Full wwPDB X-ray Structure Validation Report ⓘ

Oct 3, 2023 – 05:20 AM EDT

PDB ID	:	6Q2T
Title	:	Human sterol 14a-demethylase (CYP51) in complex with the functionally irreversible inhibitor (R)-N-(1-(3-chloro-4'-fluoro-[1,1'-biphenyl]-4-yl)-2-(1H-imidazol-1-yl)ethyl)-4-(5-(3-fluoro-5-(5-fluoropyrimidin-4-yl)phenyl)-1,3,4-oxadiazol-2-yl)benzamide
Authors	:	Friggeri, L.; Hargrove, T.Y.; Wawrzak, Z.; Lepesheva, G.I.
Deposited on	:	2019-08-08
Resolution	:	2.80 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 ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

MolProbity	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
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 2.80 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	DXC	A	603	X	-	-	-
4	DXC	A	604	X	-	-	-
4	DXC	A	605	X	-	-	-
4	DXC	A	606	X	-	-	-
4	DXC	A	607	X	-	-	-
4	DXC	A	608	X	-	-	-
4	DXC	A	609	X	-	-	-
4	DXC	A	610	X	-	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7658 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.

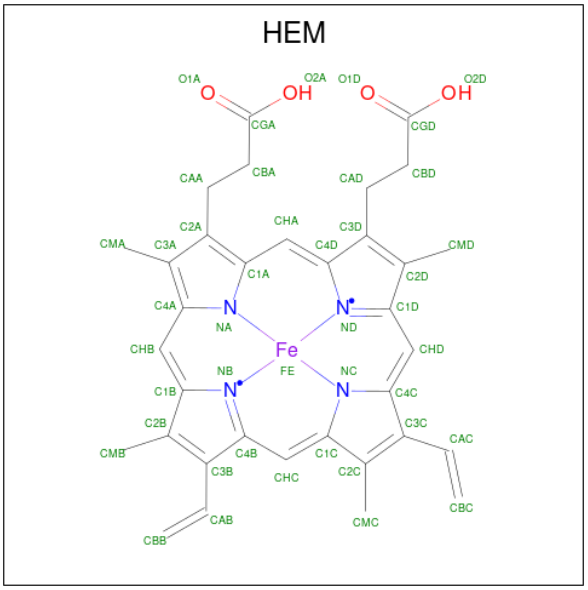
- Molecule 1 is a protein called Lanosterol 14-alpha demethylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	445	Total	C	N	O	S	0	0	0
			3588	2310	611	651	16			
1	B	444	Total	C	N	O	S	0	0	0
			3584	2308	610	650	16			

There are 6 discrepancies between the modelled and reference sequences:

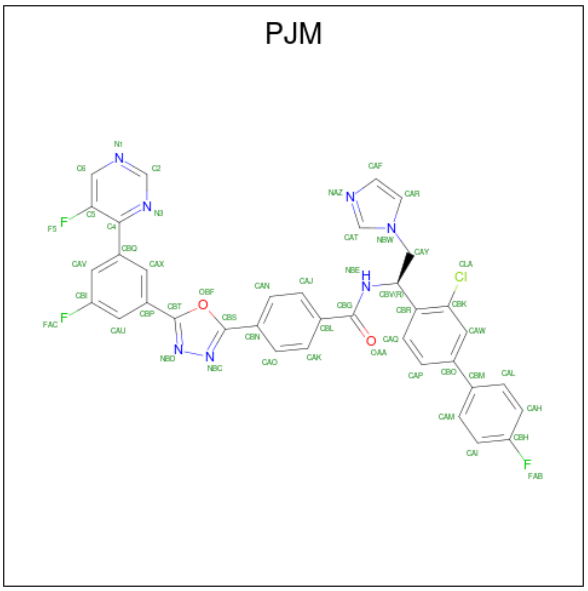
Chain	Residue	Modelled	Actual	Comment	Reference
A	58	GLY	-	expression tag	UNP Q16850
A	59	LYS	-	expression tag	UNP Q16850
A	60	LEU	-	expression tag	UNP Q16850
B	58	GLY	-	expression tag	UNP Q16850
B	59	LYS	-	expression tag	UNP Q16850
B	60	LEU	-	expression tag	UNP Q16850

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



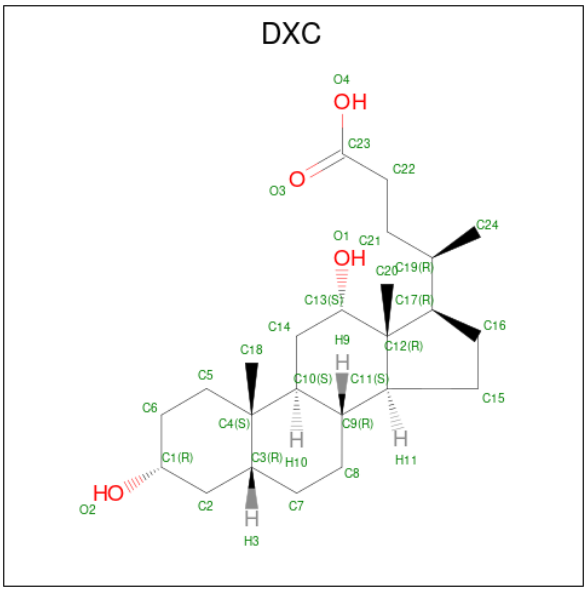
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is N-[(1R)-1-(3-chloro-4'-fluoro[1,1'-biphenyl]-4-yl)-2-(1H-imidazol-1-yl)ethyl]-4-{5-[3-fluoro-5-(5-fluoropyrimidin-4-yl)phenyl]-1,3,4-oxadiazol-2-yl}benzamide (three-letter code: PJM) (formula: $C_{36}H_{23}ClF_3N_7O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Cl	F	N	O	0	0
			49	36	1	3	7	2		
3	A	1	Total	C	Cl	F	N	O	0	0
			49	36	1	3	7	2		
3	B	1	Total	C	Cl	F	N	O	0	0
			49	36	1	3	7	2		

- Molecule 4 is (3ALPHA,5BETA,12ALPHA)-3,12-DIHYDROXYCHOLAN-24-OIC ACID (three-letter code: DXC) (formula: $C_{24}H_{40}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 28 24 4	0	0
4	A	1	Total C O 28 24 4	0	0
4	A	1	Total C O 28 24 4	0	0
4	A	1	Total C O 28 24 4	0	0
4	A	1	Total C O 28 24 4	0	0
4	A	1	Total C O 28 24 4	0	0
4	A	1	Total C O 28 24 4	0	0
4	A	1	Total C O 28 24 4	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	13	Total O 13 13	0	0
5	B	16	Total O 16 16	0	0

MolProbity and EDS failed to run properly - this section is therefore empty.

3 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α, β, γ	117.66Å 117.66Å 157.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.10 – 2.80	Depositor
% Data completeness (in resolution range)	99.6 (28.10-2.80)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.32 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.227 , 0.256	Depositor
Wilson B-factor (Å^2)	84.1	Xtriage
Anisotropy	0.048	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.015 for -h,k,-l	Xtriage
Total number of atoms	7658	wwPDB-VP
Average B, all atoms (Å^2)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.26% 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.

4 Model quality

4.1 Standard geometry

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles

4.3.1 Protein backbone

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates

There are no monosaccharides in this entry.

4.6 Ligand geometry

13 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	DXC	A	609	-	31,31,31	0.99	1 (3%)	49,49,49	2.74	20 (40%)
4	DXC	A	603	-	31,31,31	0.88	1 (3%)	49,49,49	2.42	20 (40%)
4	DXC	A	608	-	31,31,31	1.07	3 (9%)	49,49,49	2.16	12 (24%)
3	PJM	A	611	-	46,55,55	3.19	9 (19%)	67,78,78	1.97	15 (22%)
3	PJM	A	602	2	46,55,55	2.73	9 (19%)	67,78,78	1.75	11 (16%)
4	DXC	A	607	-	31,31,31	0.92	2 (6%)	49,49,49	2.62	18 (36%)
2	HEM	B	601	1,3	41,50,50	1.34	7 (17%)	45,82,82	1.88	11 (24%)
4	DXC	A	610	-	31,31,31	0.99	2 (6%)	49,49,49	2.07	16 (32%)
2	HEM	A	601	1,3	41,50,50	1.35	7 (17%)	45,82,82	1.90	10 (22%)
4	DXC	A	605	-	31,31,31	0.89	1 (3%)	49,49,49	2.21	19 (38%)
4	DXC	A	606	-	31,31,31	0.97	1 (3%)	49,49,49	2.50	16 (32%)
4	DXC	A	604	-	31,31,31	0.84	1 (3%)	49,49,49	2.18	15 (30%)
3	PJM	B	602	2	46,55,55	2.70	9 (19%)	67,78,78	1.75	9 (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
4	DXC	A	609	-	1/1/11/11	2/9/71/71	1/4/4/4
4	DXC	A	608	-	1/1/11/11	8/9/71/71	1/4/4/4
3	PJM	A	611	-	-	13/28/32/32	0/7/7/7
3	PJM	A	602	2	-	5/28/32/32	0/7/7/7
4	DXC	A	607	-	1/1/11/11	2/9/71/71	1/4/4/4
2	HEM	B	601	1,3	-	4/12/54/54	-
4	DXC	A	610	-	1/1/11/11	9/9/71/71	1/4/4/4
2	HEM	A	601	1,3	-	2/12/54/54	-
4	DXC	A	605	-	1/1/11/11	2/9/71/71	1/4/4/4
3	PJM	B	602	2	-	5/28/32/32	0/7/7/7
4	DXC	A	606	-	1/1/11/11	9/9/71/71	1/4/4/4
4	DXC	A	604	-	1/1/11/11	3/9/71/71	0/4/4/4
4	DXC	A	603	-	1/1/11/11	6/9/71/71	0/4/4/4

