



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 25, 2026 – 12:54 PM UTC

PDB ID : 9HAY / pdb\_00009hay  
Title : F420-dependent glucose-6-phosphate dehydrogenase with glucose-6-phosphate  
Authors : Palm, G.J.; Berndt, L.; Lammers, M.  
Deposited on : 2024-11-05  
Resolution : 2.39 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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

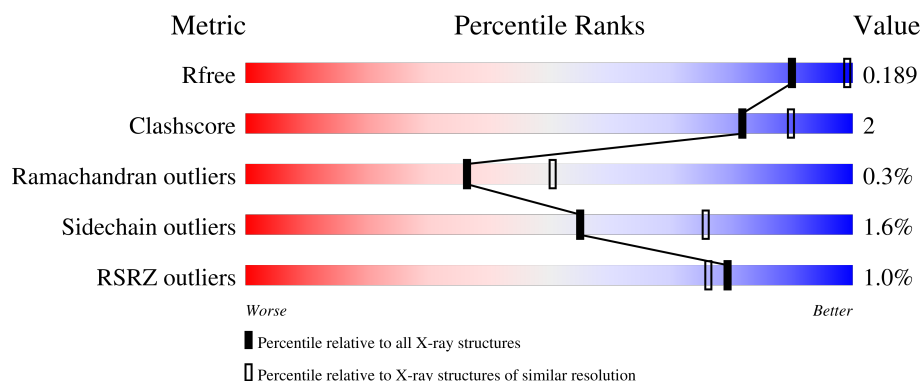
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.39 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	380	
1	B	380	
1	C	380	
1	D	380	
1	E	380	

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	380	
1	G	380	
1	H	380	
1	I	380	
1	J	380	
1	K	380	
1	L	380	
1	M	380	
1	N	380	
1	O	380	
1	P	380	
1	Q	380	
1	R	380	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PEG	J	402	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 98456 atoms, of which 47877 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 Luciferase family protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	337	Total	C	H	N	O	S	60	6	0
			5368	1731	2664	484	477	12			
1	B	338	Total	C	H	N	O	S	62	2	0
			5326	1720	2640	480	474	12			
1	C	338	Total	C	H	N	O	S	62	2	0
			5329	1721	2640	481	475	12			
1	D	340	Total	C	H	N	O	S	62	2	0
			5357	1728	2656	485	476	12			
1	E	338	Total	C	H	N	O	S	62	2	0
			5326	1720	2640	480	474	12			
1	F	337	Total	C	H	N	O	S	59	1	0
			5312	1716	2631	480	473	12			
1	G	337	Total	C	H	N	O	S	59	1	0
			5309	1715	2631	479	472	12			
1	H	337	Total	C	H	N	O	S	60	3	0
			5328	1721	2643	479	473	12			
1	I	338	Total	C	H	N	O	S	62	2	0
			5326	1720	2640	480	474	12			
1	J	338	Total	C	H	N	O	S	62	3	0
			5340	1724	2648	481	475	12			
1	K	338	Total	C	H	N	O	S	62	2	0
			5326	1720	2640	480	474	12			
1	L	338	Total	C	H	N	O	S	60	6	0
			5378	1735	2668	483	479	13			
1	M	337	Total	C	H	N	O	S	59	3	0
			5327	1720	2640	481	474	12			
1	N	338	Total	C	H	N	O	S	61	1	0
			5318	1718	2635	480	473	12			
1	O	338	Total	C	H	N	O	S	60	3	0
			5348	1726	2653	481	475	13			
1	P	338	Total	C	H	N	O	S	60	3	0
			5348	1726	2653	481	475	13			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	Q	338	Total	C	H	N	O	S	60	2	0
			5334	1722	2645	480	474	13			
1	R	338	Total	C	H	N	O	S	60	4	0
			5352	1727	2654	482	476	13			

There are 612 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-32	MET	-	initiating methionine	UNP B9L4G2
A	-31	GLY	-	expression tag	UNP B9L4G2
A	-30	SER	-	expression tag	UNP B9L4G2
A	-29	SER	-	expression tag	UNP B9L4G2
A	-28	HIS	-	expression tag	UNP B9L4G2
A	-27	HIS	-	expression tag	UNP B9L4G2
A	-26	HIS	-	expression tag	UNP B9L4G2
A	-25	HIS	-	expression tag	UNP B9L4G2
A	-24	HIS	-	expression tag	UNP B9L4G2
A	-23	HIS	-	expression tag	UNP B9L4G2
A	-22	SER	-	expression tag	UNP B9L4G2
A	-21	SER	-	expression tag	UNP B9L4G2
A	-20	GLY	-	expression tag	UNP B9L4G2
A	-19	LEU	-	expression tag	UNP B9L4G2
A	-18	VAL	-	expression tag	UNP B9L4G2
A	-17	PRO	-	expression tag	UNP B9L4G2
A	-16	ARG	-	expression tag	UNP B9L4G2
A	-15	GLY	-	expression tag	UNP B9L4G2
A	-14	SER	-	expression tag	UNP B9L4G2
A	-13	HIS	-	expression tag	UNP B9L4G2
A	-12	MET	-	expression tag	UNP B9L4G2
A	-11	ALA	-	expression tag	UNP B9L4G2
A	-10	SER	-	expression tag	UNP B9L4G2
A	-9	MET	-	expression tag	UNP B9L4G2
A	-8	THR	-	expression tag	UNP B9L4G2
A	-7	GLY	-	expression tag	UNP B9L4G2
A	-6	GLY	-	expression tag	UNP B9L4G2
A	-5	GLN	-	expression tag	UNP B9L4G2
A	-4	GLN	-	expression tag	UNP B9L4G2
A	-3	MET	-	expression tag	UNP B9L4G2
A	-2	GLY	-	expression tag	UNP B9L4G2
A	-1	ARG	-	expression tag	UNP B9L4G2
A	0	GLY	-	expression tag	UNP B9L4G2
A	1	SER	-	expression tag	UNP B9L4G2

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	-32	MET	-	initiating methionine	UNP B9L4G2
B	-31	GLY	-	expression tag	UNP B9L4G2
B	-30	SER	-	expression tag	UNP B9L4G2
B	-29	SER	-	expression tag	UNP B9L4G2
B	-28	HIS	-	expression tag	UNP B9L4G2
B	-27	HIS	-	expression tag	UNP B9L4G2
B	-26	HIS	-	expression tag	UNP B9L4G2
B	-25	HIS	-	expression tag	UNP B9L4G2
B	-24	HIS	-	expression tag	UNP B9L4G2
B	-23	HIS	-	expression tag	UNP B9L4G2
B	-22	SER	-	expression tag	UNP B9L4G2
B	-21	SER	-	expression tag	UNP B9L4G2
B	-20	GLY	-	expression tag	UNP B9L4G2
B	-19	LEU	-	expression tag	UNP B9L4G2
B	-18	VAL	-	expression tag	UNP B9L4G2
B	-17	PRO	-	expression tag	UNP B9L4G2
B	-16	ARG	-	expression tag	UNP B9L4G2
B	-15	GLY	-	expression tag	UNP B9L4G2
B	-14	SER	-	expression tag	UNP B9L4G2
B	-13	HIS	-	expression tag	UNP B9L4G2
B	-12	MET	-	expression tag	UNP B9L4G2
B	-11	ALA	-	expression tag	UNP B9L4G2
B	-10	SER	-	expression tag	UNP B9L4G2
B	-9	MET	-	expression tag	UNP B9L4G2
B	-8	THR	-	expression tag	UNP B9L4G2
B	-7	GLY	-	expression tag	UNP B9L4G2
B	-6	GLY	-	expression tag	UNP B9L4G2
B	-5	GLN	-	expression tag	UNP B9L4G2
B	-4	GLN	-	expression tag	UNP B9L4G2
B	-3	MET	-	expression tag	UNP B9L4G2
B	-2	GLY	-	expression tag	UNP B9L4G2
B	-1	ARG	-	expression tag	UNP B9L4G2
B	0	GLY	-	expression tag	UNP B9L4G2
B	1	SER	-	expression tag	UNP B9L4G2
C	-32	MET	-	initiating methionine	UNP B9L4G2
C	-31	GLY	-	expression tag	UNP B9L4G2
C	-30	SER	-	expression tag	UNP B9L4G2
C	-29	SER	-	expression tag	UNP B9L4G2
C	-28	HIS	-	expression tag	UNP B9L4G2
C	-27	HIS	-	expression tag	UNP B9L4G2
C	-26	HIS	-	expression tag	UNP B9L4G2
C	-25	HIS	-	expression tag	UNP B9L4G2

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
C	-24	HIS	-	expression tag	UNP B9L4G2
C	-23	HIS	-	expression tag	UNP B9L4G2
C	-22	SER	-	expression tag	UNP B9L4G2
C	-21	SER	-	expression tag	UNP B9L4G2
C	-20	GLY	-	expression tag	UNP B9L4G2
C	-19	LEU	-	expression tag	UNP B9L4G2
C	-18	VAL	-	expression tag	UNP B9L4G2
C	-17	PRO	-	expression tag	UNP B9L4G2
C	-16	ARG	-	expression tag	UNP B9L4G2
C	-15	GLY	-	expression tag	UNP B9L4G2
C	-14	SER	-	expression tag	UNP B9L4G2
C	-13	HIS	-	expression tag	UNP B9L4G2
C	-12	MET	-	expression tag	UNP B9L4G2
C	-11	ALA	-	expression tag	UNP B9L4G2
C	-10	SER	-	expression tag	UNP B9L4G2
C	-9	MET	-	expression tag	UNP B9L4G2
C	-8	THR	-	expression tag	UNP B9L4G2
C	-7	GLY	-	expression tag	UNP B9L4G2
C	-6	GLY	-	expression tag	UNP B9L4G2
C	-5	GLN	-	expression tag	UNP B9L4G2
C	-4	GLN	-	expression tag	UNP B9L4G2
C	-3	MET	-	expression tag	UNP B9L4G2
C	-2	GLY	-	expression tag	UNP B9L4G2
C	-1	ARG	-	expression tag	UNP B9L4G2
C	0	GLY	-	expression tag	UNP B9L4G2
C	1	SER	-	expression tag	UNP B9L4G2
D	-32	MET	-	initiating methionine	UNP B9L4G2
D	-31	GLY	-	expression tag	UNP B9L4G2
D	-30	SER	-	expression tag	UNP B9L4G2
D	-29	SER	-	expression tag	UNP B9L4G2
D	-28	HIS	-	expression tag	UNP B9L4G2
D	-27	HIS	-	expression tag	UNP B9L4G2
D	-26	HIS	-	expression tag	UNP B9L4G2
D	-25	HIS	-	expression tag	UNP B9L4G2
D	-24	HIS	-	expression tag	UNP B9L4G2
D	-23	HIS	-	expression tag	UNP B9L4G2
D	-22	SER	-	expression tag	UNP B9L4G2
D	-21	SER	-	expression tag	UNP B9L4G2
D	-20	GLY	-	expression tag	UNP B9L4G2
D	-19	LEU	-	expression tag	UNP B9L4G2
D	-18	VAL	-	expression tag	UNP B9L4G2
D	-17	PRO	-	expression tag	UNP B9L4G2

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	ARG	-	expression tag	UNP B9L4G2
D	-15	GLY	-	expression tag	UNP B9L4G2
D	-14	SER	-	expression tag	UNP B9L4G2
D	-13	HIS	-	expression tag	UNP B9L4G2
D	-12	MET	-	expression tag	UNP B9L4G2
D	-11	ALA	-	expression tag	UNP B9L4G2
D	-10	SER	-	expression tag	UNP B9L4G2
D	-9	MET	-	expression tag	UNP B9L4G2
D	-8	THR	-	expression tag	UNP B9L4G2
D	-7	GLY	-	expression tag	UNP B9L4G2
D	-6	GLY	-	expression tag	UNP B9L4G2
D	-5	GLN	-	expression tag	UNP B9L4G2
D	-4	GLN	-	expression tag	UNP B9L4G2
D	-3	MET	-	expression tag	UNP B9L4G2
D	-2	GLY	-	expression tag	UNP B9L4G2
D	-1	ARG	-	expression tag	UNP B9L4G2
D	0	GLY	-	expression tag	UNP B9L4G2
D	1	SER	-	expression tag	UNP B9L4G2
E	-32	MET	-	initiating methionine	UNP B9L4G2
E	-31	GLY	-	expression tag	UNP B9L4G2
E	-30	SER	-	expression tag	UNP B9L4G2
E	-29	SER	-	expression tag	UNP B9L4G2
E	-28	HIS	-	expression tag	UNP B9L4G2
E	-27	HIS	-	expression tag	UNP B9L4G2
E	-26	HIS	-	expression tag	UNP B9L4G2
E	-25	HIS	-	expression tag	UNP B9L4G2
E	-24	HIS	-	expression tag	UNP B9L4G2
E	-23	HIS	-	expression tag	UNP B9L4G2
E	-22	SER	-	expression tag	UNP B9L4G2
E	-21	SER	-	expression tag	UNP B9L4G2
E	-20	GLY	-	expression tag	UNP B9L4G2
E	-19	LEU	-	expression tag	UNP B9L4G2
E	-18	VAL	-	expression tag	UNP B9L4G2
E	-17	PRO	-	expression tag	UNP B9L4G2
E	-16	ARG	-	expression tag	UNP B9L4G2
E	-15	GLY	-	expression tag	UNP B9L4G2
E	-14	SER	-	expression tag	UNP B9L4G2
E	-13	HIS	-	expression tag	UNP B9L4G2
E	-12	MET	-	expression tag	UNP B9L4G2
E	-11	ALA	-	expression tag	UNP B9L4G2
E	-10	SER	-	expression tag	UNP B9L4G2
E	-9	MET	-	expression tag	UNP B9L4G2

*Continued on next page...*



*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
E	-8	THR	-	expression tag	UNP B9L4G2
E	-7	GLY	-	expression tag	UNP B9L4G2
E	-6	GLY	-	expression tag	UNP B9L4G2
E	-5	GLN	-	expression tag	UNP B9L4G2
E	-4	GLN	-	expression tag	UNP B9L4G2
E	-3	MET	-	expression tag	UNP B9L4G2
E	-2	GLY	-	expression tag	UNP B9L4G2
E	-1	ARG	-	expression tag	UNP B9L4G2
E	0	GLY	-	expression tag	UNP B9L4G2
E	1	SER	-	expression tag	UNP B9L4G2
F	-32	MET	-	initiating methionine	UNP B9L4G2
F	-31	GLY	-	expression tag	UNP B9L4G2
F	-30	SER	-	expression tag	UNP B9L4G2
F	-29	SER	-	expression tag	UNP B9L4G2
F	-28	HIS	-	expression tag	UNP B9L4G2
F	-27	HIS	-	expression tag	UNP B9L4G2
F	-26	HIS	-	expression tag	UNP B9L4G2
F	-25	HIS	-	expression tag	UNP B9L4G2
F	-24	HIS	-	expression tag	UNP B9L4G2
F	-23	HIS	-	expression tag	UNP B9L4G2
F	-22	SER	-	expression tag	UNP B9L4G2
F	-21	SER	-	expression tag	UNP B9L4G2
F	-20	GLY	-	expression tag	UNP B9L4G2
F	-19	LEU	-	expression tag	UNP B9L4G2
F	-18	VAL	-	expression tag	UNP B9L4G2
F	-17	PRO	-	expression tag	UNP B9L4G2
F	-16	ARG	-	expression tag	UNP B9L4G2
F	-15	GLY	-	expression tag	UNP B9L4G2
F	-14	SER	-	expression tag	UNP B9L4G2
F	-13	HIS	-	expression tag	UNP B9L4G2
F	-12	MET	-	expression tag	UNP B9L4G2
F	-11	ALA	-	expression tag	UNP B9L4G2
F	-10	SER	-	expression tag	UNP B9L4G2
F	-9	MET	-	expression tag	UNP B9L4G2
F	-8	THR	-	expression tag	UNP B9L4G2
F	-7	GLY	-	expression tag	UNP B9L4G2
F	-6	GLY	-	expression tag	UNP B9L4G2
F	-5	GLN	-	expression tag	UNP B9L4G2
F	-4	GLN	-	expression tag	UNP B9L4G2
F	-3	MET	-	expression tag	UNP B9L4G2
F	-2	GLY	-	expression tag	UNP B9L4G2
F	-1	ARG	-	expression tag	UNP B9L4G2

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
F	0	GLY	-	expression tag	UNP B9L4G2
F	1	SER	-	expression tag	UNP B9L4G2
G	-32	MET	-	initiating methionine	UNP B9L4G2
G	-31	GLY	-	expression tag	UNP B9L4G2
G	-30	SER	-	expression tag	UNP B9L4G2
G	-29	SER	-	expression tag	UNP B9L4G2
G	-28	HIS	-	expression tag	UNP B9L4G2
G	-27	HIS	-	expression tag	UNP B9L4G2
G	-26	HIS	-	expression tag	UNP B9L4G2
G	-25	HIS	-	expression tag	UNP B9L4G2
G	-24	HIS	-	expression tag	UNP B9L4G2
G	-23	HIS	-	expression tag	UNP B9L4G2
G	-22	SER	-	expression tag	UNP B9L4G2
G	-21	SER	-	expression tag	UNP B9L4G2
G	-20	GLY	-	expression tag	UNP B9L4G2
G	-19	LEU	-	expression tag	UNP B9L4G2
G	-18	VAL	-	expression tag	UNP B9L4G2
G	-17	PRO	-	expression tag	UNP B9L4G2
G	-16	ARG	-	expression tag	UNP B9L4G2
G	-15	GLY	-	expression tag	UNP B9L4G2
G	-14	SER	-	expression tag	UNP B9L4G2
G	-13	HIS	-	expression tag	UNP B9L4G2
G	-12	MET	-	expression tag	UNP B9L4G2
G	-11	ALA	-	expression tag	UNP B9L4G2
G	-10	SER	-	expression tag	UNP B9L4G2
G	-9	MET	-	expression tag	UNP B9L4G2
G	-8	THR	-	expression tag	UNP B9L4G2
G	-7	GLY	-	expression tag	UNP B9L4G2
G	-6	GLY	-	expression tag	UNP B9L4G2
G	-5	GLN	-	expression tag	UNP B9L4G2
G	-4	GLN	-	expression tag	UNP B9L4G2
G	-3	MET	-	expression tag	UNP B9L4G2
G	-2	GLY	-	expression tag	UNP B9L4G2
G	-1	ARG	-	expression tag	UNP B9L4G2
G	0	GLY	-	expression tag	UNP B9L4G2
G	1	SER	-	expression tag	UNP B9L4G2
H	-32	MET	-	initiating methionine	UNP B9L4G2
H	-31	GLY	-	expression tag	UNP B9L4G2
H	-30	SER	-	expression tag	UNP B9L4G2
H	-29	SER	-	expression tag	UNP B9L4G2
H	-28	HIS	-	expression tag	UNP B9L4G2
H	-27	HIS	-	expression tag	UNP B9L4G2

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
H	-26	HIS	-	expression tag	UNP B9L4G2
H	-25	HIS	-	expression tag	UNP B9L4G2
H	-24	HIS	-	expression tag	UNP B9L4G2
H	-23	HIS	-	expression tag	UNP B9L4G2
H	-22	SER	-	expression tag	UNP B9L4G2
H	-21	SER	-	expression tag	UNP B9L4G2
H	-20	GLY	-	expression tag	UNP B9L4G2
H	-19	LEU	-	expression tag	UNP B9L4G2
H	-18	VAL	-	expression tag	UNP B9L4G2
H	-17	PRO	-	expression tag	UNP B9L4G2
H	-16	ARG	-	expression tag	UNP B9L4G2
H	-15	GLY	-	expression tag	UNP B9L4G2
H	-14	SER	-	expression tag	UNP B9L4G2
H	-13	HIS	-	expression tag	UNP B9L4G2
H	-12	MET	-	expression tag	UNP B9L4G2
H	-11	ALA	-	expression tag	UNP B9L4G2
H	-10	SER	-	expression tag	UNP B9L4G2
H	-9	MET	-	expression tag	UNP B9L4G2
H	-8	THR	-	expression tag	UNP B9L4G2
H	-7	GLY	-	expression tag	UNP B9L4G2
H	-6	GLY	-	expression tag	UNP B9L4G2
H	-5	GLN	-	expression tag	UNP B9L4G2
H	-4	GLN	-	expression tag	UNP B9L4G2
H	-3	MET	-	expression tag	UNP B9L4G2
H	-2	GLY	-	expression tag	UNP B9L4G2
H	-1	ARG	-	expression tag	UNP B9L4G2
H	0	GLY	-	expression tag	UNP B9L4G2
H	1	SER	-	expression tag	UNP B9L4G2
I	-32	MET	-	initiating methionine	UNP B9L4G2
I	-31	GLY	-	expression tag	UNP B9L4G2
I	-30	SER	-	expression tag	UNP B9L4G2
I	-29	SER	-	expression tag	UNP B9L4G2
I	-28	HIS	-	expression tag	UNP B9L4G2
I	-27	HIS	-	expression tag	UNP B9L4G2
I	-26	HIS	-	expression tag	UNP B9L4G2
I	-25	HIS	-	expression tag	UNP B9L4G2
I	-24	HIS	-	expression tag	UNP B9L4G2
I	-23	HIS	-	expression tag	UNP B9L4G2
I	-22	SER	-	expression tag	UNP B9L4G2
I	-21	SER	-	expression tag	UNP B9L4G2
I	-20	GLY	-	expression tag	UNP B9L4G2
I	-19	LEU	-	expression tag	UNP B9L4G2

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
I	-18	VAL	-	expression tag	UNP B9L4G2
I	-17	PRO	-	expression tag	UNP B9L4G2
I	-16	ARG	-	expression tag	UNP B9L4G2
I	-15	GLY	-	expression tag	UNP B9L4G2
I	-14	SER	-	expression tag	UNP B9L4G2
I	-13	HIS	-	expression tag	UNP B9L4G2
I	-12	MET	-	expression tag	UNP B9L4G2
I	-11	ALA	-	expression tag	UNP B9L4G2
I	-10	SER	-	expression tag	UNP B9L4G2
I	-9	MET	-	expression tag	UNP B9L4G2
I	-8	THR	-	expression tag	UNP B9L4G2
I	-7	GLY	-	expression tag	UNP B9L4G2
I	-6	GLY	-	expression tag	UNP B9L4G2
I	-5	GLN	-	expression tag	UNP B9L4G2
I	-4	GLN	-	expression tag	UNP B9L4G2
I	-3	MET	-	expression tag	UNP B9L4G2
I	-2	GLY	-	expression tag	UNP B9L4G2
I	-1	ARG	-	expression tag	UNP B9L4G2
I	0	GLY	-	expression tag	UNP B9L4G2
I	1	SER	-	expression tag	UNP B9L4G2
J	-32	MET	-	initiating methionine	UNP B9L4G2
J	-31	GLY	-	expression tag	UNP B9L4G2
J	-30	SER	-	expression tag	UNP B9L4G2
J	-29	SER	-	expression tag	UNP B9L4G2
J	-28	HIS	-	expression tag	UNP B9L4G2
J	-27	HIS	-	expression tag	UNP B9L4G2
J	-26	HIS	-	expression tag	UNP B9L4G2
J	-25	HIS	-	expression tag	UNP B9L4G2
J	-24	HIS	-	expression tag	UNP B9L4G2
J	-23	HIS	-	expression tag	UNP B9L4G2
J	-22	SER	-	expression tag	UNP B9L4G2
J	-21	SER	-	expression tag	UNP B9L4G2
J	-20	GLY	-	expression tag	UNP B9L4G2
J	-19	LEU	-	expression tag	UNP B9L4G2
J	-18	VAL	-	expression tag	UNP B9L4G2
J	-17	PRO	-	expression tag	UNP B9L4G2
J	-16	ARG	-	expression tag	UNP B9L4G2
J	-15	GLY	-	expression tag	UNP B9L4G2
J	-14	SER	-	expression tag	UNP B9L4G2
J	-13	HIS	-	expression tag	UNP B9L4G2
J	-12	MET	-	expression tag	UNP B9L4G2
J	-11	ALA	-	expression tag	UNP B9L4G2

