



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 28, 2022 – 06:34 PM EDT

PDB ID : 7U3B  
Title : Structure of *S. venezuelae* GlgX bound to c-di-GMP and acarbose (pH 8.5)  
Authors : Schumacher, M.A.; Tschowri, N.  
Deposited on : 2022-02-26  
Resolution : 3.60 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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.31.2  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

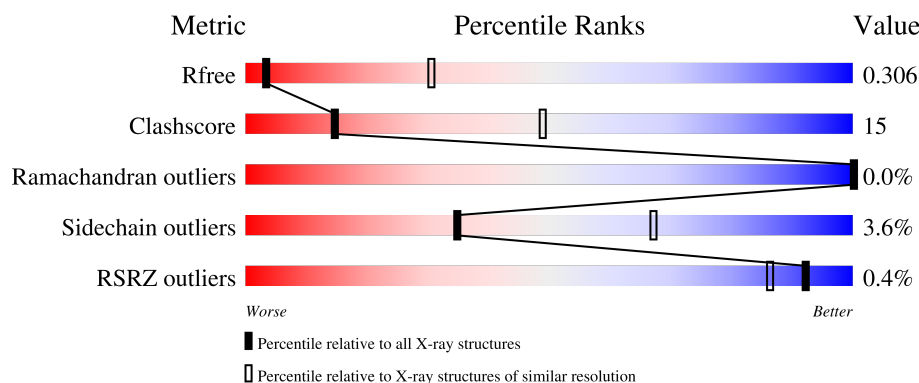
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.60 Å.

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






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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	C	709	<div> <div></div> <div>65%32%..</div> </div>
1	D	709	<div> <div>%</div> <div>64%32%..</div> </div>
1	E	709	<div> <div></div> <div>66%31%..</div> </div>
1	F	709	<div> <div>%</div> <div>63%34%..</div> </div>
1	G	709	<div> <div></div> <div>68%29%..</div> </div>

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Mol	Chain	Length	Quality of chain
1	H	709	 70%27%..
1	I	709	 %66%31%..
1	J	709	 64%32%..

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
2	A16	G	801	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 44957 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 Glycogen debranching enzyme GlgX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	696	Total	C	N	O	S	0	0	0
			5547	3485	1005	1033	24			
1	D	694	Total	C	N	O	S	0	0	0
			5535	3480	1003	1028	24			
1	E	696	Total	C	N	O	S	0	0	0
			5545	3484	1005	1033	23			
1	F	694	Total	C	N	O	S	0	0	0
			5529	3474	1000	1031	24			
1	G	693	Total	C	N	O	S	0	0	0
			5518	3468	996	1031	23			
1	H	696	Total	C	N	O	S	0	0	0
			5549	3488	1005	1032	24			
1	I	696	Total	C	N	O	S	0	0	0
			5535	3478	1002	1031	24			
1	J	694	Total	C	N	O	S	0	0	0
			5535	3480	1003	1028	24			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP A0A5P2ALW6
C	-1	SER	-	expression tag	UNP A0A5P2ALW6
C	0	HIS	-	expression tag	UNP A0A5P2ALW6
C	103	VAL	ILE	conflict	UNP A0A5P2ALW6
C	192	ARG	LYS	conflict	UNP A0A5P2ALW6
C	296	ALA	SER	conflict	UNP A0A5P2ALW6
C	297	ASP	ASN	conflict	UNP A0A5P2ALW6
C	303	MET	THR	conflict	UNP A0A5P2ALW6
C	682	GLN	GLU	conflict	UNP A0A5P2ALW6
D	-2	GLY	-	expression tag	UNP A0A5P2ALW6
D	-1	SER	-	expression tag	UNP A0A5P2ALW6
D	0	HIS	-	expression tag	UNP A0A5P2ALW6
D	103	VAL	ILE	conflict	UNP A0A5P2ALW6

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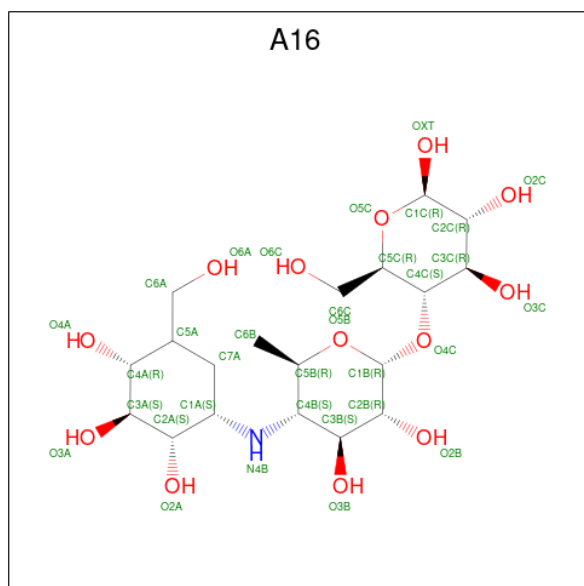
Chain	Residue	Modelled	Actual	Comment	Reference
D	192	ARG	LYS	conflict	UNP A0A5P2ALW6
D	296	ALA	SER	conflict	UNP A0A5P2ALW6
D	297	ASP	ASN	conflict	UNP A0A5P2ALW6
D	303	MET	THR	conflict	UNP A0A5P2ALW6
D	682	GLN	GLU	conflict	UNP A0A5P2ALW6
E	-2	GLY	-	expression tag	UNP A0A5P2ALW6
E	-1	SER	-	expression tag	UNP A0A5P2ALW6
E	0	HIS	-	expression tag	UNP A0A5P2ALW6
E	103	VAL	ILE	conflict	UNP A0A5P2ALW6
E	192	ARG	LYS	conflict	UNP A0A5P2ALW6
E	296	ALA	SER	conflict	UNP A0A5P2ALW6
E	297	ASP	ASN	conflict	UNP A0A5P2ALW6
E	303	MET	THR	conflict	UNP A0A5P2ALW6
E	682	GLN	GLU	conflict	UNP A0A5P2ALW6
F	-2	GLY	-	expression tag	UNP A0A5P2ALW6
F	-1	SER	-	expression tag	UNP A0A5P2ALW6
F	0	HIS	-	expression tag	UNP A0A5P2ALW6
F	103	VAL	ILE	conflict	UNP A0A5P2ALW6
F	192	ARG	LYS	conflict	UNP A0A5P2ALW6
F	296	ALA	SER	conflict	UNP A0A5P2ALW6
F	297	ASP	ASN	conflict	UNP A0A5P2ALW6
F	303	MET	THR	conflict	UNP A0A5P2ALW6
F	682	GLN	GLU	conflict	UNP A0A5P2ALW6
G	-2	GLY	-	expression tag	UNP A0A5P2ALW6
G	-1	SER	-	expression tag	UNP A0A5P2ALW6
G	0	HIS	-	expression tag	UNP A0A5P2ALW6
G	103	VAL	ILE	conflict	UNP A0A5P2ALW6
G	192	ARG	LYS	conflict	UNP A0A5P2ALW6
G	296	ALA	SER	conflict	UNP A0A5P2ALW6
G	297	ASP	ASN	conflict	UNP A0A5P2ALW6
G	303	MET	THR	conflict	UNP A0A5P2ALW6
G	682	GLN	GLU	conflict	UNP A0A5P2ALW6
H	-2	GLY	-	expression tag	UNP A0A5P2ALW6
H	-1	SER	-	expression tag	UNP A0A5P2ALW6
H	0	HIS	-	expression tag	UNP A0A5P2ALW6
H	103	VAL	ILE	conflict	UNP A0A5P2ALW6
H	192	ARG	LYS	conflict	UNP A0A5P2ALW6
H	296	ALA	SER	conflict	UNP A0A5P2ALW6
H	297	ASP	ASN	conflict	UNP A0A5P2ALW6
H	303	MET	THR	conflict	UNP A0A5P2ALW6
H	682	GLN	GLU	conflict	UNP A0A5P2ALW6
I	-2	GLY	-	expression tag	UNP A0A5P2ALW6

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-1	SER	-	expression tag	UNP A0A5P2ALW6
I	0	HIS	-	expression tag	UNP A0A5P2ALW6
I	103	VAL	ILE	conflict	UNP A0A5P2ALW6
I	192	ARG	LYS	conflict	UNP A0A5P2ALW6
I	296	ALA	SER	conflict	UNP A0A5P2ALW6
I	297	ASP	ASN	conflict	UNP A0A5P2ALW6
I	303	MET	THR	conflict	UNP A0A5P2ALW6
I	682	GLN	GLU	conflict	UNP A0A5P2ALW6
J	-2	GLY	-	expression tag	UNP A0A5P2ALW6
J	-1	SER	-	expression tag	UNP A0A5P2ALW6
J	0	HIS	-	expression tag	UNP A0A5P2ALW6
J	103	VAL	ILE	conflict	UNP A0A5P2ALW6
J	192	ARG	LYS	conflict	UNP A0A5P2ALW6
J	296	ALA	SER	conflict	UNP A0A5P2ALW6
J	297	ASP	ASN	conflict	UNP A0A5P2ALW6
J	303	MET	THR	conflict	UNP A0A5P2ALW6
J	682	GLN	GLU	conflict	UNP A0A5P2ALW6

- Molecule 2 is 4-O-(4,6-dideoxy-4-{[(1S,2S,3S,4R,5S)-2,3,4-trihydroxy-5-(hydroxymethyl)cyclohexyl]amino}-alpha-D-glucopyranosyl)-beta-D-glucopyranose (three-letter code: A16) (formula: C<sub>19</sub>H<sub>35</sub>NO<sub>13</sub>) (labeled as "Ligand of Interest" by depositor).



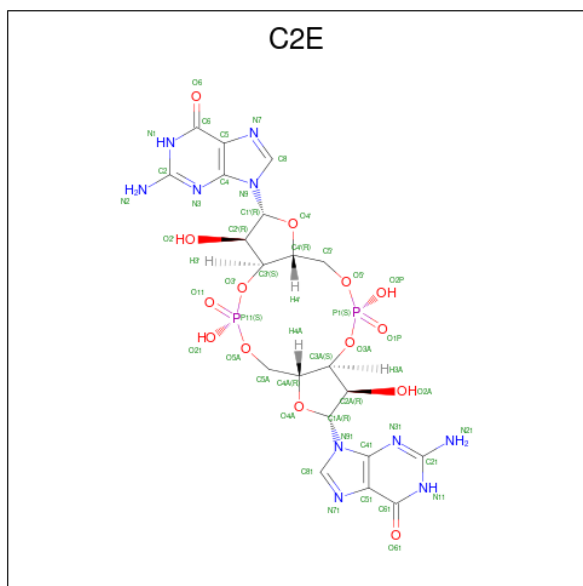
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			32	19	1	12		
2	D	1	Total	C	N	O	0	0
			32	19	1	12		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	E	1	Total	C	N	O	0	0
			32	19	1	12		
2	F	1	Total	C	N	O	0	0
			32	19	1	12		
2	G	1	Total	C	N	O	0	0
			32	19	1	12		
2	H	1	Total	C	N	O	0	0
			32	19	1	12		
2	I	1	Total	C	N	O	0	0
			32	19	1	12		
2	J	1	Total	C	N	O	0	0
			32	19	1	12		

- Molecule 3 is 9,9'-[(2R,3R,3aS,5S,7aR,9R,10R,10aS,12S,14aR)-3,5,10,12-tetrahydroxy-5,12-dioxidoctahydro-2H,7H-difuro[3,2-d:3',2'-j][1,3,7,9,2,8]tetraoxadiphosphacyclododecine-2,9-diyl]bis(2-amino-1,9-dihydro-6H-purin-6-one) (three-letter code: C2E) (formula:  $C_{20}H_{24}N_{10}O_{14}P_2$ ).



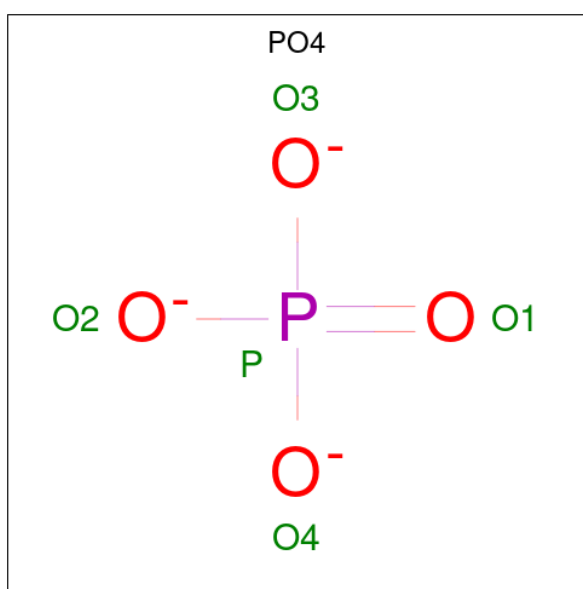
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	N	O	P	0	0
			46	20	10	14	2		
3	D	1	Total	C	N	O	P	0	0
			46	20	10	14	2		
3	E	1	Total	C	N	O	P	0	0
			46	20	10	14	2		
3	F	1	Total	C	N	O	P	0	0
			46	20	10	14	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	G	1	Total	C	N	O	P	0	0
			46	20	10	14	2		
3	H	1	Total	C	N	O	P	0	0
			46	20	10	14	2		
3	I	1	Total	C	N	O	P	0	0
			46	20	10	14	2		
3	J	1	Total	C	N	O	P	0	0
			46	20	10	14	2		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	O	P	0	0
			5	4	1		
4	D	1	Total	O	P	0	0
			5	4	1		
4	E	1	Total	O	P	0	0
			5	4	1		
4	H	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	8	Total	O	0	0
			8	8		

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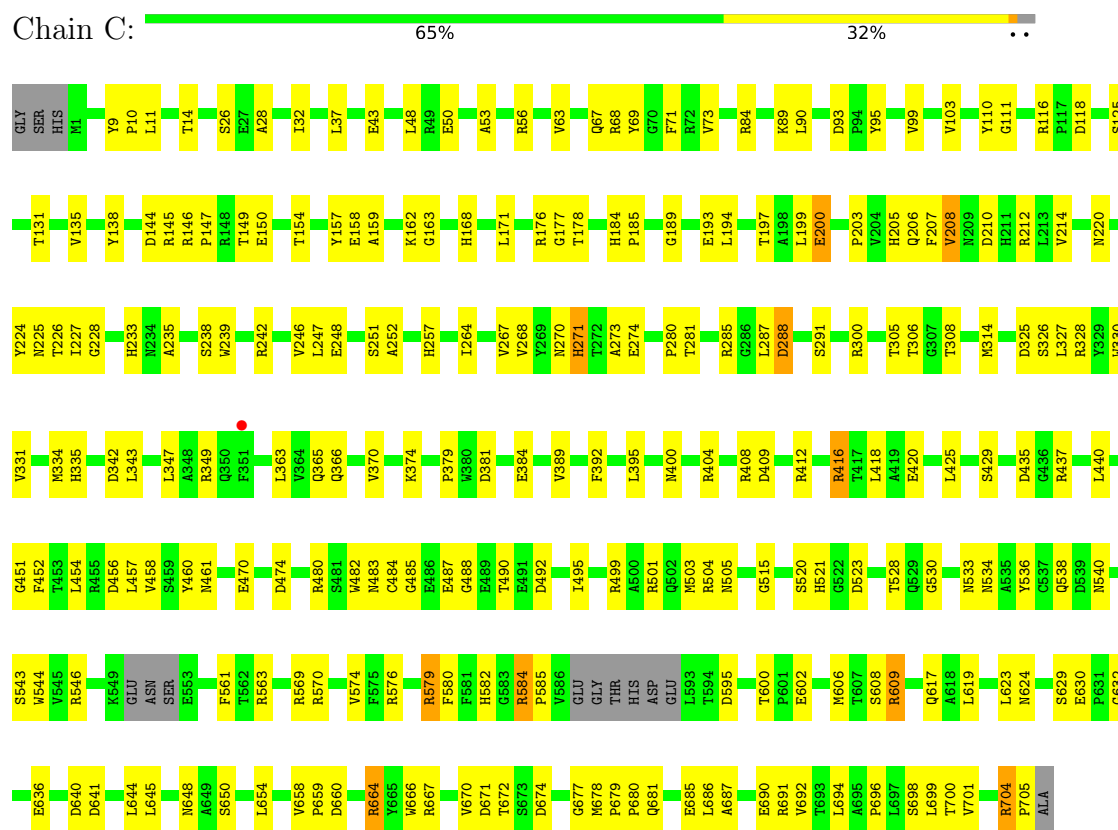
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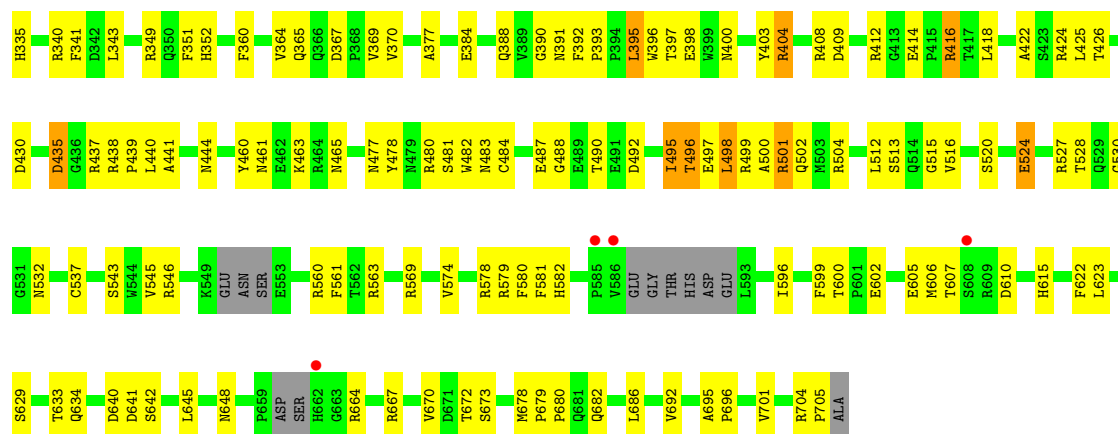
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	3	Total 3	O 3	0	0
5	F	3	Total 3	O 3	0	0
5	H	2	Total 2	O 2	0	0
5	I	4	Total 4	O 4	0	0