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	611	PJM	NBC-NBD	-15.34	1.07	1.37
3	A	602	PJM	NBC-NBD	-10.44	1.17	1.37
3	B	602	PJM	NBC-NBD	-9.66	1.18	1.37
3	A	611	PJM	CBQ-C4	-9.26	1.38	1.49
3	B	602	PJM	CBR-CBV	-8.81	1.38	1.52
3	A	602	PJM	CBR-CBV	-8.58	1.38	1.52
3	B	602	PJM	CBQ-C4	-8.49	1.39	1.49
3	A	602	PJM	CBQ-C4	-8.32	1.39	1.49
3	A	611	PJM	CBR-CBV	-7.48	1.40	1.52
3	A	611	PJM	CBL-CBG	-5.52	1.38	1.50
3	B	602	PJM	CBL-CBG	-5.31	1.39	1.50
3	A	602	PJM	CBL-CBG	-5.19	1.39	1.50
3	A	602	PJM	CBM-CBO	-4.18	1.38	1.49
3	B	602	PJM	CBM-CBO	-4.12	1.38	1.49
3	A	611	PJM	CBM-CBO	-3.69	1.39	1.49
2	A	601	HEM	C1B-NB	-3.47	1.34	1.40
2	B	601	HEM	C1B-NB	-3.45	1.34	1.40
3	B	602	PJM	C2-N3	3.45	1.40	1.33
3	A	602	PJM	C2-N3	3.44	1.40	1.33
3	B	602	PJM	C2-N1	3.42	1.40	1.33
3	A	611	PJM	C2-N1	3.42	1.40	1.33
3	A	602	PJM	C2-N1	3.39	1.40	1.33
3	A	611	PJM	C2-N3	3.31	1.40	1.33
2	B	601	HEM	C4D-ND	-3.31	1.34	1.40
2	A	601	HEM	C4D-ND	-3.29	1.34	1.40
4	A	608	DXC	C12-C11	-3.02	1.50	1.55
4	A	609	DXC	C12-C11	-2.80	1.50	1.55
3	B	602	PJM	C6-N1	2.80	1.40	1.34
2	A	601	HEM	FE-NB	2.79	2.10	1.96
2	B	601	HEM	FE-NB	2.78	2.10	1.96
3	A	611	PJM	C6-N1	2.77	1.40	1.34
3	A	602	PJM	C6-N1	2.76	1.40	1.34
4	A	606	DXC	C12-C11	-2.66	1.51	1.55
4	A	607	DXC	C12-C11	-2.62	1.51	1.55
4	A	610	DXC	C12-C11	-2.54	1.51	1.55
4	A	605	DXC	C12-C11	-2.41	1.51	1.55
3	A	602	PJM	CAR-NBW	-2.35	1.33	1.37
4	A	610	DXC	C4-C3	-2.34	1.51	1.55
4	A	604	DXC	C12-C11	-2.33	1.51	1.55
3	B	602	PJM	CAR-NBW	-2.30	1.33	1.37
4	A	608	DXC	C12-C17	-2.29	1.51	1.55
4	A	607	DXC	C8-C9	-2.24	1.49	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	HEM	C1D-ND	-2.23	1.34	1.38
3	A	611	PJM	CAR-NBW	-2.22	1.33	1.37
4	A	608	DXC	C12-C13	-2.21	1.51	1.54
4	A	603	DXC	C12-C11	-2.19	1.51	1.55
2	B	601	HEM	C1D-ND	-2.13	1.34	1.38
2	B	601	HEM	FE-ND	-2.11	1.86	1.96
2	A	601	HEM	FE-ND	-2.10	1.86	1.96
2	B	601	HEM	C4B-NB	-2.10	1.34	1.38
2	A	601	HEM	C4B-NB	-2.08	1.34	1.38
2	B	601	HEM	CHB-C1B	2.08	1.40	1.35
2	A	601	HEM	CHB-C1B	2.06	1.40	1.35