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
J	-10	SER	-	expression tag	UNP B9L4G2
J	-9	MET	-	expression tag	UNP B9L4G2
J	-8	THR	-	expression tag	UNP B9L4G2
J	-7	GLY	-	expression tag	UNP B9L4G2
J	-6	GLY	-	expression tag	UNP B9L4G2
J	-5	GLN	-	expression tag	UNP B9L4G2
J	-4	GLN	-	expression tag	UNP B9L4G2
J	-3	MET	-	expression tag	UNP B9L4G2
J	-2	GLY	-	expression tag	UNP B9L4G2
J	-1	ARG	-	expression tag	UNP B9L4G2
J	0	GLY	-	expression tag	UNP B9L4G2
J	1	SER	-	expression tag	UNP B9L4G2
K	-32	MET	-	initiating methionine	UNP B9L4G2
K	-31	GLY	-	expression tag	UNP B9L4G2
K	-30	SER	-	expression tag	UNP B9L4G2
K	-29	SER	-	expression tag	UNP B9L4G2
K	-28	HIS	-	expression tag	UNP B9L4G2
K	-27	HIS	-	expression tag	UNP B9L4G2
K	-26	HIS	-	expression tag	UNP B9L4G2
K	-25	HIS	-	expression tag	UNP B9L4G2
K	-24	HIS	-	expression tag	UNP B9L4G2
K	-23	HIS	-	expression tag	UNP B9L4G2
K	-22	SER	-	expression tag	UNP B9L4G2
K	-21	SER	-	expression tag	UNP B9L4G2
K	-20	GLY	-	expression tag	UNP B9L4G2
K	-19	LEU	-	expression tag	UNP B9L4G2
K	-18	VAL	-	expression tag	UNP B9L4G2
K	-17	PRO	-	expression tag	UNP B9L4G2
K	-16	ARG	-	expression tag	UNP B9L4G2
K	-15	GLY	-	expression tag	UNP B9L4G2
K	-14	SER	-	expression tag	UNP B9L4G2
K	-13	HIS	-	expression tag	UNP B9L4G2
K	-12	MET	-	expression tag	UNP B9L4G2
K	-11	ALA	-	expression tag	UNP B9L4G2
K	-10	SER	-	expression tag	UNP B9L4G2
K	-9	MET	-	expression tag	UNP B9L4G2
K	-8	THR	-	expression tag	UNP B9L4G2
K	-7	GLY	-	expression tag	UNP B9L4G2
K	-6	GLY	-	expression tag	UNP B9L4G2
K	-5	GLN	-	expression tag	UNP B9L4G2
K	-4	GLN	-	expression tag	UNP B9L4G2
K	-3	MET	-	expression tag	UNP B9L4G2

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
K	-2	GLY	-	expression tag	UNP B9L4G2
K	-1	ARG	-	expression tag	UNP B9L4G2
K	0	GLY	-	expression tag	UNP B9L4G2
K	1	SER	-	expression tag	UNP B9L4G2
L	-32	MET	-	initiating methionine	UNP B9L4G2
L	-31	GLY	-	expression tag	UNP B9L4G2
L	-30	SER	-	expression tag	UNP B9L4G2
L	-29	SER	-	expression tag	UNP B9L4G2
L	-28	HIS	-	expression tag	UNP B9L4G2
L	-27	HIS	-	expression tag	UNP B9L4G2
L	-26	HIS	-	expression tag	UNP B9L4G2
L	-25	HIS	-	expression tag	UNP B9L4G2
L	-24	HIS	-	expression tag	UNP B9L4G2
L	-23	HIS	-	expression tag	UNP B9L4G2
L	-22	SER	-	expression tag	UNP B9L4G2
L	-21	SER	-	expression tag	UNP B9L4G2
L	-20	GLY	-	expression tag	UNP B9L4G2
L	-19	LEU	-	expression tag	UNP B9L4G2
L	-18	VAL	-	expression tag	UNP B9L4G2
L	-17	PRO	-	expression tag	UNP B9L4G2
L	-16	ARG	-	expression tag	UNP B9L4G2
L	-15	GLY	-	expression tag	UNP B9L4G2
L	-14	SER	-	expression tag	UNP B9L4G2
L	-13	HIS	-	expression tag	UNP B9L4G2
L	-12	MET	-	expression tag	UNP B9L4G2
L	-11	ALA	-	expression tag	UNP B9L4G2
L	-10	SER	-	expression tag	UNP B9L4G2
L	-9	MET	-	expression tag	UNP B9L4G2
L	-8	THR	-	expression tag	UNP B9L4G2
L	-7	GLY	-	expression tag	UNP B9L4G2
L	-6	GLY	-	expression tag	UNP B9L4G2
L	-5	GLN	-	expression tag	UNP B9L4G2
L	-4	GLN	-	expression tag	UNP B9L4G2
L	-3	MET	-	expression tag	UNP B9L4G2
L	-2	GLY	-	expression tag	UNP B9L4G2
L	-1	ARG	-	expression tag	UNP B9L4G2
L	0	GLY	-	expression tag	UNP B9L4G2
L	1	SER	-	expression tag	UNP B9L4G2
M	-32	MET	-	initiating methionine	UNP B9L4G2
M	-31	GLY	-	expression tag	UNP B9L4G2
M	-30	SER	-	expression tag	UNP B9L4G2
M	-29	SER	-	expression tag	UNP B9L4G2

*Continued on next page...*



*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
M	-28	HIS	-	expression tag	UNP B9L4G2
M	-27	HIS	-	expression tag	UNP B9L4G2
M	-26	HIS	-	expression tag	UNP B9L4G2
M	-25	HIS	-	expression tag	UNP B9L4G2
M	-24	HIS	-	expression tag	UNP B9L4G2
M	-23	HIS	-	expression tag	UNP B9L4G2
M	-22	SER	-	expression tag	UNP B9L4G2
M	-21	SER	-	expression tag	UNP B9L4G2
M	-20	GLY	-	expression tag	UNP B9L4G2
M	-19	LEU	-	expression tag	UNP B9L4G2
M	-18	VAL	-	expression tag	UNP B9L4G2
M	-17	PRO	-	expression tag	UNP B9L4G2
M	-16	ARG	-	expression tag	UNP B9L4G2
M	-15	GLY	-	expression tag	UNP B9L4G2
M	-14	SER	-	expression tag	UNP B9L4G2
M	-13	HIS	-	expression tag	UNP B9L4G2
M	-12	MET	-	expression tag	UNP B9L4G2
M	-11	ALA	-	expression tag	UNP B9L4G2
M	-10	SER	-	expression tag	UNP B9L4G2
M	-9	MET	-	expression tag	UNP B9L4G2
M	-8	THR	-	expression tag	UNP B9L4G2
M	-7	GLY	-	expression tag	UNP B9L4G2
M	-6	GLY	-	expression tag	UNP B9L4G2
M	-5	GLN	-	expression tag	UNP B9L4G2
M	-4	GLN	-	expression tag	UNP B9L4G2
M	-3	MET	-	expression tag	UNP B9L4G2
M	-2	GLY	-	expression tag	UNP B9L4G2
M	-1	ARG	-	expression tag	UNP B9L4G2
M	0	GLY	-	expression tag	UNP B9L4G2
M	1	SER	-	expression tag	UNP B9L4G2
N	-32	MET	-	initiating methionine	UNP B9L4G2
N	-31	GLY	-	expression tag	UNP B9L4G2
N	-30	SER	-	expression tag	UNP B9L4G2
N	-29	SER	-	expression tag	UNP B9L4G2
N	-28	HIS	-	expression tag	UNP B9L4G2
N	-27	HIS	-	expression tag	UNP B9L4G2
N	-26	HIS	-	expression tag	UNP B9L4G2
N	-25	HIS	-	expression tag	UNP B9L4G2
N	-24	HIS	-	expression tag	UNP B9L4G2
N	-23	HIS	-	expression tag	UNP B9L4G2
N	-22	SER	-	expression tag	UNP B9L4G2
N	-21	SER	-	expression tag	UNP B9L4G2

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
N	-20	GLY	-	expression tag	UNP B9L4G2
N	-19	LEU	-	expression tag	UNP B9L4G2
N	-18	VAL	-	expression tag	UNP B9L4G2
N	-17	PRO	-	expression tag	UNP B9L4G2
N	-16	ARG	-	expression tag	UNP B9L4G2
N	-15	GLY	-	expression tag	UNP B9L4G2
N	-14	SER	-	expression tag	UNP B9L4G2
N	-13	HIS	-	expression tag	UNP B9L4G2
N	-12	MET	-	expression tag	UNP B9L4G2
N	-11	ALA	-	expression tag	UNP B9L4G2
N	-10	SER	-	expression tag	UNP B9L4G2
N	-9	MET	-	expression tag	UNP B9L4G2
N	-8	THR	-	expression tag	UNP B9L4G2
N	-7	GLY	-	expression tag	UNP B9L4G2
N	-6	GLY	-	expression tag	UNP B9L4G2
N	-5	GLN	-	expression tag	UNP B9L4G2
N	-4	GLN	-	expression tag	UNP B9L4G2
N	-3	MET	-	expression tag	UNP B9L4G2
N	-2	GLY	-	expression tag	UNP B9L4G2
N	-1	ARG	-	expression tag	UNP B9L4G2
N	0	GLY	-	expression tag	UNP B9L4G2
N	1	SER	-	expression tag	UNP B9L4G2
O	-32	MET	-	initiating methionine	UNP B9L4G2
O	-31	GLY	-	expression tag	UNP B9L4G2
O	-30	SER	-	expression tag	UNP B9L4G2
O	-29	SER	-	expression tag	UNP B9L4G2
O	-28	HIS	-	expression tag	UNP B9L4G2
O	-27	HIS	-	expression tag	UNP B9L4G2
O	-26	HIS	-	expression tag	UNP B9L4G2
O	-25	HIS	-	expression tag	UNP B9L4G2
O	-24	HIS	-	expression tag	UNP B9L4G2
O	-23	HIS	-	expression tag	UNP B9L4G2
O	-22	SER	-	expression tag	UNP B9L4G2
O	-21	SER	-	expression tag	UNP B9L4G2
O	-20	GLY	-	expression tag	UNP B9L4G2
O	-19	LEU	-	expression tag	UNP B9L4G2
O	-18	VAL	-	expression tag	UNP B9L4G2
O	-17	PRO	-	expression tag	UNP B9L4G2
O	-16	ARG	-	expression tag	UNP B9L4G2
O	-15	GLY	-	expression tag	UNP B9L4G2
O	-14	SER	-	expression tag	UNP B9L4G2
O	-13	HIS	-	expression tag	UNP B9L4G2

*Continued on next page...*



*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
O	-12	MET	-	expression tag	UNP B9L4G2
O	-11	ALA	-	expression tag	UNP B9L4G2
O	-10	SER	-	expression tag	UNP B9L4G2
O	-9	MET	-	expression tag	UNP B9L4G2
O	-8	THR	-	expression tag	UNP B9L4G2
O	-7	GLY	-	expression tag	UNP B9L4G2
O	-6	GLY	-	expression tag	UNP B9L4G2
O	-5	GLN	-	expression tag	UNP B9L4G2
O	-4	GLN	-	expression tag	UNP B9L4G2
O	-3	MET	-	expression tag	UNP B9L4G2
O	-2	GLY	-	expression tag	UNP B9L4G2
O	-1	ARG	-	expression tag	UNP B9L4G2
O	0	GLY	-	expression tag	UNP B9L4G2
O	1	SER	-	expression tag	UNP B9L4G2
P	-32	MET	-	initiating methionine	UNP B9L4G2
P	-31	GLY	-	expression tag	UNP B9L4G2
P	-30	SER	-	expression tag	UNP B9L4G2
P	-29	SER	-	expression tag	UNP B9L4G2
P	-28	HIS	-	expression tag	UNP B9L4G2
P	-27	HIS	-	expression tag	UNP B9L4G2
P	-26	HIS	-	expression tag	UNP B9L4G2
P	-25	HIS	-	expression tag	UNP B9L4G2
P	-24	HIS	-	expression tag	UNP B9L4G2
P	-23	HIS	-	expression tag	UNP B9L4G2
P	-22	SER	-	expression tag	UNP B9L4G2
P	-21	SER	-	expression tag	UNP B9L4G2
P	-20	GLY	-	expression tag	UNP B9L4G2
P	-19	LEU	-	expression tag	UNP B9L4G2
P	-18	VAL	-	expression tag	UNP B9L4G2
P	-17	PRO	-	expression tag	UNP B9L4G2
P	-16	ARG	-	expression tag	UNP B9L4G2
P	-15	GLY	-	expression tag	UNP B9L4G2
P	-14	SER	-	expression tag	UNP B9L4G2
P	-13	HIS	-	expression tag	UNP B9L4G2
P	-12	MET	-	expression tag	UNP B9L4G2
P	-11	ALA	-	expression tag	UNP B9L4G2
P	-10	SER	-	expression tag	UNP B9L4G2
P	-9	MET	-	expression tag	UNP B9L4G2
P	-8	THR	-	expression tag	UNP B9L4G2
P	-7	GLY	-	expression tag	UNP B9L4G2
P	-6	GLY	-	expression tag	UNP B9L4G2
P	-5	GLN	-	expression tag	UNP B9L4G2

*Continued on next page...*

*Continued from previous page...*

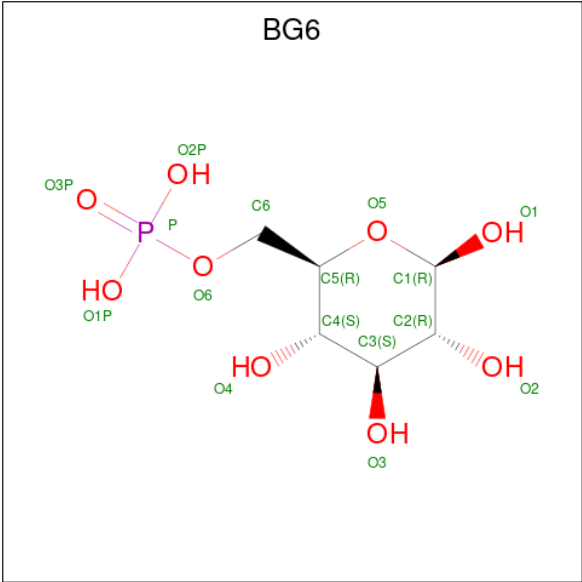
Chain	Residue	Modelled	Actual	Comment	Reference
P	-4	GLN	-	expression tag	UNP B9L4G2
P	-3	MET	-	expression tag	UNP B9L4G2
P	-2	GLY	-	expression tag	UNP B9L4G2
P	-1	ARG	-	expression tag	UNP B9L4G2
P	0	GLY	-	expression tag	UNP B9L4G2
P	1	SER	-	expression tag	UNP B9L4G2
Q	-32	MET	-	initiating methionine	UNP B9L4G2
Q	-31	GLY	-	expression tag	UNP B9L4G2
Q	-30	SER	-	expression tag	UNP B9L4G2
Q	-29	SER	-	expression tag	UNP B9L4G2
Q	-28	HIS	-	expression tag	UNP B9L4G2
Q	-27	HIS	-	expression tag	UNP B9L4G2
Q	-26	HIS	-	expression tag	UNP B9L4G2
Q	-25	HIS	-	expression tag	UNP B9L4G2
Q	-24	HIS	-	expression tag	UNP B9L4G2
Q	-23	HIS	-	expression tag	UNP B9L4G2
Q	-22	SER	-	expression tag	UNP B9L4G2
Q	-21	SER	-	expression tag	UNP B9L4G2
Q	-20	GLY	-	expression tag	UNP B9L4G2
Q	-19	LEU	-	expression tag	UNP B9L4G2
Q	-18	VAL	-	expression tag	UNP B9L4G2
Q	-17	PRO	-	expression tag	UNP B9L4G2
Q	-16	ARG	-	expression tag	UNP B9L4G2
Q	-15	GLY	-	expression tag	UNP B9L4G2
Q	-14	SER	-	expression tag	UNP B9L4G2
Q	-13	HIS	-	expression tag	UNP B9L4G2
Q	-12	MET	-	expression tag	UNP B9L4G2
Q	-11	ALA	-	expression tag	UNP B9L4G2
Q	-10	SER	-	expression tag	UNP B9L4G2
Q	-9	MET	-	expression tag	UNP B9L4G2
Q	-8	THR	-	expression tag	UNP B9L4G2
Q	-7	GLY	-	expression tag	UNP B9L4G2
Q	-6	GLY	-	expression tag	UNP B9L4G2
Q	-5	GLN	-	expression tag	UNP B9L4G2
Q	-4	GLN	-	expression tag	UNP B9L4G2
Q	-3	MET	-	expression tag	UNP B9L4G2
Q	-2	GLY	-	expression tag	UNP B9L4G2
Q	-1	ARG	-	expression tag	UNP B9L4G2
Q	0	GLY	-	expression tag	UNP B9L4G2
Q	1	SER	-	expression tag	UNP B9L4G2
R	-32	MET	-	initiating methionine	UNP B9L4G2
R	-31	GLY	-	expression tag	UNP B9L4G2

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
R	-30	SER	-	expression tag	UNP B9L4G2
R	-29	SER	-	expression tag	UNP B9L4G2
R	-28	HIS	-	expression tag	UNP B9L4G2
R	-27	HIS	-	expression tag	UNP B9L4G2
R	-26	HIS	-	expression tag	UNP B9L4G2
R	-25	HIS	-	expression tag	UNP B9L4G2
R	-24	HIS	-	expression tag	UNP B9L4G2
R	-23	HIS	-	expression tag	UNP B9L4G2
R	-22	SER	-	expression tag	UNP B9L4G2
R	-21	SER	-	expression tag	UNP B9L4G2
R	-20	GLY	-	expression tag	UNP B9L4G2
R	-19	LEU	-	expression tag	UNP B9L4G2
R	-18	VAL	-	expression tag	UNP B9L4G2
R	-17	PRO	-	expression tag	UNP B9L4G2
R	-16	ARG	-	expression tag	UNP B9L4G2
R	-15	GLY	-	expression tag	UNP B9L4G2
R	-14	SER	-	expression tag	UNP B9L4G2
R	-13	HIS	-	expression tag	UNP B9L4G2
R	-12	MET	-	expression tag	UNP B9L4G2
R	-11	ALA	-	expression tag	UNP B9L4G2
R	-10	SER	-	expression tag	UNP B9L4G2
R	-9	MET	-	expression tag	UNP B9L4G2
R	-8	THR	-	expression tag	UNP B9L4G2
R	-7	GLY	-	expression tag	UNP B9L4G2
R	-6	GLY	-	expression tag	UNP B9L4G2
R	-5	GLN	-	expression tag	UNP B9L4G2
R	-4	GLN	-	expression tag	UNP B9L4G2
R	-3	MET	-	expression tag	UNP B9L4G2
R	-2	GLY	-	expression tag	UNP B9L4G2
R	-1	ARG	-	expression tag	UNP B9L4G2
R	0	GLY	-	expression tag	UNP B9L4G2
R	1	SER	-	expression tag	UNP B9L4G2

- Molecule 2 is 6-O-phosphono-beta-D-glucopyranose (CCD ID: BG6) (formula: C<sub>6</sub>H<sub>13</sub>O<sub>9</sub>P) (labeled as "Ligand of Interest" by depositor).



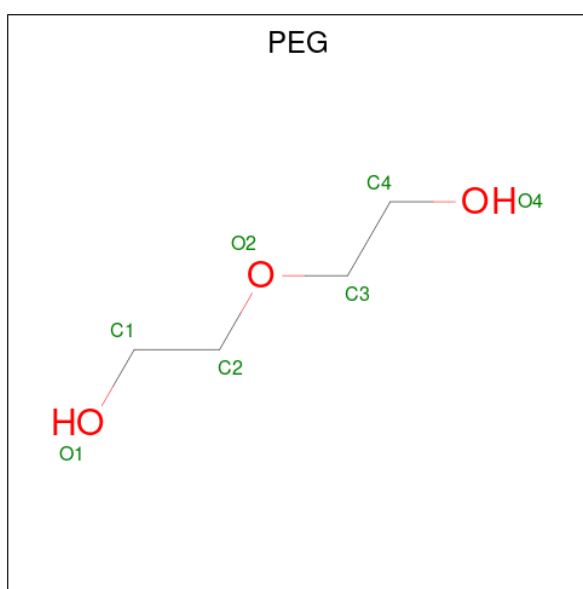
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	O	P	4	0
			27	6	11	9	1		
2	B	1	Total	C	H	O	P	4	0
			27	6	11	9	1		
2	C	1	Total	C	H	O	P	4	0
			27	6	11	9	1		
2	D	1	Total	C	H	O	P	4	0
			27	6	11	9	1		
2	E	1	Total	C	H	O	P	4	0
			27	6	11	9	1		
2	F	1	Total	C	H	O	P	4	0
			27	6	11	9	1		
2	G	1	Total	C	H	O	P	4	0
			27	6	11	9	1		
2	H	1	Total	C	H	O	P	4	0
			27	6	11	9	1		
2	I	1	Total	C	H	O	P	4	0
			27	6	11	9	1		
2	J	1	Total	C	H	O	P	4	0
			27	6	11	9	1		
2	K	1	Total	C	H	O	P	4	0
			27	6	11	9	1		
2	L	1	Total	C	H	O	P	4	0
			27	6	11	9	1		
2	M	1	Total	C	H	O	P	4	0
			27	6	11	9	1		
2	N	1	Total	C	H	O	P	4	0
			27	6	11	9	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	O	1	Total	C	H	O	P	4	0
			27	6	11	9	1		
2	P	1	Total	C	H	O	P	4	0
			27	6	11	9	1		
2	Q	1	Total	C	H	O	P	4	0
			27	6	11	9	1		
2	R	1	Total	C	H	O	P	4	0
			27	6	11	9	1		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula:  $C_4H_{10}O_3$ ).