### 3 Residue-property plots

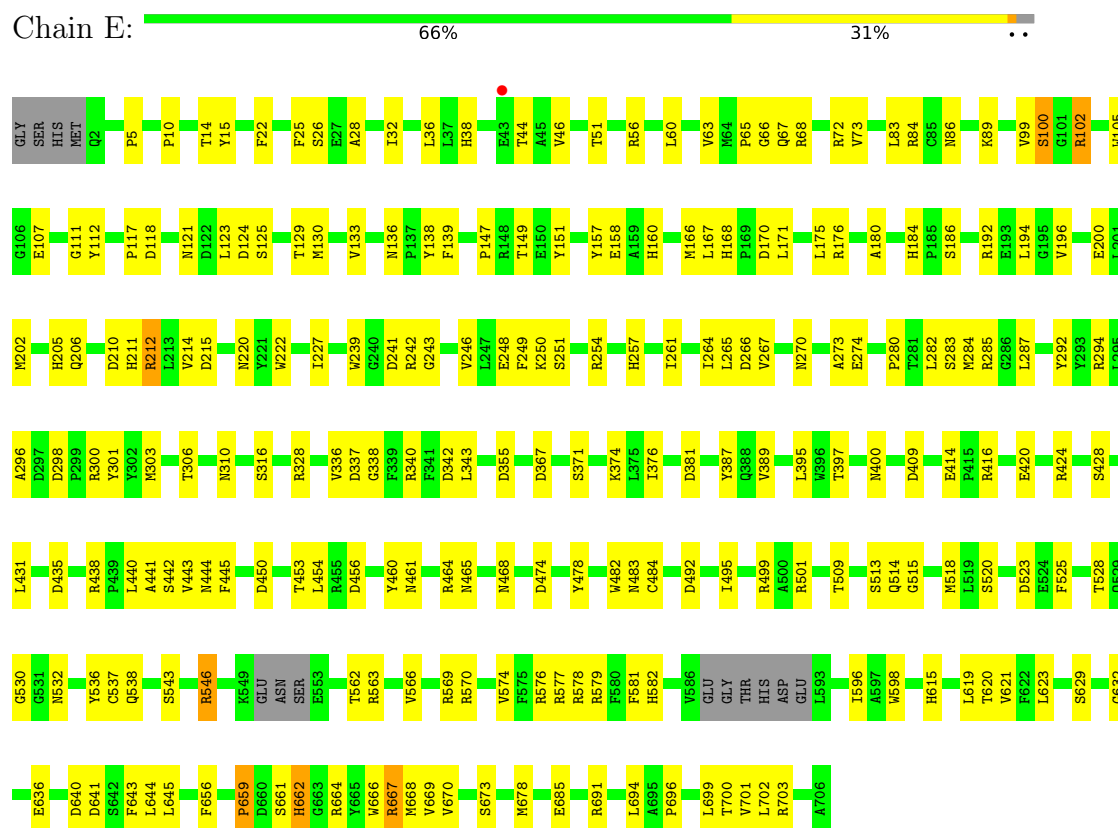
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



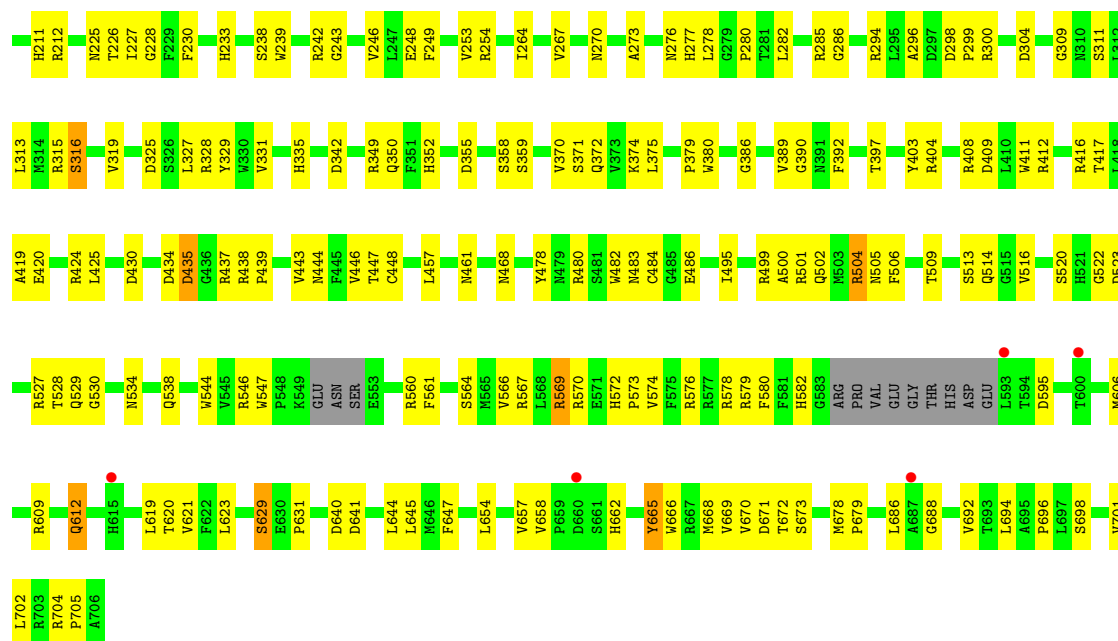


• Molecule 1: Glycogen debranching enzyme GlgX



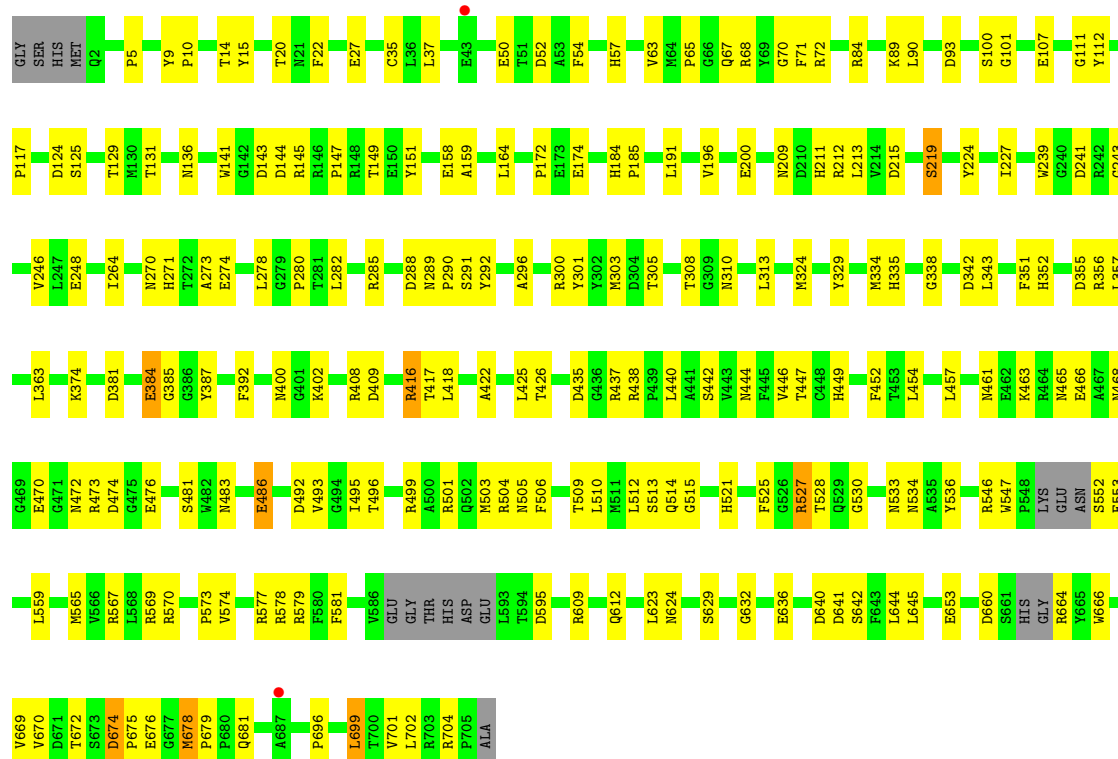
• Molecule 1: Glycogen debranching enzyme GlgX





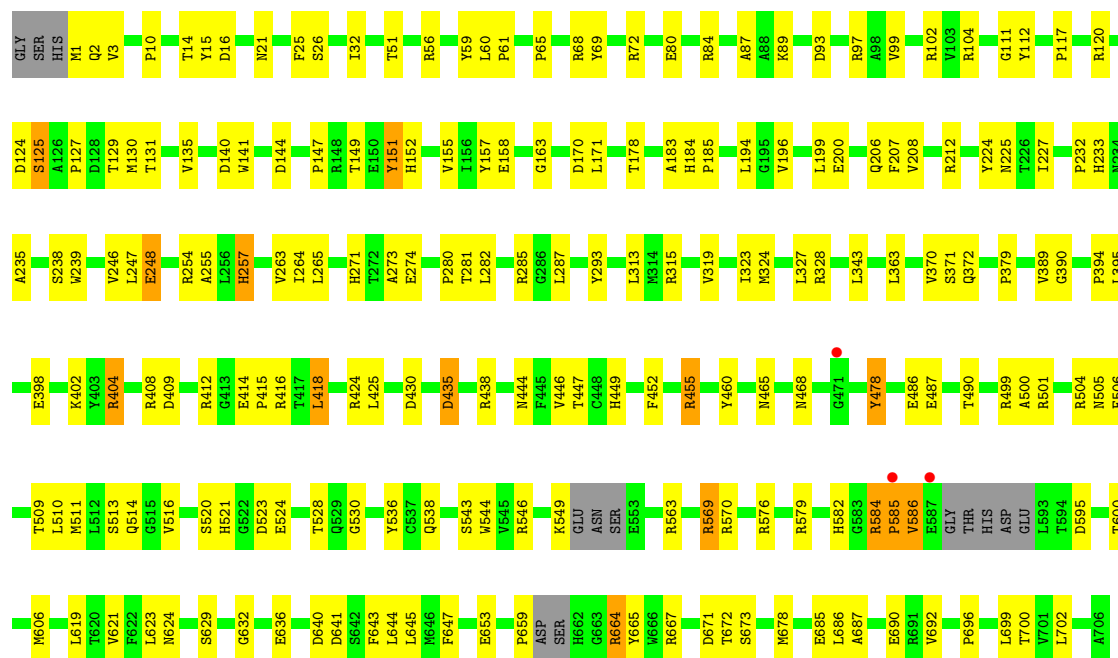
• Molecule 1: Glycogen debranching enzyme GlgX

Chain G: 68% 29% ..

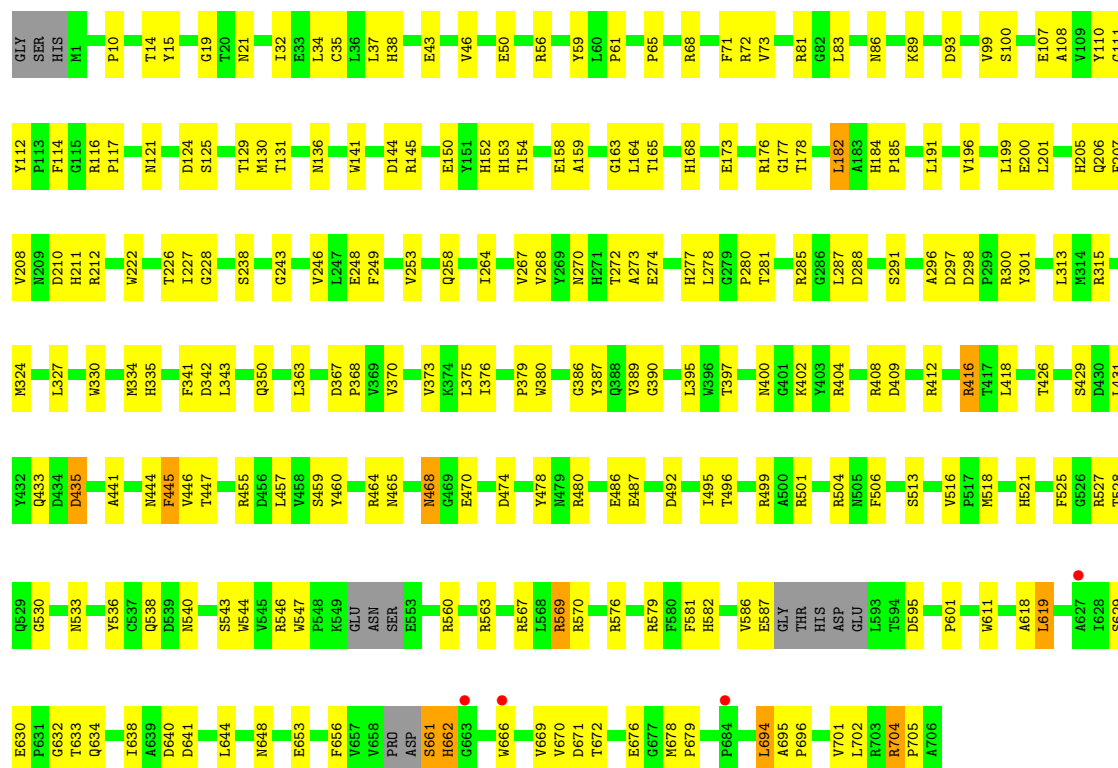


• Molecule 1: Glycogen debranching enzyme GlgX

Chain H: 70% 27% ..