All (192) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	609	DXC	C14-C10-C4	-8.85	104.60	113.73
4	A	608	DXC	C12-C17-C19	-8.45	109.41	119.50
4	A	607	DXC	C12-C17-C19	-8.43	109.43	119.50
3	A	611	PJM	N1-C2-N3	-7.66	119.28	127.70
4	A	606	DXC	C14-C10-C4	-7.57	105.92	113.73
3	B	602	PJM	N1-C2-N3	-7.43	119.53	127.70
3	A	602	PJM	N1-C2-N3	-7.01	119.99	127.70
4	A	607	DXC	C10-C4-C3	6.22	117.32	108.58
4	A	608	DXC	C12-C11-C9	-6.17	107.90	114.71
4	A	610	DXC	C17-C12-C11	-6.02	94.03	100.09
4	A	606	DXC	C17-C12-C13	-5.87	112.31	117.67
4	A	603	DXC	C10-C4-C3	5.75	116.65	108.58
4	A	609	DXC	C10-C4-C3	5.74	116.64	108.58
4	A	604	DXC	C12-C17-C19	-5.70	112.69	119.50
4	A	606	DXC	C12-C17-C19	-5.58	112.83	119.50
3	A	611	PJM	CAO-CBN-CBS	-5.57	111.94	120.44
2	B	601	HEM	CHC-C4B-NB	5.53	130.43	124.43
4	A	607	DXC	C14-C10-C4	-5.33	108.23	113.73
4	A	606	DXC	C10-C4-C3	5.31	116.03	108.58
2	A	601	HEM	CHC-C4B-NB	5.30	130.19	124.43
4	A	605	DXC	C12-C17-C19	-5.09	113.42	119.50
4	A	609	DXC	C15-C11-C9	-5.02	110.81	119.08
4	A	605	DXC	C10-C4-C3	4.94	115.52	108.58
4	A	607	DXC	C4-C10-C9	4.75	117.42	112.42
2	A	601	HEM	CHD-C1D-ND	4.66	129.50	124.43
4	A	603	DXC	C12-C17-C19	-4.66	113.93	119.50
4	A	604	DXC	C10-C4-C3	4.64	115.10	108.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	602	PJM	CAQ-CBR-CBK	4.63	121.42	116.81
4	A	603	DXC	C4-C10-C9	4.57	117.22	112.42
4	A	609	DXC	C4-C10-C9	4.55	117.20	112.42
2	B	601	HEM	CHD-C1D-ND	4.54	129.37	124.43
4	A	603	DXC	C14-C10-C4	-4.51	109.08	113.73
4	A	605	DXC	C17-C12-C13	-4.50	113.55	117.67
4	A	609	DXC	C10-C14-C13	4.37	120.07	114.30
4	A	607	DXC	C22-C21-C19	-4.30	106.66	114.52
4	A	607	DXC	C17-C12-C13	-4.30	113.74	117.67
4	A	603	DXC	C17-C12-C13	-4.28	113.75	117.67
4	A	607	DXC	C12-C11-C9	-4.26	110.01	114.71
4	A	607	DXC	C7-C8-C9	-4.25	105.14	112.14
4	A	605	DXC	C15-C11-C9	-4.19	112.18	119.08
4	A	604	DXC	C15-C11-C9	-4.18	112.19	119.08
3	A	602	PJM	CAQ-CBR-CBK	4.18	120.97	116.81
4	A	608	DXC	C17-C12-C13	-4.16	113.87	117.67
4	A	609	DXC	C17-C12-C13	-4.15	113.88	117.67
4	A	609	DXC	C8-C9-C11	-4.14	105.01	112.08
4	A	603	DXC	C15-C11-C9	-4.12	112.30	119.08
4	A	606	DXC	C8-C9-C11	-4.11	105.06	112.08
4	A	610	DXC	C2-C3-C4	-4.08	108.32	112.66
4	A	603	DXC	C7-C8-C9	-4.00	105.55	112.14
4	A	610	DXC	C15-C11-C12	-3.97	99.66	103.55
3	B	602	PJM	CBV-NBE-CBG	-3.95	117.25	122.34
4	A	610	DXC	C14-C10-C4	-3.94	109.66	113.73
4	A	610	DXC	C12-C17-C19	-3.93	114.80	119.50
4	A	609	DXC	C7-C8-C9	-3.91	105.70	112.14
4	A	603	DXC	C5-C4-C10	-3.89	105.23	111.35
4	A	604	DXC	C7-C8-C9	-3.87	105.76	112.14
4	A	603	DXC	C2-C3-C4	-3.86	108.55	112.66
4	A	603	DXC	C3-C2-C1	-3.83	107.14	112.76
3	A	602	PJM	CBV-NBE-CBG	-3.81	117.43	122.34
4	A	604	DXC	C2-C1-C6	-3.79	106.03	110.55
4	A	605	DXC	C2-C3-C4	-3.75	108.67	112.66
4	A	605	DXC	C7-C8-C9	-3.71	106.02	112.14
2	B	601	HEM	CHA-C4D-ND	3.71	128.96	124.38
4	A	607	DXC	C15-C11-C9	-3.70	112.99	119.08
4	A	606	DXC	C15-C11-C9	-3.69	113.00	119.08
2	A	601	HEM	CHA-C4D-ND	3.69	128.94	124.38
4	A	609	DXC	C11-C9-C10	3.65	113.98	109.09
4	A	609	DXC	C2-C3-C4	-3.64	108.79	112.66
4	A	604	DXC	C10-C14-C13	-3.63	109.50	114.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	HEM	CHB-C1B-NB	3.62	128.85	124.38
4	A	606	DXC	C20-C12-C13	3.54	112.67	109.07
4	A	609	DXC	C8-C7-C3	-3.54	104.74	111.84
4	A	605	DXC	C8-C9-C11	-3.52	106.07	112.08
3	A	611	PJM	CAU-CBI-CAV	-3.49	119.11	123.52
4	A	608	DXC	C15-C11-C9	-3.49	113.33	119.08
4	A	604	DXC	C17-C12-C13	-3.45	114.52	117.67
4	A	610	DXC	C12-C11-C9	-3.44	110.92	114.71
4	A	608	DXC	C14-C10-C4	-3.43	110.19	113.73
4	A	606	DXC	C22-C21-C19	-3.42	108.27	114.52
4	A	604	DXC	C18-C4-C10	-3.42	106.47	111.18
4	A	605	DXC	C14-C10-C4	-3.40	110.22	113.73
4	A	609	DXC	C14-C10-C9	3.40	116.33	110.82
2	B	601	HEM	CHB-C1B-NB	3.37	128.54	124.38
4	A	605	DXC	C3-C2-C1	-3.36	107.83	112.76
4	A	610	DXC	C8-C9-C10	3.33	114.62	110.49
4	A	606	DXC	C5-C6-C1	-3.31	106.22	110.47
2	A	601	HEM	C1B-NB-C4B	3.31	108.49	105.07
3	A	611	PJM	CBL-CBG-NBE	-3.30	110.74	117.06
4	A	609	DXC	C12-C17-C19	-3.30	115.56	119.50
2	B	601	HEM	C1B-NB-C4B	3.29	108.47	105.07
4	A	610	DXC	C16-C17-C12	-3.25	100.36	103.55
4	A	604	DXC	C12-C11-C9	-3.24	111.14	114.71
4	A	605	DXC	C4-C10-C9	3.23	115.81	112.42
2	A	601	HEM	CHD-C1D-C2D	-3.22	119.94	124.98
4	A	606	DXC	C18-C4-C10	-3.16	106.82	111.18
2	B	601	HEM	CHD-C1D-C2D	-3.14	120.07	124.98
4	A	607	DXC	C2-C3-C4	-3.14	109.32	112.66
3	A	602	PJM	CAY-NBW-CAT	-3.11	119.63	125.76
3	A	611	PJM	CAU-CBP-CAX	3.08	122.87	118.31
4	A	606	DXC	C2-C3-C4	-3.04	109.43	112.66
4	A	604	DXC	C8-C9-C11	-3.03	106.91	112.08
4	A	603	DXC	C8-C9-C11	-3.01	106.94	112.08
3	A	611	PJM	C6-N1-C2	3.00	119.64	115.80
3	A	602	PJM	CAY-NBW-CAR	2.99	132.08	125.92
4	A	608	DXC	C14-C10-C9	2.95	115.60	110.82
4	A	607	DXC	C8-C9-C11	-2.94	107.07	112.08
3	A	611	PJM	CAN-CBN-CAO	2.93	123.43	117.59
3	A	611	PJM	CAX-CBP-CBT	-2.93	115.77	120.06
4	A	609	DXC	C3-C2-C1	-2.87	108.54	112.76
4	A	605	DXC	C12-C11-C9	-2.87	111.54	114.71
4	A	610	DXC	C24-C19-C17	-2.87	108.53	112.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	604	DXC	C5-C6-C1	-2.87	106.79	110.47
4	A	604	DXC	C8-C7-C3	-2.86	106.11	111.84
4	A	609	DXC	C5-C4-C10	-2.85	106.88	111.35
4	A	603	DXC	C6-C5-C4	2.79	117.57	112.78
3	A	602	PJM	CAU-CBI-CAV	-2.74	120.06	123.52
4	A	603	DXC	C12-C11-C9	-2.69	111.74	114.71
3	B	602	PJM	CAU-CBI-CAV	-2.68	120.13	123.52
3	A	611	PJM	CAJ-CBL-CAK	2.68	122.40	118.59
4	A	605	DXC	C20-C12-C13	2.68	111.79	109.07
3	A	611	PJM	CBN-CBS-NBC	-2.67	119.60	124.12
2	A	601	HEM	CHA-C4D-C3D	-2.64	120.37	125.33
4	A	609	DXC	C20-C12-C13	2.62	111.73	109.07
2	B	601	HEM	CHA-C4D-C3D	-2.62	120.41	125.33
4	A	608	DXC	C24-C19-C17	-2.58	108.98	112.92
4	A	609	DXC	C18-C4-C10	-2.55	107.67	111.18
4	A	605	DXC	C8-C7-C3	-2.54	106.75	111.84
3	A	602	PJM	CBK-CBR-CBV	-2.54	118.46	121.71
4	A	607	DXC	C17-C12-C11	2.53	102.64	100.09
4	A	604	DXC	C3-C2-C1	-2.51	109.07	112.76
3	A	611	PJM	CAK-CBL-CBG	-2.50	112.51	120.62
4	A	607	DXC	C8-C7-C3	-2.50	106.82	111.84
3	A	611	PJM	CAN-CBN-CBS	2.50	124.25	120.44
4	A	606	DXC	C7-C3-C4	2.49	116.77	112.31
4	A	603	DXC	C18-C4-C10	-2.46	107.80	111.18
4	A	603	DXC	C8-C9-C10	2.45	113.53	110.49
3	A	602	PJM	CAP-CBO-CAW	2.45	121.62	118.16
3	B	602	PJM	CAW-CBK-CBR	-2.44	119.50	122.41
3	A	611	PJM	CBP-CAX-CBQ	-2.43	117.47	121.31
3	B	602	PJM	C6-N1-C2	2.41	118.88	115.80
4	A	610	DXC	C14-C13-C12	-2.41	108.77	111.24
4	A	610	DXC	C20-C12-C13	2.40	111.51	109.07
4	A	605	DXC	C18-C4-C10	-2.39	107.88	111.18
4	A	606	DXC	C12-C11-C9	-2.39	112.07	114.71
4	A	608	DXC	C20-C12-C13	2.38	111.49	109.07
3	A	611	PJM	CAI-CBH-CAH	-2.38	119.67	122.83
3	B	602	PJM	CAP-CBO-CAW	2.38	121.52	118.16
4	A	610	DXC	C10-C14-C13	-2.37	111.17	114.30
4	A	606	DXC	C11-C12-C13	2.37	109.61	107.40
4	A	606	DXC	C2-C3-C7	-2.36	107.41	111.74
4	A	609	DXC	C8-C9-C10	2.34	113.39	110.49
4	A	607	DXC	C3-C2-C1	-2.33	109.33	112.76
4	A	607	DXC	C20-C12-C13	2.33	111.44	109.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	609	DXC	C16-C17-C19	-2.31	108.58	112.15
3	A	611	PJM	CAJ-CAN-CBN	-2.30	117.82	121.13
4	A	603	DXC	C16-C17-C19	-2.28	108.61	112.15
2	B	601	HEM	CHC-C4B-C3B	-2.28	121.08	124.57
2	A	601	HEM	CHB-C1B-C2B	-2.27	120.45	126.72
3	A	602	PJM	C6-N1-C2	2.25	118.68	115.80
3	B	602	PJM	CAO-CBN-CBS	-2.25	117.00	120.44
2	A	601	HEM	CAD-CBD-CGD	-2.25	108.76	113.60
3	B	602	PJM	C2-N3-C4	2.25	121.28	117.78
4	A	605	DXC	C8-C9-C10	2.24	113.28	110.49
4	A	610	DXC	C18-C4-C10	-2.23	108.11	111.18
4	A	608	DXC	C18-C4-C10	-2.22	108.13	111.18
4	A	605	DXC	C10-C14-C13	-2.20	111.40	114.30
4	A	607	DXC	C24-C19-C17	-2.19	109.57	112.92
4	A	610	DXC	C8-C9-C11	-2.17	108.38	112.08
4	A	605	DXC	C22-C21-C19	-2.17	110.56	114.52
2	B	601	HEM	CBA-CAA-C2A	-2.16	108.94	112.62
4	A	608	DXC	C5-C4-C3	2.15	110.95	107.77
4	A	603	DXC	C8-C7-C3	-2.15	107.53	111.84
3	A	602	PJM	CAY-CBV-NBE	-2.14	106.72	110.45
2	B	601	HEM	CHB-C1B-C2B	-2.13	120.82	126.72
4	A	607	DXC	C18-C4-C10	-2.13	108.25	111.18
4	A	603	DXC	C24-C19-C17	-2.13	109.66	112.92
4	A	605	DXC	C16-C17-C19	-2.11	108.88	112.15
4	A	609	DXC	C21-C22-C23	-2.10	106.94	112.51
4	A	610	DXC	C11-C9-C10	-2.10	106.28	109.09
4	A	610	DXC	C16-C15-C11	-2.10	100.97	105.13
3	A	602	PJM	C2-N3-C4	2.09	121.04	117.78
4	A	604	DXC	C16-C17-C19	-2.08	108.93	112.15
4	A	603	DXC	O3-C23-C22	-2.08	116.41	123.08
4	A	608	DXC	C21-C22-C23	-2.07	107.02	112.51
4	A	605	DXC	C21-C22-C23	-2.06	107.03	112.51
4	A	603	DXC	C10-C14-C13	-2.05	111.59	114.30
4	A	607	DXC	C5-C4-C10	-2.05	108.14	111.35
4	A	604	DXC	C5-C4-C3	2.04	110.79	107.77
2	B	601	HEM	C4B-C3B-C2B	-2.04	105.50	107.11
4	A	608	DXC	C16-C17-C12	-2.03	101.56	103.55
4	A	606	DXC	C21-C22-C23	-2.02	107.15	112.51
2	A	601	HEM	CHC-C4B-C3B	-2.02	121.48	124.57

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	603	DXC	C10
4	A	604	DXC	C10
4	A	605	DXC	C10
4	A	606	DXC	C10
4	A	607	DXC	C10
4	A	608	DXC	C10
4	A	609	DXC	C10
4	A	610	DXC	C10

All (70) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	611	PJM	CAY-CBV-NBE-CBG
3	B	602	PJM	CBR-CBV-NBE-CBG
4	A	608	DXC	C12-C17-C19-C24
4	A	606	DXC	C16-C17-C19-C24
4	A	606	DXC	C12-C17-C19-C24
4	A	606	DXC	C16-C17-C19-C21
4	A	608	DXC	C12-C17-C19-C21
4	A	608	DXC	C24-C19-C21-C22
4	A	610	DXC	C24-C19-C21-C22
4	A	608	DXC	C16-C17-C19-C24
4	A	606	DXC	C12-C17-C19-C21
4	A	608	DXC	C16-C17-C19-C21
4	A	604	DXC	C24-C19-C21-C22
4	A	610	DXC	C12-C17-C19-C24
4	A	608	DXC	C17-C19-C21-C22
4	A	603	DXC	C24-C19-C21-C22
4	A	604	DXC	C17-C19-C21-C22
4	A	606	DXC	C17-C19-C21-C22
4	A	610	DXC	C17-C19-C21-C22
4	A	606	DXC	C24-C19-C21-C22
4	A	603	DXC	C12-C17-C19-C24
4	A	610	DXC	C12-C17-C19-C21
3	A	611	PJM	CAN-CBN-CBS-NBC
4	A	607	DXC	C19-C21-C22-C23
4	A	609	DXC	C16-C17-C19-C21
3	A	602	PJM	CBR-CBV-NBE-CBG
3	A	611	PJM	CAO-CBN-CBS-NBC
4	A	603	DXC	C12-C17-C19-C21
3	A	611	PJM	C5-C4-CBQ-CAX
3	B	602	PJM	N3-C4-CBQ-CAV
3	A	611	PJM	C5-C4-CBQ-CAV

