



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 10, 2023 – 01:46 AM 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

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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.35.1
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) : 2.35.1

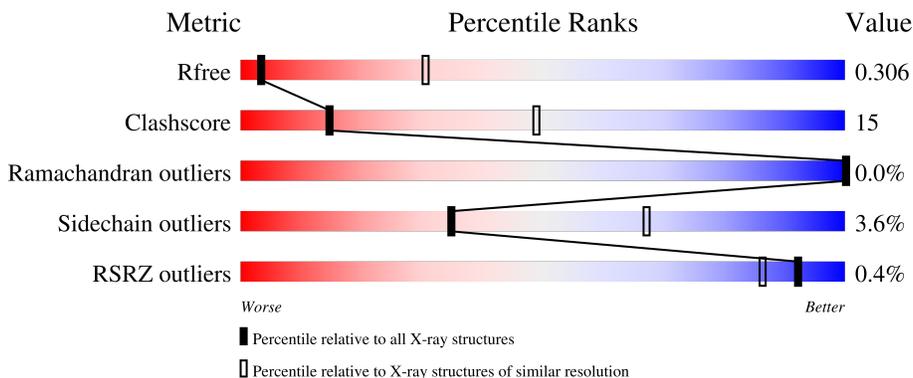
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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 ≥ 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	 65% 32% ..
1	D	709	 64% 32% ..
1	E	709	 66% 31% ..
1	F	709	 63% 34% ..
1	G	709	 68% 29% ..

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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 [i](#)

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

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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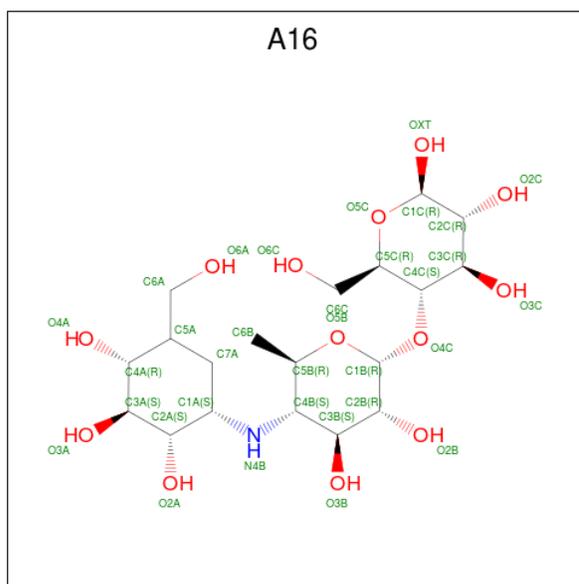
Chain	Residue	Modelled	Actual	Comment	Reference
D	192	ARG	LYS	conflict	UNP A0A5P2ALW6
D	296	ALA	SER	conflict	UNP A0A5P2ALW6
D	297	ASP	ASN	conflict	UNP A0A5P2ALW6
D	303	MET	THR	conflict	UNP A0A5P2ALW6
D	682	GLN	GLU	conflict	UNP A0A5P2ALW6
E	-2	GLY	-	expression tag	UNP A0A5P2ALW6
E	-1	SER	-	expression 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: C₁₉H₃₅NO₁₃) (labeled as "Ligand of Interest" by depositor).



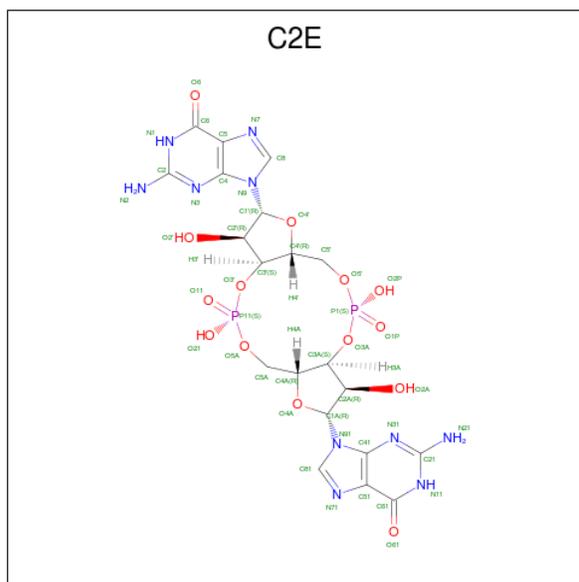
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	N			O
2	C	1	Total	C	N	O	0	0
			32	19	1	12		
2	D	1	Total	C	N	O	0	0
			32	19	1	12		

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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-dioxidooctahydro-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: C₂₀H₂₄N₁₀O₁₄P₂).



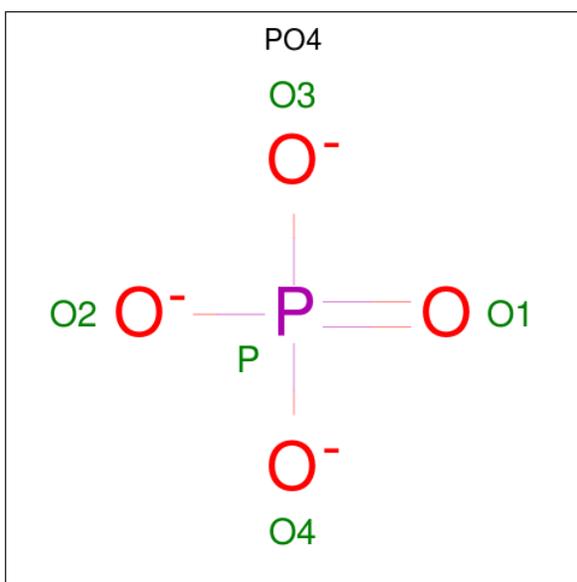
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	N	O	P	0	0
			46	20	10	14	2		
3	D	1	Total	C	N	O	P	0	0
			46	20	10	14	2		
3	E	1	Total	C	N	O	P	0	0
			46	20	10	14	2		
3	F	1	Total	C	N	O	P	0	0
			46	20	10	14	2		

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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: O₄P).



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		

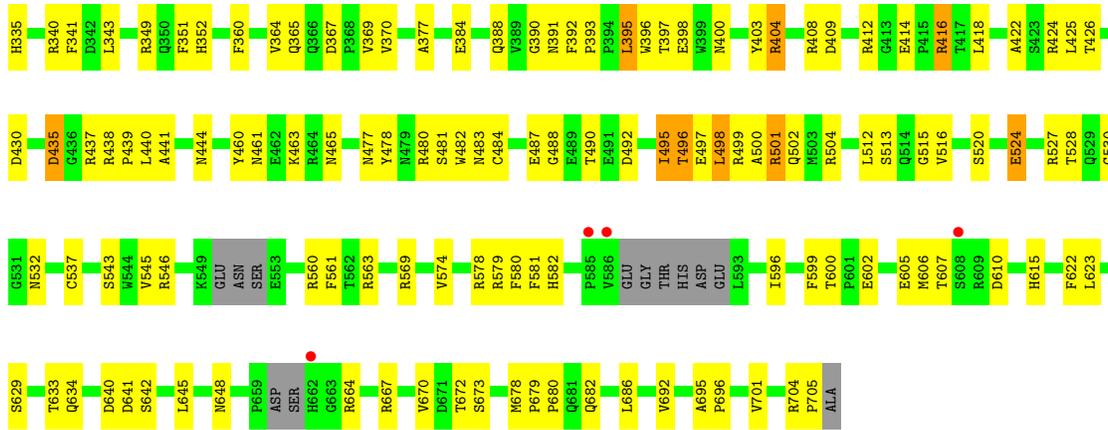
- Molecule 5 is water.

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

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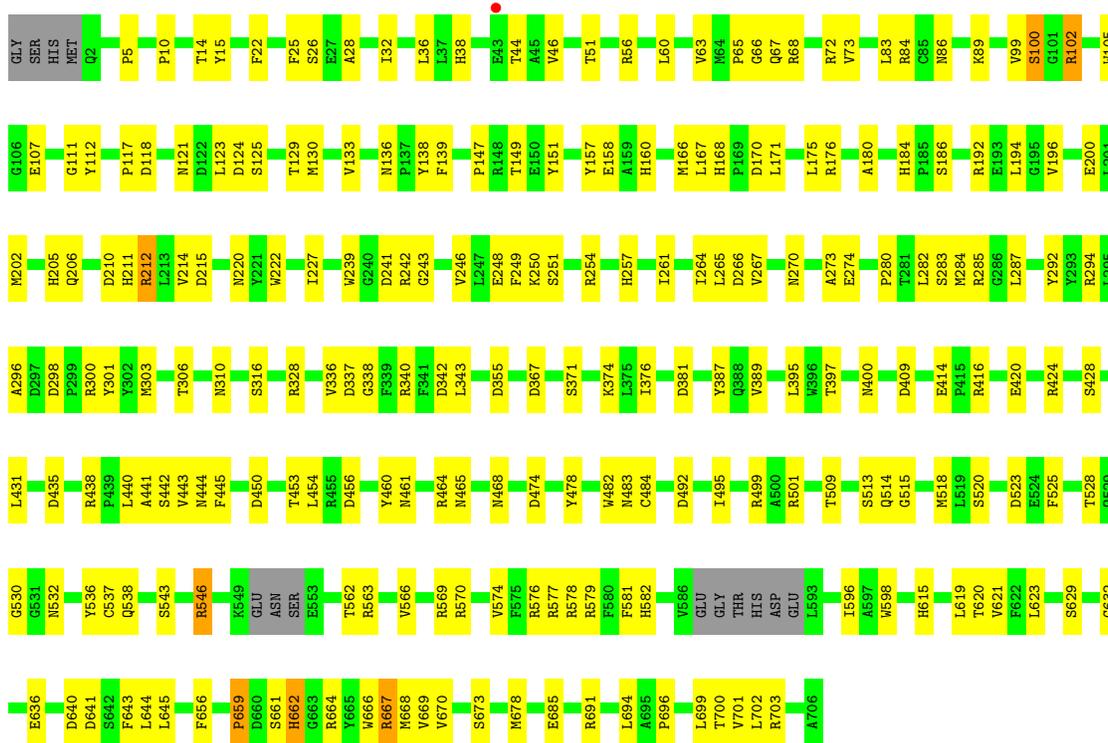
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	3	Total O 3 3	0	0
5	F	3	Total O 3 3	0	0
5	H	2	Total O 2 2	0	0
5	I	4	Total O 4 4	0	0



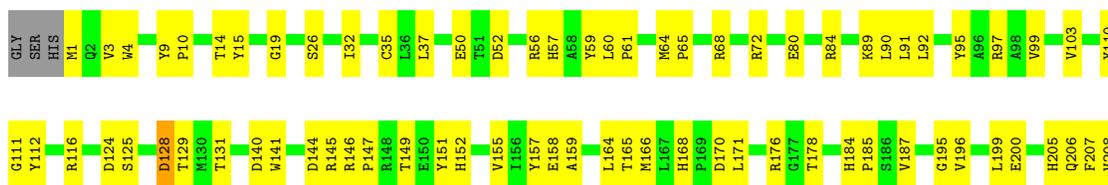
● Molecule 1: Glycogen debranching enzyme GlgX

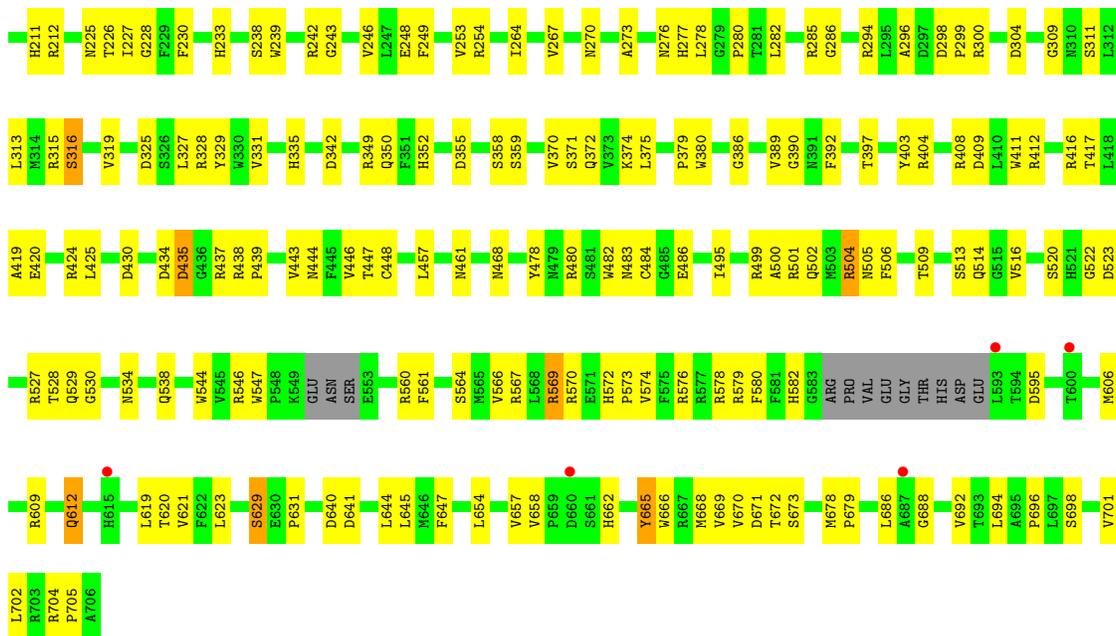
Chain E: 66% 31% ..