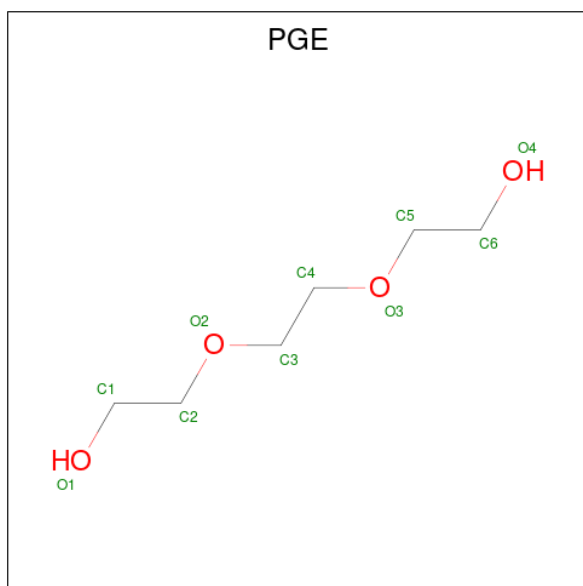
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	J	1	Total	C	H	O	2	0
			17	4	10	3		
3	N	1	Total	C	H	O	2	0
			17	4	10	3		

- Molecule 4 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula:  $C_8H_{18}O_5$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	K	1	Total	C	H	O	2	0
			31	8	18	5		

- Molecule 5 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula:  $C_6H_{14}O_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	O	1	Total	C	H	O	2	0
			24	6	14	4		

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	Q	1	Total	C	H	O	2	0
			10	2	6	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	138	Total	O	0	1
			139	139		
7	B	160	Total	O	0	2
			162	162		
7	C	107	Total	O	0	2
			109	109		
7	D	120	Total	O	0	2
			122	122		
7	E	70	Total	O	0	1
			71	71		
7	F	67	Total	O	0	1
			68	68		
7	G	63	Total	O	0	2
			65	65		
7	H	85	Total	O	0	1
			86	86		
7	I	128	Total	O	0	2
			130	130		
7	J	104	Total	O	0	4
			108	108		
7	K	100	Total	O	0	2
			102	102		

*Continued on next page...*

*Continued from previous page...*

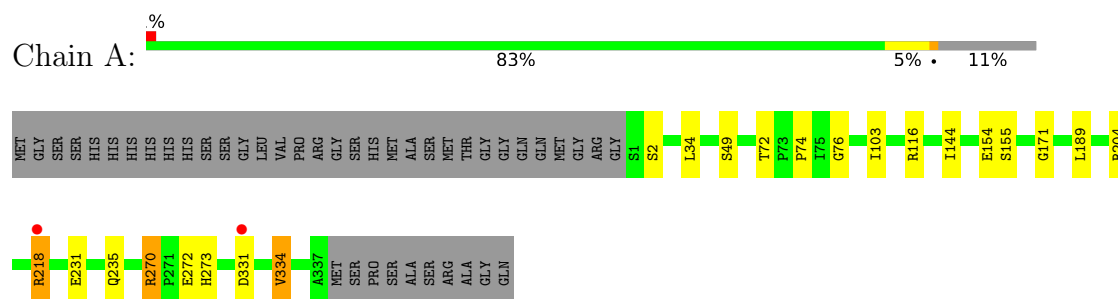
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	L	149	Total 151	O 151	0	2
7	M	58	Total 60	O 60	0	2
7	N	54	Total 55	O 55	0	1
7	O	117	Total 119	O 119	0	2
7	P	56	Total 57	O 57	0	1
7	Q	110	Total 112	O 112	0	2
7	R	101	Total 103	O 103	0	2



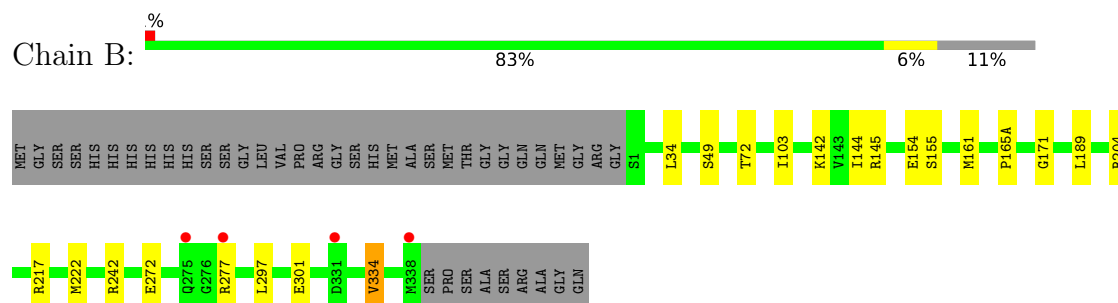
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

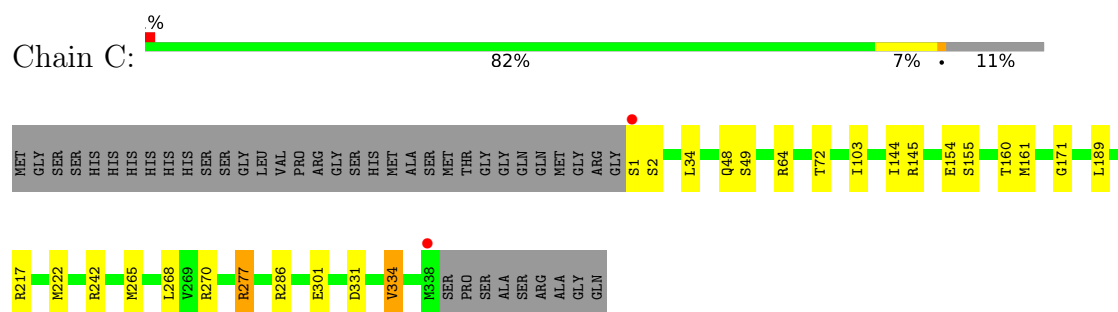
- Molecule 1: Luciferase family protein



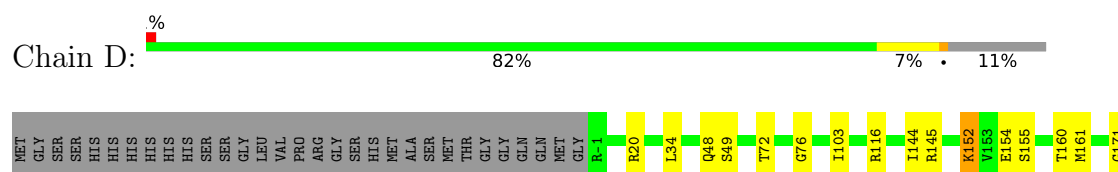
- Molecule 1: Luciferase family protein



- Molecule 1: Luciferase family protein

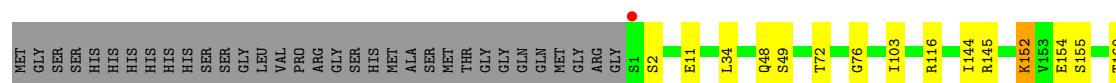
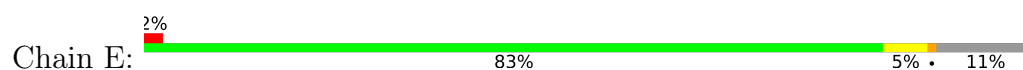


- Molecule 1: Luciferase family protein

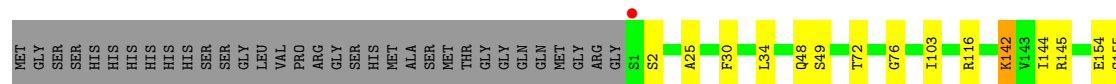
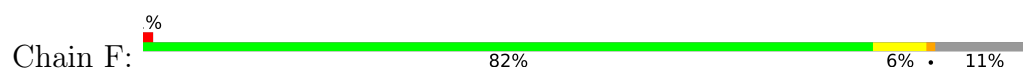




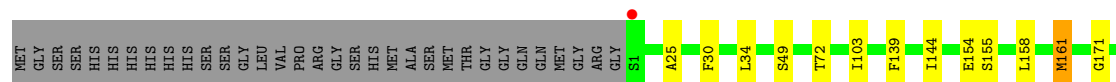
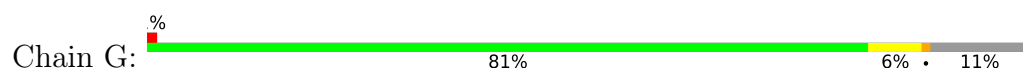
- Molecule 1: Luciferase family protein



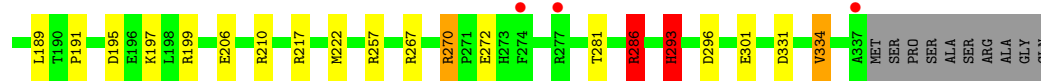
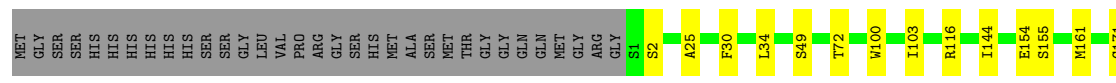
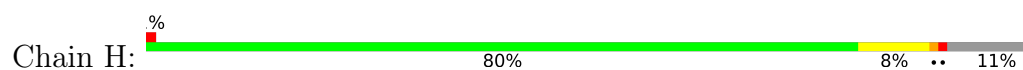
- Molecule 1: Luciferase family protein



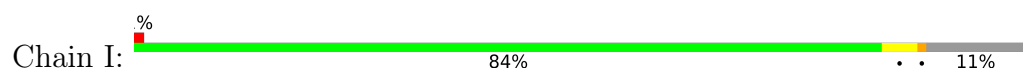
- Molecule 1: Luciferase family protein

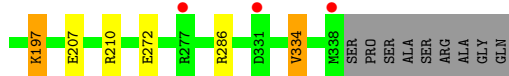
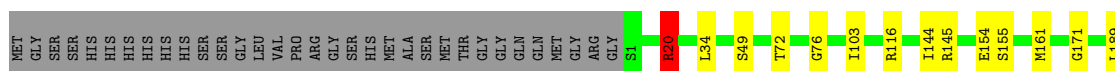


- Molecule 1: Luciferase family protein

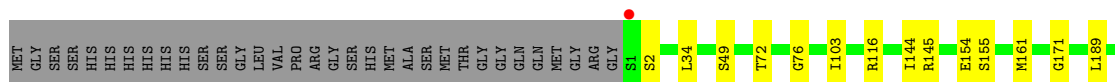
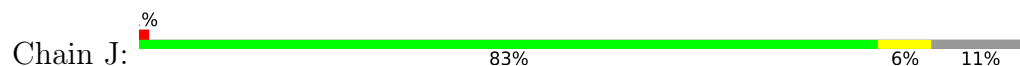


- Molecule 1: Luciferase family protein

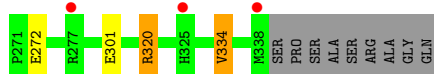
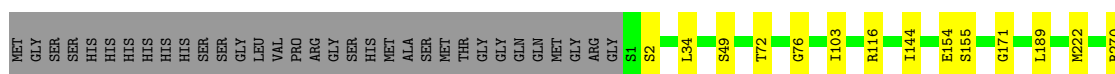
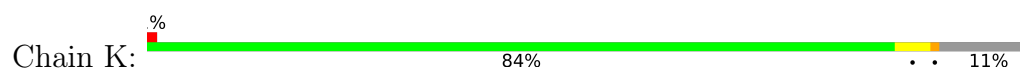




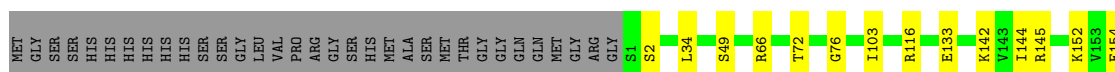
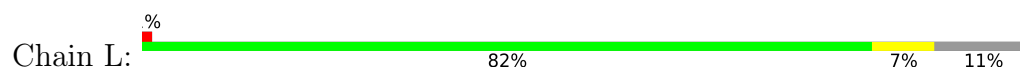
- Molecule 1: Luciferase family protein



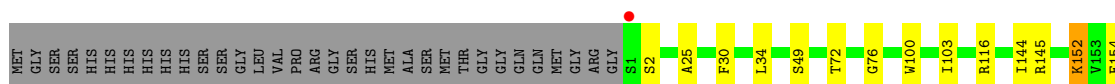
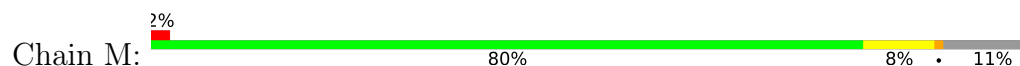
- Molecule 1: Luciferase family protein



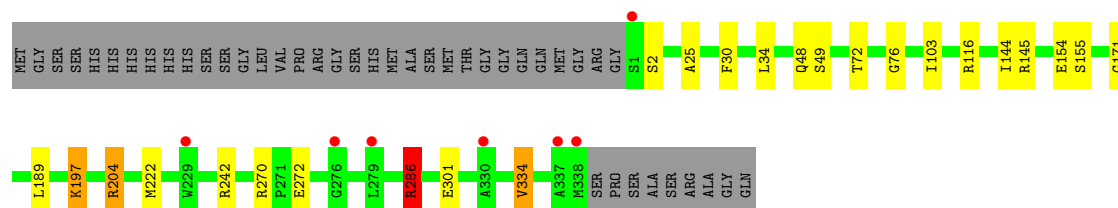
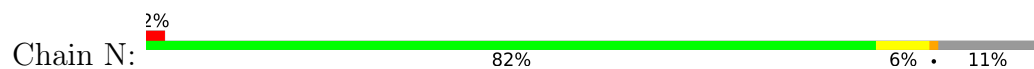
- Molecule 1: Luciferase family protein



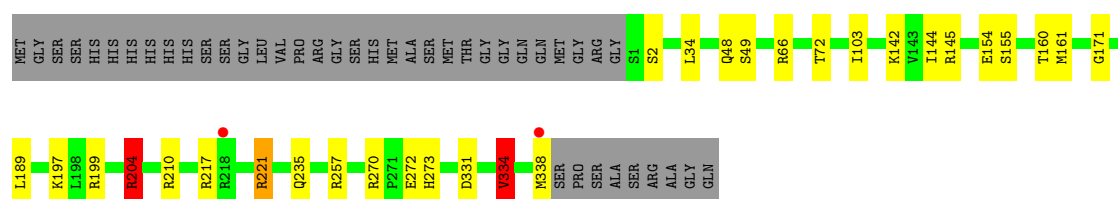
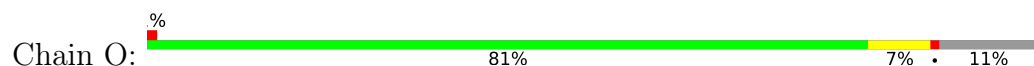
- Molecule 1: Luciferase family protein



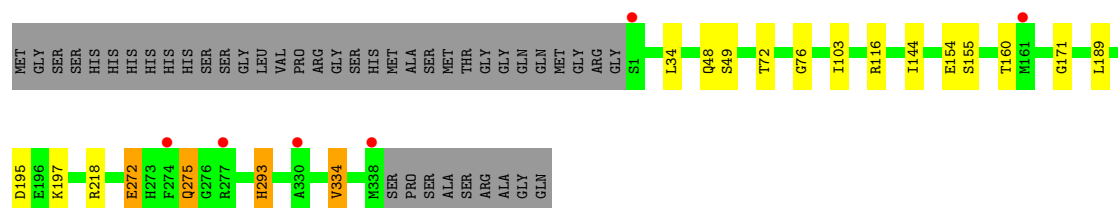
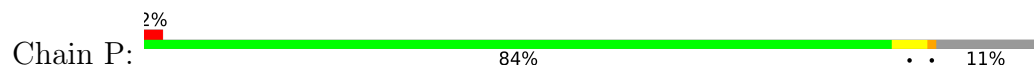
- Molecule 1: Luciferase family protein



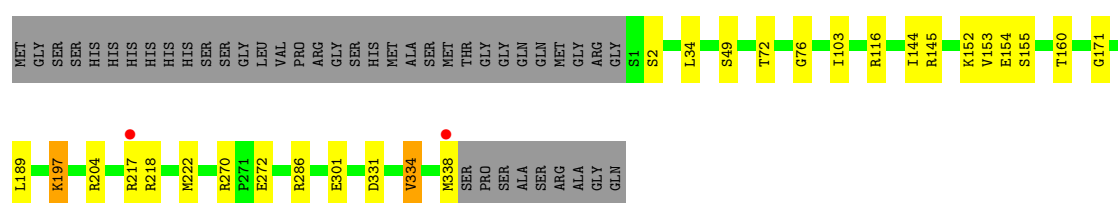
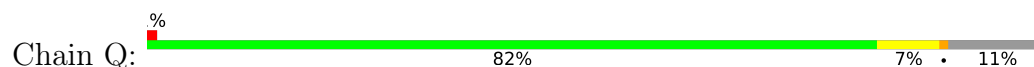
- Molecule 1: Luciferase family protein



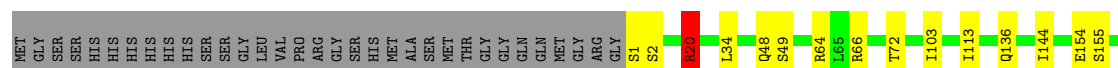
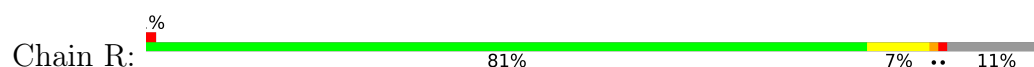
- Molecule 1: Luciferase family protein



- Molecule 1: Luciferase family protein



- Molecule 1: Luciferase family protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	199.75Å 372.95Å 104.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.99 – 2.39 49.99 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.99-2.39) 95.0 (49.99-2.39)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.15	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.72 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, $R_{free}$	0.173 , 0.191 0.172 , 0.189	Depositor DCC
$R_{free}$ test set	15389 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.9	Xtriage
Anisotropy	0.367	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 45.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	98456	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.04% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PGE, EDO, PG4, BG6, PEG

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	0.62	0/2803	0.97	4/3806 (0.1%)
1	B	0.62	0/2771	0.96	4/3764 (0.1%)
1	C	0.60	0/2771	0.98	6/3764 (0.2%)
1	D	0.62	0/2786	1.02	9/3783 (0.2%)
1	E	0.58	0/2771	0.95	5/3764 (0.1%)
1	F	0.57	0/2760	0.95	5/3749 (0.1%)
1	G	0.57	0/2760	0.98	6/3749 (0.2%)
1	H	0.66	0/2774	1.01	13/3768 (0.3%)
1	I	0.61	0/2771	1.00	7/3764 (0.2%)
1	J	0.62	0/2780	0.96	4/3776 (0.1%)
1	K	0.59	0/2771	0.95	4/3764 (0.1%)
1	L	0.69	0/2810	1.02	5/3814 (0.1%)
1	M	0.68	2/2774 (0.1%)	1.01	9/3768 (0.2%)
1	N	0.57	0/2765	0.95	6/3756 (0.2%)
1	O	0.66	0/2783	1.00	7/3779 (0.2%)
1	P	0.57	0/2783	0.94	5/3779 (0.1%)
1	Q	0.61	0/2774	0.99	7/3767 (0.2%)
1	R	0.63	0/2792	1.00	9/3790 (0.2%)
All	All	0.61	2/49999 (0.0%)	0.98	115/67904 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	5
1	D	0	3
1	E	0	1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1
1	G	0	2
1	H	0	4
1	I	0	3
1	J	0	3
1	K	0	1
1	L	0	5
1	M	0	5
1	N	0	3
1	O	0	5
1	Q	0	4
1	R	0	3
All	All	0	52

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	166	PRO	C-O	-5.80	1.19	1.24
1	M	293	HIS	CG-CD2	-5.12	1.30	1.35

The worst 5 of 115 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	234	GLU	CB-CG-CD	-9.52	96.41	112.60
1	F	197	LYS	CB-CG-CD	9.26	132.61	111.30
1	H	286	ARG	CA-CB-CG	9.22	132.55	114.10
1	I	207	GLU	CB-CA-C	8.90	125.57	110.79
1	A	270	ARG	CB-CG-CD	8.80	131.54	111.30

There are no chirality outliers.

5 of 52 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	204	ARG	Sidechain
1	A	218[A]	ARG	Sidechain
1	B	145	ARG	Sidechain
1	B	204	ARG	Sidechain
1	C	145	ARG	Sidechain



## 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	2704	2664	2644	12	0
1	B	2686	2640	2628	12	0
1	C	2689	2640	2628	18	0
1	D	2701	2656	2644	14	0
1	E	2686	2640	2628	11	0
1	F	2681	2631	2621	11	0
1	G	2678	2631	2621	18	0
1	H	2685	2643	2633	13	1
1	I	2686	2640	2628	11	0
1	J	2692	2648	2636	17	0
1	K	2686	2640	2628	9	0
1	L	2710	2668	2644	15	0
1	M	2687	2640	2624	19	1
1	N	2683	2635	2623	12	0
1	O	2695	2653	2643	15	0
1	P	2695	2653	2643	13	0
1	Q	2689	2645	2635	13	0
1	R	2698	2654	2630	19	0
2	A	16	11	11	1	0
2	B	16	11	11	0	0
2	C	16	11	11	0	0
2	D	16	11	11	0	0
2	E	16	11	11	0	0
2	F	16	11	11	0	0
2	G	16	11	11	0	0
2	H	16	11	11	0	0
2	I	16	11	11	0	0
2	J	16	11	11	0	0
2	K	16	11	11	0	0
2	L	16	11	11	1	0
2	M	16	11	11	0	0
2	N	16	11	11	0	0
2	O	16	11	10	0	0
2	P	16	11	11	0	0
2	Q	16	11	11	0	0
2	R	16	11	11	2	0
3	J	7	10	10	4	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	N	7	10	10	1	0
4	K	13	18	18	3	0
5	O	10	14	14	0	0
6	Q	4	6	6	0	0
7	A	139	0	0	1	0
7	B	162	0	0	9	0
7	C	109	0	0	7	0
7	D	122	0	0	4	0
7	E	71	0	0	1	0
7	F	68	0	0	0	0
7	G	65	0	0	2	0
7	H	86	0	0	3	0
7	I	130	0	0	4	0
7	J	108	0	0	6	0
7	K	102	0	0	1	0
7	L	151	0	0	6	0
7	M	60	0	0	8	0
7	N	55	0	0	0	0
7	O	119	0	0	3	0
7	P	57	0	0	0	0
7	Q	112	0	0	0	0
7	R	103	0	0	10	0
All	All	50579	47877	47636	238	1

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 2.

