



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 29, 2026 – 03:52 AM UTC

PDB ID : 7U3B / pdb_00007u3b
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

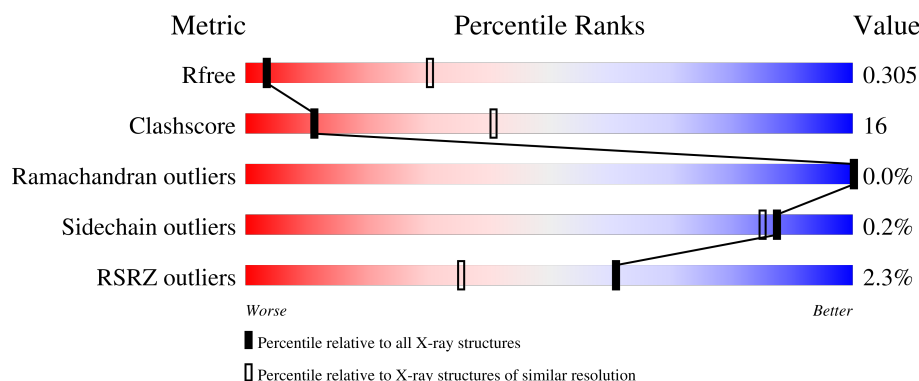
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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}	180053	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (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	2% 65% 33% .
1	D	709	2% 65% 32% .
1	E	709	2% 68% 30% .
1	F	709	2% 63% 35% .
1	G	709	3% 68% 29% .

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Mol	Chain	Length	Quality of chain
1	H	709	2% 70% 28%
1	I	709	3% 66% 32%
1	J	709	2% 65% 32%

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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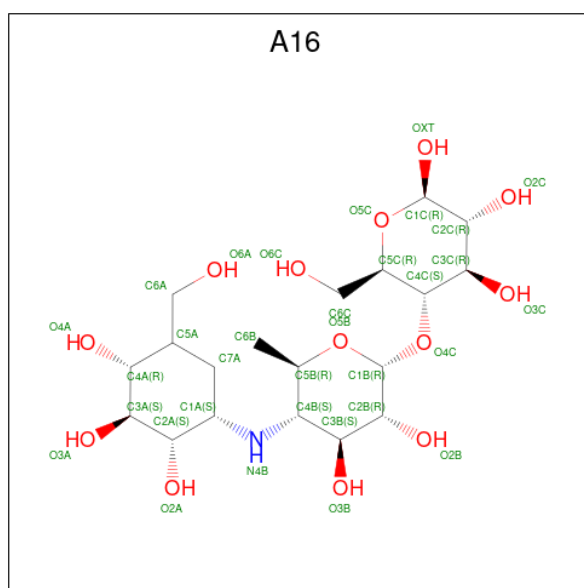
Chain	Residue	Modelled	Actual	Comment	Reference
D	192	ARG	LYS	conflict	UNP A0A5P2ALW6
D	296	ALA	SER	conflict	UNP A0A5P2ALW6
D	297	ASP	ASN	conflict	UNP A0A5P2ALW6
D	303	MET	THR	conflict	UNP A0A5P2ALW6
D	682	GLN	GLU	conflict	UNP A0A5P2ALW6
E	-2	GLY	-	expression tag	UNP A0A5P2ALW6
E	-1	SER	-	expression 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 (CCD ID: A16) (formula: C₁₉H₃₅NO₁₃) (labeled as "Ligand of Interest" by depositor).



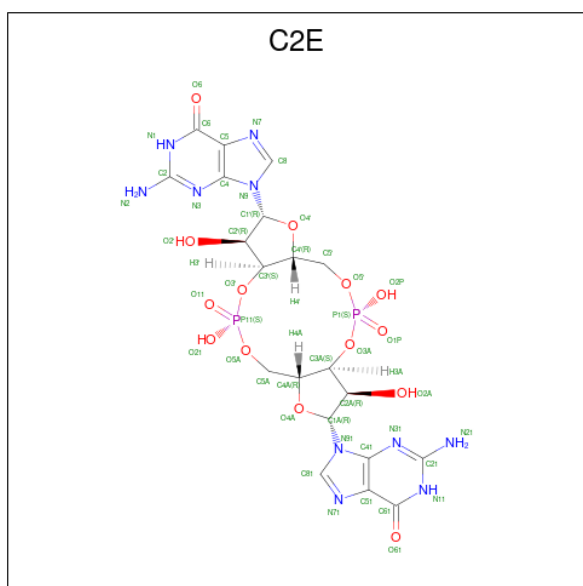
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			32	19	1	12		
2	D	1	Total	C	N	O	0	0
			32	19	1	12		

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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) (CCD ID: C2E) (formula: C₂₀H₂₄N₁₀O₁₄P₂).



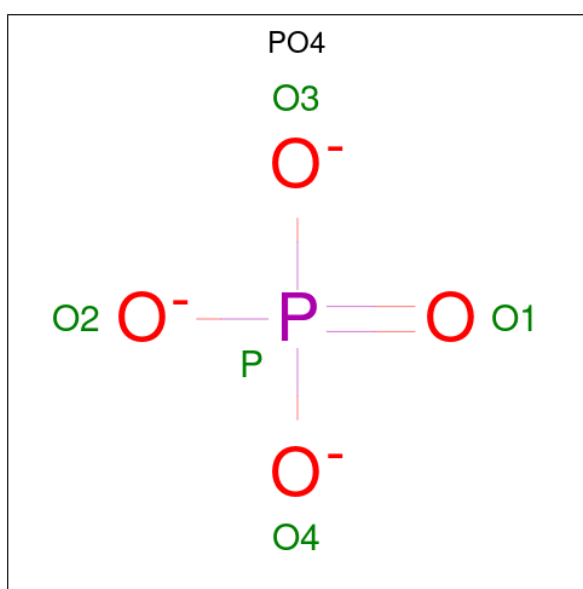
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	N	O	P	0	0
			46	20	10	14	2		
3	D	1	Total	C	N	O	P	0	0
			46	20	10	14	2		
3	E	1	Total	C	N	O	P	0	0
			46	20	10	14	2		
3	F	1	Total	C	N	O	P	0	0
			46	20	10	14	2		

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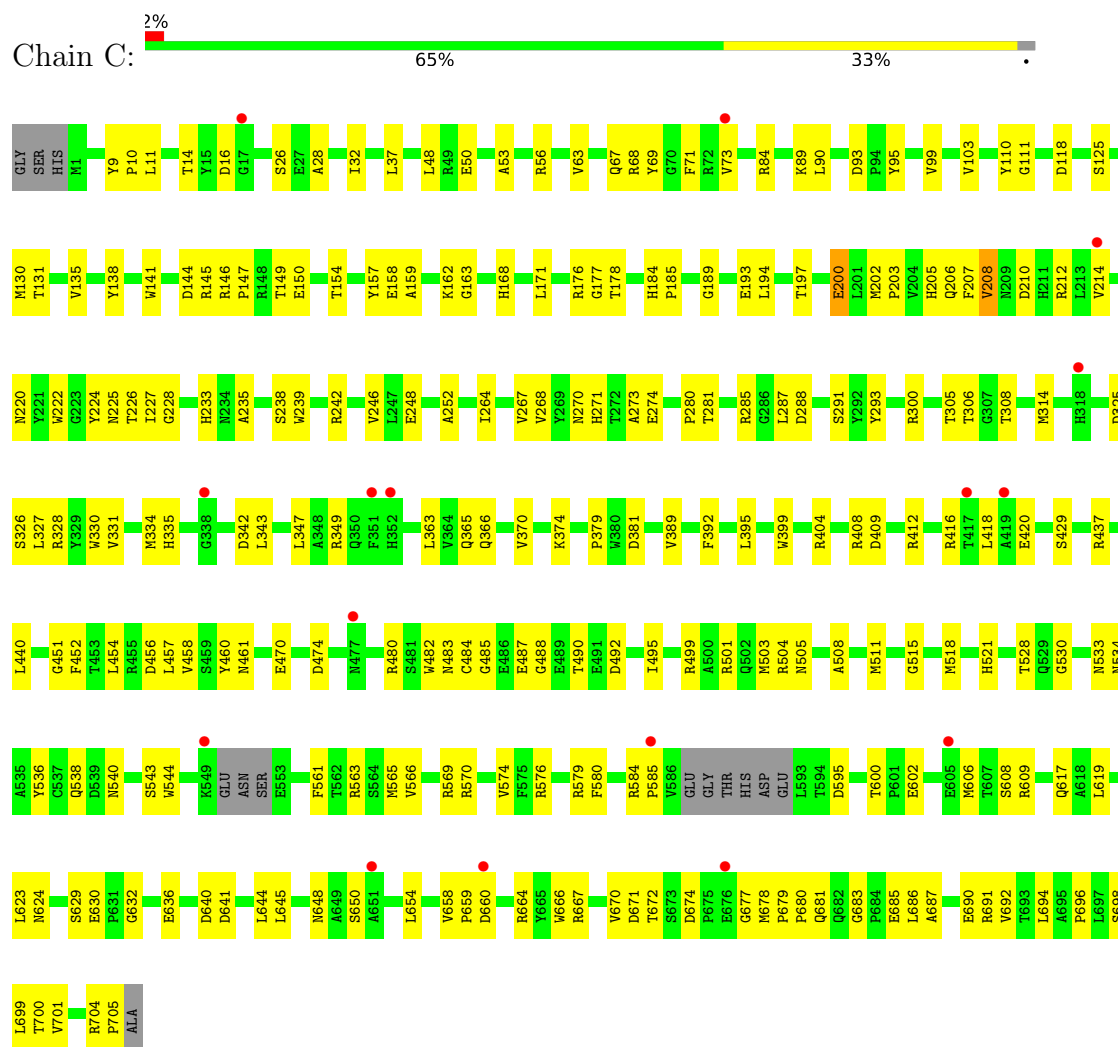
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	3	Total 3	O 3	0	0
5	F	3	Total 3	O 3	0	0
5	H	2	Total 2	O 2	0	0
5	I	4	Total 4	O 4	0	0

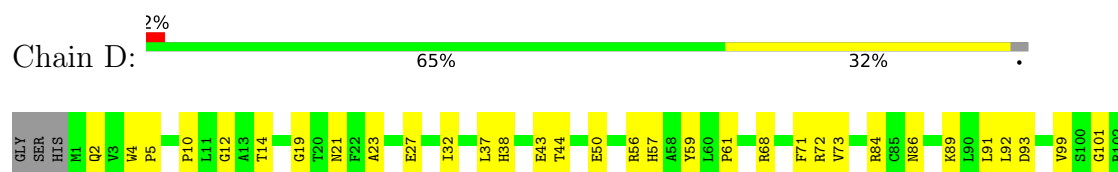
3 Residue-property plots

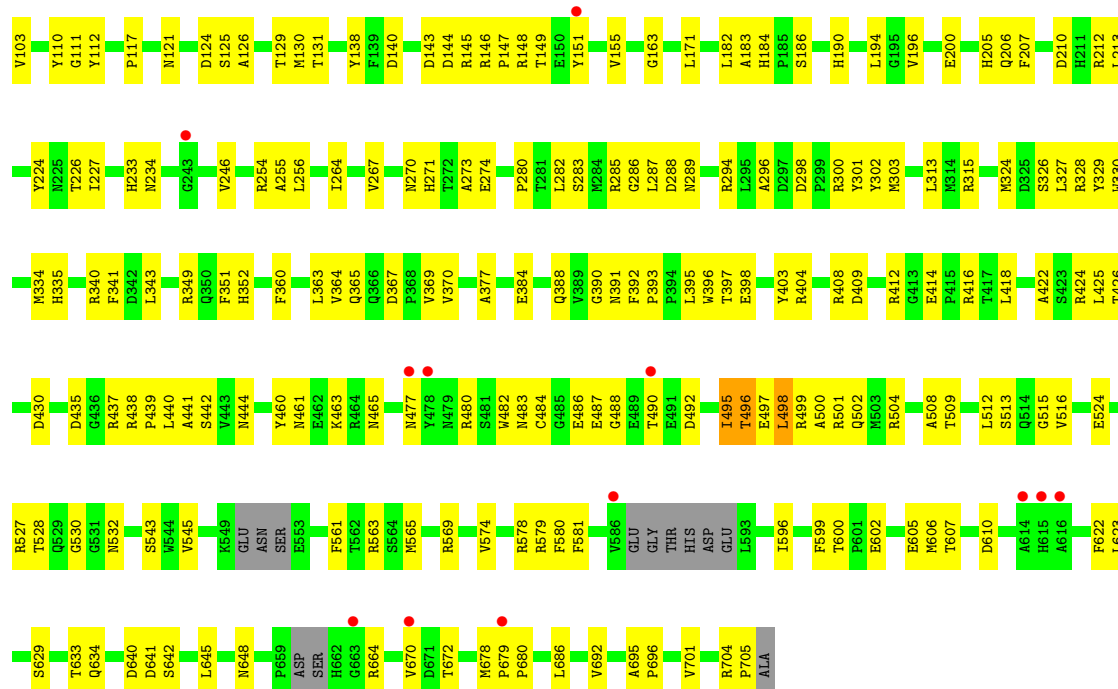
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

