Full wwPDB X-ray Structure Validation Report (i)

Sep 19, 2023 – 07:17 AM EDT

PDB ID	:	5C8E
Title	:	Crystal structure of Thermus thermophilus CarH bound to adenosylcobalamin and a 26-bp DNA segment
Authors	:	Jost, M.; Drennan, C.L.
Deposited on	:	2015-06-25
Resolution	:	3.89 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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:

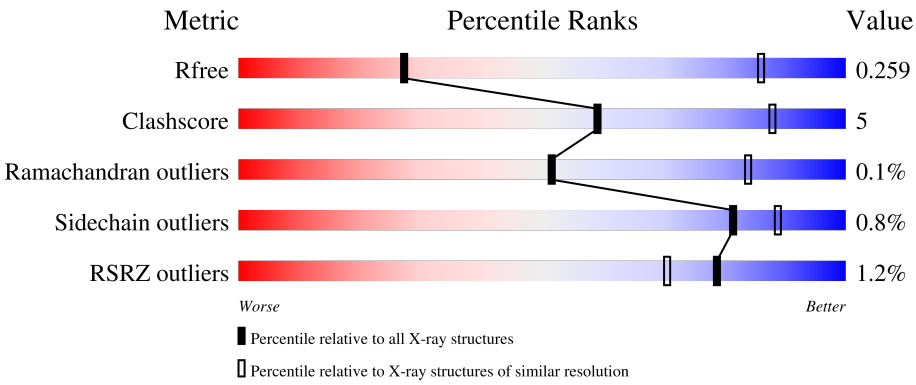
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 3.89 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	1002 (4.14-3.66)
Clashscore	141614	1004 (4.12-3.68)
Ramachandran outliers	138981	1021 (4.14-3.66)
Sidechain outliers	138945	1014 (4.14-3.66)
RSRZ outliers	127900	1275 (4.20-3.60)

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	305	83% 6% 10%
1	B	305	% 81% 9% 10%
1	C	305	% 84% 7% 9%
1	D	305	% 62% 5% 33%
1	E	305	% 85% • 10%

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Mol	Chain	Length	Quality of chain
1	F	305	%, 81%, 8%, 11%
1	G	305	85%, 7%, 8%
1	H	305	3%, 61%, 34%
2	I	26	54%, 46%
2	K	26	62%, 38%
3	J	26	50%, 50%
3	L	26	35%, 65%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 17492 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 Light-dependent transcriptional regulator CarH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	273	1895	1220	340	332	3	0	0	0
			Total	C	N	O	S			
1	B	276	1951	1257	344	347	3	0	0	0
			Total	C	N	O	S			
1	C	279	1982	1271	361	347	3	0	0	0
			Total	C	N	O	S			
1	D	205	1465	944	259	260	2	0	0	0
			Total	C	N	O	S			
1	E	273	1909	1221	346	340	2	0	0	0
			Total	C	N	O	S			
1	F	270	1880	1206	338	333	3	0	0	0
			Total	C	N	O	S			
1	G	280	2000	1280	364	353	3	0	0	0
			Total	C	N	O	S			
1	H	201	1418	908	254	254	2	0	0	0

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q746J7
A	-18	GLY	-	expression tag	UNP Q746J7
A	-17	SER	-	expression tag	UNP Q746J7
A	-16	SER	-	expression tag	UNP Q746J7
A	-15	HIS	-	expression tag	UNP Q746J7
A	-14	HIS	-	expression tag	UNP Q746J7
A	-13	HIS	-	expression tag	UNP Q746J7
A	-12	HIS	-	expression tag	UNP Q746J7
A	-11	HIS	-	expression tag	UNP Q746J7
A	-10	HIS	-	expression tag	UNP Q746J7
A	-9	SER	-	expression tag	UNP Q746J7
A	-8	SER	-	expression tag	UNP Q746J7
A	-7	GLY	-	expression tag	UNP Q746J7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	LEU	-	expression tag	UNP Q746J7
A	-5	VAL	-	expression tag	UNP Q746J7
A	-4	PRO	-	expression tag	UNP Q746J7
A	-3	ARG	-	expression tag	UNP Q746J7
A	-2	GLY	-	expression tag	UNP Q746J7
A	-1	SER	-	expression tag	UNP Q746J7
A	0	HIS	-	expression tag	UNP Q746J7
B	-19	MET	-	initiating methionine	UNP Q746J7
B	-18	GLY	-	expression tag	UNP Q746J7
B	-17	SER	-	expression tag	UNP Q746J7
B	-16	SER	-	expression tag	UNP Q746J7
B	-15	HIS	-	expression tag	UNP Q746J7
B	-14	HIS	-	expression tag	UNP Q746J7
B	-13	HIS	-	expression tag	UNP Q746J7
B	-12	HIS	-	expression tag	UNP Q746J7
B	-11	HIS	-	expression tag	UNP Q746J7
B	-10	HIS	-	expression tag	UNP Q746J7
B	-9	SER	-	expression tag	UNP Q746J7
B	-8	SER	-	expression tag	UNP Q746J7
B	-7	GLY	-	expression tag	UNP Q746J7
B	-6	LEU	-	expression tag	UNP Q746J7
B	-5	VAL	-	expression tag	UNP Q746J7
B	-4	PRO	-	expression tag	UNP Q746J7
B	-3	ARG	-	expression tag	UNP Q746J7
B	-2	GLY	-	expression tag	UNP Q746J7
B	-1	SER	-	expression tag	UNP Q746J7
B	0	HIS	-	expression tag	UNP Q746J7
C	-19	MET	-	initiating methionine	UNP Q746J7
C	-18	GLY	-	expression tag	UNP Q746J7
C	-17	SER	-	expression tag	UNP Q746J7
C	-16	SER	-	expression tag	UNP Q746J7
C	-15	HIS	-	expression tag	UNP Q746J7
C	-14	HIS	-	expression tag	UNP Q746J7
C	-13	HIS	-	expression tag	UNP Q746J7
C	-12	HIS	-	expression tag	UNP Q746J7
C	-11	HIS	-	expression tag	UNP Q746J7
C	-10	HIS	-	expression tag	UNP Q746J7
C	-9	SER	-	expression tag	UNP Q746J7
C	-8	SER	-	expression tag	UNP Q746J7
C	-7	GLY	-	expression tag	UNP Q746J7
C	-6	LEU	-	expression tag	UNP Q746J7
C	-5	VAL	-	expression tag	UNP Q746J7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	PRO	-	expression tag	UNP Q746J7
C	-3	ARG	-	expression tag	UNP Q746J7
C	-2	GLY	-	expression tag	UNP Q746J7
C	-1	SER	-	expression tag	UNP Q746J7
C	0	HIS	-	expression tag	UNP Q746J7
D	-19	MET	-	initiating methionine	UNP Q746J7
D	-18	GLY	-	expression tag	UNP Q746J7
D	-17	SER	-	expression tag	UNP Q746J7
D	-16	SER	-	expression tag	UNP Q746J7
D	-15	HIS	-	expression tag	UNP Q746J7
D	-14	HIS	-	expression tag	UNP Q746J7
D	-13	HIS	-	expression tag	UNP Q746J7
D	-12	HIS	-	expression tag	UNP Q746J7
D	-11	HIS	-	expression tag	UNP Q746J7
D	-10	HIS	-	expression tag	UNP Q746J7
D	-9	SER	-	expression tag	UNP Q746J7
D	-8	SER	-	expression tag	UNP Q746J7
D	-7	GLY	-	expression tag	UNP Q746J7
D	-6	LEU	-	expression tag	UNP Q746J7
D	-5	VAL	-	expression tag	UNP Q746J7
D	-4	PRO	-	expression tag	UNP Q746J7
D	-3	ARG	-	expression tag	UNP Q746J7
D	-2	GLY	-	expression tag	UNP Q746J7
D	-1	SER	-	expression tag	UNP Q746J7
D	0	HIS	-	expression tag	UNP Q746J7
E	-19	MET	-	initiating methionine	UNP Q746J7
E	-18	GLY	-	expression tag	UNP Q746J7
E	-17	SER	-	expression tag	UNP Q746J7
E	-16	SER	-	expression tag	UNP Q746J7
E	-15	HIS	-	expression tag	UNP Q746J7
E	-14	HIS	-	expression tag	UNP Q746J7
E	-13	HIS	-	expression tag	UNP Q746J7
E	-12	HIS	-	expression tag	UNP Q746J7
E	-11	HIS	-	expression tag	UNP Q746J7
E	-10	HIS	-	expression tag	UNP Q746J7
E	-9	SER	-	expression tag	UNP Q746J7
E	-8	SER	-	expression tag	UNP Q746J7
E	-7	GLY	-	expression tag	UNP Q746J7
E	-6	LEU	-	expression tag	UNP Q746J7
E	-5	VAL	-	expression tag	UNP Q746J7
E	-4	PRO	-	expression tag	UNP Q746J7
E	-3	ARG	-	expression tag	UNP Q746J7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	expression tag	UNP Q746J7
E	-1	SER	-	expression tag	UNP Q746J7
E	0	HIS	-	expression tag	UNP Q746J7
F	-19	MET	-	initiating methionine	UNP Q746J7
F	-18	GLY	-	expression tag	UNP Q746J7
F	-17	SER	-	expression tag	UNP Q746J7
F	-16	SER	-	expression tag	UNP Q746J7
F	-15	HIS	-	expression tag	UNP Q746J7
F	-14	HIS	-	expression tag	UNP Q746J7
F	-13	HIS	-	expression tag	UNP Q746J7
F	-12	HIS	-	expression tag	UNP Q746J7
F	-11	HIS	-	expression tag	UNP Q746J7
F	-10	HIS	-	expression tag	UNP Q746J7
F	-9	SER	-	expression tag	UNP Q746J7
F	-8	SER	-	expression tag	UNP Q746J7
F	-7	GLY	-	expression tag	UNP Q746J7
F	-6	LEU	-	expression tag	UNP Q746J7
F	-5	VAL	-	expression tag	UNP Q746J7
F	-4	PRO	-	expression tag	UNP Q746J7
F	-3	ARG	-	expression tag	UNP Q746J7
F	-2	GLY	-	expression tag	UNP Q746J7
F	-1	SER	-	expression tag	UNP Q746J7
F	0	HIS	-	expression tag	UNP Q746J7
G	-19	MET	-	initiating methionine	UNP Q746J7
G	-18	GLY	-	expression tag	UNP Q746J7
G	-17	SER	-	expression tag	UNP Q746J7
G	-16	SER	-	expression tag	UNP Q746J7
G	-15	HIS	-	expression tag	UNP Q746J7
G	-14	HIS	-	expression tag	UNP Q746J7
G	-13	HIS	-	expression tag	UNP Q746J7
G	-12	HIS	-	expression tag	UNP Q746J7
G	-11	HIS	-	expression tag	UNP Q746J7
G	-10	HIS	-	expression tag	UNP Q746J7
G	-9	SER	-	expression tag	UNP Q746J7
G	-8	SER	-	expression tag	UNP Q746J7
G	-7	GLY	-	expression tag	UNP Q746J7
G	-6	LEU	-	expression tag	UNP Q746J7
G	-5	VAL	-	expression tag	UNP Q746J7
G	-4	PRO	-	expression tag	UNP Q746J7
G	-3	ARG	-	expression tag	UNP Q746J7
G	-2	GLY	-	expression tag	UNP Q746J7
G	-1	SER	-	expression tag	UNP Q746J7

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Chain	Residue	Modelled	Actual	Comment	Reference
G	0	HIS	-	expression tag	UNP Q746J7
H	-19	MET	-	initiating methionine	UNP Q746J7
H	-18	GLY	-	expression tag	UNP Q746J7
H	-17	SER	-	expression tag	UNP Q746J7
H	-16	SER	-	expression tag	UNP Q746J7
H	-15	HIS	-	expression tag	UNP Q746J7
H	-14	HIS	-	expression tag	UNP Q746J7
H	-13	HIS	-	expression tag	UNP Q746J7
H	-12	HIS	-	expression tag	UNP Q746J7
H	-11	HIS	-	expression tag	UNP Q746J7
H	-10	HIS	-	expression tag	UNP Q746J7
H	-9	SER	-	expression tag	UNP Q746J7
H	-8	SER	-	expression tag	UNP Q746J7
H	-7	GLY	-	expression tag	UNP Q746J7
H	-6	LEU	-	expression tag	UNP Q746J7
H	-5	VAL	-	expression tag	UNP Q746J7
H	-4	PRO	-	expression tag	UNP Q746J7
H	-3	ARG	-	expression tag	UNP Q746J7
H	-2	GLY	-	expression tag	UNP Q746J7
H	-1	SER	-	expression tag	UNP Q746J7
H	0	HIS	-	expression tag	UNP Q746J7

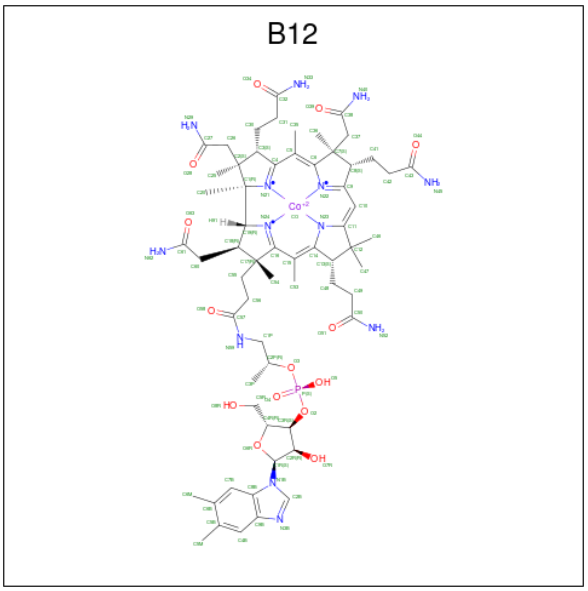
- Molecule 2 is a DNA chain called 26-mer DNA segment containing the CarH operator sequence (antisense strand).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	I	26	530	257	88	160	25	0	0	0
2	K	26	530	257	88	160	25	0	0	0

- Molecule 3 is a DNA chain called 26-mer DNA segment containing the CarH operator sequence (sense strand).

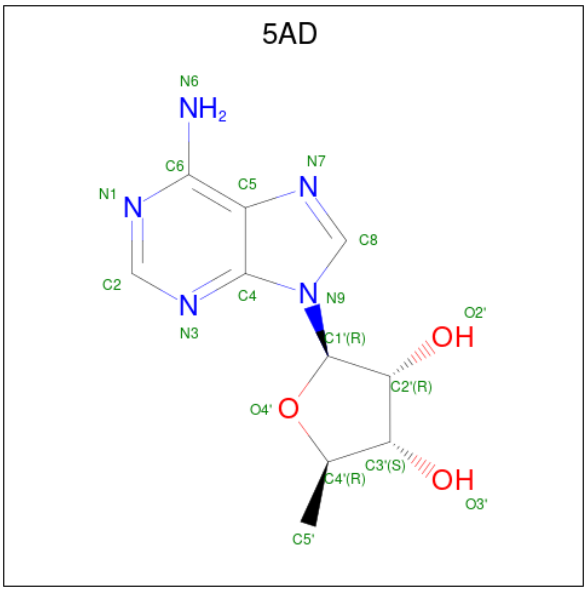
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	J	26	530	255	102	148	25	0	0	0
3	L	26	530	255	102	148	25	0	0	0

- Molecule 4 is COBALAMIN (three-letter code: B12) (formula: $C_{62}H_{89}CoN_{13}O_{14}P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Co	N	O	P		
4	A	1	91	62	1	13	14	1	0	0
4	B	1	91	62	1	13	14	1	0	0
4	C	1	91	62	1	13	14	1	0	0
4	D	1	91	62	1	13	14	1	0	0
4	E	1	91	62	1	13	14	1	0	0
4	F	1	91	62	1	13	14	1	0	0
4	G	1	91	62	1	13	14	1	0	0
4	H	1	91	62	1	13	14	1	0	0

- Molecule 5 is 5'-DEOXYADENOSINE (three-letter code: 5AD) (formula: $C_{10}H_{13}N_5O_3$).



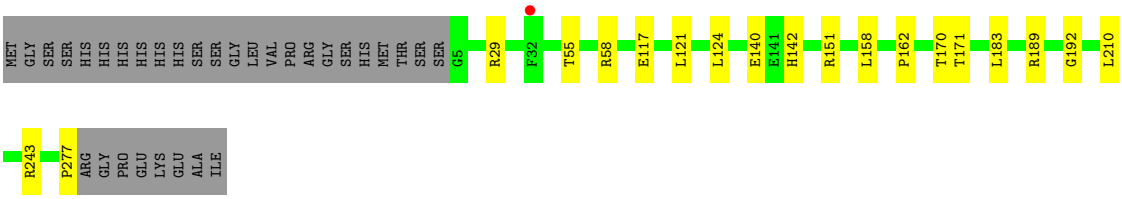
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	18	10	5	3	0	0
5	B	1	18	10	5	3	0	0
5	C	1	18	10	5	3	0	0
5	D	1	18	10	5	3	0	0
5	E	1	18	10	5	3	0	0
5	F	1	18	10	5	3	0	0
5	G	1	18	10	5	3	0	0
5	H	1	18	10	5	3	0	0

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.