The worst 5 of 238 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:O:161[B]:MET:HE2	7:O:566[B]:HOH:O	1.22	1.39
1:C:161[A]:MET:HE2	7:C:585[A]:HOH:O	1.12	1.26
1:M:161[B]:MET:CE	7:M:557[B]:HOH:O	1.81	1.23
1:I:161[B]:MET:HE2	7:I:1825[B]:HOH:O	1.39	1.20
1:D:161[B]:MET:HE2	7:D:618[B]:HOH:O	1.40	1.18

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:296:ASP:OD2	1:M:296:ASP:OD2[1_554]	1.83	0.37

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	341/380 (90%)	331 (97%)	9 (3%)	1 (0%)	36	50
1	B	338/380 (89%)	328 (97%)	9 (3%)	1 (0%)	36	50
1	C	338/380 (89%)	328 (97%)	9 (3%)	1 (0%)	36	50
1	D	340/380 (90%)	330 (97%)	9 (3%)	1 (0%)	36	50
1	E	338/380 (89%)	328 (97%)	9 (3%)	1 (0%)	36	50
1	F	336/380 (88%)	327 (97%)	8 (2%)	1 (0%)	36	50
1	G	336/380 (88%)	326 (97%)	9 (3%)	1 (0%)	36	50
1	H	338/380 (89%)	329 (97%)	8 (2%)	1 (0%)	36	50
1	I	338/380 (89%)	328 (97%)	9 (3%)	1 (0%)	36	50
1	J	339/380 (89%)	329 (97%)	9 (3%)	1 (0%)	36	50
1	K	338/380 (89%)	328 (97%)	9 (3%)	1 (0%)	36	50
1	L	342/380 (90%)	333 (97%)	8 (2%)	1 (0%)	36	50
1	M	338/380 (89%)	328 (97%)	9 (3%)	1 (0%)	36	50
1	N	337/380 (89%)	327 (97%)	9 (3%)	1 (0%)	36	50
1	O	339/380 (89%)	330 (97%)	8 (2%)	1 (0%)	36	50
1	P	339/380 (89%)	329 (97%)	9 (3%)	1 (0%)	36	50
1	Q	338/380 (89%)	328 (97%)	9 (3%)	1 (0%)	36	50
1	R	340/380 (90%)	329 (97%)	10 (3%)	1 (0%)	36	50
All	All	6093/6840 (89%)	5916 (97%)	159 (3%)	18 (0%)	36	50

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	49	SER
1	B	49	SER
1	C	49	SER
1	D	49	SER
1	E	49	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	276/302 (91%)	270 (98%)	6 (2%)	45	67
1	B	272/302 (90%)	269 (99%)	3 (1%)	65	82
1	C	272/302 (90%)	269 (99%)	3 (1%)	65	82
1	D	273/302 (90%)	271 (99%)	2 (1%)	76	88
1	E	272/302 (90%)	267 (98%)	5 (2%)	51	73
1	F	271/302 (90%)	266 (98%)	5 (2%)	51	73
1	G	271/302 (90%)	264 (97%)	7 (3%)	40	63
1	H	273/302 (90%)	268 (98%)	5 (2%)	51	73
1	I	272/302 (90%)	269 (99%)	3 (1%)	65	82
1	J	273/302 (90%)	269 (98%)	4 (2%)	57	77
1	K	272/302 (90%)	270 (99%)	2 (1%)	76	88
1	L	277/302 (92%)	274 (99%)	3 (1%)	65	82
1	M	272/302 (90%)	267 (98%)	5 (2%)	51	73
1	N	271/302 (90%)	266 (98%)	5 (2%)	51	73
1	O	274/302 (91%)	266 (97%)	8 (3%)	37	60
1	P	274/302 (91%)	270 (98%)	4 (2%)	57	77
1	Q	273/302 (90%)	269 (98%)	4 (2%)	57	77
1	R	275/302 (91%)	271 (98%)	4 (2%)	57	77
All	All	4913/5436 (90%)	4835 (98%)	78 (2%)	55	76

5 of 78 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	334	VAL
1	Q	197	LYS
1	O	142	LYS
1	O	338	MET
1	R	20	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	N	235	GLN
1	Q	235	GLN
1	O	48	GLN
1	P	235	GLN
1	R	224	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

23 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	BG6	N	401	-	16,16,16	0.56	0	23,24,24	0.99	1 (4%)
2	BG6	P	401	-	16,16,16	0.61	0	23,24,24	0.62	0
2	BG6	B	401	-	16,16,16	0.52	0	23,24,24	0.70	0
2	BG6	Q	401	-	16,16,16	0.56	0	23,24,24	0.93	0
6	EDO	Q	402	-	3,3,3	0.15	0	2,2,2	0.08	0
2	BG6	K	401	-	16,16,16	0.48	0	23,24,24	0.88	0
2	BG6	G	401	-	16,16,16	0.44	0	23,24,24	0.83	0
3	PEG	J	402	-	6,6,6	0.41	0	5,5,5	0.35	0
2	BG6	C	401	-	16,16,16	0.57	0	23,24,24	0.59	0
2	BG6	F	401	-	16,16,16	0.48	0	23,24,24	0.78	0
2	BG6	O	401	-	16,16,16	0.81	0	23,24,24	1.19	3 (13%)
2	BG6	J	401	-	16,16,16	0.52	0	23,24,24	1.04	2 (8%)
2	BG6	A	401	-	16,16,16	0.50	0	23,24,24	0.77	0
5	PGE	O	402	-	9,9,9	0.39	0	8,8,8	0.26	0
2	BG6	R	401	-	16,16,16	0.41	0	23,24,24	0.68	0
2	BG6	M	401	-	16,16,16	0.55	0	23,24,24	0.82	0
2	BG6	I	401	-	16,16,16	0.57	0	23,24,24	1.09	1 (4%)
2	BG6	H	401	-	16,16,16	0.50	0	23,24,24	0.79	0
2	BG6	D	401	-	16,16,16	0.66	0	23,24,24	0.58	0
2	BG6	E	401	-	16,16,16	0.52	0	23,24,24	0.72	0
3	PEG	N	402	-	6,6,6	0.19	0	5,5,5	0.16	0
4	PG4	K	402	-	12,12,12	0.47	0	11,11,11	0.33	0
2	BG6	L	401	-	16,16,16	0.52	0	23,24,24	0.80	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BG6	N	401	-	-	2/6/26/26	0/1/1/1
2	BG6	P	401	-	-	1/6/26/26	0/1/1/1
2	BG6	B	401	-	-	3/6/26/26	0/1/1/1
2	BG6	Q	401	-	-	0/6/26/26	0/1/1/1
6	EDO	Q	402	-	-	1/1/1/1	-
2	BG6	K	401	-	-	3/6/26/26	0/1/1/1
2	BG6	G	401	-	-	0/6/26/26	0/1/1/1
3	PEG	J	402	-	-	1/4/4/4	-
2	BG6	C	401	-	-	0/6/26/26	0/1/1/1
2	BG6	F	401	-	-	5/6/26/26	0/1/1/1
2	BG6	O	401	-	-	6/6/26/26	0/1/1/1

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BG6	J	401	-	-	0/6/26/26	0/1/1/1
2	BG6	A	401	-	-	3/6/26/26	0/1/1/1
5	PGE	O	402	-	-	4/7/7/7	-
2	BG6	R	401	-	-	3/6/26/26	0/1/1/1
2	BG6	M	401	-	-	5/6/26/26	0/1/1/1
2	BG6	I	401	-	-	3/6/26/26	0/1/1/1
2	BG6	H	401	-	-	2/6/26/26	0/1/1/1
2	BG6	D	401	-	-	0/6/26/26	0/1/1/1
2	BG6	E	401	-	-	4/6/26/26	0/1/1/1
3	PEG	N	402	-	-	1/4/4/4	-
4	PG4	K	402	-	-	7/10/10/10	-
2	BG6	L	401	-	-	1/6/26/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	401	BG6	O1-C1-O5	-2.63	102.61	110.41
2	O	401	BG6	O5-C5-C4	2.52	114.23	109.70
2	N	401	BG6	O1-C1-C2	2.43	116.04	108.98
2	O	401	BG6	O1-C1-O5	-2.36	103.40	110.41
2	O	401	BG6	C1-O5-C5	2.17	117.85	113.65

There are no chirality outliers.

5 of 55 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	BG6	C6-O6-P-O1P
2	A	401	BG6	C6-O6-P-O2P
2	B	401	BG6	C6-O6-P-O2P
2	E	401	BG6	O5-C5-C6-O6
2	E	401	BG6	C4-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 12 short contacts:

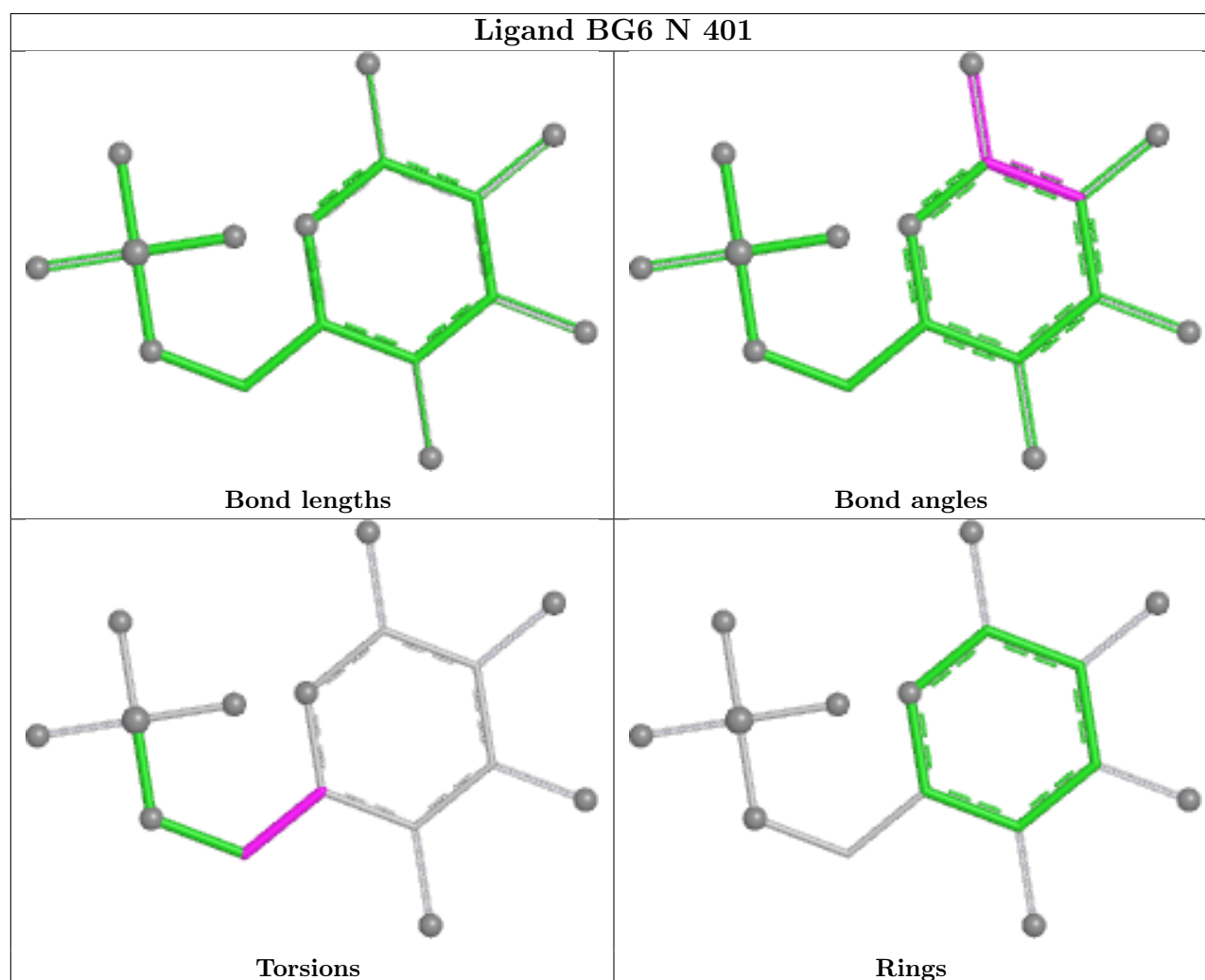
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	402	PEG	4	0
2	A	401	BG6	1	0

*Continued on next page...*

*Continued from previous page...*

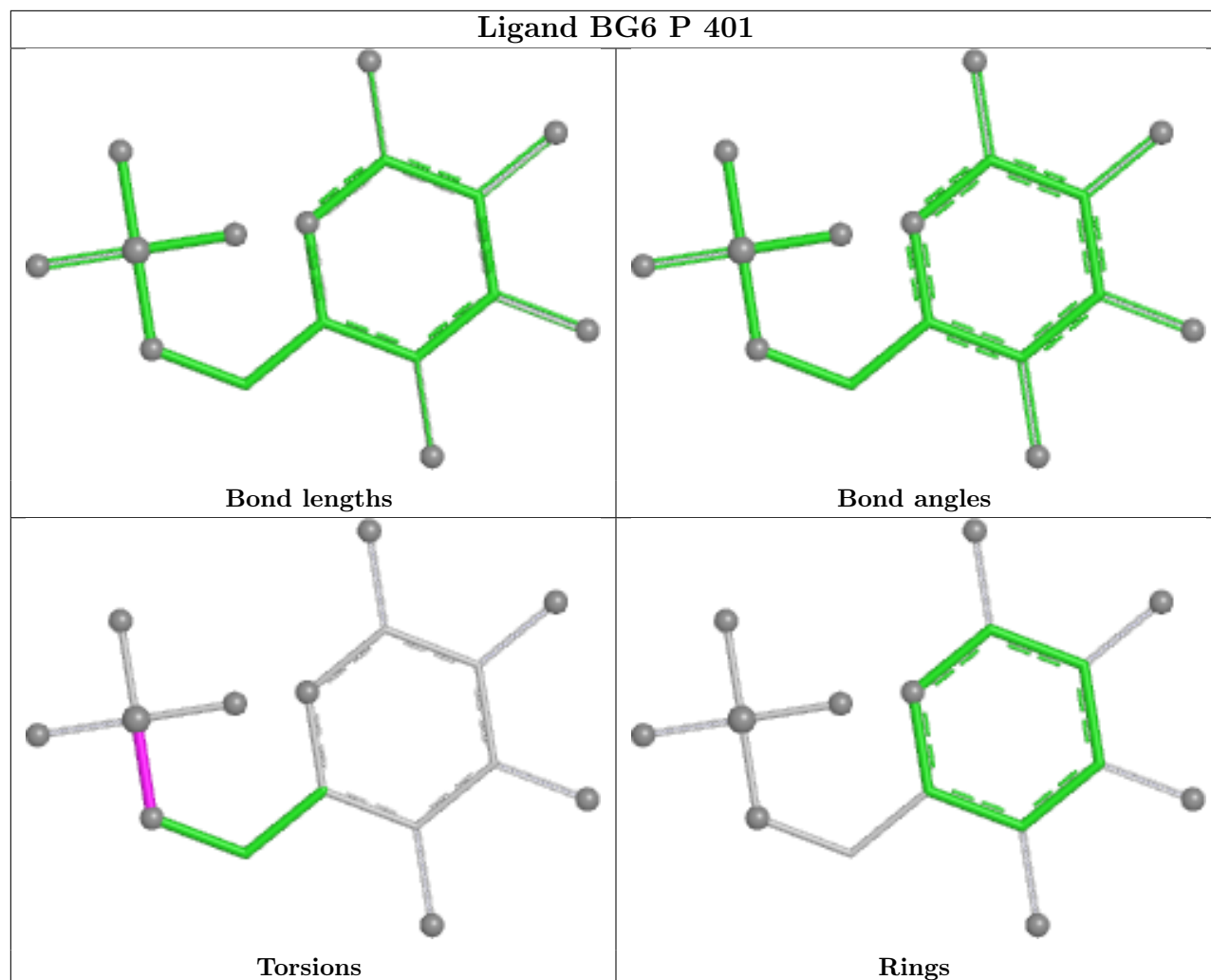
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	R	401	BG6	2	0
3	N	402	PEG	1	0
4	K	402	PG4	3	0
2	L	401	BG6	1	0