• Molecule 1: Glycogen debranching enzyme GlgX



• Molecule 1: Glycogen debranching enzyme GlgX



S543	F643	L644	V544	V545	V546	K549	GLU	ASN	SER	E553	L558	M565	Y566	R567	L568	R569	R570	N483	C484	G485	E486	E487	G488	D492	I495	R499	A500	R501	Q502	M503	R504	N505	L512	S513	Q514	G515	V516	P517	M518	H521	G522	R527	T528	Q529	G530	G534	A535	Y536	C537	Q538																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
F643	L644	L645	H646	F647	N648	A649	L654	E655	P659	ASP	SER	H662	G663	G664	Y665	W666	R667	R668	V669	V670	D671	T672	G673	S674	D674	P675	N678	P679	G683	P684	R691	P696	L697	S698	L699	T700	V701	L702	R703	R704	P705	ALA																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
F452	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322	L322

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.84Å 185.59Å 184.67Å 90.00° 98.08° 90.00°	Depositor
Resolution (Å)	48.50 – 3.60 48.49 – 3.61	Depositor EDS
% Data completeness (in resolution range)	98.2 (48.50-3.60) 98.2 (48.49-3.61)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.20	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.79 (at 3.57Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.237 , 0.307 0.236 , 0.306	Depositor DCC
$R_{free}$ test set	1986 reflections (2.40%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.5	Xtriage
Anisotropy	0.475	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 51.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.83	EDS
Total number of atoms	44957	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 13.08% 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: PO4, A16, C2E

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	C	0.28	1/5699 (0.0%)	0.51	3/7750 (0.0%)
1	D	0.27	0/5686	0.49	3/7731 (0.0%)
1	E	0.33	1/5697 (0.0%)	0.50	2/7748 (0.0%)
1	F	0.30	2/5680 (0.0%)	0.49	1/7724 (0.0%)
1	G	0.26	0/5668	0.48	1/7710 (0.0%)
1	H	0.32	2/5700 (0.0%)	0.52	4/7750 (0.1%)
1	I	0.26	0/5684	0.48	2/7727 (0.0%)
1	J	0.32	2/5686 (0.0%)	0.49	2/7731 (0.0%)
All	All	0.29	8/45500 (0.0%)	0.50	18/61871 (0.0%)

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	D	0	1
1	E	0	1
1	G	0	1
1	H	0	1
1	J	0	1
All	All	0	5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	659	PRO	N-CA	13.08	1.69	1.47
1	J	675	PRO	N-CA	12.54	1.68	1.47
1	H	585	PRO	N-CA	12.40	1.68	1.47
1	C	208	VAL	C-N	7.28	1.50	1.34
1	F	657	VAL	C-N	6.49	1.49	1.34



The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	200	GLU	O-C-N	8.06	135.59	122.70
1	J	675	PRO	CA-N-CD	-7.29	101.30	111.50
1	H	585	PRO	CA-N-CD	-6.86	101.90	111.50
1	C	200	GLU	CA-C-N	-6.80	102.23	117.20
1	E	659	PRO	CA-N-CD	-6.74	102.07	111.50

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	678	MET	Peptide
1	E	678	MET	Peptide
1	G	678	MET	Peptide
1	H	678	MET	Peptide
1	J	678	MET	Peptide

## 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	C	5547	0	5252	177	0
1	D	5535	0	5249	173	0
1	E	5545	0	5251	144	0
1	F	5529	0	5235	194	0
1	G	5518	0	5217	157	0
1	H	5549	0	5260	140	0
1	I	5535	0	5236	157	0
1	J	5535	0	5249	169	0
2	C	32	0	33	5	0
2	D	32	0	33	7	0
2	E	32	0	33	7	0
2	F	32	0	33	7	0
2	G	32	0	33	10	0
2	H	32	0	33	5	0
2	I	32	0	32	5	0
2	J	32	0	33	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	46	0	22	9	0
3	D	46	0	22	18	0
3	E	46	0	22	5	0
3	F	46	0	22	3	0
3	G	46	0	22	5	0
3	H	46	0	22	7	0
3	I	46	0	22	7	0
3	J	46	0	22	4	0
4	D	10	0	0	1	0
4	E	5	0	0	0	0
4	H	5	0	0	0	0
5	C	8	0	0	0	0
5	E	3	0	0	0	0
5	F	3	0	0	0	0
5	H	2	0	0	0	0
5	I	4	0	0	0	0
All	All	44957	0	42388	1335	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 15.

The worst 5 of 1335 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:H:585:PRO:N	1:H:585:PRO:CA	1.68	1.47
1:J:675:PRO:N	1:J:675:PRO:CA	1.68	1.44
1:E:659:PRO:N	1:E:659:PRO:CA	1.69	1.37
1:F:411:TRP:CD1	1:F:506:PHE:CE1	2.12	1.37
1:F:500:ALA:O	1:F:504:ARG:NH1	1.62	1.32

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	690/709 (97%)	630 (91%)	60 (9%)	0	100	100
1	D	686/709 (97%)	637 (93%)	49 (7%)	0	100	100
1	E	690/709 (97%)	638 (92%)	52 (8%)	0	100	100
1	F	688/709 (97%)	635 (92%)	53 (8%)	0	100	100
1	G	685/709 (97%)	629 (92%)	56 (8%)	0	100	100
1	H	688/709 (97%)	639 (93%)	49 (7%)	0	100	100
1	I	688/709 (97%)	628 (91%)	59 (9%)	1 (0%)	51	83
1	J	686/709 (97%)	641 (93%)	45 (7%)	0	100	100
All	All	5501/5672 (97%)	5077 (92%)	423 (8%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	679	PRO

### 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	C	577/590 (98%)	561 (97%)	16 (3%)	43	72
1	D	576/590 (98%)	548 (95%)	28 (5%)	25	59
1	E	577/590 (98%)	550 (95%)	27 (5%)	26	61
1	F	575/590 (98%)	557 (97%)	18 (3%)	40	71
1	G	575/590 (98%)	561 (98%)	14 (2%)	49	75
1	H	577/590 (98%)	554 (96%)	23 (4%)	31	65
1	I	574/590 (97%)	553 (96%)	21 (4%)	34	66
1	J	576/590 (98%)	556 (96%)	20 (4%)	36	68
All	All	4607/4720 (98%)	4440 (96%)	167 (4%)	35	67

5 of 167 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	404	ARG
1	I	661	SER
1	H	546	ARG
1	I	210	ASP
1	J	199	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	350	GLN
1	J	205	HIS
1	J	681	GLN
1	E	538	GLN
1	G	205	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

20 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	A16	F	801	-	33,34,35	0.79	1 (3%)	44,50,52	1.14	2 (4%)
3	C2E	J	802	-	44,52,52	1.11	6 (13%)	52,82,82	1.13	3 (5%)
2	A16	G	801	1	33,34,35	0.57	0	44,50,52	1.15	5 (11%)
2	A16	J	801	-	33,34,35	0.57	0	44,50,52	1.14	3 (6%)
3	C2E	I	802	-	44,52,52	1.14	6 (13%)	52,82,82	1.35	8 (15%)
2	A16	H	801	-	33,34,35	0.67	1 (3%)	44,50,52	1.53	6 (13%)
3	C2E	G	802	-	44,52,52	1.13	6 (13%)	52,82,82	1.02	2 (3%)
2	A16	C	801	-	33,34,35	0.49	0	44,50,52	1.07	2 (4%)
2	A16	E	801	-	33,34,35	0.41	0	44,50,52	1.07	1 (2%)
2	A16	D	801	-	33,34,35	0.56	0	44,50,52	1.16	5 (11%)
3	C2E	F	802	-	44,52,52	1.22	6 (13%)	52,82,82	1.19	5 (9%)
3	C2E	H	803	-	44,52,52	1.23	6 (13%)	52,82,82	1.26	5 (9%)
4	PO4	D	803	-	4,4,4	0.94	0	6,6,6	0.48	0
3	C2E	D	804	-	44,52,52	1.15	6 (13%)	52,82,82	1.35	7 (13%)
2	A16	I	801	-	33,34,35	0.62	1 (3%)	44,50,52	1.03	2 (4%)
3	C2E	C	802	-	44,52,52	1.15	6 (13%)	52,82,82	1.13	3 (5%)
3	C2E	E	803	-	44,52,52	1.06	6 (13%)	52,82,82	1.12	4 (7%)
4	PO4	D	802	-	4,4,4	0.95	0	6,6,6	0.53	0
4	PO4	E	802	-	4,4,4	0.94	0	6,6,6	0.46	0
4	PO4	H	802	-	4,4,4	0.94	0	6,6,6	0.44	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
3	C2E	F	802	-	-	6/22/62/62	0/6/7/7
2	A16	J	801	-	-	5/12/69/72	1/3/3/3
3	C2E	D	804	-	-	2/22/62/62	0/6/7/7
3	C2E	H	803	-	-	10/22/62/62	0/6/7/7
2	A16	F	801	-	-	7/12/69/72	1/3/3/3
3	C2E	I	802	-	-	13/22/62/62	0/6/7/7
2	A16	H	801	-	-	4/12/69/72	0/3/3/3
2	A16	I	801	-	-	6/12/69/72	1/3/3/3
3	C2E	C	802	-	-	7/22/62/62	0/6/7/7
3	C2E	G	802	-	-	12/22/62/62	0/6/7/7

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A16	C	801	-	-	5/12/69/72	1/3/3/3
2	A16	E	801	-	-	5/12/69/72	1/3/3/3
3	C2E	E	803	-	-	5/22/62/62	0/6/7/7
2	A16	D	801	-	-	3/12/69/72	1/3/3/3
3	C2E	J	802	-	-	5/22/62/62	0/6/7/7
2	A16	G	801	1	-	3/12/69/72	1/3/3/3

The worst 5 of 51 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	802	C2E	C51-C61	-3.39	1.40	1.47
3	I	802	C2E	C5-C6	-3.26	1.40	1.47
3	C	802	C2E	C51-C61	-3.23	1.40	1.47
3	D	804	C2E	C51-C61	-3.22	1.40	1.47
3	F	802	C2E	C5-C6	-3.16	1.41	1.47

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	801	A16	C5A-C7A-C1A	7.04	117.32	108.49
2	C	801	A16	C1C-C2C-C3C	4.35	115.02	109.67
3	D	804	C2E	O2A-C2A-C1A	-4.31	94.92	110.85
3	J	802	C2E	P1-O3A-C3A	-4.16	104.27	119.41
2	J	801	A16	C5A-C7A-C1A	4.03	113.54	108.49

There are no chirality outliers.

5 of 98 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	801	A16	C3B-C4B-N4B-C1A
2	D	801	A16	C3B-C4B-N4B-C1A
2	E	801	A16	C3B-C4B-N4B-C1A
2	F	801	A16	C3B-C4B-N4B-C1A
2	F	801	A16	C7A-C5A-C6A-O6A

5 of 7 ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	801	A16	C1A-C2A-C3A-C4A-C5A-C7A
2	J	801	A16	C1A-C2A-C3A-C4A-C5A-C7A

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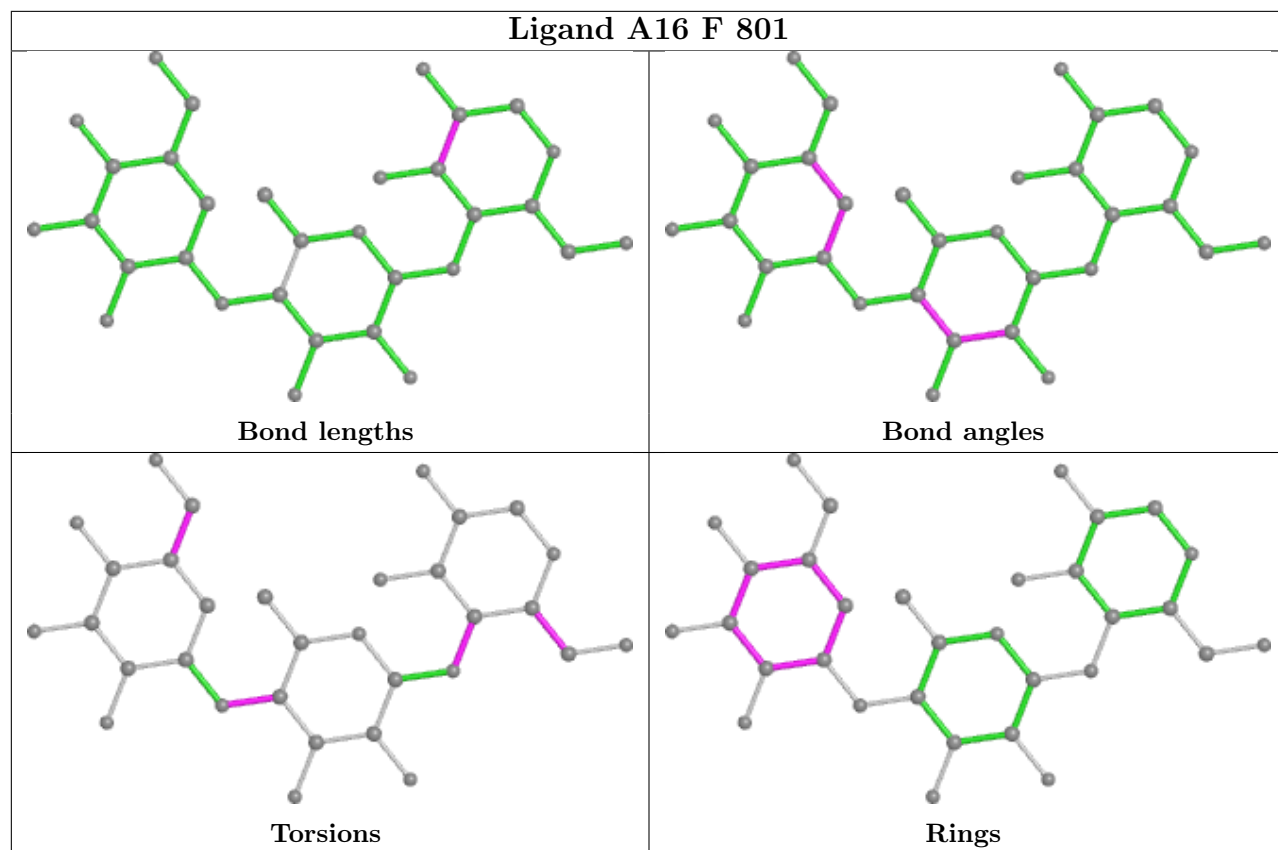
Mol	Chain	Res	Type	Atoms
2	F	801	A16	C1A-C2A-C3A-C4A-C5A-C7A
2	I	801	A16	C1A-C2A-C3A-C4A-C5A-C7A
2	C	801	A16	C1A-C2A-C3A-C4A-C5A-C7A

17 monomers are involved in 115 short contacts:

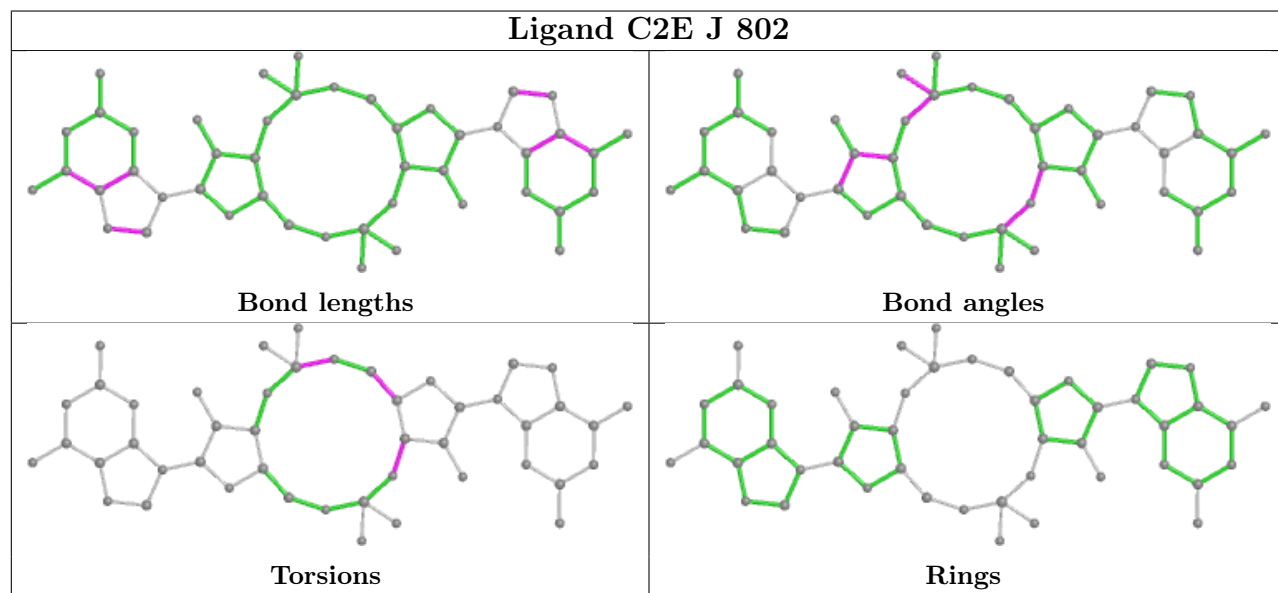
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	801	A16	7	0
3	J	802	C2E	4	0
2	G	801	A16	10	0
2	J	801	A16	10	0
3	I	802	C2E	7	0
2	H	801	A16	5	0
3	G	802	C2E	5	0
2	C	801	A16	5	0
2	E	801	A16	7	0
2	D	801	A16	7	0
3	F	802	C2E	3	0
3	H	803	C2E	7	0
3	D	804	C2E	18	0
2	I	801	A16	5	0
3	C	802	C2E	9	0
3	E	803	C2E	5	0
4	D	802	PO4	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 A16 F 801

