wwPDB X-ray Structure Validation Summary Report (i)

Jul 11, 2022 – 04:53 pm BST

PDB ID	:	6GS8
Title	:	Crystal structure of SmbA in complex with c-di-GMP
Authors	:	Dubey, B.N.; Schirmer, T.
Deposited on	:	2018-06-13
Resolution	:	2.80 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 (i) 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 (i)) were used in the production of this report:

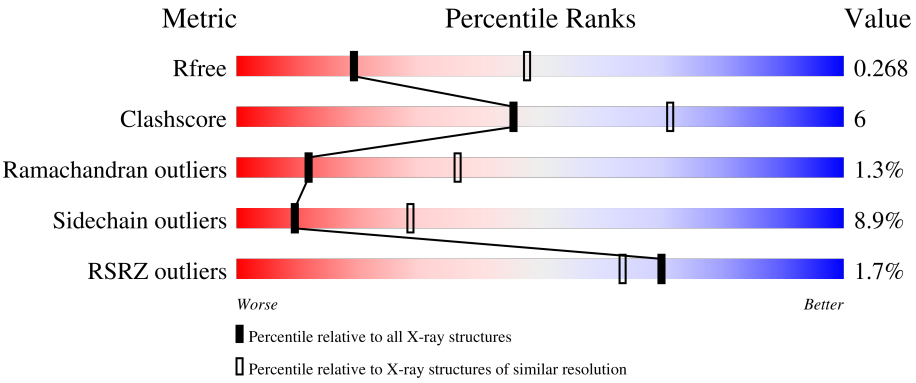
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	308	77% 16%
1	B	308	3% 78% 17%
1	C	308	2% 74% 17% 8%
1	D	308	2% 75% 14% 8%
1	E	308	79% 10% 8%

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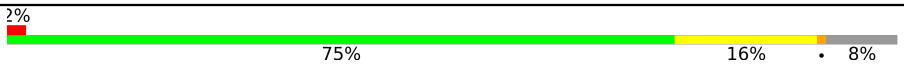
Mol	Chain	Length	Quality of chain
1	F	308	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 14110 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 Uncharacterized protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	301	Total	C	N	O	S	Se	0	0	0
			2345	1471	432	437	2	3			
1	B	301	Total	C	N	O	S	Se	0	0	0
			2345	1471	432	437	2	3			
1	C	284	Total	C	N	O	S	Se	0	0	0
			2208	1386	399	418	2	3			
1	D	284	Total	C	N	O	S	Se	0	0	0
			2208	1386	399	418	2	3			
1	E	284	Total	C	N	O	S	Se	0	0	0
			2208	1386	399	418	2	3			
1	F	284	Total	C	N	O	S	Se	0	0	0
			2208	1386	399	418	2	3			

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	initiating methionine	UNP Q9A5E6
A	198	VAL	-	insertion	UNP Q9A5E6
A	297	LYS	-	expression tag	UNP Q9A5E6
A	298	LEU	-	expression tag	UNP Q9A5E6
A	299	ALA	-	expression tag	UNP Q9A5E6
A	300	ALA	-	expression tag	UNP Q9A5E6
A	301	ALA	-	expression tag	UNP Q9A5E6
A	302	LEU	-	expression tag	UNP Q9A5E6
A	303	GLU	-	expression tag	UNP Q9A5E6
A	304	HIS	-	expression tag	UNP Q9A5E6
A	305	HIS	-	expression tag	UNP Q9A5E6
A	306	HIS	-	expression tag	UNP Q9A5E6
A	307	HIS	-	expression tag	UNP Q9A5E6
B	1	MSE	-	initiating methionine	UNP Q9A5E6
B	198	VAL	-	insertion	UNP Q9A5E6
B	297	LYS	-	expression tag	UNP Q9A5E6
B	298	LEU	-	expression tag	UNP Q9A5E6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	299	ALA	-	expression tag	UNP Q9A5E6
B	300	ALA	-	expression tag	UNP Q9A5E6
B	301	ALA	-	expression tag	UNP Q9A5E6
B	302	LEU	-	expression tag	UNP Q9A5E6
B	303	GLU	-	expression tag	UNP Q9A5E6
B	304	HIS	-	expression tag	UNP Q9A5E6
B	305	HIS	-	expression tag	UNP Q9A5E6
B	306	HIS	-	expression tag	UNP Q9A5E6
B	307	HIS	-	expression tag	UNP Q9A5E6
C	1	MSE	-	initiating methionine	UNP Q9A5E6
C	198	VAL	-	insertion	UNP Q9A5E6
C	297	LYS	-	expression tag	UNP Q9A5E6
C	298	LEU	-	expression tag	UNP Q9A5E6
C	299	ALA	-	expression tag	UNP Q9A5E6
C	300	ALA	-	expression tag	UNP Q9A5E6
C	301	ALA	-	expression tag	UNP Q9A5E6
C	302	LEU	-	expression tag	UNP Q9A5E6
C	303	GLU	-	expression tag	UNP Q9A5E6
C	304	HIS	-	expression tag	UNP Q9A5E6
C	305	HIS	-	expression tag	UNP Q9A5E6
C	306	HIS	-	expression tag	UNP Q9A5E6
C	307	HIS	-	expression tag	UNP Q9A5E6
D	1	MSE	-	initiating methionine	UNP Q9A5E6
D	198	VAL	-	insertion	UNP Q9A5E6
D	297	LYS	-	expression tag	UNP Q9A5E6
D	298	LEU	-	expression tag	UNP Q9A5E6
D	299	ALA	-	expression tag	UNP Q9A5E6
D	300	ALA	-	expression tag	UNP Q9A5E6
D	301	ALA	-	expression tag	UNP Q9A5E6
D	302	LEU	-	expression tag	UNP Q9A5E6
D	303	GLU	-	expression tag	UNP Q9A5E6
D	304	HIS	-	expression tag	UNP Q9A5E6
D	305	HIS	-	expression tag	UNP Q9A5E6
D	306	HIS	-	expression tag	UNP Q9A5E6
D	307	HIS	-	expression tag	UNP Q9A5E6
E	1	MSE	-	initiating methionine	UNP Q9A5E6
E	198	VAL	-	insertion	UNP Q9A5E6
E	297	LYS	-	expression tag	UNP Q9A5E6
E	298	LEU	-	expression tag	UNP Q9A5E6
E	299	ALA	-	expression tag	UNP Q9A5E6
E	300	ALA	-	expression tag	UNP Q9A5E6
E	301	ALA	-	expression tag	UNP Q9A5E6