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

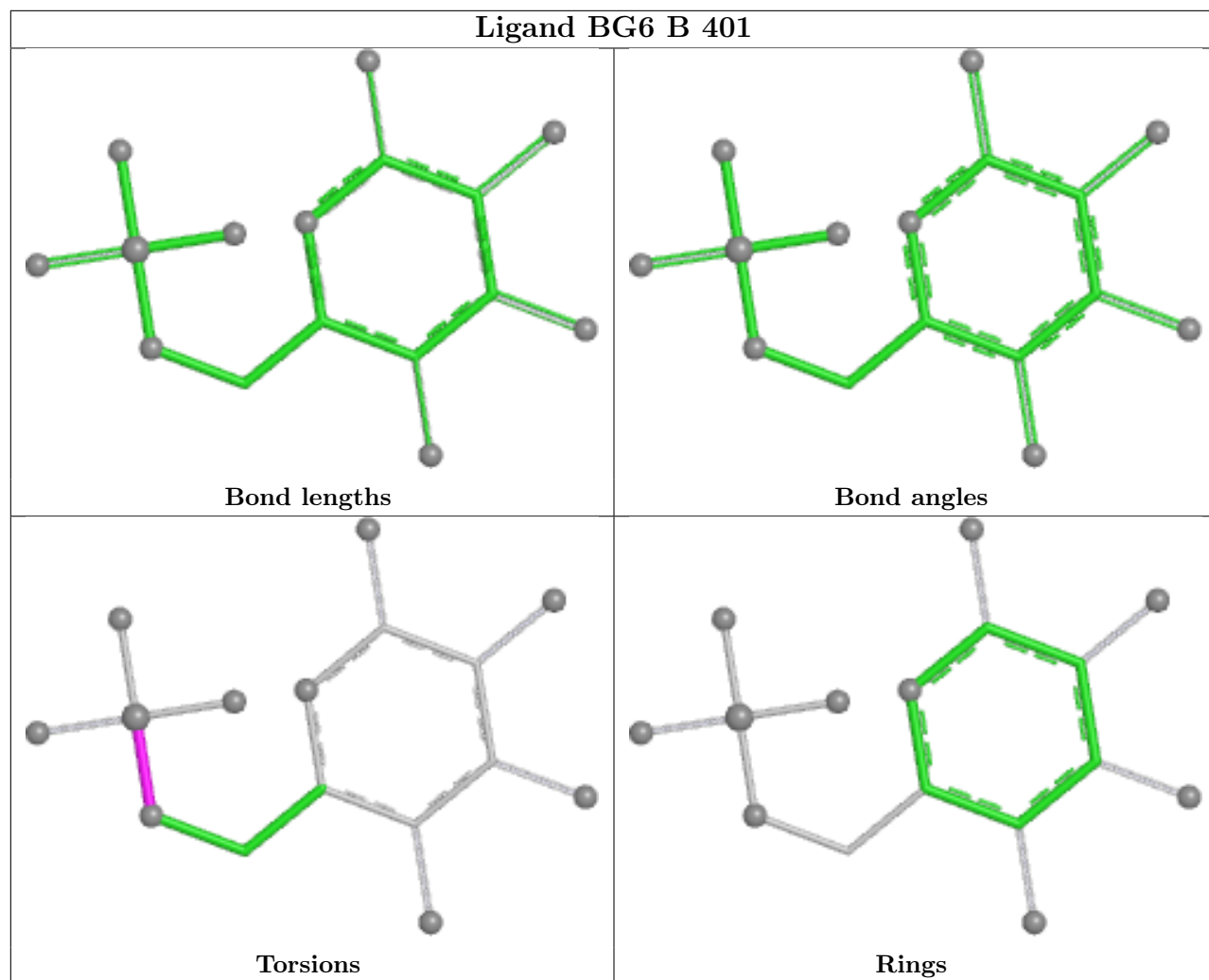




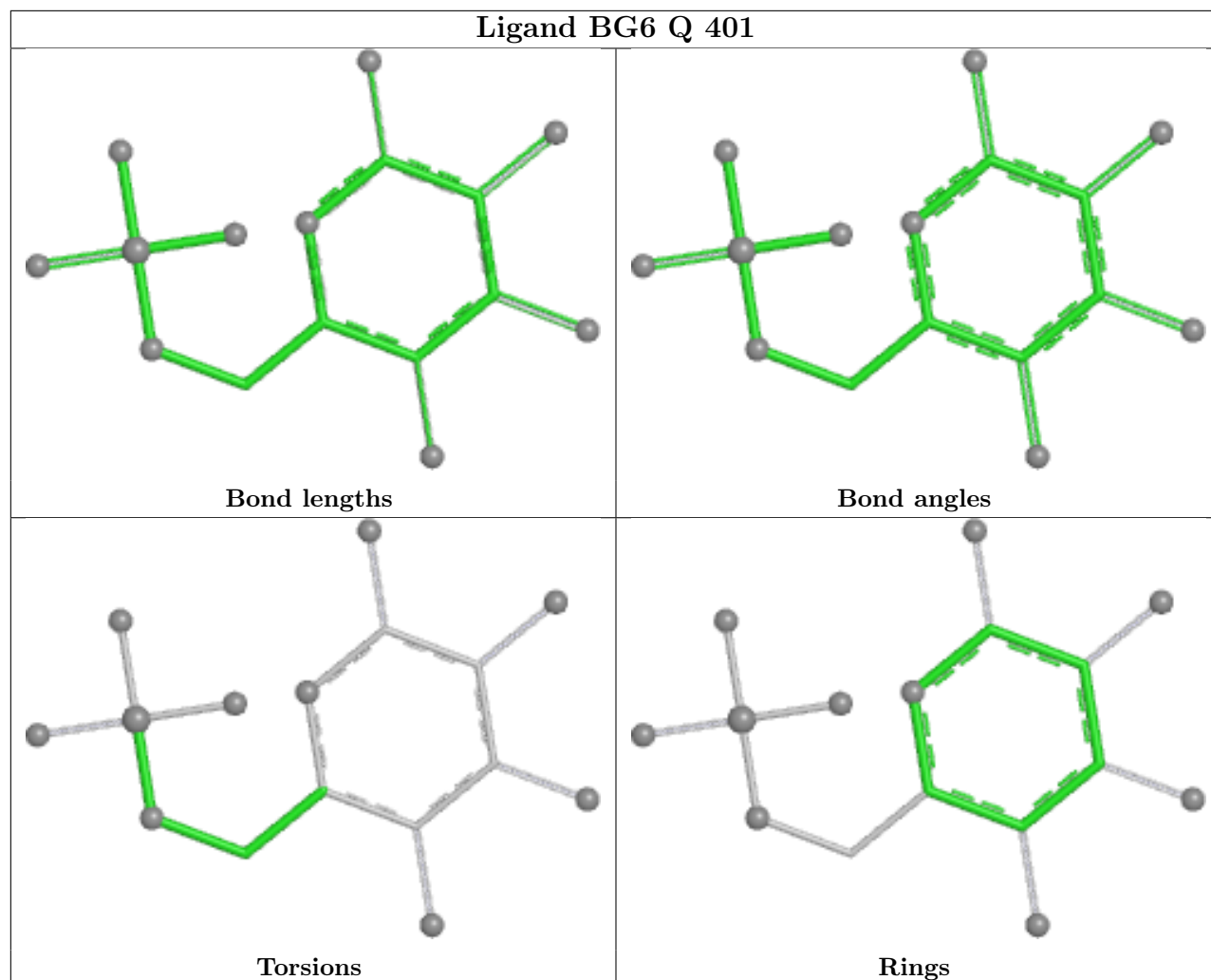
## Ligand BG6 P 401



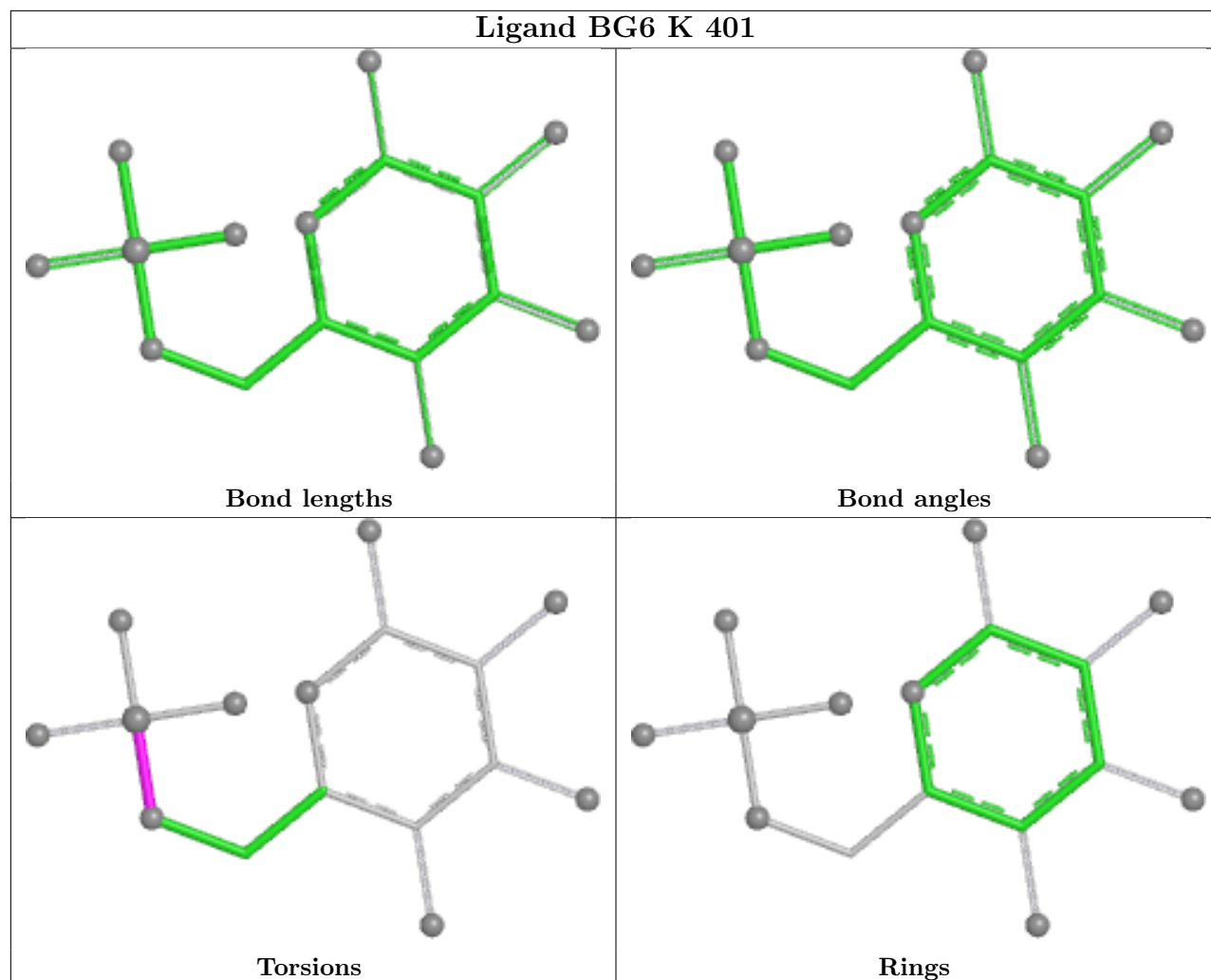
## Ligand BG6 B 401



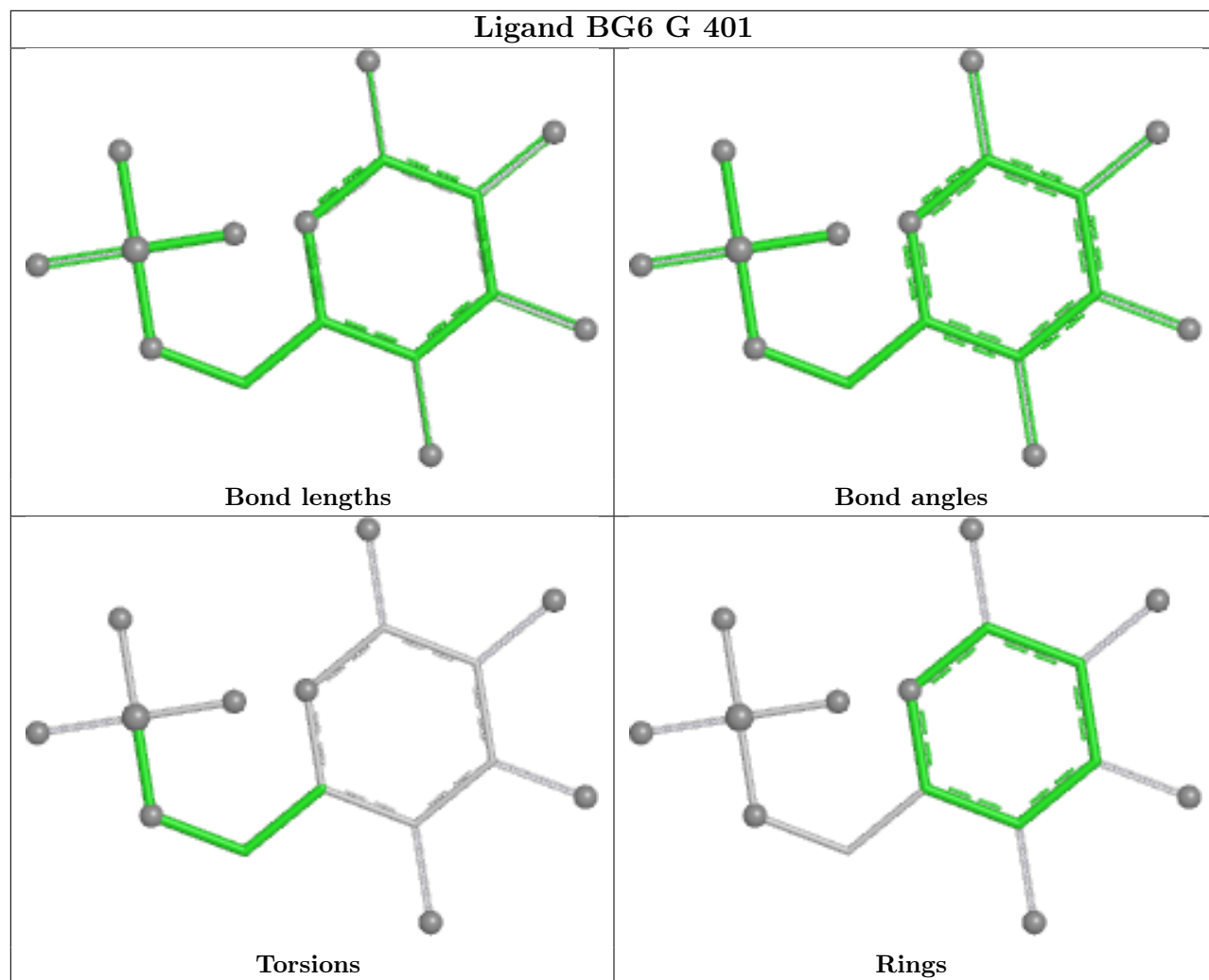
## Ligand BG6 Q 401



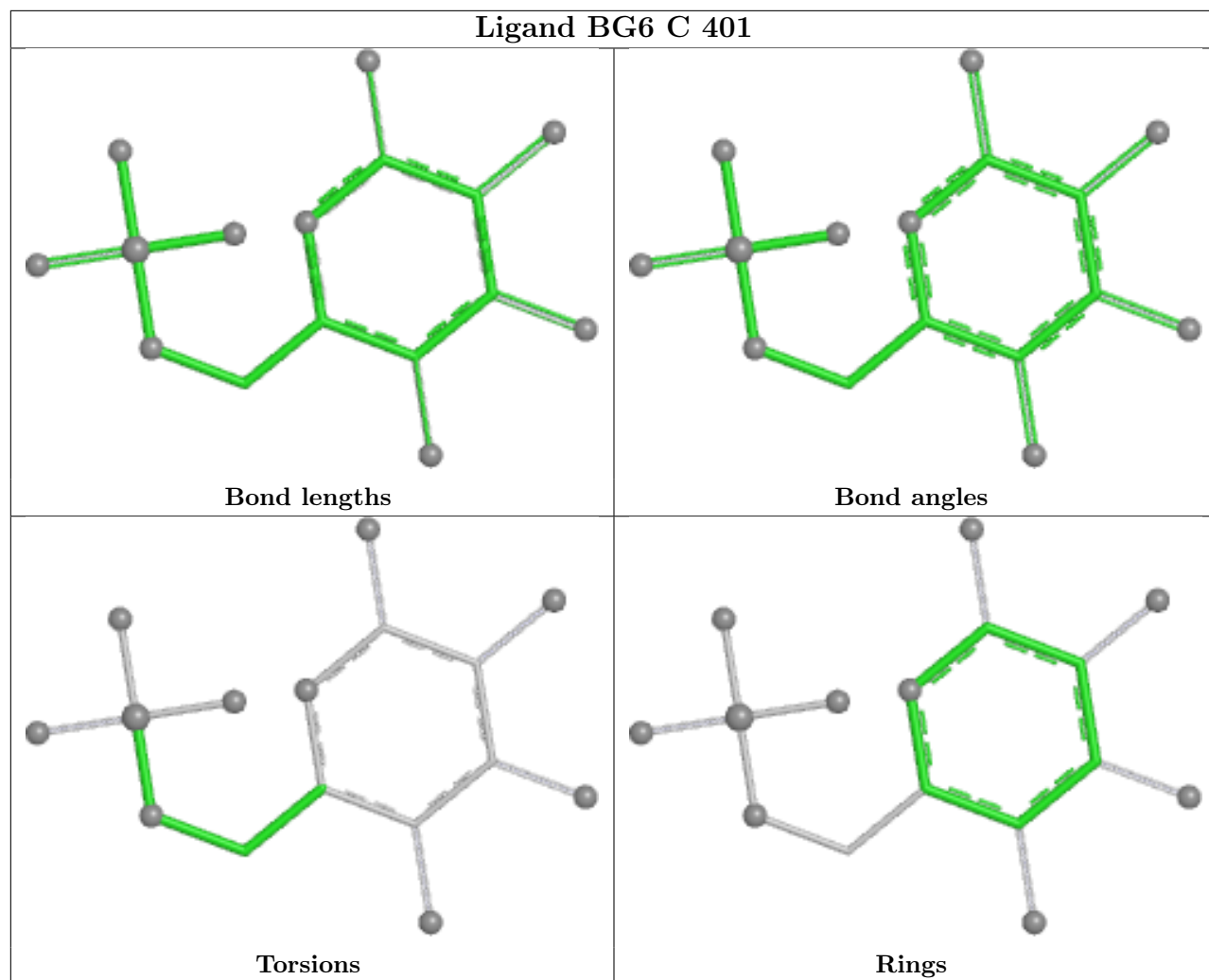
## Ligand BG6 K 401



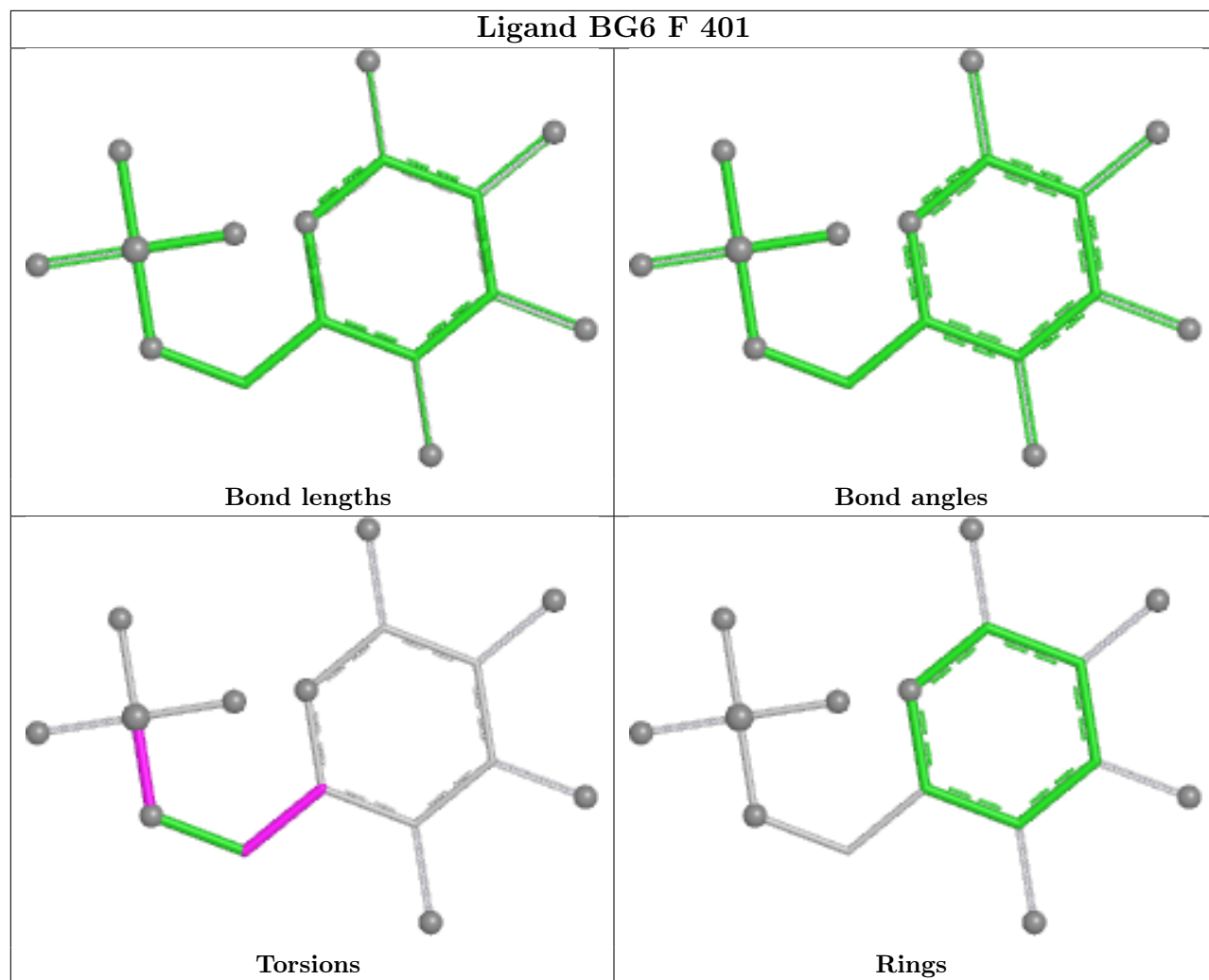
## Ligand BG6 G 401



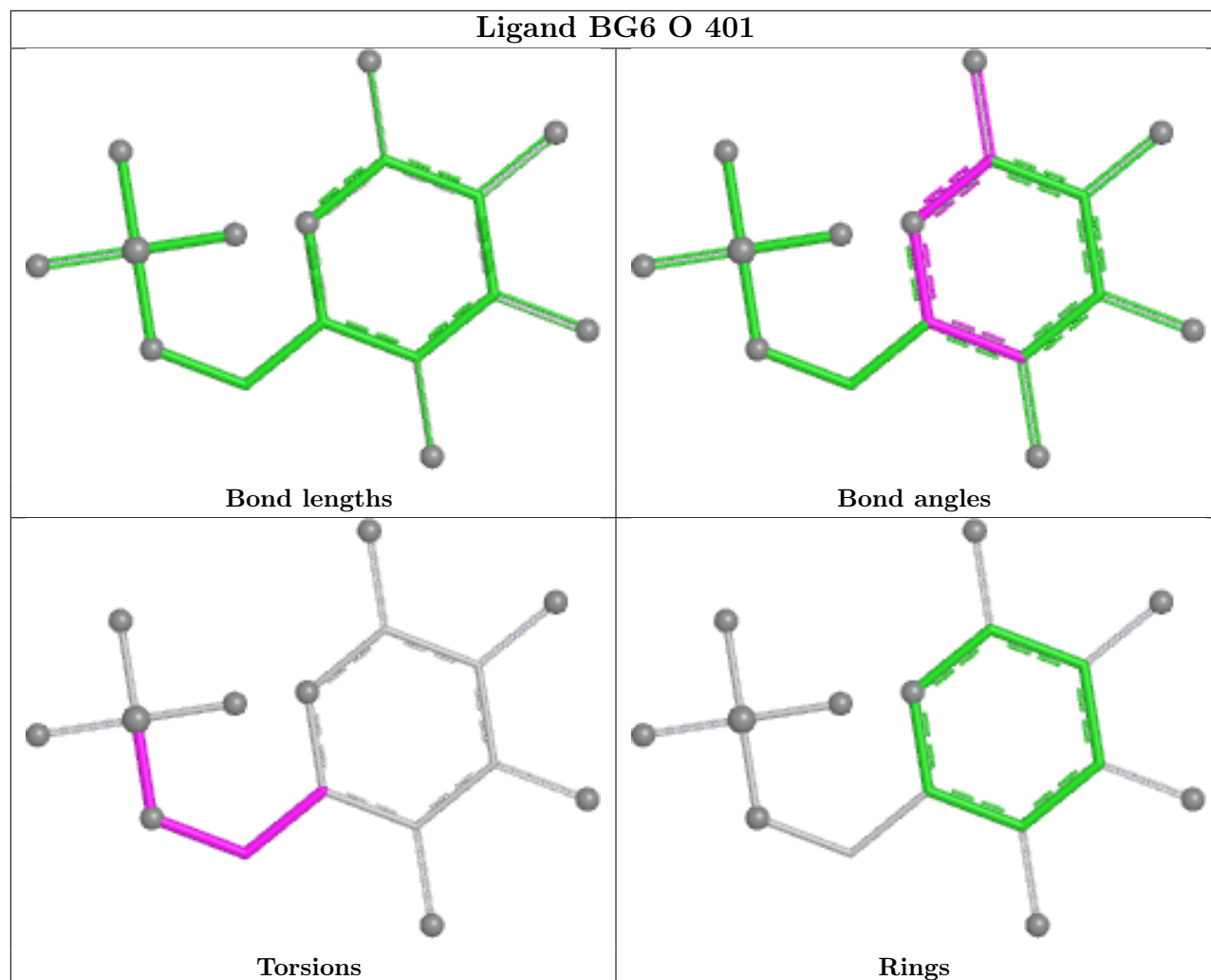
## Ligand BG6 C 401



## Ligand BG6 F 401

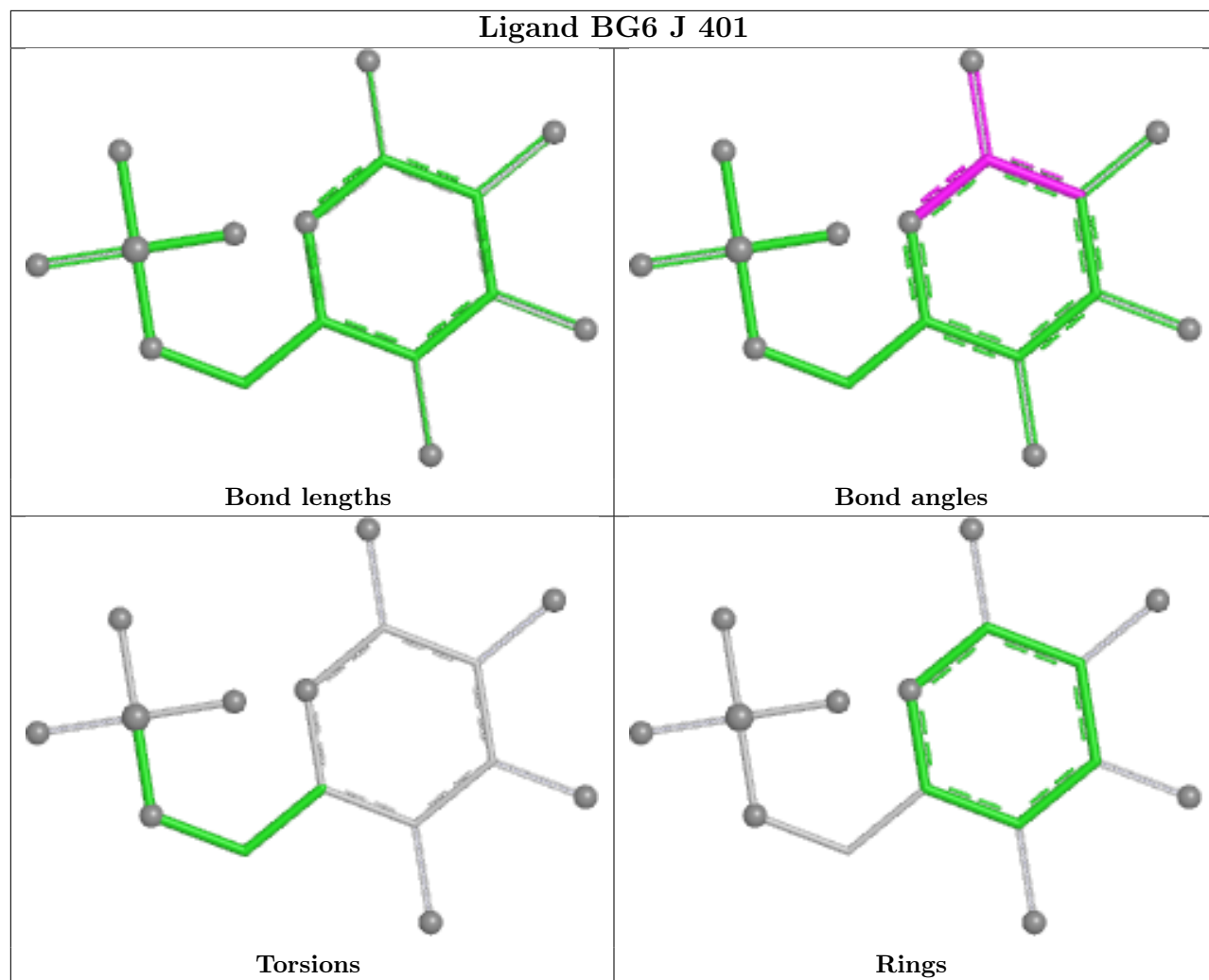


## Ligand BG6 O 401

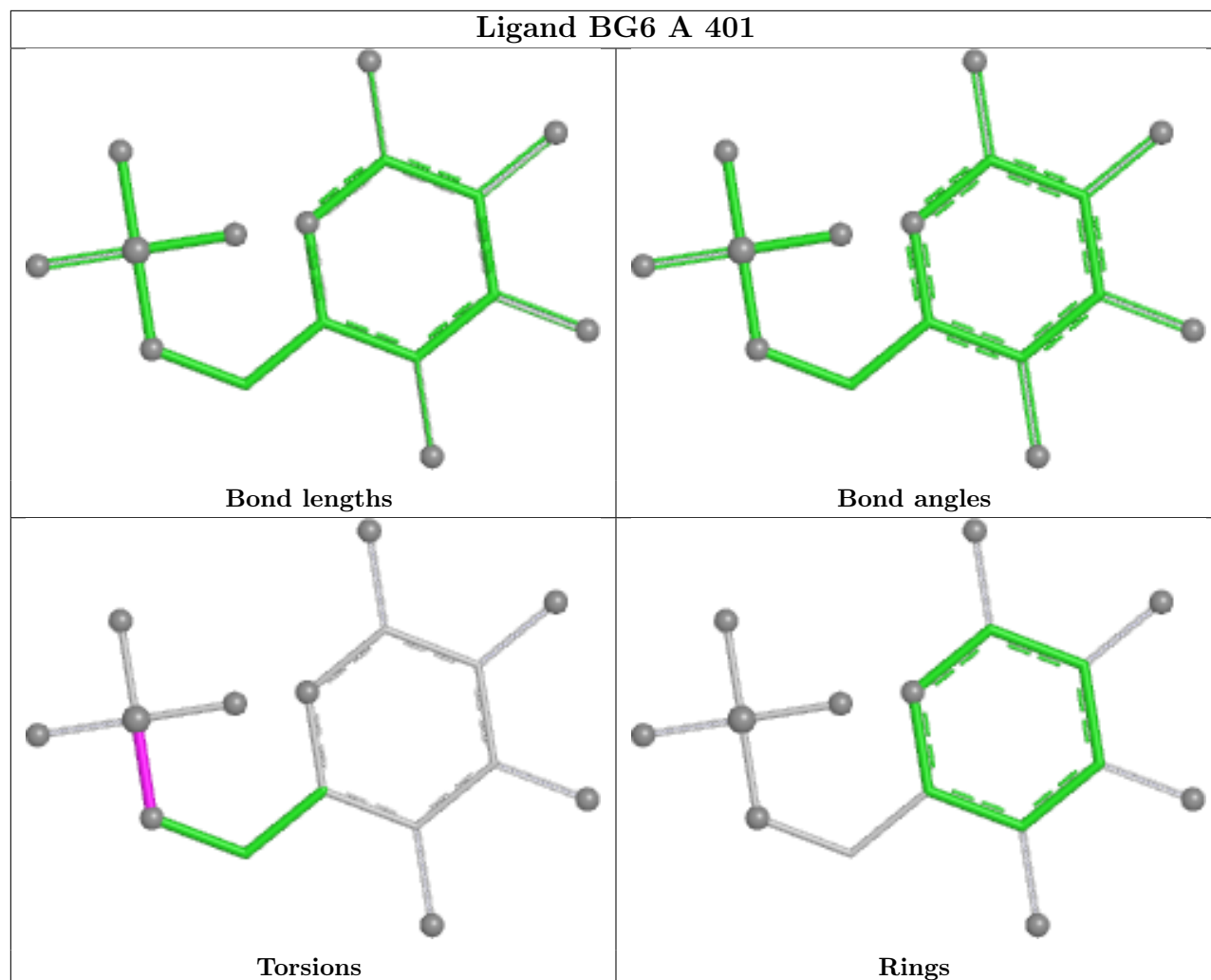




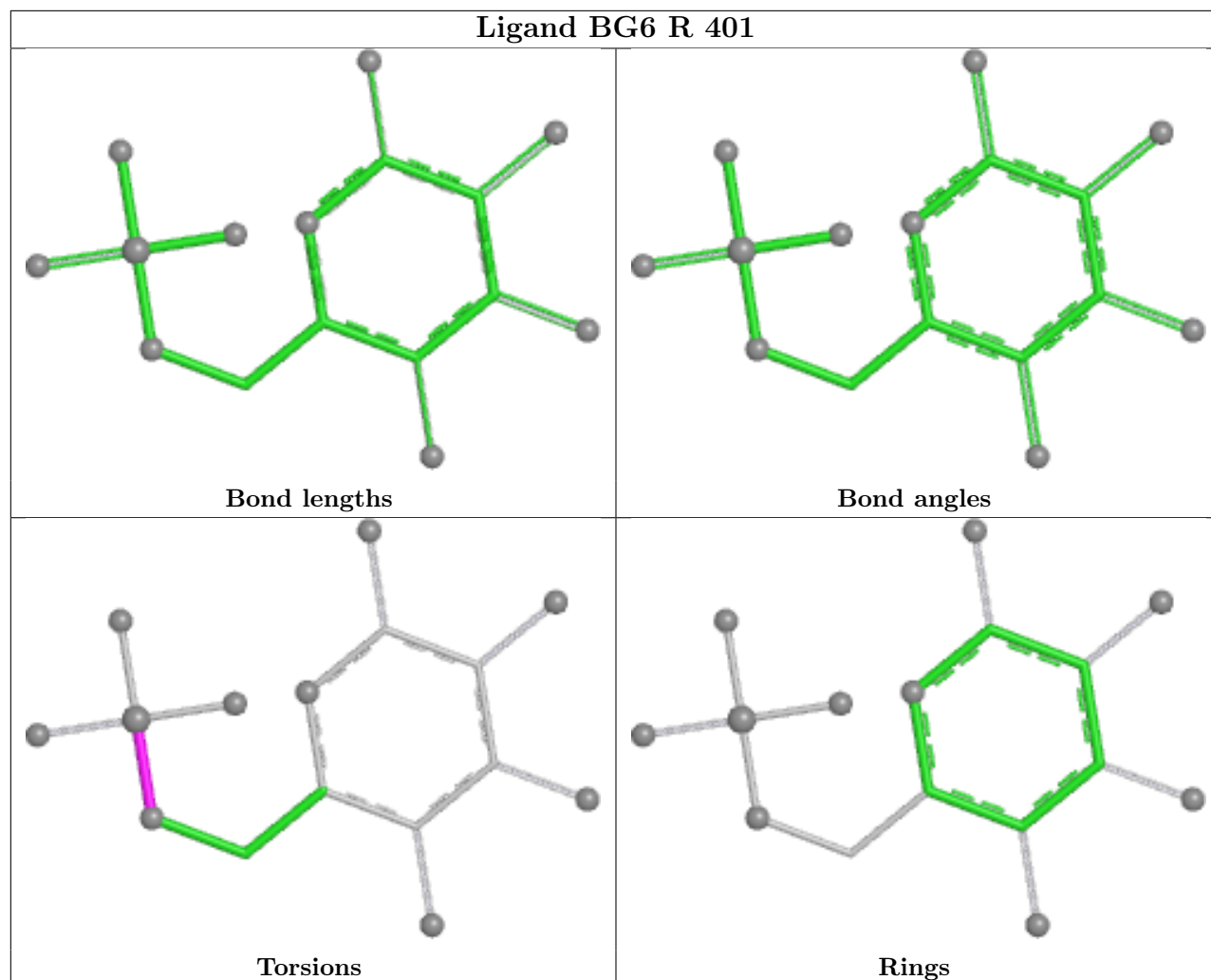
## Ligand BG6 J 401

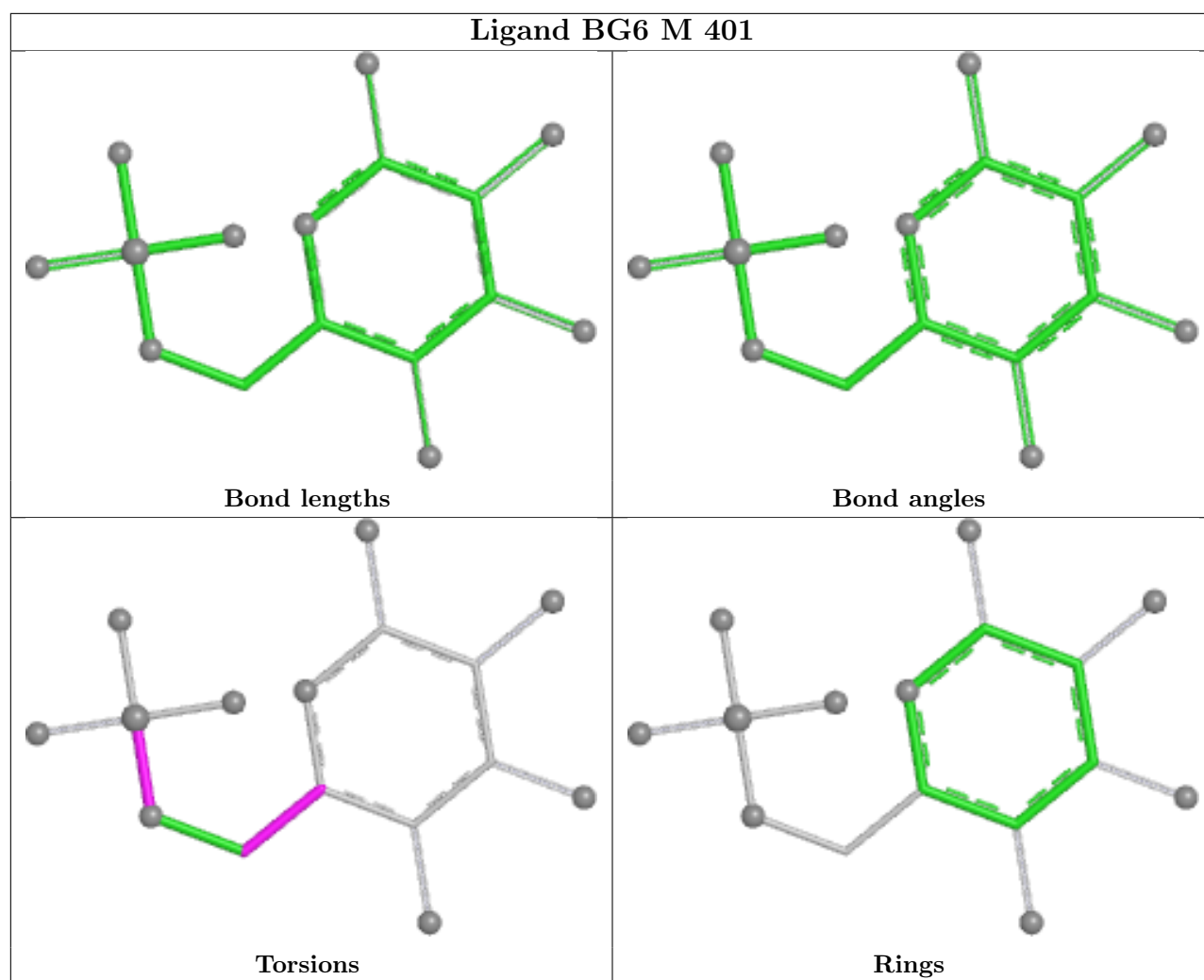


## Ligand BG6 A 401

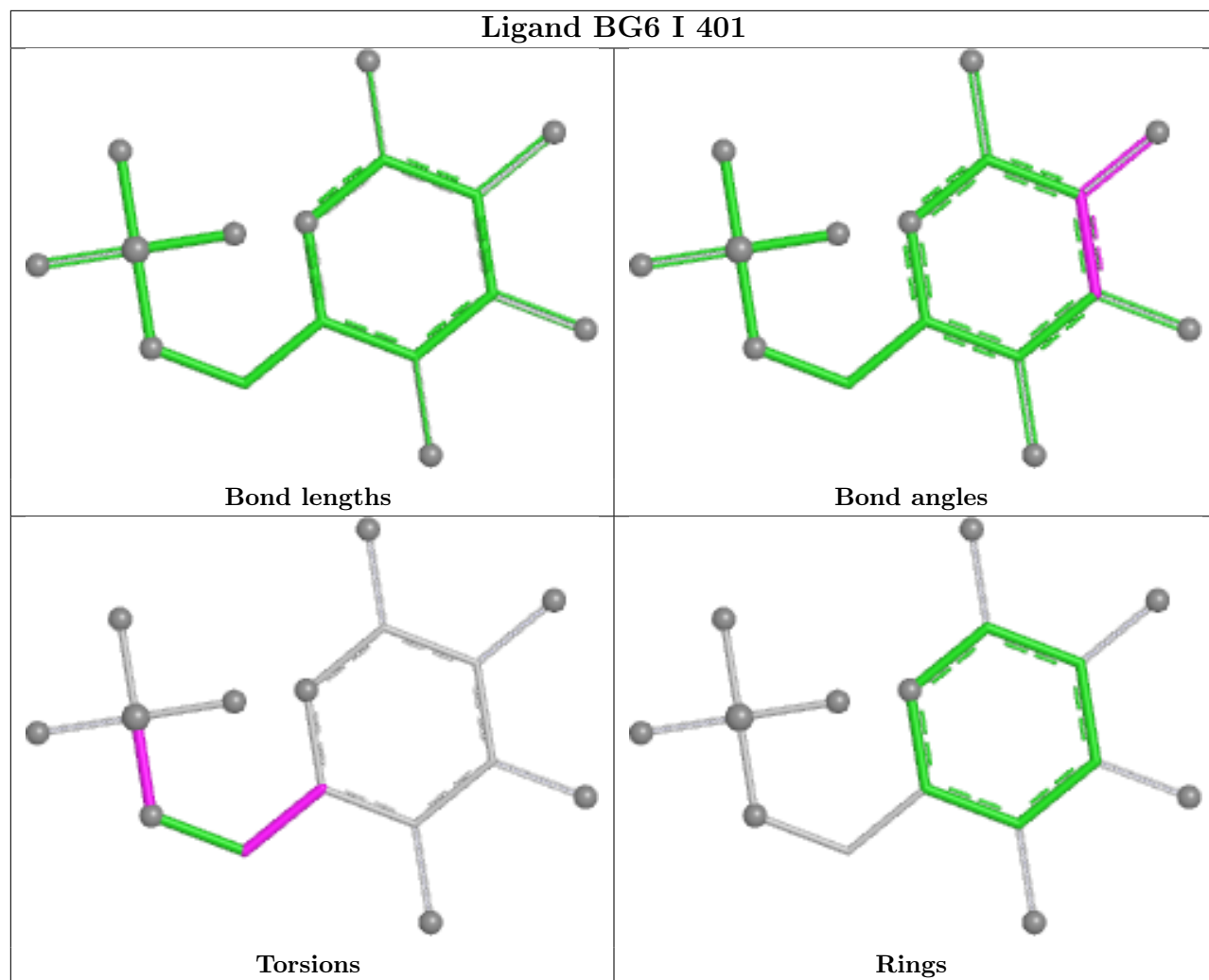


## Ligand BG6 R 401

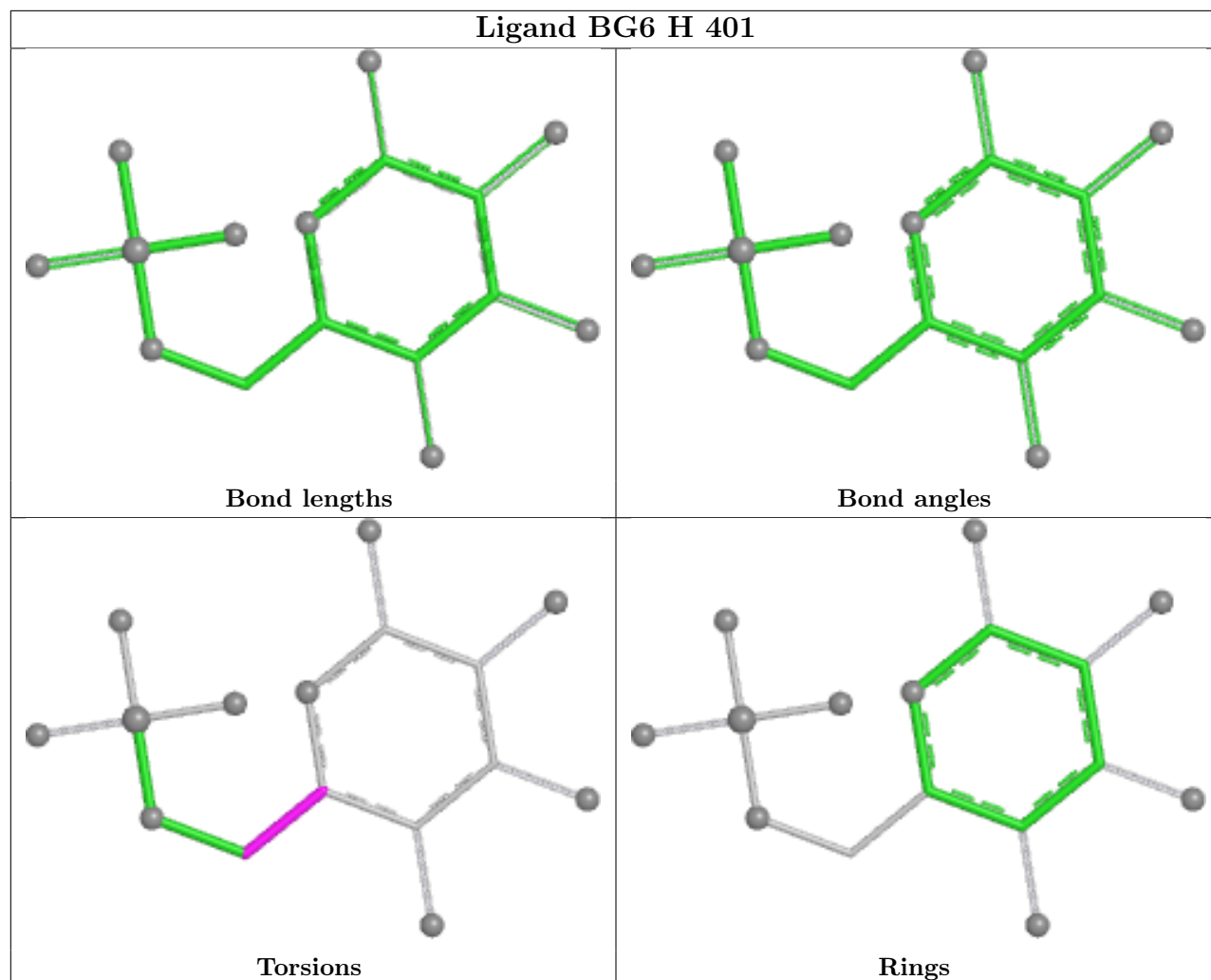




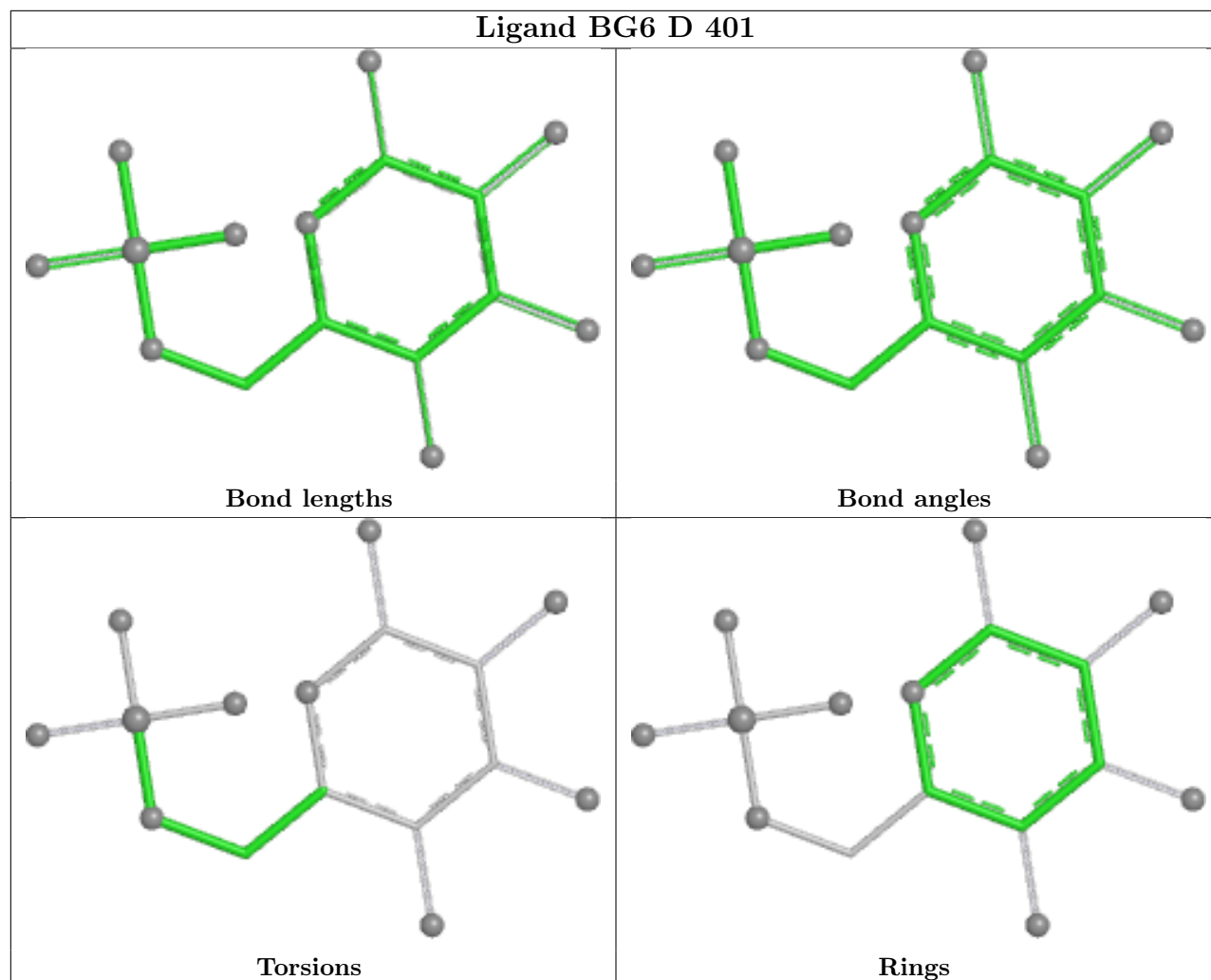
## Ligand BG6 I 401



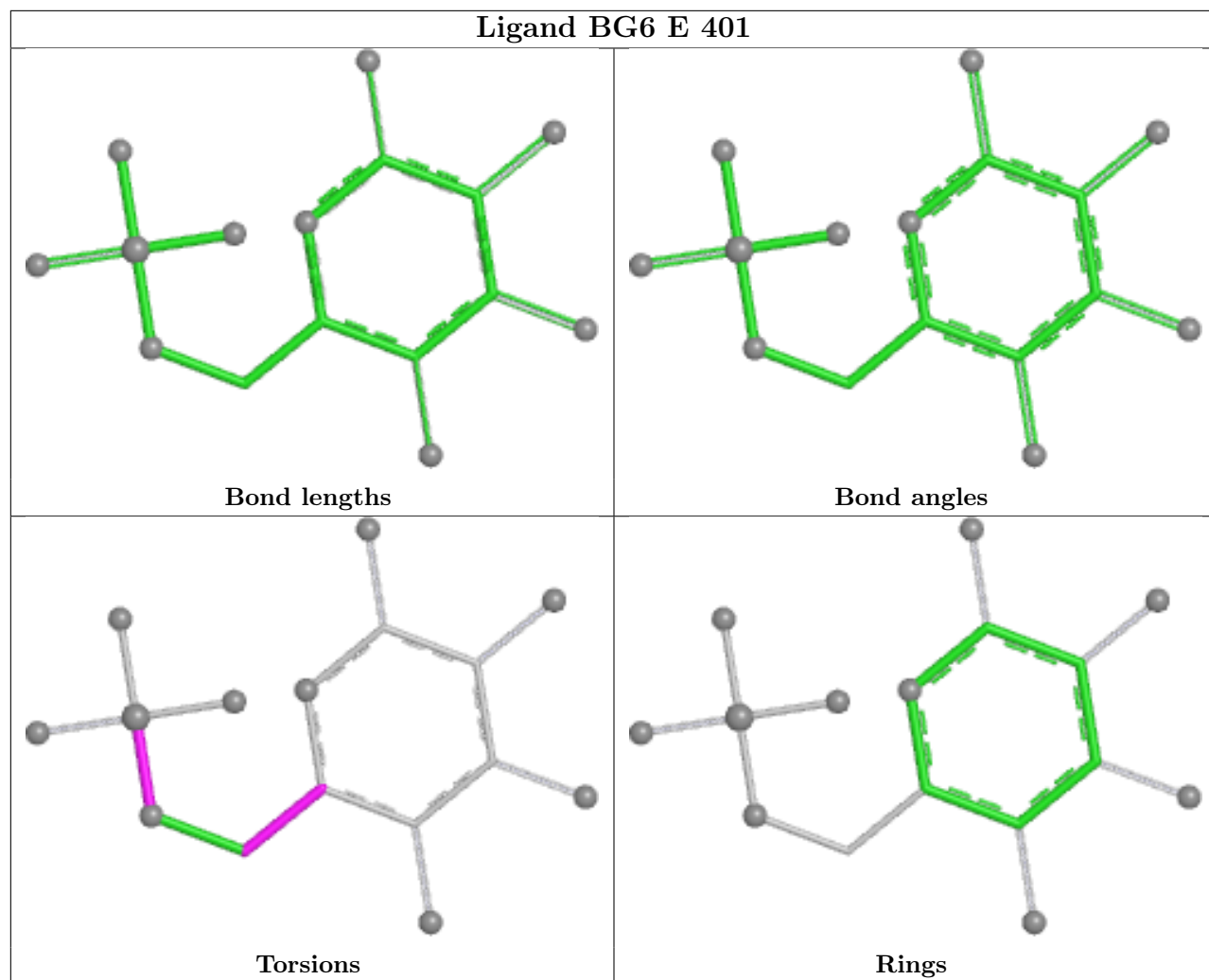
## Ligand BG6 H 401



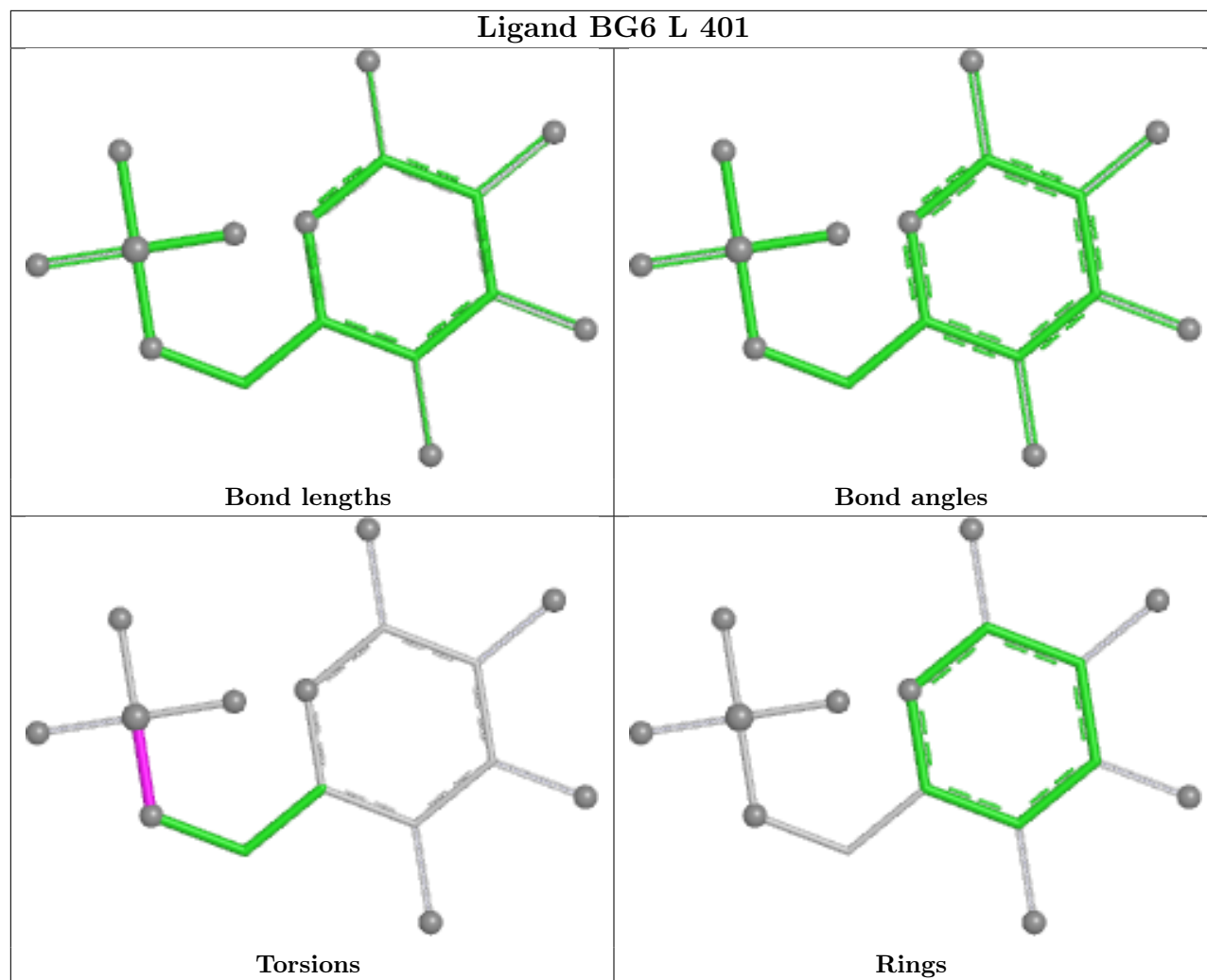
## Ligand BG6 D 401



## Ligand BG6 E 401







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	337/380 (88%)	-0.62	2 (0%) 85 83	16, 31, 60, 94	5 (1%)