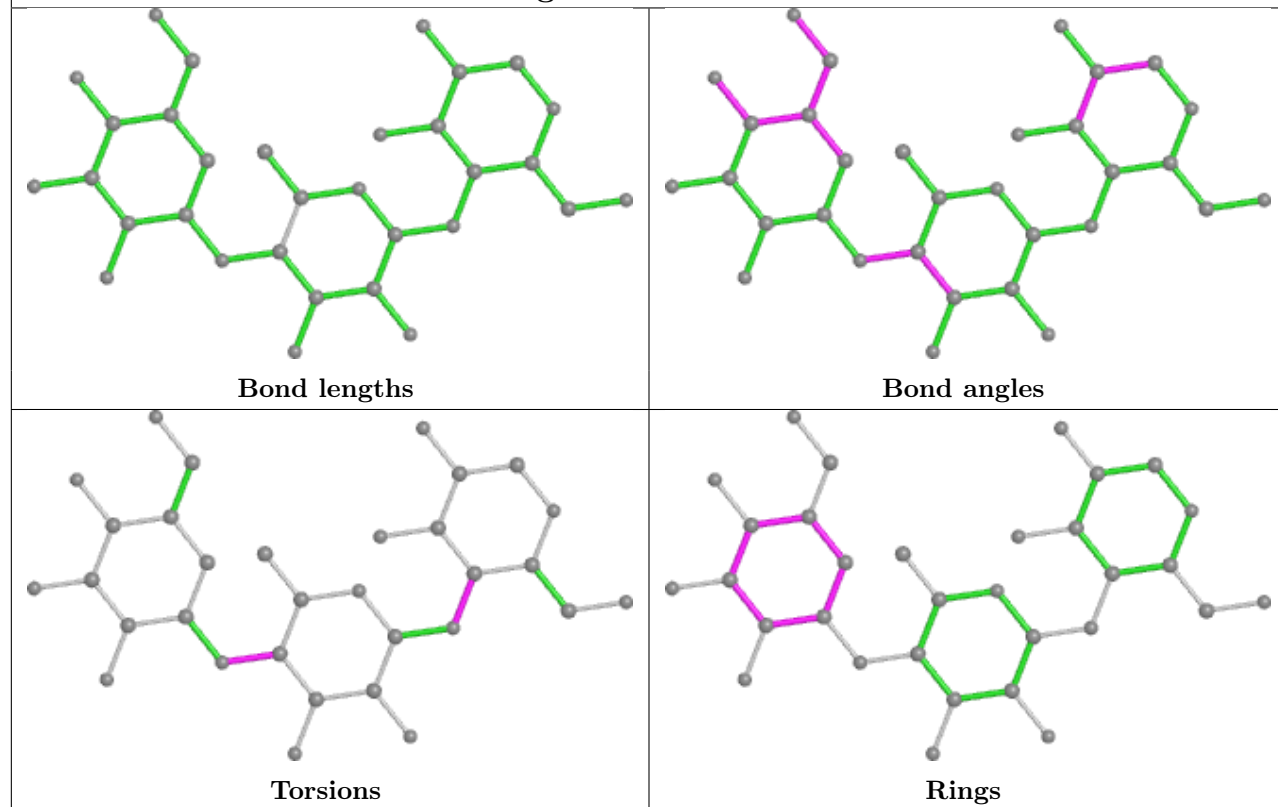


## Ligand C2E J 802

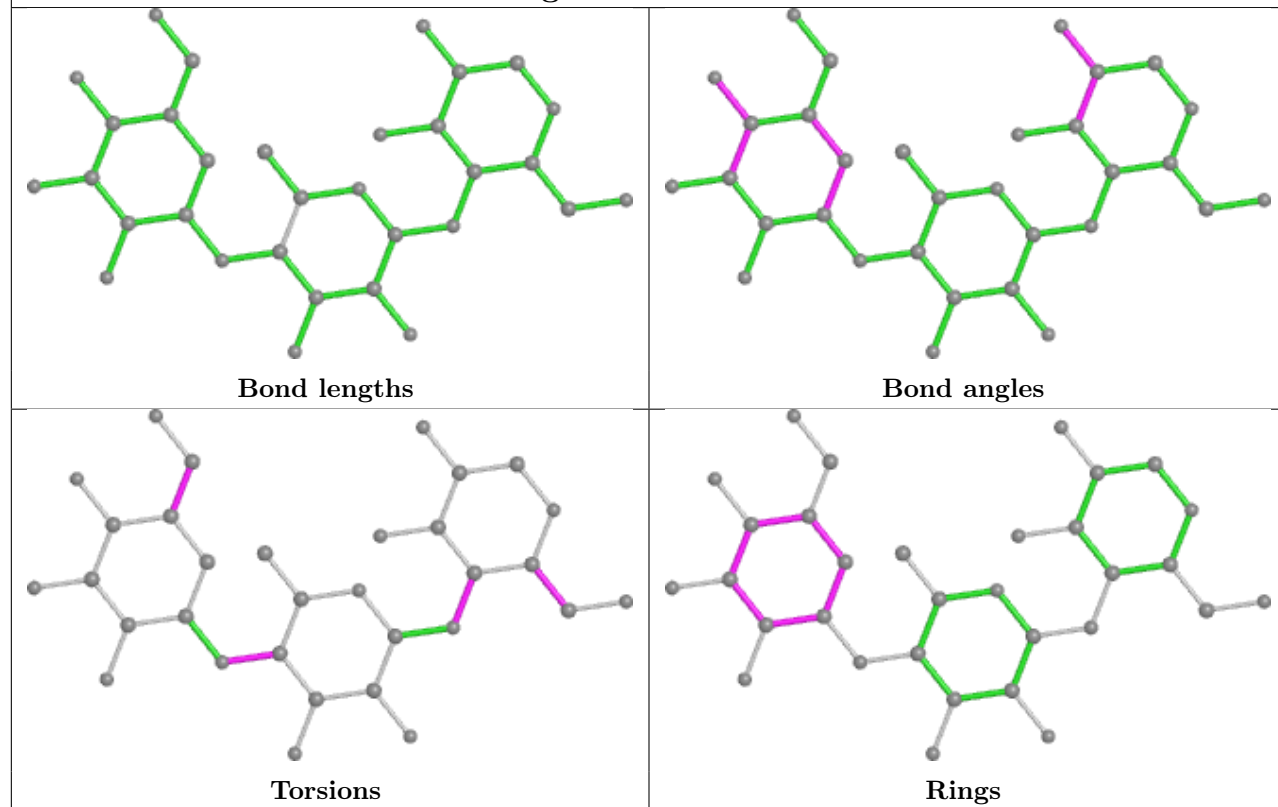




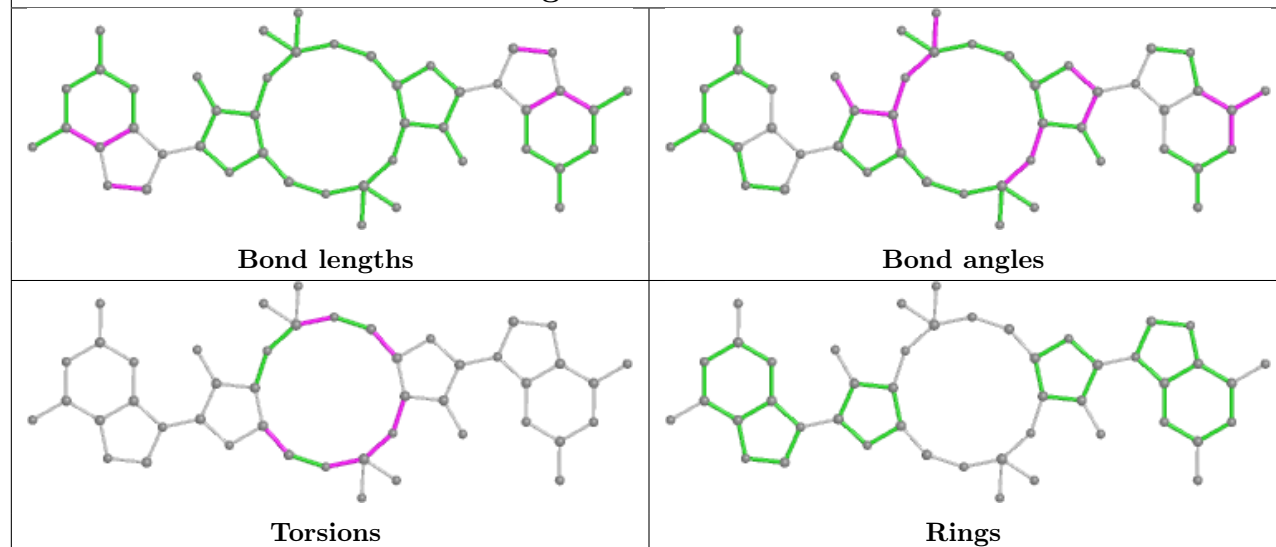
## Ligand A16 G 801



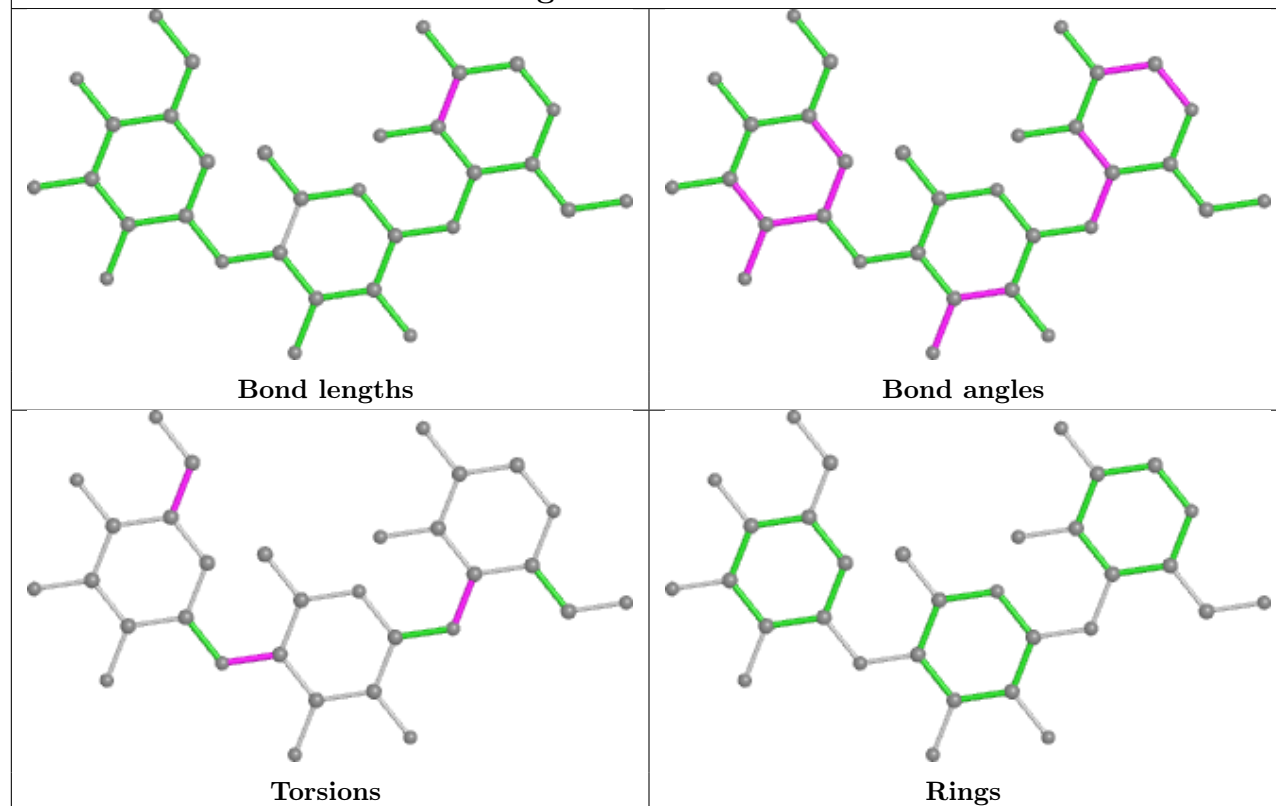
## Ligand A16 J 801



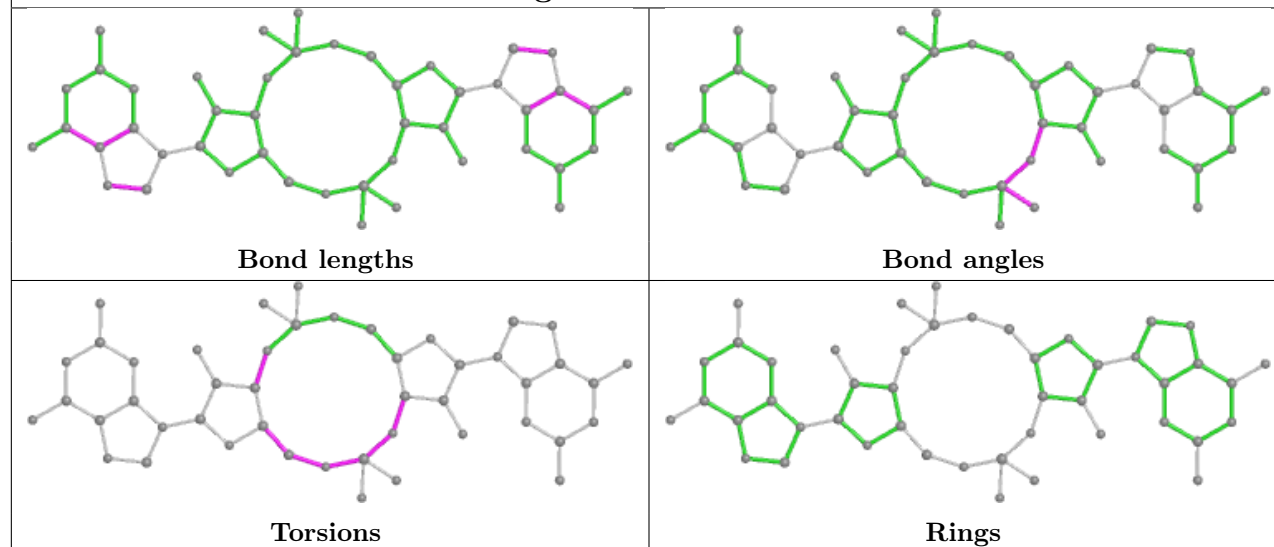
## Ligand C2E I 802



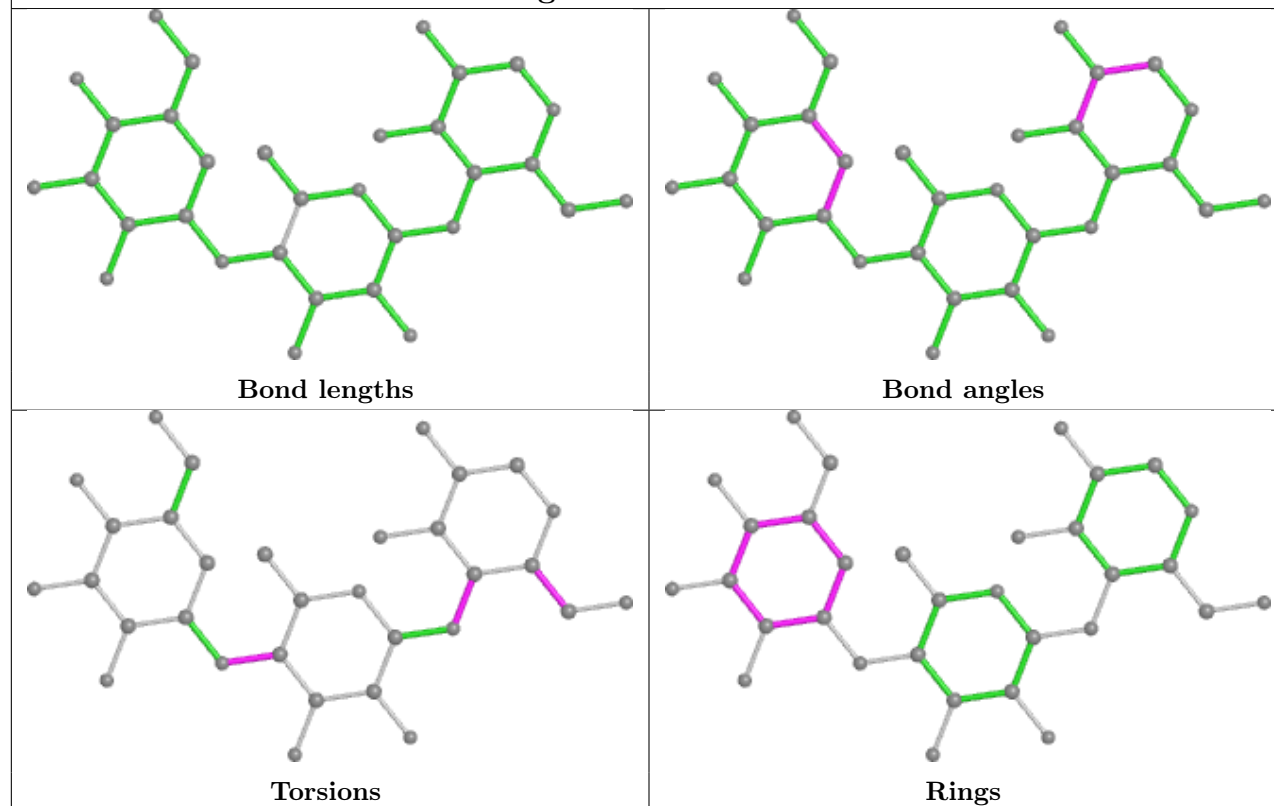
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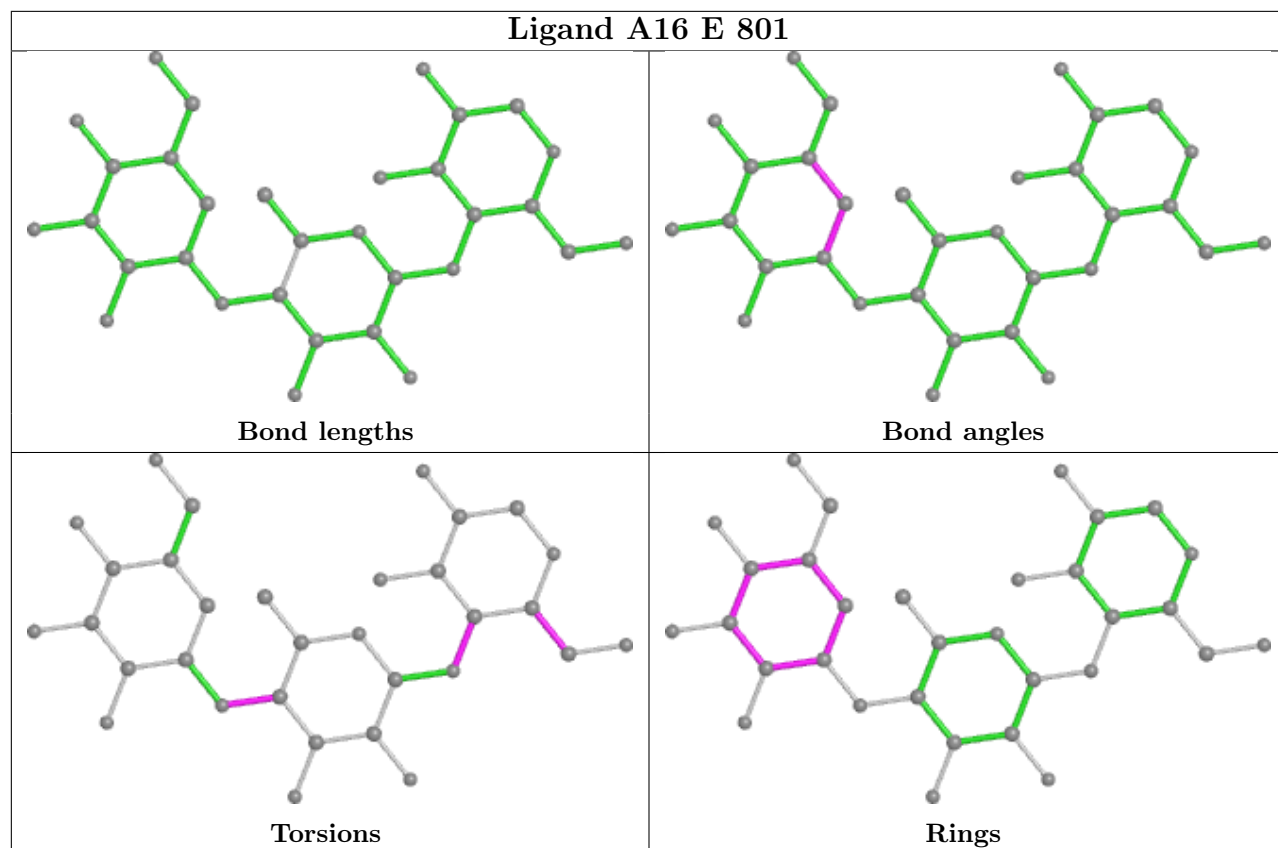
