

Full wwPDB X-ray Structure Validation Report (i)

Oct 5, 2023 – 02:15 AM EDT

PDB ID	:	6VGC
Title	:	Crystal Structures of FLAP bound to DG-031
Authors	:	Ho, J.D.; Lee, M.R.; Rauch, C.T.; Aznavour, K.; Park, J.S.; Luz, J.G.;
		Antonysamy, S.; Condon, B.; Maletic, M.; Zhang, A.; Hickey, M.J.; Hughes,
		N.E.; Chandrasekhar, S.; Sloan, A.V.; Gooding, K.; Harvey, A.; Yu, X.P.;
		Kahl, S.D.; Norman, B.H.
Deposited on		
Resolution	:	2.37 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 (1)) were used in the production of this report:

MolProbity		
		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: $X\hbox{-}RAY\,DIFFRACTION$

The reported resolution of this entry is 2.37 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.



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7340 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.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	А	144	Total	С	Ν	0	S	0	0	0
	A	144	1134	757	175	198	4	0	0	0
1	В	149	Total	С	Ν	0	S	0	0	0
	D	149	1174	782	184	204	4		0	0
1	С	151	Total	С	Ν	0	S	0	0	0
	U	101	1191	796	183	208	4			
1	D	155	Total	С	Ν	0	S	0	0	0
	D	100	1221	815	187	215	4	0	0	U
1	Е	154	Total	С	Ν	0	S	0	0	0
	Ľ	104	1225	815	194	212	4	0	0	0
1	F	148	Total	С	Ν	0	S	0	0	0
	Г	140	1152	772	174	202	4		0	U

• Molecule 1 is a protein called 5-lipoxygenase-activating protein.

There are 72 discrepancies between the modelled and reference sequences:

A0SER-expression tagUNPA1LEU-expression tagUNPA148ALALYSconflictUNPA162GLU-expression tagUNPA163GLY-expression tagUNPA164HIS-expression tagUNPA165HIS-expression tagUNPA166HIS-expression tagUNPA166HIS-expression tagUNPA167HIS-expression tagUNPA168HIS-expression tagUNPA169HIS-expression tagUNP	Chain	Residue	Modelled	Actual	Comment	Reference
A1LEU-expression tagUNPA148ALALYSconflictUNPA162GLU-expression tagUNPA163GLY-expression tagUNPA164HIS-expression tagUNPA165HIS-expression tagUNPA166HIS-expression tagUNPA166HIS-expression tagUNPA167HIS-expression tagUNPA168HIS-expression tagUNPA169HIS-expression tagUNP	А	-1	MET	-	initiating methionine	UNP P20292
A148ALALYSconflictUNPA162GLU-expression tagUNPA163GLY-expression tagUNPA164HIS-expression tagUNPA165HIS-expression tagUNPA166HIS-expression tagUNPA166HIS-expression tagUNPA167HIS-expression tagUNPA168HIS-expression tagUNPA169HIS-expression tagUNP	А	0	SER	-	expression tag	UNP P20292
A162GLU-expression tagUNPA163GLY-expression tagUNPA164HIS-expression tagUNPA165HIS-expression tagUNPA166HIS-expression tagUNPA166HIS-expression tagUNPA167HIS-expression tagUNPA168HIS-expression tagUNPA169HIS-expression tagUNP	А	1	LEU	-	expression tag	UNP P20292
A163GLY-expression tagUNPA164HIS-expression tagUNPA165HIS-expression tagUNPA166HIS-expression tagUNPA167HIS-expression tagUNPA168HIS-expression tagUNPA169HIS-expression tagUNP	А	148	ALA	LYS	conflict	UNP P20292
A164HIS-expression tagUNPA165HIS-expression tagUNPA166HIS-expression tagUNPA167HIS-expression tagUNPA168HIS-expression tagUNPA169HIS-expression tagUNP	А	162	GLU	-	expression tag	UNP P20292
A165HIS-expression tagUNPA166HIS-expression tagUNPA167HIS-expression tagUNPA168HIS-expression tagUNPA169HIS-expression tagUNP	A	163	GLY	-	expression tag	UNP P20292
A166HIS-expression tagUNPA167HIS-expression tagUNPA168HIS-expression tagUNPA169HIS-expression tagUNP	А	164	HIS	-	expression tag	UNP P20292
A167HIS-expression tagUNPA168HIS-expression tagUNPA169HIS-expression tagUNP	А	165	HIS	-	expression tag	UNP P20292
A168HIS-expression tagUNPA169HIS-expression tagUNP	А	166	HIS	-	expression tag	UNP P20292
A 169 HIS - expression tag UNP	А	167	HIS	-	expression tag	UNP P20292
1 0	А	168	HIS	-	expression tag	UNP P20292
B -1 MET - initiating methionine UNP	А	169	HIS	-	expression tag	UNP P20292
	В	-1	MET	-	initiating methionine	UNP P20292
B0SER-expression tagUNP	В	0	SER	-	expression tag	UNP P20292
B1LEU-expression tagUNP	В	1	LEU	-	expression tag	UNP P20292
B 148 ALA LYS conflict UNP	В	148	ALA	LYS	conflict	UNP P20292
B 162 GLU - expression tag UNP	В	162	GLU	-	expression tag	UNP P20292