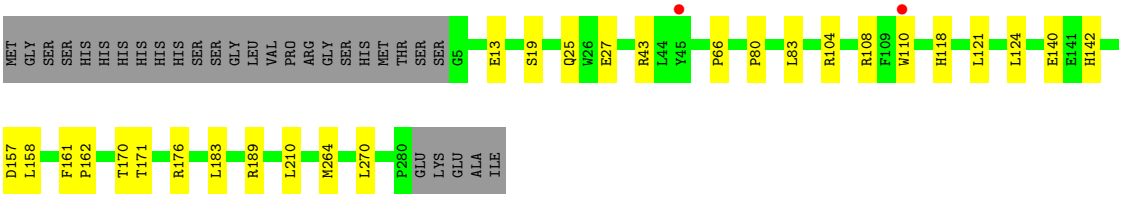
• Molecule 1: Light-dependent transcriptional regulator CarH

Chain A:



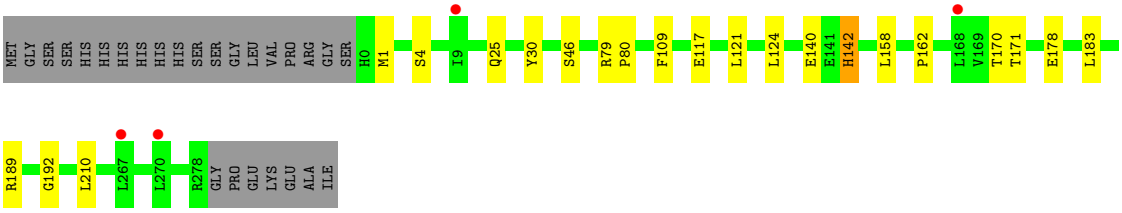
• Molecule 1: Light-dependent transcriptional regulator CarH

Chain B:



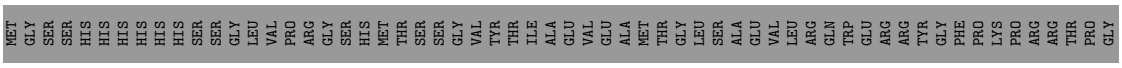
• Molecule 1: Light-dependent transcriptional regulator CarH

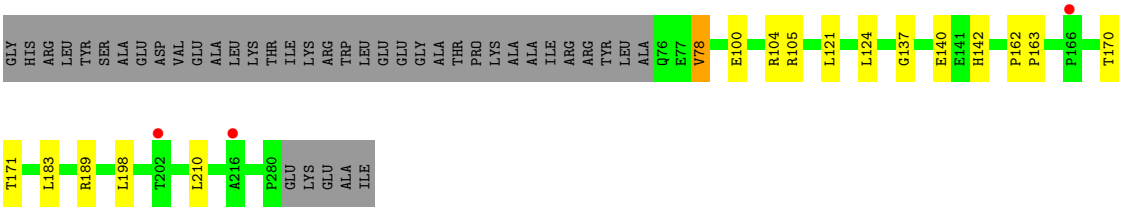
Chain C:



• Molecule 1: Light-dependent transcriptional regulator CarH

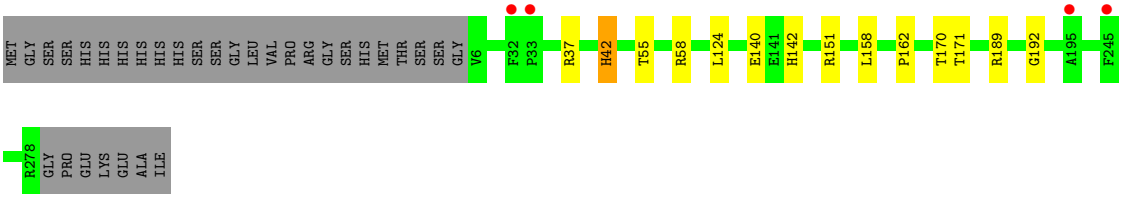
Chain D:





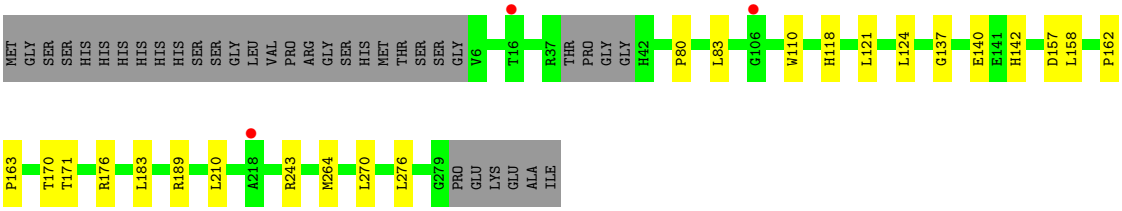
• Molecule 1: Light-dependent transcriptional regulator CarH

Chain E:



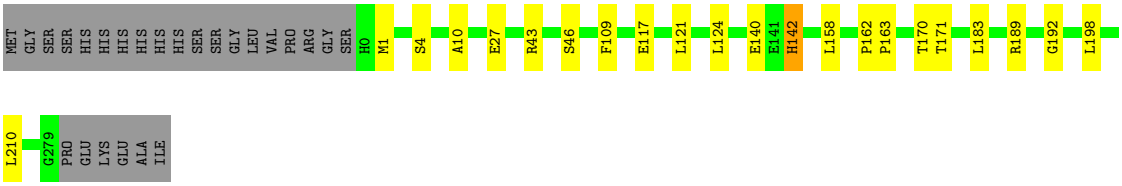
• Molecule 1: Light-dependent transcriptional regulator CarH

Chain F:



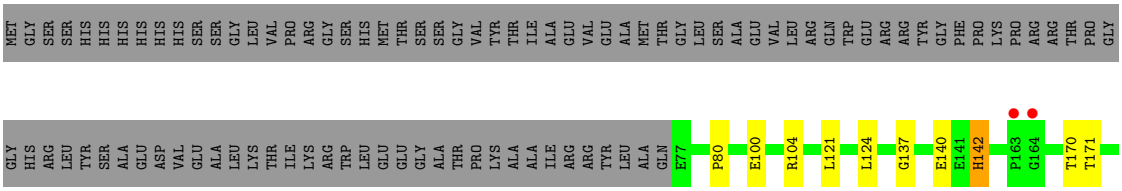
• Molecule 1: Light-dependent transcriptional regulator CarH

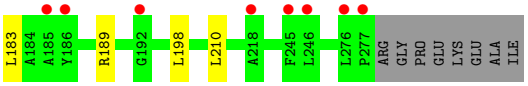
Chain G:



• Molecule 1: Light-dependent transcriptional regulator CarH

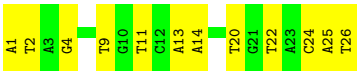
Chain H:





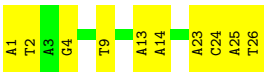
• Molecule 2: 26-mer DNA segment containing the CarH operator sequence (antisense strand)

Chain I:



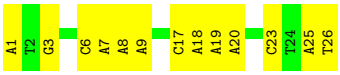
• Molecule 2: 26-mer DNA segment containing the CarH operator sequence (antisense strand)

Chain K:



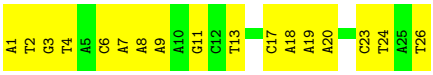
• Molecule 3: 26-mer DNA segment containing the CarH operator sequence (sense strand)

Chain J:



• Molecule 3: 26-mer DNA segment containing the CarH operator sequence (sense strand)

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	177.94Å 141.82Å 162.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.64 – 3.89 91.64 – 3.89	Depositor EDS
% Data completeness (in resolution range)	99.6 (91.64-3.89) 99.9 (91.64-3.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.17 (at 3.89Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.250 , 0.257 0.253 , 0.259	Depositor DCC
R_{free} test set	1869 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å^2)	161.0	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 136.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	17492	wwPDB-VP
Average B, all atoms (Å^2)	172.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.78 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0901e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 5AD, B12

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	0.22	0/1944	0.55	3/2669 (0.1%)
1	B	0.24	0/2002	0.52	2/2748 (0.1%)
1	C	0.21	0/2031	0.45	2/2780 (0.1%)
1	D	0.25	0/1502	0.58	2/2058 (0.1%)
1	E	0.21	0/1957	0.54	3/2686 (0.1%)
1	F	0.27	0/1923	0.53	2/2635 (0.1%)
1	G	0.21	0/2050	0.45	2/2806 (0.1%)
1	H	0.25	0/1452	0.58	2/1989 (0.1%)
2	I	0.49	0/592	1.01	0/913
2	K	0.48	0/592	1.01	0/913
3	J	0.47	0/596	0.87	0/917
3	L	0.47	0/596	0.87	0/917
All	All	0.28	0/17237	0.61	18/24031 (0.1%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	189	ARG	NE-CZ-NH2	-12.55	114.03	120.30
1	E	189	ARG	NE-CZ-NH2	-12.50	114.05	120.30
1	F	189	ARG	NE-CZ-NH1	-11.55	114.53	120.30
1	E	189	ARG	NE-CZ-NH1	11.06	125.83	120.30
1	A	189	ARG	NE-CZ-NH1	11.04	125.82	120.30
1	H	189	ARG	NE-CZ-NH1	-10.94	114.83	120.30
1	D	189	ARG	NE-CZ-NH1	-10.90	114.85	120.30
1	B	189	ARG	NE-CZ-NH1	-10.75	114.93	120.30
1	D	189	ARG	NE-CZ-NH2	9.99	125.29	120.30
1	H	189	ARG	NE-CZ-NH2	9.97	125.29	120.30
1	B	189	ARG	NE-CZ-NH2	9.88	125.24	120.30
1	F	189	ARG	NE-CZ-NH2	9.14	124.87	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	189	ARG	NE-CZ-NH2	-7.55	116.53	120.30
1	G	189	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	G	189	ARG	NE-CZ-NH1	6.79	123.70	120.30
1	C	189	ARG	NE-CZ-NH1	6.71	123.66	120.30
1	E	189	ARG	CD-NE-CZ	6.63	132.88	123.60
1	A	189	ARG	CD-NE-CZ	6.59	132.82	123.60

There are no chirality outliers.

There are no planarity outliers.

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	1895	0	1767	13	0
1	B	1951	0	1842	18	0
1	C	1982	0	1886	17	0
1	D	1465	0	1425	11	0
1	E	1909	0	1772	10	0
1	F	1880	0	1758	13	0
1	G	2000	0	1898	19	0
1	H	1418	0	1361	9	0
2	I	530	0	300	12	1
2	K	530	0	300	10	1
3	J	530	0	294	13	1
3	L	530	0	294	17	1
4	A	91	0	88	5	0
4	B	91	0	88	7	0
4	C	91	0	88	7	0
4	D	91	0	88	6	0
4	E	91	0	88	6	0
4	F	91	0	88	5	0
4	G	91	0	88	6	0
4	H	91	0	88	6	0
5	A	18	0	12	0	0
5	B	18	0	12	0	0
5	C	18	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	18	0	12	0	0
5	E	18	0	12	0	0
5	F	18	0	12	0	0
5	G	18	0	12	0	0
5	H	18	0	12	0	0
All	All	17492	0	15697	157	2

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 5.

All (157) 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:A:29:ARG:NH2	2:K:24:DC:OP2	2.17	0.77
2:I:4:DG:H1	3:J:23:DC:H42	1.36	0.74
1:E:158:LEU:HD13	1:G:158:LEU:HD13	1.77	0.65
1:B:25:GLN:NE2	2:I:22:DT:O4	2.28	0.63
1:A:158:LEU:HD13	1:C:158:LEU:HD13	1.80	0.63
1:F:243:ARG:NH1	1:F:276:LEU:O	2.32	0.62
2:K:4:DG:H1	3:L:23:DC:H42	1.48	0.60
1:B:66:PRO:HD2	2:I:20:DT:H5"	1.84	0.58
2:I:1:DA:O5'	2:K:26:DT:O2	2.22	0.58
1:E:140:GLU:HG3	1:F:210:LEU:HD13	1.86	0.57
1:F:83:LEU:HD12	1:F:110:TRP:CH2	2.39	0.56
3:J:26:DT:O2	3:L:1:DA:O5'	2.22	0.56
2:K:24:DC:H42	3:L:3:DG:H1	1.53	0.56
1:B:158:LEU:HD11	1:C:109:PHE:HB2	1.88	0.56
3:J:17:DC:H2"	3:J:18:DA:C8	2.41	0.56
1:G:43:ARG:NH2	3:L:13:DT:OP2	2.38	0.55
1:F:176:ARG:HG3	4:F:300:B12:C43	2.37	0.54
1:F:158:LEU:HD11	1:G:109:PHE:HB2	1.88	0.54
1:D:78:VAL:N	1:D:105:ARG:HH22	2.05	0.53
1:G:210:LEU:HD13	1:H:140:GLU:HG3	1.90	0.53
3:L:17:DC:H2"	3:L:18:DA:C8	2.43	0.53
1:E:151:ARG:NH1	1:F:157:ASP:OD2	2.39	0.52
3:J:6:DC:H2"	3:J:7:DA:C8	2.44	0.52
3:L:6:DC:H2"	3:L:7:DA:C8	2.44	0.52
1:G:117:GLU:HA	1:G:121:LEU:HD12	1.92	0.51
1:A:192:GLY:HA3	1:C:162:PRO:HB3	1.92	0.51
2:K:13:DA:H2"	2:K:14:DA:C8	2.46	0.51
1:H:121:LEU:HD21	1:H:183:LEU:HD11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:142:HIS:HB3	1:D:198:LEU:O	2.11	0.50
2:I:4:DG:H1	3:J:23:DC:N4	2.06	0.50
2:I:13:DA:H2"	2:I:14:DA:C8	2.46	0.50
1:A:117:GLU:HA	1:A:121:LEU:HD12	1.94	0.50
1:F:121:LEU:HD21	1:F:183:LEU:HD11	1.93	0.50
2:K:24:DC:H2"	2:K:25:DA:C8	2.47	0.50
1:B:121:LEU:HD21	1:B:183:LEU:HD11	1.93	0.49
1:C:117:GLU:HA	1:C:121:LEU:HD12	1.94	0.49
1:G:142:HIS:HB3	1:H:198:LEU:O	2.11	0.49
1:D:121:LEU:HD21	1:D:183:LEU:HD11	1.92	0.49
1:C:121:LEU:HD21	1:C:183:LEU:HD11	1.94	0.49
1:A:121:LEU:HD21	1:A:183:LEU:HD11	1.95	0.49
1:F:118:HIS:CE1	1:G:1:MET:HB3	2.47	0.49
2:I:24:DC:H2"	2:I:25:DA:C8	2.48	0.49
1:A:140:GLU:HG3	1:B:210:LEU:HD13	1.95	0.49
1:E:55:THR:HA	1:E:58:ARG:HD3	1.94	0.49
1:E:192:GLY:HA3	1:G:162:PRO:HB3	1.94	0.49
1:G:121:LEU:HD21	1:G:183:LEU:HD11	1.94	0.49
4:G:300:B12:H301	4:G:300:B12:H253	1.68	0.48
3:L:1:DA:C8	3:L:2:DT:H72	2.48	0.48
1:E:37:ARG:NH1	3:L:24:DT:OP1	2.46	0.48
1:B:66:PRO:HG2	2:I:20:DT:H3'	1.95	0.48
1:C:140:GLU:HG3	1:D:210:LEU:HD13	1.96	0.48
1:A:55:THR:HA	1:A:58:ARG:HD3	1.94	0.47
1:B:118:HIS:CE1	1:C:1:MET:HB3	2.49	0.47
4:B:300:B12:H262	4:B:300:B12:H91	1.75	0.47
1:C:4:SER:HA	1:C:46:SER:HB2	1.95	0.47
1:C:210:LEU:HD13	1:D:140:GLU:HG3	1.97	0.47
1:G:140:GLU:HG3	1:H:210:LEU:HD13	1.96	0.47
4:H:300:B12:H91	4:H:300:B12:H262	1.75	0.47
4:B:300:B12:H262	4:B:300:B12:H601	1.97	0.47
2:K:23:DA:N1	3:L:4:DT:O4	2.47	0.47
4:A:300:B12:H601	4:A:300:B12:H262	1.97	0.47
1:B:264:MET:HG3	1:B:270:LEU:HD13	1.97	0.47
4:C:300:B12:H262	4:C:300:B12:H91	1.75	0.47
4:C:300:B12:H262	4:C:300:B12:H601	1.97	0.47
4:E:300:B12:H601	4:E:300:B12:H262	1.97	0.47
4:G:300:B12:H601	4:G:300:B12:H262	1.97	0.47
4:A:300:B12:H362	4:A:300:B12:H351	1.97	0.47
1:F:264:MET:HG3	1:F:270:LEU:HD13	1.97	0.47
4:F:300:B12:H351	4:F:300:B12:H362	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:PRO:HB3	1:C:192:GLY:HA3	1.97	0.46
4:C:300:B12:H362	4:C:300:B12:H351	1.97	0.46
4:D:300:B12:H601	4:D:300:B12:H262	1.97	0.46
4:H:300:B12:H473	4:H:300:B12:H481	1.74	0.46
4:F:300:B12:H601	4:F:300:B12:H262	1.97	0.46
4:G:300:B12:H362	4:G:300:B12:H351	1.97	0.46
4:B:300:B12:H473	4:B:300:B12:H481	1.74	0.46
4:D:300:B12:H362	4:D:300:B12:H351	1.97	0.46
1:E:162:PRO:HB3	1:G:192:GLY:HA3	1.98	0.46
1:D:78:VAL:H	1:D:105:ARG:HH22	1.63	0.46
1:C:25:GLN:HG3	2:I:11:DT:H73	1.98	0.46
4:D:300:B12:H253	4:D:300:B12:H301	1.68	0.46
4:E:300:B12:H262	4:E:300:B12:H91	1.75	0.46
4:G:300:B12:H262	4:G:300:B12:H91	1.75	0.46
2:I:24:DC:H42	3:J:3:DG:H1	1.63	0.46
3:J:8:DA:H2"	3:J:9:DA:C8	2.51	0.46
4:E:300:B12:H362	4:E:300:B12:H351	1.97	0.45
1:D:137:GLY:N	1:D:140:GLU:OE1	2.31	0.45
4:H:300:B12:H262	4:H:300:B12:H601	1.97	0.45
2:K:1:DA:H1'	2:K:2:DT:C6	2.52	0.45
4:B:300:B12:H362	4:B:300:B12:H351	1.98	0.45
4:C:300:B12:H473	4:C:300:B12:H481	1.74	0.45
4:H:300:B12:H362	4:H:300:B12:H351	1.97	0.45
4:D:300:B12:H473	4:D:300:B12:H481	1.74	0.45
1:F:170:THR:OG1	1:F:171:THR:N	2.50	0.45
1:A:151:ARG:NH1	1:B:157:ASP:OD2	2.40	0.45
4:A:300:B12:H262	4:A:300:B12:H91	1.75	0.44
1:H:137:GLY:N	1:H:140:GLU:OE1	2.31	0.44
4:C:300:B12:H301	4:C:300:B12:H253	1.68	0.44
1:G:4:SER:HA	1:G:46:SER:HB2	1.98	0.44
3:L:8:DA:H2"	3:L:9:DA:H8	1.83	0.44
4:E:300:B12:H473	4:E:300:B12:H481	1.74	0.44
1:C:30:TYR:OH	2:I:9:DT:OP2	2.34	0.44
3:J:8:DA:H2"	3:J:9:DA:H8	1.81	0.44
1:B:170:THR:OG1	1:B:171:THR:N	2.50	0.43
1:C:170:THR:OG1	1:C:171:THR:N	2.52	0.43
1:D:100:GLU:O	1:D:104:ARG:HG2	2.18	0.43
1:H:170:THR:OG1	1:H:171:THR:N	2.50	0.43
2:K:9:DT:H3	3:L:18:DA:H61	1.66	0.43
1:G:198:LEU:O	1:H:142:HIS:HB3	2.17	0.43
3:J:19:DA:H2"	3:J:20:DA:C8	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:8:DA:H2"	3:L:9:DA:C8	2.53	0.43
1:A:210:LEU:HD13	1:B:140:GLU:HG3	2.00	0.43
1:B:13:GLU:HG3	1:B:19:SER:HA	1.99	0.43
1:E:170:THR:OG1	1:E:171:THR:N	2.51	0.43
4:A:300:B12:H473	4:A:300:B12:H481	1.74	0.43
1:B:27:GLU:OE1	1:B:43:ARG:NH2	2.52	0.43
1:G:10:ALA:HB2	3:L:11:DG:OP1	2.19	0.43
1:B:104:ARG:O	1:B:108:ARG:HG2	2.19	0.43
1:G:170:THR:OG1	1:G:171:THR:N	2.52	0.43
4:B:300:B12:H253	4:B:300:B12:H301	1.68	0.42
1:D:162:PRO:HA	1:D:163:PRO:HD3	1.87	0.42
1:D:170:THR:OG1	1:D:171:THR:N	2.50	0.42
2:K:4:DG:H1	3:L:23:DC:N4	2.17	0.42
3:L:7:DA:H2"	3:L:8:DA:C8	2.55	0.42
1:B:124:LEU:O	4:B:300:B12:H541	2.20	0.42
4:G:300:B12:H473	4:G:300:B12:H481	1.74	0.42
1:E:42:HIS:HA	3:L:23:DC:H5"	2.02	0.42
4:E:300:B12:H253	4:E:300:B12:H301	1.68	0.42
1:F:124:LEU:O	4:F:300:B12:H541	2.20	0.42
1:B:83:LEU:HD12	1:B:110:TRP:CH2	2.55	0.42
1:B:176:ARG:HG3	4:B:300:B12:C43	2.50	0.42
3:L:19:DA:H2"	3:L:20:DA:C8	2.54	0.42
1:G:27:GLU:OE1	1:G:43:ARG:NE	2.40	0.42
1:H:124:LEU:O	4:H:300:B12:H541	2.20	0.41
3:J:7:DA:H2"	3:J:8:DA:C8	2.55	0.41
1:E:124:LEU:O	4:E:300:B12:H541	2.21	0.41
1:G:162:PRO:HA	1:G:163:PRO:HD3	1.90	0.41
1:C:178:GLU:HG2	4:C:300:B12:H522	1.85	0.41
1:A:243:ARG:HH22	1:A:277:PRO:HG2	1.85	0.41
1:G:1:MET:SD	1:G:1:MET:N	2.94	0.41
1:A:170:THR:OG1	1:A:171:THR:N	2.51	0.41
1:F:137:GLY:N	1:F:140:GLU:OE1	2.32	0.41
1:F:162:PRO:HA	1:F:163:PRO:HD3	1.94	0.41
4:H:300:B12:H253	4:H:300:B12:H301	1.68	0.41
1:C:79:ARG:HA	1:C:80:PRO:HD3	1.96	0.41
3:J:18:DA:H2"	3:J:19:DA:H8	1.86	0.41
1:A:124:LEU:O	4:A:300:B12:H541	2.20	0.41
1:H:100:GLU:O	1:H:104:ARG:HG2	2.20	0.41
4:D:300:B12:H262	4:D:300:B12:H91	1.75	0.41
1:G:124:LEU:O	4:G:300:B12:H541	2.21	0.41
2:I:1:DA:H1'	2:I:2:DT:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:LEU:O	4:C:300:B12:H541	2.21	0.40
1:D:124:LEU:O	4:D:300:B12:H541	2.20	0.40
3:J:25:DA:H2"	3:J:26:DT:H71	2.02	0.40
1:B:161:PHE:HA	1:B:162:PRO:HD2	1.93	0.40
4:F:300:B12:H253	4:F:300:B12:H301	1.68	0.40
3:J:7:DA:H2"	3:J:8:DA:H8	1.87	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:26:DT:O2	2:K:1:DA:O5'[1_556]	2.19	0.01
3:J:1:DA:O5'	3:L:26:DT:O2[1_556]	2.19	0.01