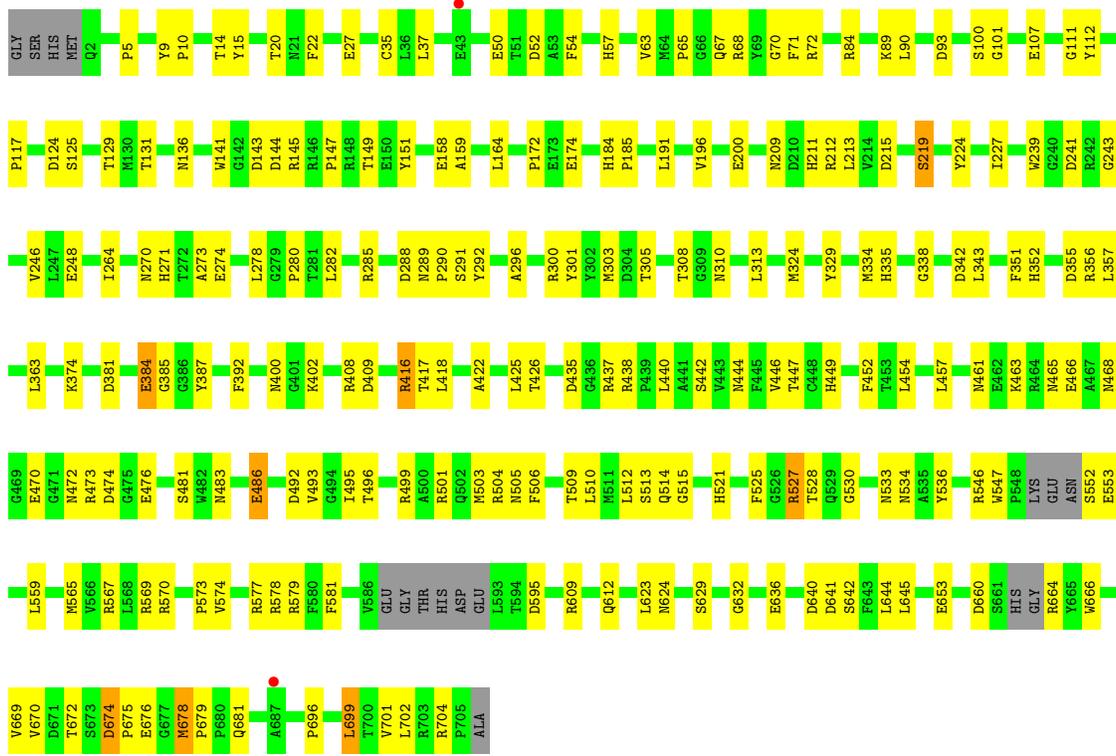
● Molecule 1: Glycogen debranching enzyme GlgX

Chain F: 63% 34% ..



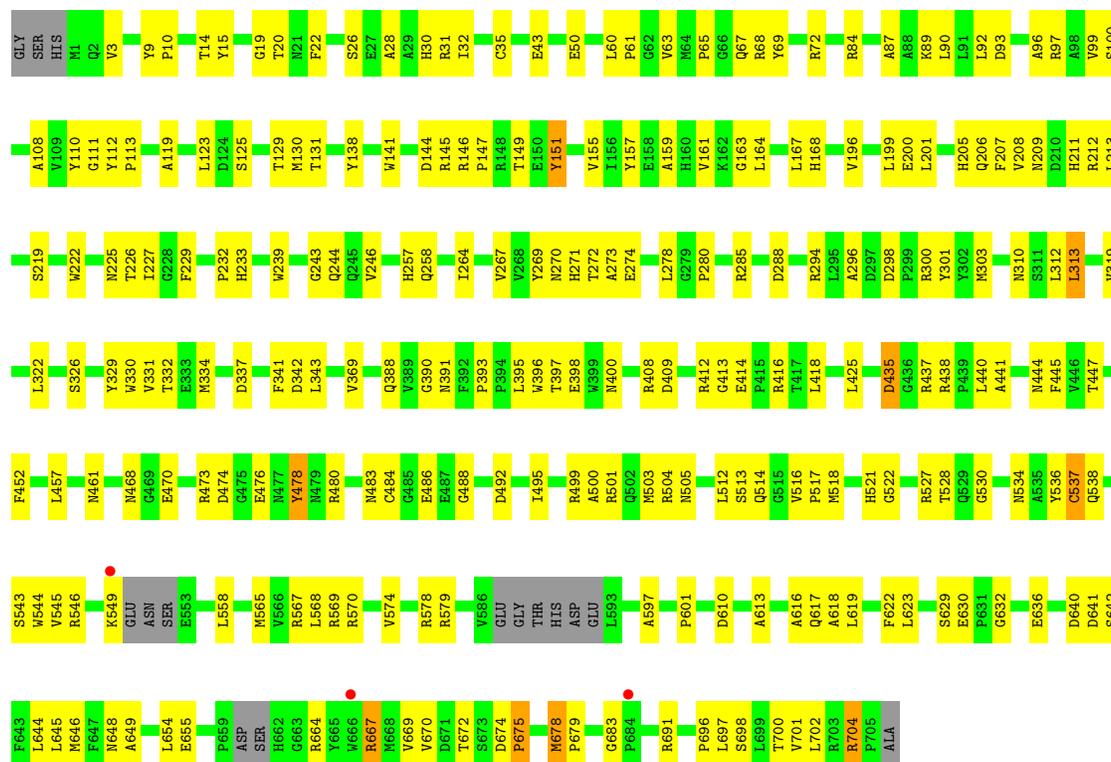


• Molecule 1: Glycogen debranching enzyme GlgX



• Molecule 1: Glycogen debranching enzyme GlgX





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 3.57Å)	Xtrriage
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 ²)	42.5	Xtrriage
Anisotropy	0.475	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 51.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	44957	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtrriage'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.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: A16, PO4, 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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	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
3	C2E	E	803	-	44,52,52	1.06	6 (13%)	52,82,82	1.12	4 (7%)
4	PO4	D	803	-	4,4,4	0.94	0	6,6,6	0.48	0
3	C2E	G	802	-	44,52,52	1.13	6 (13%)	52,82,82	1.02	2 (3%)
3	C2E	J	802	-	44,52,52	1.11	6 (13%)	52,82,82	1.13	3 (5%)
4	PO4	E	802	-	4,4,4	0.94	0	6,6,6	0.46	0
3	C2E	D	804	-	44,52,52	1.15	6 (13%)	52,82,82	1.35	7 (13%)
2	A16	F	801	-	33,34,35	0.79	1 (3%)	44,50,52	1.14	2 (4%)
3	C2E	F	802	-	44,52,52	1.22	6 (13%)	52,82,82	1.19	5 (9%)
2	A16	H	801	-	33,34,35	0.67	1 (3%)	44,50,52	1.53	6 (13%)
2	A16	G	801	1	33,34,35	0.57	0	44,50,52	1.15	5 (11%)
2	A16	C	801	-	33,34,35	0.49	0	44,50,52	1.07	2 (4%)
2	A16	J	801	-	33,34,35	0.57	0	44,50,52	1.14	3 (6%)
3	C2E	H	803	-	44,52,52	1.23	6 (13%)	52,82,82	1.26	5 (9%)
4	PO4	D	802	-	4,4,4	0.95	0	6,6,6	0.53	0
2	A16	I	801	-	33,34,35	0.62	1 (3%)	44,50,52	1.03	2 (4%)
3	C2E	I	802	-	44,52,52	1.14	6 (13%)	52,82,82	1.35	8 (15%)
3	C2E	C	802	-	44,52,52	1.15	6 (13%)	52,82,82	1.13	3 (5%)
2	A16	D	801	-	33,34,35	0.56	0	44,50,52	1.16	5 (11%)
2	A16	E	801	-	33,34,35	0.41	0	44,50,52	1.07	1 (2%)
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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	C2E	E	803	-	-	5/22/62/62	0/6/7/7
3	C2E	F	802	-	-	6/22/62/62	0/6/7/7
3	C2E	H	803	-	-	10/22/62/62	0/6/7/7
2	A16	D	801	-	-	3/12/69/72	1/3/3/3
3	C2E	G	802	-	-	12/22/62/62	0/6/7/7
2	A16	H	801	-	-	4/12/69/72	0/3/3/3
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
2	A16	C	801	-	-	5/12/69/72	1/3/3/3
2	A16	I	801	-	-	6/12/69/72	1/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	C2E	D	804	-	-	2/22/62/62	0/6/7/7
2	A16	E	801	-	-	5/12/69/72	1/3/3/3
2	A16	F	801	-	-	7/12/69/72	1/3/3/3
3	C2E	I	802	-	-	13/22/62/62	0/6/7/7
3	C2E	C	802	-	-	7/22/62/62	0/6/7/7
2	A16	J	801	-	-	5/12/69/72	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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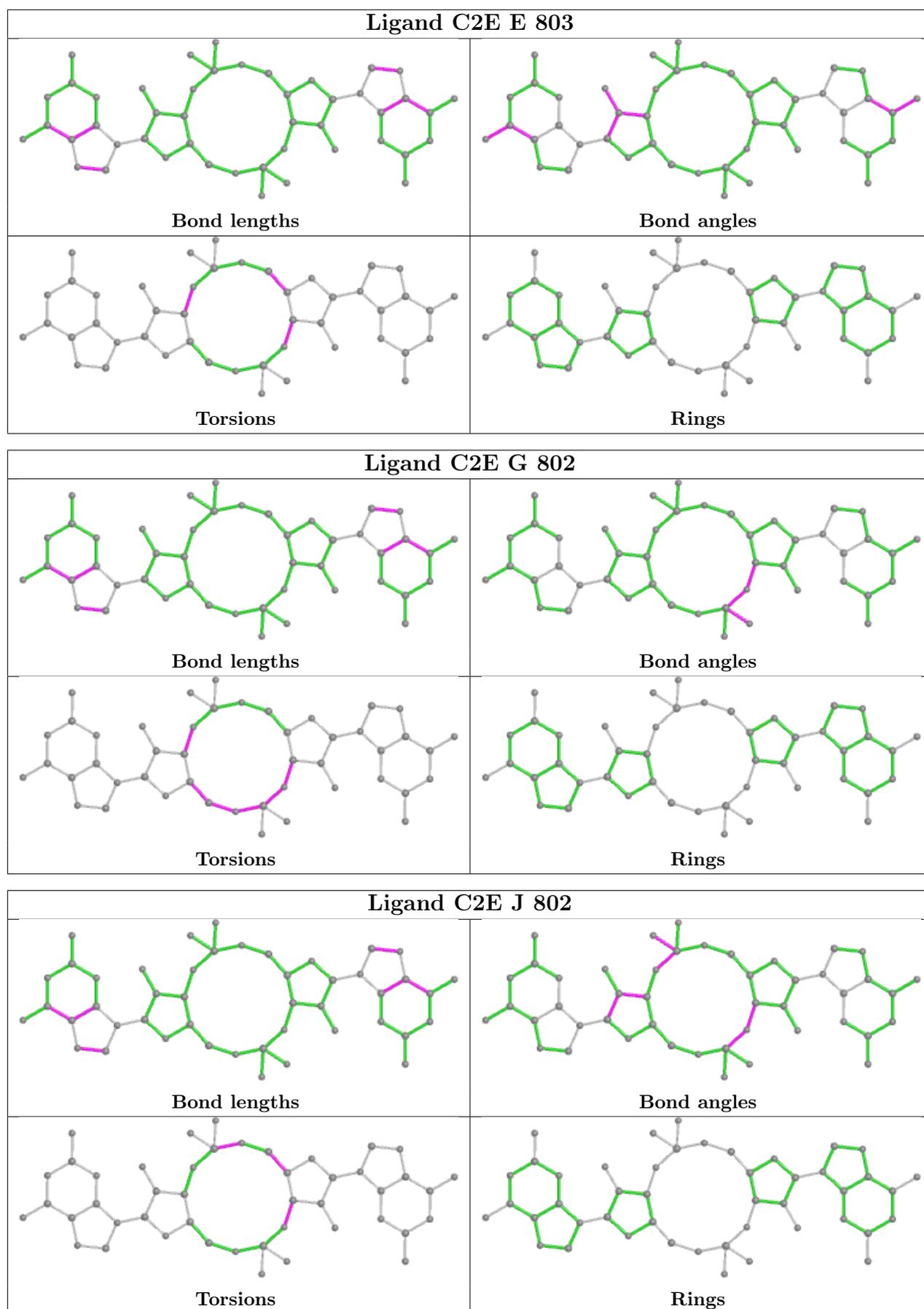
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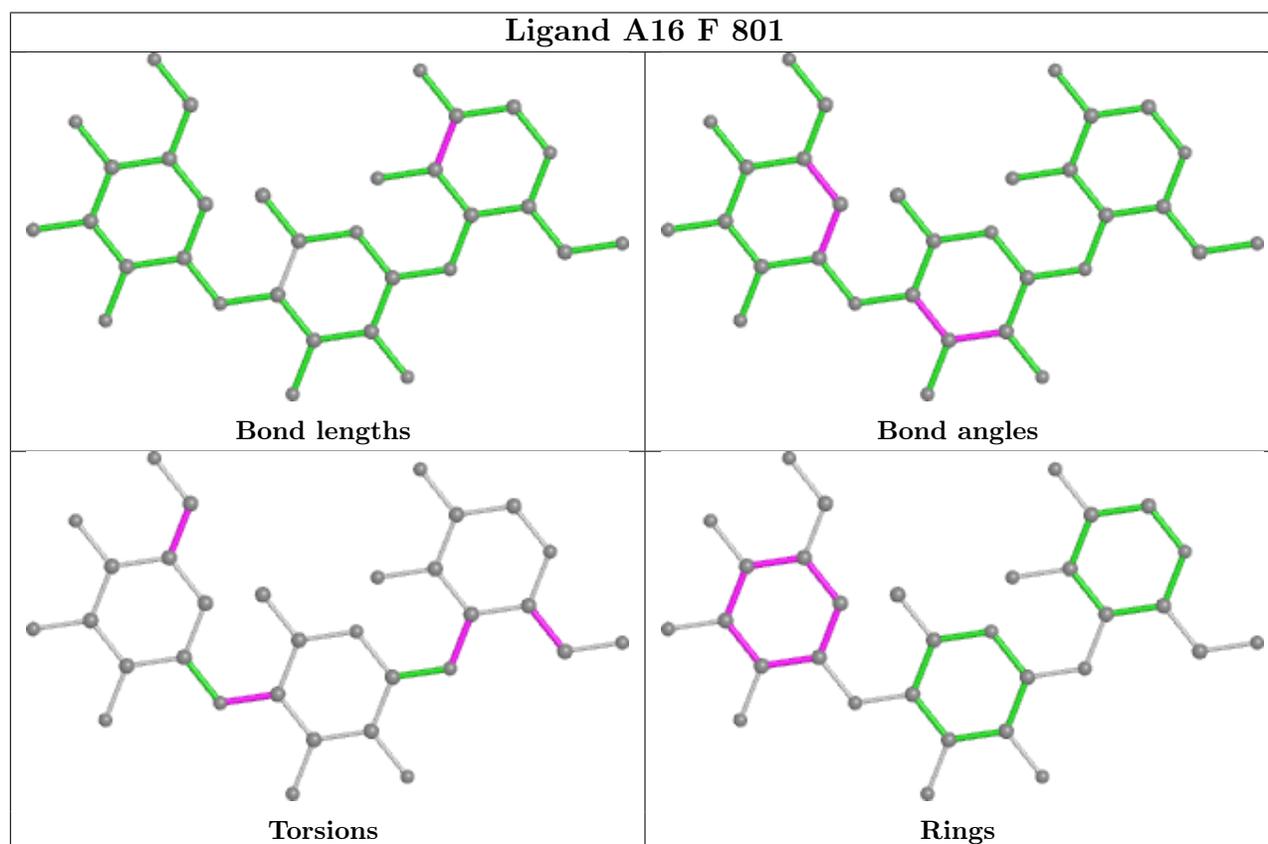
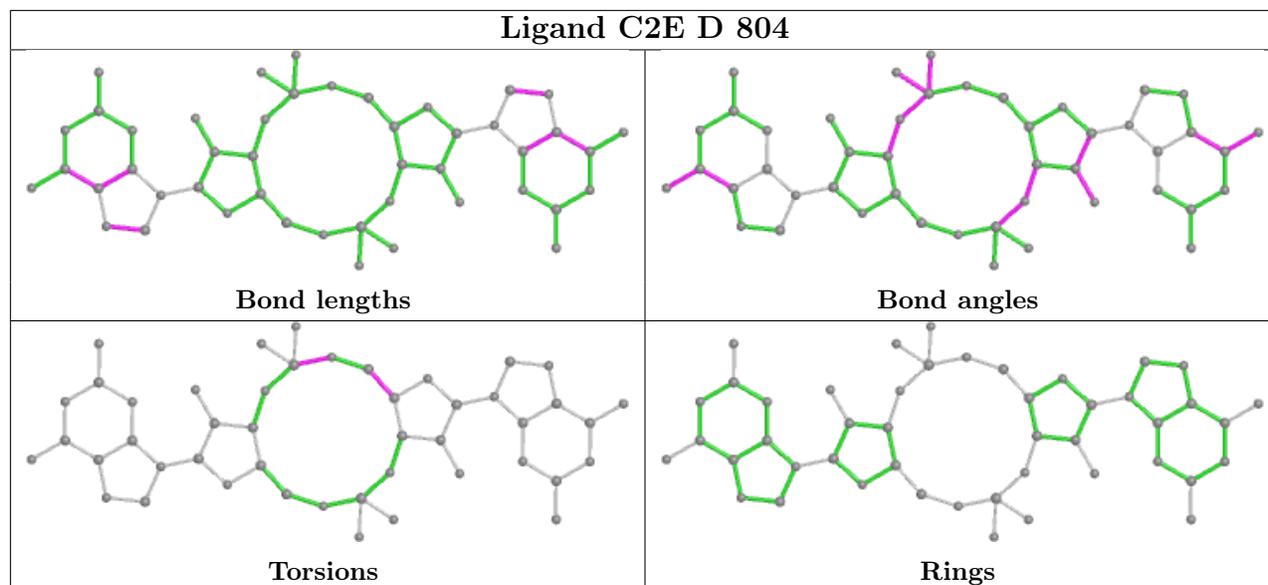
Mol	Chain	Res	Type	Atoms
2	F	801	A16	C1A-C2A-C3A-C4A-C5A-C7A
2	I	801	A16	C1A-C2A-C3A-C4A-C5A-C7A
2	C	801	A16	C1A-C2A-C3A-C4A-C5A-C7A

