wwPDB X-ray Structure Validation Summary Report (i)

May 15, 2020 – 10:29 pm BST

PDB ID	:	1PFX
Title	:	PORCINE FACTOR IXA
Authors	:	Brandstetter, H.; Bauer, M.; Huber, R.; Lollar, P.; Bode, W.
Deposited on	:	1995-07-19
Resolution	:	3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

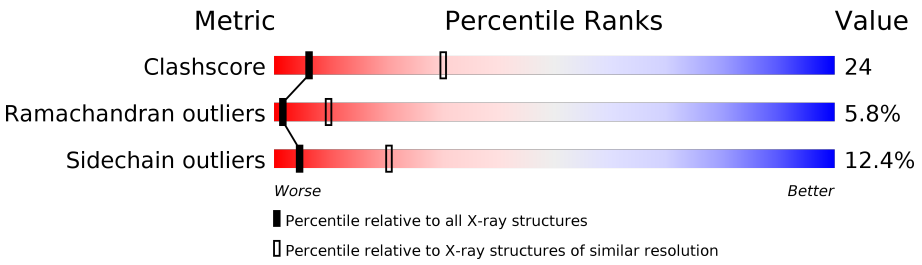
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.00 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))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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 on 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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	235	49% 41% 8% •
2	L	146	64% 29% 8%

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
3	0G6	C	301[A]	X	-	-	-
3	0G6	C	301[B]	X	-	-	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3738 atoms, of which 692 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 FACTOR IXA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	C	235	2249	1170	414	312	345	8	444	0	0

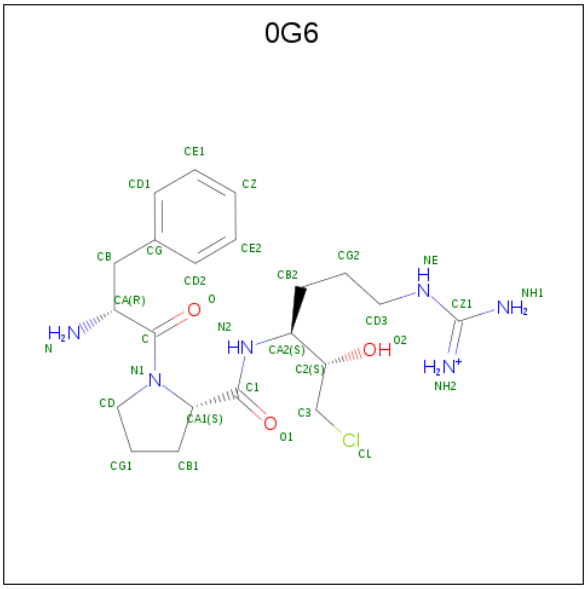
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	174	PHE	VAL	CONFLICT	UNP P16293
C	192	GLN	LEU	CONFLICT	UNP P16293

- Molecule 2 is a protein called FACTOR IXA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	L	146	1449	712	269	198	255	15	805	0	0

- Molecule 3 is D-phenylalanyl-N-[(2S,3S)-6-{[amino(iminio)methyl]amino}-1-chloro-2-hydroxyhexan-3-yl]-L-prolinamide (three-letter code: 0G6) (formula: $C_{21}H_{34}ClN_6O_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
3	C	1	40	21	9	6	4	11	1

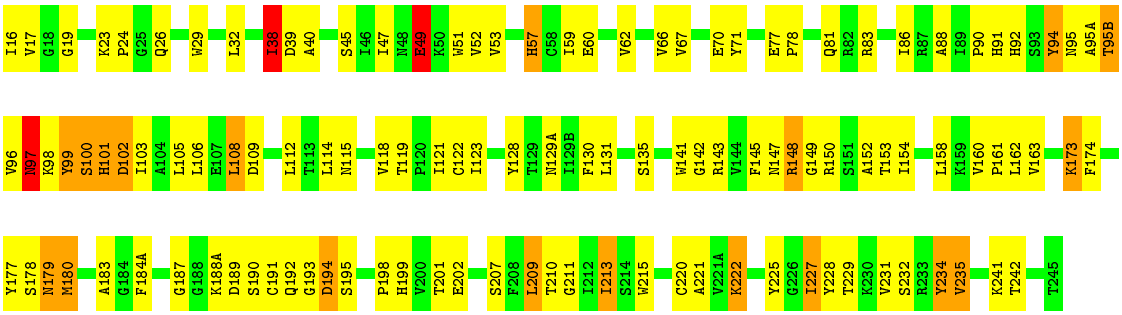
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

Note EDS was not executed.