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	602	PJM	C5-C4-CBQ-CAV
3	B	602	PJM	N3-C4-CBQ-CAX
3	A	602	PJM	N3-C4-CBQ-CAV
3	A	611	PJM	N3-C4-CBQ-CAX
3	A	602	PJM	N3-C4-CBQ-CAX
4	A	610	DXC	C16-C17-C19-C24
4	A	603	DXC	C16-C17-C19-C24
3	B	602	PJM	C5-C4-CBQ-CAX
4	A	606	DXC	C19-C21-C22-C23
3	A	611	PJM	CAQ-CBR-CBV-CAY
3	A	602	PJM	C5-C4-CBQ-CAV
4	A	603	DXC	C16-C17-C19-C21
4	A	610	DXC	C16-C17-C19-C21
4	A	610	DXC	C19-C21-C22-C23
3	A	611	PJM	OAA-CBG-CBL-CAJ
4	A	606	DXC	C21-C22-C23-O3
3	A	611	PJM	CBV-CAY-NBW-CAT
3	A	602	PJM	C5-C4-CBQ-CAX
3	A	611	PJM	N3-C4-CBQ-CAV
2	B	601	HEM	CAA-CBA-CGA-O2A
2	B	601	HEM	CAD-CBD-CGD-O2D
4	A	608	DXC	C21-C22-C23-O4
4	A	604	DXC	C19-C21-C22-C23
3	A	611	PJM	CBK-CBR-CBV-CAY
2	B	601	HEM	CAA-CBA-CGA-O1A
2	A	601	HEM	CAD-CBD-CGD-O2D
4	A	608	DXC	C21-C22-C23-O3
2	B	601	HEM	CAD-CBD-CGD-O1D
4	A	606	DXC	C21-C22-C23-O4
4	A	610	DXC	C21-C22-C23-O4
4	A	607	DXC	C21-C22-C23-O3
2	A	601	HEM	CAD-CBD-CGD-O1D
4	A	605	DXC	C21-C22-C23-O4
4	A	610	DXC	C21-C22-C23-O3
3	A	611	PJM	CAU-CBP-CBT-NBD
4	A	605	DXC	C21-C22-C23-O3
4	A	609	DXC	C16-C17-C19-C24
4	A	603	DXC	C21-C22-C23-O3
3	A	611	PJM	CBV-CAY-NBW-CAR

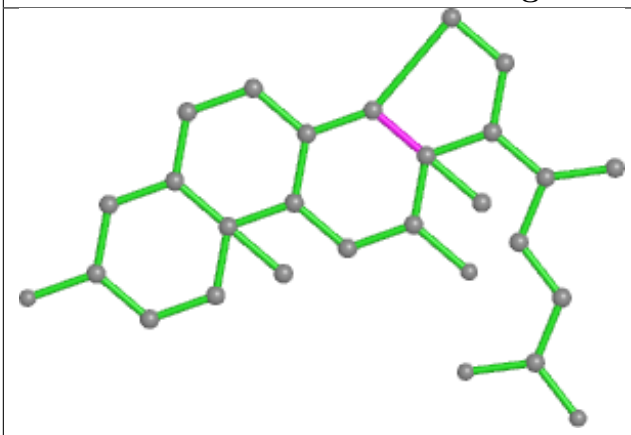
All (6) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	609	DXC	C1-C2-C3-C4-C5-C6
4	A	610	DXC	C1-C2-C3-C4-C5-C6
4	A	606	DXC	C1-C2-C3-C4-C5-C6
4	A	608	DXC	C1-C2-C3-C4-C5-C6
4	A	605	DXC	C1-C2-C3-C4-C5-C6
4	A	607	DXC	C1-C2-C3-C4-C5-C6

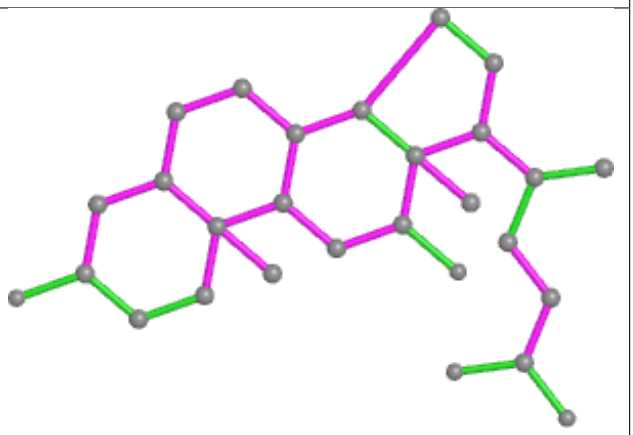
No monomer is involved in short contacts.

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.