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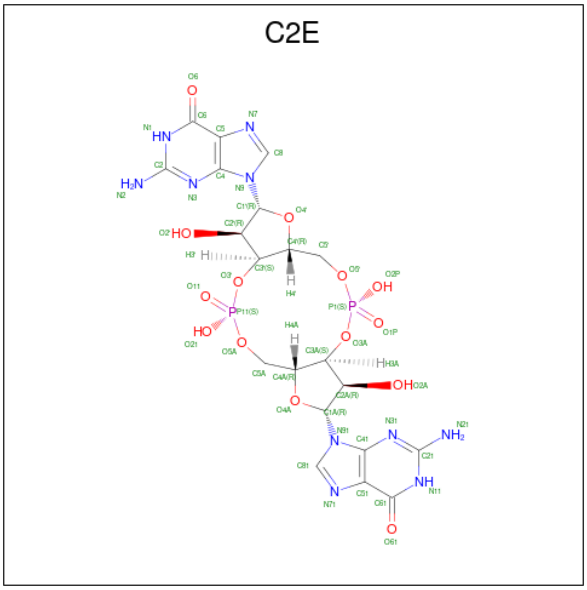
Chain	Residue	Modelled	Actual	Comment	Reference
E	302	LEU	-	expression tag	UNP Q9A5E6
E	303	GLU	-	expression tag	UNP Q9A5E6
E	304	HIS	-	expression tag	UNP Q9A5E6
E	305	HIS	-	expression tag	UNP Q9A5E6
E	306	HIS	-	expression tag	UNP Q9A5E6
E	307	HIS	-	expression tag	UNP Q9A5E6
F	1	MSE	-	initiating methionine	UNP Q9A5E6
F	198	VAL	-	insertion	UNP Q9A5E6
F	297	LYS	-	expression tag	UNP Q9A5E6
F	298	LEU	-	expression tag	UNP Q9A5E6
F	299	ALA	-	expression tag	UNP Q9A5E6
F	300	ALA	-	expression tag	UNP Q9A5E6
F	301	ALA	-	expression tag	UNP Q9A5E6
F	302	LEU	-	expression tag	UNP Q9A5E6
F	303	GLU	-	expression tag	UNP Q9A5E6
F	304	HIS	-	expression tag	UNP Q9A5E6
F	305	HIS	-	expression tag	UNP Q9A5E6
F	306	HIS	-	expression tag	UNP Q9A5E6
F	307	HIS	-	expression tag	UNP Q9A5E6

- Molecule 2 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: $C_{20}H_{24}N_{10}O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 4 is water.

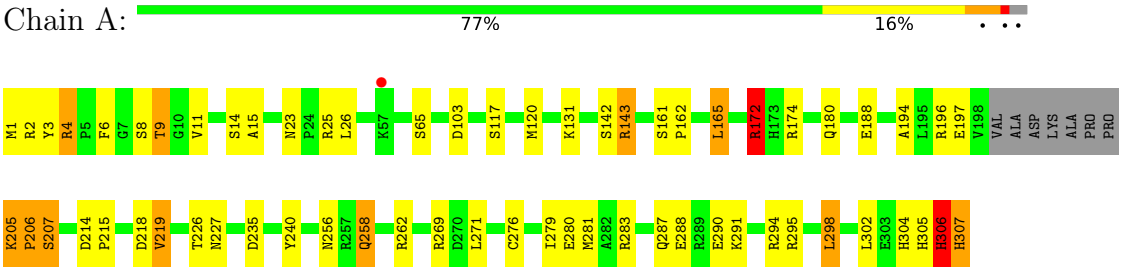
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	5	Total O 5 5	0	0
4	B	5	Total O 5 5	0	0
4	C	5	Total O 5 5	0	0
4	D	5	Total O 5 5	0	0
4	E	5	Total O 5 5	0	0
4	F	5	Total O 5 5	0	0

3 Residue-property plots (i)

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

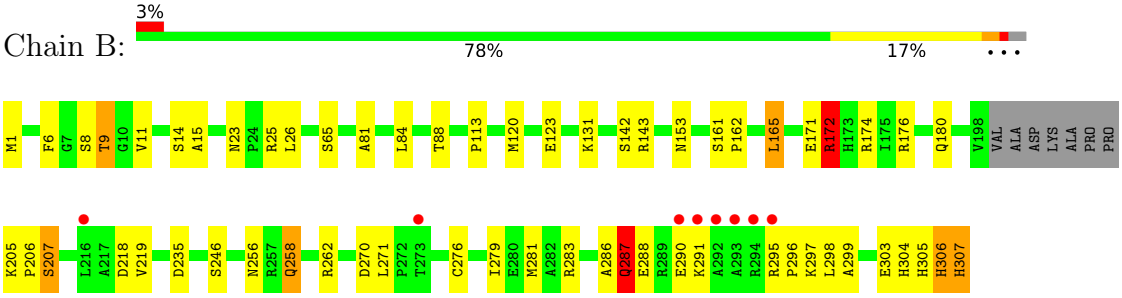
• Molecule 1: Uncharacterized protein

Chain A:



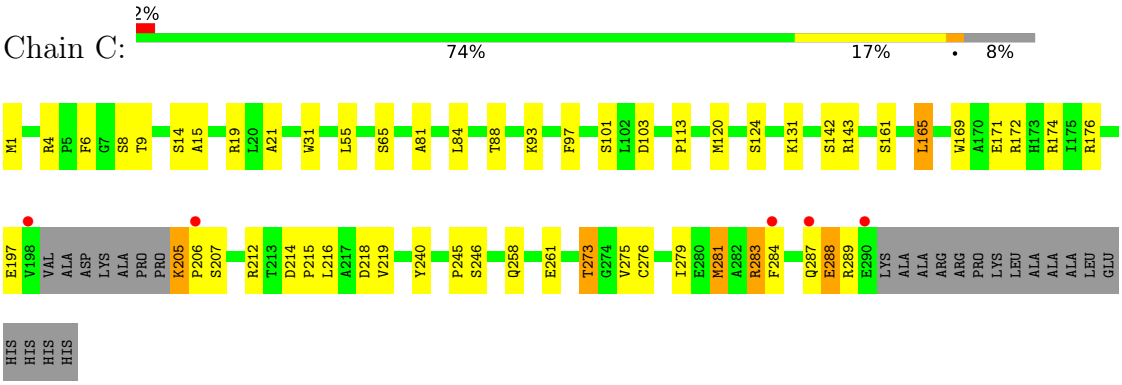
• Molecule 1: Uncharacterized protein

Chain B:



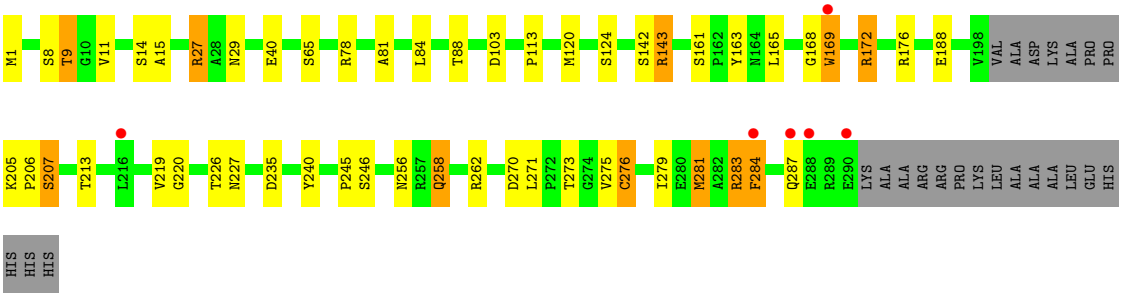
• Molecule 1: Uncharacterized protein

Chain C:

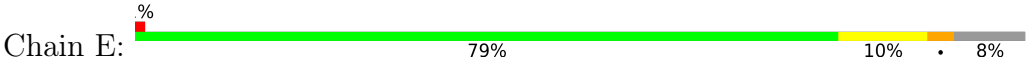


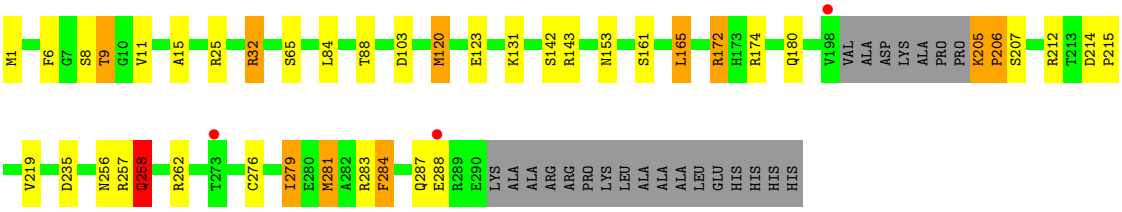
• Molecule 1: Uncharacterized protein

Chain D:

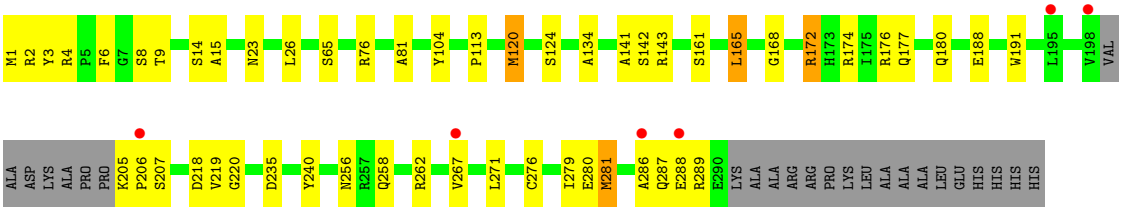


• Molecule 1: Uncharacterized protein





• Molecule 1: Uncharacterized protein



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	127.91Å 87.42Å 130.27Å 90.00° 119.48° 90.00°	Depositor
Resolution (Å)	29.57 – 2.80 113.40 – 2.70	Depositor EDS
% Data completeness (in resolution range)	91.8 (29.57-2.80) 91.3 (113.40-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.63 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.219 , 0.268 0.221 , 0.268	Depositor DCC
R_{free} test set	1998 reflections (3.06%)	wwPDB-VP
Wilson B-factor (Å^2)	66.8	Xtriage
Anisotropy	0.464	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.002 for l,k,-h-l 0.002 for -h-l,k,h 0.014 for h,-k,-h-l 0.014 for l,-k,h 0.014 for -h-l,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14110	wwPDB-VP
Average B, all atoms (Å^2)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.58% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: C2E, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.82	0/2392	1.09	9/3242 (0.3%)
1	B	0.79	0/2391	1.03	6/3239 (0.2%)
1	C	0.91	3/2250 (0.1%)	1.12	7/3051 (0.2%)
1	D	0.81	1/2250 (0.0%)	1.07	7/3051 (0.2%)
1	E	0.83	0/2250	1.09	10/3051 (0.3%)
1	F	0.81	2/2250 (0.1%)	1.05	7/3051 (0.2%)
All	All	0.83	6/13783 (0.0%)	1.07	46/18685 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
1	C	0	3
1	D	0	1
1	E	0	1
1	F	0	1
All	All	0	9

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	288	GLU	C-N	10.92	1.59	1.34
1	F	188	GLU	CD-OE2	-5.45	1.19	1.25
1	D	188	GLU	CD-OE1	-5.38	1.19	1.25
1	C	261	GLU	CD-OE2	5.25	1.31	1.25
1	F	141	ALA	C-O	5.18	1.33	1.23

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	281	MSE	CG-SE-CE	13.67	128.98	98.90
1	E	120	MSE	CG-SE-CE	13.55	128.71	98.90
1	A	143	ARG	NE-CZ-NH2	-10.96	114.82	120.30
1	B	143	ARG	NE-CZ-NH2	-10.49	115.06	120.30
1	D	143	ARG	NE-CZ-NH2	-9.99	115.30	120.30

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	306	HIS	Peptide
1	A	6	PHE	Peptide
1	B	6	PHE	Peptide
1	C	288	GLU	Mainchain
1	C	6	PHE	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	A	2345	0	2313	30	0
1	B	2345	0	2312	36	0
1	C	2208	0	2173	37	0
1	D	2208	0	2173	39	0
1	E	2208	0	2173	30	0
1	F	2208	0	2173	30	0
2	A	92	0	44	1	0
2	B	92	0	44	0	0
2	C	92	0	44	1	0
2	D	92	0	44	2	0
2	E	92	0	44	2	0
2	F	92	0	44	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
4	E	5	0	0	0	0
4	F	5	0	0	0	0
All	All	14110	0	13581	177	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 6.