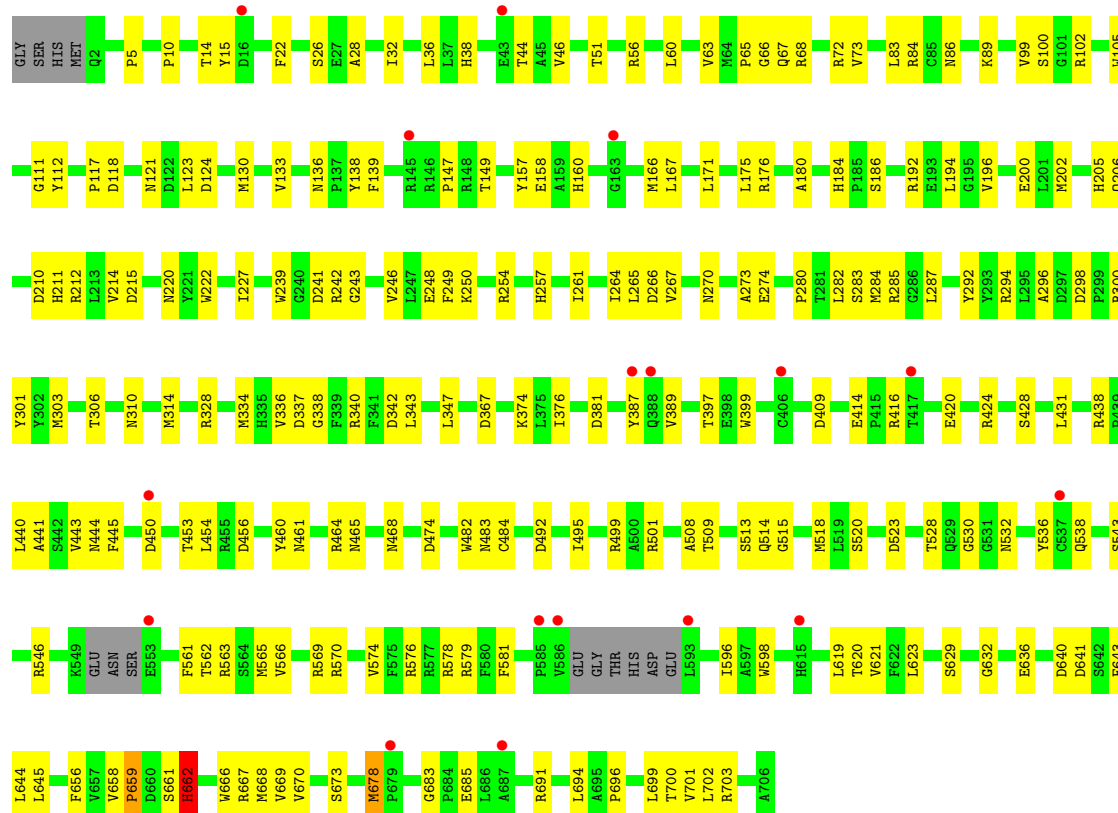


• Molecule 1: Glycogen debranching enzyme GlgX

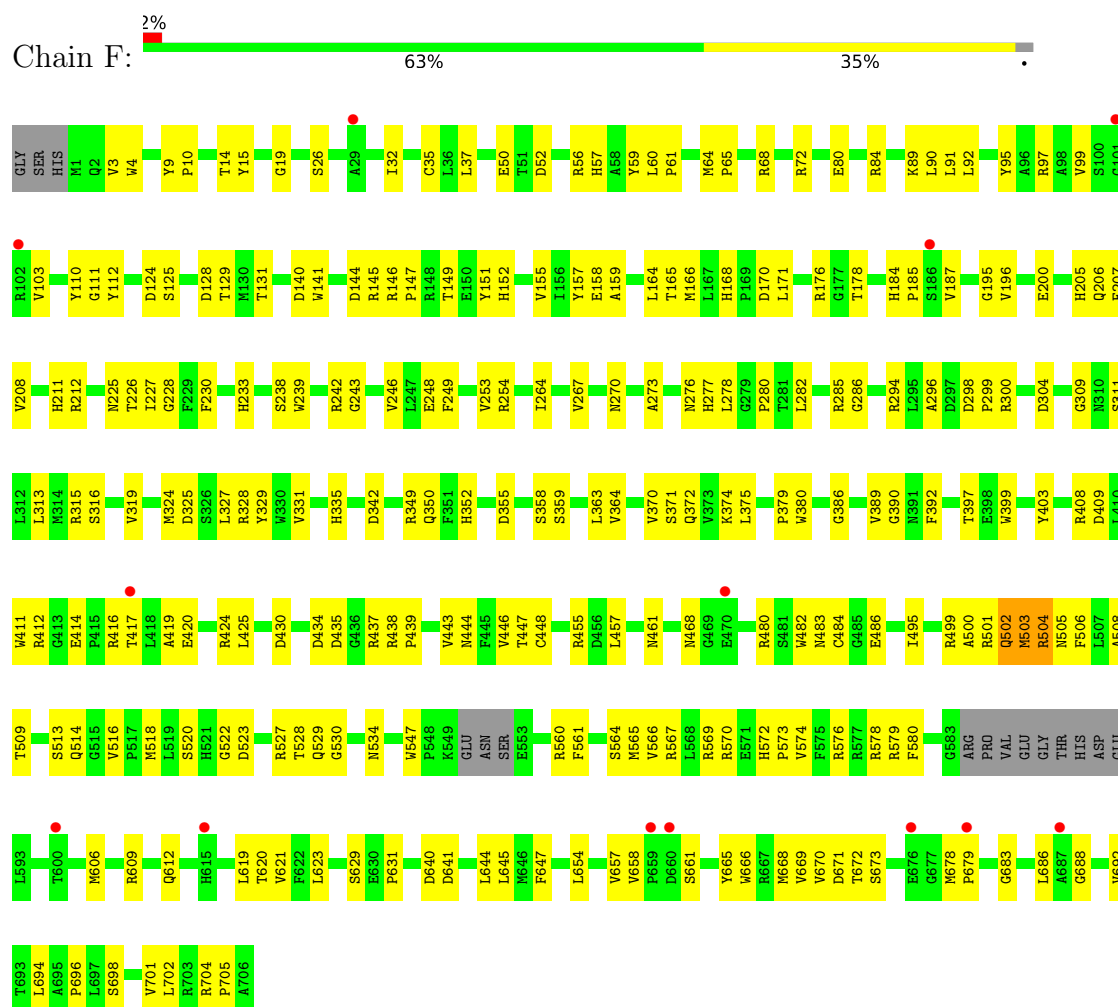




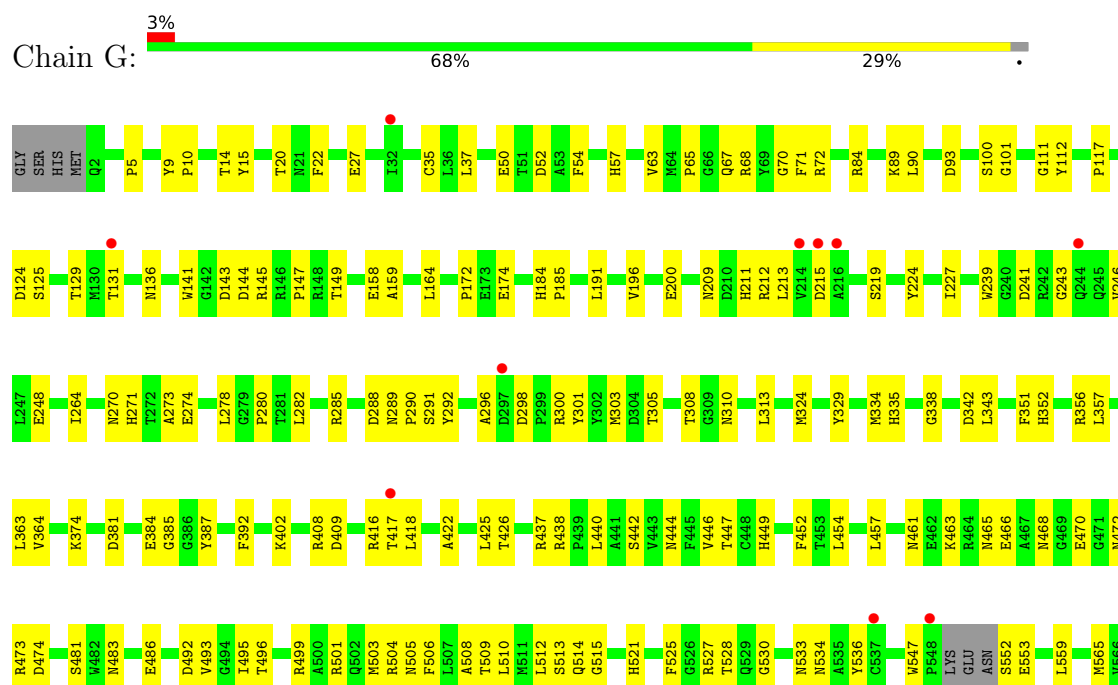
• Molecule 1: Glycogen debranching enzyme GlgX