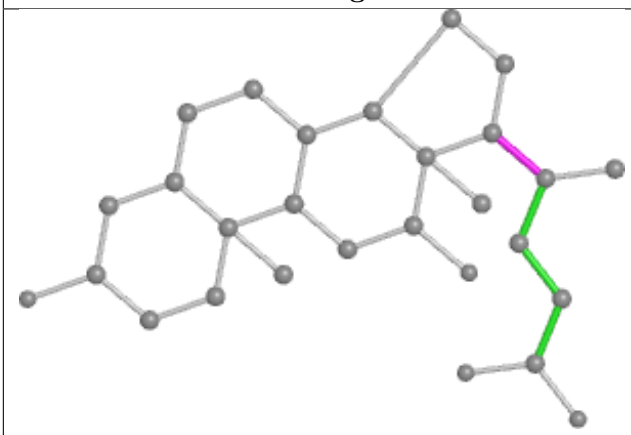
Ligand DXC A 609



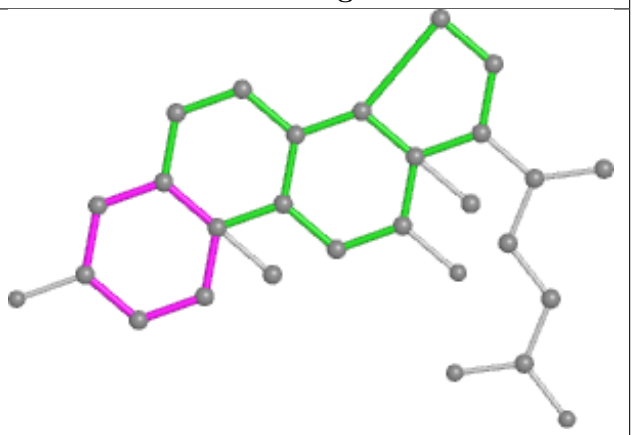
Bond lengths



Bond angles

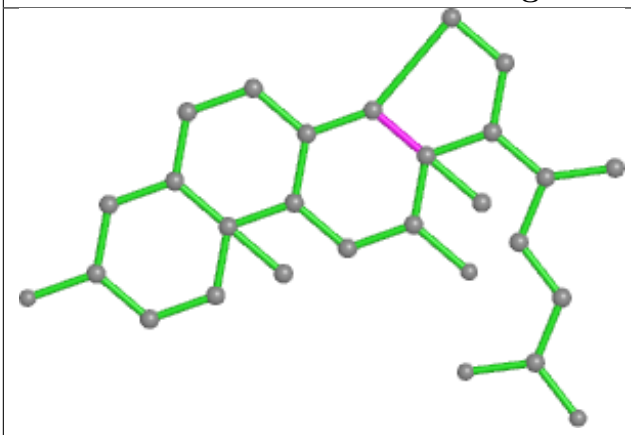


Torsions

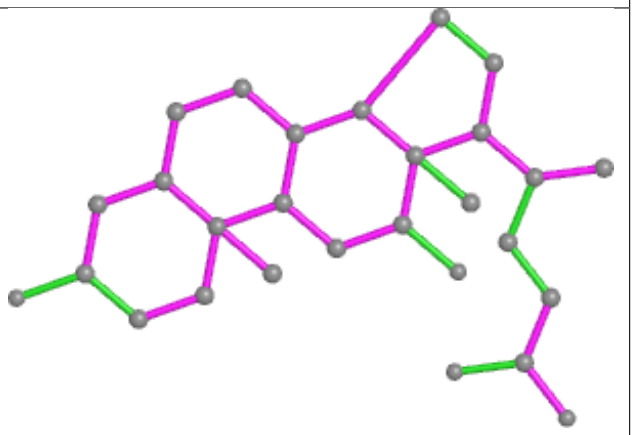


Rings

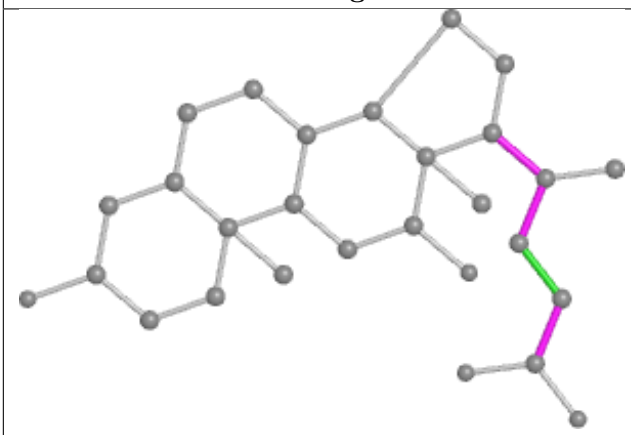
Ligand DXC A 603



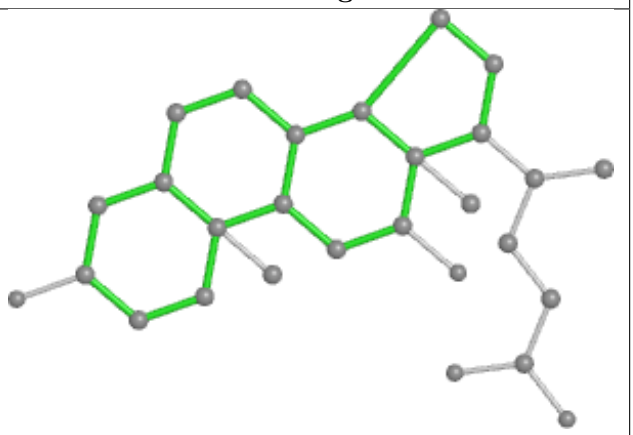
Bond lengths



Bond angles

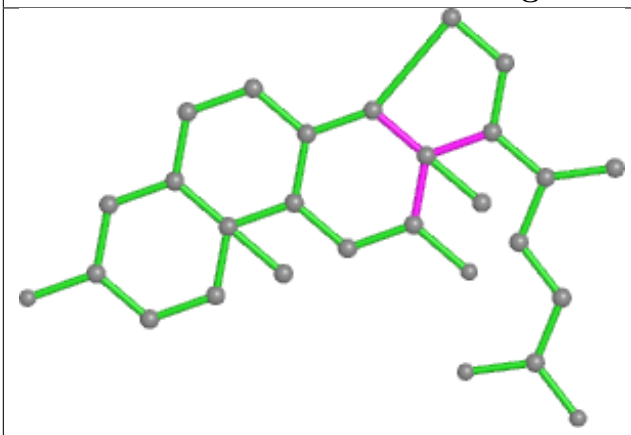


Torsions

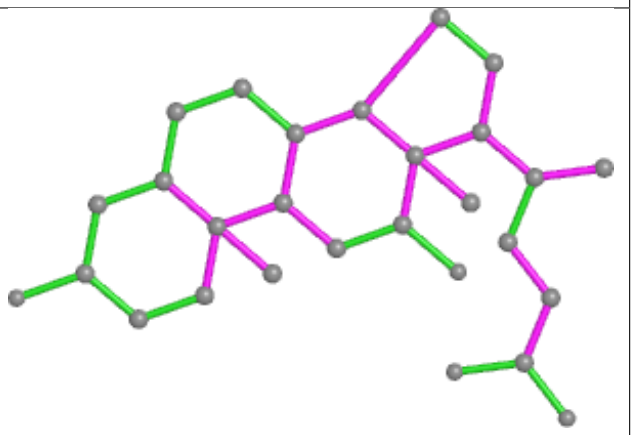


Rings

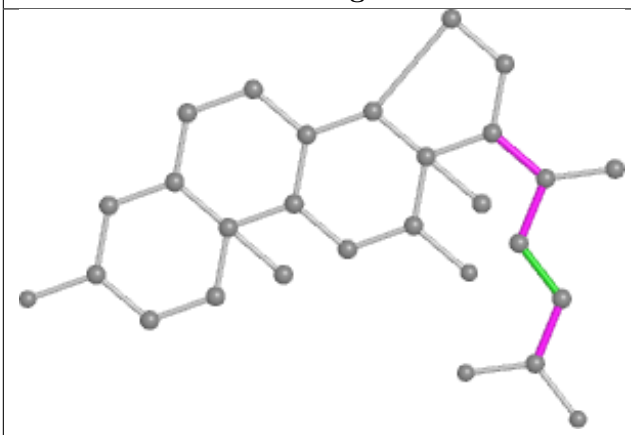
Ligand DXC A 608



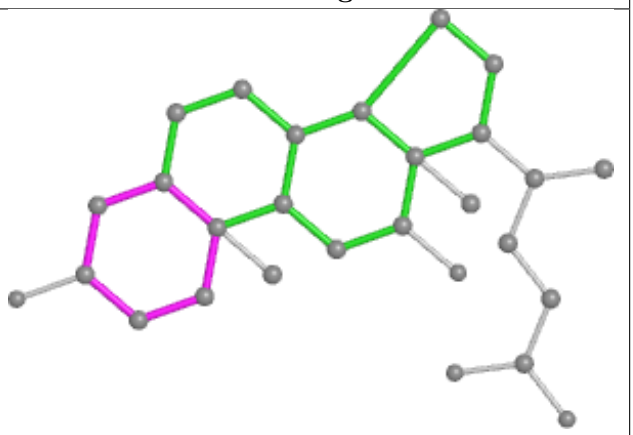
Bond lengths



Bond angles

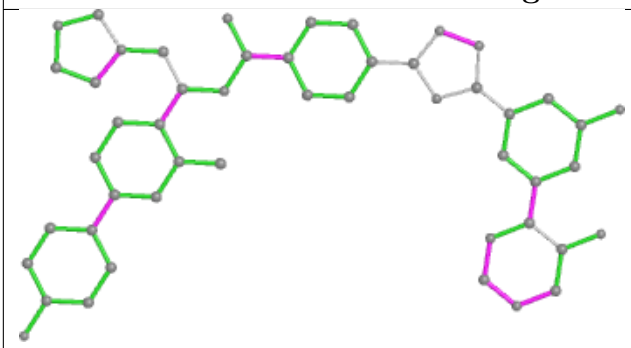


Torsions

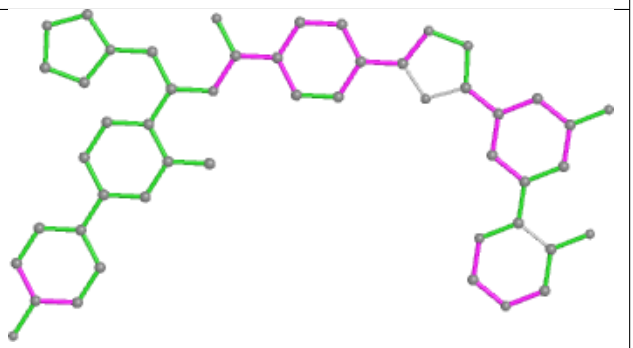


Rings

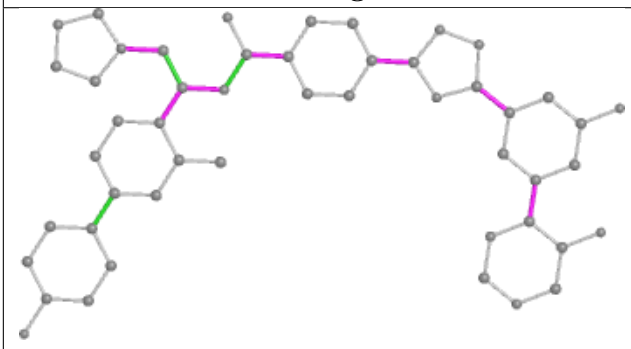
Ligand PJM A 611



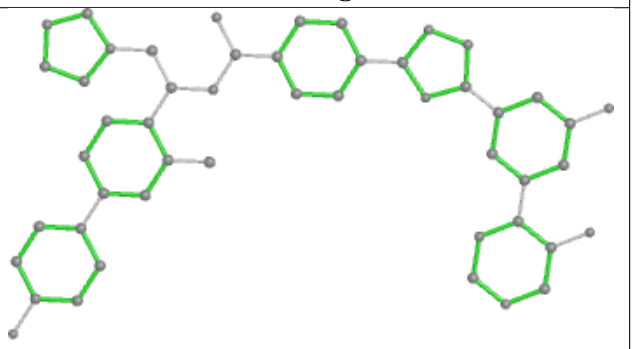