The worst 5 of 177 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:D:172:ARG:NH2	1:D:240:TYR:OH	1.90	1.02
1:B:286:ALA:C	1:B:287:GLN:HA	1.79	1.02
1:E:284:PHE:CZ	1:F:180:GLN:HG3	1.94	1.02
1:C:172:ARG:NH2	1:C:240:TYR:OH	1.94	1.00
1:E:256:ASN:ND2	1:E:258:GLN:HG2	1.80	0.96

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	297/308 (96%)	273 (92%)	20 (7%)	4 (1%)	12 36
1	B	295/308 (96%)	264 (90%)	26 (9%)	5 (2%)	9 29
1	C	280/308 (91%)	255 (91%)	22 (8%)	3 (1%)	14 41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	280/308 (91%)	260 (93%)	17 (6%)	3 (1%)	14 41
1	E	280/308 (91%)	261 (93%)	16 (6%)	3 (1%)	14 41
1	F	280/308 (91%)	260 (93%)	16 (6%)	4 (1%)	11 34
All	All	1712/1848 (93%)	1573 (92%)	117 (7%)	22 (1%)	12 36

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	306	HIS
1	B	295	ARG
1	B	306	HIS
1	A	206	PRO
1	B	8	SER

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	A	241/243 (99%)	215 (89%)	26 (11%)	6 19
1	B	241/243 (99%)	218 (90%)	23 (10%)	8 25
1	C	229/243 (94%)	210 (92%)	19 (8%)	11 32
1	D	229/243 (94%)	205 (90%)	24 (10%)	7 20
1	E	229/243 (94%)	212 (93%)	17 (7%)	13 37
1	F	229/243 (94%)	213 (93%)	16 (7%)	15 40
All	All	1398/1458 (96%)	1273 (91%)	125 (9%)	9 28

5 of 125 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	161	SER
1	F	14	SER
1	D	29	ASN
1	F	9	THR

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Mol	Chain	Res	Type
1	F	174	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	181	ASN
1	F	193	GLN
1	D	227	ASN
1	E	256	ASN
1	D	193	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	C2E	F	401	-	44,52,52	1.36	8 (18%)	52,82,82	1.60	13 (25%)
2	C2E	E	401	-	44,52,52	0.94	2 (4%)	52,82,82	1.06	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	C2E	F	402	-	44,52,52	1.37	6 (13%)	52,82,82	1.31	8 (15%)
2	C2E	B	401	-	44,52,52	1.14	5 (11%)	52,82,82	1.32	4 (7%)
2	C2E	D	401	-	44,52,52	1.20	4 (9%)	52,82,82	1.38	8 (15%)
2	C2E	B	402	-	44,52,52	1.06	4 (9%)	52,82,82	1.21	6 (11%)
2	C2E	A	401	-	44,52,52	0.99	3 (6%)	52,82,82	1.23	6 (11%)
2	C2E	D	402	-	44,52,52	1.06	3 (6%)	52,82,82	1.27	7 (13%)
2	C2E	C	401	-	44,52,52	0.96	2 (4%)	52,82,82	1.43	9 (17%)
2	C2E	C	402	-	44,52,52	1.43	4 (9%)	52,82,82	1.28	6 (11%)
2	C2E	E	402	-	44,52,52	0.95	2 (4%)	52,82,82	1.05	3 (5%)
2	C2E	A	402	-	44,52,52	1.09	5 (11%)	52,82,82	1.22	7 (13%)

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	C2E	F	401	-	-	3/22/62/62	0/6/7/7
2	C2E	E	401	-	-	0/22/62/62	0/6/7/7
2	C2E	F	402	-	-	6/22/62/62	0/6/7/7
2	C2E	B	401	-	-	1/22/62/62	0/6/7/7
2	C2E	D	401	-	-	0/22/62/62	0/6/7/7
2	C2E	B	402	-	-	7/22/62/62	0/6/7/7
2	C2E	A	401	-	-	2/22/62/62	0/6/7/7
2	C2E	D	402	-	-	0/22/62/62	0/6/7/7
2	C2E	C	401	-	-	0/22/62/62	0/6/7/7
2	C2E	C	402	-	-	5/22/62/62	0/6/7/7
2	C2E	E	402	-	-	4/22/62/62	0/6/7/7
2	C2E	A	402	-	-	0/22/62/62	0/6/7/7

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	402	C2E	C81-N71	-5.10	1.26	1.35
2	F	402	C2E	C8-N7	-4.11	1.28	1.35
2	C	402	C2E	C51-C61	-4.07	1.39	1.47
2	C	402	C2E	C51-C41	-4.06	1.32	1.43
2	D	401	C2E	C5-C6	-3.59	1.40	1.47

The worst 5 of 81 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	401	C2E	O6-C6-N1	-4.54	115.29	120.65
2	C	401	C2E	O6-C6-C5	3.89	131.97	124.37
2	A	402	C2E	O2P-P1-O1P	3.82	131.14	112.24
2	F	401	C2E	C51-C61-N11	-3.67	107.47	113.95
2	F	401	C2E	O3A-P1-O1P	-3.56	96.11	109.47

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	402	C2E	C5'-O5'-P1-O1P
2	C	402	C2E	C5'-O5'-P1-O1P
2	C	402	C2E	O4'-C4'-C5'-O5'
2	E	402	C2E	C2'-C3'-O3'-P11
2	F	402	C2E	C4'-C3'-O3'-P11

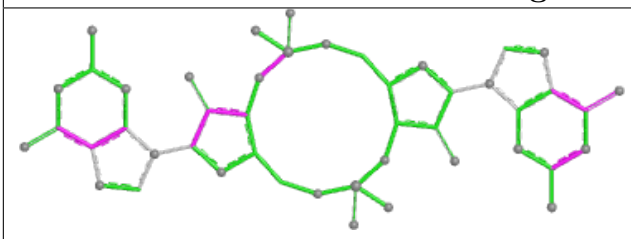
There are no ring outliers.

5 monomers are involved in 6 short contacts:

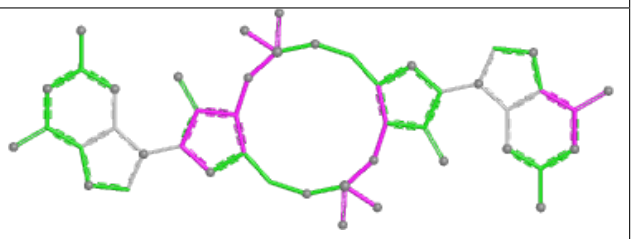
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	401	C2E	1	0
2	D	401	C2E	2	0
2	A	401	C2E	1	0
2	C	402	C2E	1	0
2	E	402	C2E	1	0

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 then 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.

