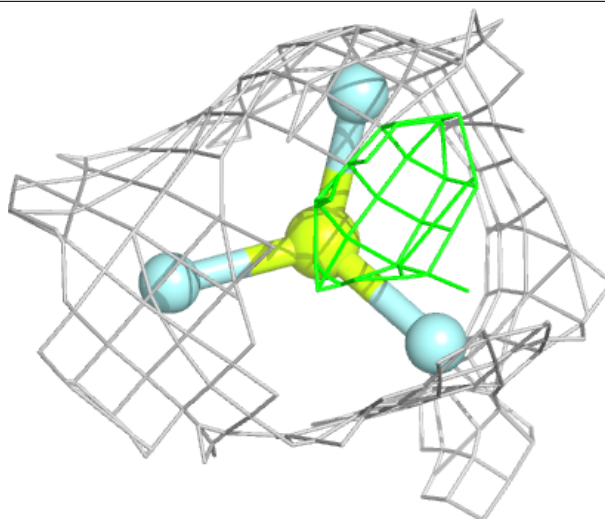
Electron density around BEF B 1001:

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



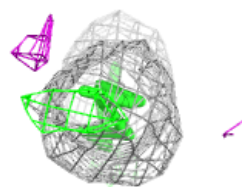
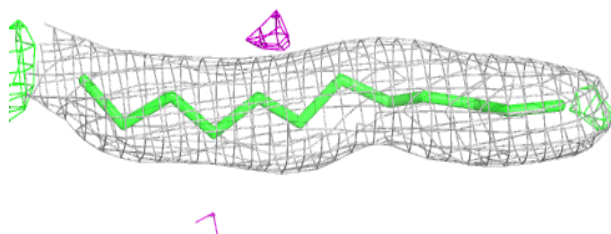
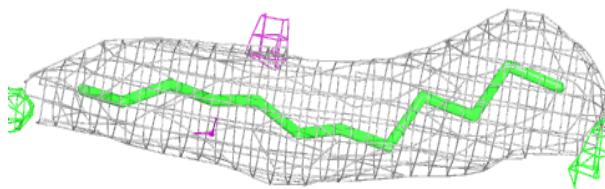
Electron density around BEF A 1001:

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



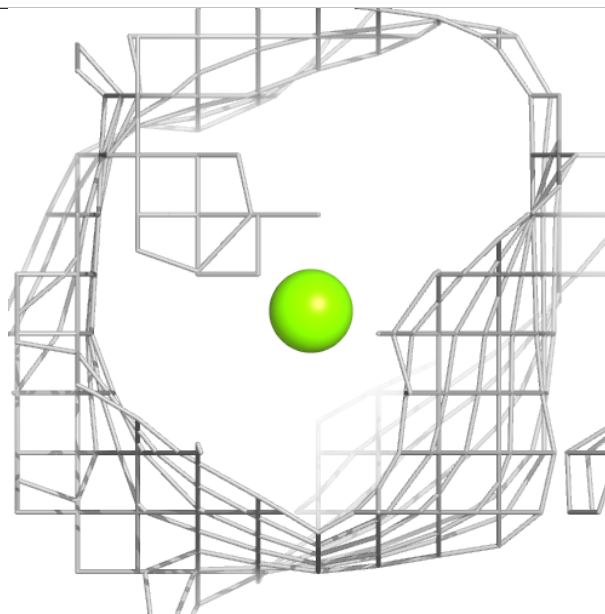
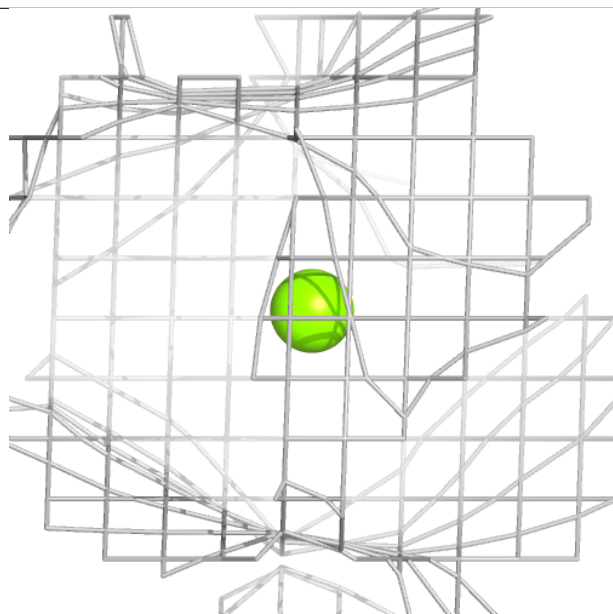
Electron density around CE1 D 1007:

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



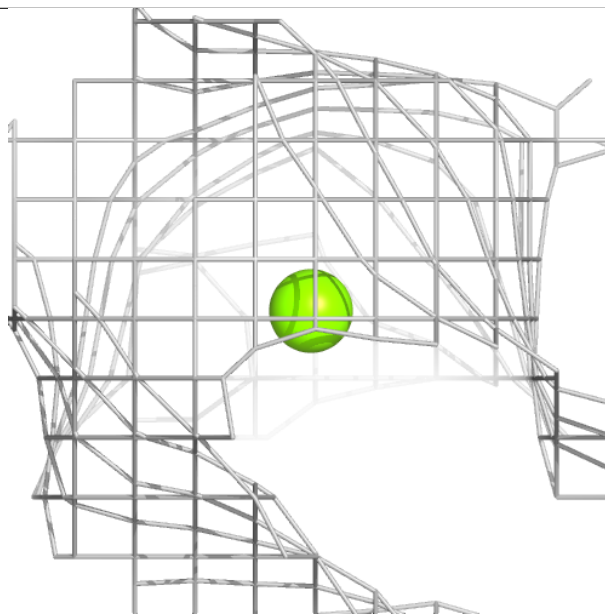
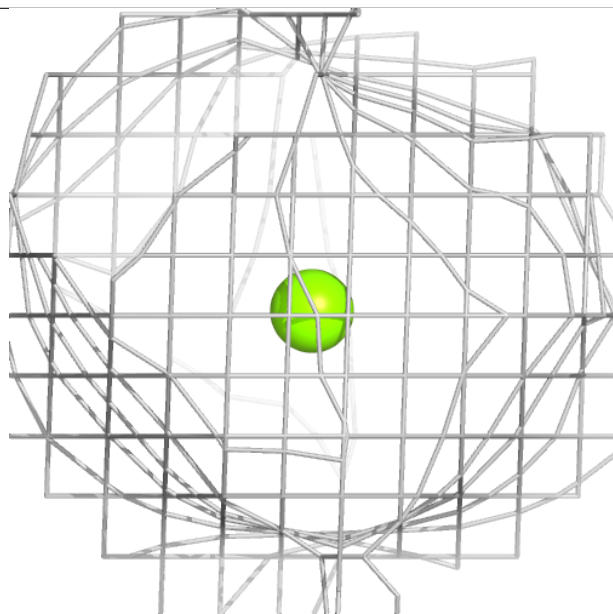
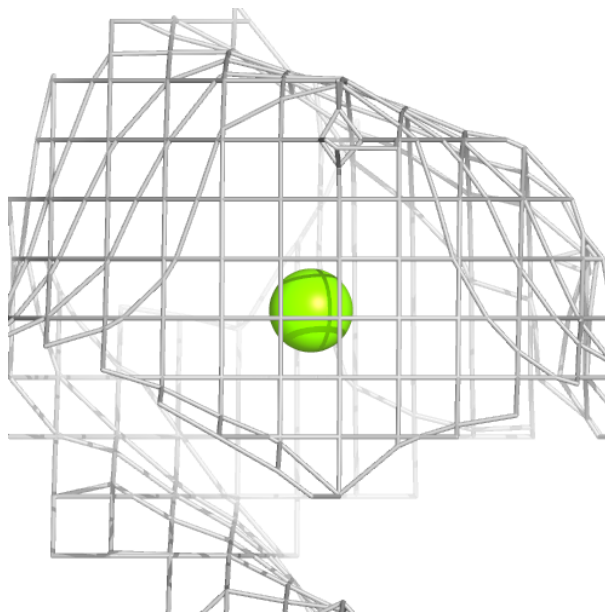
Electron density around MG C 1002:

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



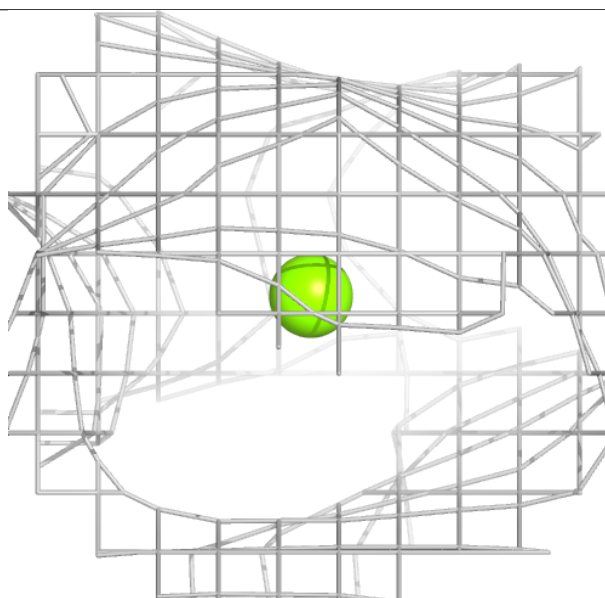
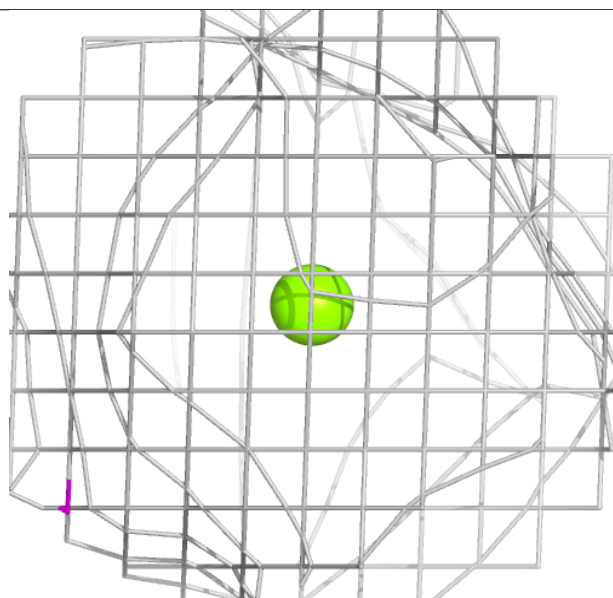
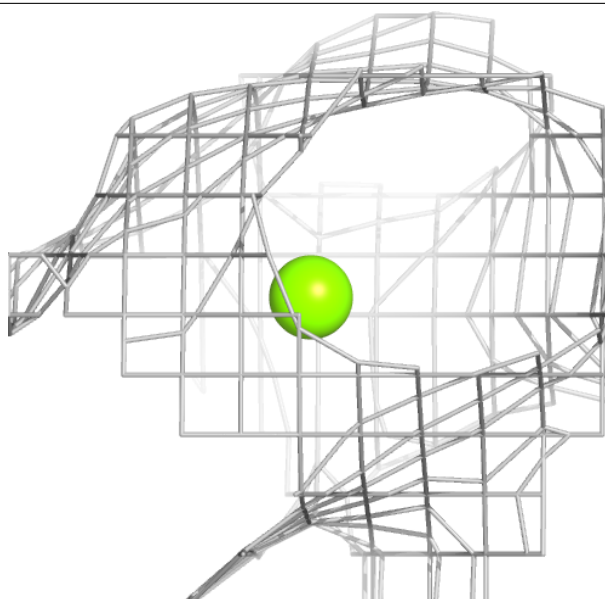
Electron density around MG D 1002:

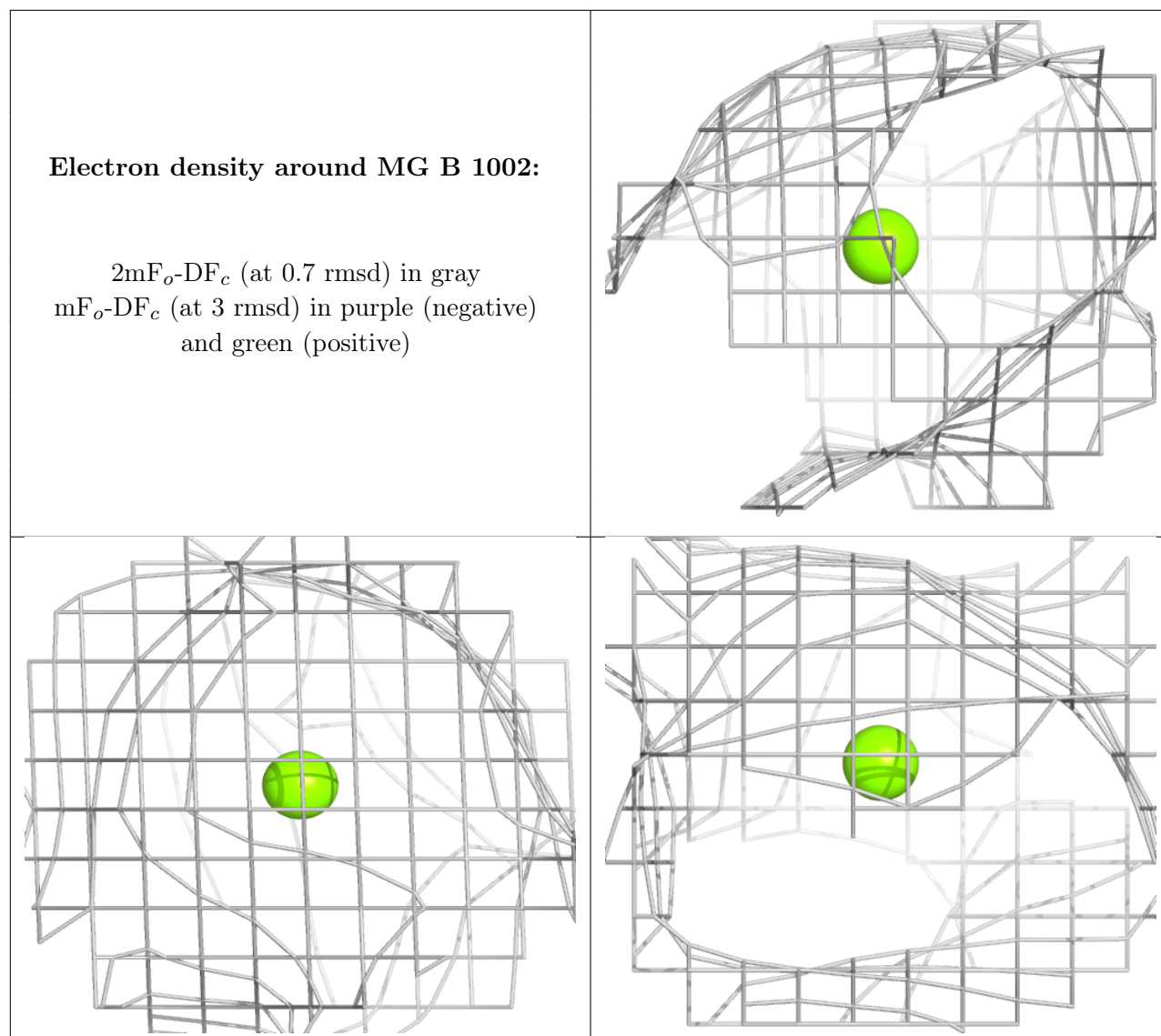
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MG A 1002:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.