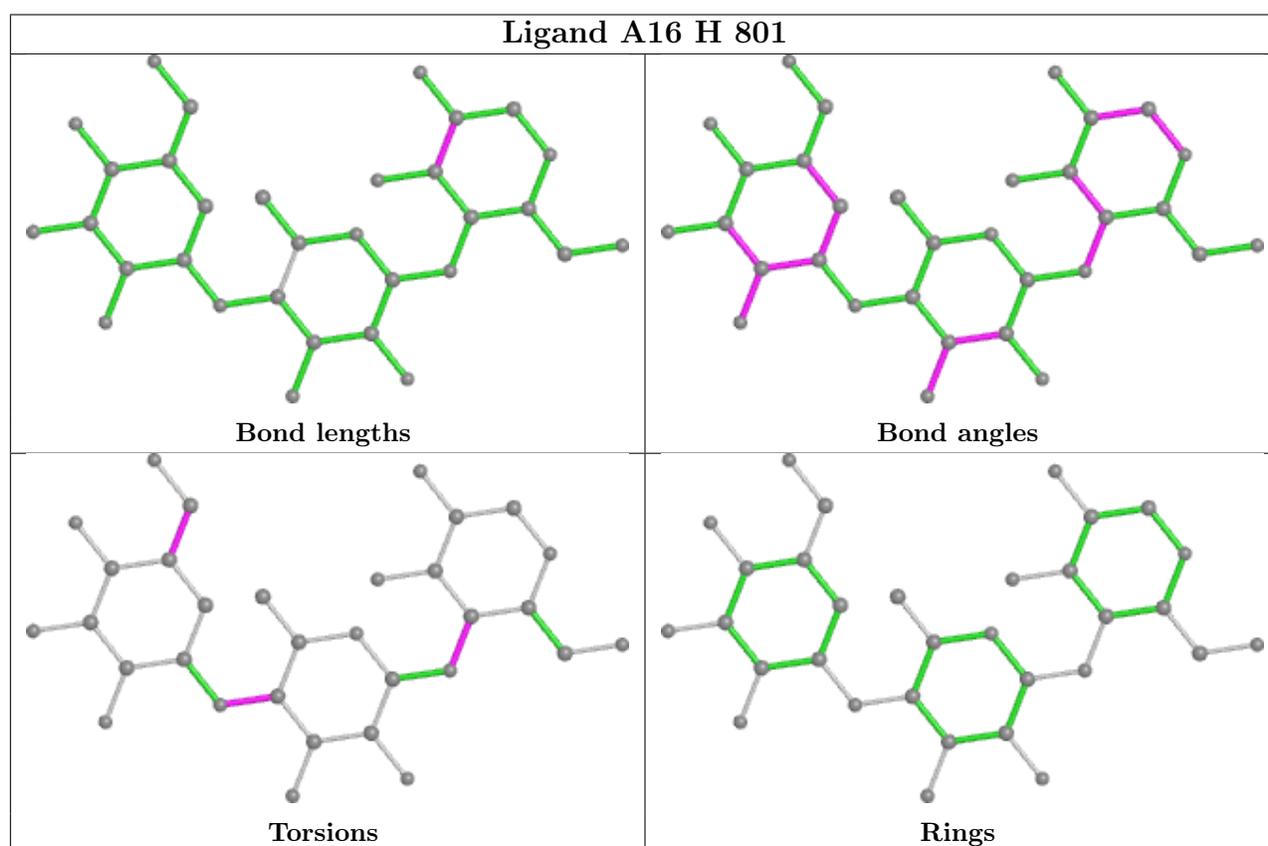
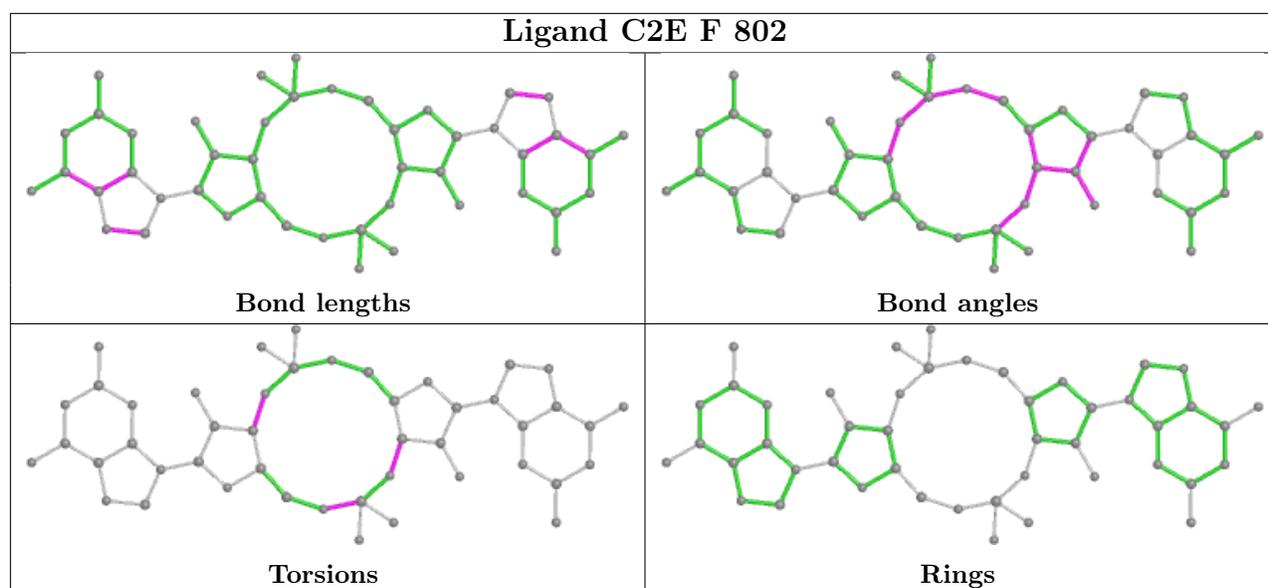
17 monomers are involved in 115 short contacts:

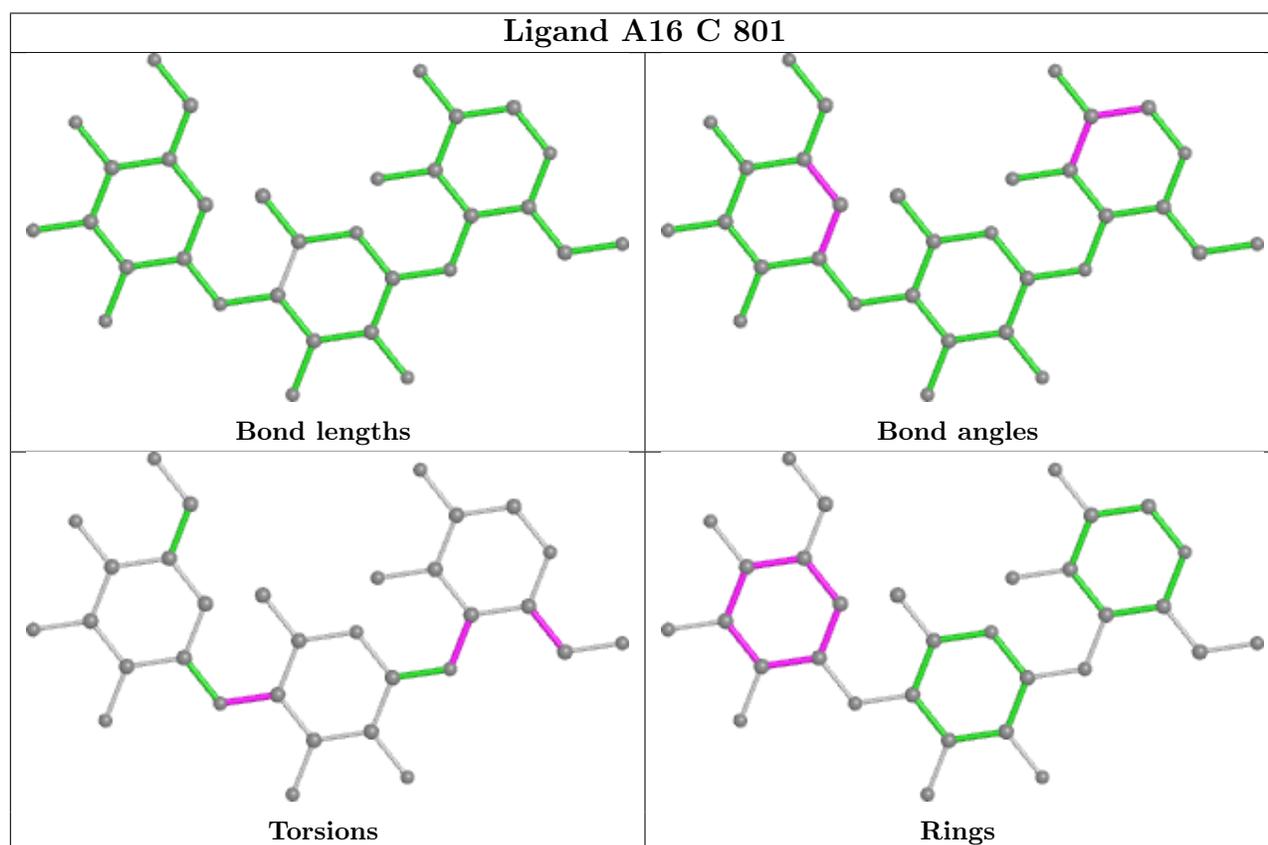
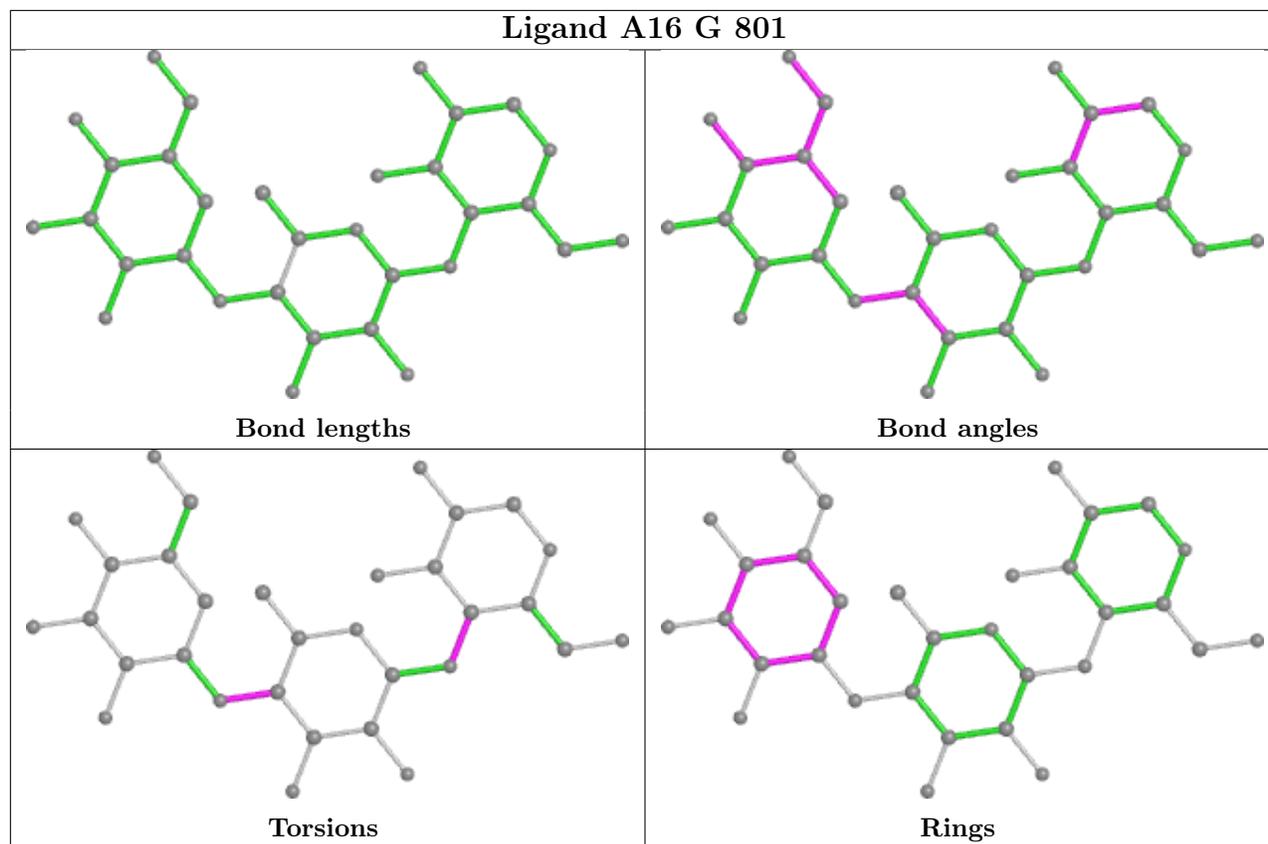
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	803	C2E	5	0
3	G	802	C2E	5	0
3	J	802	C2E	4	0
3	D	804	C2E	18	0
2	F	801	A16	7	0
3	F	802	C2E	3	0
2	H	801	A16	5	0
2	G	801	A16	10	0
2	C	801	A16	5	0
2	J	801	A16	10	0
3	H	803	C2E	7	0
4	D	802	PO4	1	0
2	I	801	A16	5	0
3	I	802	C2E	7	0
3	C	802	C2E	9	0
2	D	801	A16	7	0
2	E	801	A16	7	0

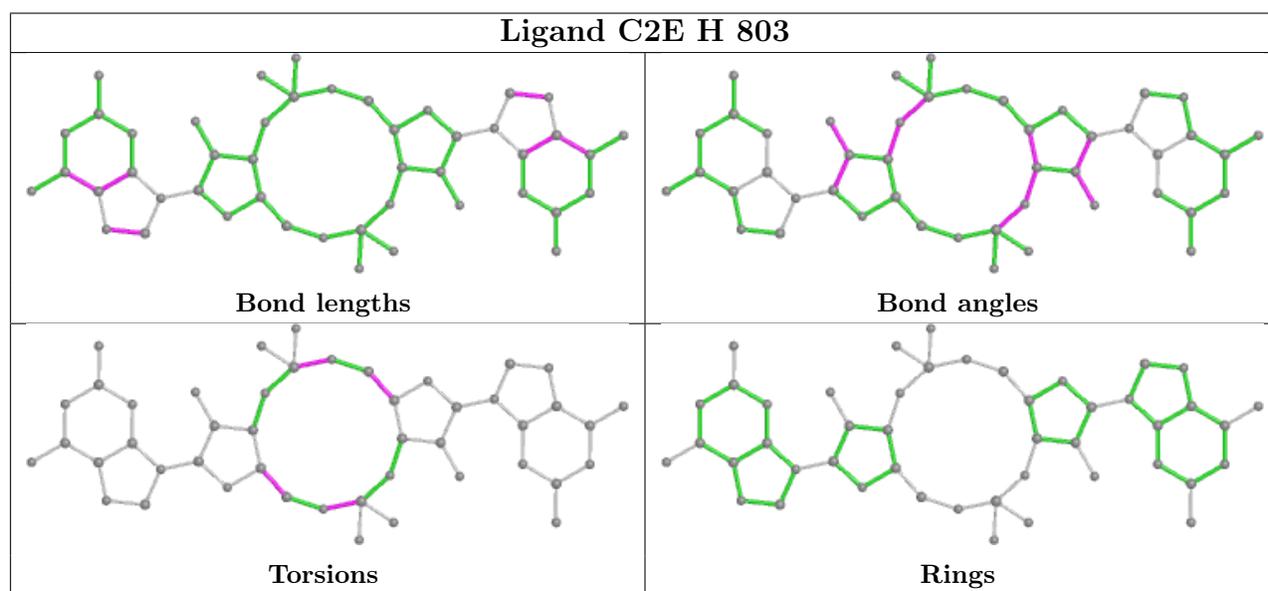
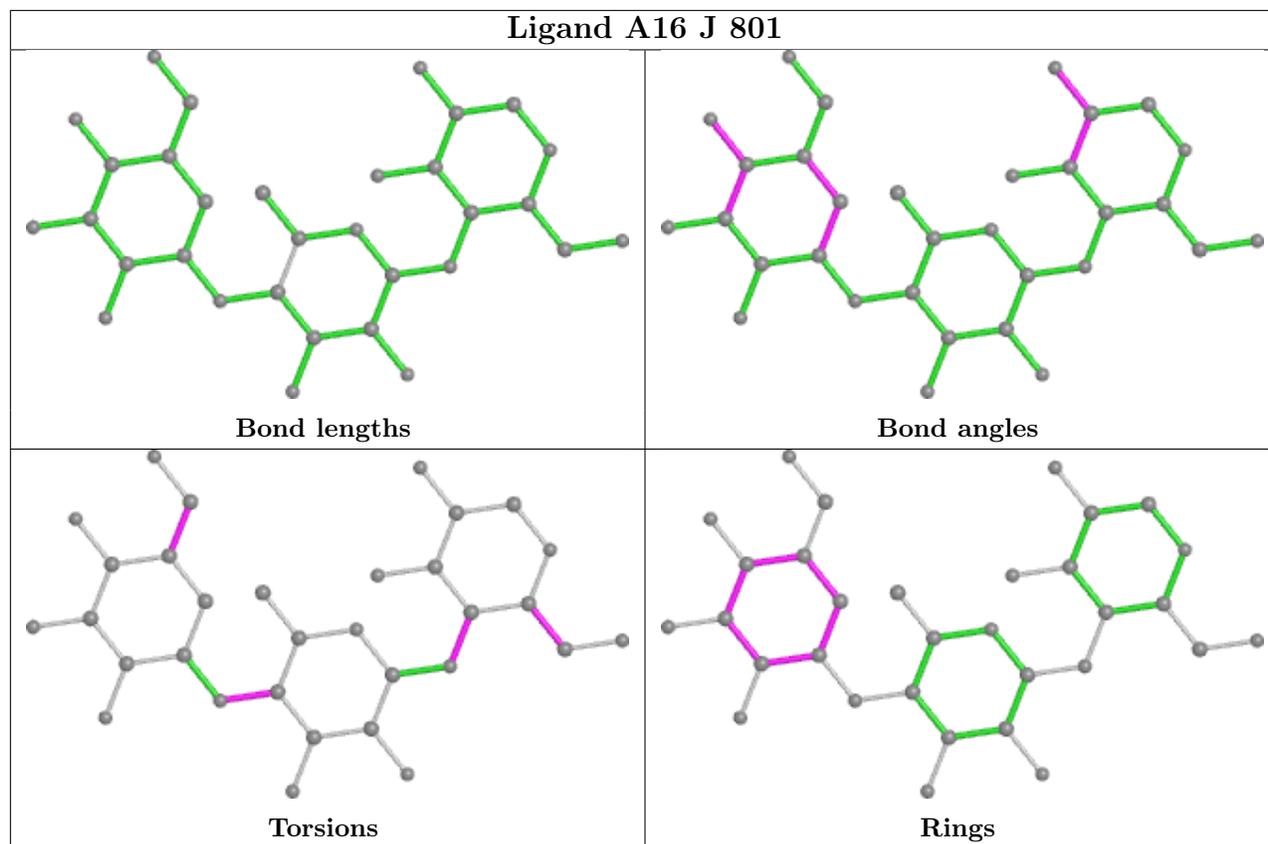
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