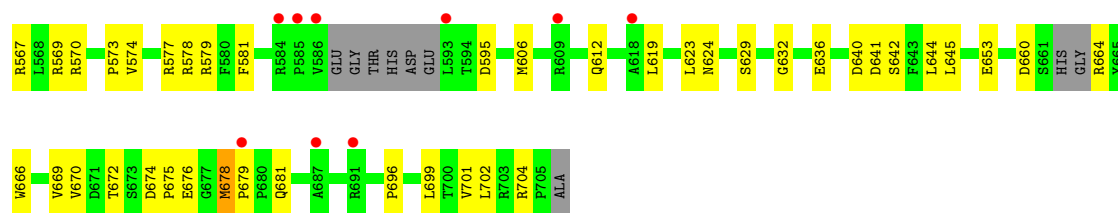


• Molecule 1: Glycogen debranching enzyme GlgX

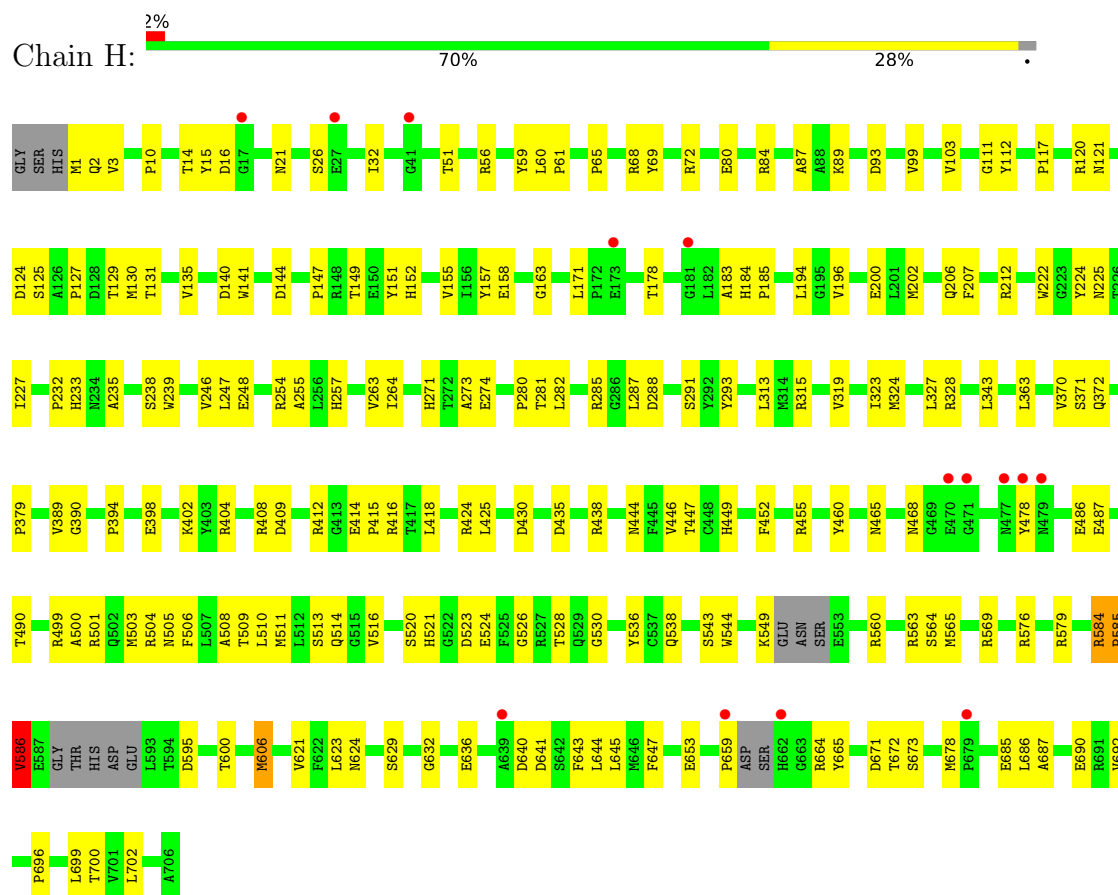


• Molecule 1: Glycogen debranching enzyme GlgX

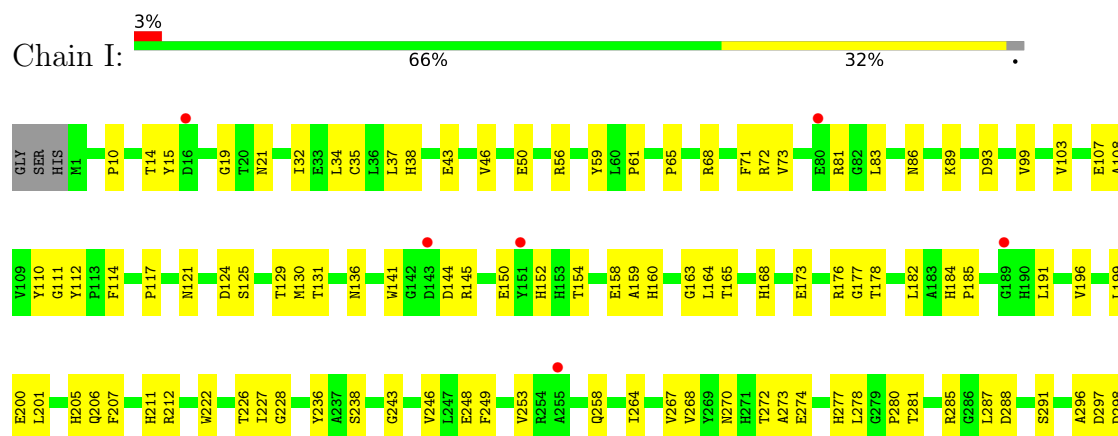


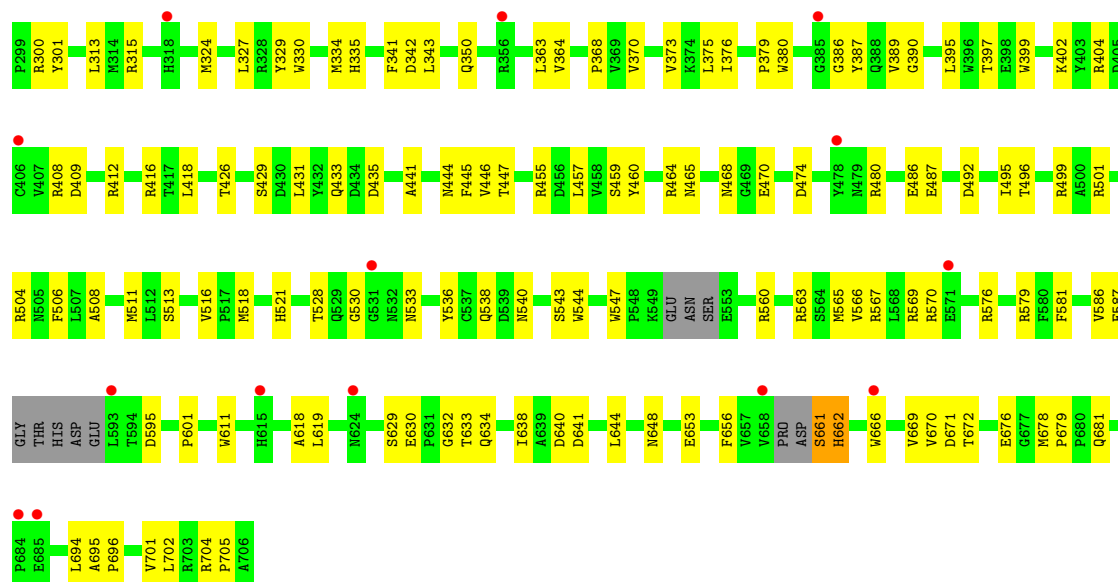


• Molecule 1: Glycogen debranching enzyme GlgX

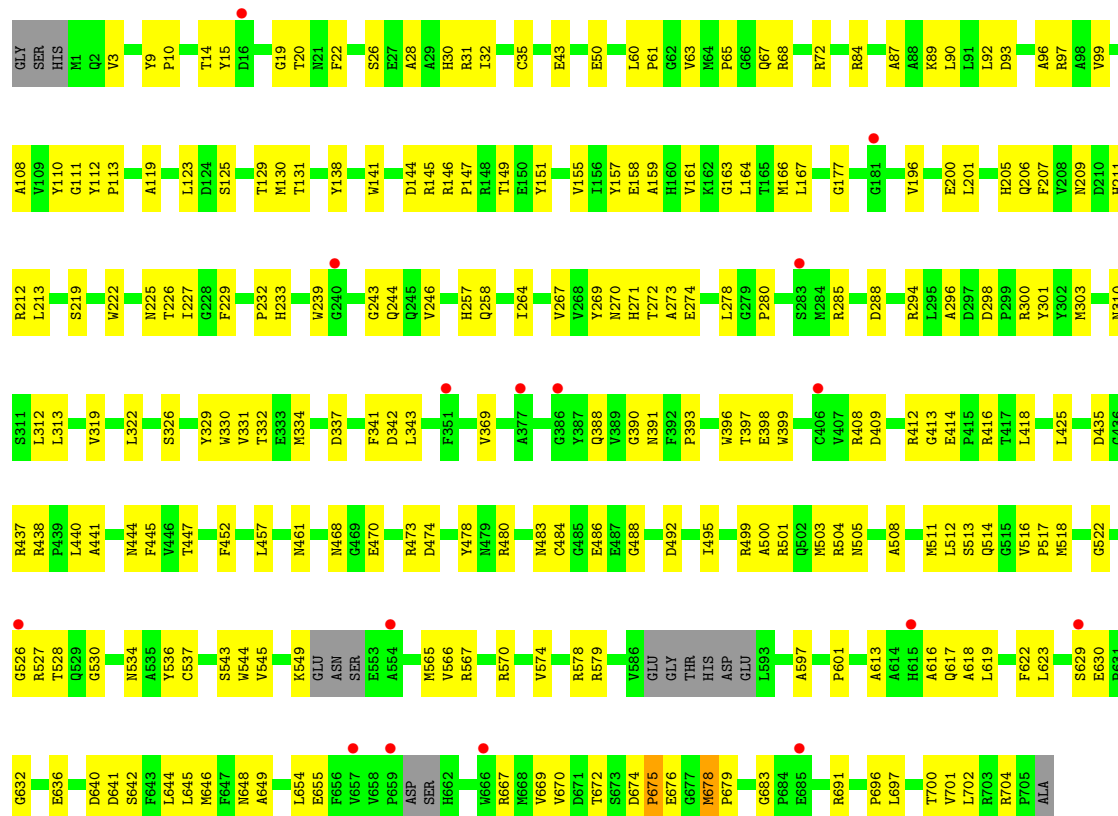


• Molecule 1: Glycogen debranching enzyme GlgX





● 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 48.50 – 3.60	Depositor EDS
% Data completeness (in resolution range)	98.2 (48.50-3.60) 98.1 (48.50-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.20	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 3.57Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.237 , 0.307 0.238 , 0.305	Depositor DCC
R_{free} test set	2000 reflections (2.36%)	wwPDB-VP
Wilson B-factor (Å ²)	42.5	Xtriage
Anisotropy	0.475	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A16, C2E, PO4

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	0.23	1/5699 (0.0%)	0.47	5/7750 (0.1%)
1	D	0.19	0/5686	0.45	1/7731 (0.0%)
1	E	0.30	2/5697 (0.0%)	0.50	5/7748 (0.1%)
1	F	0.33	4/5680 (0.1%)	0.44	2/7724 (0.0%)
1	G	0.14	0/5668	0.41	0/7710
1	H	0.28	1/5700 (0.0%)	0.53	6/7750 (0.1%)
1	I	0.16	0/5684	0.43	1/7727 (0.0%)
1	J	0.28	2/5686 (0.0%)	0.51	4/7731 (0.1%)
All	All	0.25	10/45500 (0.0%)	0.47	24/61871 (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 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	657	VAL	C-N	18.26	1.49	1.33
1	E	659	PRO	N-CA	17.32	1.69	1.47
1	H	585	PRO	N-CA	16.41	1.68	1.47
1	J	675	PRO	N-CA	15.95	1.68	1.47
1	C	208	VAL	C-N	12.15	1.50	1.33

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	674	ASP	CA-C-N	16.91	137.88	119.28
1	J	674	ASP	C-N-CA	16.91	137.88	119.28
1	H	584	ARG	CA-C-N	14.04	137.39	119.84
1	H	584	ARG	C-N-CA	14.04	137.39	119.84
1	E	658	VAL	CA-C-N	13.60	136.84	119.84

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	186	0
1	D	5535	0	5249	185	0
1	E	5545	0	5251	154	0
1	F	5529	0	5235	206	0
1	G	5518	0	5217	163	0
1	H	5549	0	5260	150	0
1	I	5535	0	5236	168	0
1	J	5535	0	5249	176	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	6	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	1411	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 16.

The worst 5 of 1411 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%)	48	79
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%)	577 (100%)	0	100	100
1	D	576/590 (98%)	574 (100%)	2 (0%)	86	83
1	E	577/590 (98%)	575 (100%)	2 (0%)	86	83
1	F	575/590 (98%)	574 (100%)	1 (0%)	87	85
1	G	575/590 (98%)	575 (100%)	0	100	100
1	H	577/590 (98%)	575 (100%)	2 (0%)	86	83
1	I	574/590 (97%)	572 (100%)	2 (0%)	86	83
1	J	576/590 (98%)	575 (100%)	1 (0%)	87	85
All	All	4607/4720 (98%)	4597 (100%)	10 (0%)	87	85

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	661	SER
1	I	662	HIS
1	J	676	GLU
1	E	662	HIS
1	F	504	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	514	GLN
1	G	681	GLN
1	J	612	GLN
1	G	74	HIS
1	G	372	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	I	801	-	33,34,35	0.60	1 (3%)	46,50,52	1.16	3 (6%)
2	A16	H	801	-	33,34,35	0.65	0	46,50,52	1.75	6 (13%)
2	A16	J	801	-	33,34,35	0.56	0	46,50,52	1.27	4 (8%)
3	C2E	E	803	-	52,52,52	0.50	0	78,82,82	0.82	3 (3%)
2	A16	F	801	-	33,34,35	0.77	1 (3%)	46,50,52	1.27	3 (6%)
3	C2E	H	803	-	52,52,52	0.66	0	78,82,82	0.95	3 (3%)
3	C2E	I	802	-	52,52,52	0.62	0	78,82,82	0.88	3 (3%)
4	PO4	D	803	-	4,4,4	0.98	0	6,6,6	0.51	0
4	PO4	D	802	-	4,4,4	1.00	0	6,6,6	0.57	0
3	C2E	G	802	-	52,52,52	0.59	0	78,82,82	0.78	1 (1%)
2	A16	G	801	-	33,34,35	0.55	0	46,50,52	1.32	7 (15%)
4	PO4	E	802	-	4,4,4	0.98	0	6,6,6	0.49	0
4	PO4	H	802	-	4,4,4	0.99	0	6,6,6	0.48	0
2	A16	C	801	-	33,34,35	0.49	0	46,50,52	1.11	3 (6%)
2	A16	D	801	-	33,34,35	0.54	0	46,50,52	1.32	7 (15%)
3	C2E	C	802	-	52,52,52	0.55	0	78,82,82	0.79	1 (1%)
3	C2E	D	804	-	52,52,52	0.60	0	78,82,82	0.96	4 (5%)
3	C2E	J	802	-	52,52,52	0.55	0	78,82,82	0.81	2 (2%)
2	A16	E	801	-	33,34,35	0.40	0	46,50,52	1.29	2 (4%)
3	C2E	F	802	-	52,52,52	0.65	0	78,82,82	0.88	3 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A16	I	801	-	-	6/12/69/72	1/3/3/3
3	C2E	G	802	-	-	13/30/62/62	0/6/7/7
2	A16	H	801	-	-	4/12/69/72	0/3/3/3
3	C2E	I	802	-	-	14/30/62/62	0/6/7/7
2	A16	D	801	-	-	3/12/69/72	1/3/3/3
2	A16	J	801	-	-	5/12/69/72	1/3/3/3
3	C2E	H	803	-	-	10/30/62/62	0/6/7/7
3	C2E	E	803	-	-	5/30/62/62	0/6/7/7
3	C2E	C	802	-	-	7/30/62/62	0/6/7/7
2	A16	F	801	-	-	7/12/69/72	1/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	C2E	D	804	-	-	1/30/62/62	0/6/7/7
2	A16	G	801	-	-	3/12/69/72	1/3/3/3
2	A16	E	801	-	-	5/12/69/72	1/3/3/3
3	C2E	F	802	-	-	6/30/62/62	0/6/7/7
3	C2E	J	802	-	-	3/30/62/62	0/6/7/7
2	A16	C	801	-	-	5/12/69/72	1/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	801	A16	C2C-C3C	-2.91	1.48	1.52
2	I	801	A16	C2C-C3C	-2.20	1.49	1.52

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	801	A16	C5A-C7A-C1A	6.80	117.32	108.53
2	H	801	A16	C1A-N4B-C4B	6.64	127.19	116.13
2	E	801	A16	C1A-N4B-C4B	5.24	124.85	116.13
2	G	801	A16	C1A-N4B-C4B	4.59	123.77	116.13
2	D	801	A16	C1A-N4B-C4B	4.57	123.73	116.13

There are no chirality outliers.

5 of 97 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:

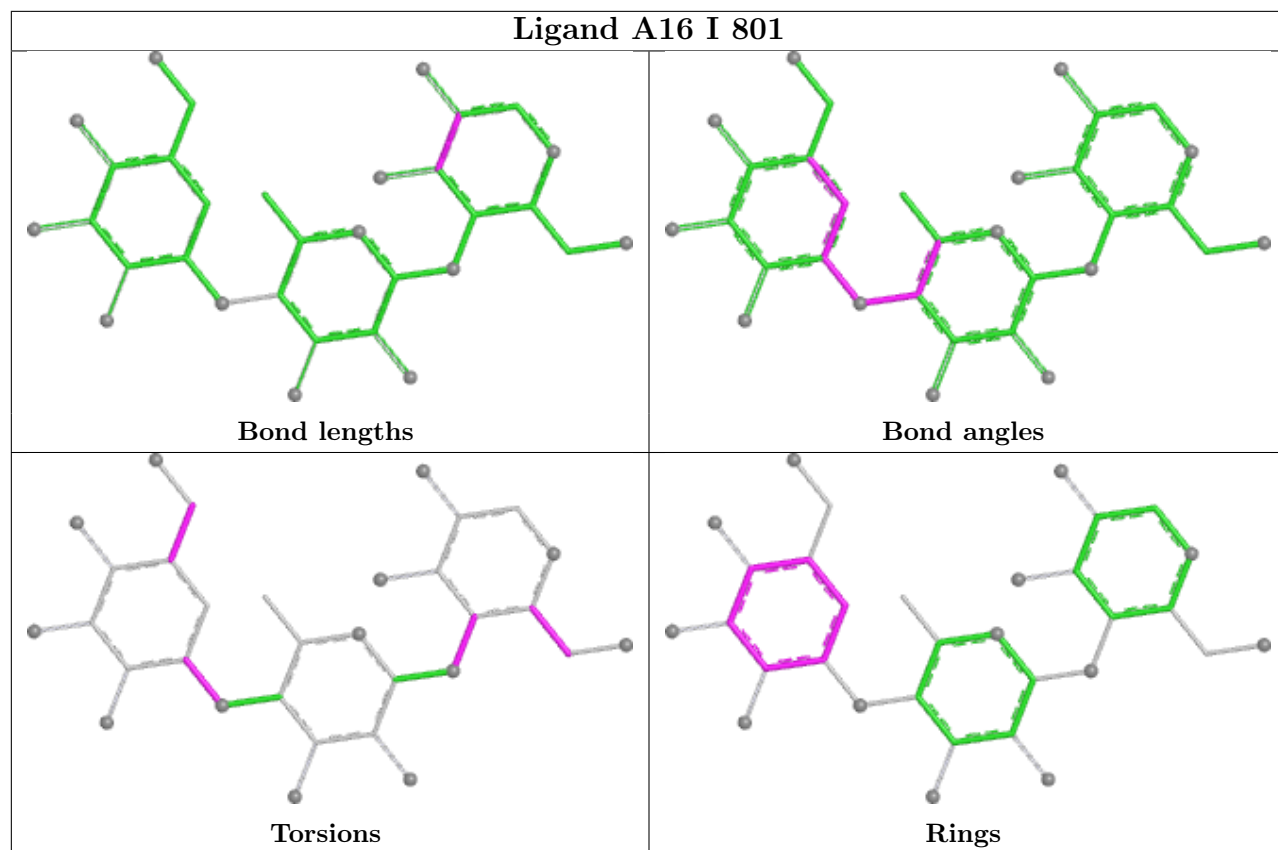
Mol	Chain	Res	Type	Atoms
2	E	801	A16	C1A-C2A-C3A-C4A-C5A-C7A
2	J	801	A16	C1A-C2A-C3A-C4A-C5A-C7A
2	F	801	A16	C1A-C2A-C3A-C4A-C5A-C7A
2	I	801	A16	C1A-C2A-C3A-C4A-C5A-C7A
2	C	801	A16	C1A-C2A-C3A-C4A-C5A-C7A

17 monomers are involved in 116 short contacts:

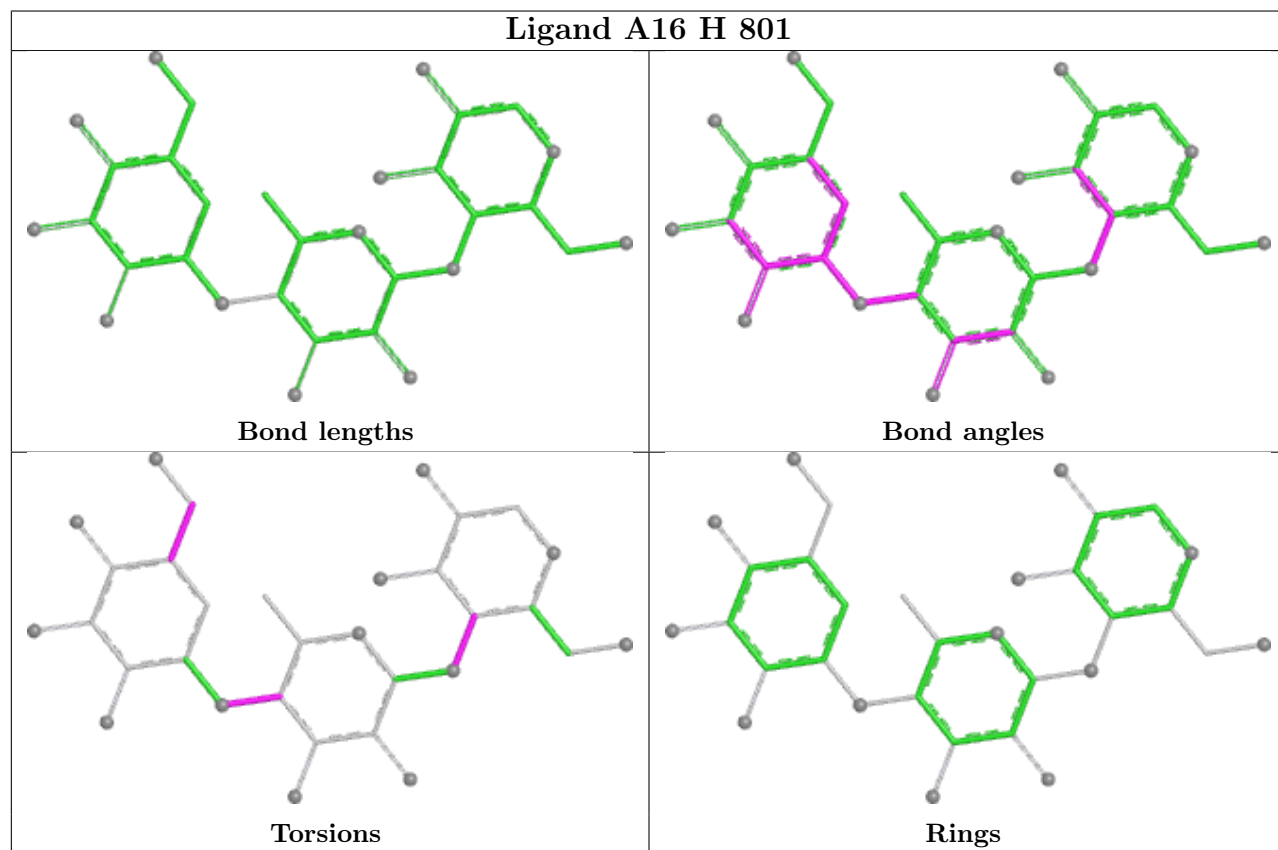
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	801	A16	5	0
2	H	801	A16	6	0
2	J	801	A16	10	0
3	E	803	C2E	5	0
2	F	801	A16	7	0
3	H	803	C2E	7	0
3	I	802	C2E	7	0
4	D	802	PO4	1	0
3	G	802	C2E	5	0
2	G	801	A16	10	0
2	C	801	A16	5	0
2	D	801	A16	7	0
3	C	802	C2E	9	0
3	D	804	C2E	18	0
3	J	802	C2E	4	0
2	E	801	A16	7	0
3	F	802	C2E	3	0

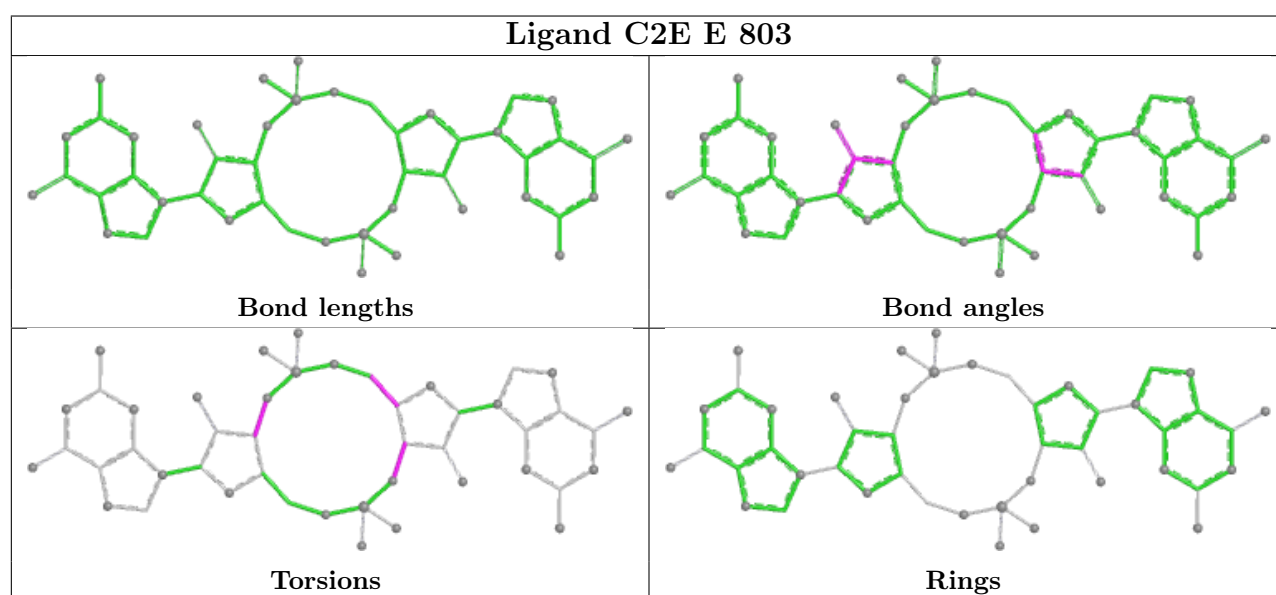
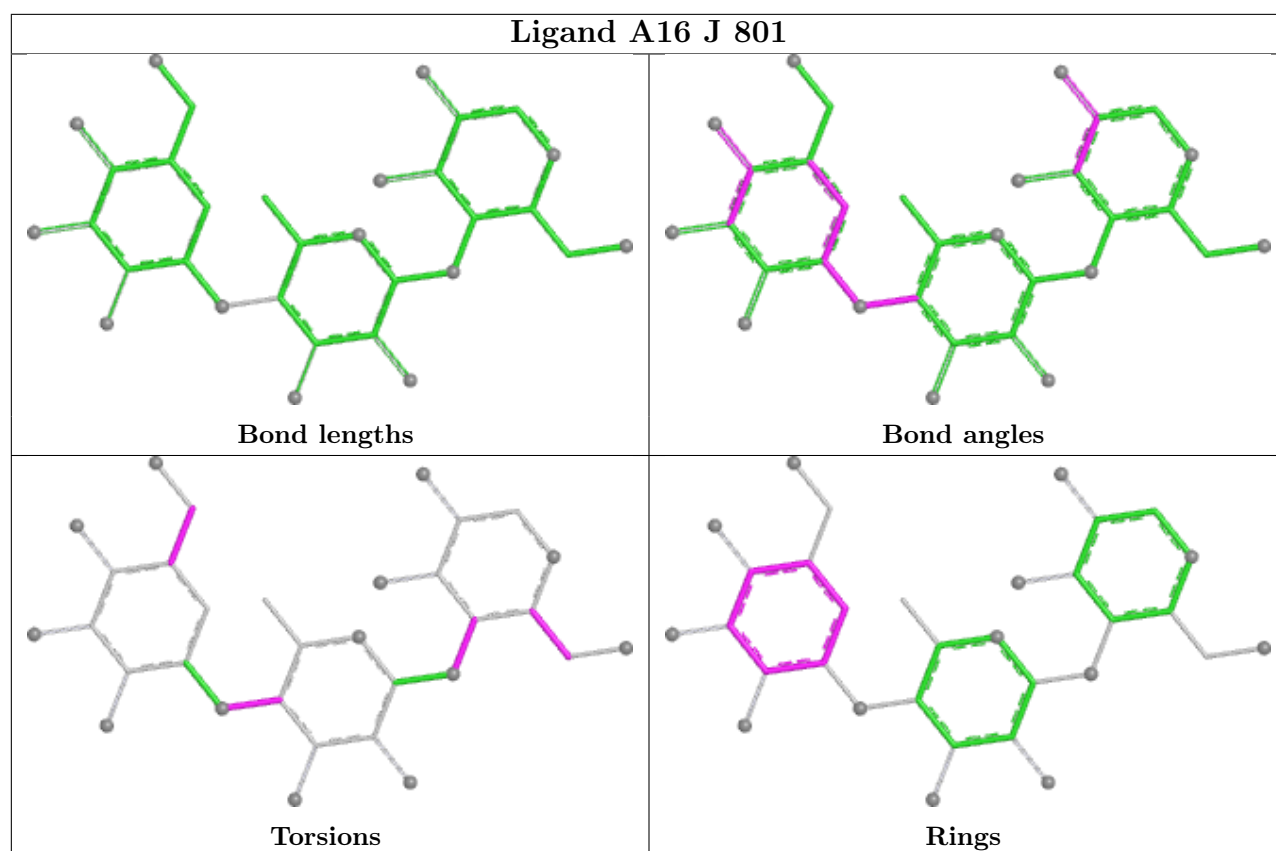
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 I 801