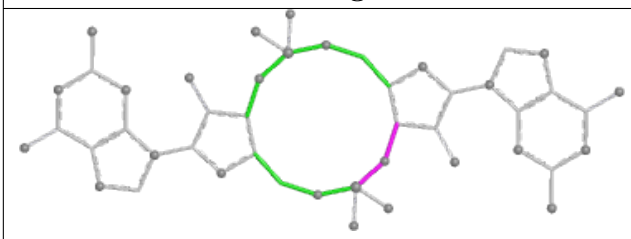
Ligand C2E F 401



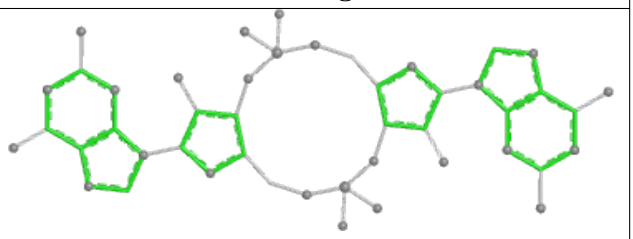
Bond lengths



Bond angles

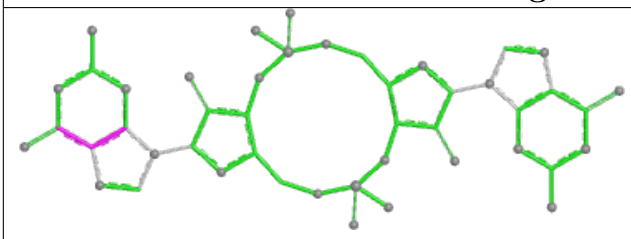


Torsions



Rings

Ligand C2E E 401



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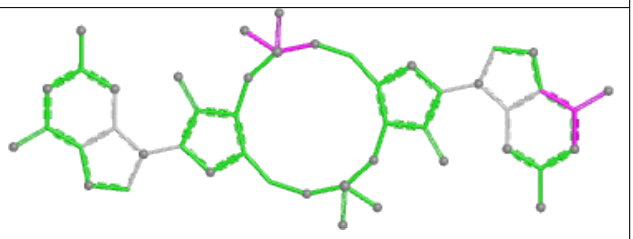

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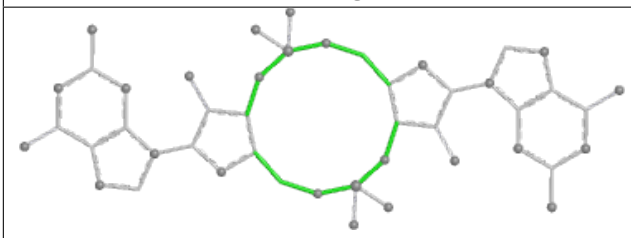

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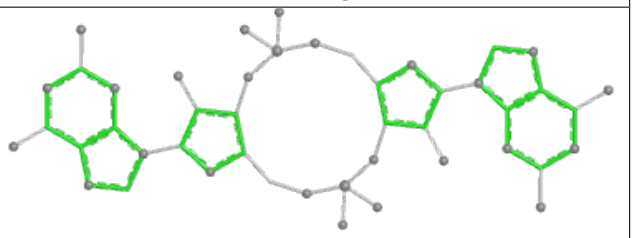
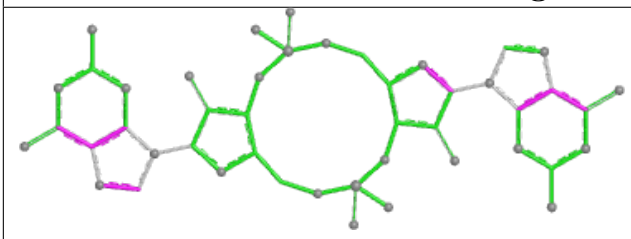


Rings

Ligand C2E F 402



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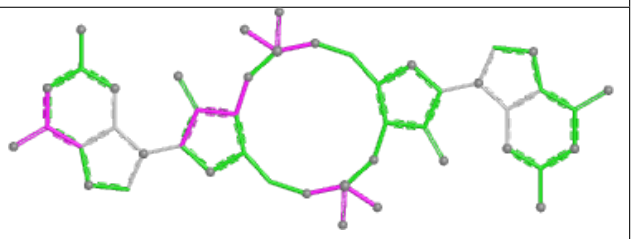

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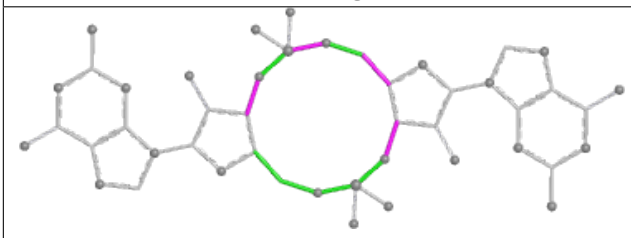

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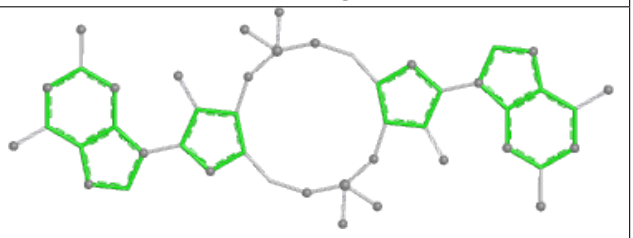
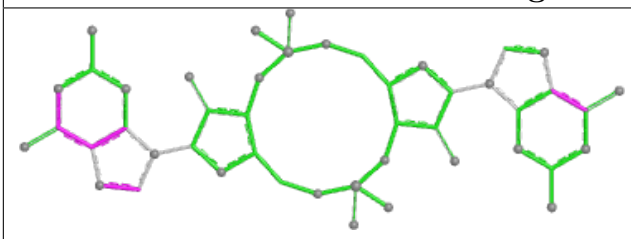


Rings

Ligand C2E B 401



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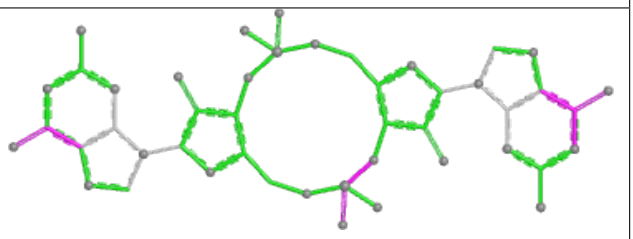