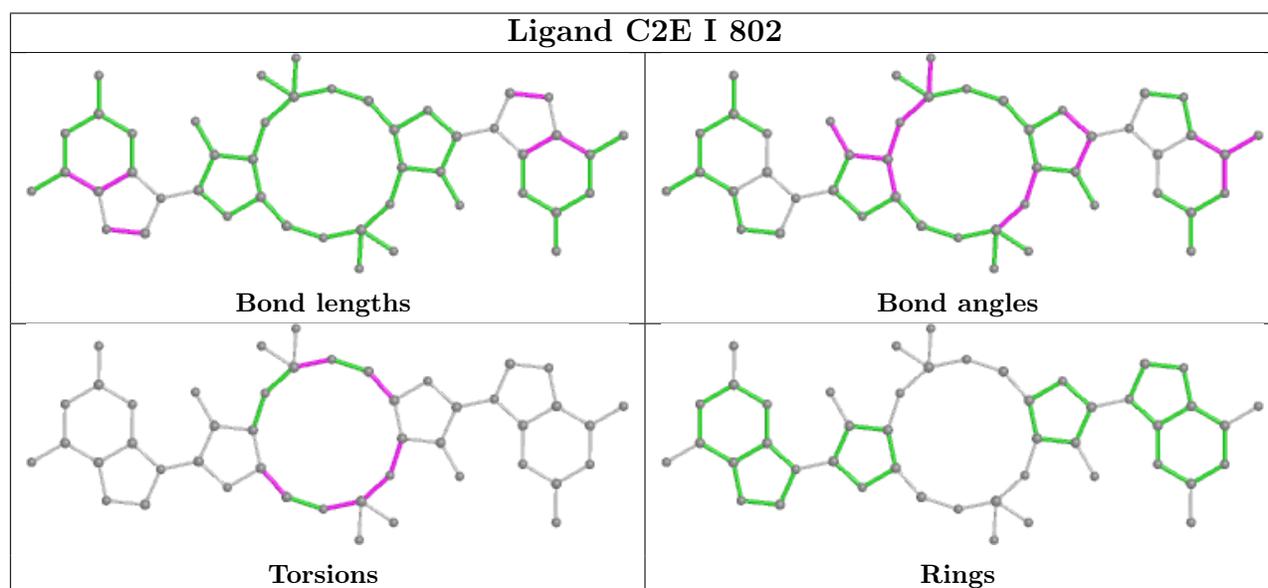
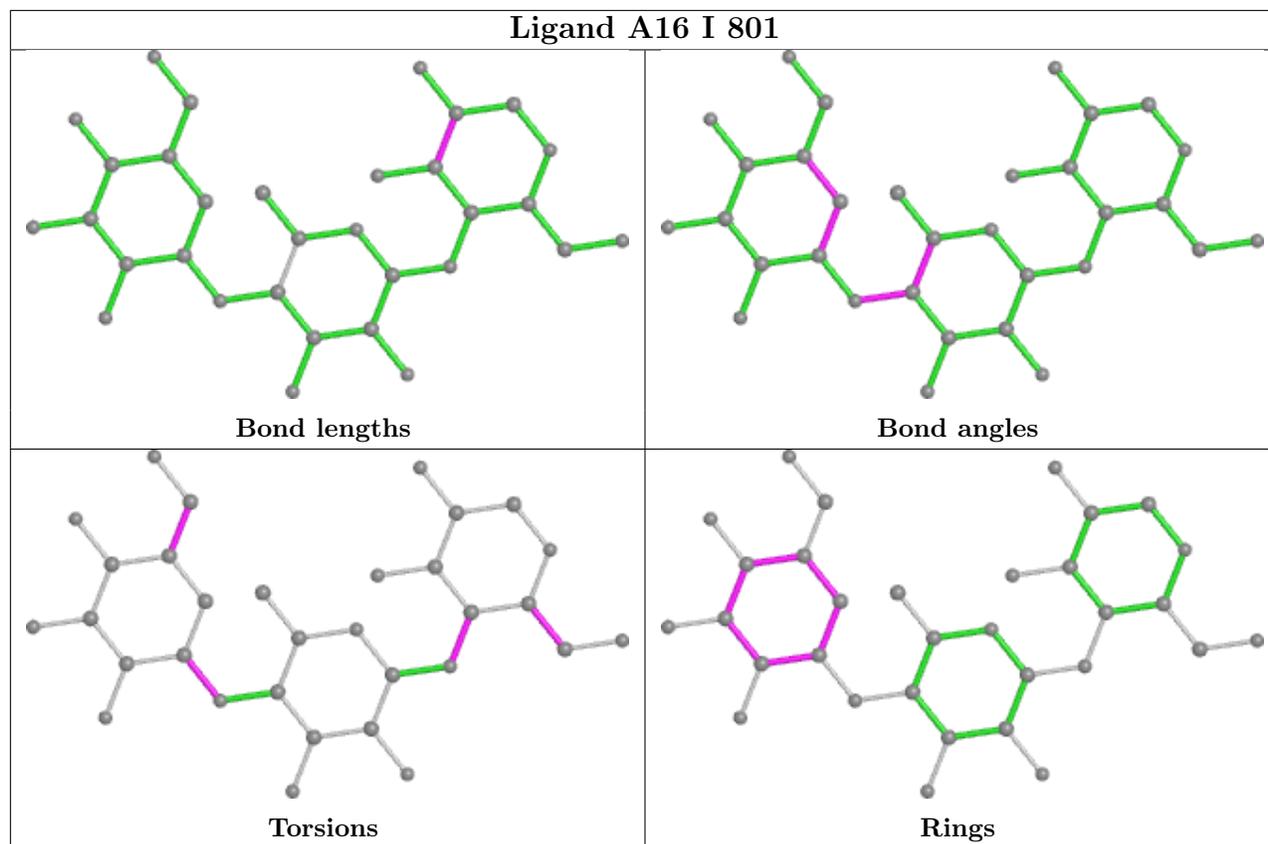


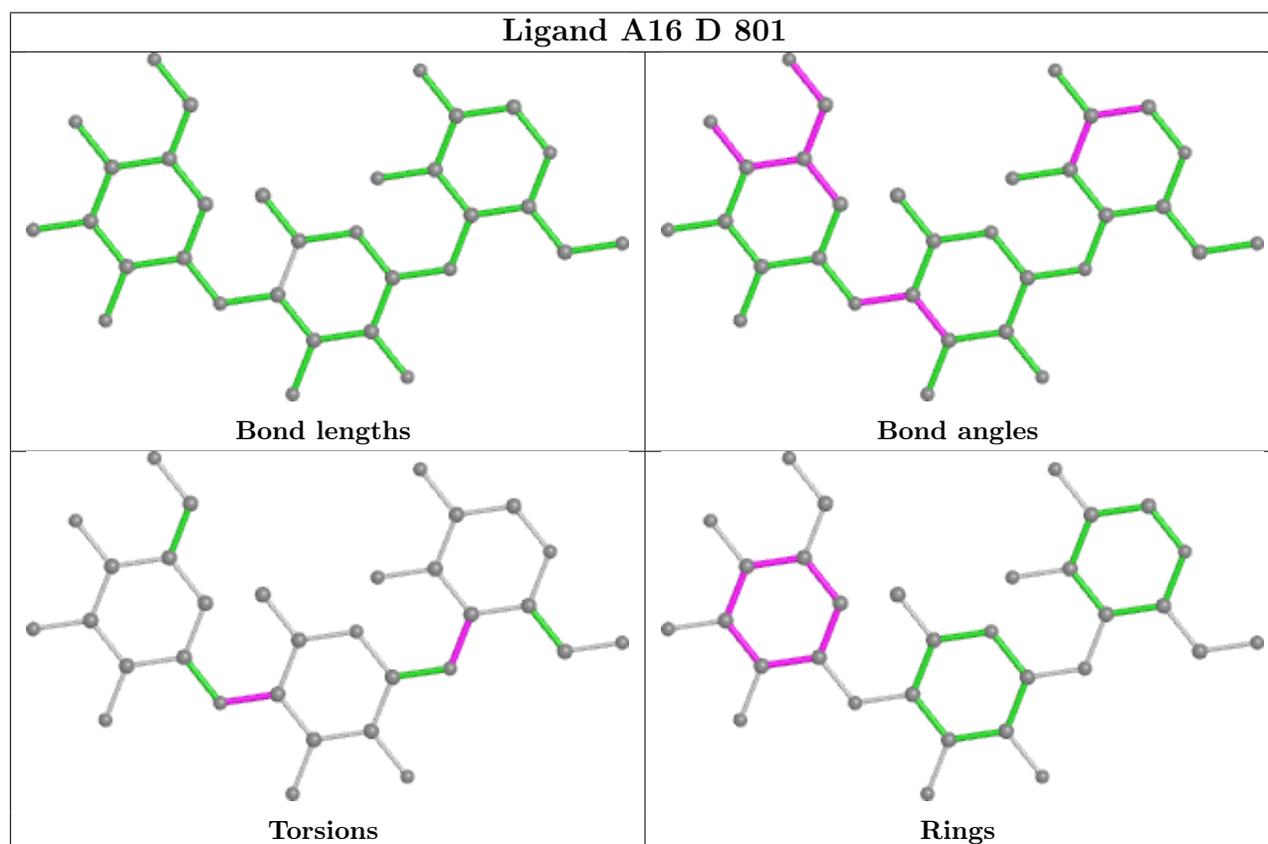
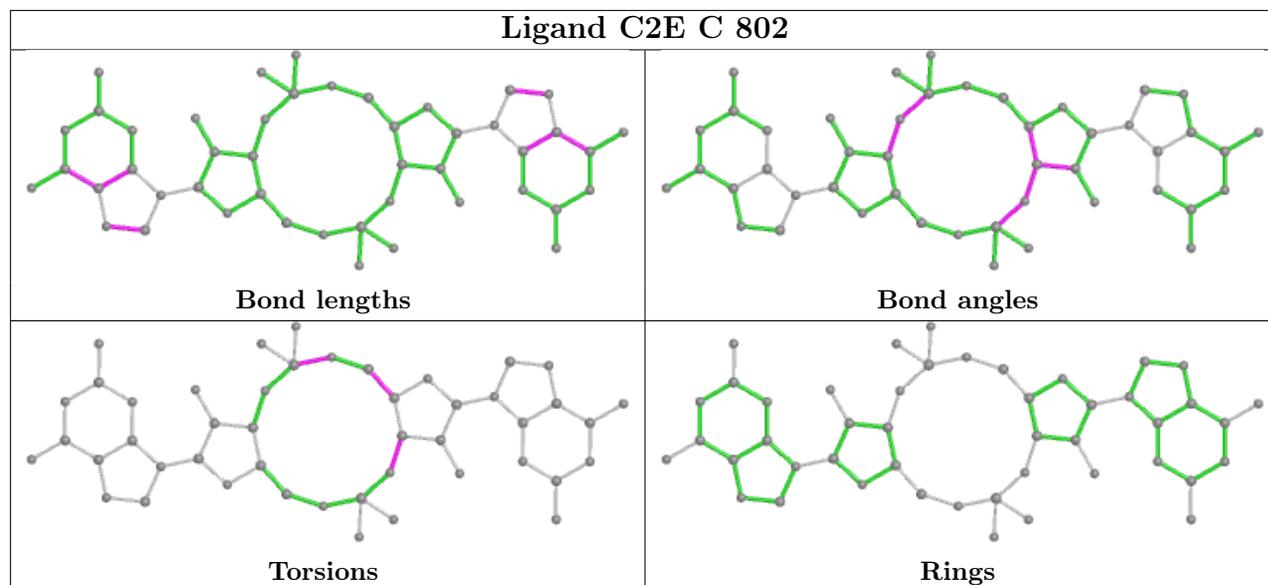