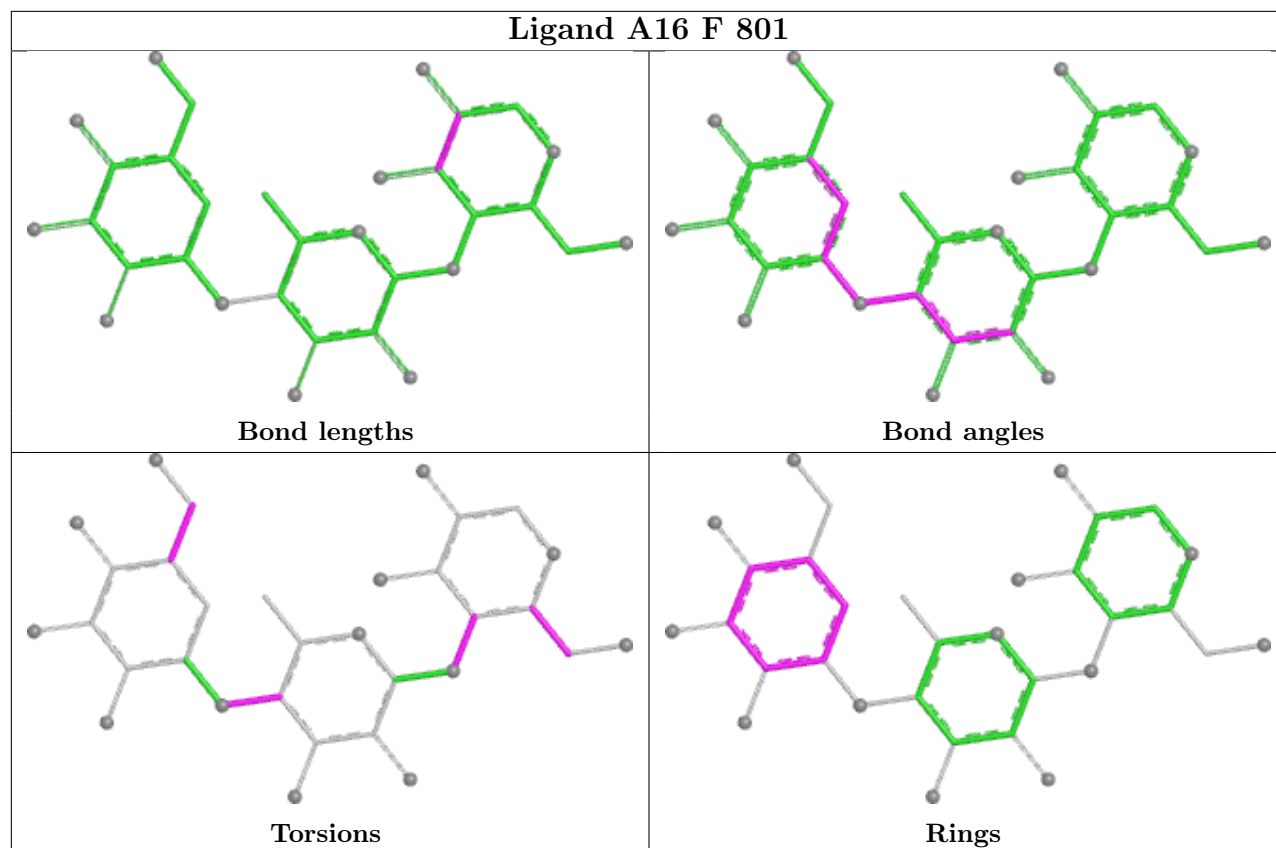


Ligand A16 H 801

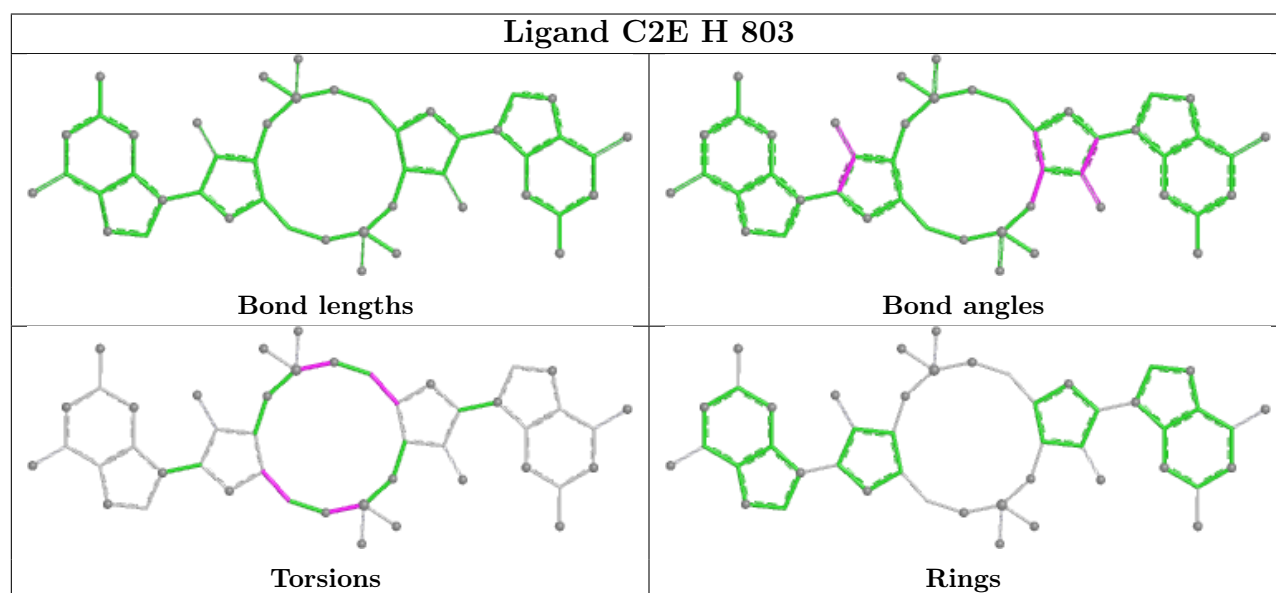


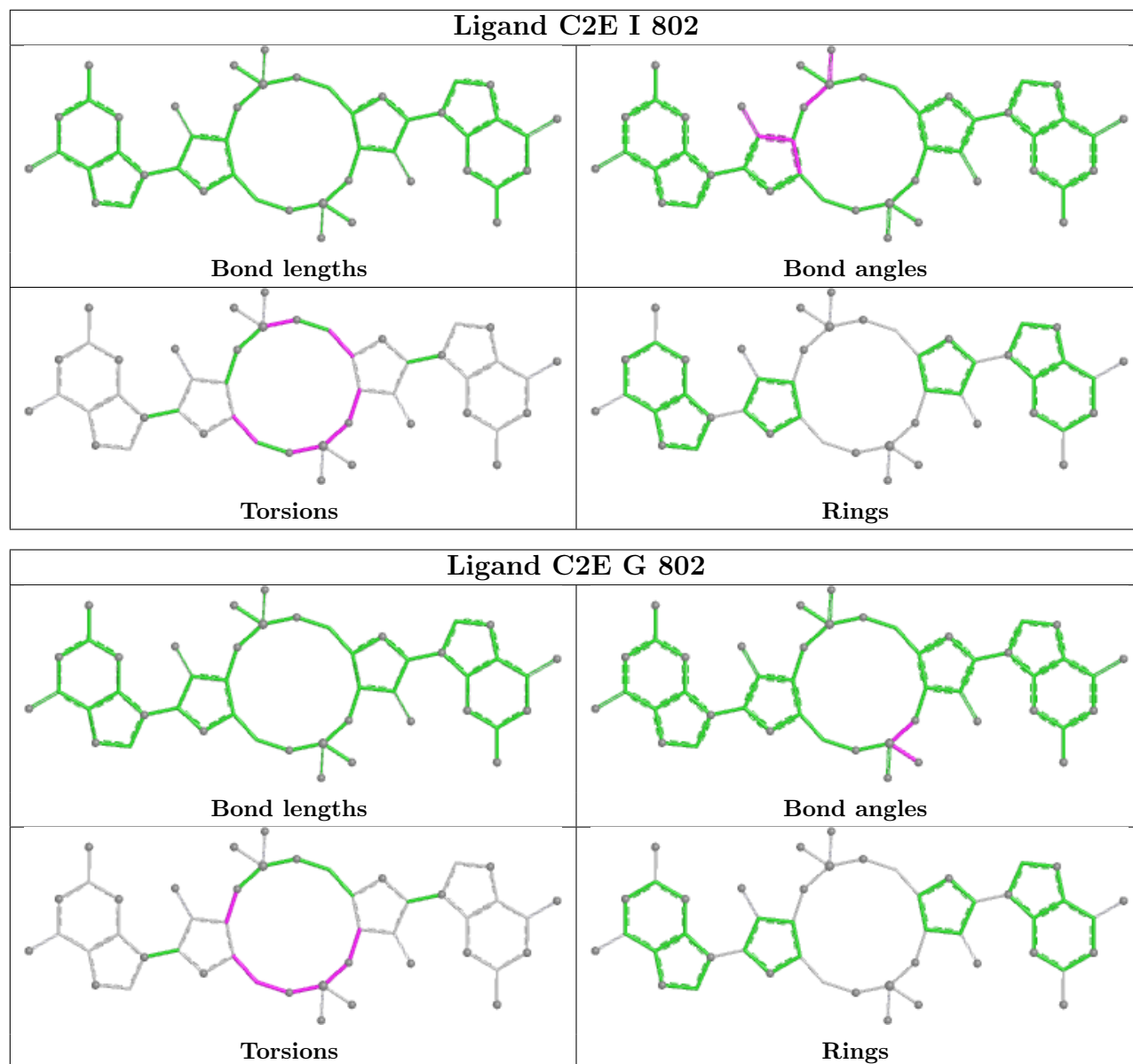


Ligand A16 F 801

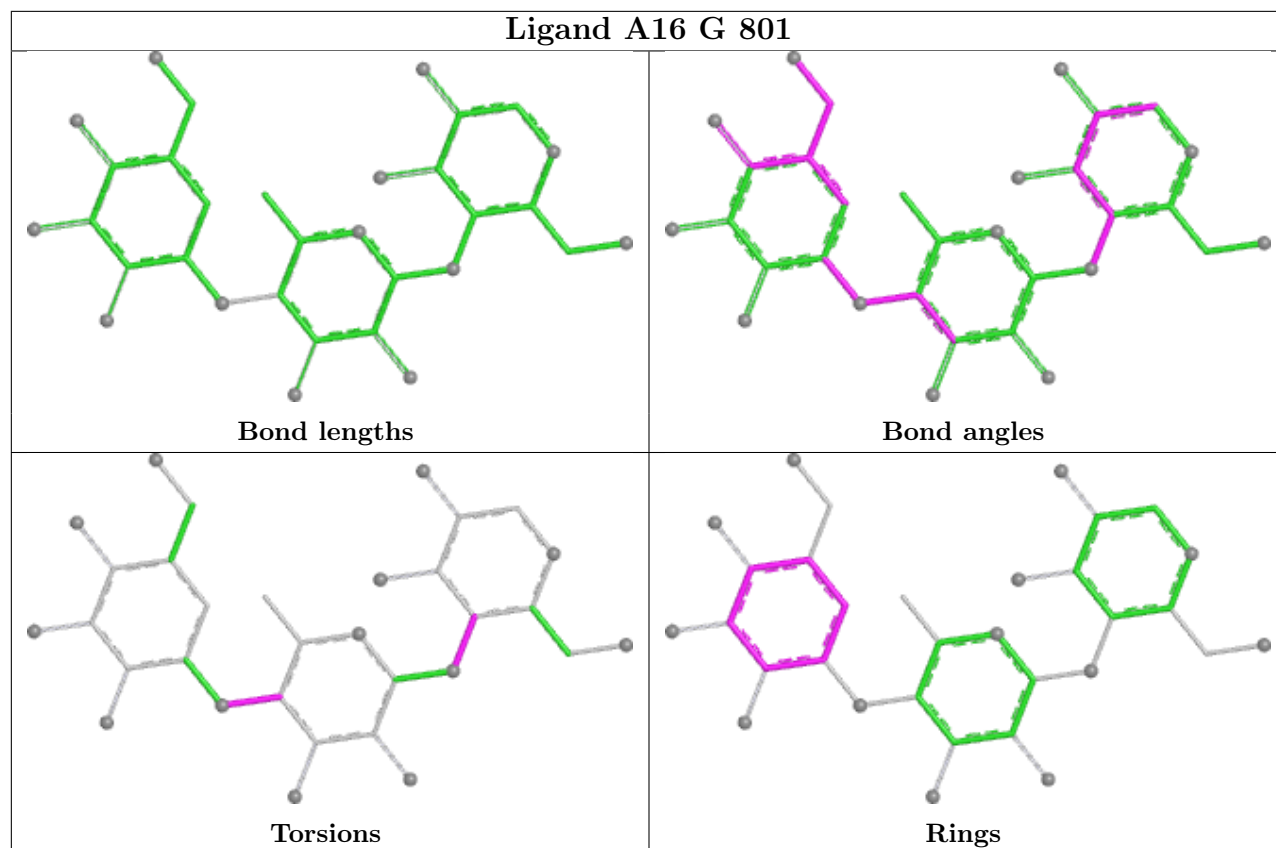


Ligand C2E H 803

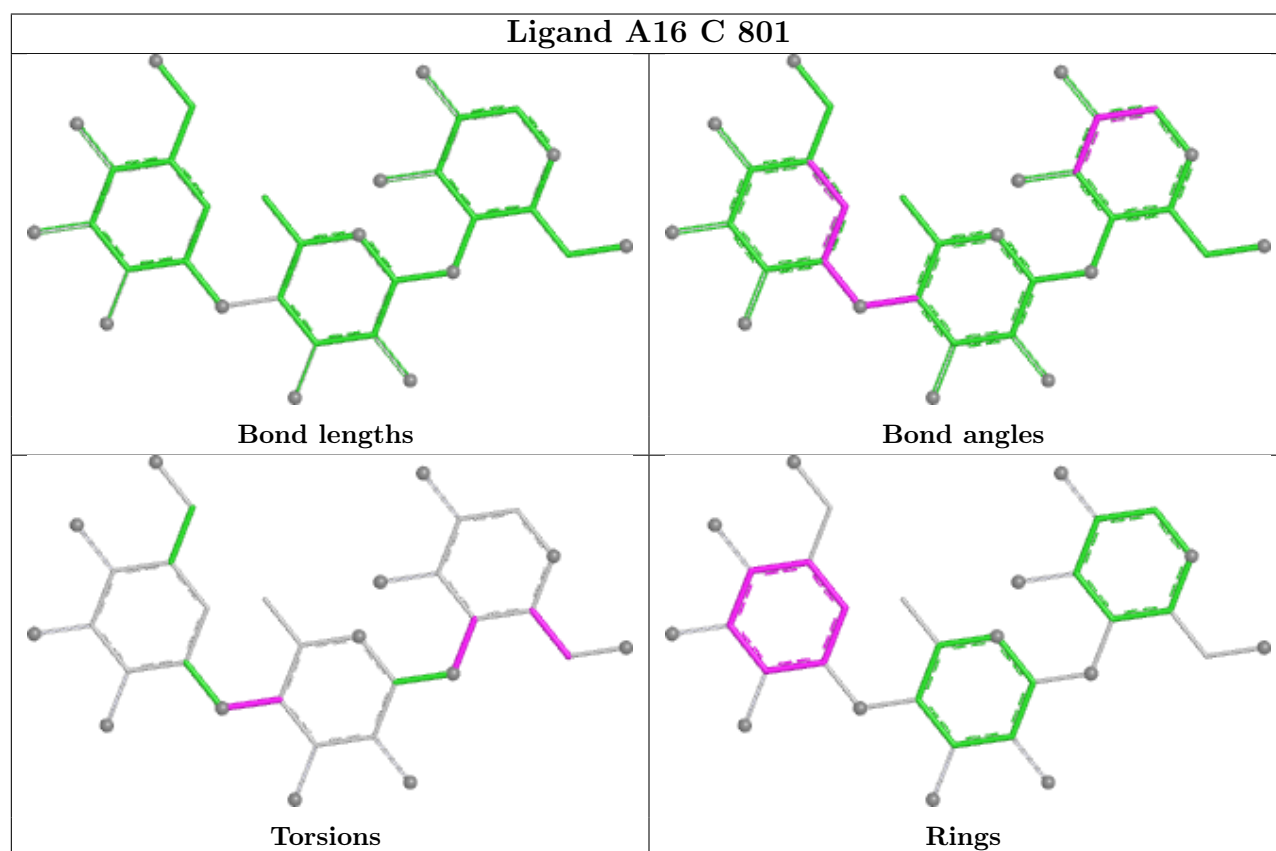




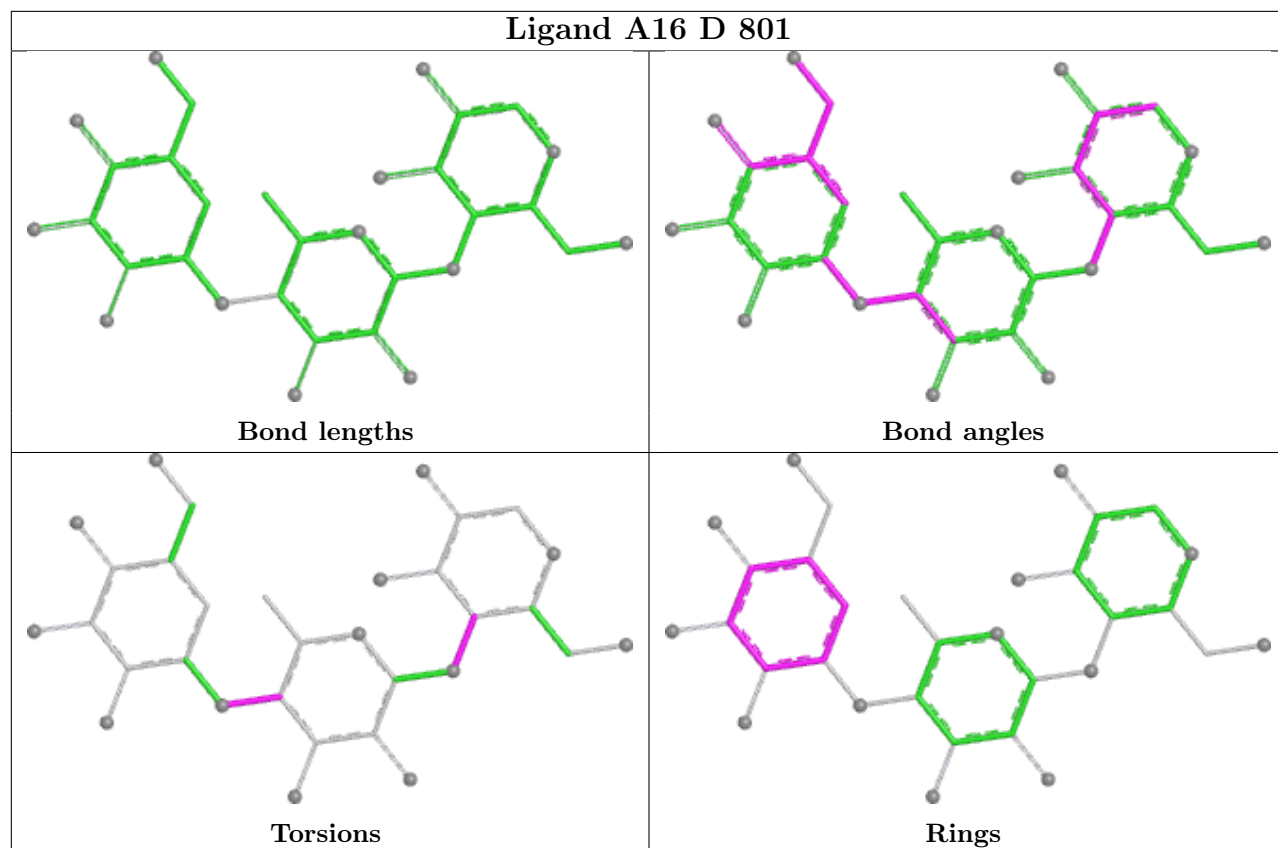
Ligand A16 G 801



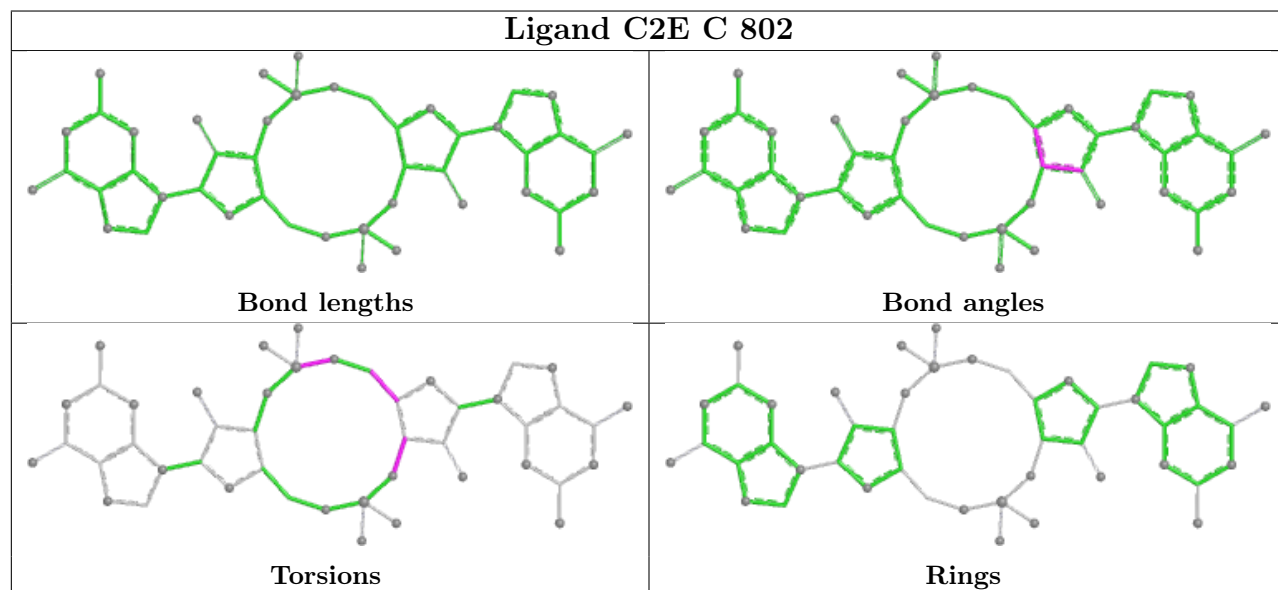
Ligand A16 C 801



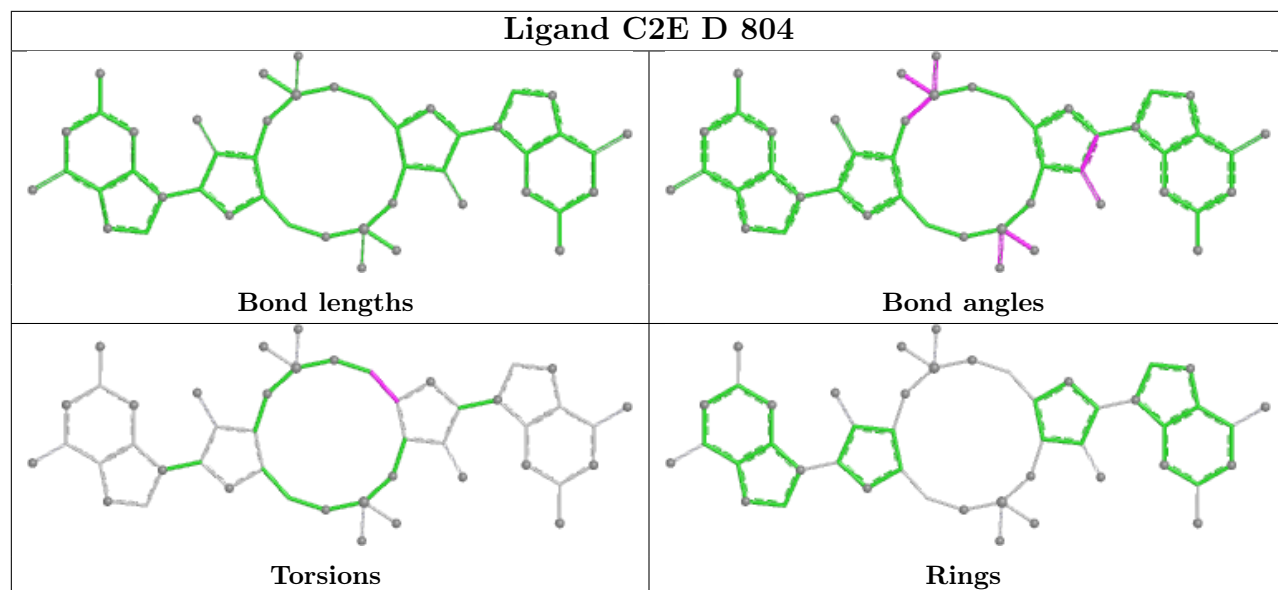
Ligand A16 D 801



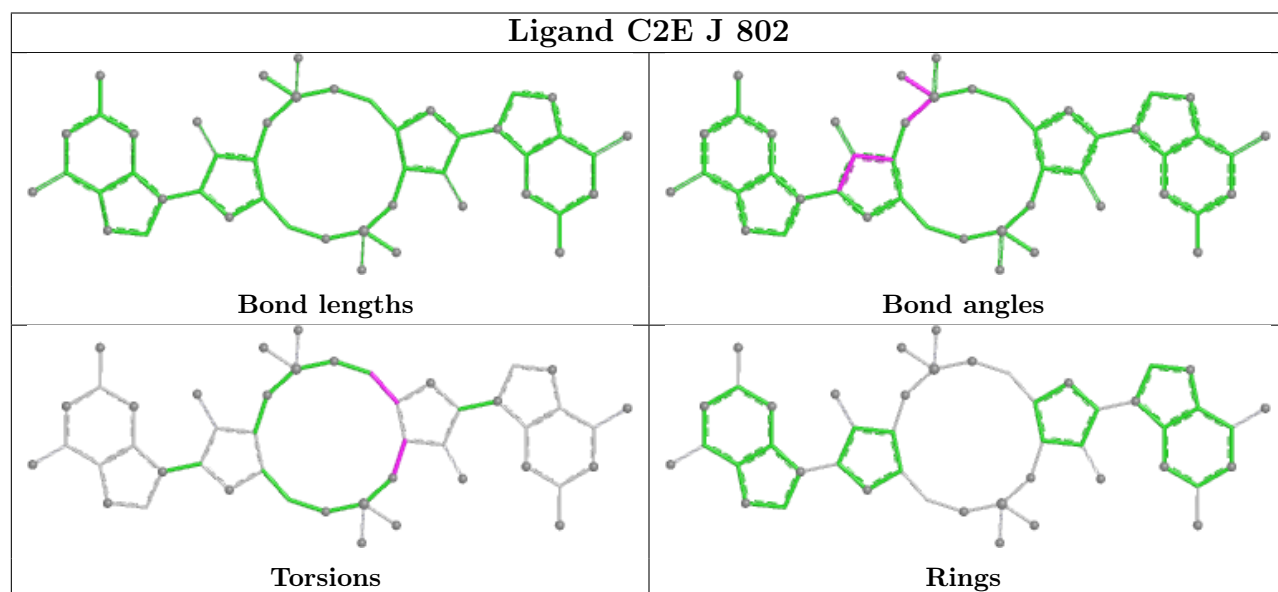
Ligand C2E C 802

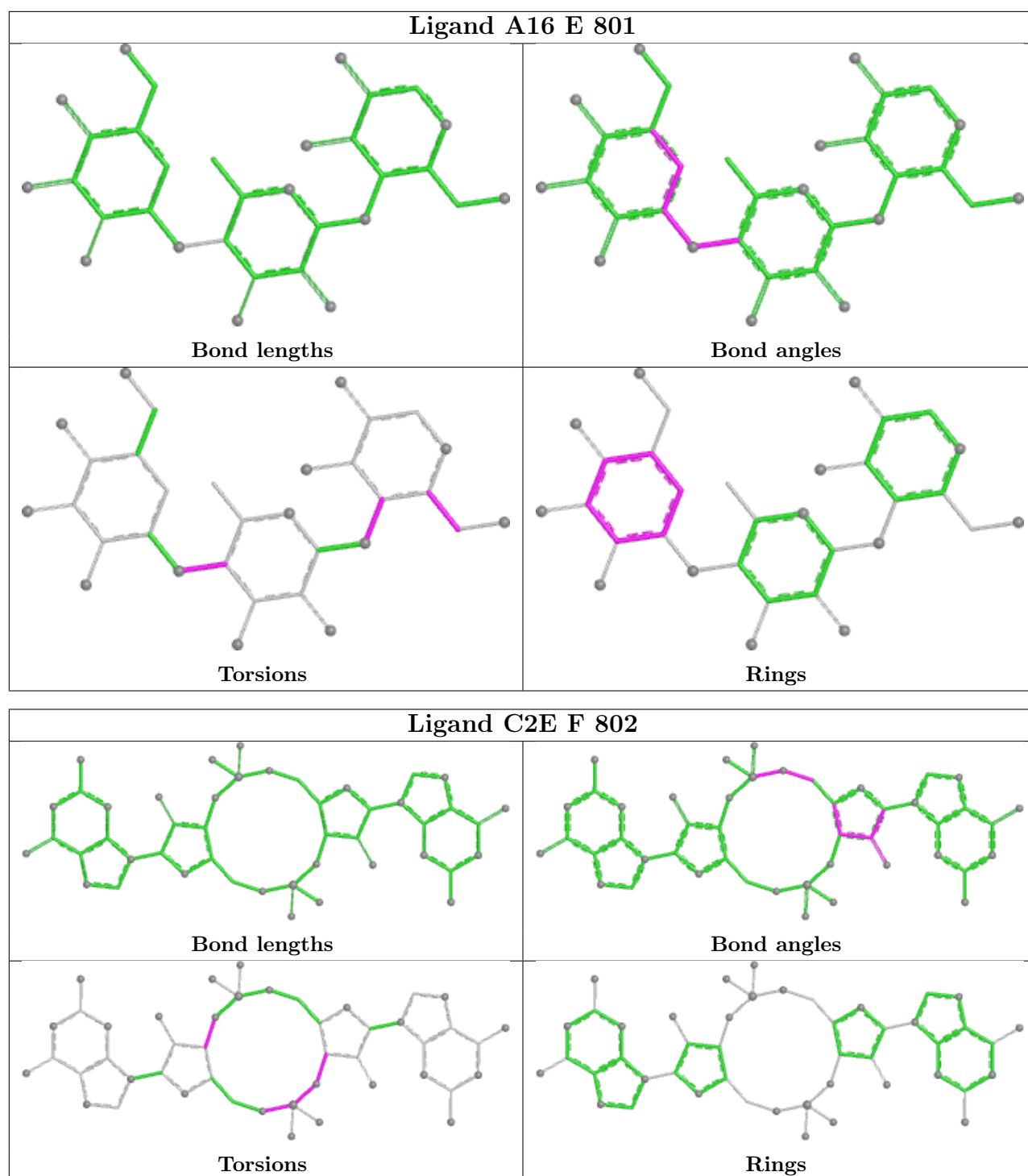


Ligand C2E D 804



Ligand C2E J 802





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [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%)	0.46	16 (2%) 61 35	23, 40, 64, 95	0
1	D	694/709 (97%)	0.34	12 (1%) 69 41	19, 38, 66, 115	0
1	E	696/709 (98%)	0.44	17 (2%) 59 34	22, 39, 62, 102	0
1	F	694/709 (97%)	0.45	13 (1%) 66 39	17, 42, 67, 128	0
1	G	693/709 (97%)	0.49	19 (2%) 56 32	23, 44, 75, 127	0
1	H	696/709 (98%)	0.48	14 (2%) 65 38	24, 47, 76, 114	0
1	I	696/709 (98%)	0.56	20 (2%) 53 30	23, 51, 80, 122	0
1	J	694/709 (97%)	0.53	16 (2%) 61 35	23, 49, 83, 128	0
All	All	5559/5672 (98%)	0.47	127 (2%) 61 35	17, 43, 74, 128	0

The worst 5 of 127 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	215	ASP	4.5
1	I	684	PRO	4.3