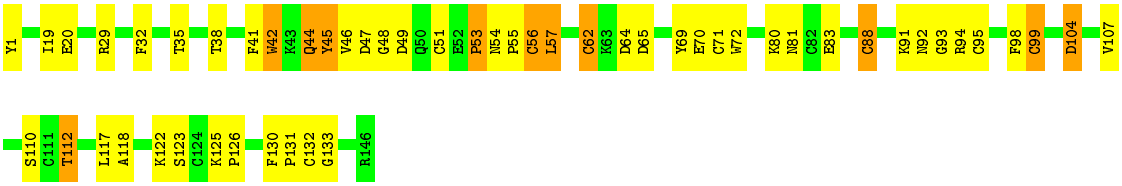
- Molecule 1: FACTOR IXA

Chain C:



- Molecule 2: FACTOR IXA

Chain L:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	128.75Å 128.75Å 77.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-3.00)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.198 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3738	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

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: 0G6, CGU, BHD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	C	0.38	0/1879	0.67	1/2548 (0.0%)
2	L	0.53	2/1039 (0.2%)	1.07	7/1383 (0.5%)
All	All	0.44	2/2918 (0.1%)	0.84	8/3931 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	L	0	7

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	42	TRP	CD2-CE2	-6.13	1.33	1.41
2	L	42	TRP	CD1-NE1	-5.37	1.28	1.38

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	42	TRP	CB-CG-CD1	-9.77	114.30	127.00
2	L	42	TRP	CA-CB-CG	-9.32	96.00	113.70
2	L	29	ARG	NE-CZ-NH1	-7.47	116.56	120.30
2	L	42	TRP	CE2-CD2-CG	-5.99	102.50	107.30
2	L	29	ARG	NE-CZ-NH2	5.69	123.15	120.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	L	19	ILE	Mainchain,Peptide
2	L	20	CGU	Mainchain
2	L	32	PHE	Mainchain
2	L	35	THR	Peptide
2	L	45	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1835	414	1800	97	1
2	L	1180	269	1043	25	1
3	C	31	9	3	1	0
All	All	3046	692	2846	119	1

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 24.

The worst 5 of 119 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:C:47:ILE:HD13	1:C:53:VAL:HB	1.59	0.85
1:C:59:ILE:HD12	1:C:90:PRO:HG3	1.62	0.79
1:C:143:ARG:HA	1:C:150:ARG:O	1.86	0.76
1:C:19:GLY:HA2	1:C:158:LEU:HD13	1.68	0.76
2:L:51:CYS:HB2	2:L:64:BHD:HB	1.69	0.75

All (1) 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)
1:C:129(A):ASN:ND2	2:L:44:GLN:NE2[7_558]	2.14	0.06

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	233/235 (99%)	188 (81%)	33 (14%)	12 (5%)	2 12
2	L	131/146 (90%)	89 (68%)	33 (25%)	9 (7%)	1 6
All	All	364/381 (96%)	277 (76%)	66 (18%)	21 (6%)	1 10

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	38	ILE
1	C	49	GLU
1	C	95(B)	THR
1	C	100	SER
2	L	53	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	198/198 (100%)	174 (88%)	24 (12%)	5 21
2	L	117/117 (100%)	102 (87%)	15 (13%)	4 19
All	All	315/315 (100%)	276 (88%)	39 (12%)	4 20

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	213	ILE

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Mol	Chain	Res	Type
1	C	232	SER
2	L	99	CYS
1	C	220	CYS
1	C	222	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	26	GLN
1	C	91	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

13 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	CGU	L	7	-	3,11,12	0.70	0	1,14,16	0.04	0
2	CGU	L	33	2	3,11,12	0.55	0	1,14,16	0.60	0
2	CGU	L	27	2	3,11,12	0.73	0	1,14,16	0.26	0
2	CGU	L	36	2	3,11,12	0.92	0	1,14,16	1.33	0
2	CGU	L	15	2	3,11,12	0.70	0	1,14,16	0.05	0
2	CGU	L	40	2	3,11,12	1.40	1 (33%)	1,14,16	0.42	0
2	CGU	L	20	-	3,11,12	1.02	0	1,14,16	0.47	0
2	CGU	L	21	2	3,11,12	0.94	0	1,14,16	1.66	0
2	BHD	L	64	2	3,8,9	0.63	0	4,10,12	1.09	0
2	CGU	L	17	2	3,11,12	0.69	0	1,14,16	0.10	0
2	CGU	L	26	-	3,11,12	0.77	0	1,14,16	0.27	0
2	CGU	L	8	2	3,11,12	0.75	0	1,14,16	0.02	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	CGU	L	30	2	3,11,12	0.66	0	1,14,16	0.27	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CGU	L	7	-	-	0/5/14/16	-
2	CGU	L	33	2	-	0/5/14/16	-
2	CGU	L	27	2	-	1/5/14/16	-
2	CGU	L	36	2	-	2/5/14/16	-
2	CGU	L	15	2	-	2/5/14/16	-
2	CGU	L	40	2	-	4/5/14/16	-
2	CGU	L	20	-	-	2/5/14/16	-
2	CGU	L	21	2	-	4/5/14/16	-
2	BHD	L	64	2	-	2/5/10/12	-
2	CGU	L	17	2	-	2/5/14/16	-
2	CGU	L	26	-	-	0/5/14/16	-
2	CGU	L	8	2	-	2/5/14/16	-
2	CGU	L	30	2	-	4/5/14/16	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	40	CGU	CB-CG	-2.17	1.49	1.53