1	B	338/380 (88%)	-0.63	4 (1%) 76 73	16, 32, 55, 95	2 (0%)
1	C	338/380 (88%)	-0.34	2 (0%) 85 83	20, 41, 73, 94	2 (0%)
1	D	340/380 (89%)	-0.55	2 (0%) 85 83	17, 35, 66, 93	2 (0%)
1	E	338/380 (88%)	0.02	6 (1%) 67 63	27, 52, 83, 101	2 (0%)
1	F	337/380 (88%)	-0.15	2 (0%) 85 83	25, 52, 83, 111	1 (0%)
1	G	337/380 (88%)	-0.02	3 (0%) 81 78	29, 54, 86, 106	1 (0%)
1	H	337/380 (88%)	-0.18	3 (0%) 81 78	27, 47, 75, 110	3 (0%)
1	I	338/380 (88%)	-0.55	3 (0%) 81 78	17, 35, 63, 90	2 (0%)
1	J	338/380 (88%)	-0.50	3 (0%) 81 78	18, 36, 64, 91	3 (0%)
1	K	338/380 (88%)	-0.42	3 (0%) 81 78	21, 39, 70, 100	2 (0%)
1	L	338/380 (88%)	-0.60	2 (0%) 85 83	15, 33, 55, 101	5 (1%)
1	M	337/380 (88%)	0.02	7 (2%) 63 59	30, 51, 76, 105	2 (0%)
1	N	338/380 (88%)	0.15	7 (2%) 63 59	33, 59, 89, 104	1 (0%)
1	O	338/380 (88%)	-0.48	2 (0%) 85 83	17, 36, 58, 92	3 (0%)
1	P	338/380 (88%)	-0.03	6 (1%) 67 63	25, 53, 88, 117	3 (0%)
1	Q	338/380 (88%)	-0.39	2 (0%) 85 83	20, 39, 64, 98	2 (0%)
1	R	338/380 (88%)	-0.30	3 (0%) 81 78	21, 41, 69, 99	3 (0%)
All	All	6081/6840 (88%)	-0.31	62 (1%) 79 76	15, 42, 78, 117	44 (0%)