Bond lengths



Bond angles

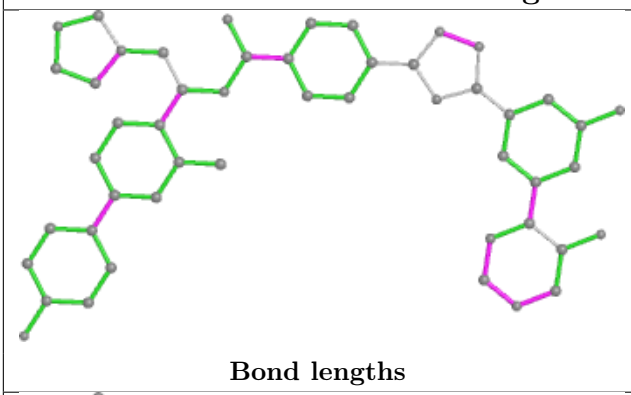


Torsions

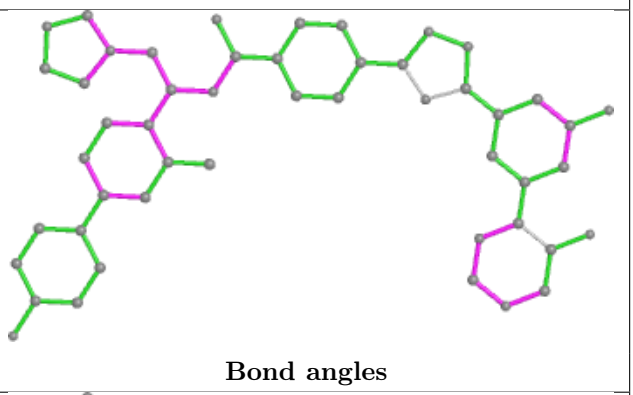


Rings

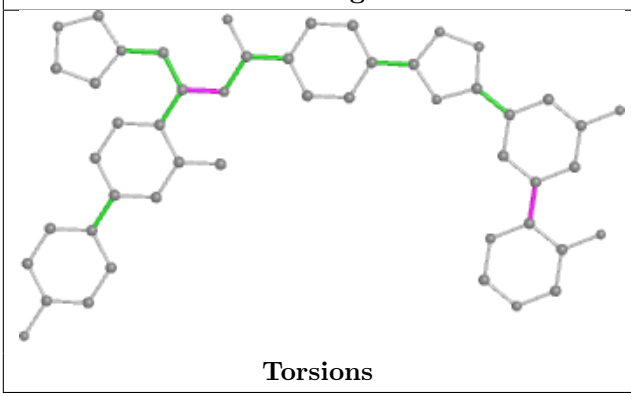
Ligand PJM A 602



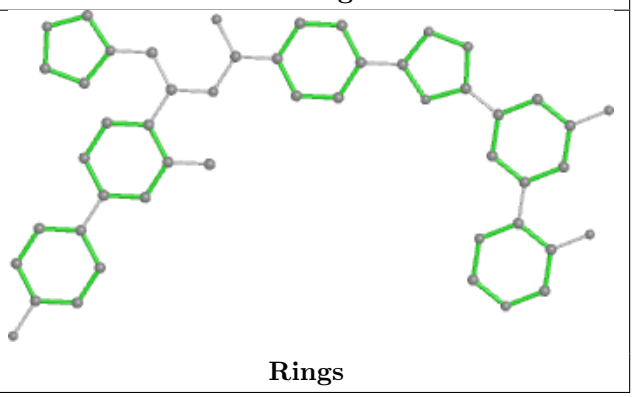
Bond lengths



Bond angles

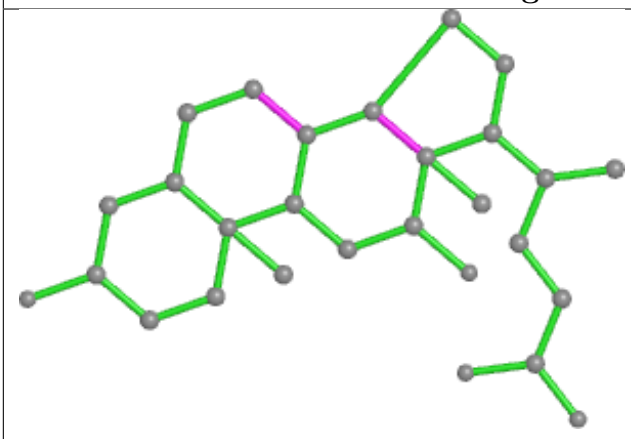


Torsions

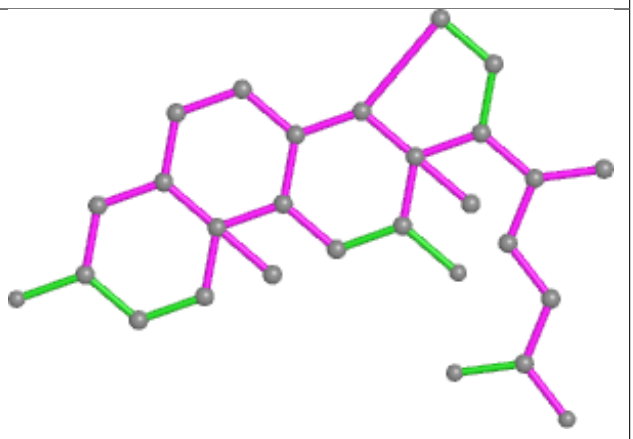


Rings

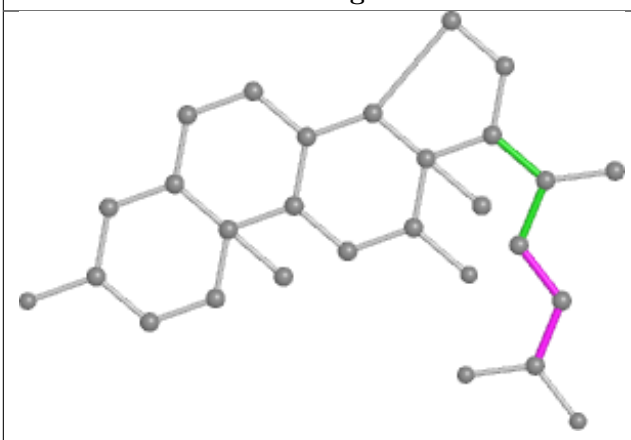
Ligand DXC A 607



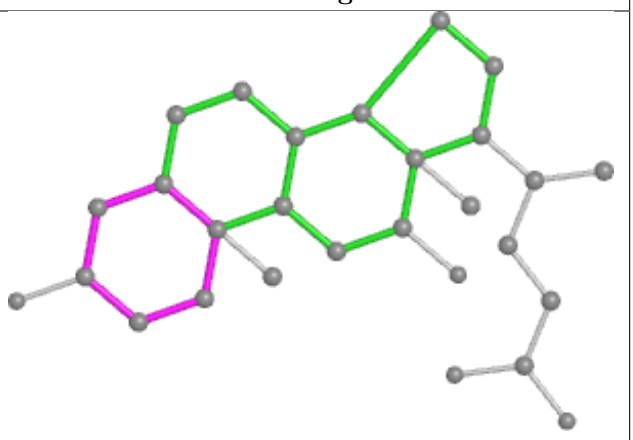
Bond lengths



Bond angles

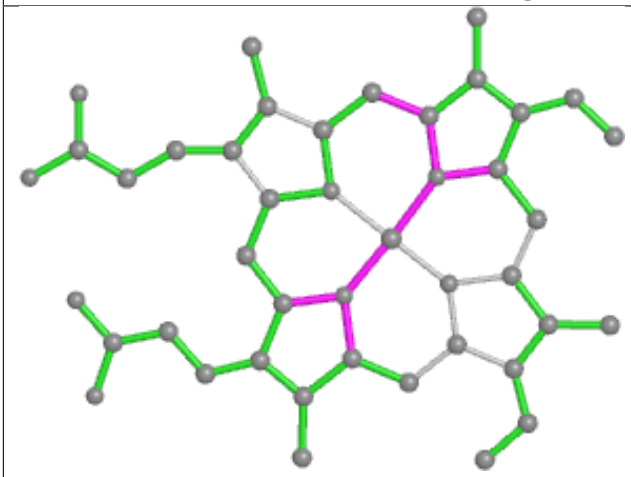


Torsions

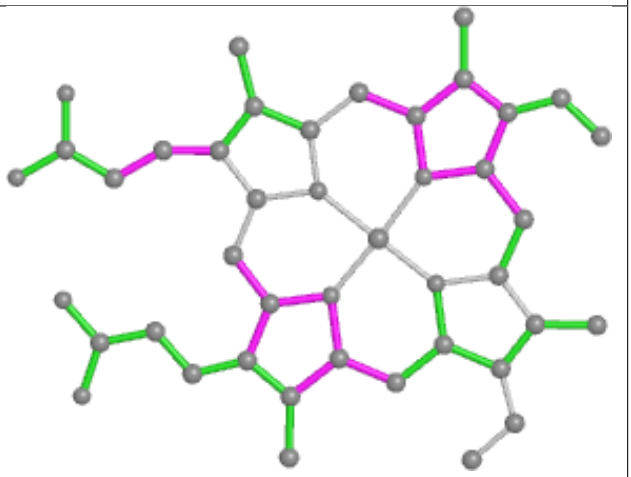


Rings

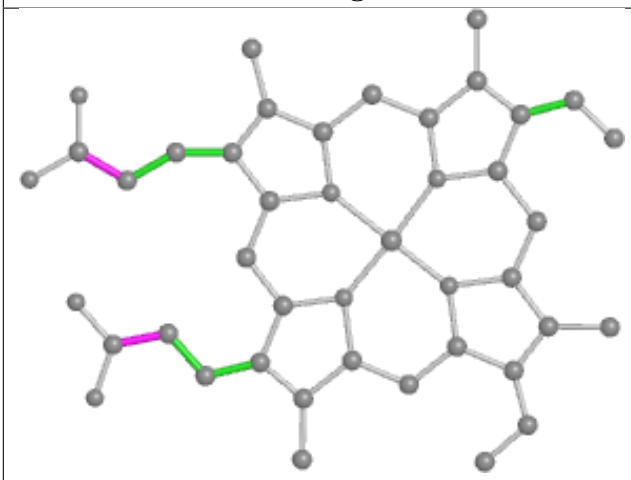
Ligand HEM B 601



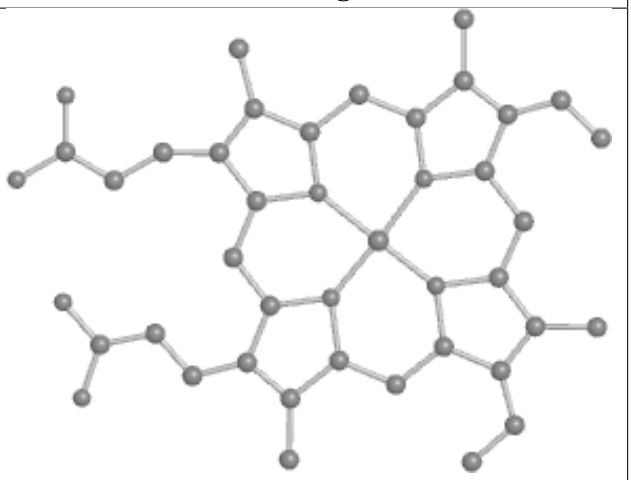
Bond lengths



Bond angles

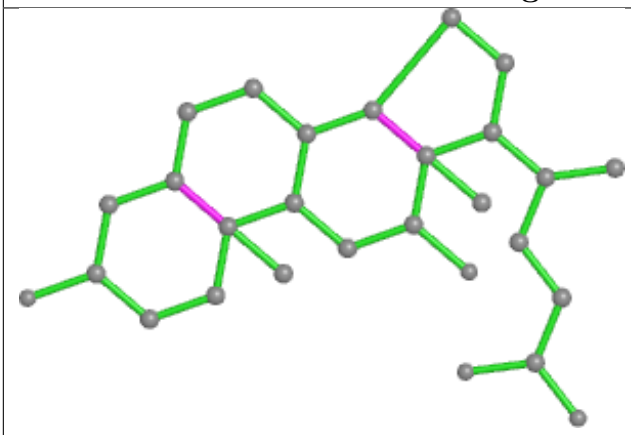