There are no bond angle outliers.

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L	36	CGU	CA-CB-CG-CD1
2	L	36	CGU	CA-CB-CG-CD2
2	L	40	CGU	N-CA-CB-CG
2	L	40	CGU	C-CA-CB-CG
2	L	40	CGU	CA-CB-CG-CD1

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	64	BHD	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	0G6	C	301[B]	-	30,30,32	13.48	2 (6%)	38,39,42	4.44	3 (7%)
3	0G6	C	301[A]	1	30,30,32	0.38	0	38,39,42	1.00	1 (2%)

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
3	0G6	C	301[B]	-	1/1/9/10	6/29/39/43	0/2/2/2
3	0G6	C	301[A]	1	1/1/9/10	4/29/39/43	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	301[B]	0G6	C2-CA2	69.52	2.66	1.52
3	C	301[B]	0G6	O2-C2	24.85	2.47	1.42

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	301[B]	0G6	O2-C2-CA2	-18.51	64.12	111.95
3	C	301[B]	0G6	CB2-CA2-C2	17.12	137.52	111.78
3	C	301[B]	0G6	C2-CA2-N2	-10.12	86.92	109.60
3	C	301[A]	0G6	O2-C2-CA2	-4.91	99.27	111.95

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	301[B]	0G6	C2
3	C	301[A]	0G6	C2

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	301[B]	0G6	N-CA-CB-CG
3	C	301[B]	0G6	C-CA-CB-CG
3	C	301[A]	0G6	N-CA-CB-CG
3	C	301[A]	0G6	C-CA-CB-CG
3	C	301[B]	0G6	O2-C2-CA2-CB2

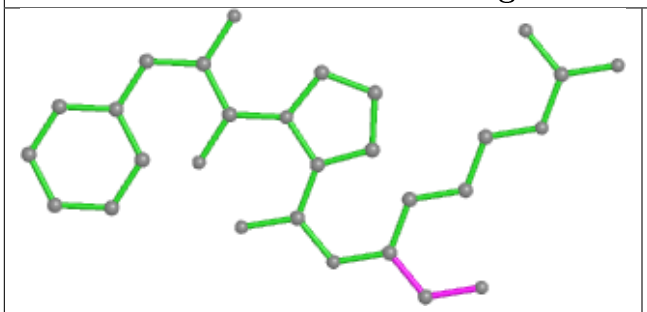
There are no ring outliers.

1 monomer is involved in 1 short contact:

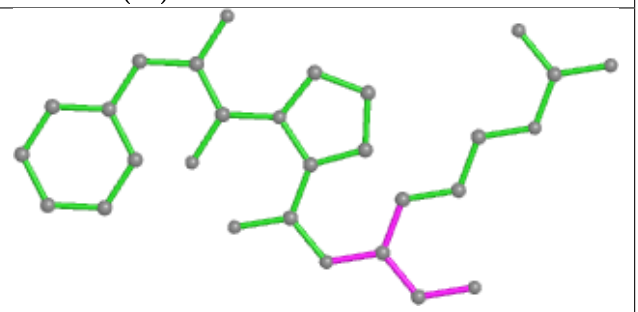
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	301[A]	0G6	1	0

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

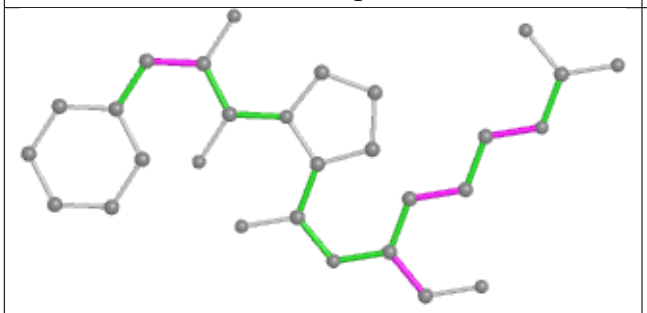
Ligand 0G6 C 301 (B)