The worst 5 of 62 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	338	MET	7.7
1	E	338	MET	6.3
1	J	338	MET	5.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	Q	338	MET	5.6
1	N	338	MET	5.5

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	BG6	O	401	16/16	0.79	0.31	23,49,68,74	27
2	BG6	L	401	16/16	0.80	0.34	49,71,81,81	27
5	PGE	O	402	10/10	0.81	0.24	62,86,93,101	2
2	BG6	R	401	16/16	0.83	0.35	16,34,37,38	27
3	PEG	N	402	7/7	0.84	0.27	67,104,108,109	2
2	BG6	P	401	16/16	0.84	0.30	13,39,48,49	27
4	PG4	K	402	13/13	0.85	0.21	57,81,99,102	2
2	BG6	Q	401	16/16	0.86	0.23	11,29,34,36	27
2	BG6	I	401	16/16	0.87	0.18	22,43,47,50	27
2	BG6	N	401	16/16	0.89	0.20	20,50,52,53	27
2	BG6	G	401	16/16	0.91	0.16	15,40,42,45	27
3	PEG	J	402	7/7	0.91	0.15	45,69,74,76	2
2	BG6	E	401	16/16	0.91	0.14	26,58,62,63	27
2	BG6	K	401	16/16	0.91	0.13	22,38,49,51	27
2	BG6	F	401	16/16	0.91	0.14	24,47,49,50	27
6	EDO	Q	402	4/4	0.91	0.16	49,64,64,67	2
2	BG6	C	401	16/16	0.93	0.10	22,41,43,44	27
2	BG6	J	401	16/16	0.93	0.11	22,36,37,39	27
2	BG6	A	401	16/16	0.93	0.11	23,36,45,52	27
2	BG6	H	401	16/16	0.93	0.14	16,38,40,40	27
2	BG6	M	401	16/16	0.93	0.12	24,50,52,53	27

*Continued on next page...*

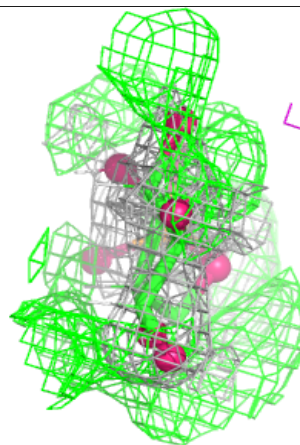
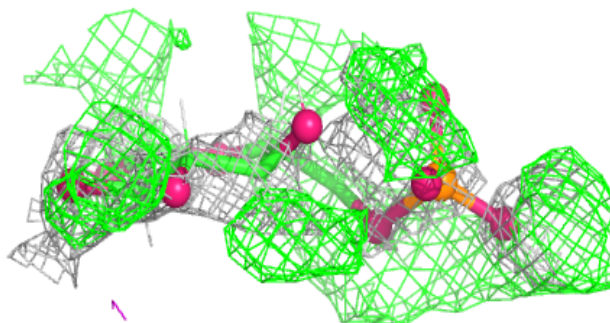
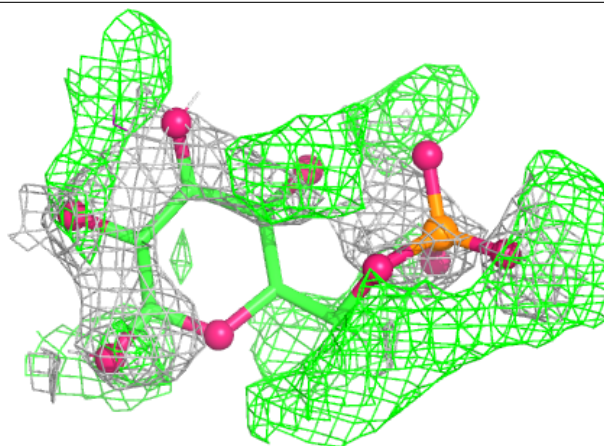
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	BG6	B	401	16/16	0.94	0.10	21,31,34,36	27
2	BG6	D	401	16/16	0.95	0.09	22,35,42,44	27

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.

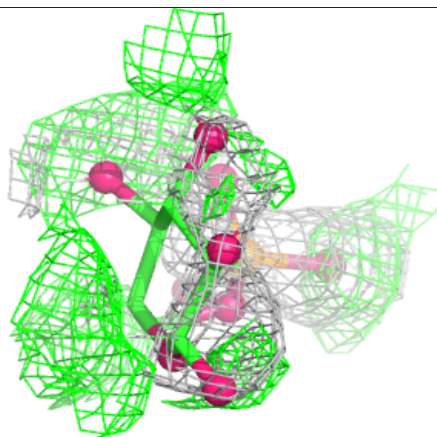
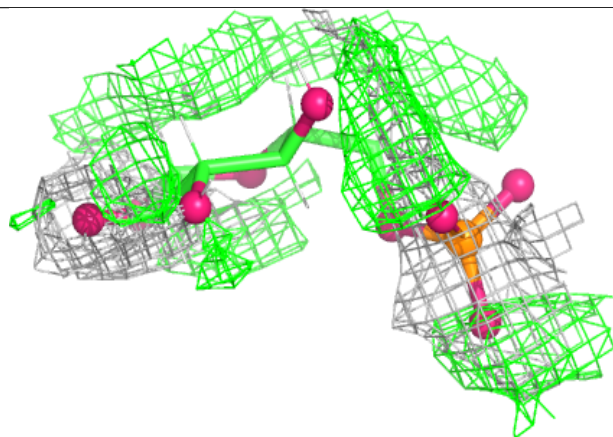
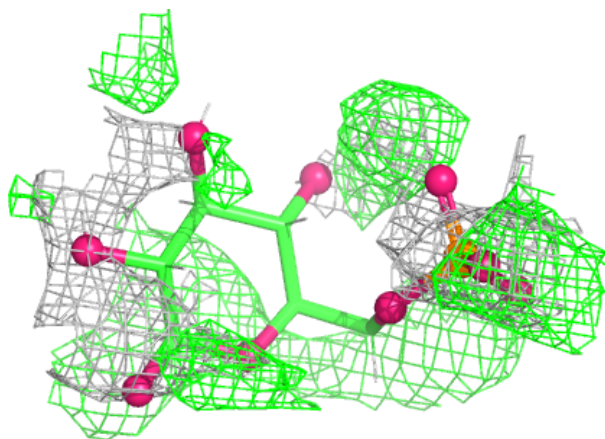
**Electron density around BG6 O 401:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



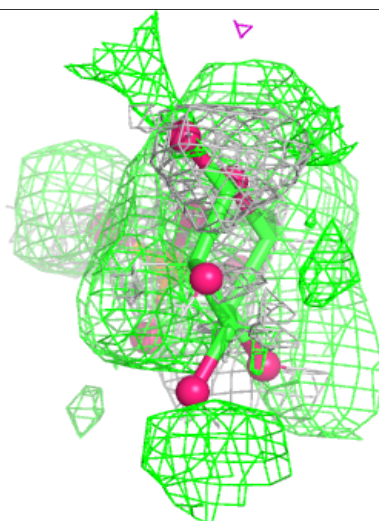
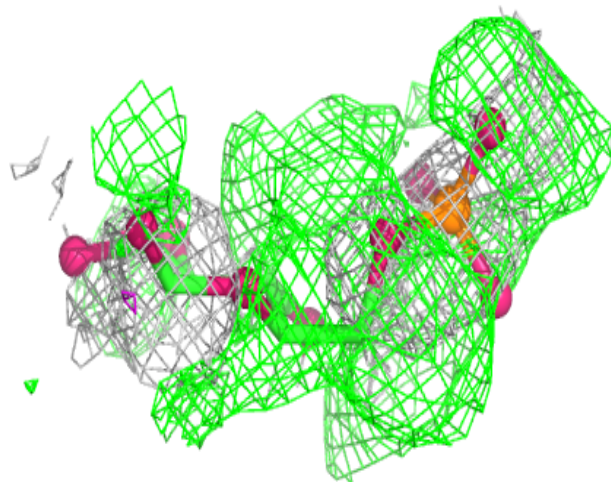
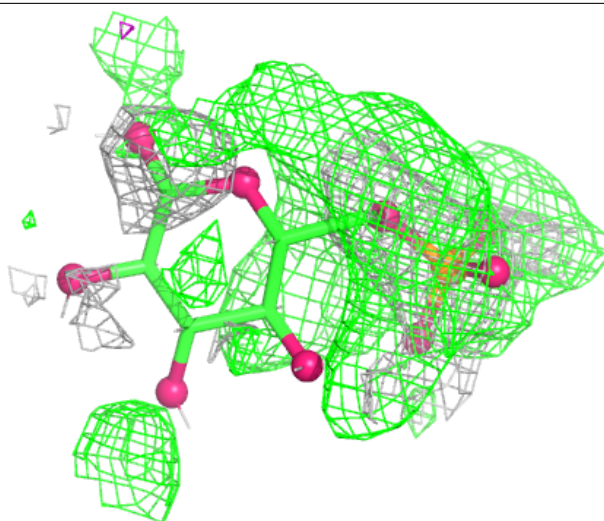
**Electron density around BG6 L 401:**

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



**Electron density around BG6 R 401:**

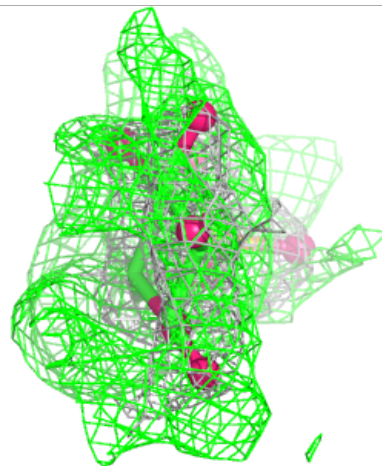
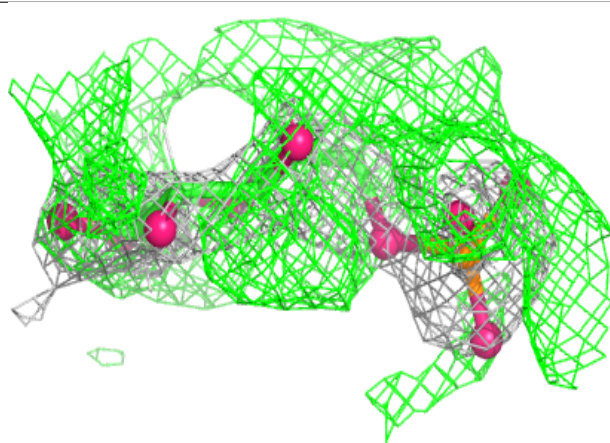
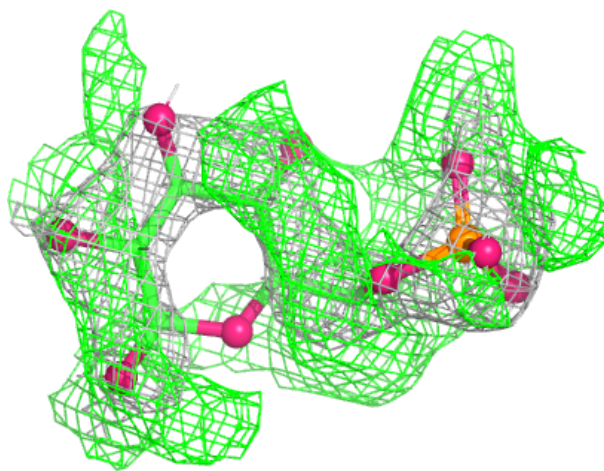
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





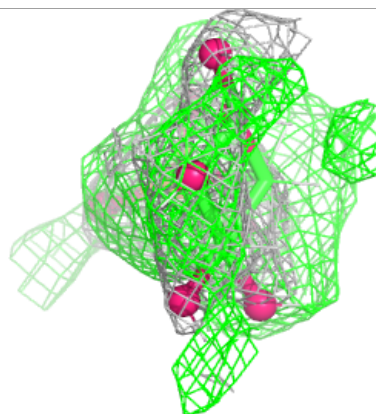
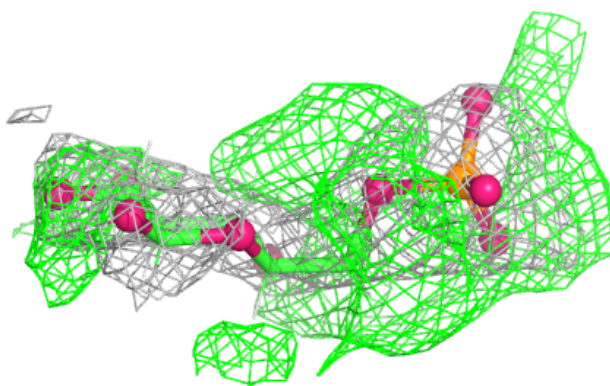
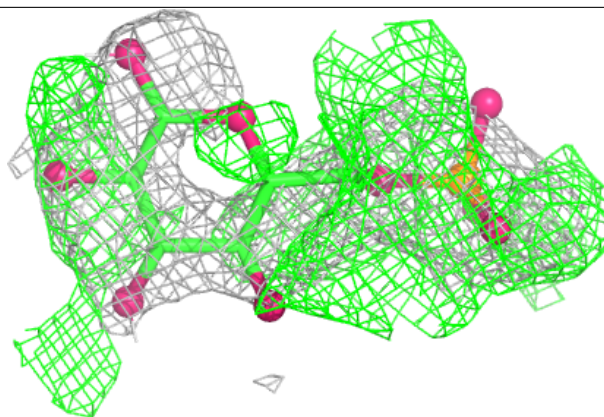
**Electron density around BG6 P 401:**

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



**Electron density around BG6 Q 401:**

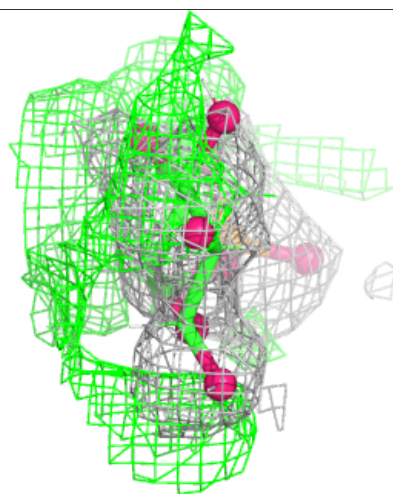
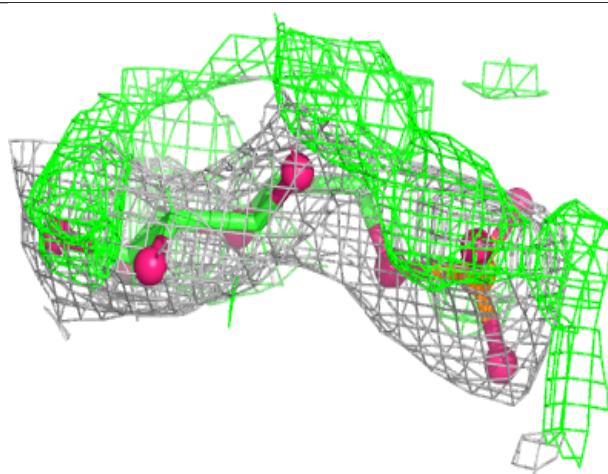
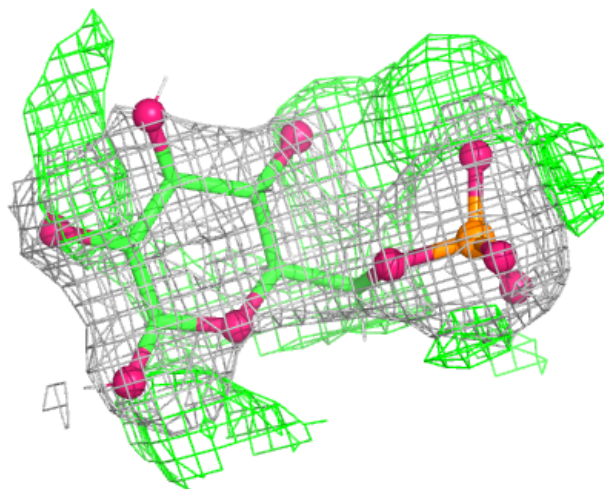
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





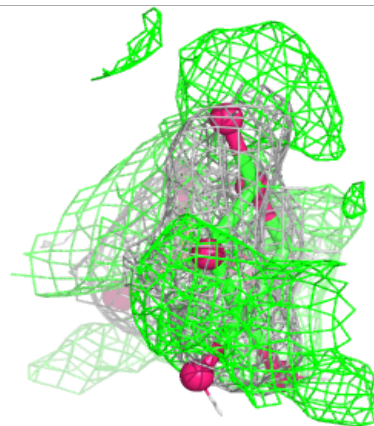
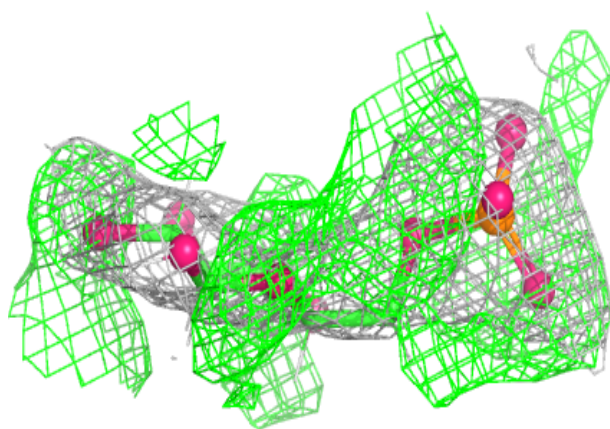
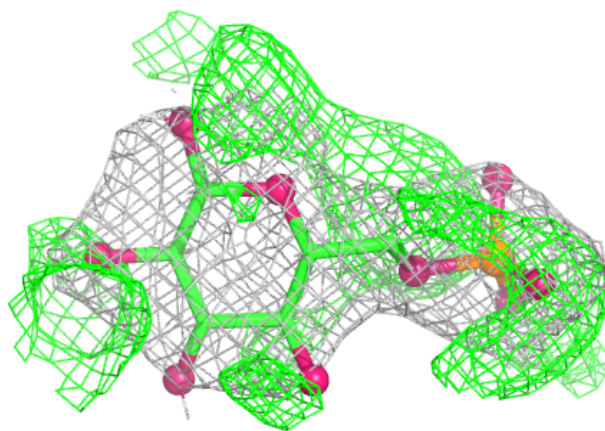
**Electron density around BG6 I 401:**

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



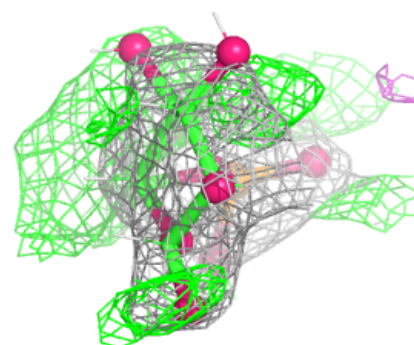
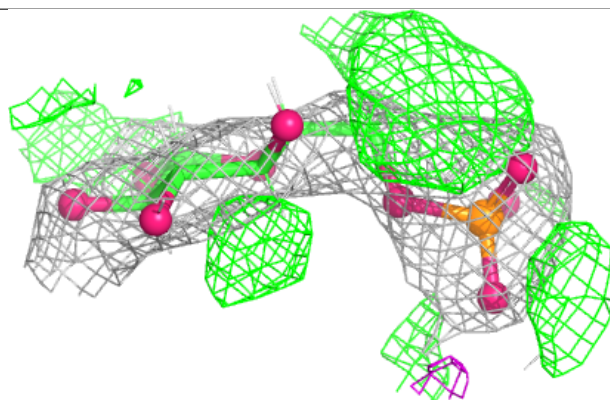
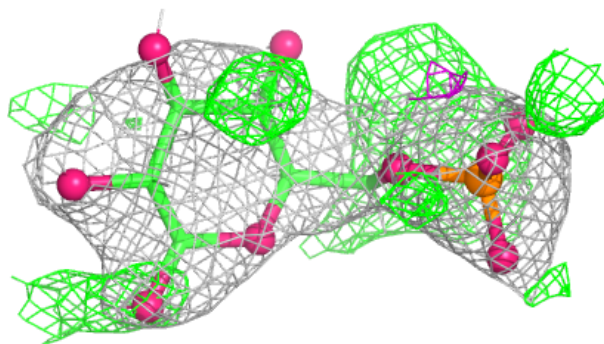
**Electron density around BG6 N 401:**