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	271/305 (89%)	264 (97%)	7 (3%)	0	100	100
1	B	274/305 (90%)	265 (97%)	8 (3%)	1 (0%)	34	71
1	C	277/305 (91%)	269 (97%)	8 (3%)	0	100	100
1	D	203/305 (67%)	196 (97%)	7 (3%)	0	100	100
1	E	271/305 (89%)	264 (97%)	7 (3%)	0	100	100
1	F	266/305 (87%)	256 (96%)	9 (3%)	1 (0%)	34	71
1	G	278/305 (91%)	272 (98%)	6 (2%)	0	100	100
1	H	199/305 (65%)	193 (97%)	5 (2%)	1 (0%)	29	67
All	All	2039/2440 (84%)	1979 (97%)	57 (3%)	3 (0%)	51	84

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	80	PRO
1	F	80	PRO
1	H	80	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	A	155/234 (66%)	154 (99%)	1 (1%)	86	91
1	B	167/234 (71%)	166 (99%)	1 (1%)	86	91
1	C	168/234 (72%)	167 (99%)	1 (1%)	86	91
1	D	132/234 (56%)	130 (98%)	2 (2%)	65	80
1	E	158/234 (68%)	156 (99%)	2 (1%)	69	82
1	F	154/234 (66%)	153 (99%)	1 (1%)	86	91
1	G	171/234 (73%)	170 (99%)	1 (1%)	86	91
1	H	125/234 (53%)	124 (99%)	1 (1%)	81	89
All	All	1230/1872 (66%)	1220 (99%)	10 (1%)	81	89

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	142	HIS
1	B	142	HIS
1	C	142	HIS
1	D	78	VAL
1	D	142	HIS
1	E	42	HIS
1	E	142	HIS
1	F	142	HIS
1	G	142	HIS
1	H	142	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	GLN
1	B	153	GLN
1	C	153	GLN
1	D	153	GLN
1	E	153	GLN
1	F	153	GLN
1	G	153	GLN
1	H	153	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)

16 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	$\#\|Z\| > 2$
4	B12	C	300	1,5	90,101,101	0.80	3 (3%)	137,166,166	1.01	10 (7%)
5	5AD	C	301	4	17,20,20	0.63	0	15,30,30	0.87	1 (6%)
5	5AD	A	301	4	17,20,20	0.63	0	15,30,30	0.89	1 (6%)
5	5AD	E	301	4	17,20,20	0.64	0	15,30,30	0.88	1 (6%)
5	5AD	B	301	4	17,20,20	0.63	0	15,30,30	0.87	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	5AD	D	301	4	17,20,20	0.64	0	15,30,30	0.87	1 (6%)
4	B12	A	300	1,5	90,101,101	0.80	3 (3%)	137,166,166	1.01	10 (7%)
4	B12	E	300	1,5	90,101,101	0.80	3 (3%)	137,166,166	1.01	10 (7%)
5	5AD	G	301	4	17,20,20	0.65	0	15,30,30	0.88	1 (6%)
5	5AD	F	301	4	17,20,20	0.64	0	15,30,30	0.88	1 (6%)
5	5AD	H	301	4	17,20,20	0.64	0	15,30,30	0.87	1 (6%)
4	B12	H	300	1,5	90,101,101	0.80	3 (3%)	137,166,166	1.01	10 (7%)
4	B12	F	300	1,5	90,101,101	0.80	3 (3%)	137,166,166	1.01	10 (7%)
4	B12	D	300	1,5	90,101,101	0.80	3 (3%)	137,166,166	1.01	10 (7%)
4	B12	G	300	1,5	90,101,101	0.80	3 (3%)	137,166,166	1.01	10 (7%)
4	B12	B	300	1,5	90,101,101	0.80	3 (3%)	137,166,166	1.01	10 (7%)

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
4	B12	C	300	1,5	-	15/52/223/223	0/3/11/11
5	5AD	C	301	4	-	0/0/20/20	0/3/3/3
5	5AD	A	301	4	-	0/0/20/20	0/3/3/3
5	5AD	E	301	4	-	0/0/20/20	0/3/3/3
5	5AD	B	301	4	-	0/0/20/20	0/3/3/3
5	5AD	D	301	4	-	0/0/20/20	0/3/3/3
4	B12	A	300	1,5	-	15/52/223/223	0/3/11/11
4	B12	E	300	1,5	-	15/52/223/223	0/3/11/11
5	5AD	G	301	4	-	0/0/20/20	0/3/3/3
5	5AD	F	301	4	-	0/0/20/20	0/3/3/3
5	5AD	H	301	4	-	0/0/20/20	0/3/3/3
4	B12	H	300	1,5	-	15/52/223/223	0/3/11/11
4	B12	F	300	1,5	-	15/52/223/223	0/3/11/11
4	B12	D	300	1,5	-	15/52/223/223	0/3/11/11
4	B12	G	300	1,5	-	15/52/223/223	0/3/11/11
4	B12	B	300	1,5	-	15/52/223/223	0/3/11/11

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	300	B12	C14-N23	4.61	1.41	1.35
4	H	300	B12	C14-N23	4.60	1.41	1.35
4	G	300	B12	C14-N23	4.58	1.40	1.35
4	C	300	B12	C14-N23	4.56	1.40	1.35
4	B	300	B12	C14-N23	4.55	1.40	1.35
4	F	300	B12	C14-N23	4.55	1.40	1.35
4	A	300	B12	C14-N23	4.55	1.40	1.35
4	D	300	B12	C14-N23	4.55	1.40	1.35
4	E	300	B12	C16-C15	2.77	1.52	1.44
4	F	300	B12	C16-C15	2.76	1.52	1.44
4	G	300	B12	C16-C15	2.75	1.52	1.44
4	C	300	B12	C16-C15	2.75	1.52	1.44
4	D	300	B12	C16-C15	2.75	1.52	1.44
4	B	300	B12	C16-C15	2.74	1.52	1.44
4	A	300	B12	C16-C15	2.73	1.52	1.44
4	H	300	B12	C16-C15	2.71	1.52	1.44
4	A	300	B12	C1P-C2P	2.05	1.56	1.51
4	H	300	B12	C1P-C2P	2.05	1.56	1.51
4	G	300	B12	C1P-C2P	2.04	1.56	1.51
4	B	300	B12	C1P-C2P	2.04	1.56	1.51
4	D	300	B12	C1P-C2P	2.04	1.56	1.51
4	E	300	B12	C1P-C2P	2.04	1.56	1.51
4	C	300	B12	C1P-C2P	2.03	1.56	1.51
4	F	300	B12	C1P-C2P	2.02	1.56	1.51

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	300	B12	C55-C17-C18	-3.47	104.45	111.15
4	A	300	B12	C55-C17-C18	-3.46	104.46	111.15
4	H	300	B12	C55-C17-C18	-3.46	104.47	111.15
4	E	300	B12	C55-C17-C18	-3.45	104.49	111.15
4	G	300	B12	C55-C17-C18	-3.44	104.50	111.15
4	C	300	B12	C55-C17-C18	-3.43	104.52	111.15
4	F	300	B12	C55-C17-C18	-3.42	104.53	111.15
4	D	300	B12	C55-C17-C18	-3.42	104.53	111.15
4	H	300	B12	C30-C3-C2	-3.18	112.36	119.09
4	B	300	B12	C30-C3-C2	-3.16	112.40	119.09
4	F	300	B12	C30-C3-C2	-3.16	112.41	119.09
4	C	300	B12	C30-C3-C2	-3.16	112.41	119.09
4	D	300	B12	C30-C3-C2	-3.15	112.42	119.09
4	A	300	B12	C30-C3-C2	-3.15	112.43	119.09
4	E	300	B12	C30-C3-C2	-3.14	112.44	119.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	300	B12	C30-C3-C2	-3.13	112.46	119.09
4	B	300	B12	C10-C9-N22	2.72	128.85	125.73
4	H	300	B12	C10-C9-N22	2.70	128.83	125.73
4	E	300	B12	C10-C9-N22	2.69	128.82	125.73
4	A	300	B12	C10-C9-N22	2.67	128.79	125.73
4	D	300	B12	C10-C9-N22	2.66	128.78	125.73
4	F	300	B12	C10-C9-N22	2.66	128.78	125.73
4	G	300	B12	C10-C9-N22	2.65	128.77	125.73
4	C	300	B12	C10-C9-N22	2.65	128.77	125.73
4	E	300	B12	C56-C55-C17	-2.38	110.92	115.52
4	G	300	B12	C56-C55-C17	-2.38	110.93	115.52
4	C	300	B12	C56-C55-C17	-2.38	110.94	115.52
4	B	300	B12	C56-C55-C17	-2.36	110.96	115.52
4	A	300	B12	C56-C55-C17	-2.36	110.97	115.52
4	F	300	B12	C56-C55-C17	-2.34	111.00	115.52
4	H	300	B12	C56-C55-C17	-2.34	111.00	115.52
4	D	300	B12	C56-C55-C17	-2.33	111.03	115.52
5	A	301	5AD	C5-C6-N6	2.31	123.87	120.35
5	G	301	5AD	C5-C6-N6	2.29	123.83	120.35
5	E	301	5AD	C5-C6-N6	2.28	123.82	120.35
5	F	301	5AD	C5-C6-N6	2.28	123.82	120.35
5	H	301	5AD	C5-C6-N6	2.28	123.82	120.35
5	B	301	5AD	C5-C6-N6	2.26	123.78	120.35
5	C	301	5AD	C5-C6-N6	2.25	123.78	120.35
5	D	301	5AD	C5-C6-N6	2.25	123.77	120.35
4	G	300	B12	C35-C5-C6	2.19	125.92	122.43
4	D	300	B12	P-O2-C3R	2.19	127.37	119.41
4	E	300	B12	P-O2-C3R	2.18	127.36	119.41
4	H	300	B12	P-O2-C3R	2.18	127.34	119.41
4	H	300	B12	C35-C5-C4	-2.18	112.35	116.79
4	G	300	B12	P-O2-C3R	2.18	127.33	119.41
4	F	300	B12	C35-C5-C6	2.18	125.90	122.43
4	A	300	B12	P-O2-C3R	2.17	127.32	119.41
4	C	300	B12	P-O2-C3R	2.17	127.32	119.41
4	A	300	B12	C35-C5-C6	2.17	125.89	122.43
4	A	300	B12	C1-C19-N24	2.17	108.68	106.24
4	A	300	B12	C35-C5-C4	-2.17	112.37	116.79
4	E	300	B12	C35-C5-C4	-2.17	112.37	116.79
4	G	300	B12	C1-C19-N24	2.17	108.68	106.24
4	D	300	B12	C35-C5-C6	2.17	125.88	122.43
4	G	300	B12	C35-C5-C4	-2.16	112.38	116.79
4	F	300	B12	C35-C5-C4	-2.16	112.38	116.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	300	B12	C35-C5-C4	-2.16	112.39	116.79
4	B	300	B12	C35-C5-C4	-2.16	112.39	116.79
4	H	300	B12	C35-C5-C6	2.16	125.87	122.43
4	H	300	B12	C1-C19-N24	2.16	108.67	106.24
4	B	300	B12	P-O2-C3R	2.16	127.26	119.41
4	B	300	B12	C35-C5-C6	2.15	125.86	122.43
4	C	300	B12	C35-C5-C6	2.15	125.86	122.43
4	E	300	B12	C35-C5-C6	2.15	125.86	122.43
4	D	300	B12	C35-C5-C4	-2.15	112.41	116.79
4	F	300	B12	P-O2-C3R	2.15	127.22	119.41
4	F	300	B12	C1-C19-N24	2.14	108.65	106.24
4	E	300	B12	C1-C19-N24	2.13	108.64	106.24
4	C	300	B12	C1-C19-N24	2.12	108.62	106.24
4	B	300	B12	C1-C19-N24	2.11	108.62	106.24
4	D	300	B12	C1-C19-N24	2.11	108.62	106.24
4	H	300	B12	C2-C1-N21	2.11	104.71	101.77
4	B	300	B12	C2-C1-N21	2.09	104.69	101.77
4	G	300	B12	C2-C1-N21	2.09	104.68	101.77
4	F	300	B12	C2-C1-N21	2.08	104.67	101.77
4	A	300	B12	C2-C1-N21	2.08	104.67	101.77
4	G	300	B12	C15-C16-N24	-2.08	119.43	122.42
4	C	300	B12	C2-C1-N21	2.07	104.66	101.77
4	F	300	B12	C15-C16-N24	-2.07	119.44	122.42
4	E	300	B12	C15-C16-N24	-2.06	119.45	122.42
4	E	300	B12	C2-C1-N21	2.06	104.64	101.77
4	A	300	B12	C15-C16-N24	-2.06	119.45	122.42
4	D	300	B12	C15-C16-N24	-2.05	119.46	122.42
4	D	300	B12	C2-C1-N21	2.05	104.62	101.77
4	B	300	B12	C15-C16-N24	-2.05	119.47	122.42
4	H	300	B12	C15-C16-N24	-2.04	119.48	122.42
4	C	300	B12	C15-C16-N24	-2.04	119.49	122.42

There are no chirality outliers.

All (120) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	300	B12	C2-C3-C30-C31
4	A	300	B12	N59-C1P-C2P-O3
4	A	300	B12	C1P-C2P-O3-P
4	B	300	B12	C2-C3-C30-C31
4	B	300	B12	N59-C1P-C2P-C3P
4	B	300	B12	N59-C1P-C2P-O3

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Mol	Chain	Res	Type	Atoms
4	B	300	B12	C1P-C2P-O3-P
4	C	300	B12	C2-C3-C30-C31
4	C	300	B12	N59-C1P-C2P-O3
4	C	300	B12	C1P-C2P-O3-P
4	D	300	B12	C2-C3-C30-C31
4	D	300	B12	N59-C1P-C2P-O3
4	D	300	B12	C1P-C2P-O3-P
4	E	300	B12	C2-C3-C30-C31
4	E	300	B12	N59-C1P-C2P-O3
4	E	300	B12	C1P-C2P-O3-P
4	F	300	B12	C2-C3-C30-C31
4	F	300	B12	N59-C1P-C2P-C3P
4	F	300	B12	N59-C1P-C2P-O3
4	G	300	B12	C2-C3-C30-C31
4	G	300	B12	N59-C1P-C2P-O3
4	G	300	B12	C1P-C2P-O3-P
4	H	300	B12	C2-C3-C30-C31
4	H	300	B12	N59-C1P-C2P-C3P
4	H	300	B12	N59-C1P-C2P-O3
4	H	300	B12	C1P-C2P-O3-P
4	A	300	B12	C12-C13-C48-C49
4	B	300	B12	C12-C13-C48-C49
4	C	300	B12	C12-C13-C48-C49
4	D	300	B12	C12-C13-C48-C49
4	E	300	B12	C12-C13-C48-C49
4	F	300	B12	C12-C13-C48-C49
4	G	300	B12	C12-C13-C48-C49
4	H	300	B12	C12-C13-C48-C49
4	A	300	B12	C4-C3-C30-C31
4	B	300	B12	C4-C3-C30-C31
4	C	300	B12	C4-C3-C30-C31
4	D	300	B12	C4-C3-C30-C31
4	E	300	B12	C4-C3-C30-C31
4	F	300	B12	C4-C3-C30-C31
4	G	300	B12	C4-C3-C30-C31
4	H	300	B12	C4-C3-C30-C31
4	A	300	B12	C14-C13-C48-C49
4	B	300	B12	C14-C13-C48-C49
4	C	300	B12	C14-C13-C48-C49
4	D	300	B12	C14-C13-C48-C49
4	E	300	B12	C14-C13-C48-C49
4	F	300	B12	C14-C13-C48-C49