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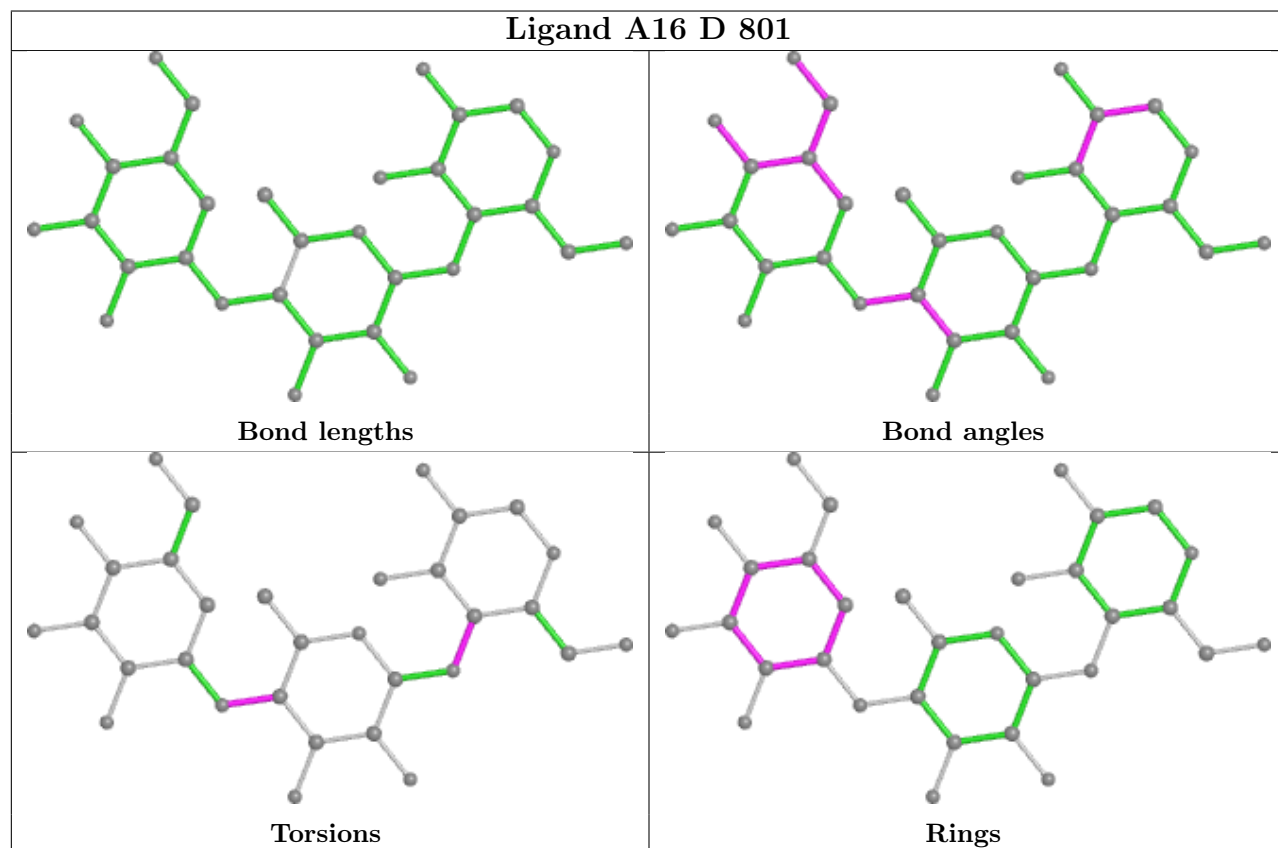
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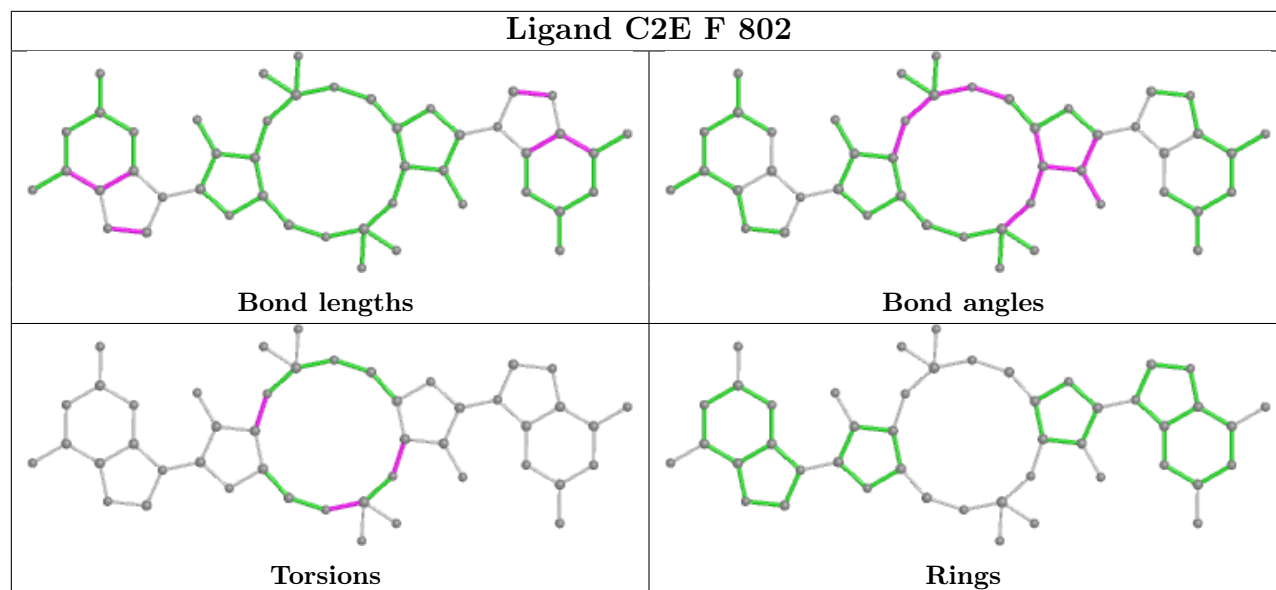
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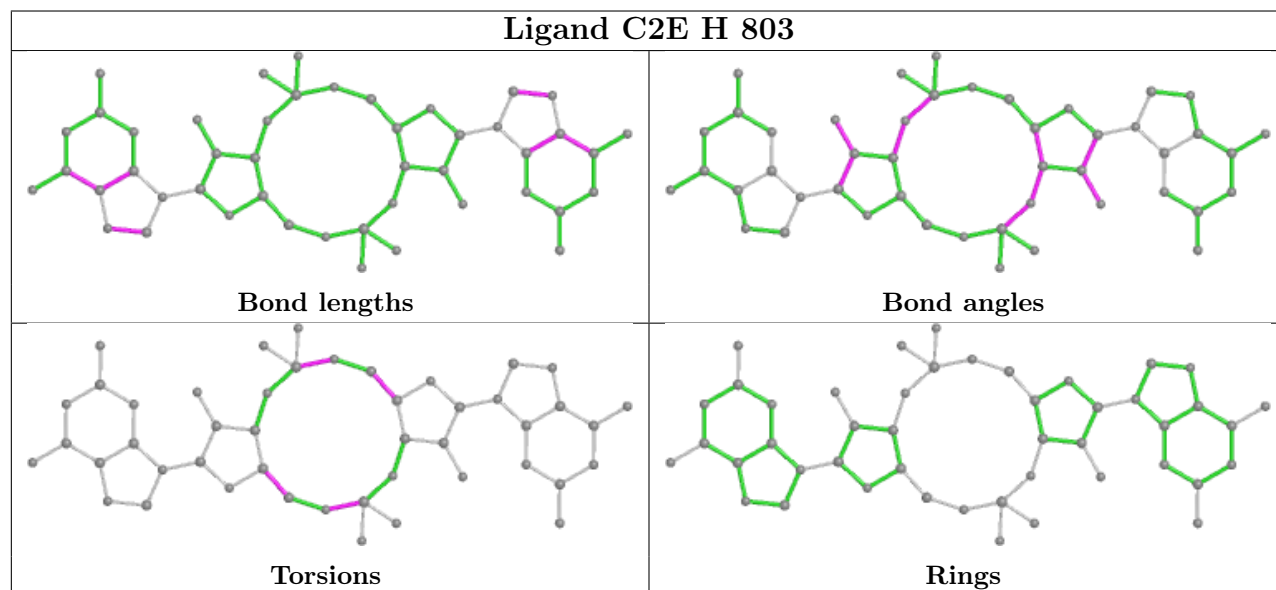
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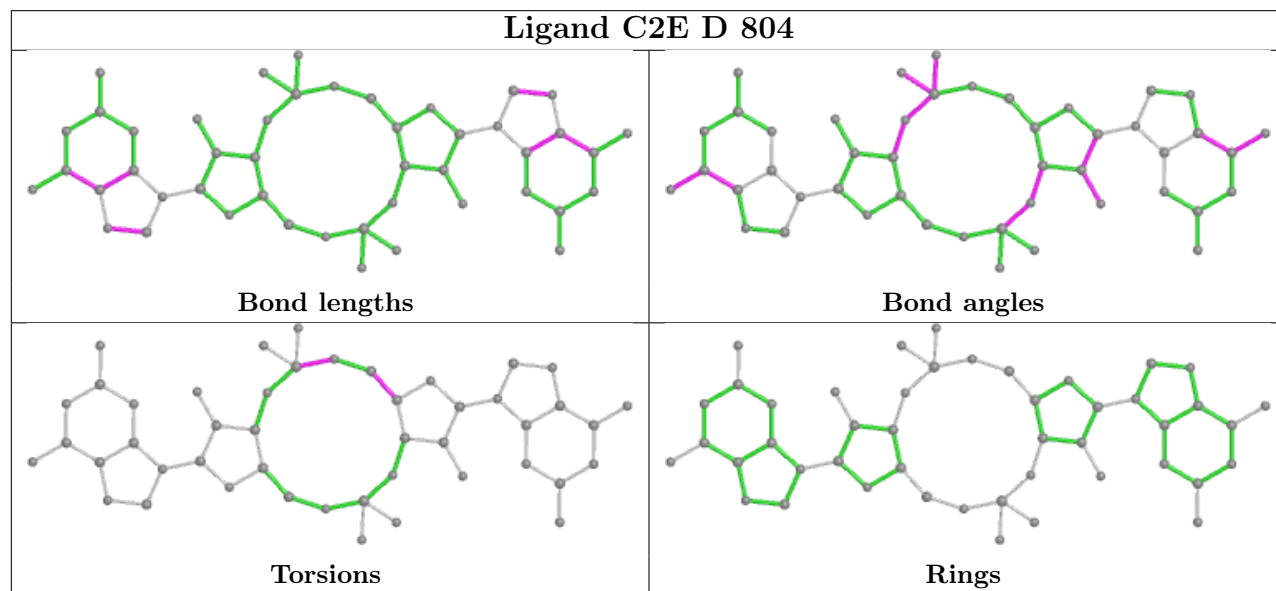
## Ligand C2E F 802