6VGC

	Continued from previous page Chain Residue Modelled Actual Comment						
Chain	Residue		Actual	Comment	Reference		
B	163	GLY	-	expression tag	UNP P20292		
B	164	HIS	-	expression tag	UNP P20292		
B	165	HIS	-	expression tag	UNP P20292		
B	166	HIS	-	expression tag	UNP P20292		
B	167	HIS	-	expression tag	UNP P20292		
В	168	HIS	-	expression tag	UNP P20292		
В	169	HIS	-	expression tag	UNP P20292		
С	-1	MET	-	initiating methionine	UNP P20292		
С	0	SER	-	expression tag	UNP P20292		
С	1	LEU	-	expression tag	UNP P20292		
С	148	ALA	LYS	conflict	UNP P20292		
С	162	GLU	-	expression tag	UNP P20292		
С	163	GLY	-	expression tag	UNP P20292		
С	164	HIS	-	expression tag	UNP P20292		
С	165	HIS	-	expression tag	UNP P20292		
С	166	HIS	-	expression tag	UNP P20292		
С	167	HIS	-	expression tag	UNP P20292		
С	168	HIS	-	expression tag	UNP P20292		
С	169	HIS	-	expression tag	UNP P20292		
D	-1	MET	-	initiating methionine	UNP P20292		
D	0	SER	-	expression tag	UNP P20292		
D	1	LEU	-	expression tag	UNP P20292		
D	148	ALA	LYS	conflict	UNP P20292		
D	162	GLU	-	expression tag	UNP P20292		
D	163	GLY	-	expression tag	UNP P20292		
D	164	HIS	-	expression tag	UNP P20292		
D	165	HIS	-	expression tag	UNP P20292		
D	166	HIS	-	expression tag	UNP P20292		
D	167	HIS	-	expression tag	UNP P20292		
D	168	HIS	-	expression tag	UNP P20292		
D	169	HIS	-	expression tag	UNP P20292		
Е	-1	MET	-	initiating methionine	UNP P20292		
Е	0	SER	-	expression tag	UNP P20292		
Е	1	LEU	-	expression tag	UNP P20292		
Е	148	ALA	LYS	conflict	UNP P20292		
Е	162	GLU	-	expression tag	UNP P20292		
Е	163	GLY	-	expression tag	UNP P20292		
Е	164	HIS	-	expression tag	UNP P20292		
Е	165	HIS	-	expression tag	UNP P20292		
Е	166	HIS	-	expression tag	UNP P20292		
Е	167	HIS	-	expression tag	UNP P20292		
Е	168	HIS	-	expression tag	UNP P20292		
	· · · · ·	1	1	· · · · · · · · · · · · · · · · ·			

Continued from previous page...

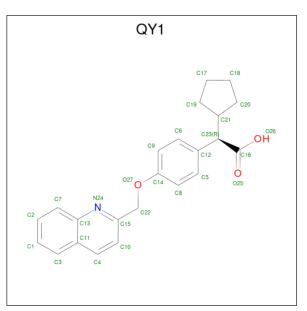


G	۲7	0	\cap
υ	v	G	U

Chain	Residue	Modelled	Actual	Comment	Reference
Е	169	HIS	-	expression tag	UNP P20292
F	-1	MET	-	initiating methionine	UNP P20292
F	0	SER	-	expression tag	UNP P20292
F	1	LEU	-	expression tag	UNP P20292
F	148	ALA	LYS	conflict	UNP P20292
F	162	GLU	-	expression tag	UNP P20292
F	163	GLY	-	expression tag	UNP P20292
F	164	HIS	-	expression tag	UNP P20292
F	165	HIS	-	expression tag	UNP P20292
F	166	HIS	-	expression tag	UNP P20292
F	167	HIS	-	expression tag	UNP P20292
F	168	HIS	-	expression tag	UNP P20292
F	169	HIS	-	expression tag	UNP P20292

Continued from previous page...