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Mol	Chain	Res	Type	Atoms
4	G	300	B12	C14-C13-C48-C49
4	H	300	B12	C14-C13-C48-C49
4	A	300	B12	N59-C1P-C2P-C3P
4	C	300	B12	N59-C1P-C2P-C3P
4	D	300	B12	N59-C1P-C2P-C3P
4	E	300	B12	N59-C1P-C2P-C3P
4	G	300	B12	N59-C1P-C2P-C3P
4	C	300	B12	C3P-C2P-O3-P
4	D	300	B12	C3P-C2P-O3-P
4	F	300	B12	C1P-C2P-O3-P
4	H	300	B12	C3P-C2P-O3-P
4	A	300	B12	C3R-O2-P-O3
4	B	300	B12	C3R-O2-P-O3
4	C	300	B12	C3R-O2-P-O3
4	D	300	B12	C3R-O2-P-O3
4	E	300	B12	C3R-O2-P-O3
4	F	300	B12	C3R-O2-P-O3
4	G	300	B12	C3R-O2-P-O3
4	H	300	B12	C3R-O2-P-O3
4	A	300	B12	C55-C56-C57-O58
4	B	300	B12	C55-C56-C57-O58
4	C	300	B12	C55-C56-C57-O58
4	D	300	B12	C55-C56-C57-O58
4	E	300	B12	C55-C56-C57-O58
4	F	300	B12	C55-C56-C57-O58
4	H	300	B12	C55-C56-C57-O58
4	G	300	B12	C55-C56-C57-O58
4	A	300	B12	C55-C56-C57-N59
4	B	300	B12	C55-C56-C57-N59
4	C	300	B12	C55-C56-C57-N59
4	D	300	B12	C55-C56-C57-N59
4	E	300	B12	C55-C56-C57-N59
4	F	300	B12	C55-C56-C57-N59
4	G	300	B12	C55-C56-C57-N59
4	H	300	B12	C55-C56-C57-N59
4	A	300	B12	C3P-C2P-O3-P
4	B	300	B12	C3P-C2P-O3-P
4	E	300	B12	C3P-C2P-O3-P
4	F	300	B12	C3P-C2P-O3-P
4	G	300	B12	C3P-C2P-O3-P
4	A	300	B12	C30-C31-C32-O34
4	B	300	B12	C30-C31-C32-O34

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Mol	Chain	Res	Type	Atoms
4	C	300	B12	C30-C31-C32-O34
4	D	300	B12	C30-C31-C32-O34
4	E	300	B12	C30-C31-C32-O34
4	F	300	B12	C30-C31-C32-O34
4	G	300	B12	C30-C31-C32-O34
4	H	300	B12	C30-C31-C32-O34
4	B	300	B12	C30-C31-C32-N33
4	C	300	B12	C30-C31-C32-N33
4	D	300	B12	C30-C31-C32-N33
4	F	300	B12	C30-C31-C32-N33
4	H	300	B12	C30-C31-C32-N33
4	A	300	B12	C30-C31-C32-N33
4	E	300	B12	C30-C31-C32-N33
4	G	300	B12	C30-C31-C32-N33
4	A	300	B12	C42-C41-C8-C9
4	B	300	B12	C42-C41-C8-C9
4	C	300	B12	C42-C41-C8-C9
4	D	300	B12	C42-C41-C8-C9
4	E	300	B12	C42-C41-C8-C9
4	F	300	B12	C42-C41-C8-C9
4	H	300	B12	C42-C41-C8-C9
4	G	300	B12	C42-C41-C8-C9
4	A	300	B12	C3R-O2-P-O5
4	B	300	B12	C3R-O2-P-O5
4	C	300	B12	C3R-O2-P-O5
4	D	300	B12	C3R-O2-P-O5
4	E	300	B12	C3R-O2-P-O5
4	F	300	B12	C3R-O2-P-O5
4	G	300	B12	C3R-O2-P-O5
4	H	300	B12	C3R-O2-P-O5

There are no ring outliers.

8 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	300	B12	7	0
4	A	300	B12	5	0
4	E	300	B12	6	0
4	H	300	B12	6	0
4	F	300	B12	5	0
4	D	300	B12	6	0
4	G	300	B12	6	0

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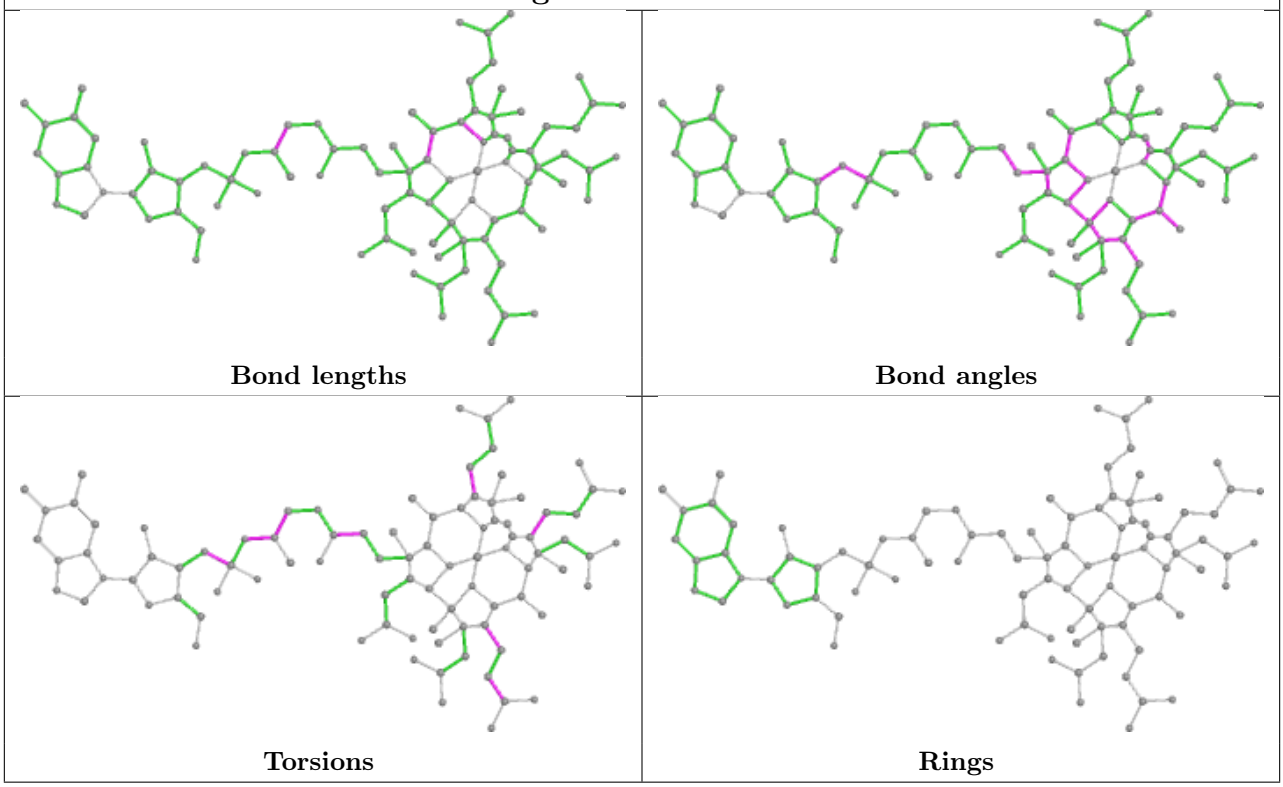
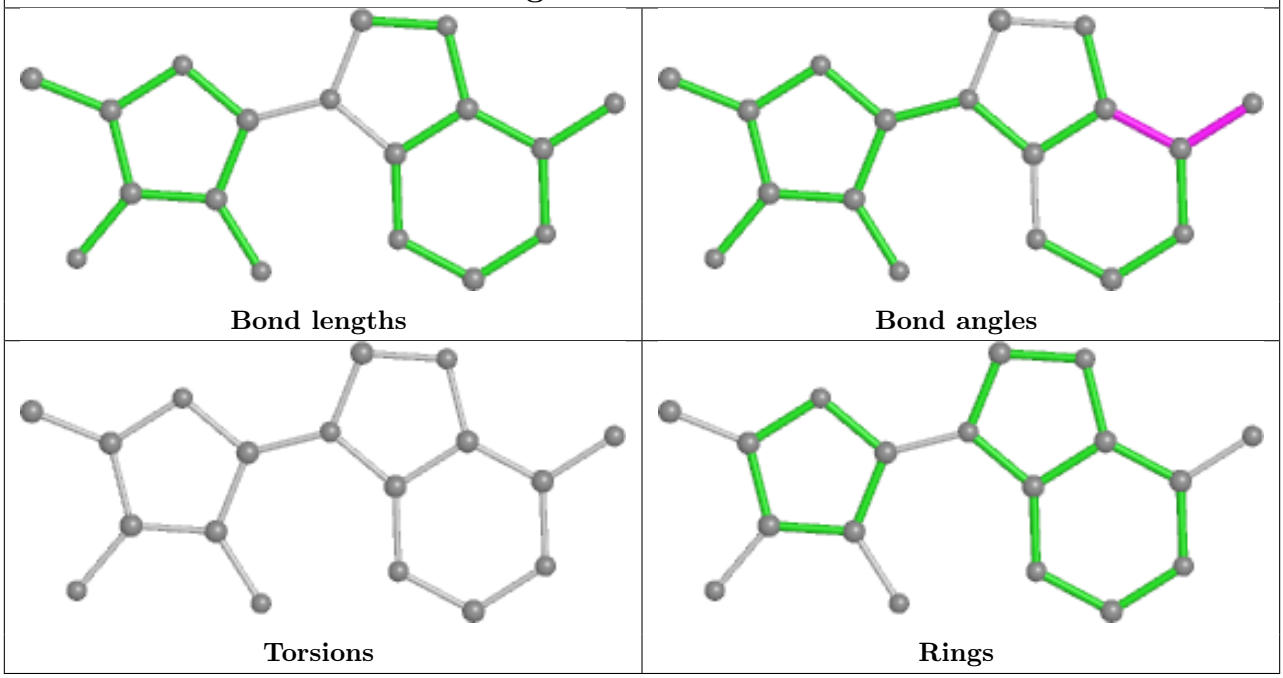
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	300	B12	7	0

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 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.