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

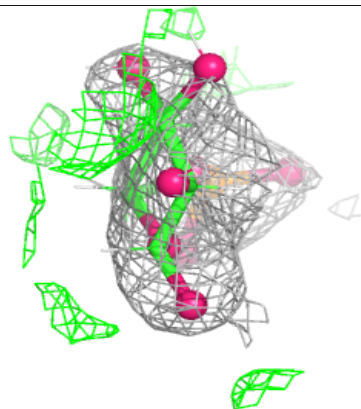
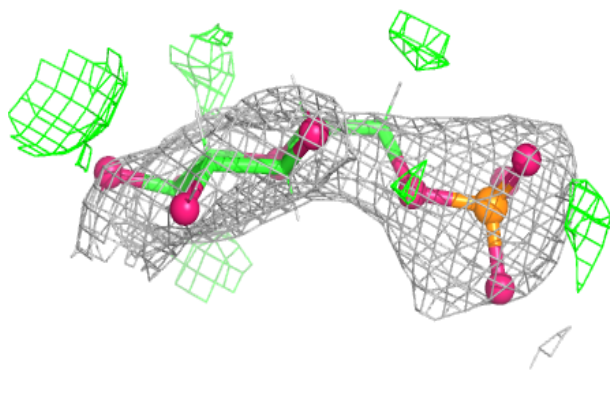
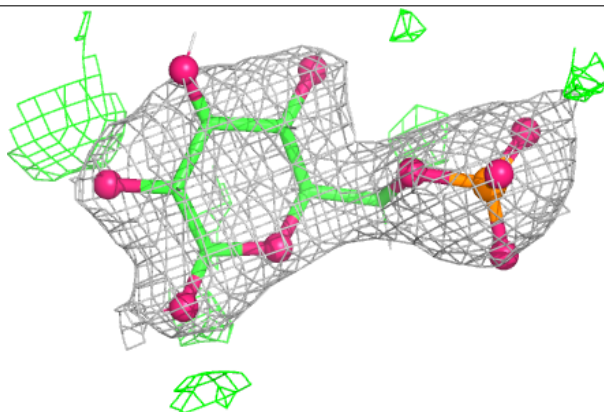


**Electron density around BG6 G 401:**

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

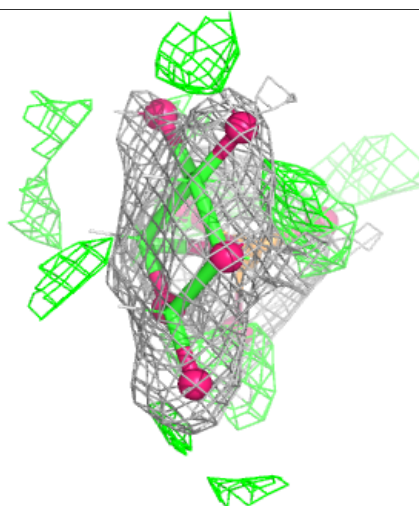
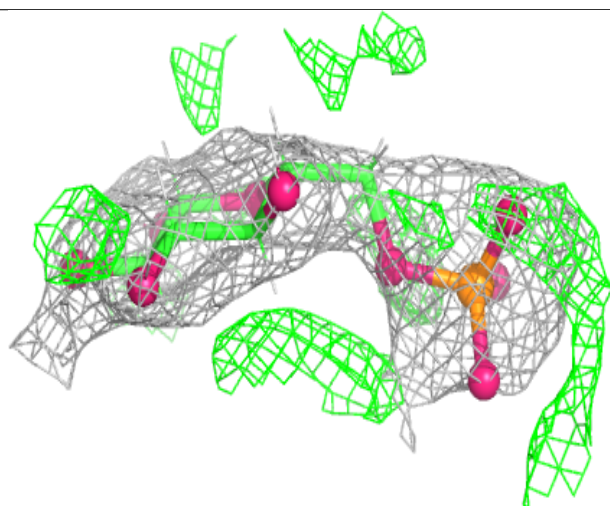
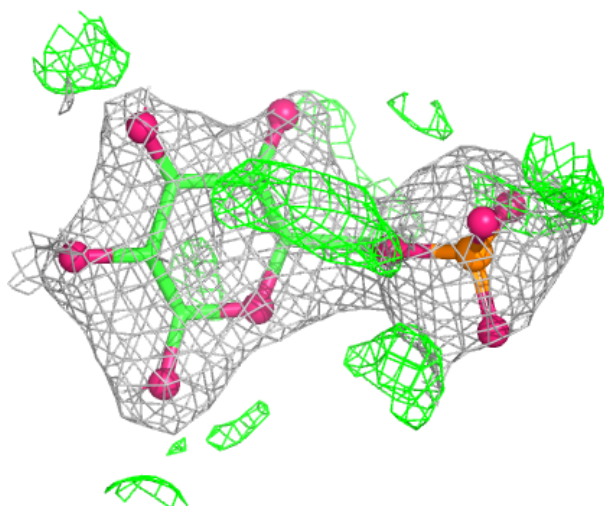
**Electron density around BG6 E 401:**

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



**Electron density around BG6 K 401:**

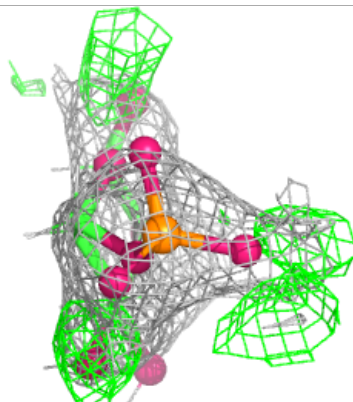
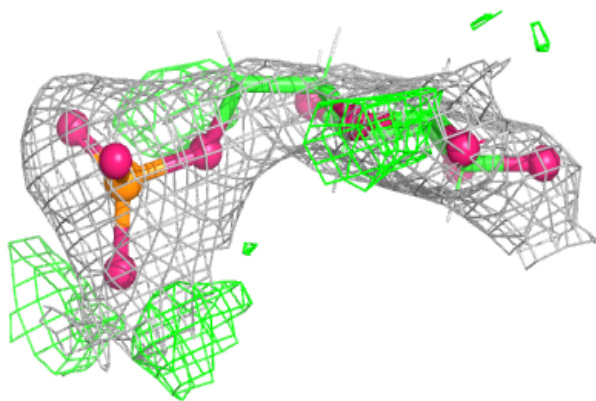
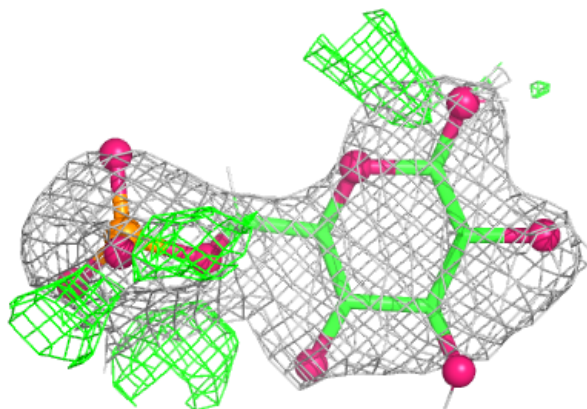
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





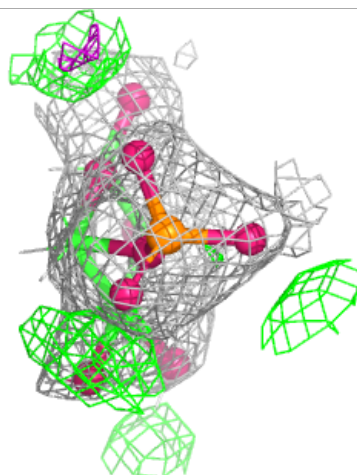
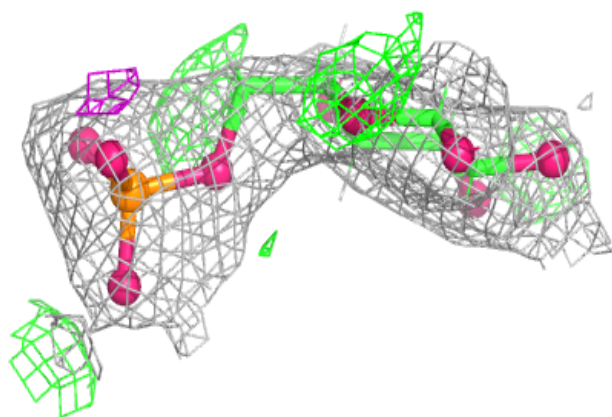
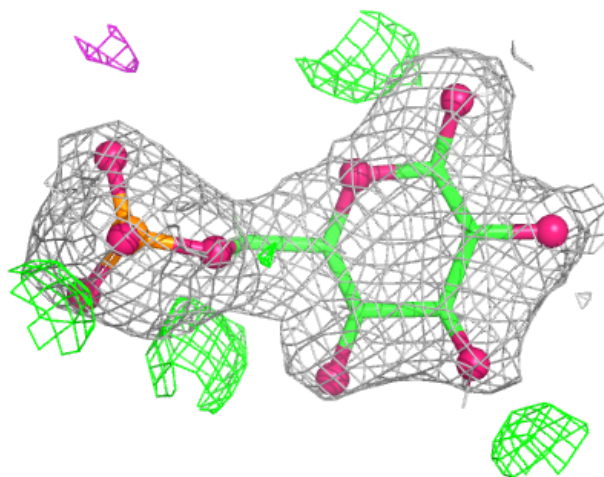
**Electron density around BG6 F 401:**

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



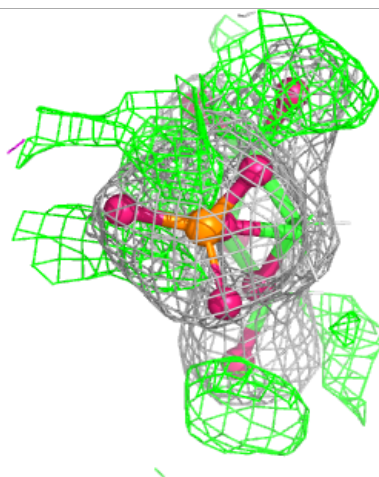
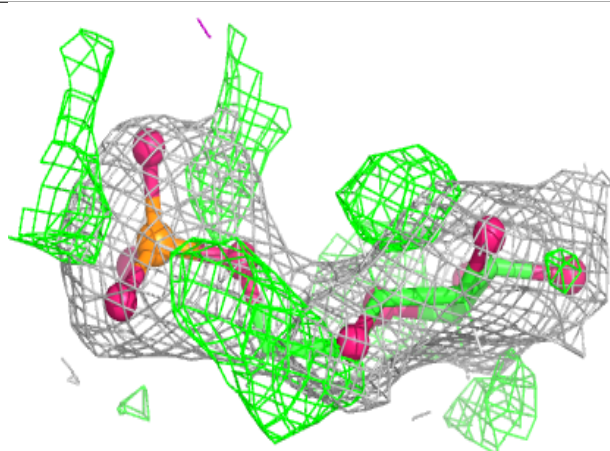
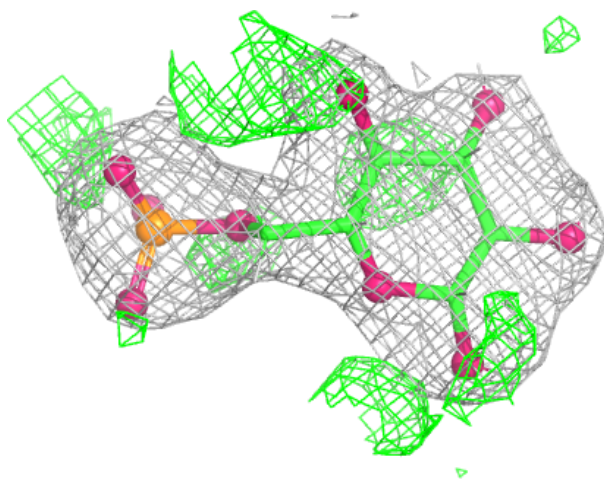
**Electron density around BG6 C 401:**

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



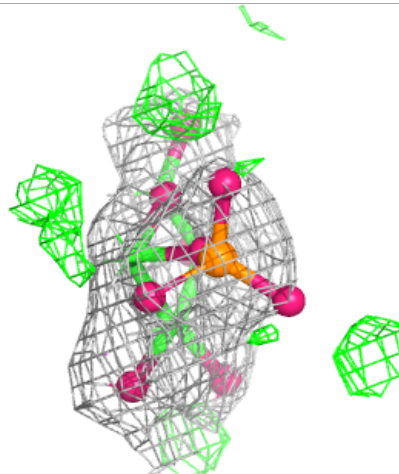
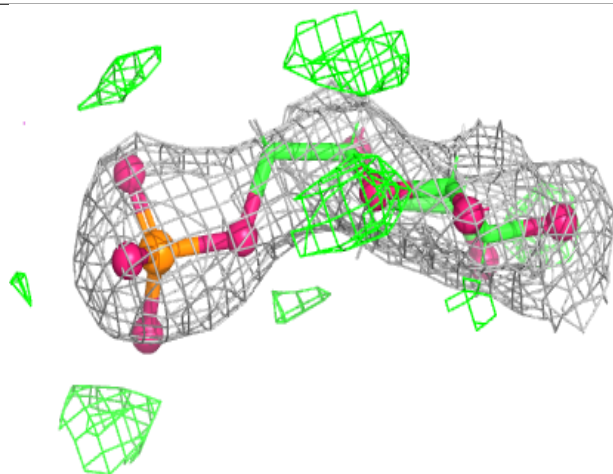
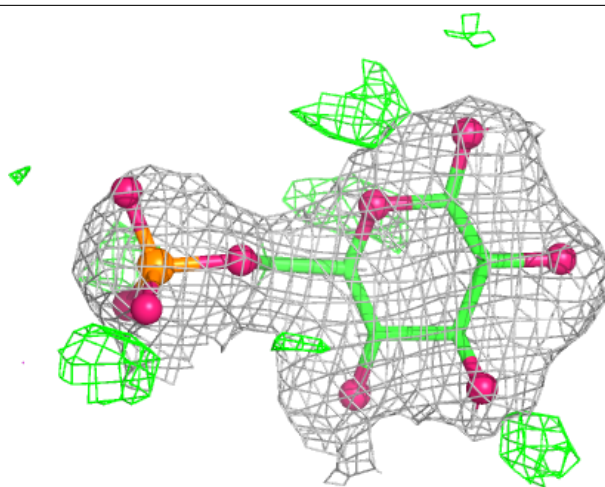
**Electron density around BG6 J 401:**

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



**Electron density around BG6 A 401:**

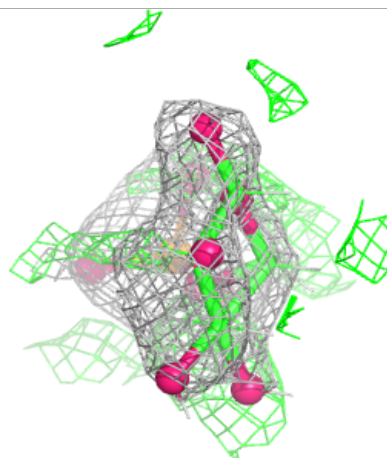
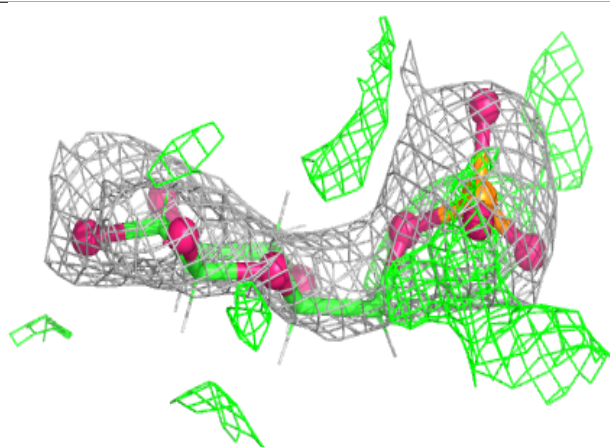
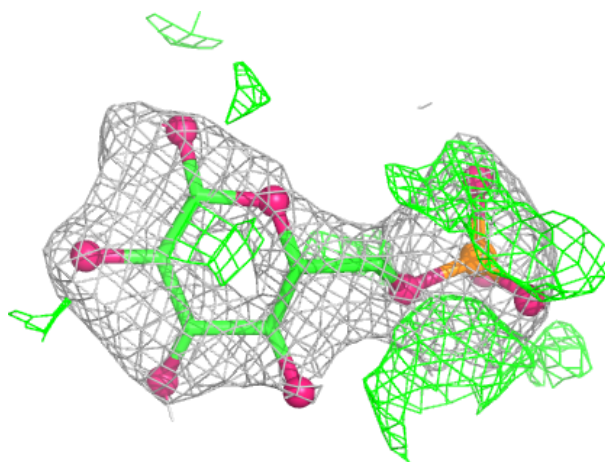
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





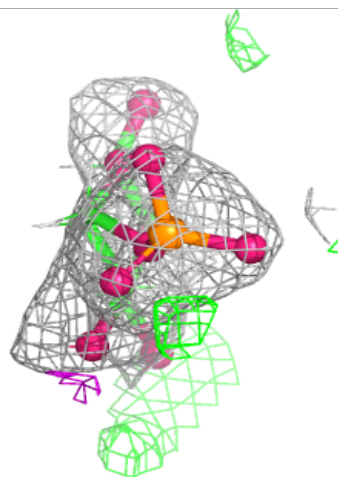
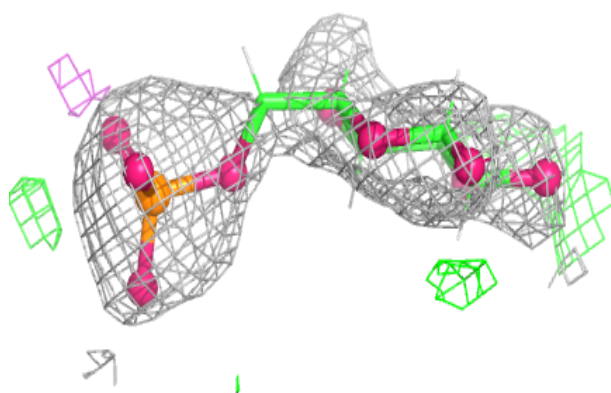
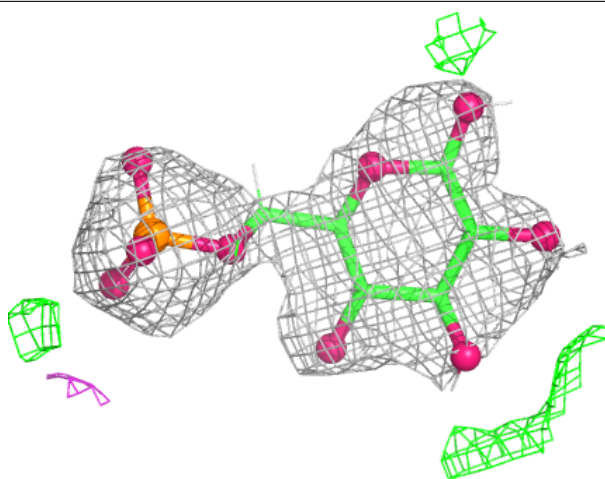
**Electron density around BG6 H 401:**

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



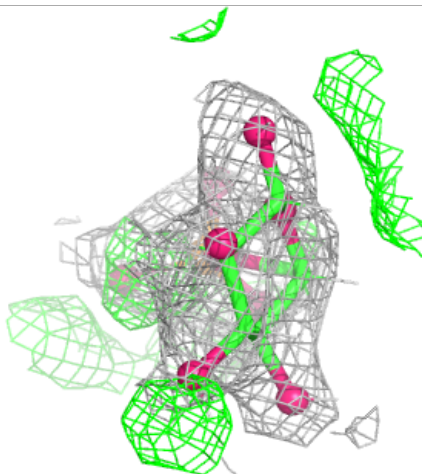
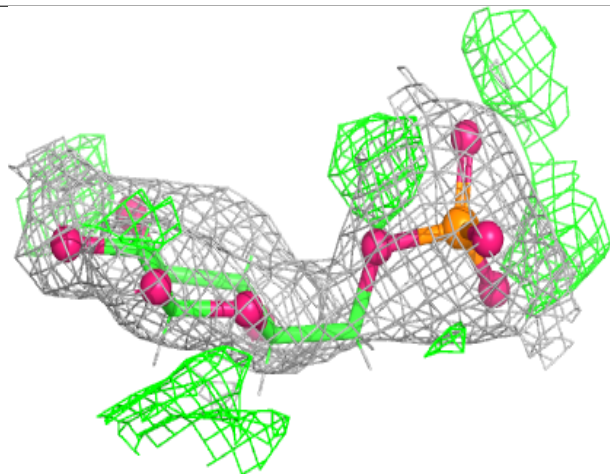
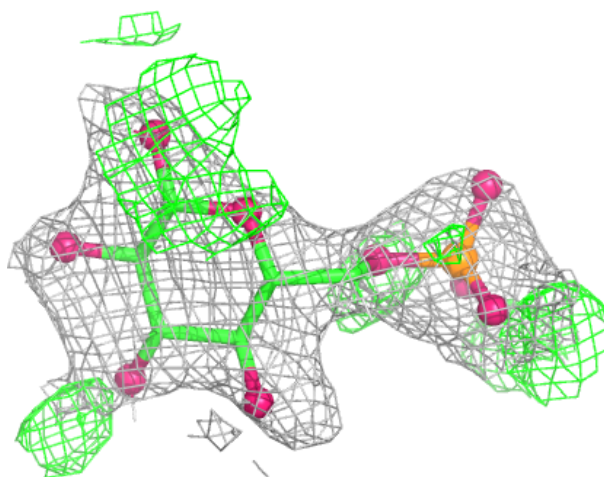
**Electron density around BG6 M 401:**

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



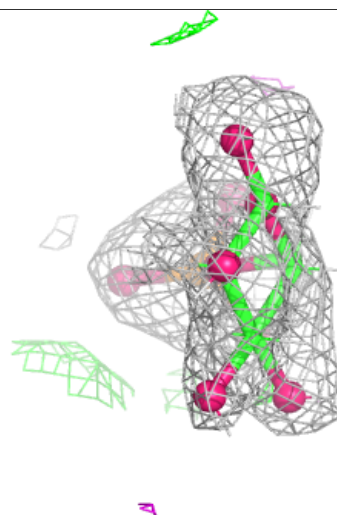
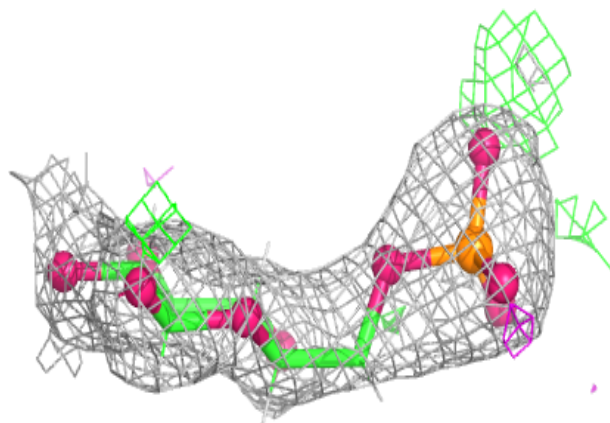
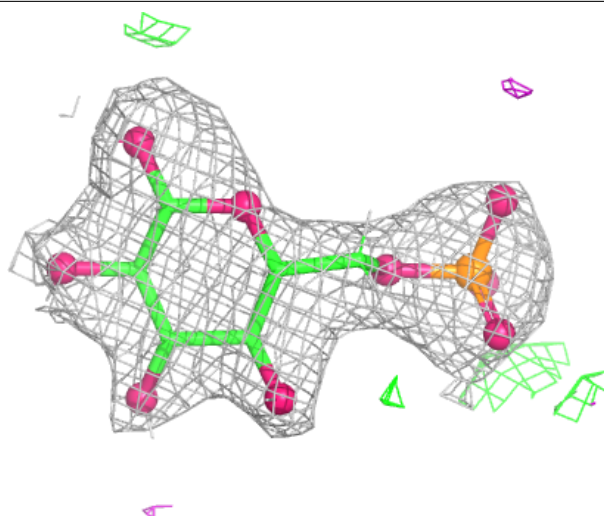
**Electron density around BG6 B 401:**

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



**Electron density around BG6 D 401:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.