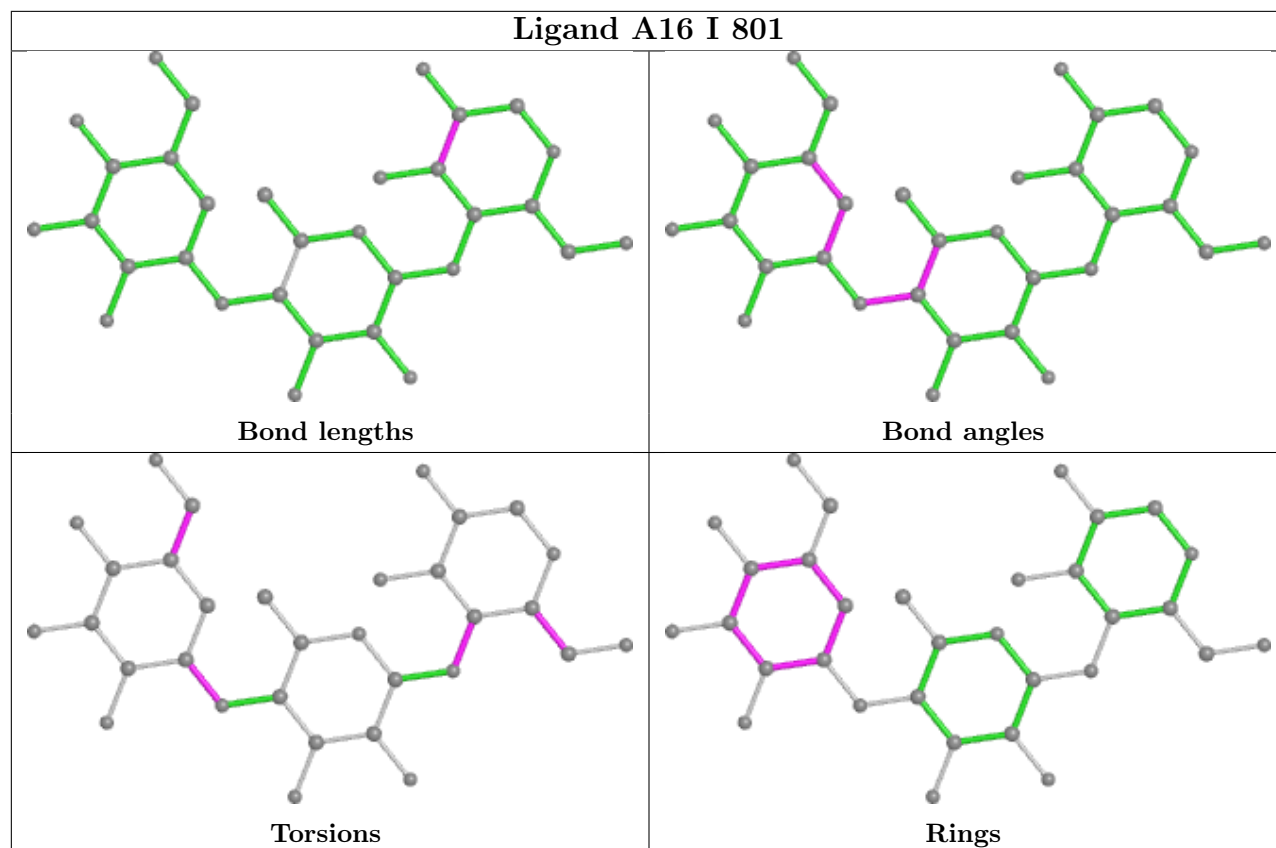
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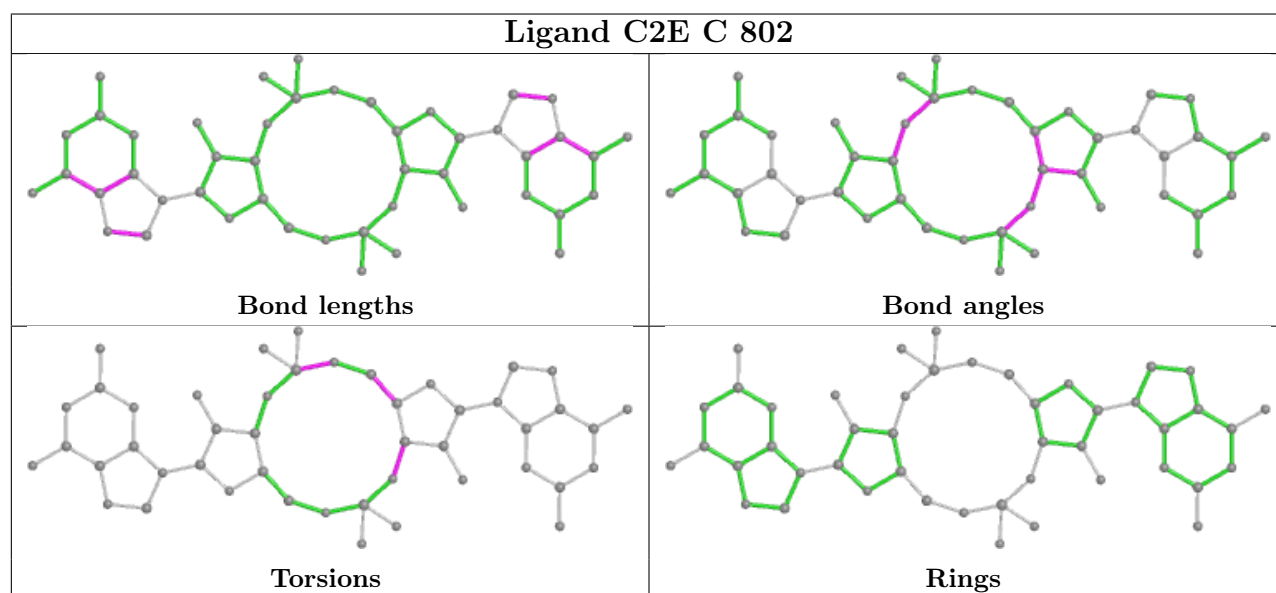
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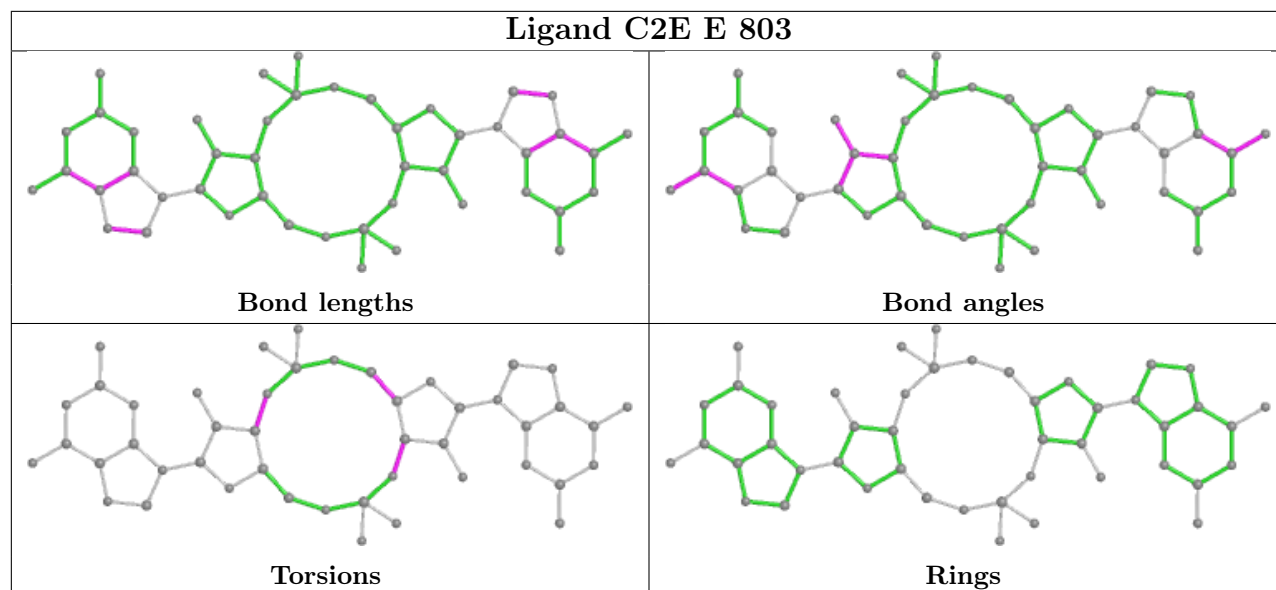


## Ligand A16 I 801



## Ligand C2E C 802





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	C	696/709 (98%)	-0.38	1 (0%) 95 93	23, 40, 64, 95	0
1	D	694/709 (97%)	-0.43	4 (0%) 89 81	19, 38, 66, 115	0
1	E	696/709 (98%)	-0.40	1 (0%) 95 93	22, 39, 62, 102	0
1	F	694/709 (97%)	-0.32	5 (0%) 87 78	17, 42, 67, 128	0
1	G	693/709 (97%)	-0.31	2 (0%) 94 88	23, 44, 75, 127	0
1	H	696/709 (98%)	-0.27	3 (0%) 92 86	24, 47, 76, 114	0
1	I	696/709 (98%)	-0.11	4 (0%) 89 81	23, 51, 80, 122	0
1	J	694/709 (97%)	-0.17	3 (0%) 92 86	23, 49, 83, 128	0
All	All	5559/5672 (98%)	-0.30	23 (0%) 92 86	17, 43, 74, 128	0

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	684	PRO	4.2
1	D	586	VAL	3.5
1	I	663	GLY	3.2
1	F	615	HIS	3.1
1	F	600	THR	3.0

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.



## 6.4 Ligands ⓘ

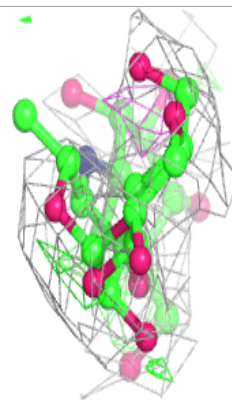
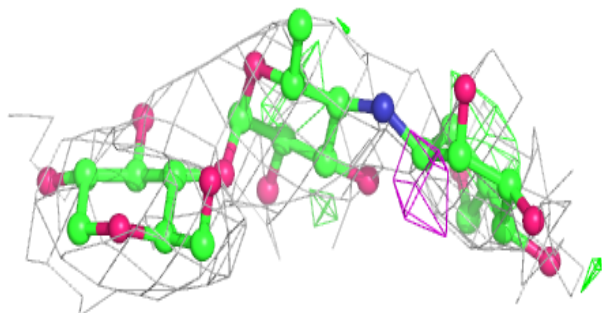
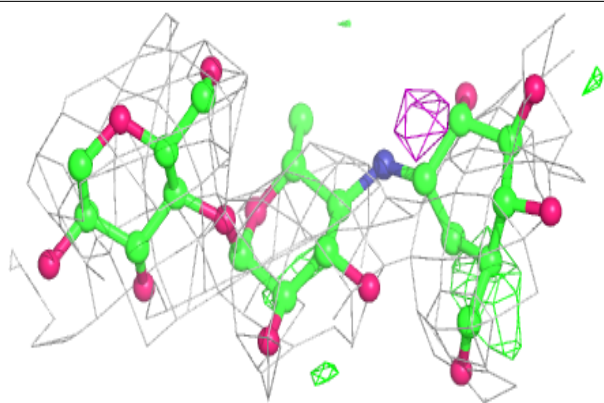
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<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	A16	G	801	32/33	0.69	0.43	77,107,116,124	0
2	A16	I	801	32/33	0.74	0.32	77,107,116,124	0
2	A16	D	801	32/33	0.79	0.33	77,107,116,124	0
2	A16	J	801	32/33	0.79	0.33	78,107,116,124	0
2	A16	E	801	32/33	0.80	0.37	77,108,116,124	0
2	A16	H	801	32/33	0.83	0.28	78,107,120,124	0
4	PO4	D	802	5/5	0.84	0.41	70,72,82,88	0
2	A16	F	801	32/33	0.86	0.24	27,42,63,83	0
2	A16	C	801	32/33	0.87	0.28	70,82,105,114	0
4	PO4	D	803	5/5	0.88	0.24	66,70,75,84	0
3	C2E	D	804	46/46	0.89	0.24	96,101,117,122	0
3	C2E	E	803	46/46	0.92	0.22	39,47,59,66	0
3	C2E	G	802	46/46	0.93	0.19	28,49,58,65	0
3	C2E	I	802	46/46	0.93	0.22	38,46,55,59	0
4	PO4	E	802	5/5	0.93	0.24	44,45,61,76	0
3	C2E	J	802	46/46	0.94	0.20	29,49,60,63	0
3	C2E	C	802	46/46	0.94	0.17	45,52,60,66	0
3	C2E	H	803	46/46	0.96	0.15	29,39,55,61	0
3	C2E	F	802	46/46	0.96	0.15	29,39,45,51	0
4	PO4	H	802	5/5	0.97	0.29	55,58,67,70	0

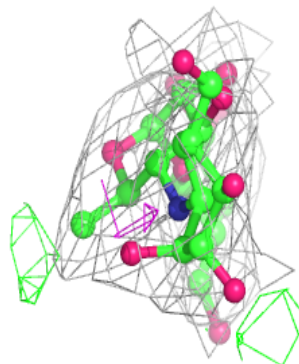
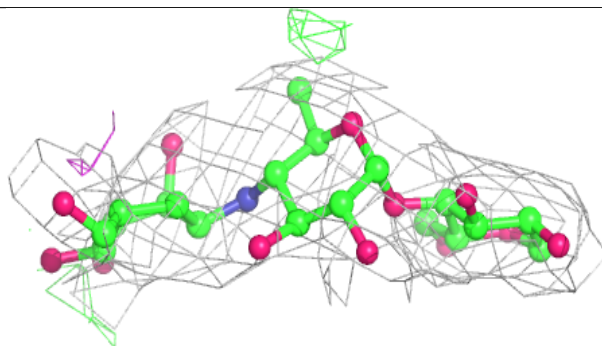
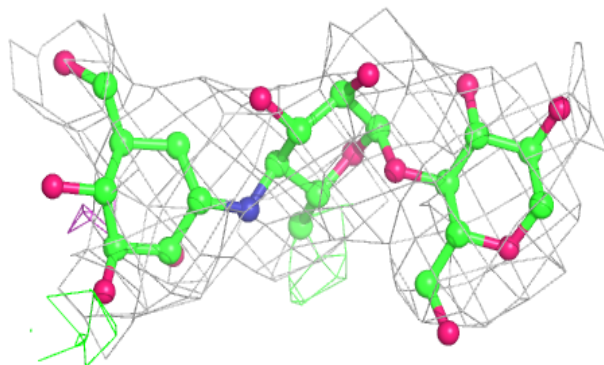
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around A16 G 801:**