1	H	27	GLU	4.2
1	E	586	VAL	3.9
1	J	377	ALA	3.9

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

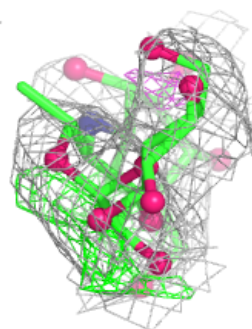
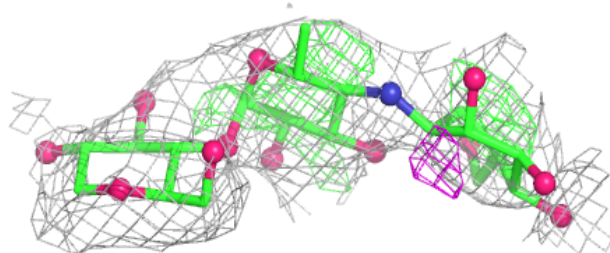
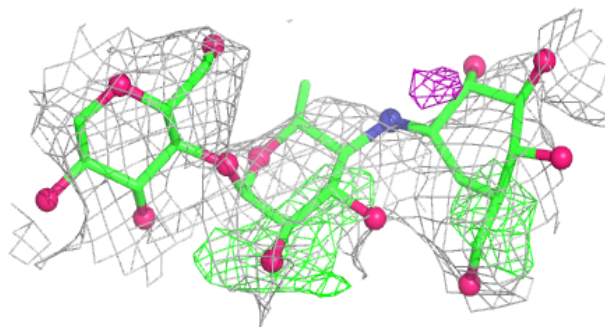
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	0.70	0.31	77,107,116,124	0
2	A16	I	801	32/33	0.74	0.23	77,107,116,124	0
2	A16	H	801	32/33	0.77	0.27	78,107,120,124	0
2	A16	J	801	32/33	0.77	0.26	78,107,116,124	0
2	A16	E	801	32/33	0.79	0.28	77,108,116,124	0
4	PO4	D	802	5/5	0.79	0.21	70,72,82,88	0
2	A16	C	801	32/33	0.80	0.23	70,82,105,114	0
4	PO4	E	802	5/5	0.80	0.19	44,45,61,76	0
4	PO4	D	803	5/5	0.81	0.17	66,70,75,84	0
2	A16	F	801	32/33	0.81	0.16	27,42,63,83	0
2	A16	D	801	32/33	0.82	0.30	77,107,116,124	0
3	C2E	D	804	46/46	0.86	0.18	96,101,117,122	0
3	C2E	E	803	46/46	0.88	0.10	39,47,59,66	0
4	PO4	H	802	5/5	0.89	0.18	55,58,67,70	0
3	C2E	I	802	46/46	0.90	0.11	38,46,55,59	0
3	C2E	J	802	46/46	0.90	0.11	29,49,60,63	0
3	C2E	G	802	46/46	0.90	0.10	28,49,58,65	0
3	C2E	H	803	46/46	0.93	0.09	29,39,55,61	0
3	C2E	C	802	46/46	0.94	0.08	45,52,60,66	0
3	C2E	F	802	46/46	0.94	0.09	29,39,45,51	0

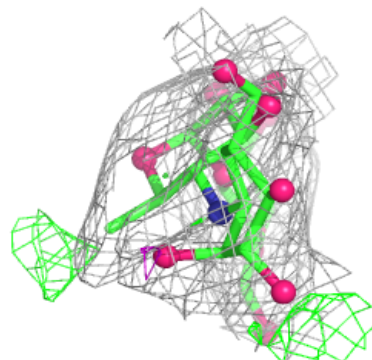
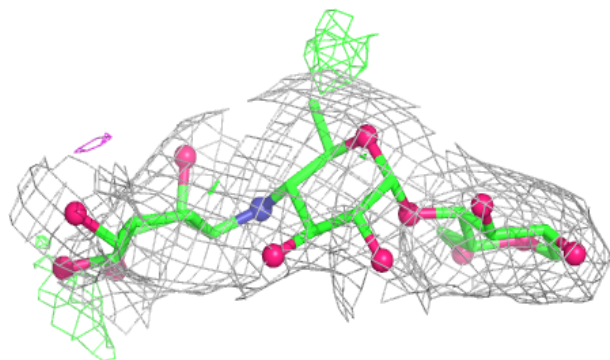
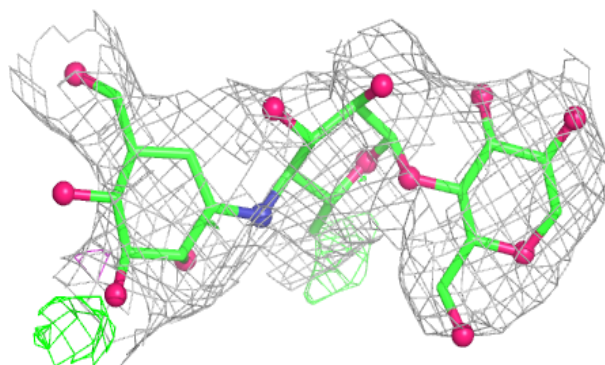
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