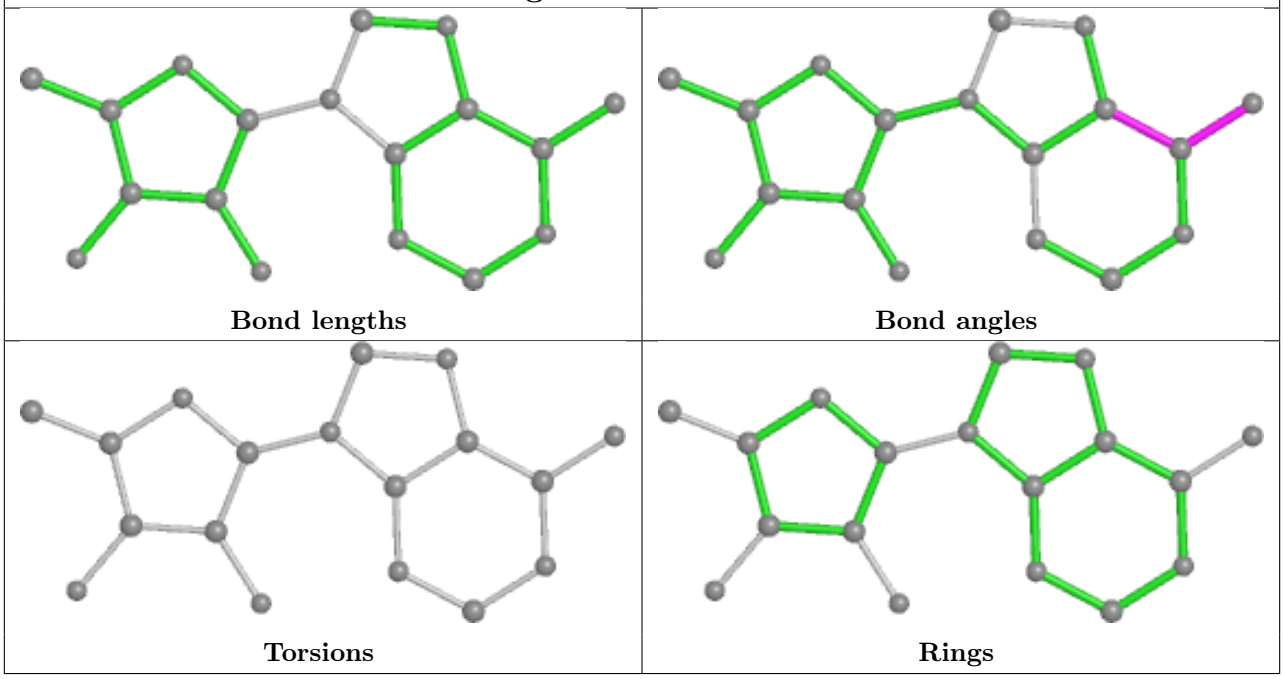
Ligand B12 C 300



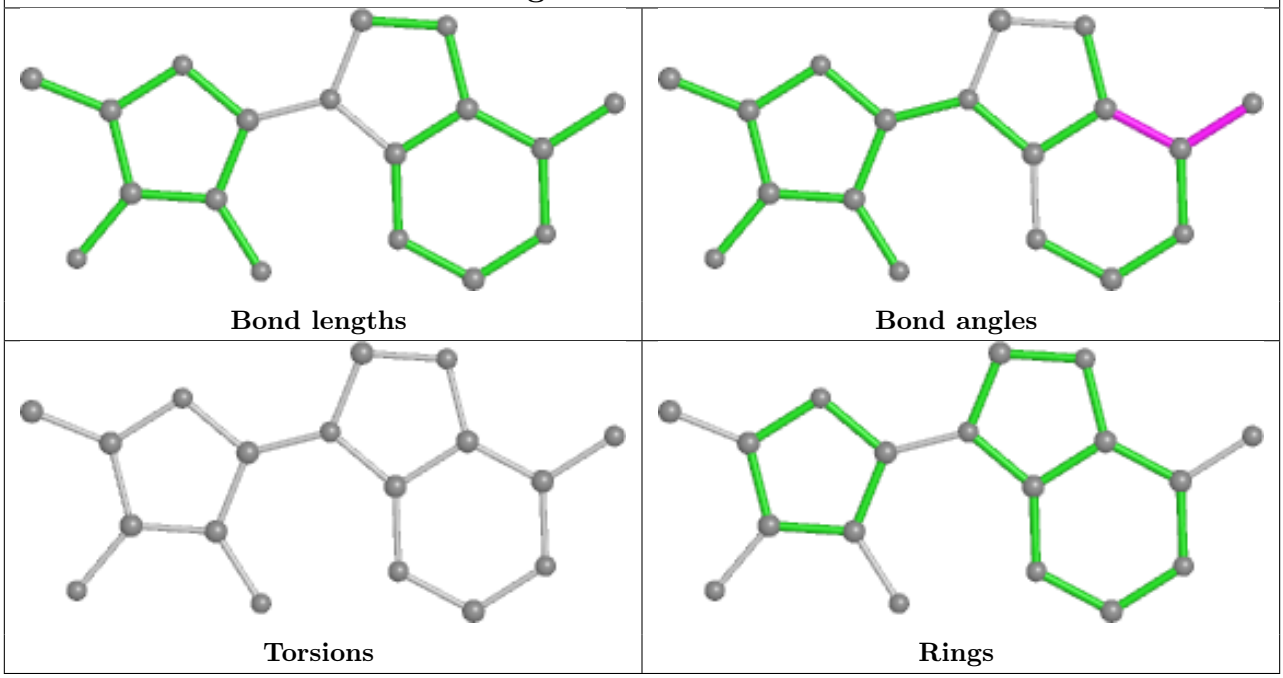
Ligand 5AD C 301



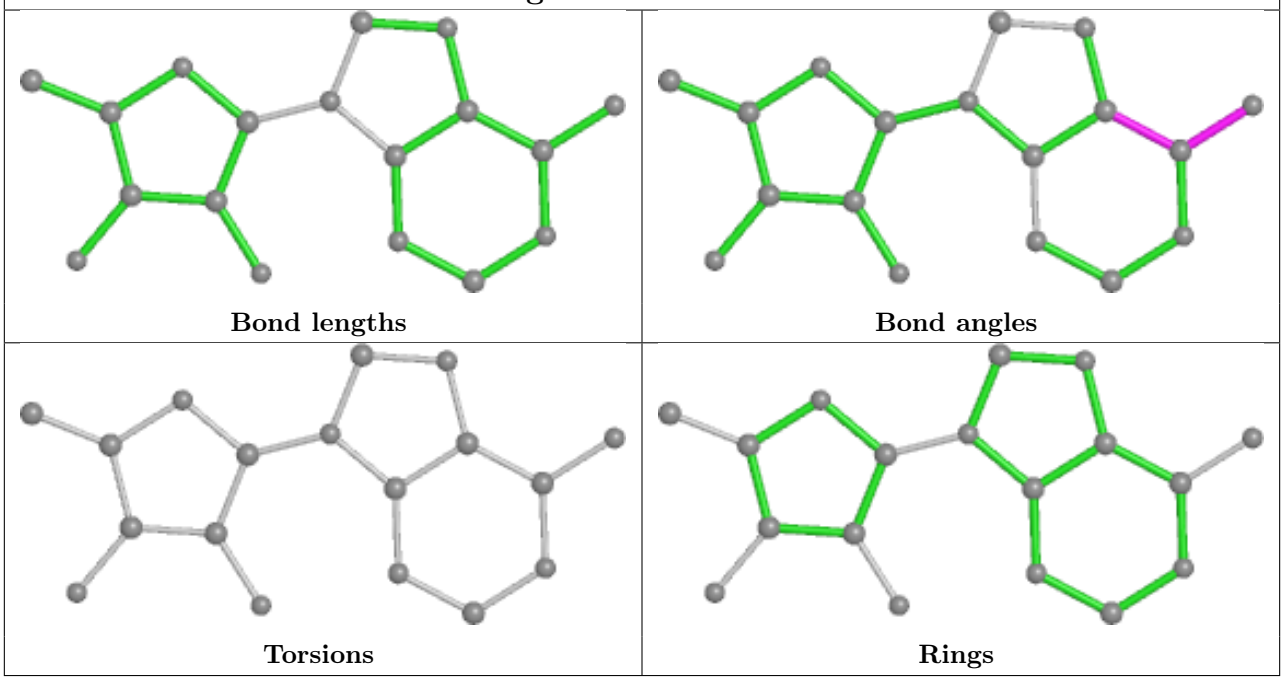
Ligand 5AD A 301



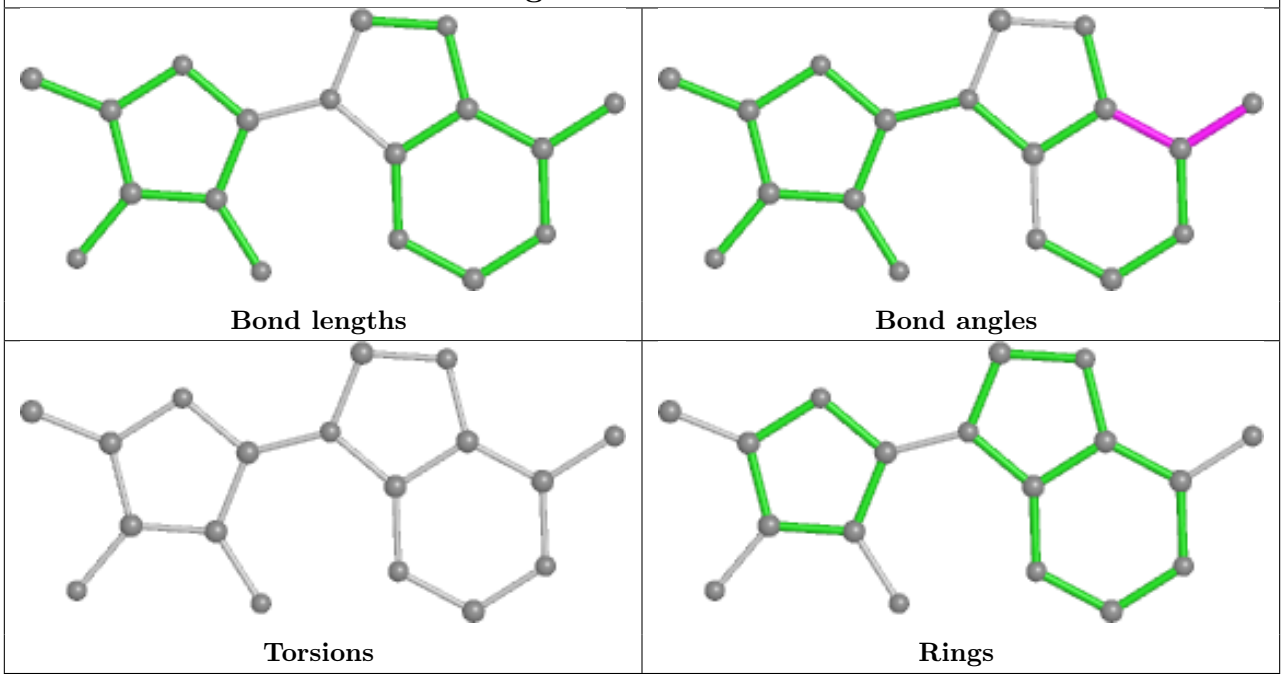
Ligand 5AD E 301



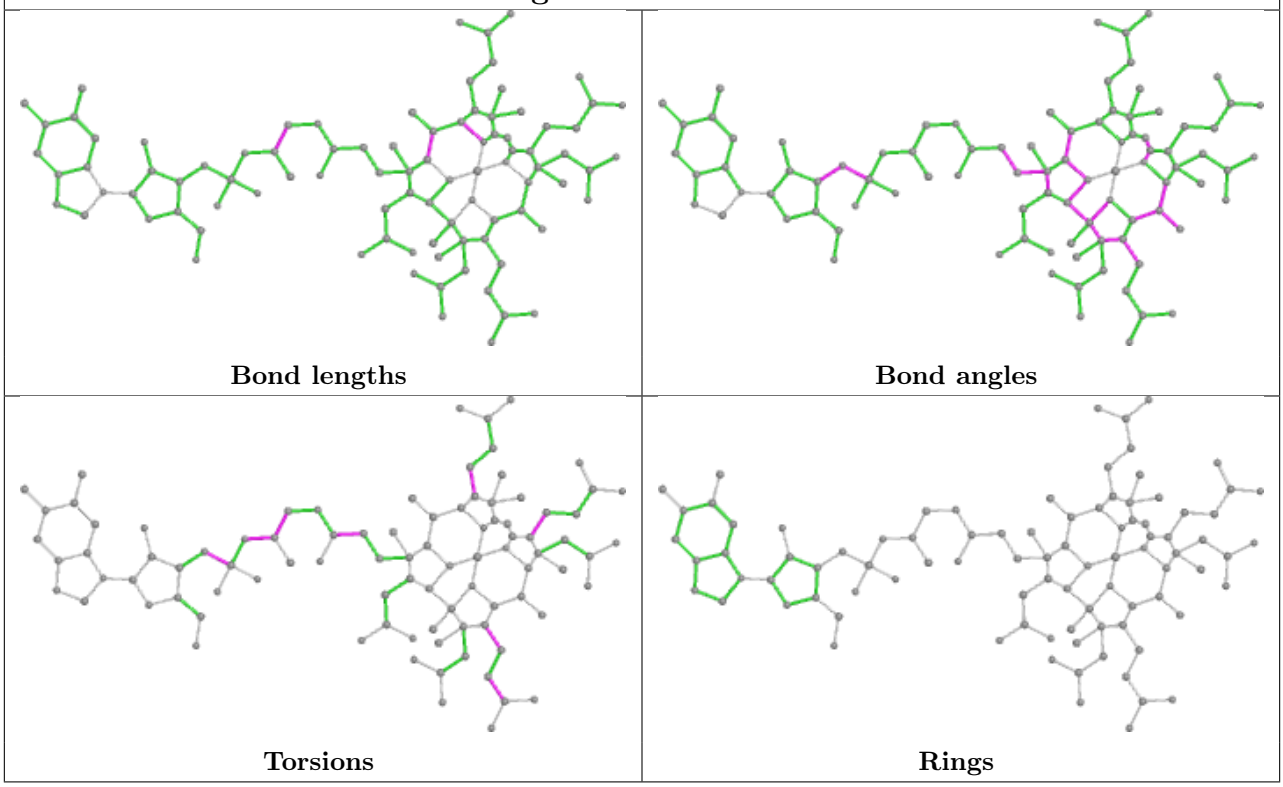
Ligand 5AD B 301



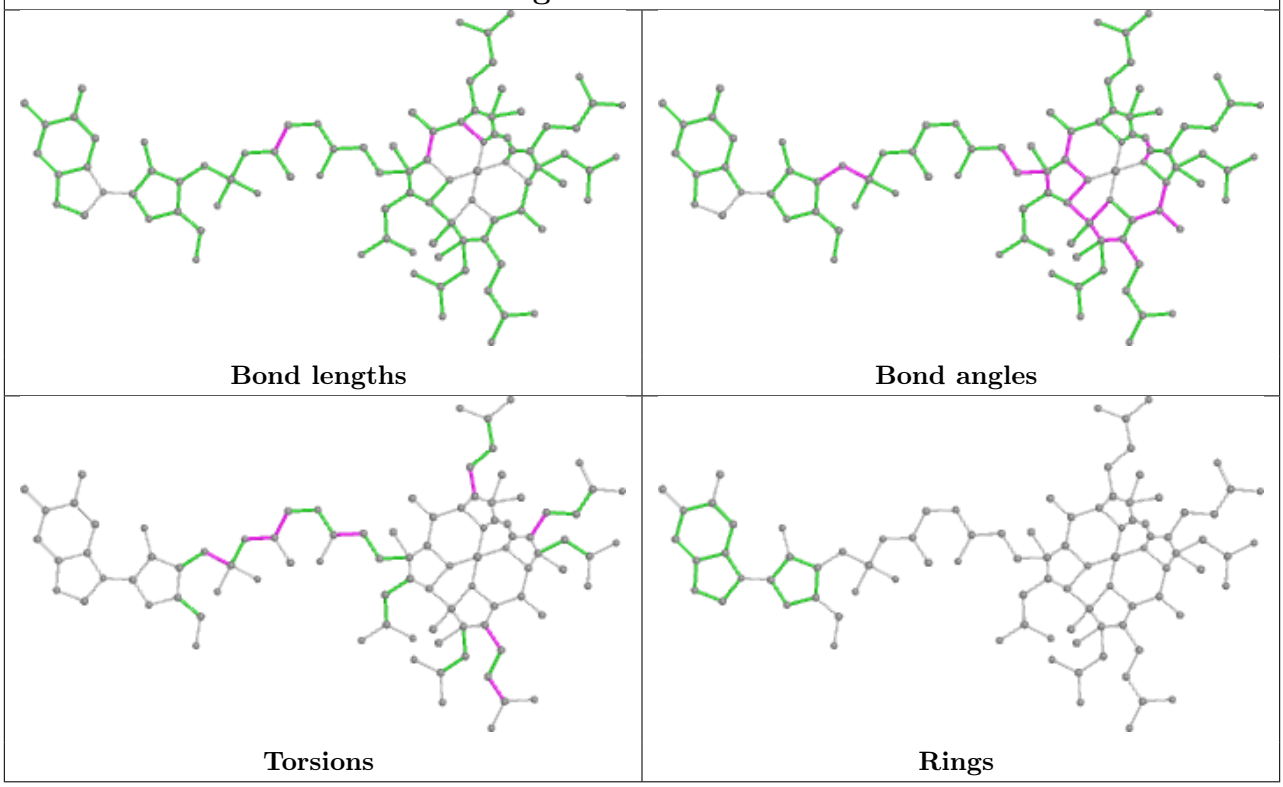
Ligand 5AD D 301



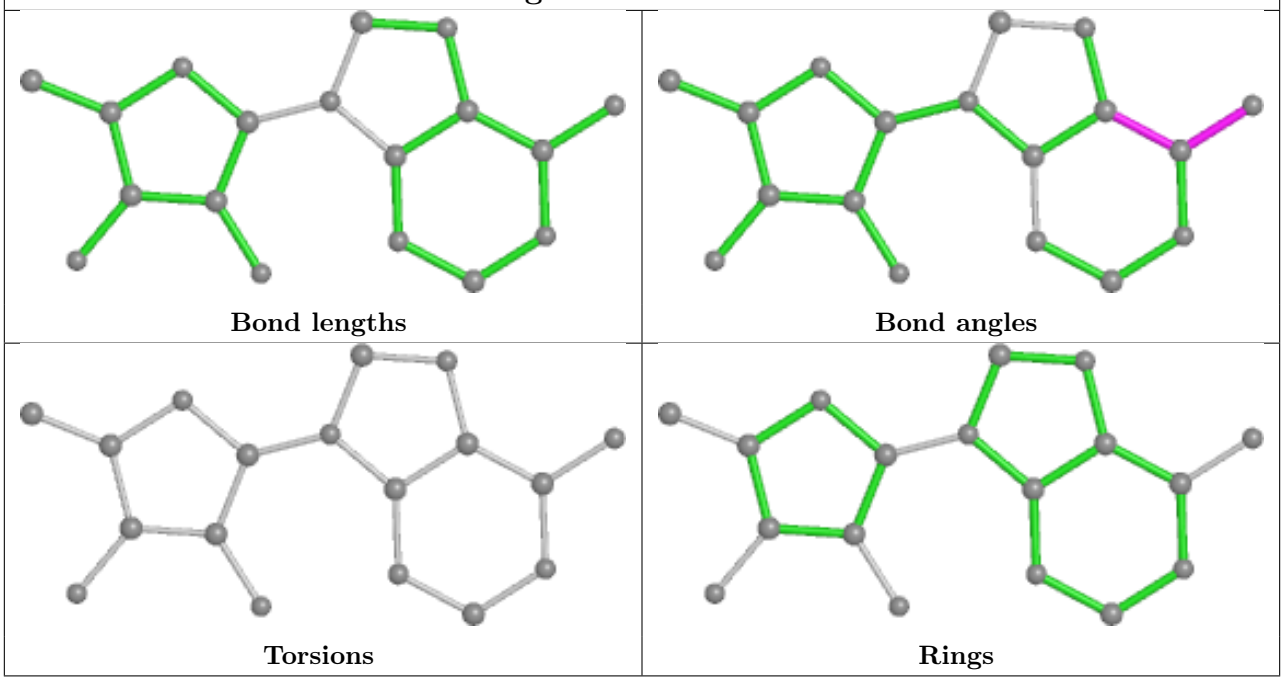
Ligand B12 A 300



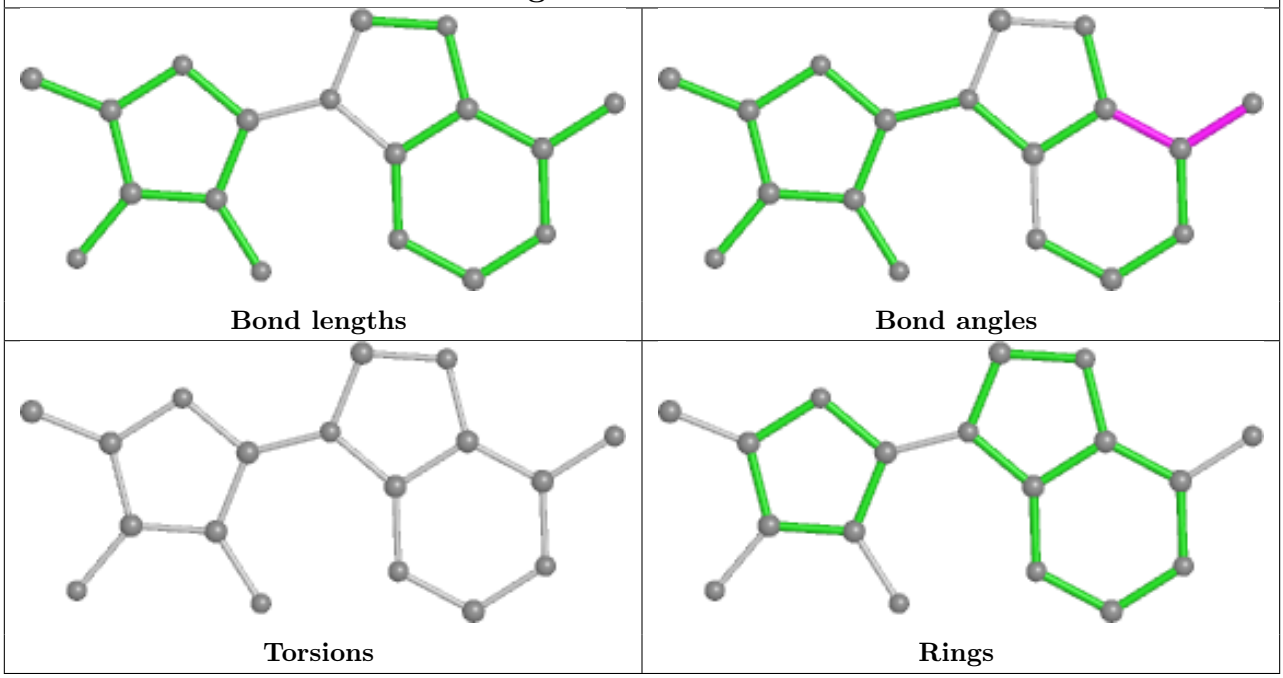
Ligand B12 E 300



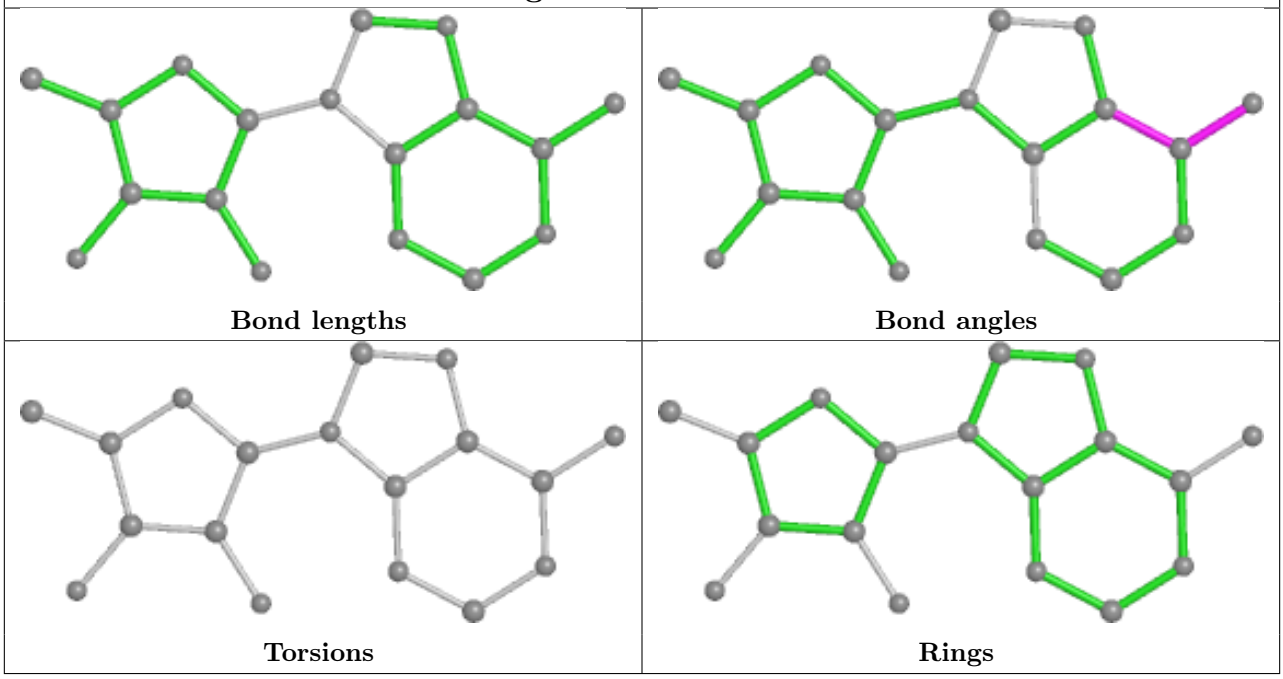
Ligand 5AD G 301



Ligand 5AD F 301



Ligand 5AD H 301



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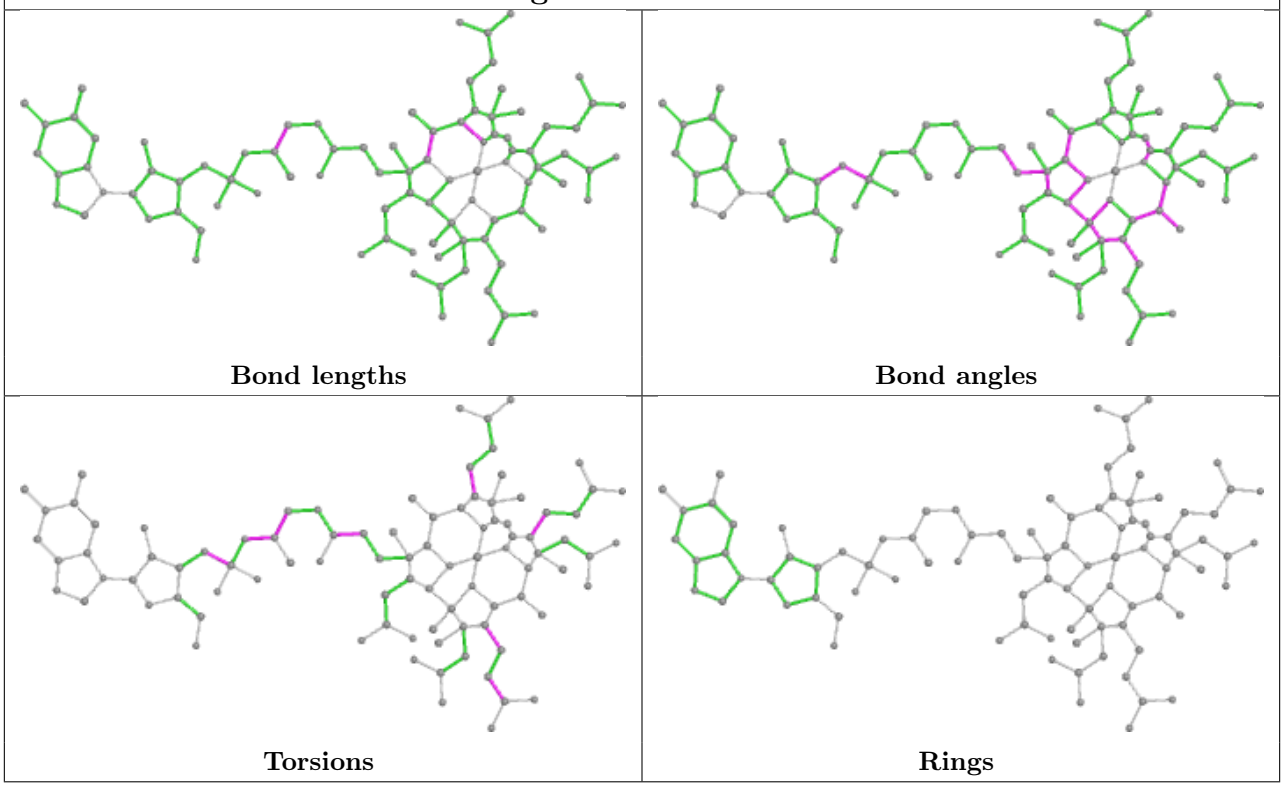
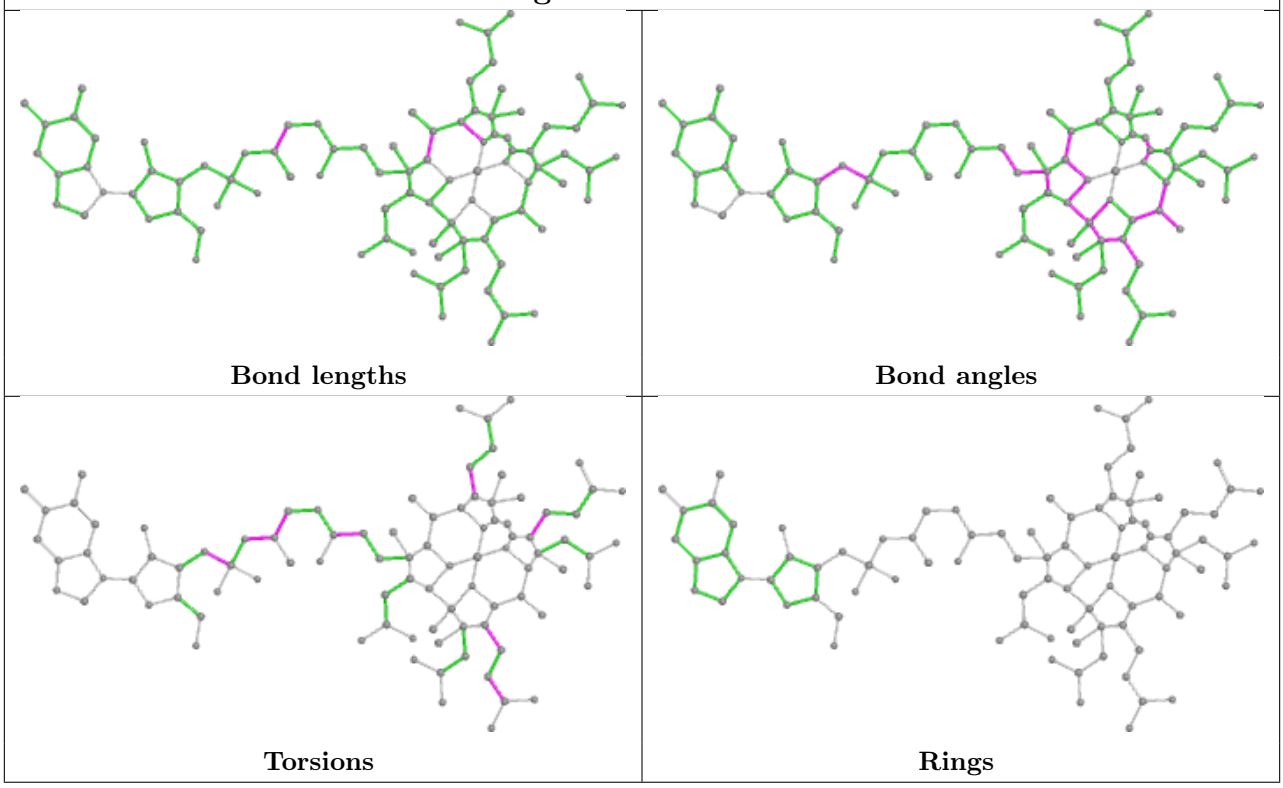
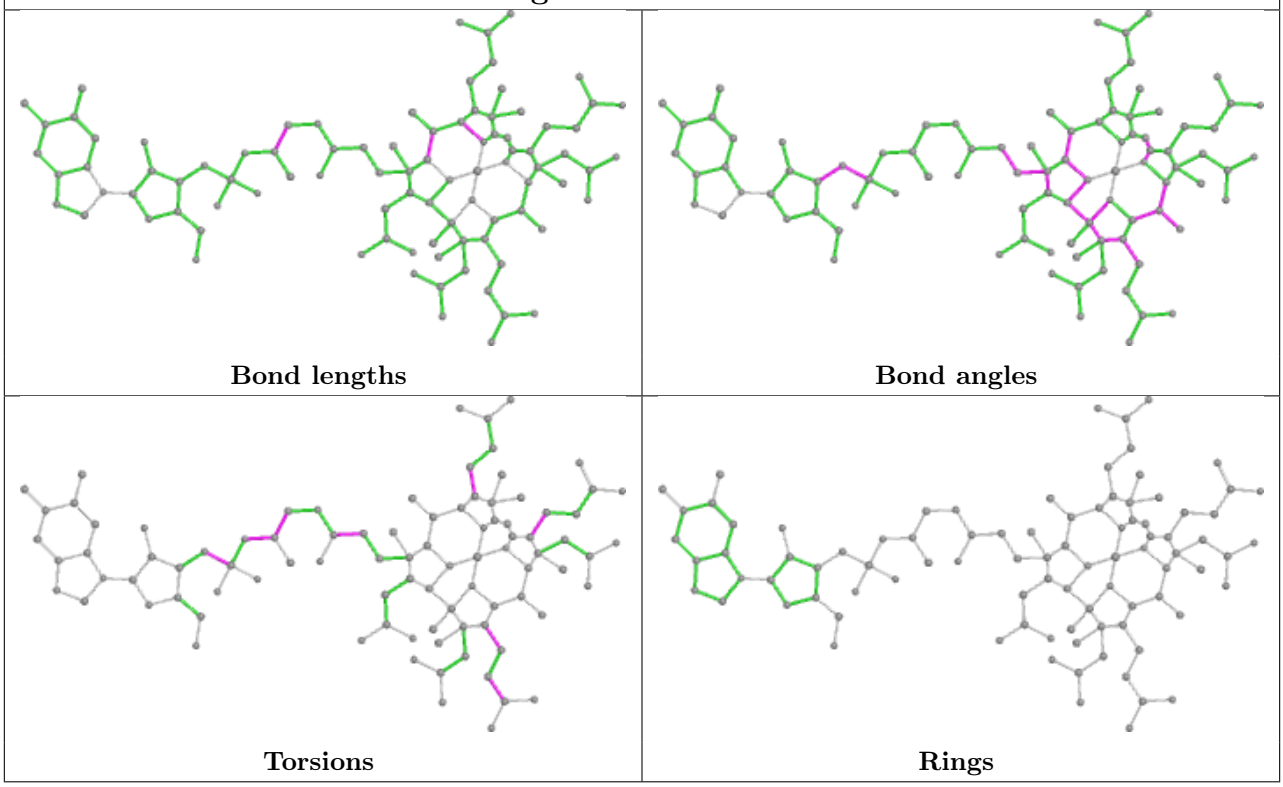


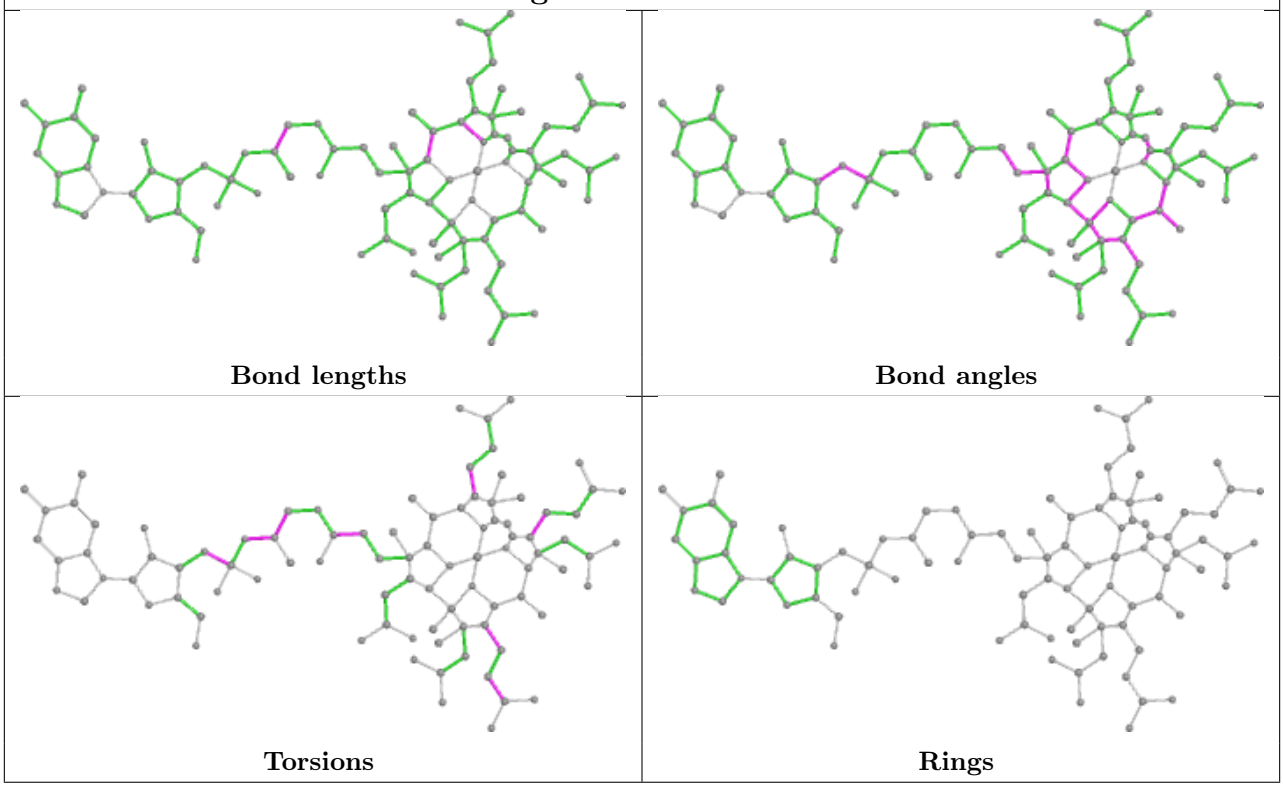
Ligand B12 F 300



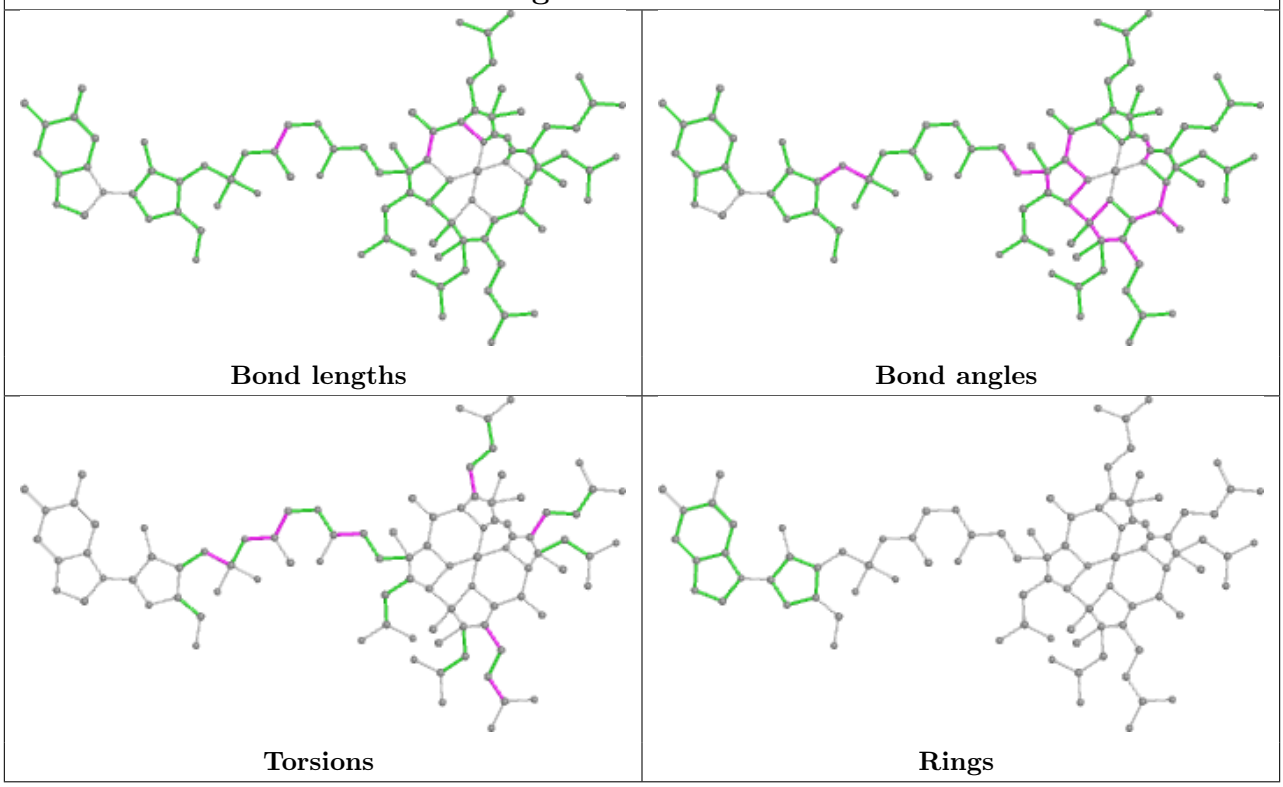
Ligand B12 D 300



Ligand B12 G 300



Ligand B12 B 300



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	A	273/305 (89%)	-0.22	1 (0%)	92	87	120, 159, 219, 235	0
1	B	276/305 (90%)	0.02	2 (0%)	87	82	135, 155, 216, 224	0
1	C	279/305 (91%)	0.01	4 (1%)	75	66	136, 156, 183, 200	0
1	D	205/305 (67%)	-0.15	3 (1%)	73	64	154, 177, 214, 244	0
1	E	273/305 (89%)	0.05	4 (1%)	73	64	116, 148, 214, 229	0
1	F	270/305 (88%)	0.01	3 (1%)	80	73	134, 158, 266, 296	0
1	G	280/305 (91%)	-0.14	0	100	100	125, 146, 190, 215	0
1	H	201/305 (65%)	0.27	10 (4%)	28	24	140, 163, 194, 210	0
2	I	26/26 (100%)	-0.82	0	100	100	199, 226, 272, 278	0
2	K	26/26 (100%)	-0.61	0	100	100	196, 229, 257, 284	0
3	J	26/26 (100%)	-0.84	0	100	100	208, 226, 254, 275	0
3	L	26/26 (100%)	-0.70	0	100	100	208, 222, 275, 276	0