• Molecule 2 is (2R)-cyclopentyl{4-[(quinolin-2-yl)methoxy]phenyl}acetic acid (three-letter code: QY1) (formula: C₂₃H₂₃NO₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total C N O 27 23 1 3	0	0
			$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		
2	В	1	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	0	0
2	С	1	Total C N O	0	0
			27 23 1 3		
2	D	1	Total C N O	0	0
			27 23 1 3		



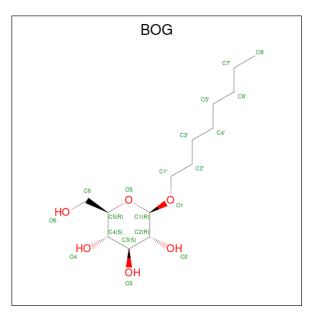
Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	Е	1	Total 0 27 2				0	0
2	F	1	Total 0 27 2	C 2 23			0	0

• Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	В	1	Total Ca 1 1	0	0
3	D	1	Total Ca 1 1	0	0

• Molecule 4 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	F	1	Total 20	C 14	O 6	0	0

• Molecule 5 is water.

-	Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
	5	А	11	Total O 11 11	0	0
	5	В	14	Total O 14 14	0	0



Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	С	10	Total O 10 10	0	0
5	D	8	Total O 8 8	0	0
5	Е	7	Total O 7 7	0	0
5	F	9	Total O 9 9	0	0

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



3 Data and refinement statistics (i)

Property	Value	Source	
Space group	P 1 21 1	Depositor	
Cell constants	65.91Å 101.49Å 111.86Å	Depositor	
a, b, c, α , β , γ	90.00° 99.83° 90.00°	Depositor	
Resolution (Å)	30.00 - 2.37	Depositor	
% Data completeness	97.7 (30.00-2.37)	Depositor	
(in resolution range)		-	
R _{merge}	(Not available)	Depositor	
R_{sym}	0.04	Depositor	
$< I/\sigma(I) > 1$	$3.43 (at 2.37 \text{\AA})$	Xtriage	
Refinement program	REFMAC 5.5.0109	Depositor	
R, R_{free}	0.254 , 0.285	Depositor	
Wilson B-factor $(Å^2)$	47.2	Xtriage	
Anisotropy	0.247	Xtriage	
L-test for twinning ²	$ < L >=0.49, < L^2>=0.32$	Xtriage	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	7340	wwPDB-VP	
Average B, all atoms $(Å^2)$	57.0	wwPDB-VP	

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

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.84% of the height of the origin peak. No significant pseudotranslation is detected.

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



¹Intensities estimated from amplitudes.

4 Model quality (i)

4.1 Standard geometry (i)

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

4.2 Too-close contacts (i)

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

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

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

4.3.2 Protein sidechains (i)

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

4.3.3 RNA (i)

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

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

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

4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond



Mol	Type Chain Res Li		Link	Bo	ond lengths		Bond angles		les	
	Type	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
2	QY1	D	201	-	29,30,30	0.85	0	38,41,41	0.71	0
2	QY1	В	201	-	29,30,30	0.86	0	38,41,41	0.76	1 (2%)
2	QY1	Е	201	-	29,30,30	0.85	0	38,41,41	0.75	1 (2%)
2	QY1	С	201	-	29,30,30	0.85	0	38,41,41	0.76	1 (2%)
4	BOG	F	202	-	20,20,20	0.51	0	$25,\!25,\!25$	0.60	0
2	QY1	А	201	-	29,30,30	0.85	0	38,41,41	0.81	1 (2%)
2	QY1	F	201	-	29,30,30	0.86	0	38,41,41	0.75	0

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).