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

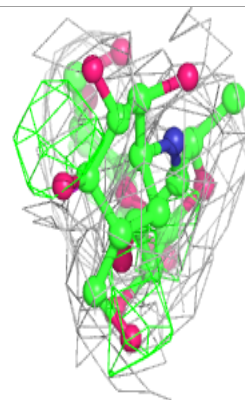
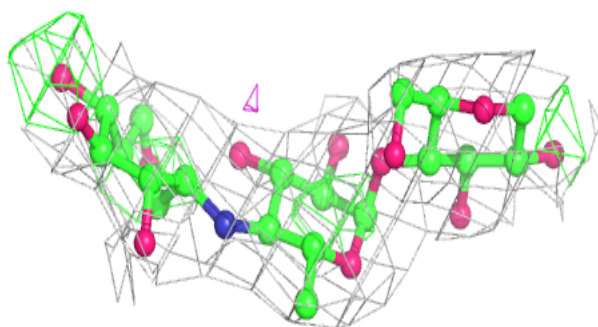
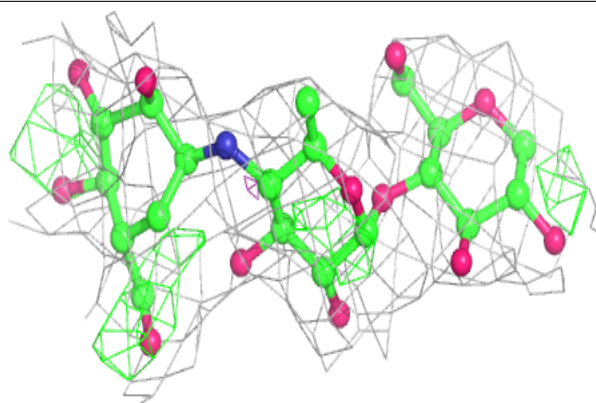
**Electron density around A16 I 801:**

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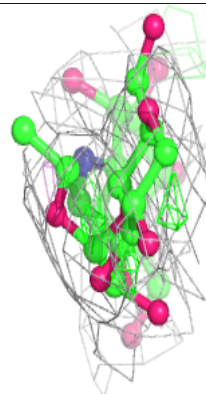
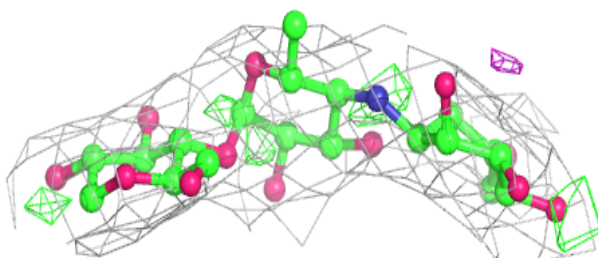
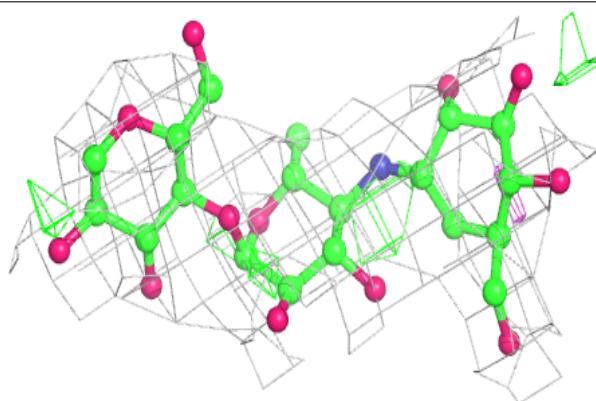


**Electron density around A16 D 801:**

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

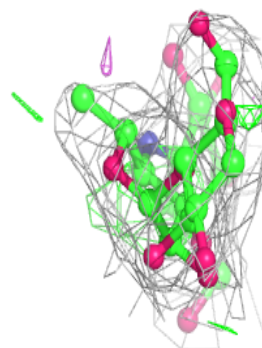
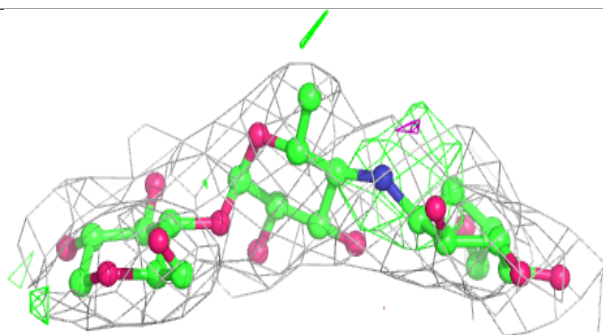
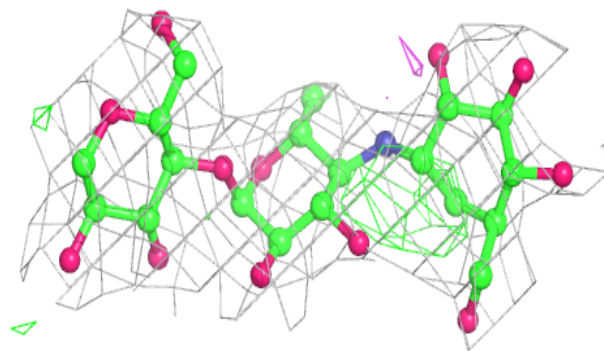
**Electron density around A16 J 801:**

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

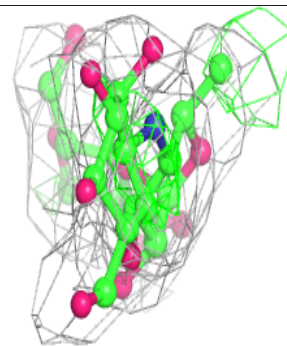
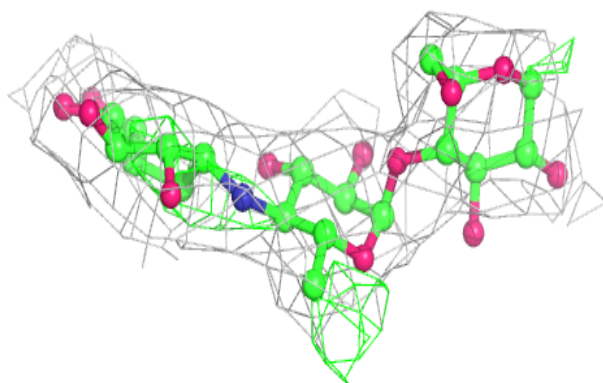
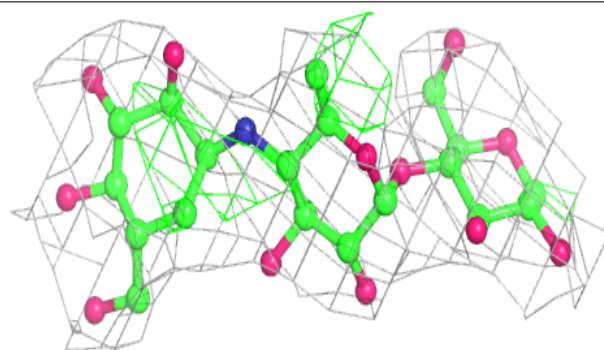


**Electron density around A16 E 801:**

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and green (positive)

**Electron density around A16 H 801:**

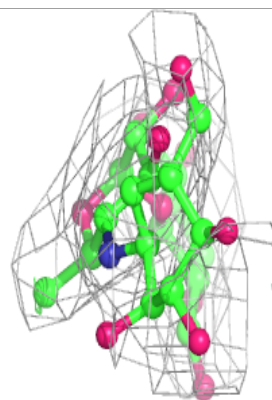
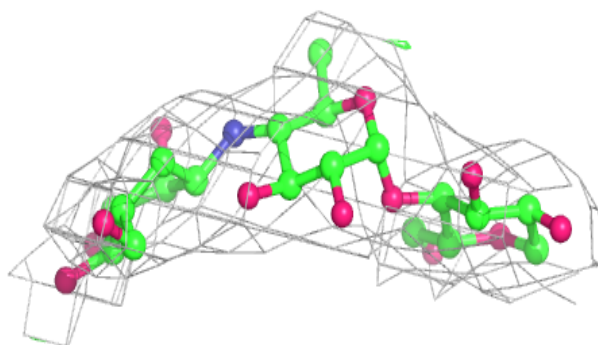
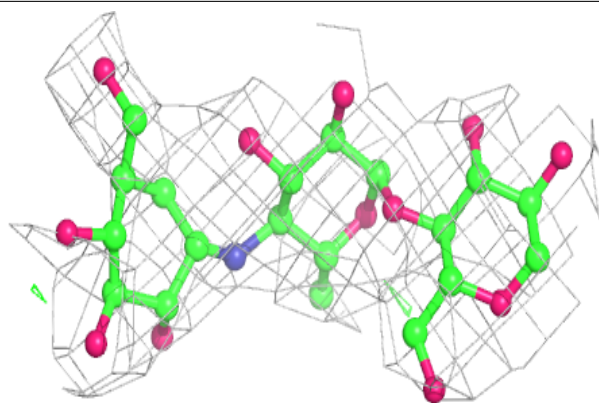
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and green (positive)



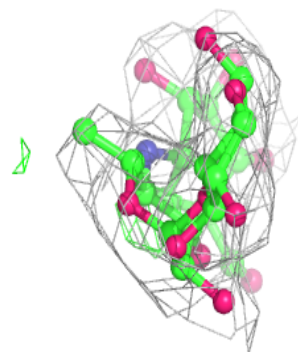
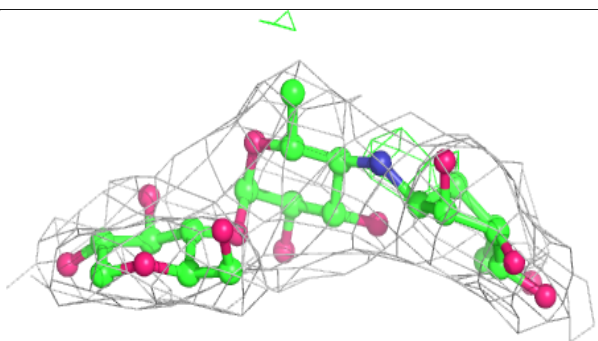
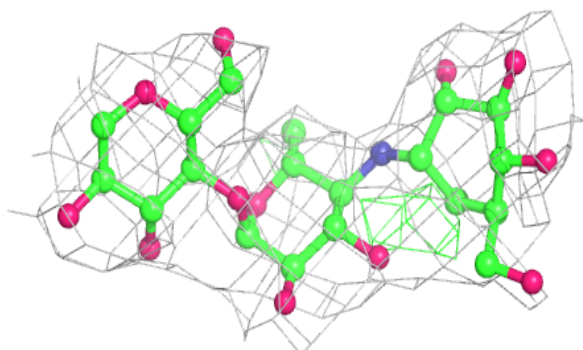


**Electron density around A16 F 801:**

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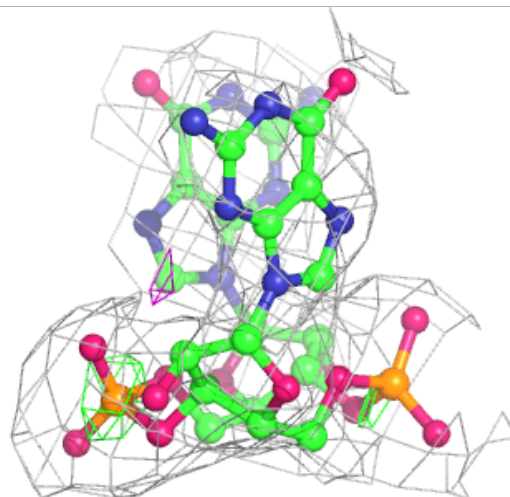
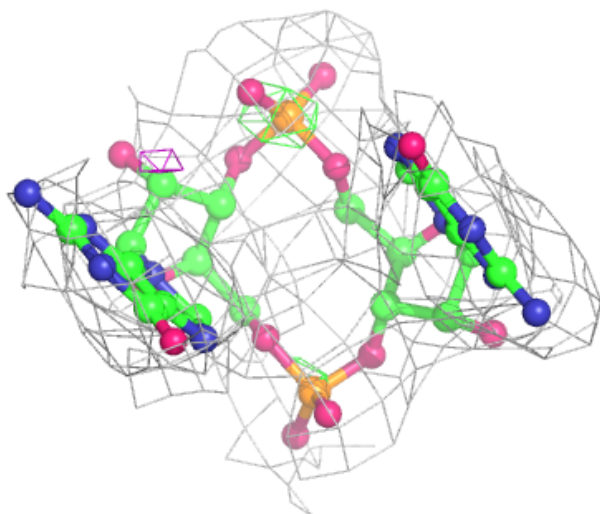
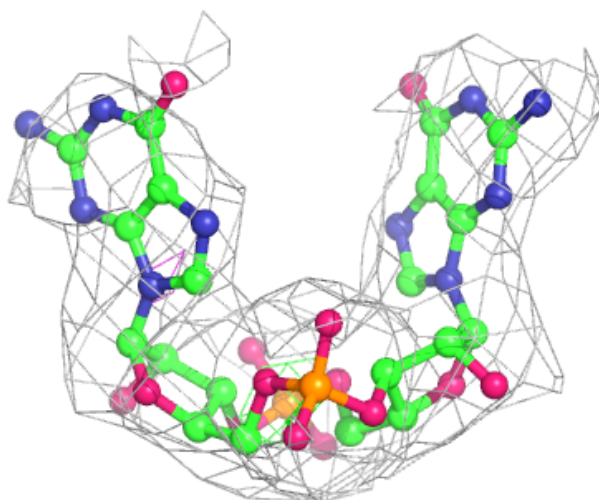
**Electron density around A16 C 801:**

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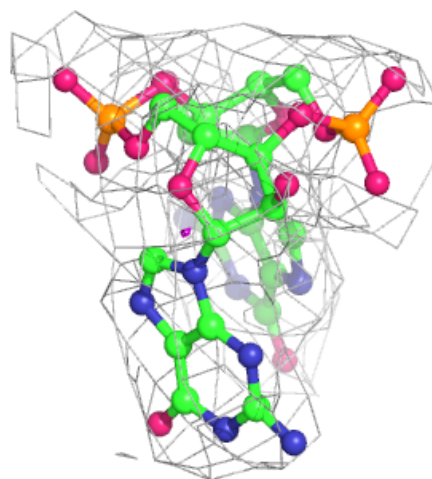
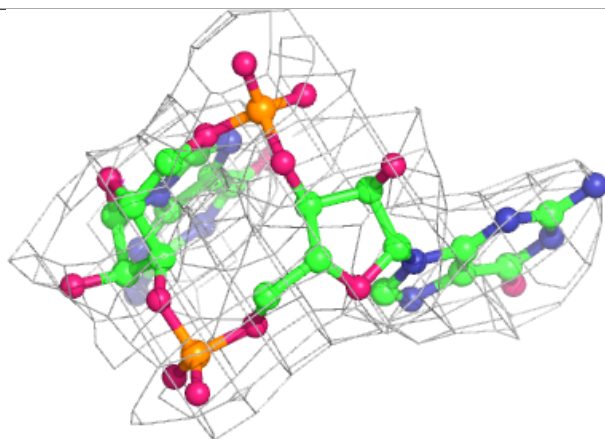
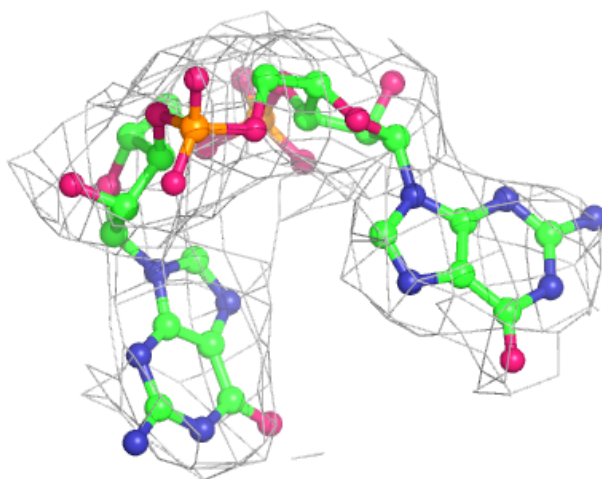
**Electron density around C2E D 804:**