Torsions

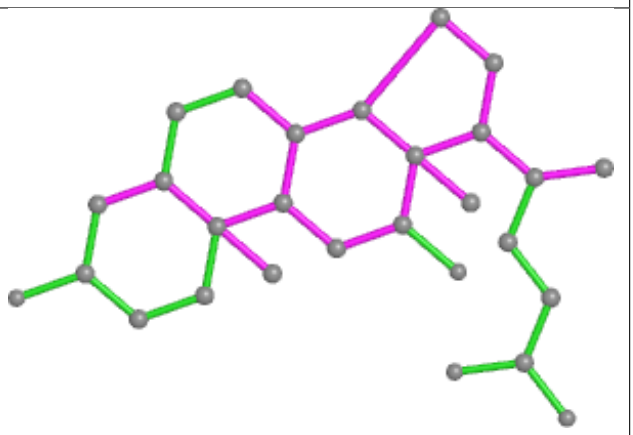


Rings

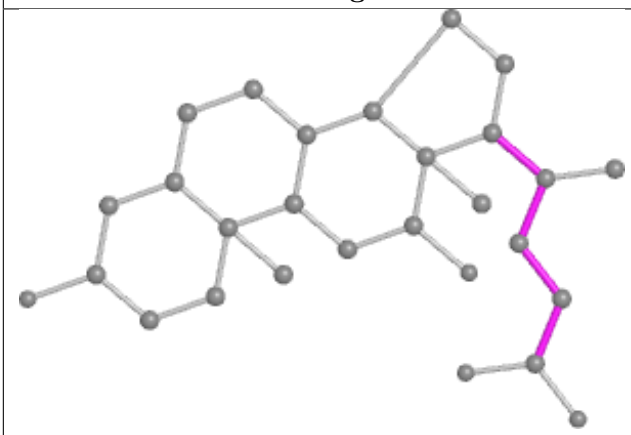
Ligand DXC A 610



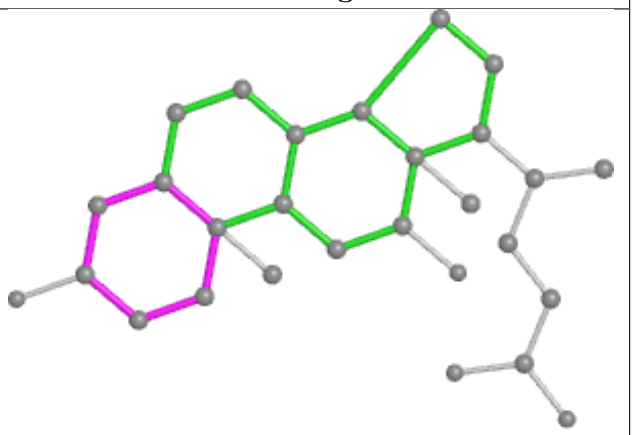
Bond lengths



Bond angles

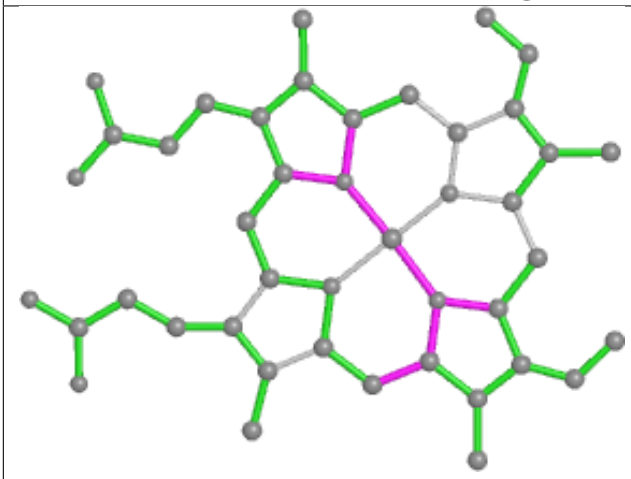


Torsions

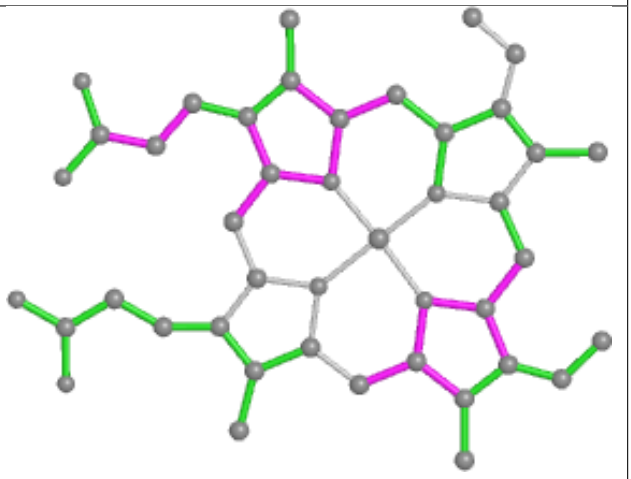


Rings

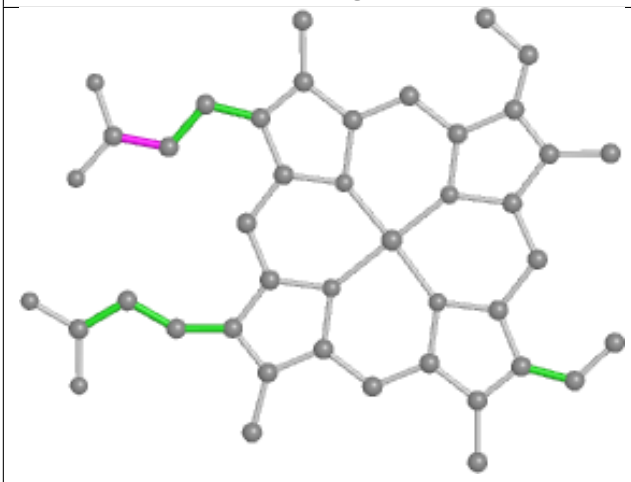
Ligand HEM A 601



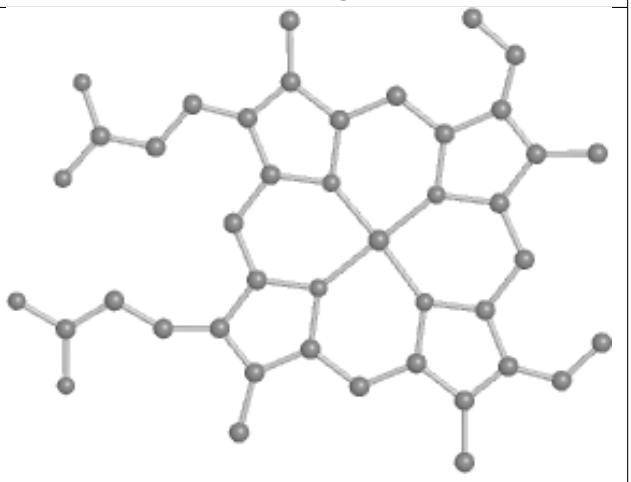
Bond lengths



Bond angles

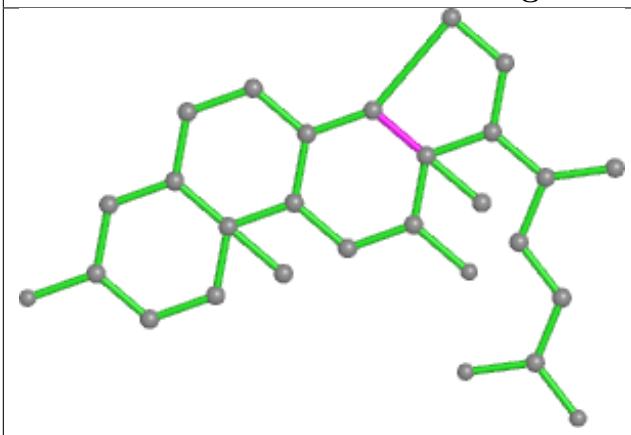


Torsions

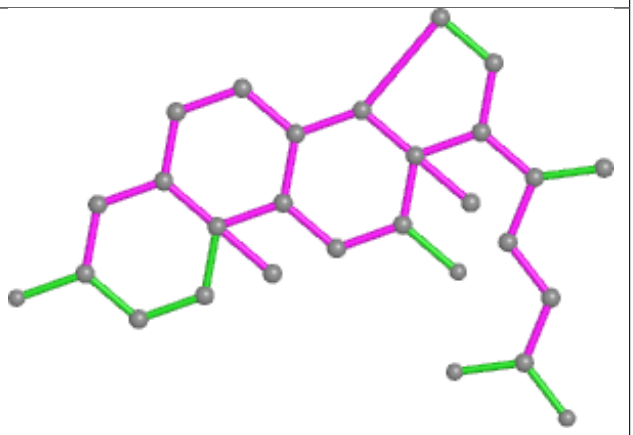


Rings

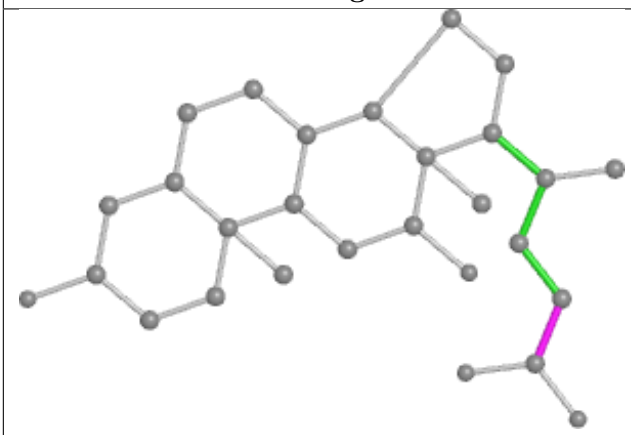
Ligand DXC A 605



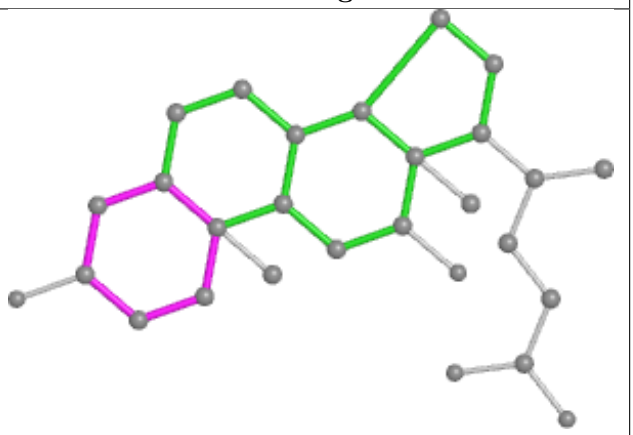
Bond lengths



Bond angles

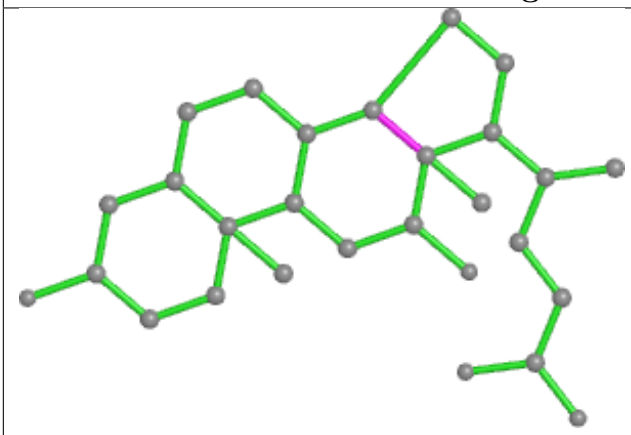


Torsions

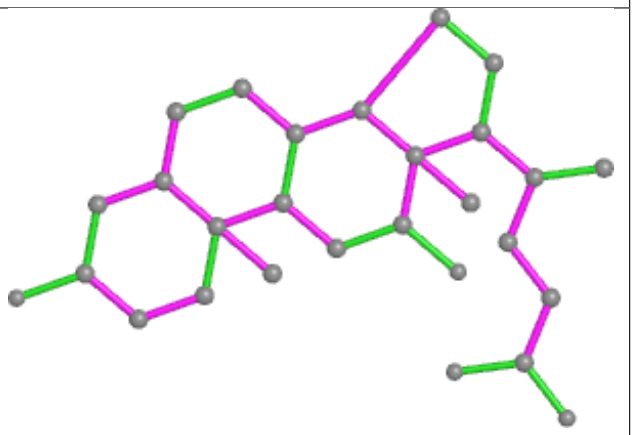


Rings