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	QY1	D	201	-	-	0/17/24/24	0/4/4/4
2	QY1	В	201	-	-	0/17/24/24	0/4/4/4
2	QY1	Е	201	-	-	9/17/24/24	0/4/4/4
2	QY1	С	201	-	-	5/17/24/24	0/4/4/4
4	BOG	F	202	-	-	7/11/31/31	0/1/1/1
2	QY1	А	201	-	-	0/17/24/24	0/4/4/4
2	QY1	\mathbf{F}	201	-	-	7/17/24/24	0/4/4/4

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
2	А	201	QY1	C12-C23-C16	2.84	112.98	107.97
2	В	201	QY1	C12-C23-C16	2.42	112.23	107.97
2	Е	201	QY1	C12-C23-C16	2.21	111.86	107.97
2	С	201	QY1	C12-C23-C16	2.07	111.62	107.97

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms				
2	С	201	QY1	C19-C21-C23-C16				

Mol	Chain	Res	Type	Atoms
2	Е	201	QY1	C19-C21-C23-C12
2	Е	201	QY1	C19-C21-C23-C16
2	Е	201	QY1	C20-C21-C23-C12
2	Е	201	QY1	C20-C21-C23-C16
2	F	201	QY1	C20-C21-C23-C12
2	F	201	QY1	C20-C21-C23-C16
4	F	202	BOG	O5-C5-C6-O6
4	F	202	BOG	C4-C5-C6-O6
2	С	201	QY1	C9-C14-O27-C22
2	С	201	QY1	C8-C14-O27-C22
2	F	201	QY1	C8-C14-O27-C22
2	F	201	QY1	C9-C14-O27-C22
4	F	202	BOG	C2'-C1'-O1-C1
4	F	202	BOG	C3'-C4'-C5'-C6'
2	F	201	QY1	C6-C12-C23-C21
4	F	202	BOG	O1-C1'-C2'-C3'
2	F	201	QY1	C5-C12-C23-C21
2	С	201	QY1	C20-C21-C23-C12
2	F	201	QY1	C19-C21-C23-C12
2	С	201	QY1	C20-C21-C23-C16
4	F	202	BOG	C2'-C3'-C4'-C5'
2	Е	201	QY1	O25-C16-C23-C12
2	Е	201	QY1	O26-C16-C23-C12
4	F	202	BOG	C5'-C6'-C7'-C8'
2	Е	201	QY1	C5-C12-C23-C16
2	Е	201	QY1	C6-C12-C23-C21
2	Е	201	QY1	C6-C12-C23-C16

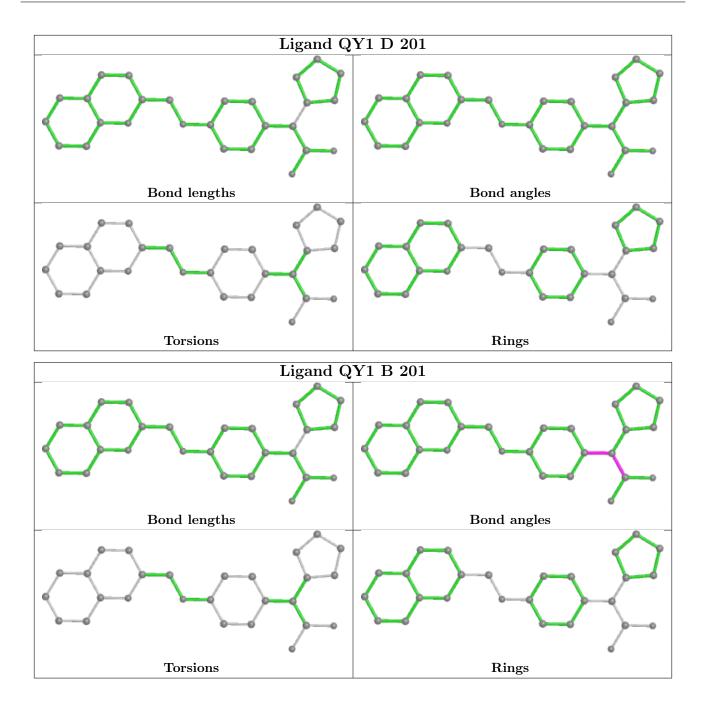
Continued from previous page...

There are no ring outliers.