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and green (positive)



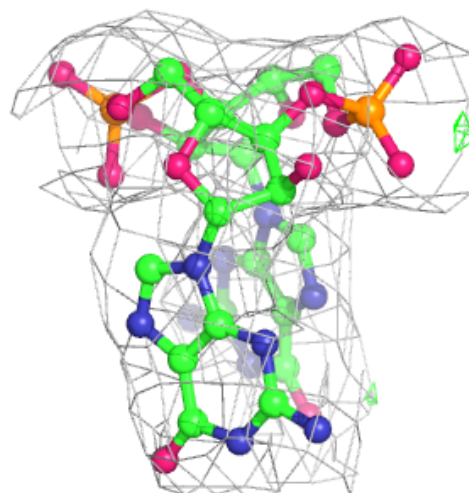
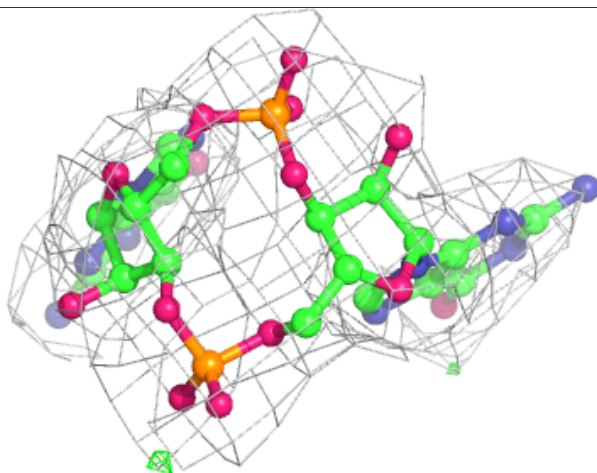
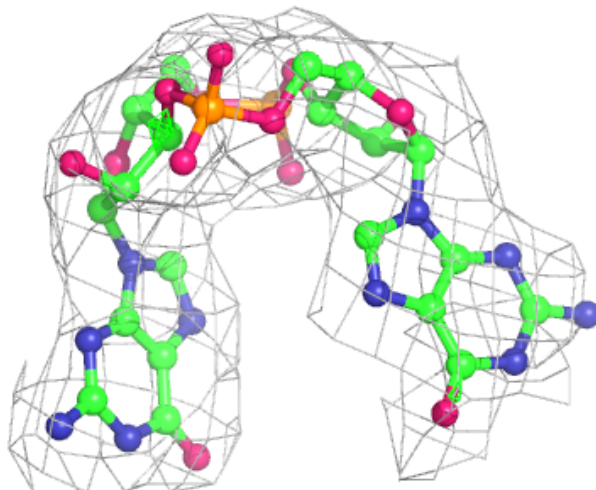
**Electron density around C2E E 803:**

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and green (positive)



**Electron density around C2E G 802:**

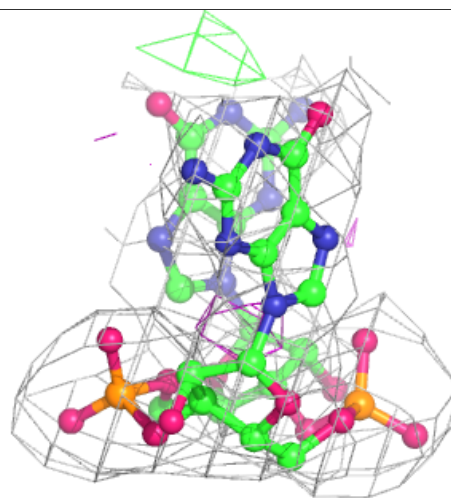
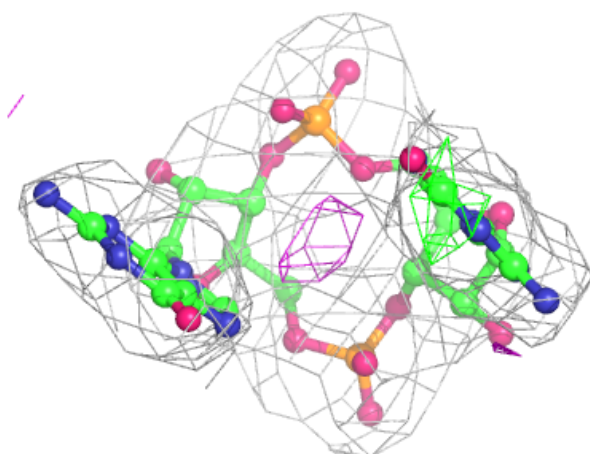
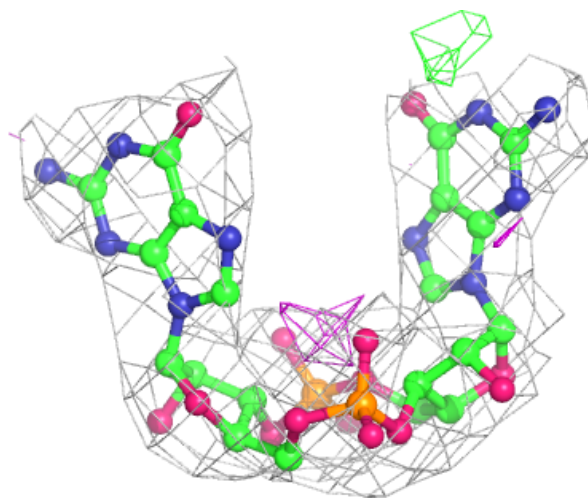
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





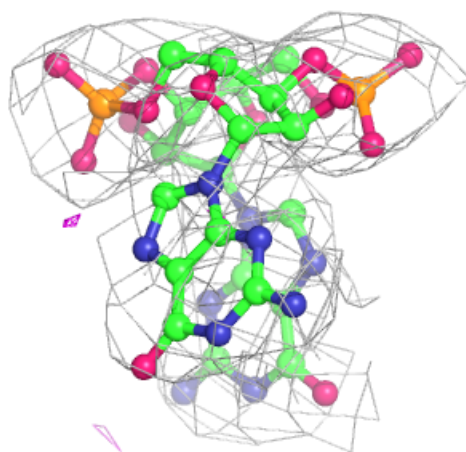
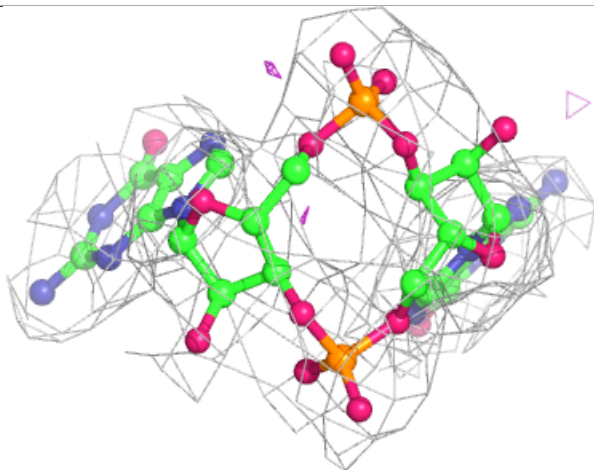
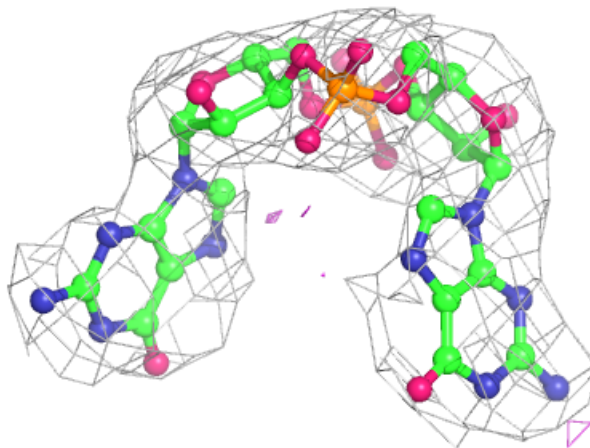
**Electron density around C2E I 802:**

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



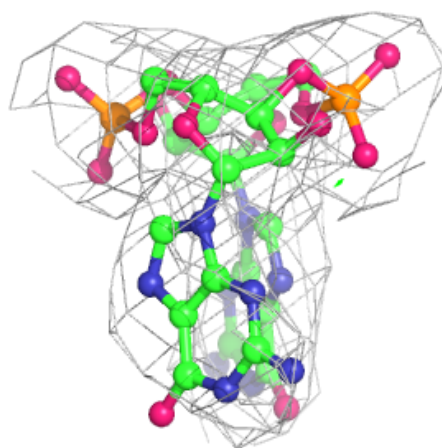
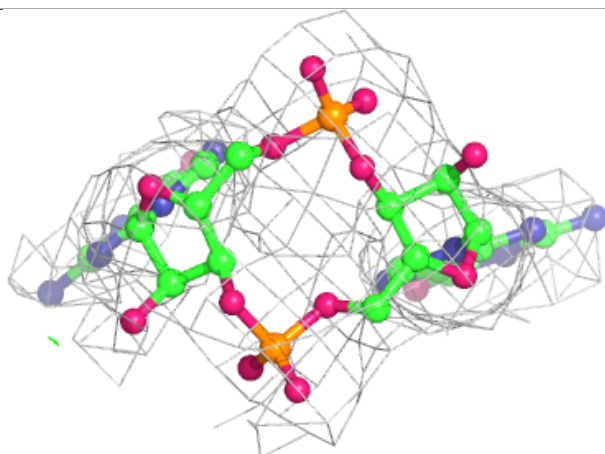
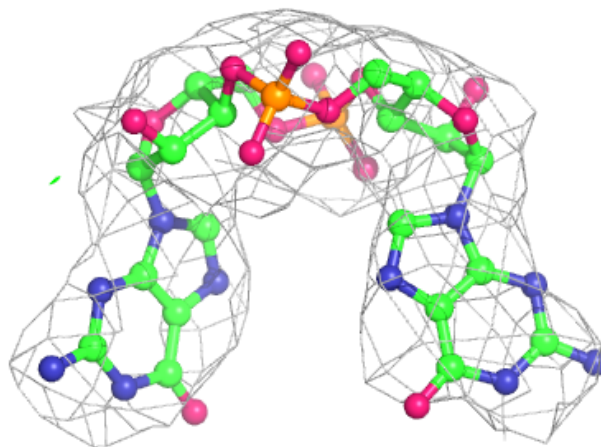
**Electron density around C2E J 802:**

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



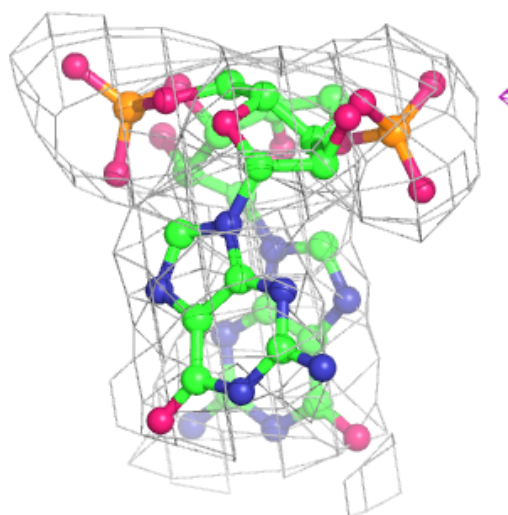
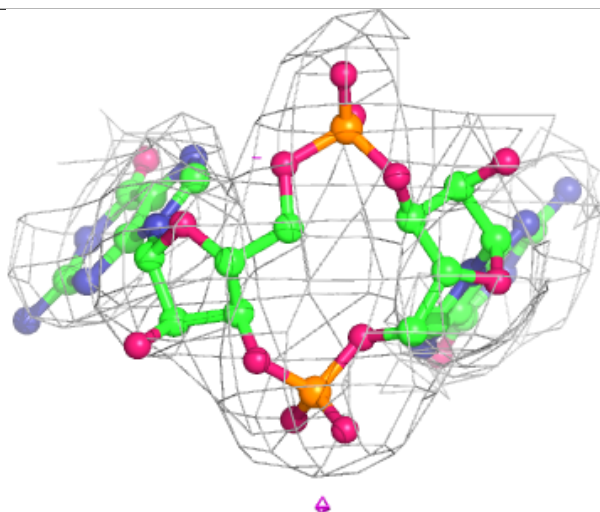
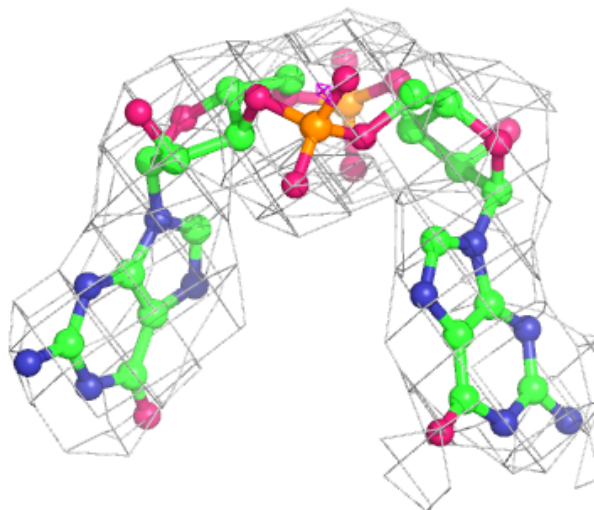
**Electron density around C2E C 802:**

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



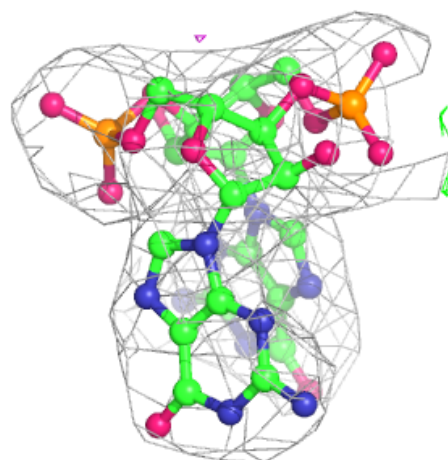
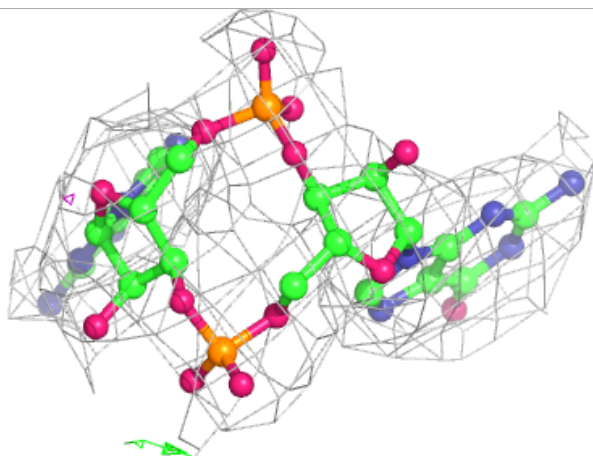
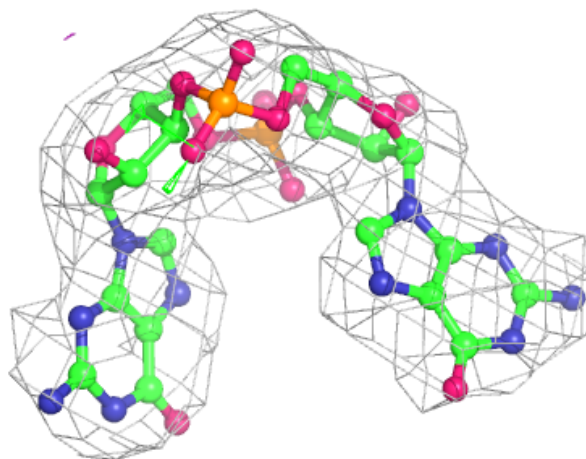
**Electron density around C2E H 803:**

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



**Electron density around C2E F 802:**

$2mF_o-DF_c$  (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.