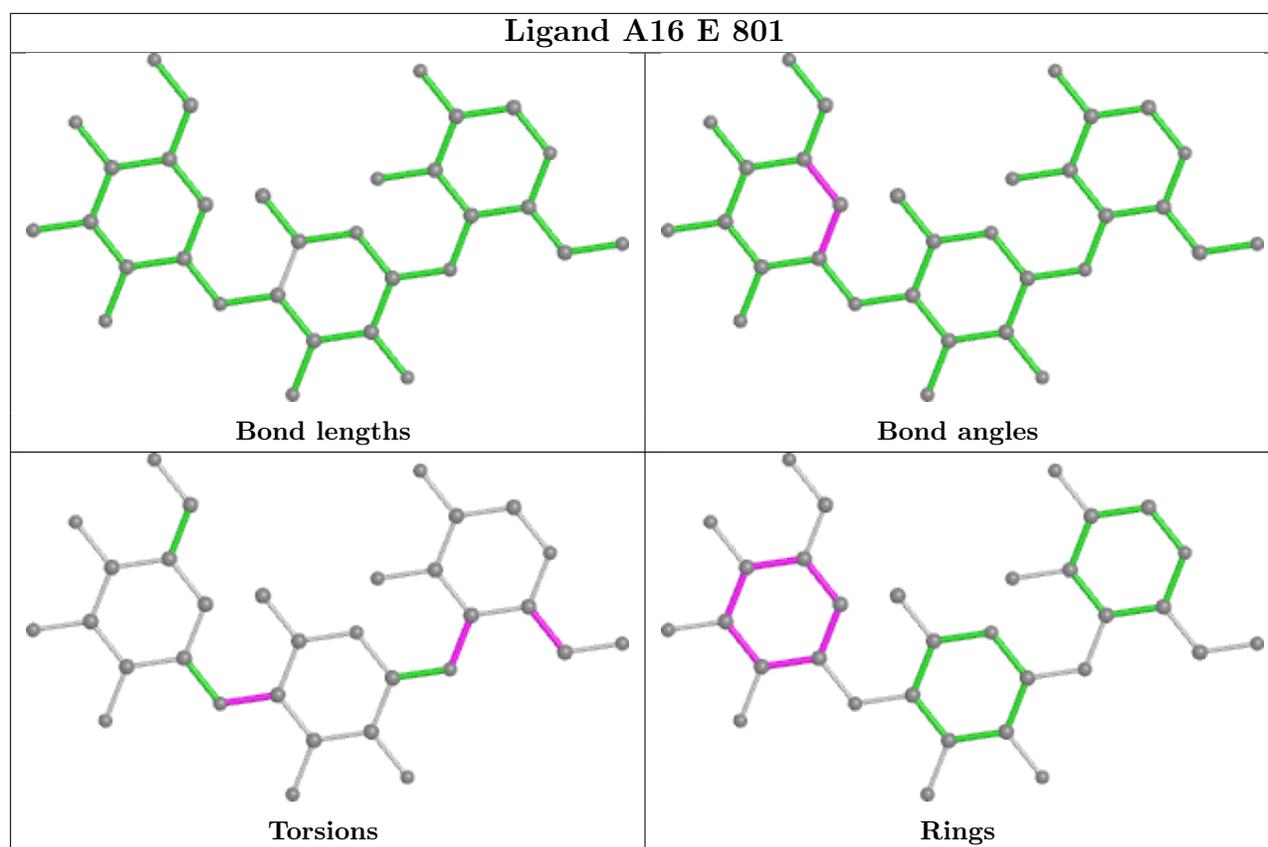












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	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

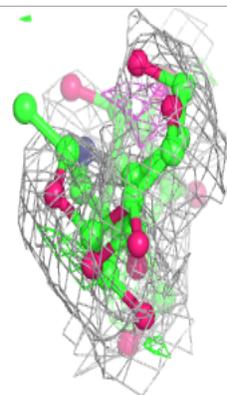
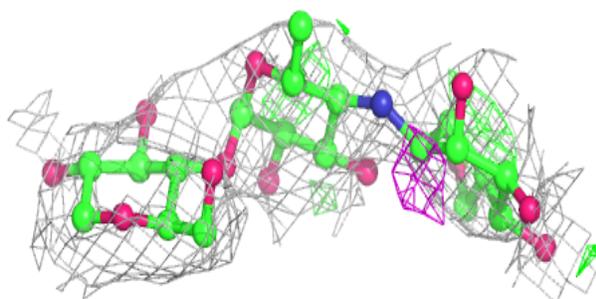
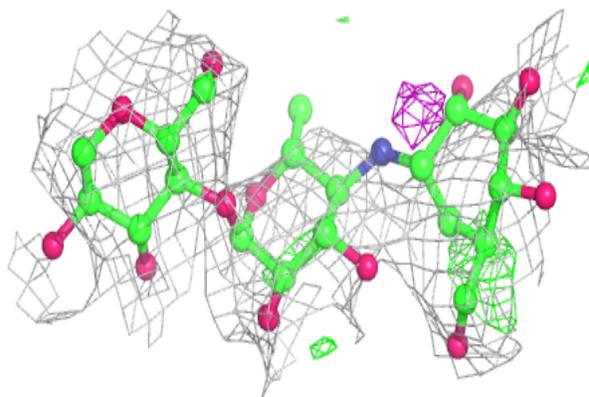
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
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

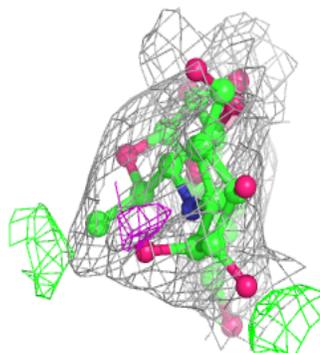
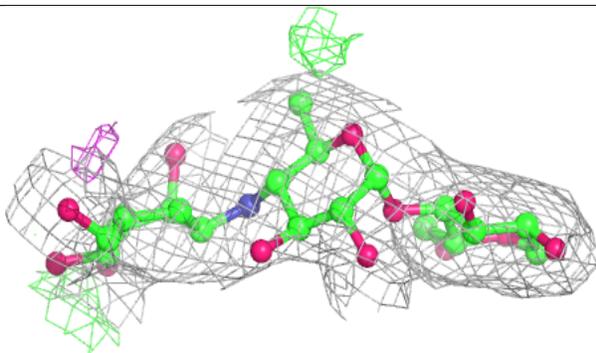
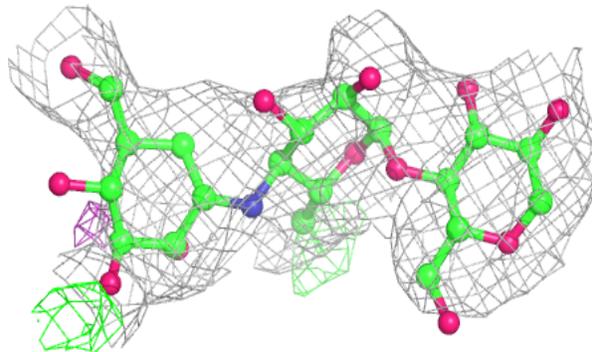
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

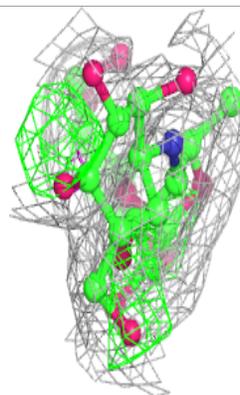
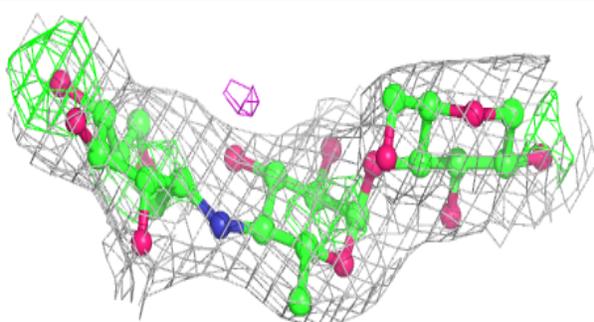
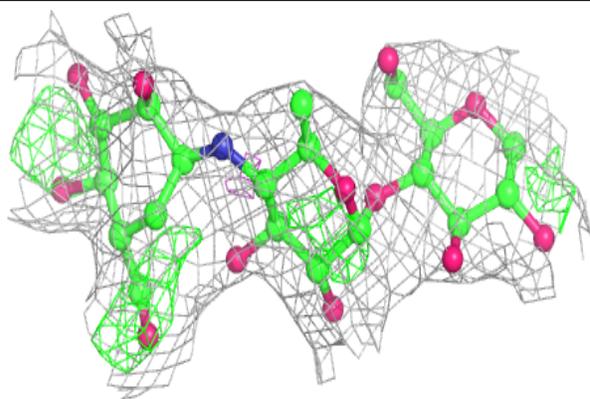
**Electron density around A16 I 801:**

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

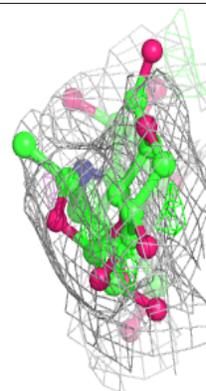
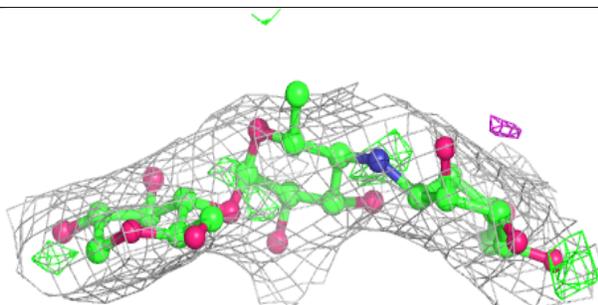
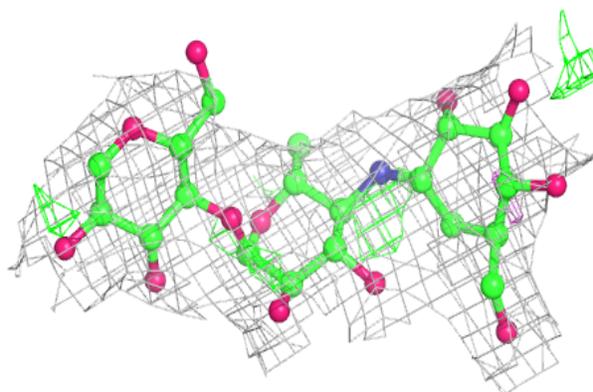


Electron density around A16 D 801:

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

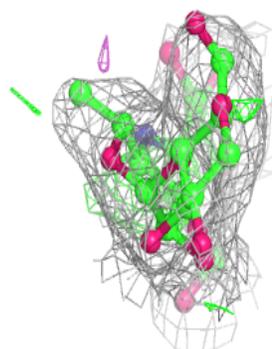
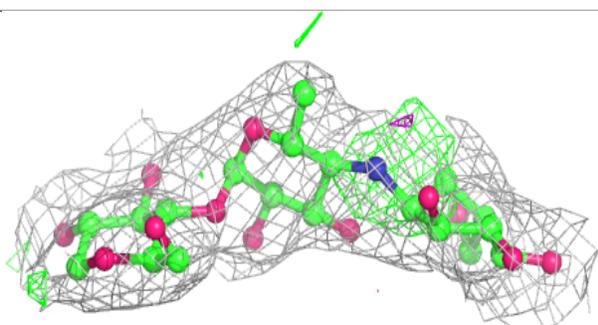
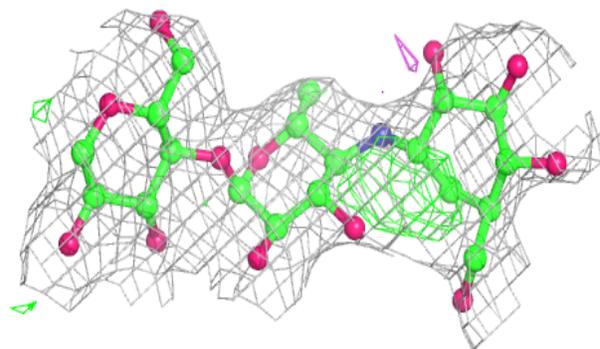
**Electron density around A16 J 801:**

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

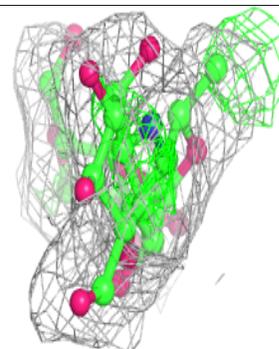
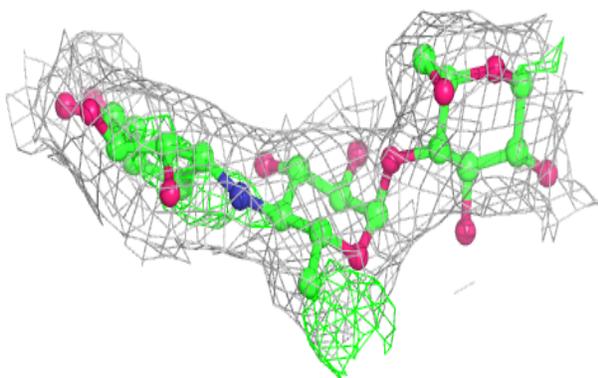
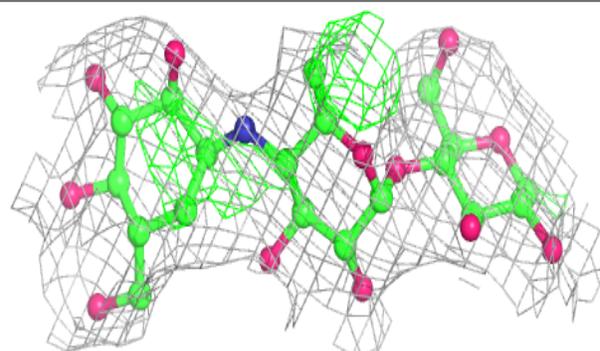


Electron density around A16 E 801:

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

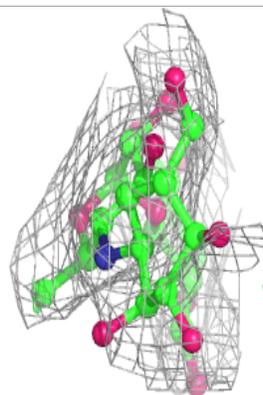
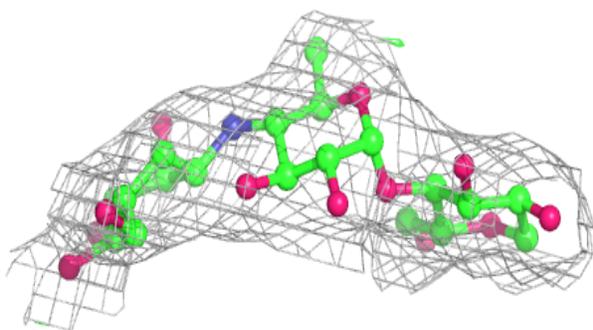
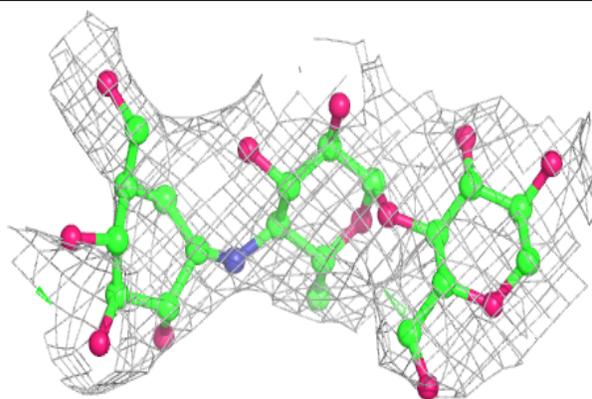
**Electron density around A16 H 801:**

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

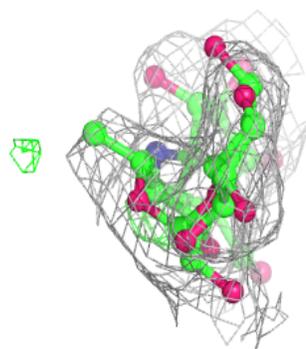
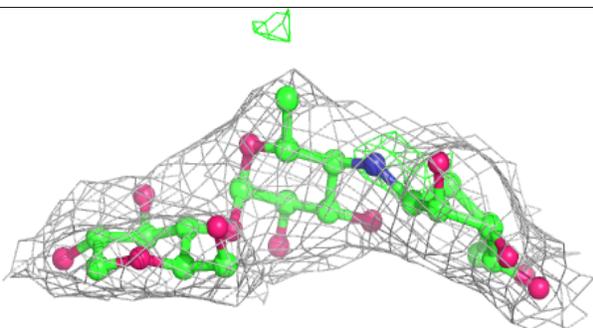
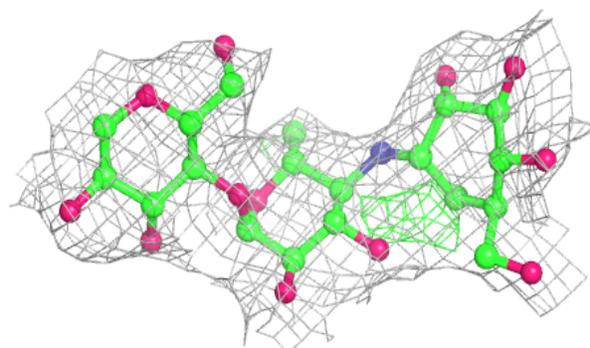


Electron density around A16 F 801:

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

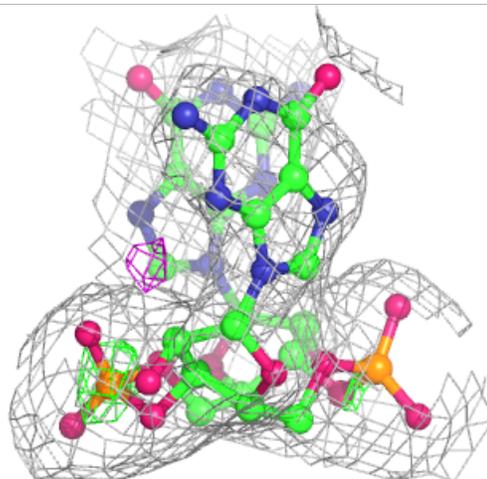
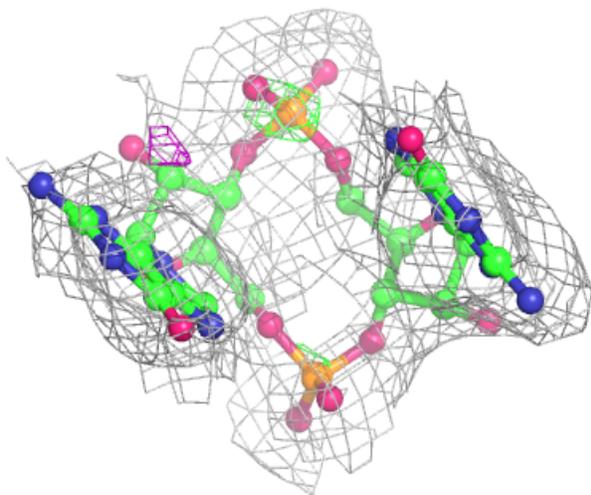
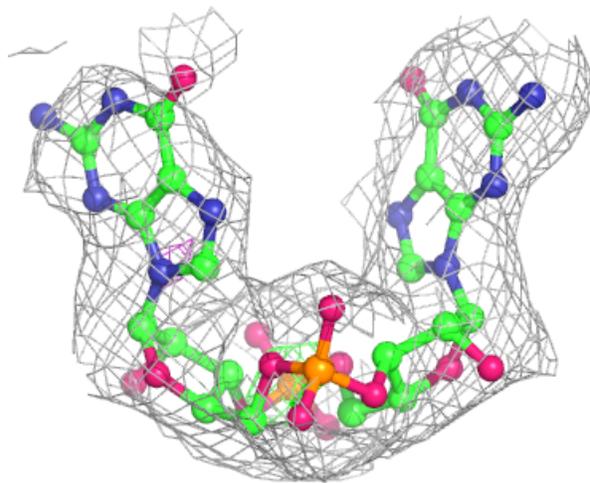
**Electron density around A16 C 801:**

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



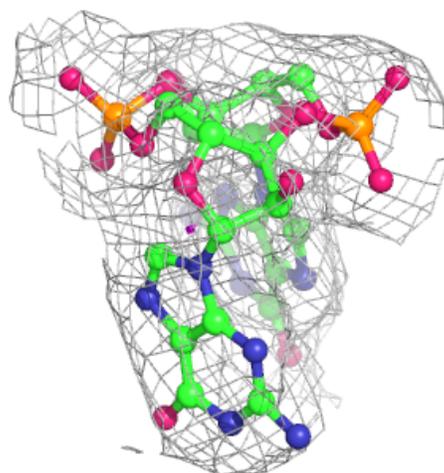
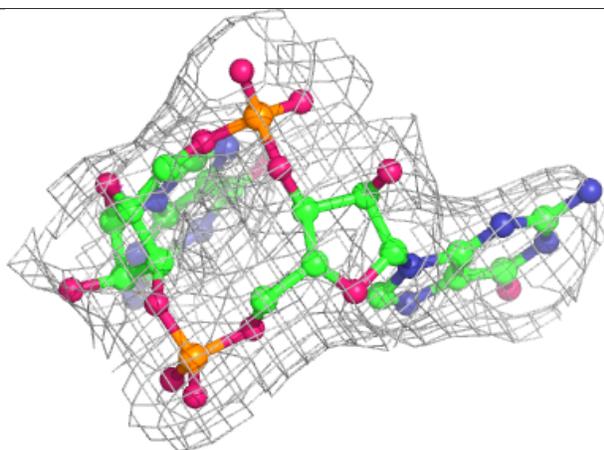
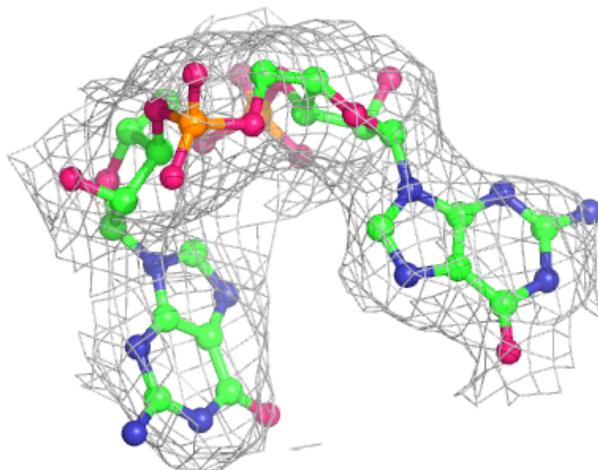
Electron density around C2E D 804:

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



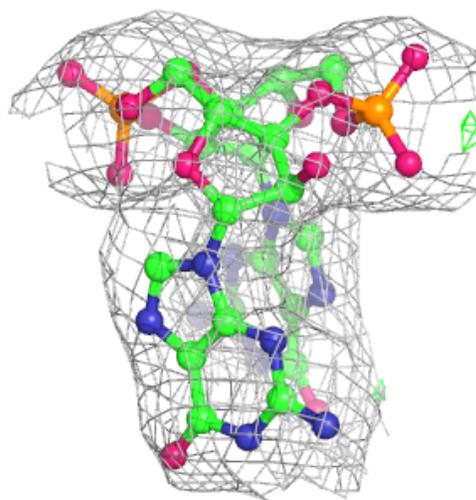
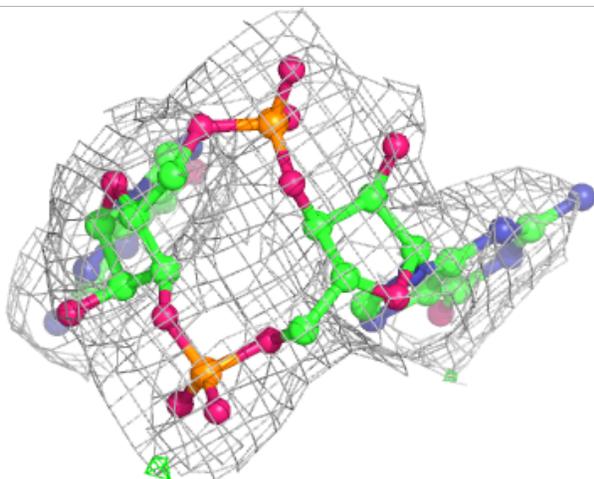
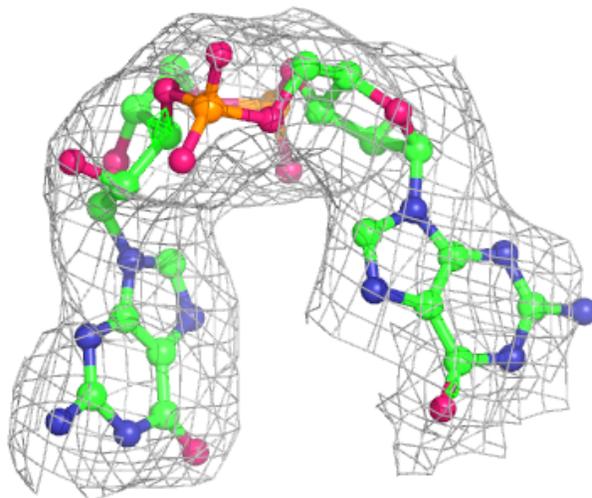
Electron density around C2E E 803:

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



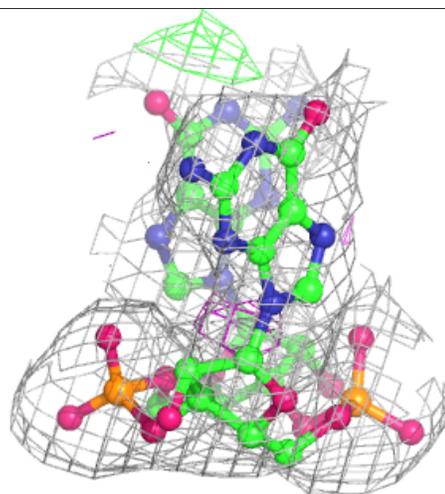
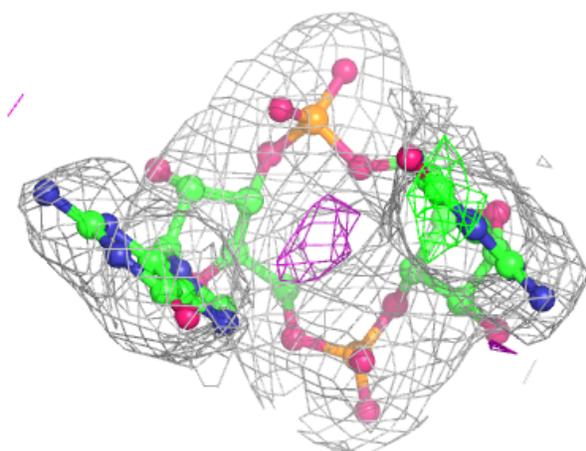
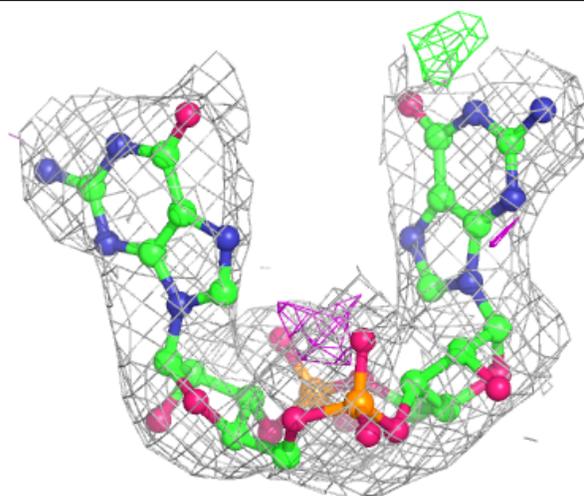
Electron density around C2E G 802:

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



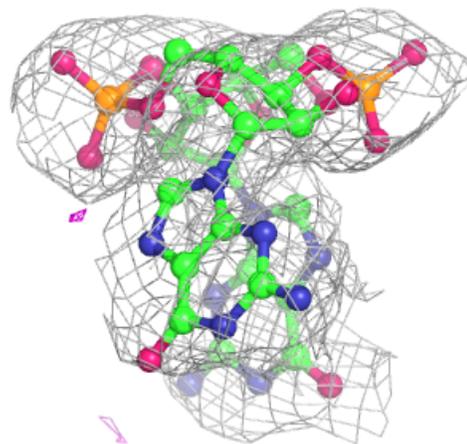
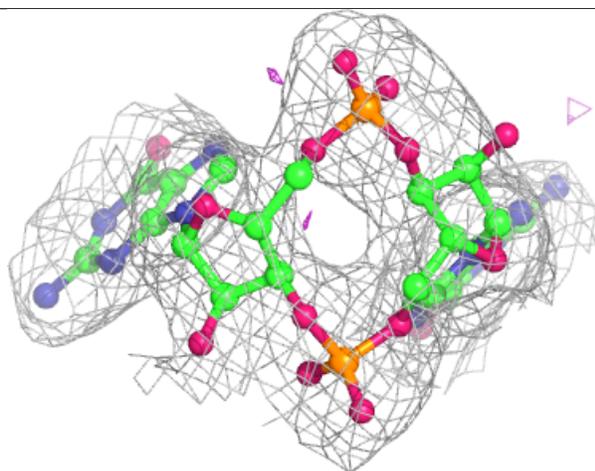
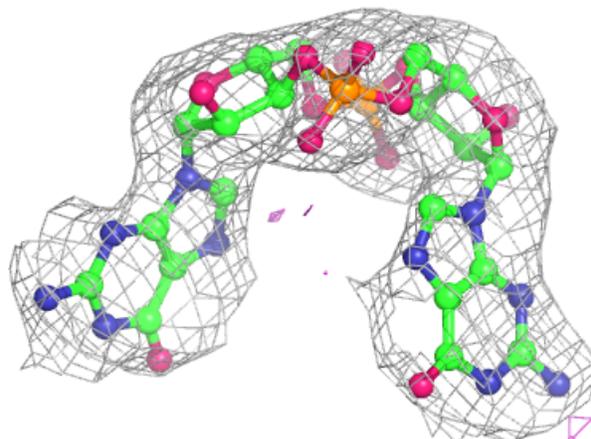
Electron density around C2E I 802:

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



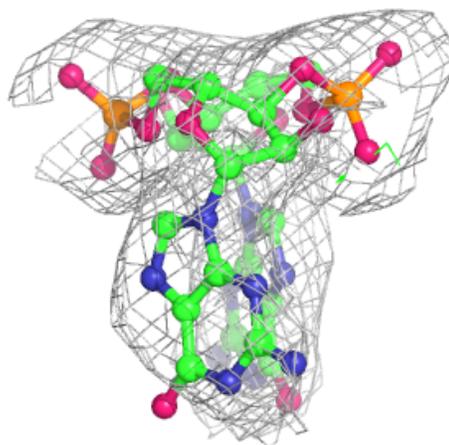
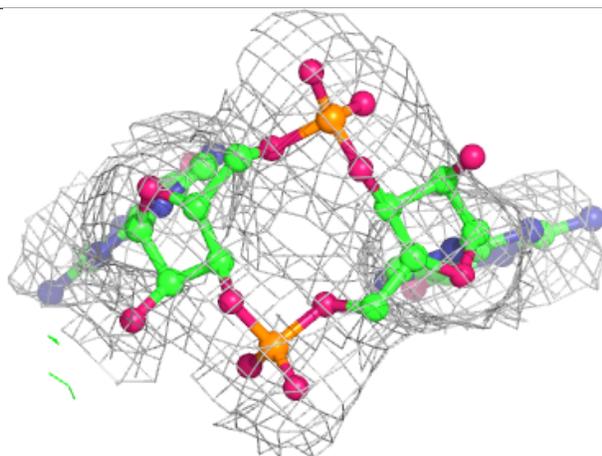
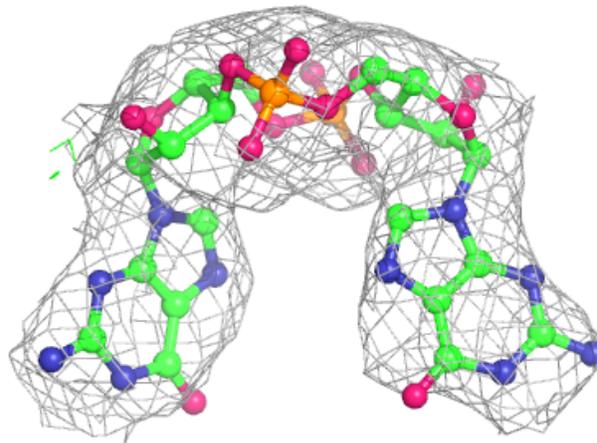
Electron density around C2E J 802:

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



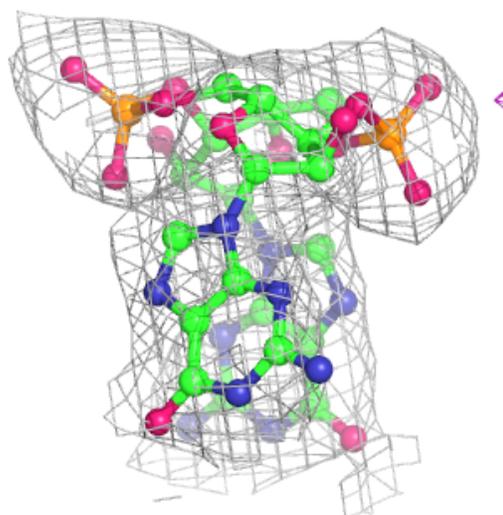
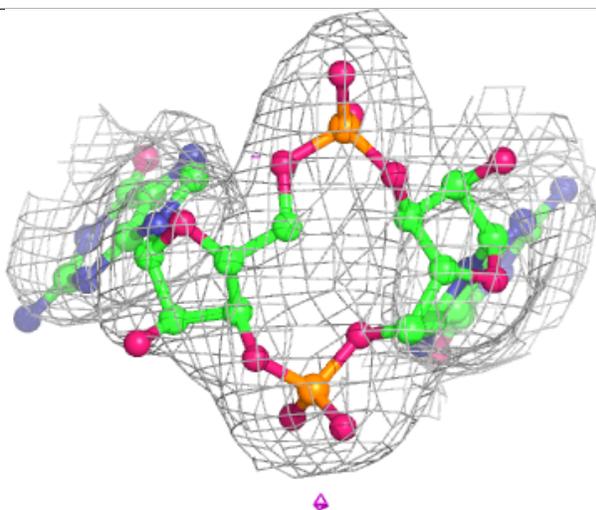
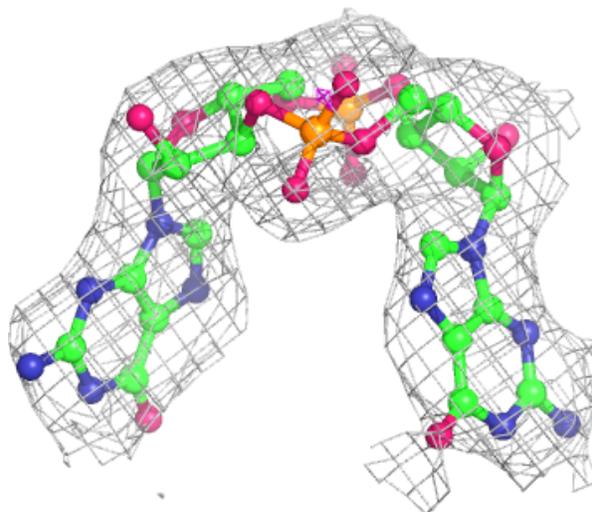
Electron density around C2E C 802:

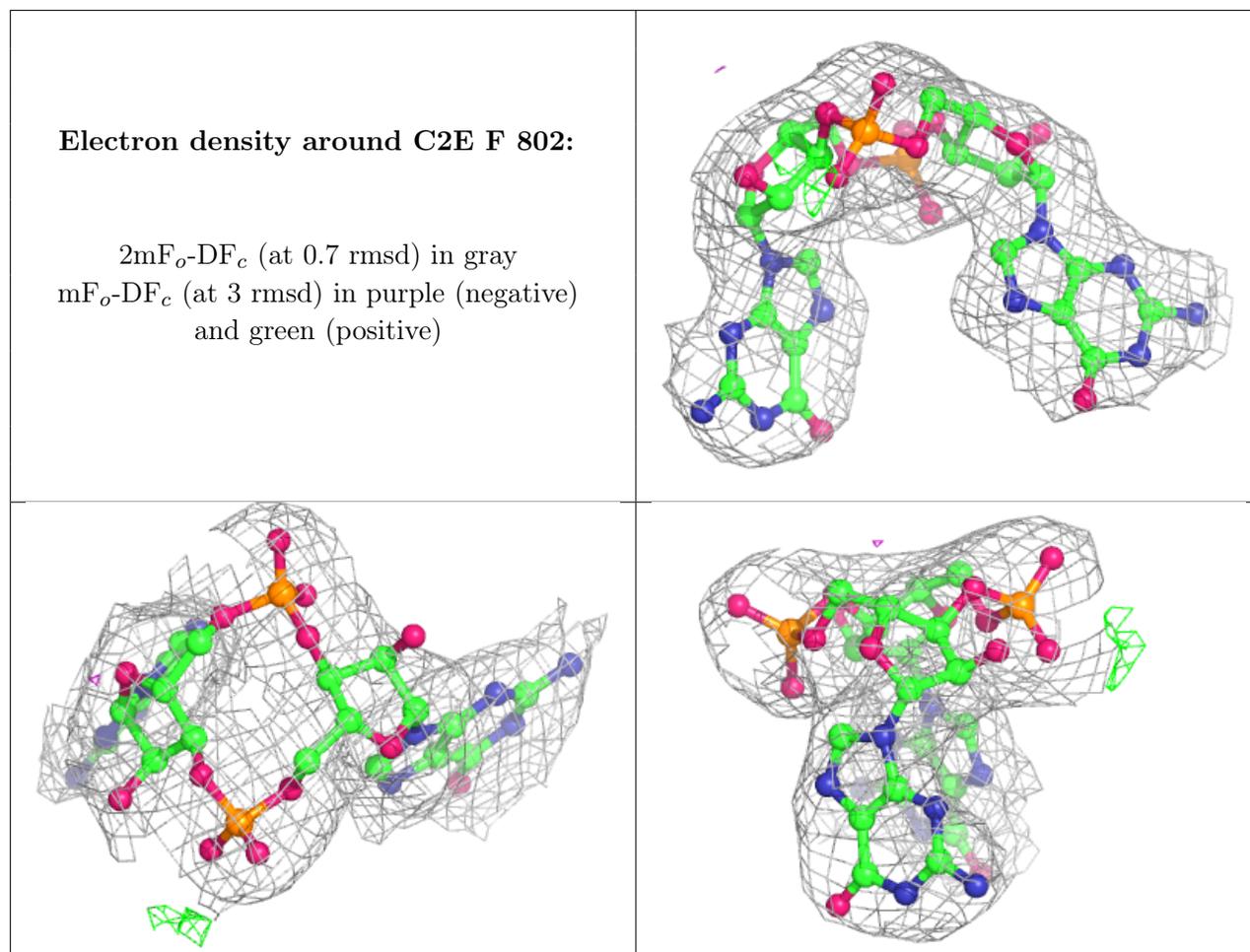
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers [i](#)

There are no such residues in this entry.