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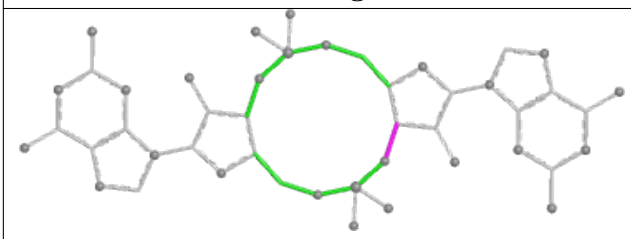

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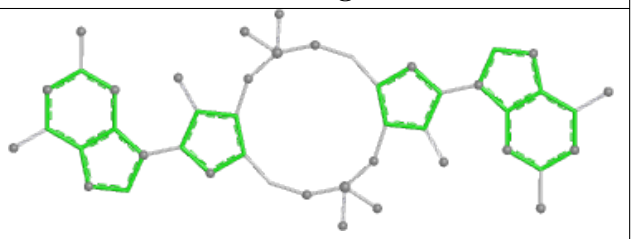
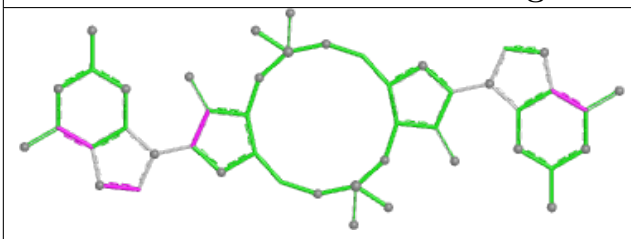


Rings

Ligand C2E D 401



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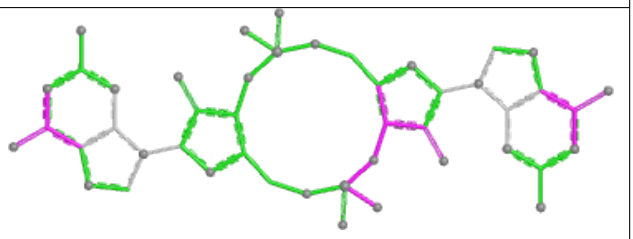

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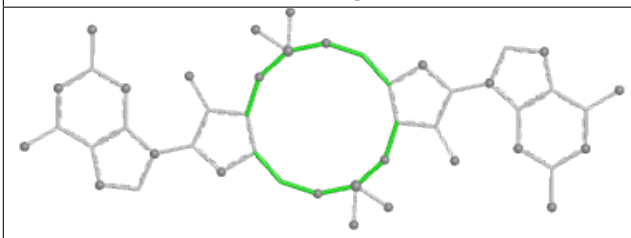

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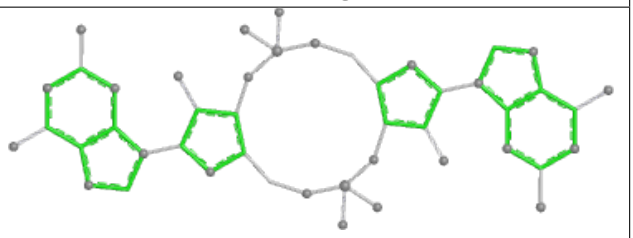
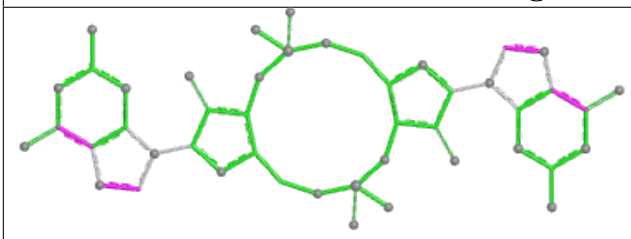


Rings

Ligand C2E B 402



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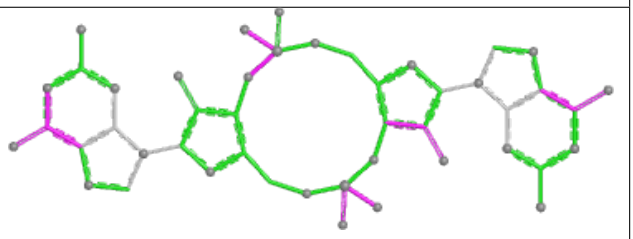

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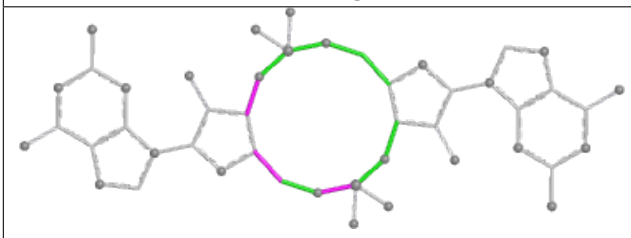

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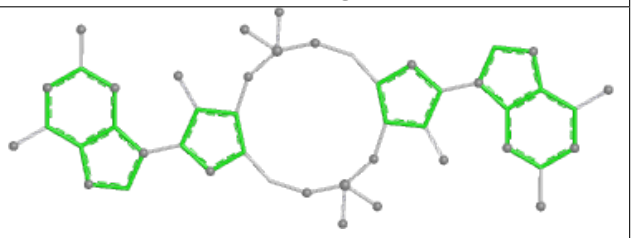
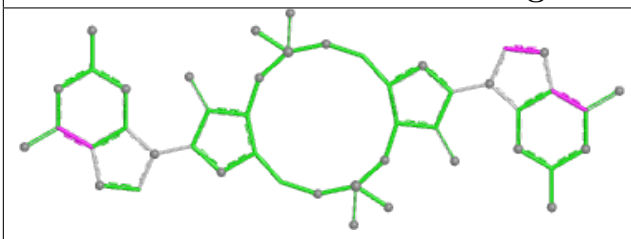


Rings

Ligand C2E A 401



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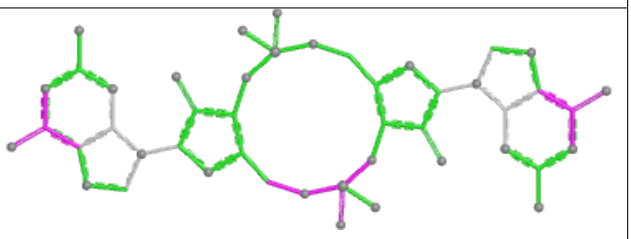