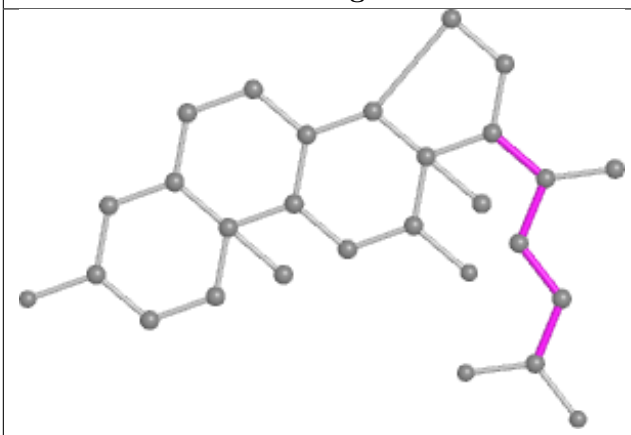
Ligand DXC A 606



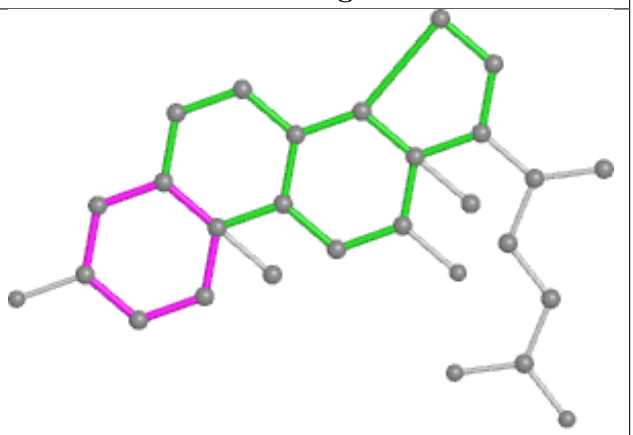
Bond lengths



Bond angles

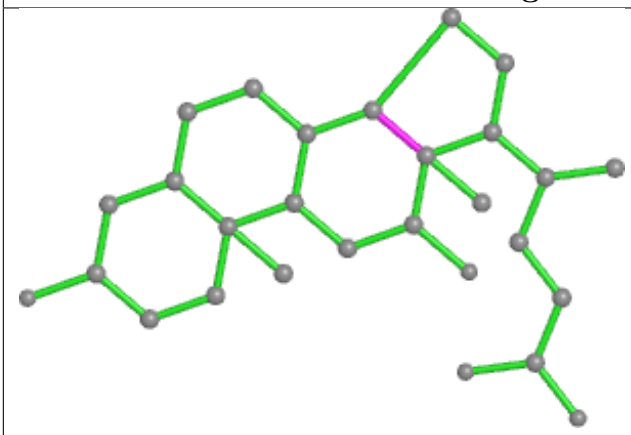


Torsions

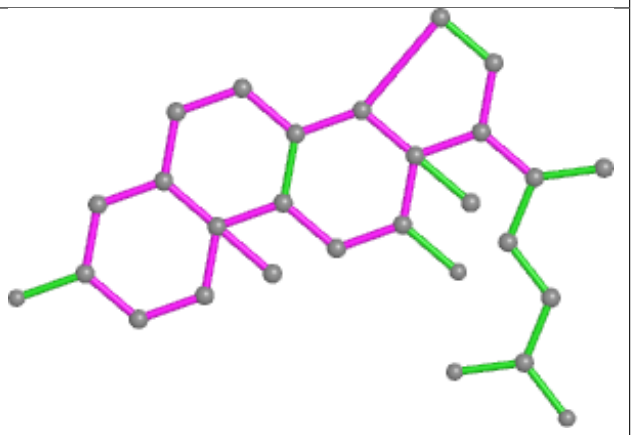


Rings

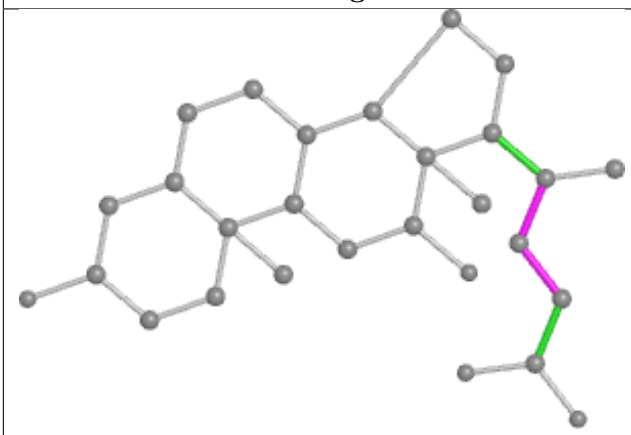
Ligand DXC A 604



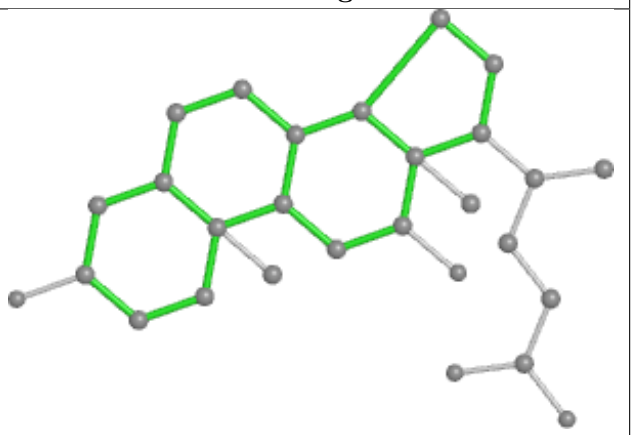
Bond lengths



Bond angles

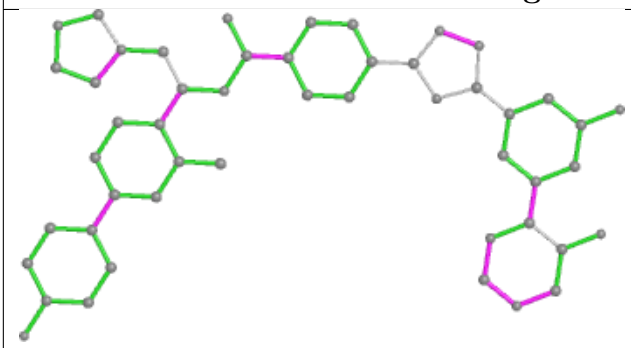


Torsions

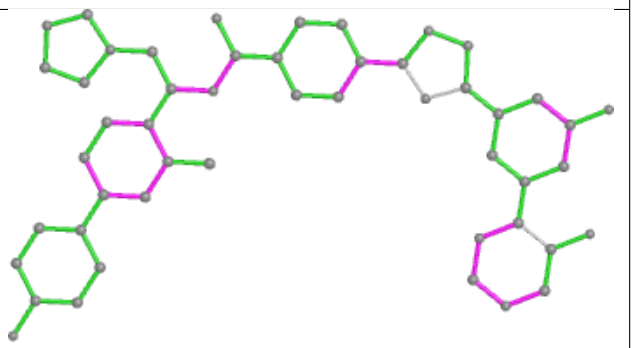


Rings

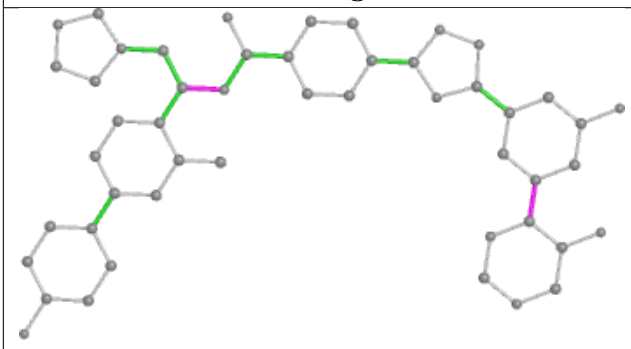
Ligand PJM B 602



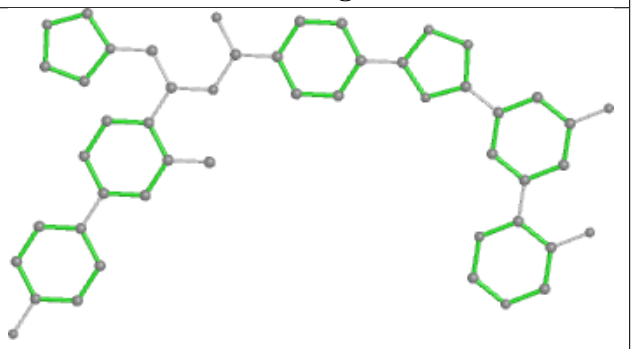
Bond lengths



Bond angles



Torsions



Rings

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

5.4 Ligands

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers

EDS failed to run properly - this section is therefore empty.