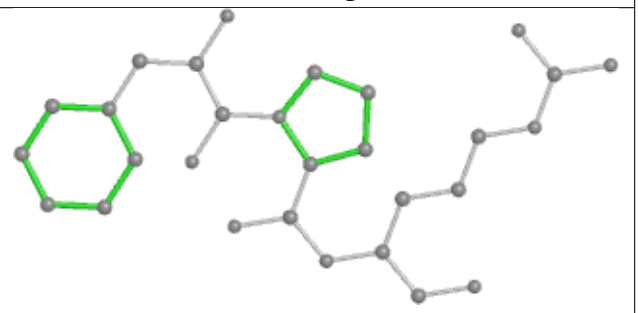
Bond lengths



Bond angles

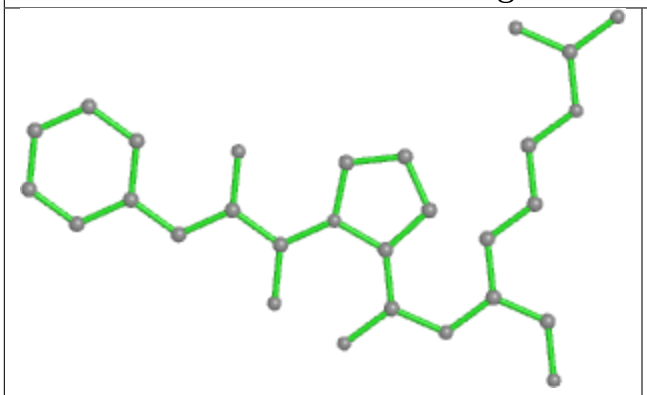


Torsions

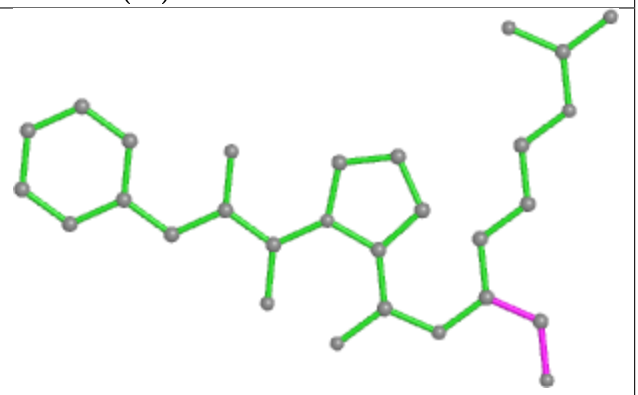


Rings

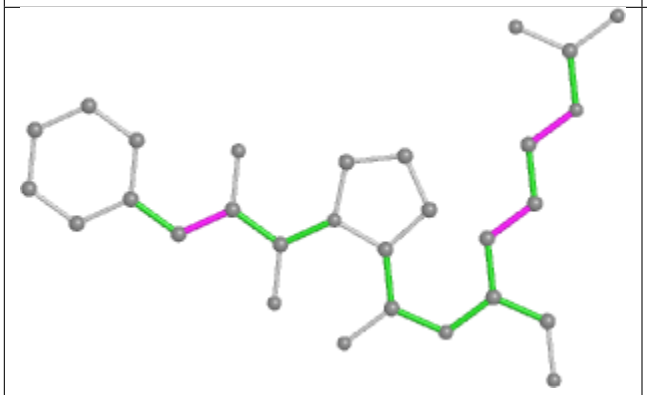
Ligand 0G6 C 301 (A)



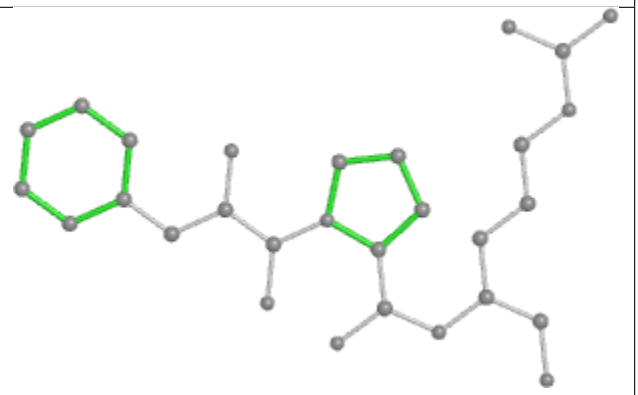
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.