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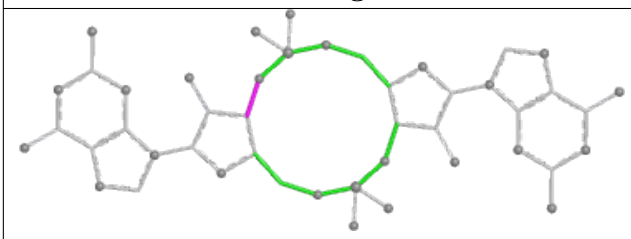

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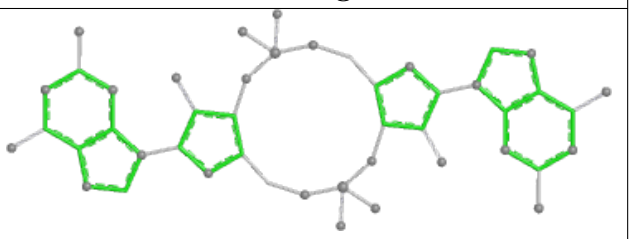
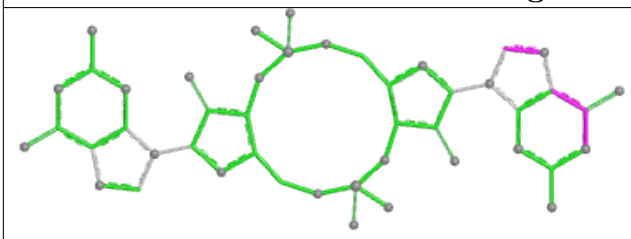


Rings

Ligand C2E D 402



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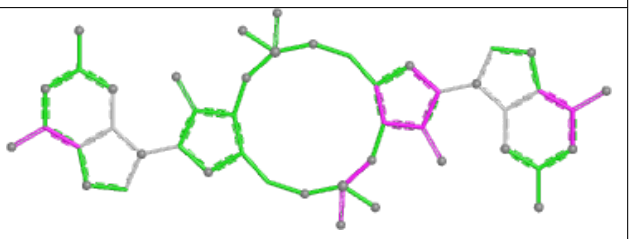

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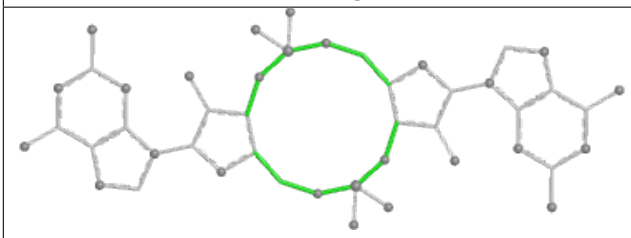

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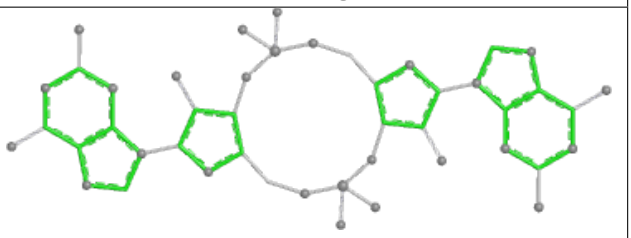
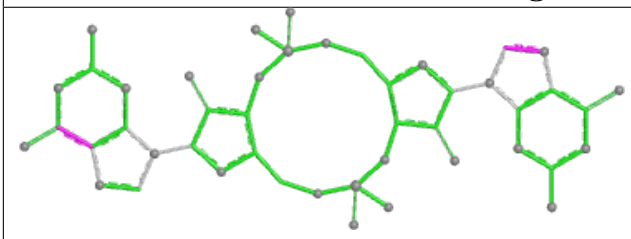
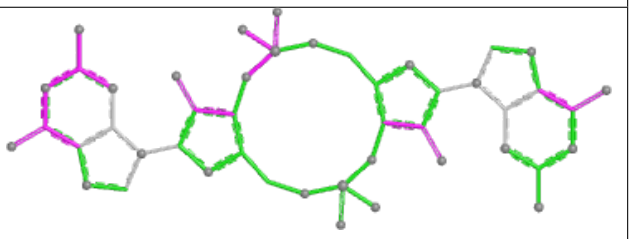


Rings

Ligand C2E C 401



Bond lengths



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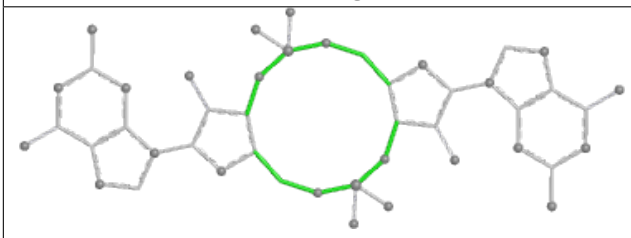

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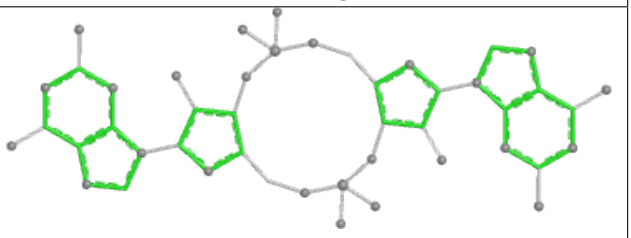
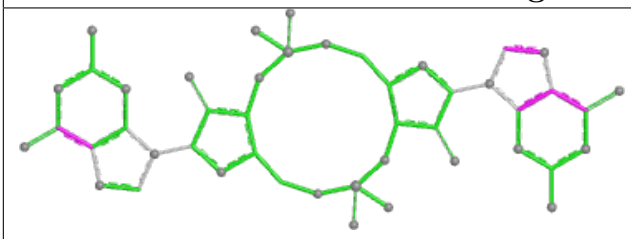
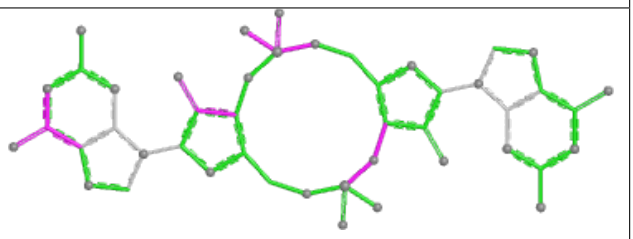