All	All	2161/2544 (84%)	-0.06	27 (1%)	79	70	116, 159, 229, 296	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	16	THR	5.5
1	H	277	PRO	3.2
1	H	163	PRO	3.0
1	H	164	GLY	2.9
1	H	186	TYR	2.9
1	D	202	THR	2.8
1	H	185	ALA	2.7
1	C	168	LEU	2.7
1	F	218	ALA	2.6
1	D	216	ALA	2.5
1	H	218	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	246	LEU	2.3
1	E	245	PHE	2.3
1	B	45	TYR	2.2
1	D	166	PRO	2.2
1	E	32	PHE	2.2
1	H	192	GLY	2.2
1	H	245	PHE	2.2
1	B	110	TRP	2.2
1	H	276	LEU	2.2
1	E	33	PRO	2.1
1	F	106	GLY	2.1
1	E	195	ALA	2.0
1	A	32	PHE	2.0
1	C	270	LEU	2.0
1	C	9	ILE	2.0
1	C	267	LEU	2.0

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 (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
5	5AD	D	301	18/18	0.89	0.23	164,168,171,171	0
5	5AD	H	301	18/18	0.91	0.17	155,170,176,177	0
4	B12	E	300	91/91	0.92	0.38	131,148,159,162	0
5	5AD	E	301	18/18	0.92	0.41	149,160,166,166	0
5	5AD	B	301	18/18	0.92	0.29	150,153,155,156	0
4	B12	B	300	91/91	0.93	0.34	130,149,154,155	0
4	B12	D	300	91/91	0.93	0.30	164,172,182,186	0

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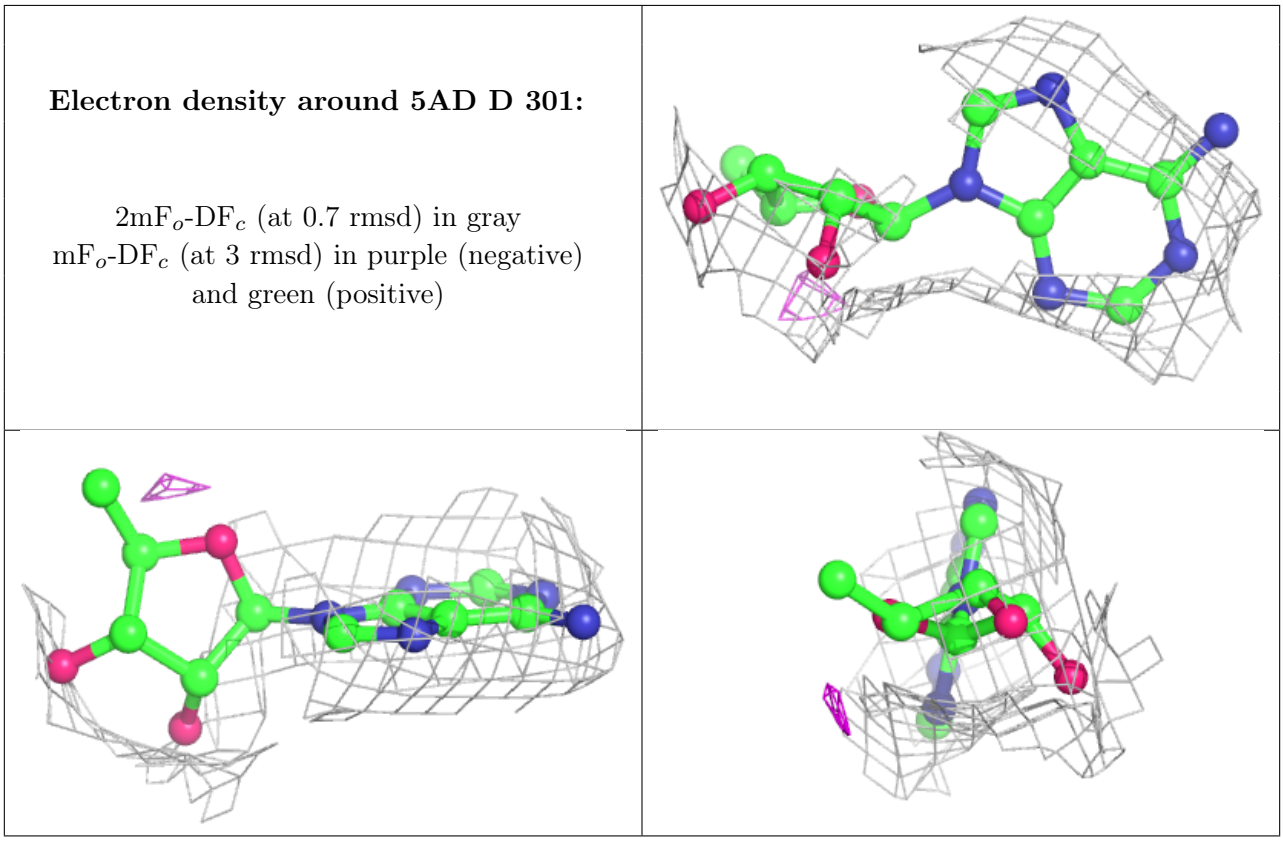
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	B12	A	300	91/91	0.93	0.36	143,156,173,179	0
5	5AD	F	301	18/18	0.93	0.31	141,152,157,157	0
5	5AD	G	301	18/18	0.93	0.32	141,143,147,149	0
4	B12	H	300	91/91	0.93	0.34	141,174,181,183	0
4	B12	C	300	91/91	0.94	0.39	139,146,156,160	0
5	5AD	A	301	18/18	0.94	0.36	160,164,175,179	0
4	B12	F	300	91/91	0.94	0.35	140,148,158,165	0
4	B12	G	300	91/91	0.94	0.33	132,138,144,146	0
5	5AD	C	301	18/18	0.95	0.33	150,156,161,163	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.