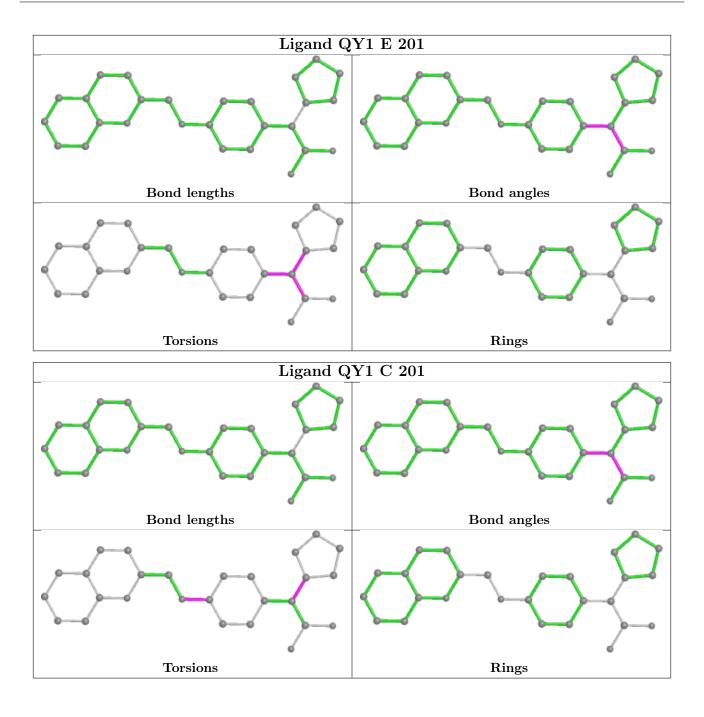
No monomer is involved in short contacts.

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.

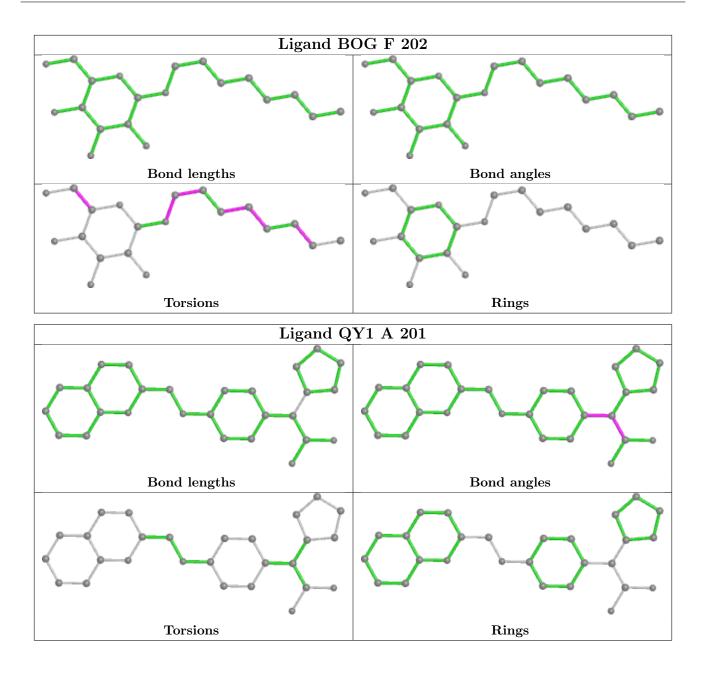




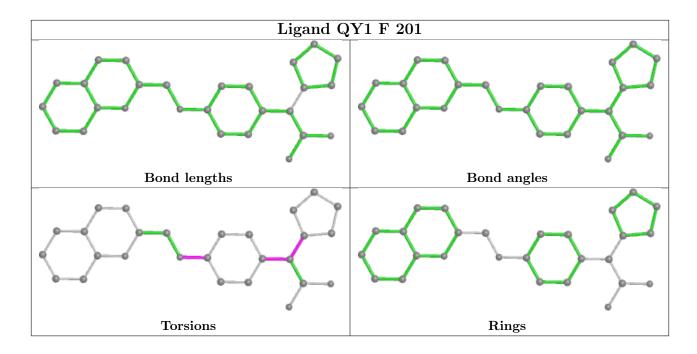












4.7 Other polymers (i)

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 (i)

5.1 Protein, DNA and RNA chains (i)

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

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

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

5.3 Carbohydrates (i)

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

5.4 Ligands (i)

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

5.5 Other polymers (i)

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