Rings

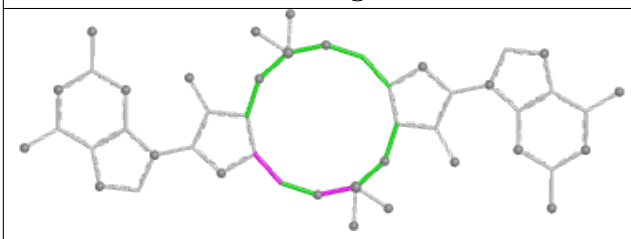
Ligand C2E C 402



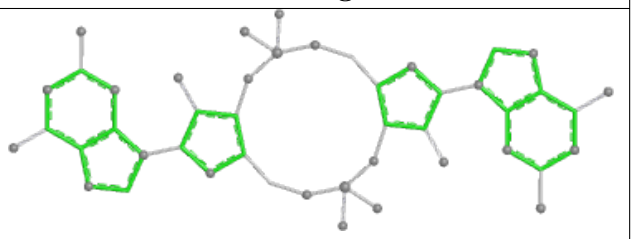
Bond lengths



Bond angles

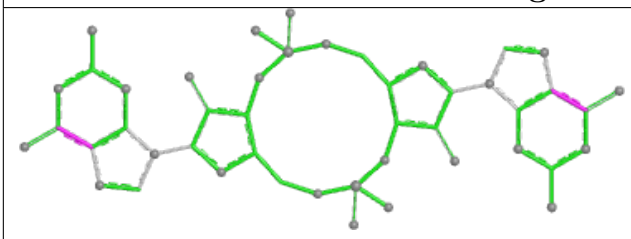


Torsions

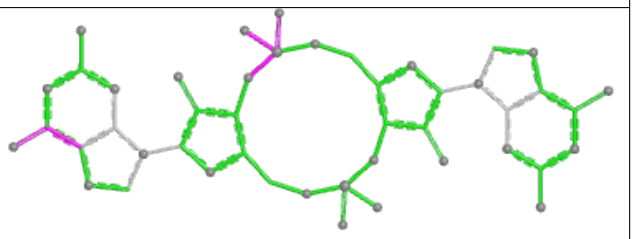


Rings

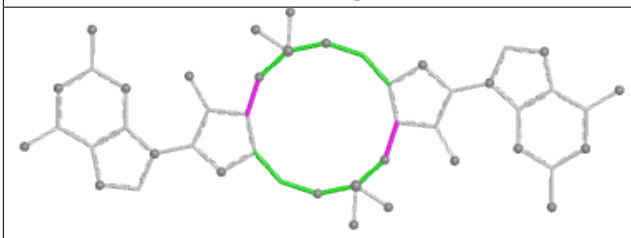
Ligand C2E E 402



Bond lengths



Bond angles



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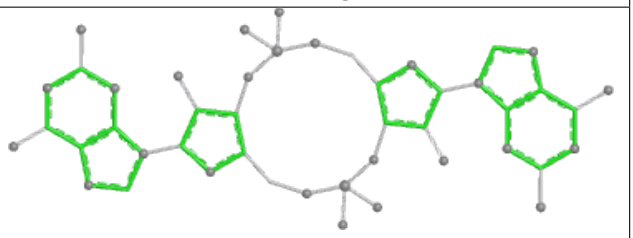
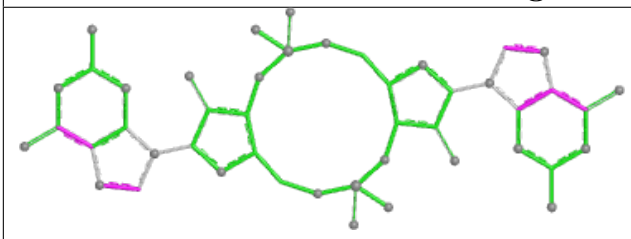
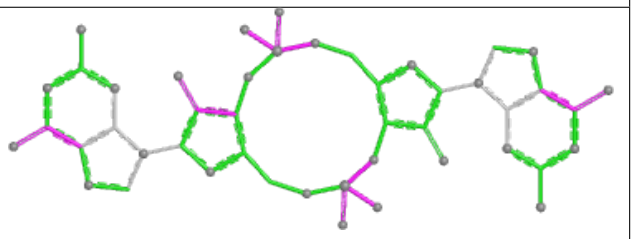


Rings

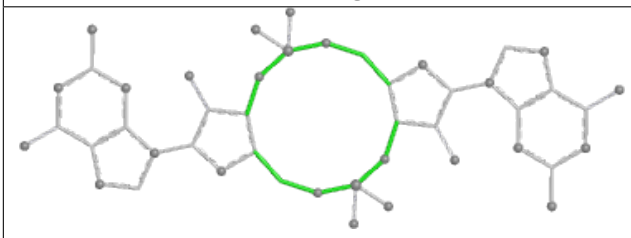
Ligand C2E A 402



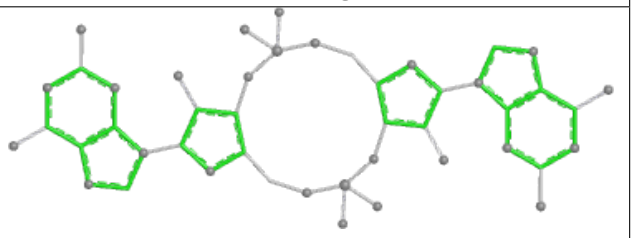
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	286:ALA	C	287:GLN	N	2.50

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	298/308 (96%)	-0.03	1 (0%)	94	93	43, 73, 113, 135	0
1	B	298/308 (96%)	-0.12	8 (2%)	54	44	52, 84, 147, 184	0
1	C	281/308 (91%)	-0.00	5 (1%)	68	61	41, 68, 128, 161	0
1	D	281/308 (91%)	-0.10	6 (2%)	63	54	48, 81, 137, 165	0
1	E	281/308 (91%)	-0.08	3 (1%)	80	75	45, 75, 129, 170	0
1	F	281/308 (91%)	0.02	6 (2%)	63	54	54, 98, 134, 157	0
All	All	1720/1848 (93%)	-0.05	29 (1%)	70	63	41, 80, 132, 184	0

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	284	PHE	7.6
1	B	292	ALA	7.0
1	B	293	ALA	6.7
1	C	287	GLN	5.2
1	F	288	GLU	4.5

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

LIGAND-RSR INFOmissingINFO

6.5 Other polymers (i)

There are no such residues in this entry.