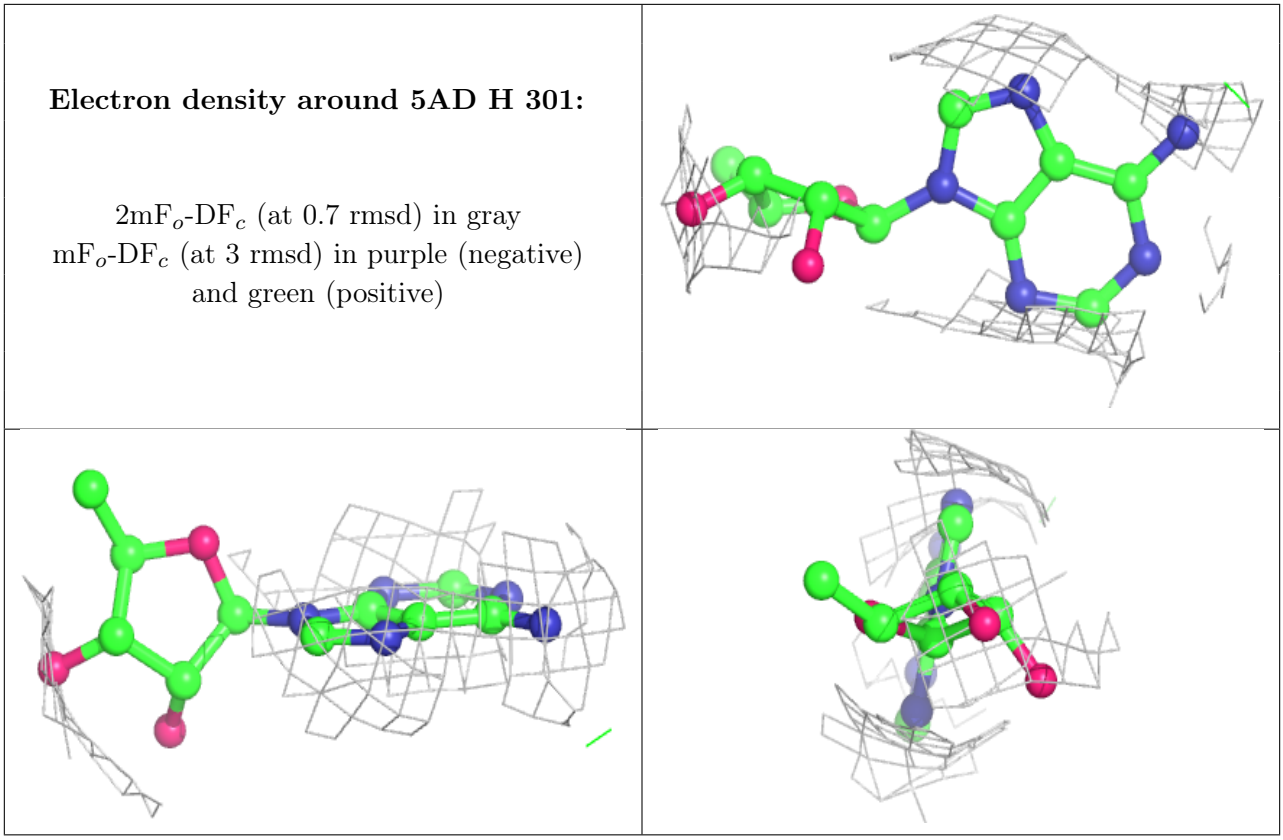
Electron density around 5AD D 301:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)



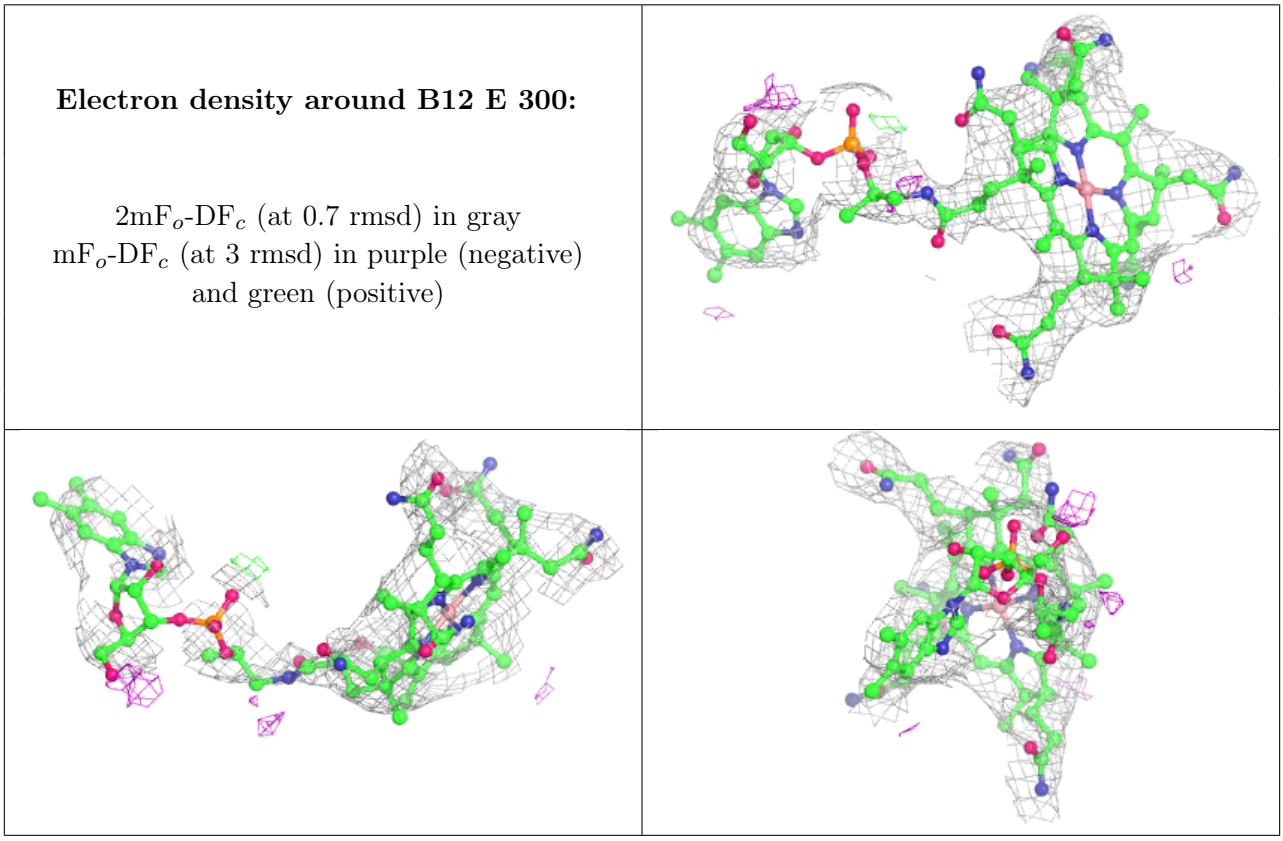
Electron density around 5AD H 301:

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



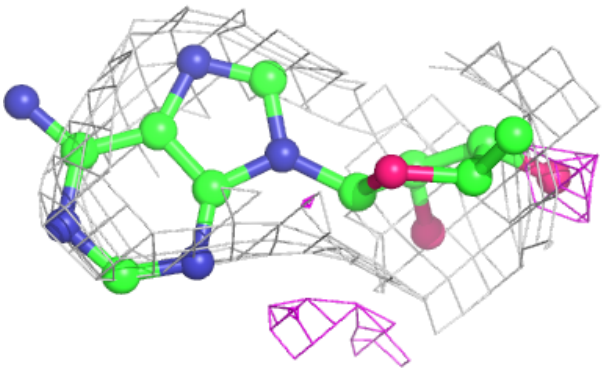
Electron density around B12 E 300:

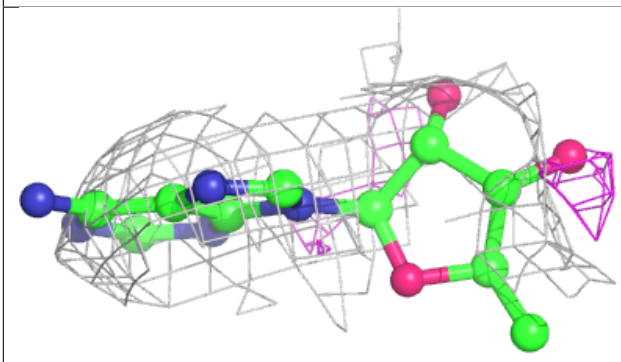
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

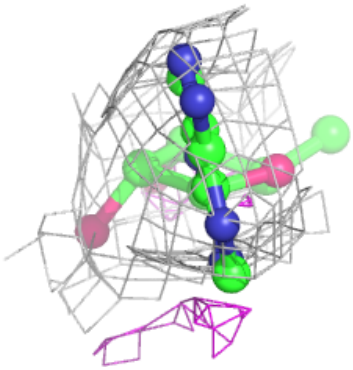


Electron density around 5AD E 301:

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

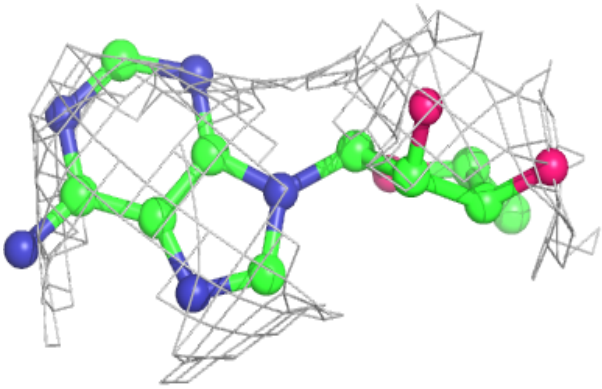


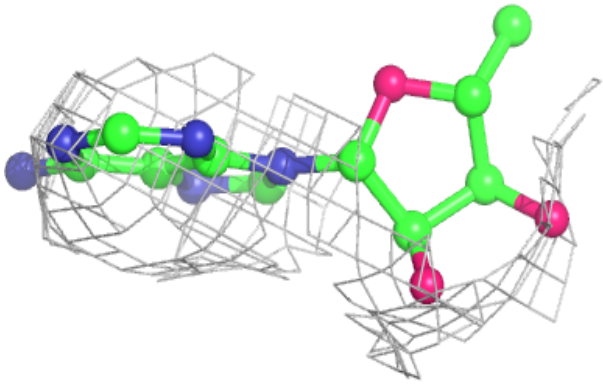


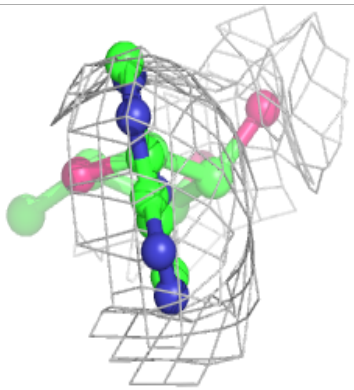


Electron density around 5AD B 301:

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

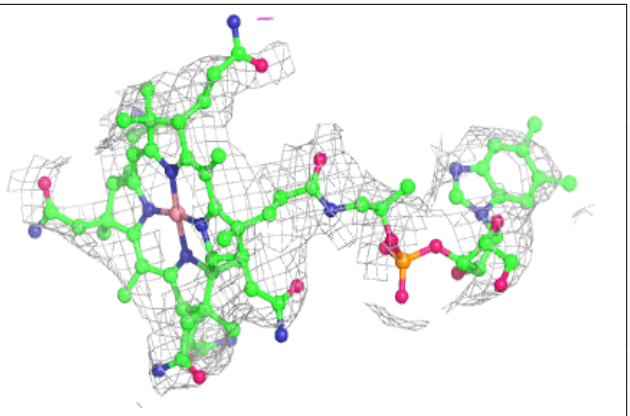


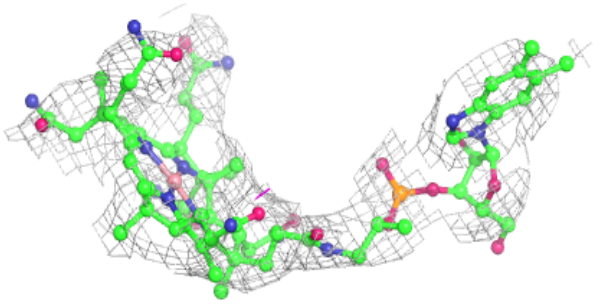


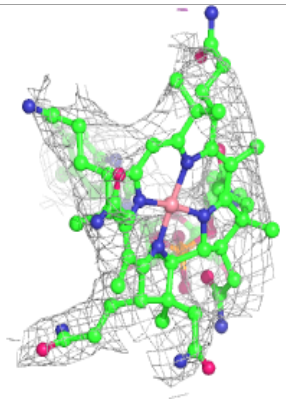


Electron density around B12 B 300:

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

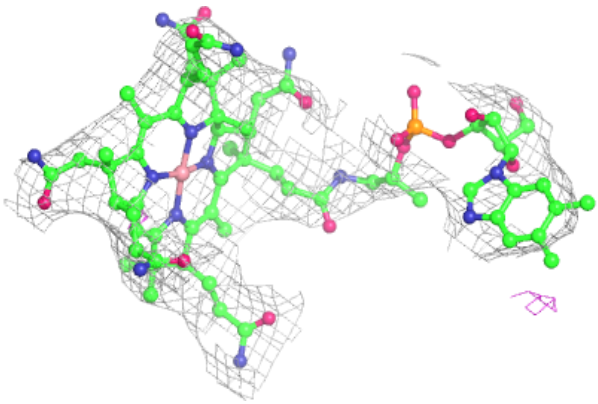


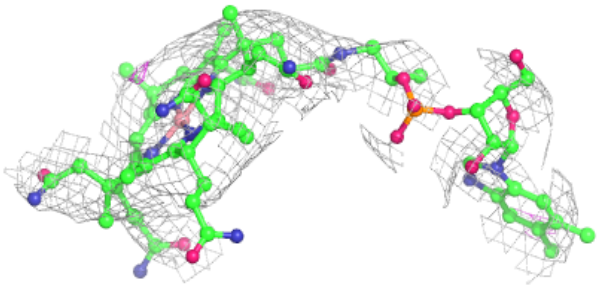


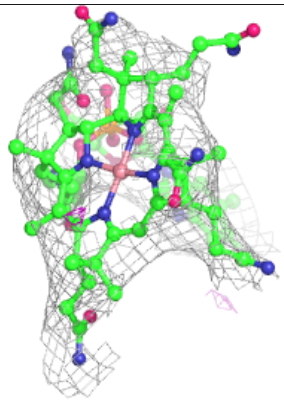


Electron density around B12 D 300:

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

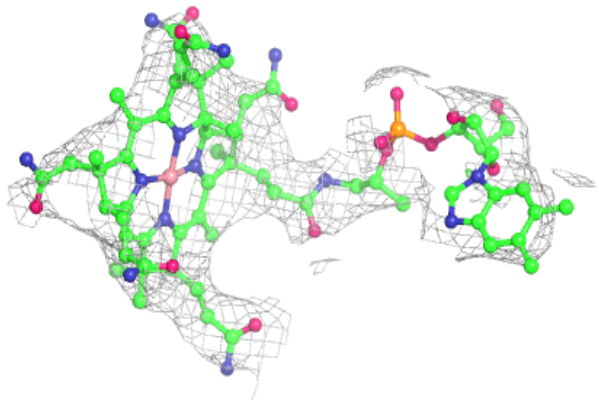


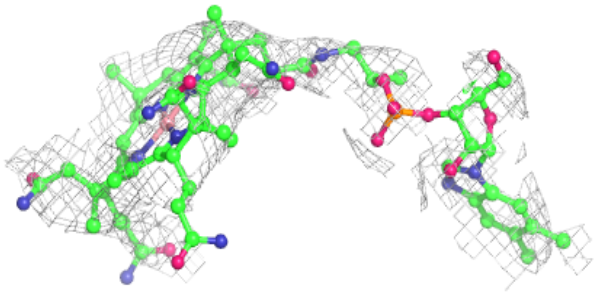


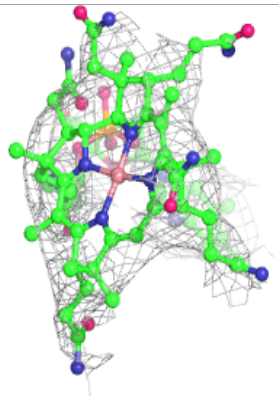


Electron density around B12 A 300:

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

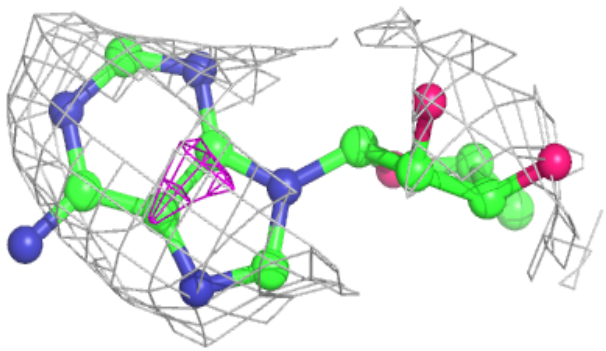


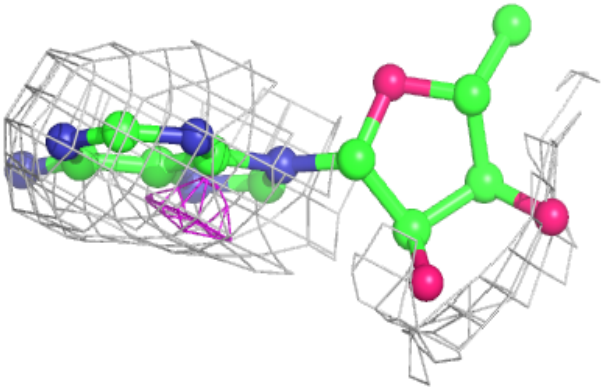


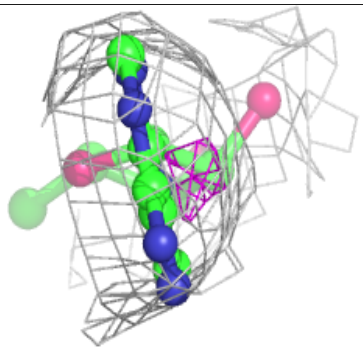


Electron density around 5AD F 301:

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

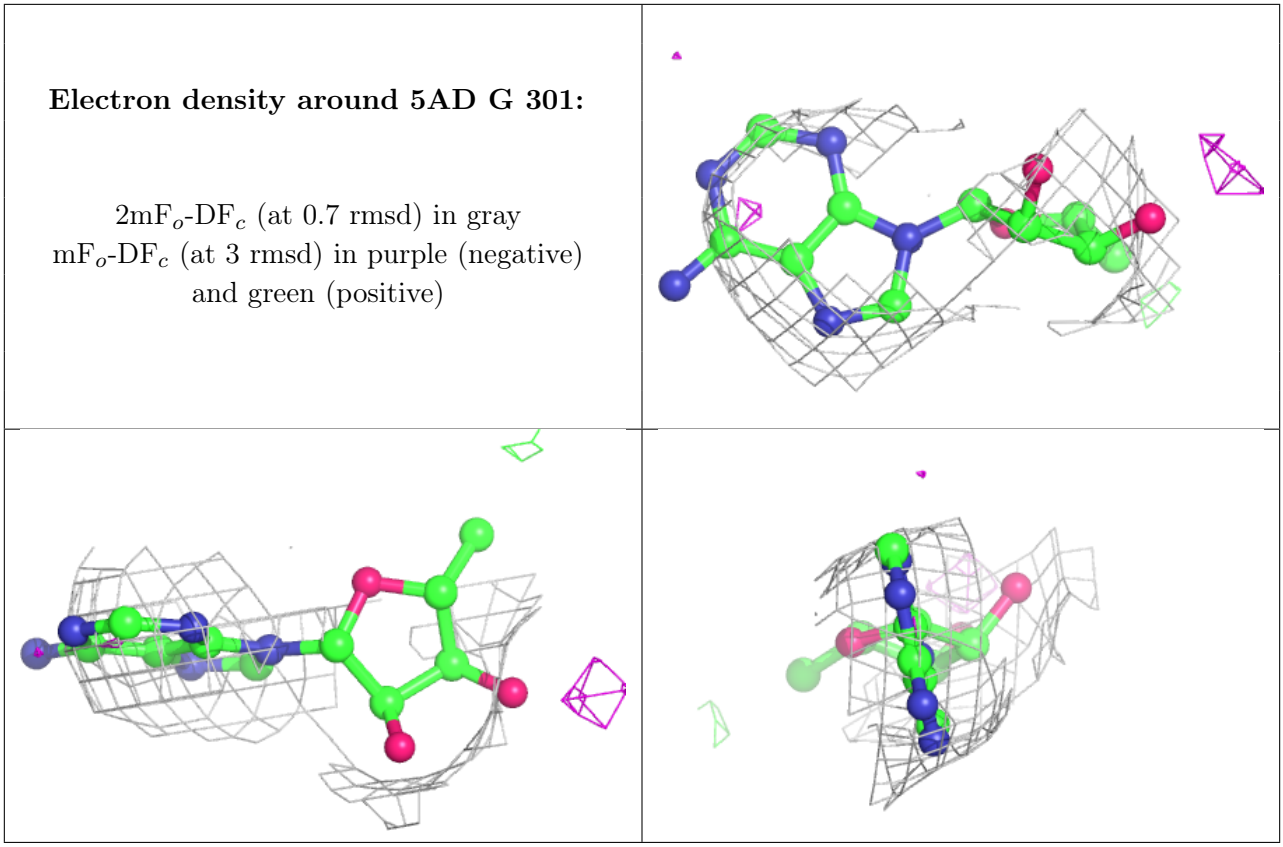






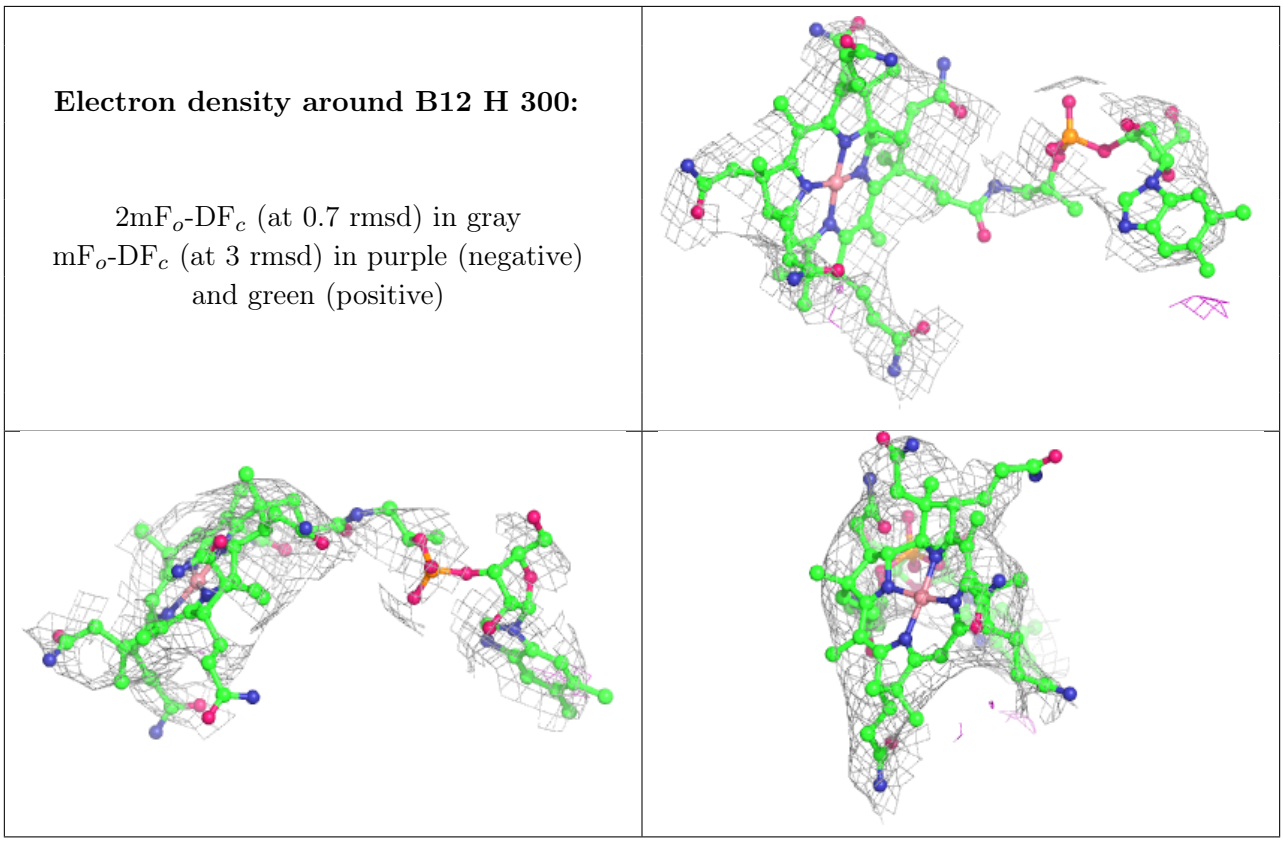
Electron density around 5AD G 301:

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



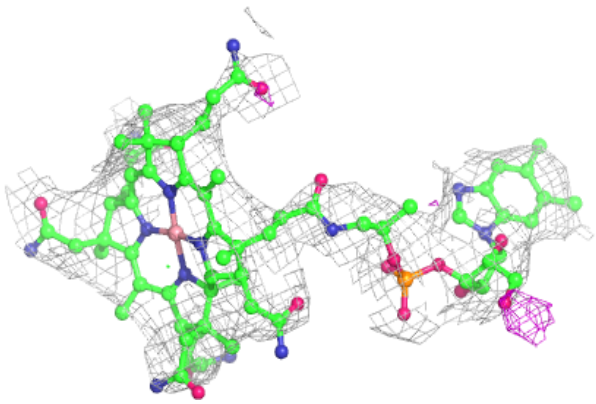
Electron density around B12 H 300:

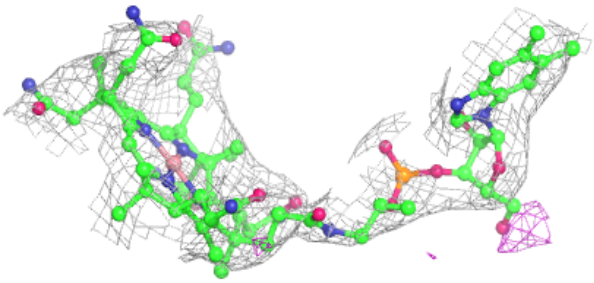
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

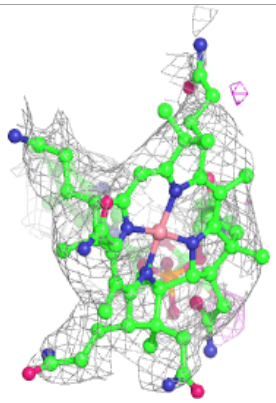


Electron density around B12 C 300:

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

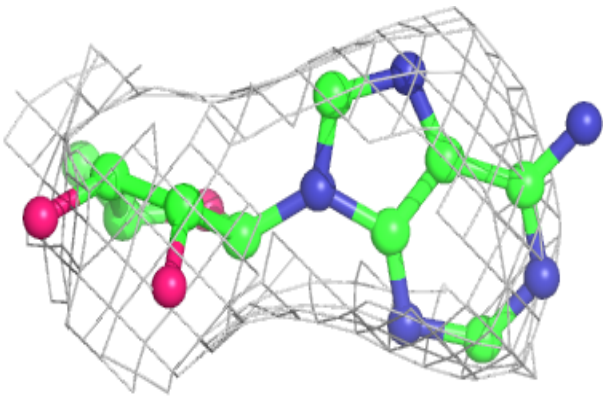


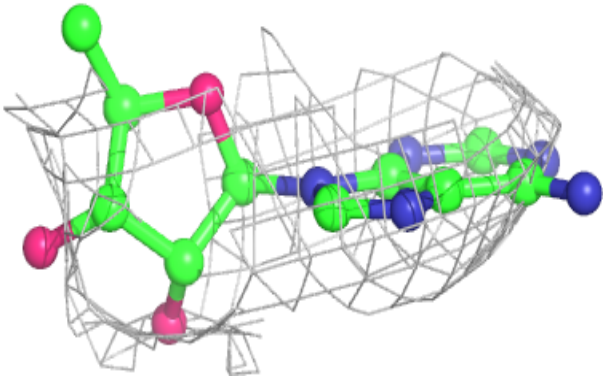


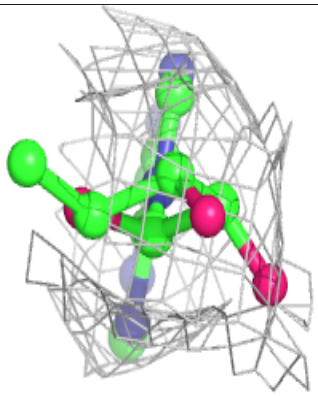


Electron density around 5AD A 301:

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

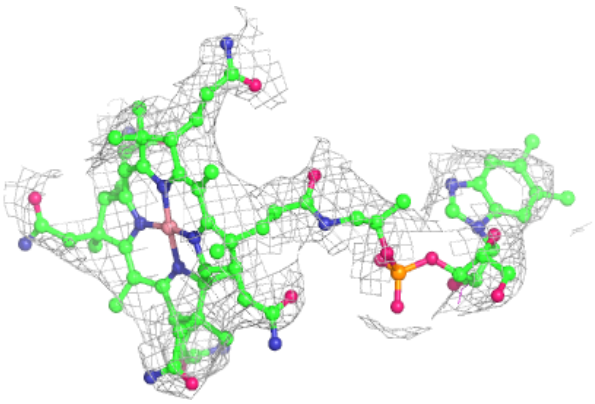


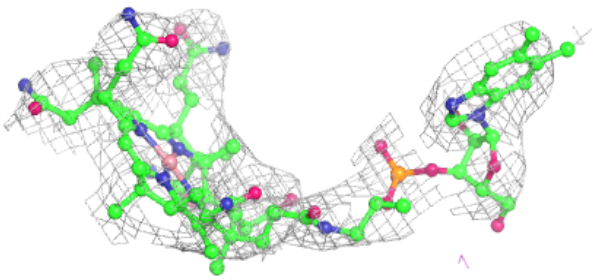


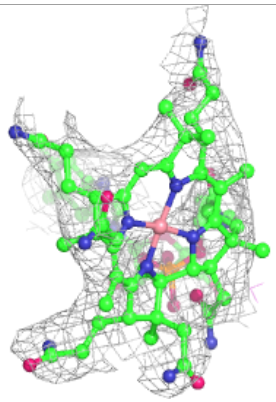


Electron density around B12 F 300:

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

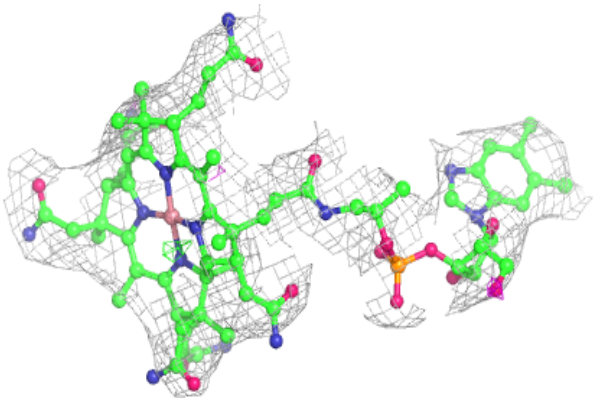


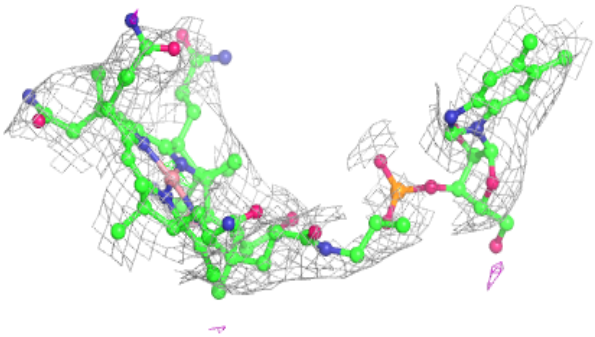


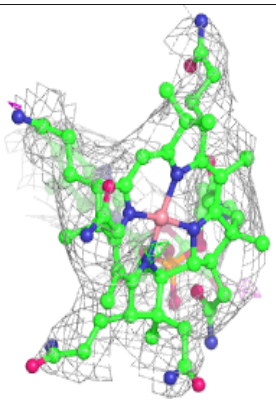


Electron density around B12 G 300:

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

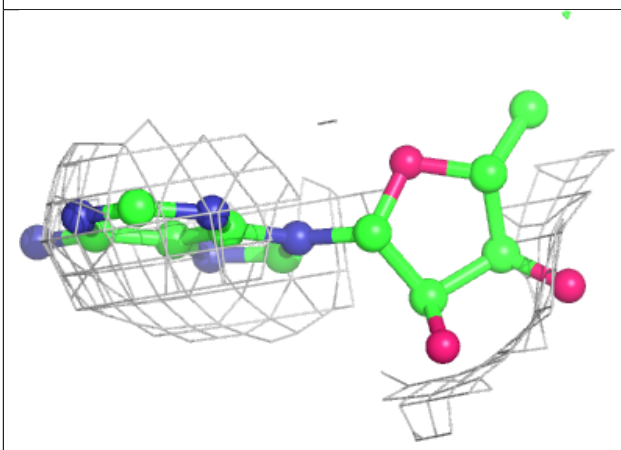


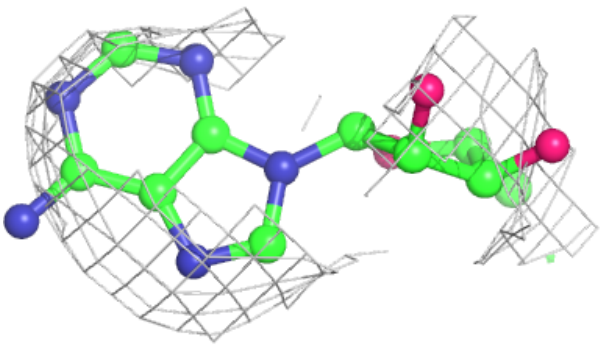


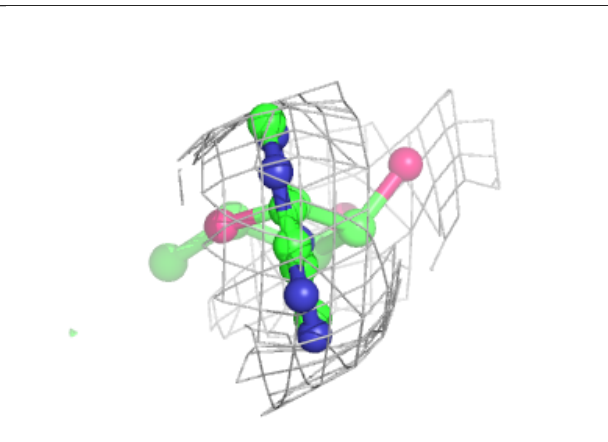


Electron density around 5AD C 301:

$2mF_o$-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.