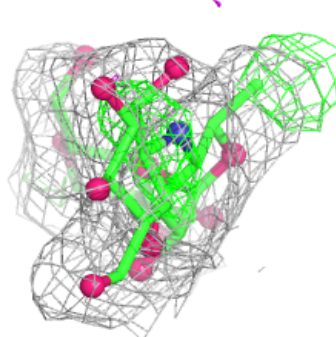
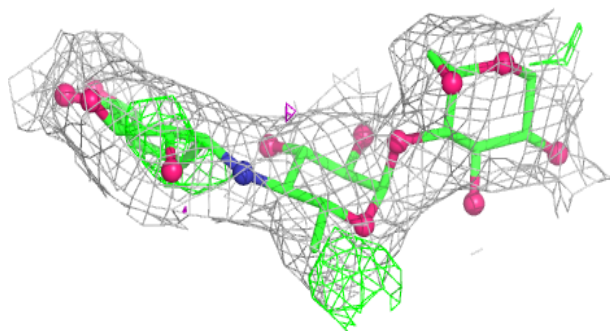
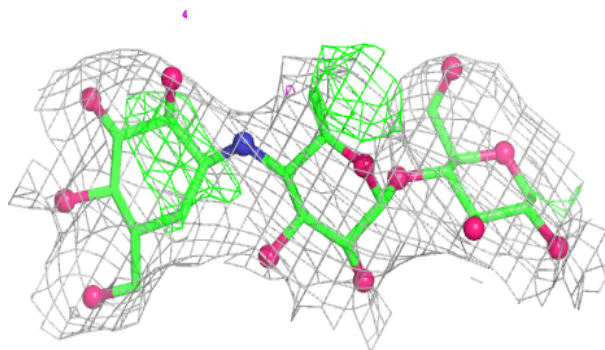
**Electron density around A16 I 801:**

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

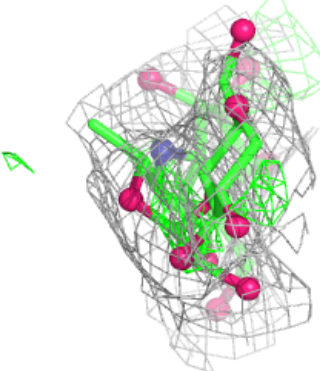
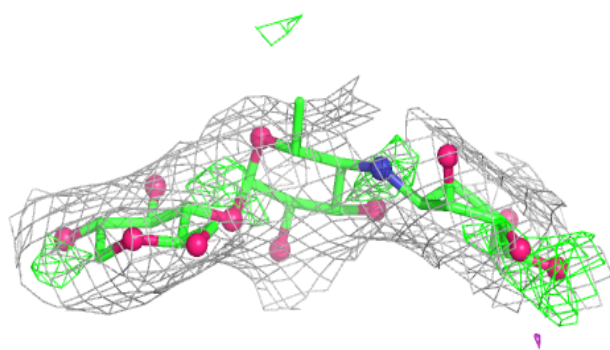
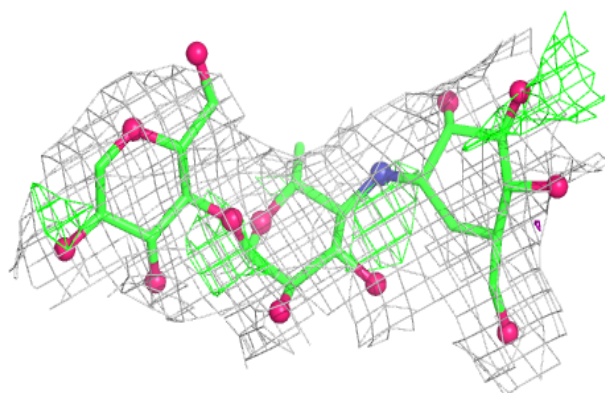


Electron density around A16 H 801:

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

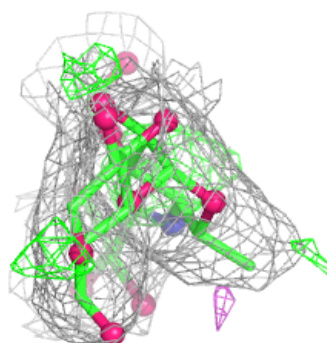
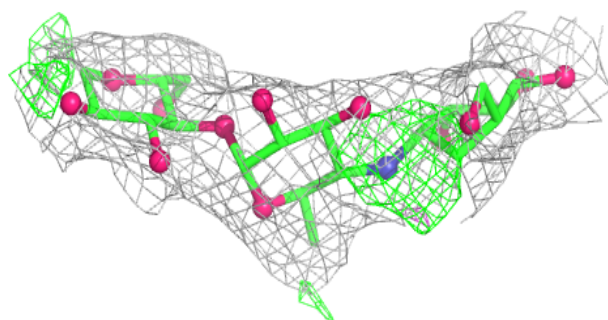
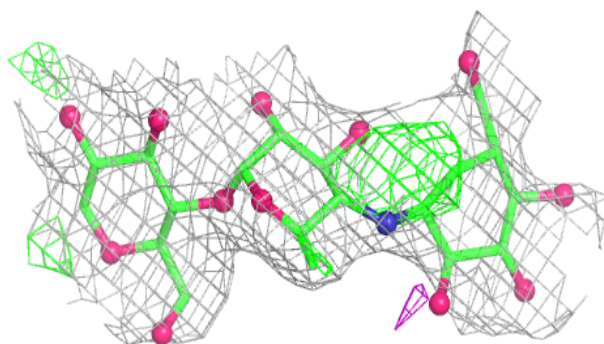
**Electron density around A16 J 801:**

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

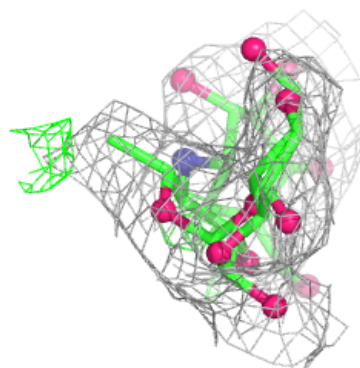
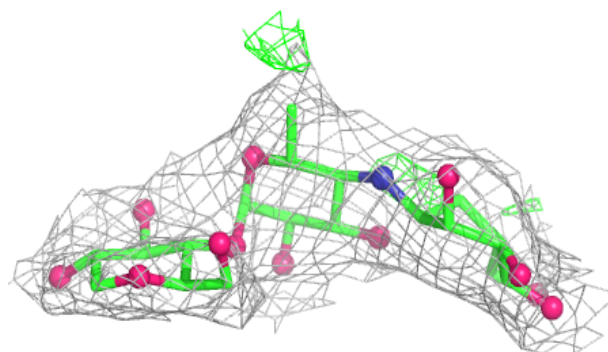
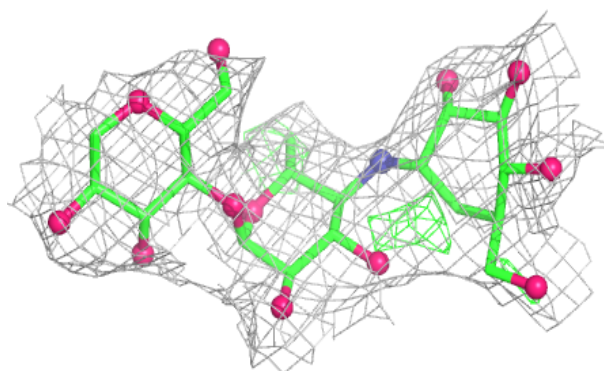


Electron density around A16 E 801:

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

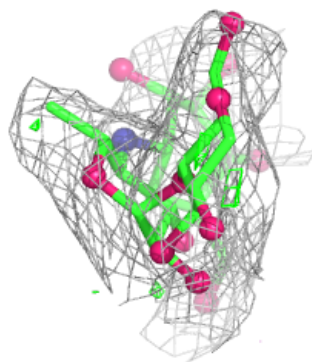
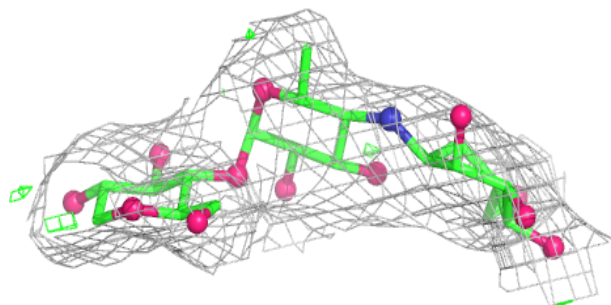
**Electron density around A16 C 801:**

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

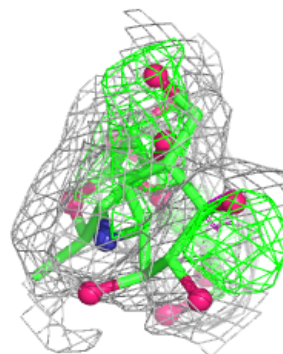
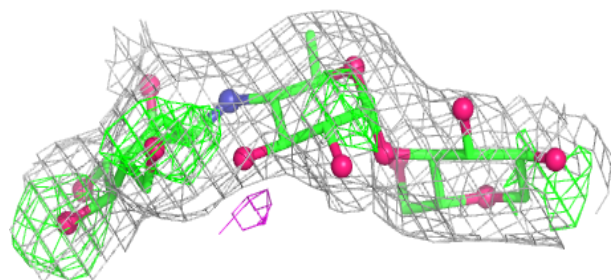
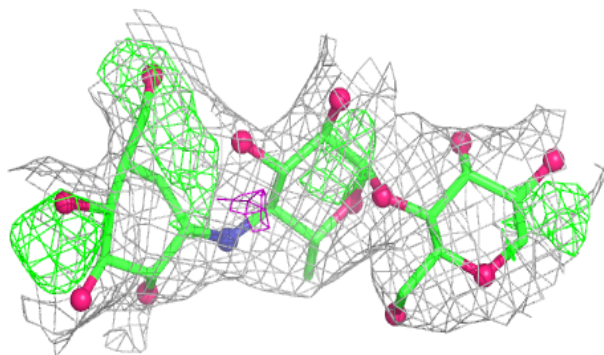


Electron density around A16 F 801:

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

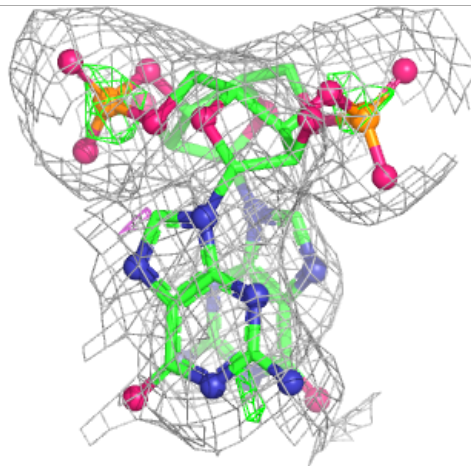
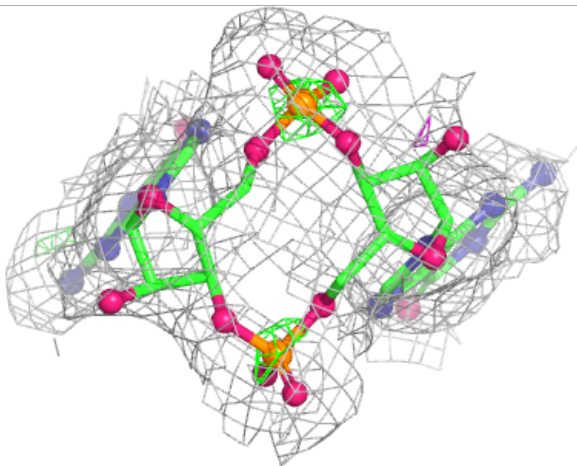
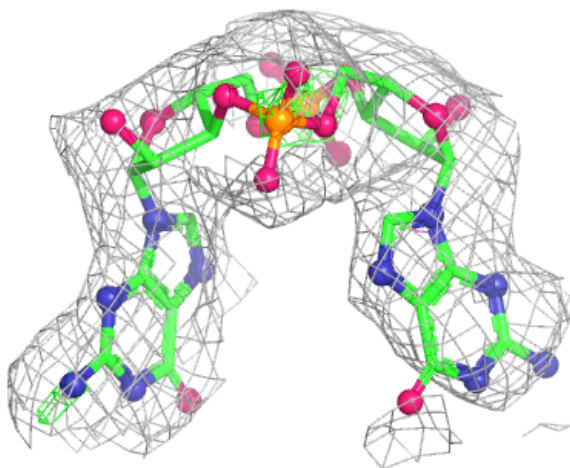
**Electron density around A16 D 801:**

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



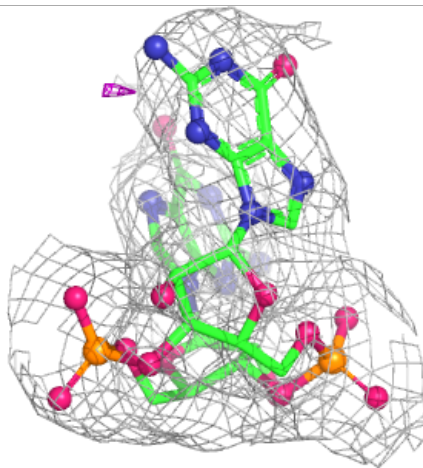
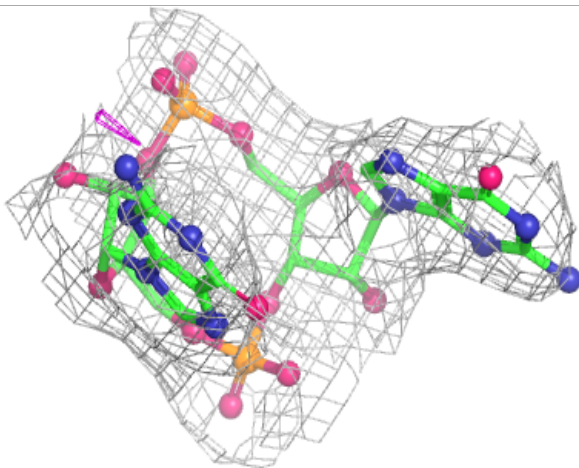
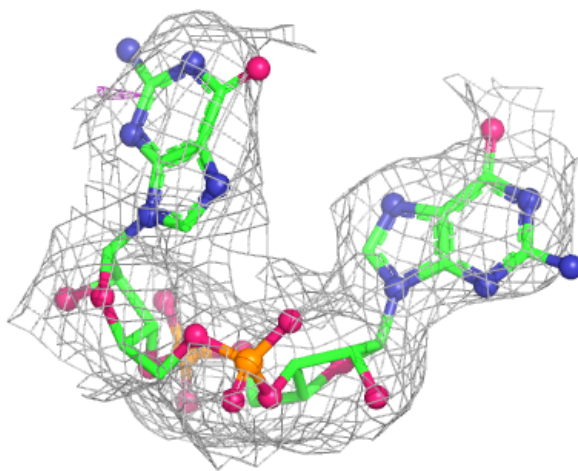
Electron density around C2E D 804:

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



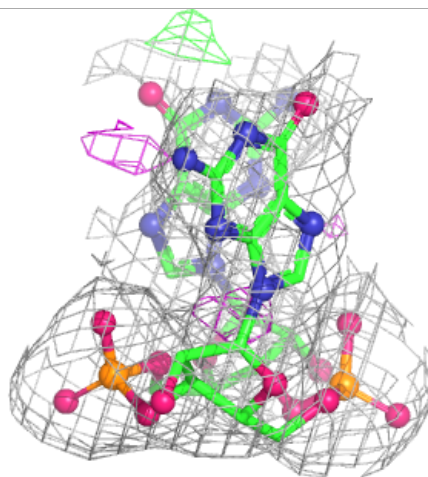
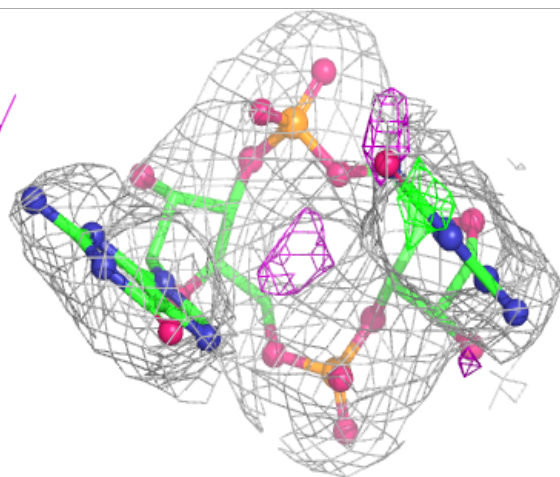
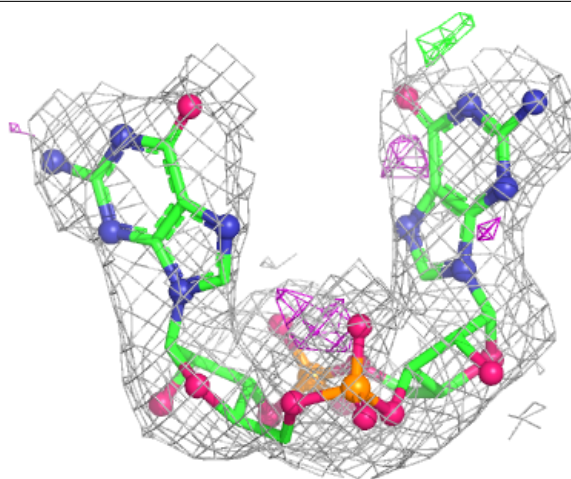
Electron density around C2E E 803:

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



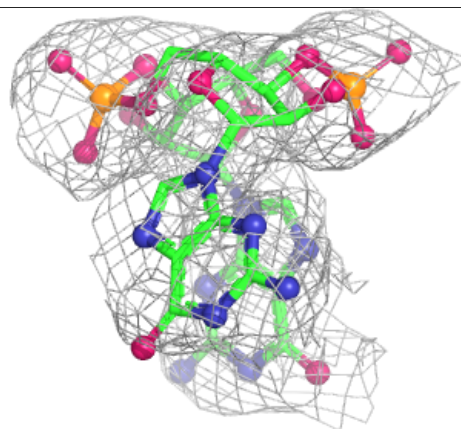
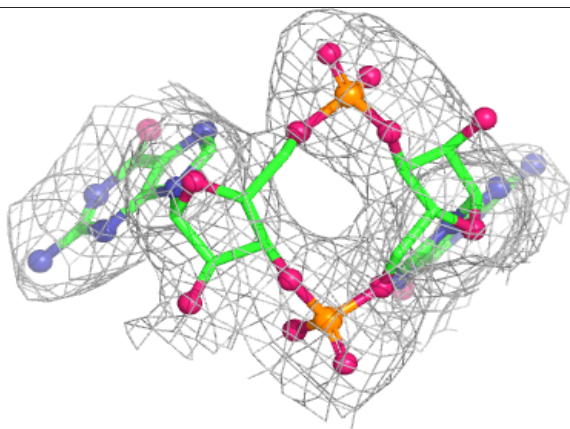
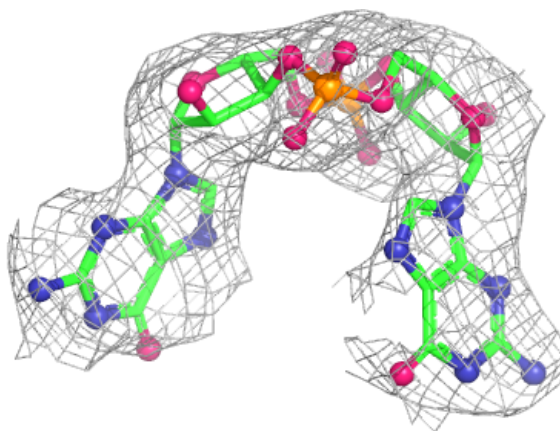
Electron density around C2E I 802:

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



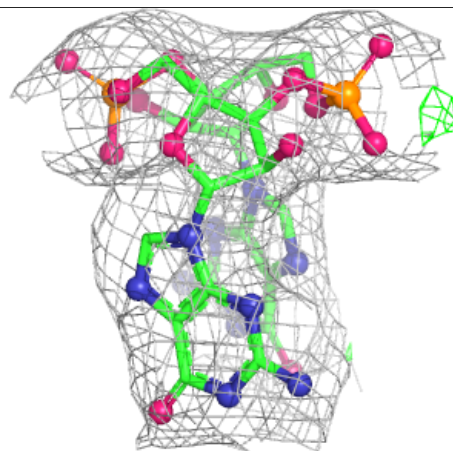
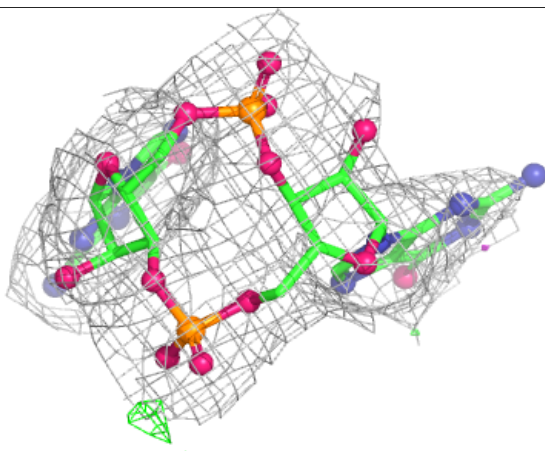
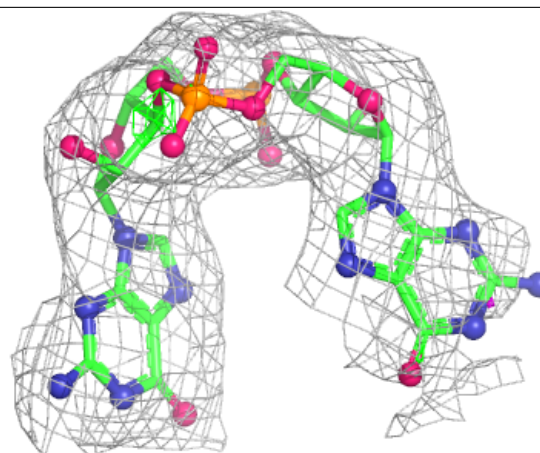
Electron density around C2E J 802:

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



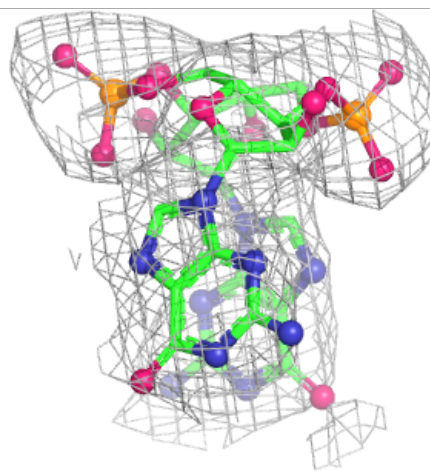
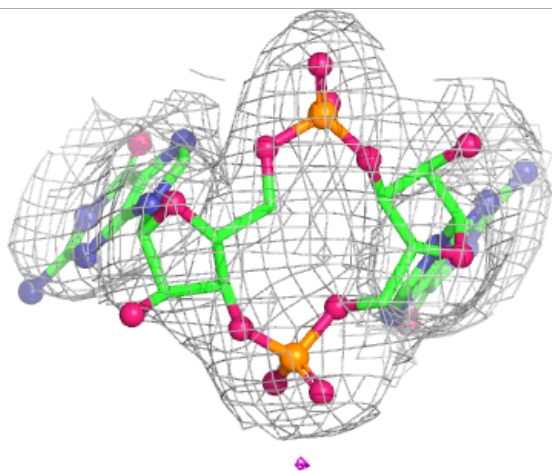
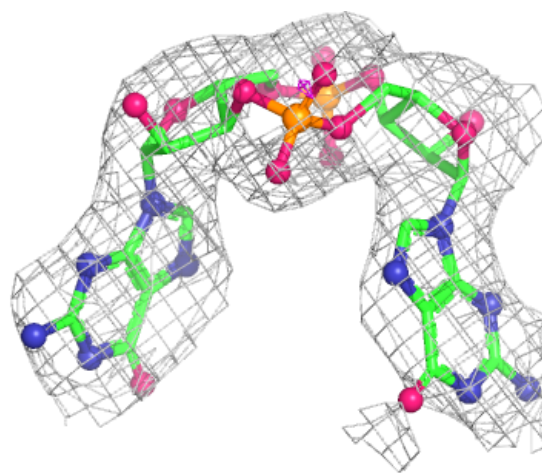
Electron density around C2E G 802:

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



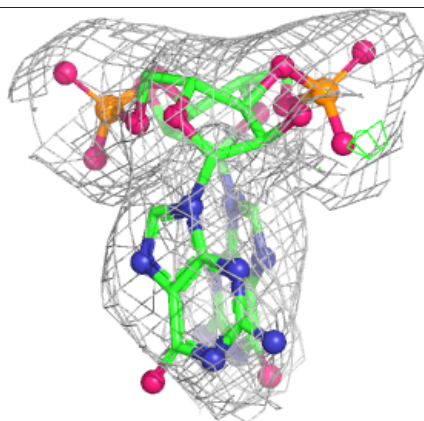
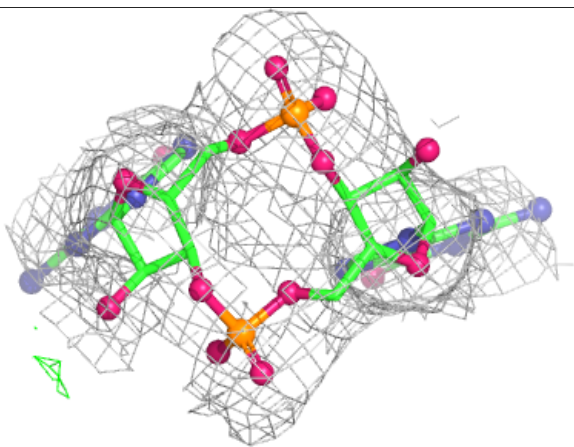
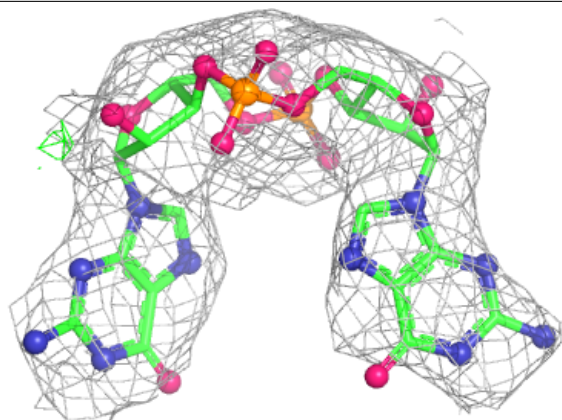
Electron density around C2E H 803:

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



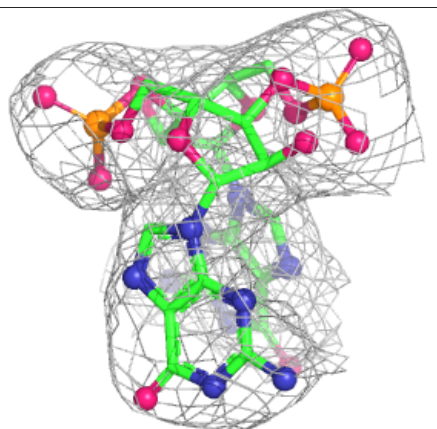
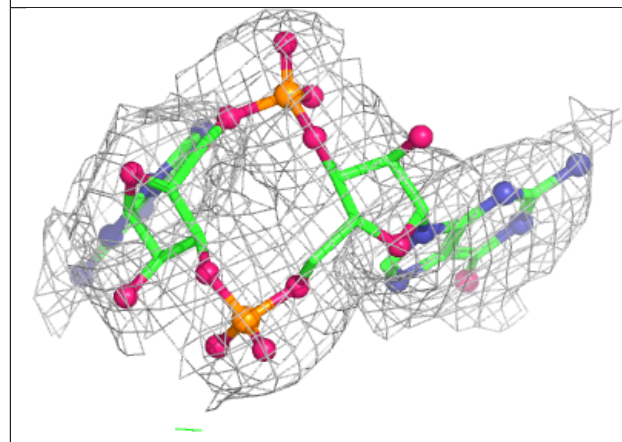
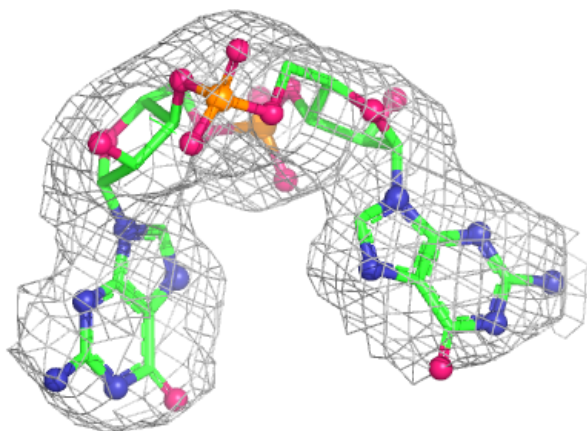
Electron density around C2E C 802:

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



Electron density around C2E 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.