

# Full wwPDB X-ray Structure Validation Report (i)

#### Nov 9, 2023 – 12:15 PM EST

PDB ID : 8GD8

Title : Porous framework formed by assembly of a bipyridyl-conjugated helical peptide

Authors: Hess, S.S.; Nguyen, A.I.

Deposited on : 2023-03-03

Resolution : 1.04 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 : 4.02b-467

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.36

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$ 

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

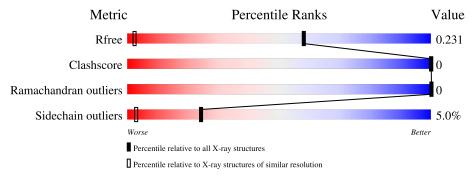
Validation Pipeline (wwPDB-VP) : 2.36

## 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 1.04 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	Similar resolution
1,13,113	$(\# \mathrm{Entries})$	$(\#  ext{Entries},  ext{ resolution range}( ext{Å}))$
$R_{free}$	130704	1596 (1.10-0.98)
Clashscore	141614	1677 (1.10-0.98)
Ramachandran outliers	138981	1591 (1.10-0.98)
Sidechain outliers	138945	1589 (1.10-0.98)

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%

Mol	Chain	Length	Quality of chain		
1	A	11	82%		18%
1	В	11	73%	9%	18%
1	С	11	82%		18%
1	D	11	82%		18%



## 2 Entry composition (i)

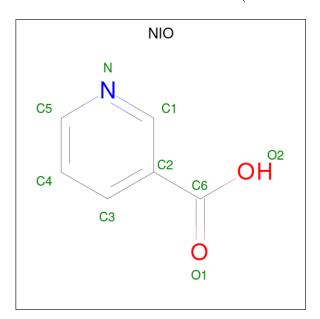
There are 4 unique types of molecules in this entry. The entry contains 742 atoms, of which 352 are hydrogens and 0 are deuteriums.

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 NIO-LEU-AIB-ALA-CYS-LEU-AIB-GLN-AIB-LEU-BPH.

Mol	Chain	Residues		Atoms			ZeroOcc	AltConf	Trace		
1	1 A	9	Total	С	Н	N	О	S	0	1	0
1			142	44	74	11	11	2	U	1	0
1	В	9	Total	С	Н	N	О	S	0	1	0
1	Ъ	9	142	44	74	11	11	2			
1	С	С 9	Total	С	Н	N	О	S	0	1	0
1			142	44	74	11	11	2	U		
1	1 D	0	Total	С	Н	N	О	S	0	1	0
	9	142	44	74	11	11	2	0	1		

• Molecule 2 is NICOTINIC ACID (three-letter code: NIO) (formula: C<sub>6</sub>H<sub>5</sub>NO<sub>2</sub>).



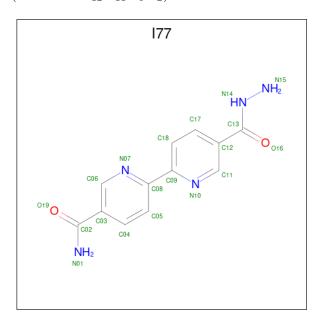
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
9	Λ	1	Total	С	Н	N	О	0	0
Z A	1	12	6	4	1	1			
9	D	1	Total	С	Н	N	О	0	0
2 B	1	12	6	4	1	1	U	U	



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$\mathbf{N}$	Iol	Chain	Residues	Atoms				ZeroOcc	AltConf	
	9	С	1	Total	С	Н	N	О	0	0
		1	12	6	4	1	1	0	0	
	2	D	1	Total	С	Н	N	О	0	0
		1	12	6	4	1	1	0	U	

 $\bullet$  Molecule 3 is 5'-(hydrazinecarbonyl) [2,2'-bipyridine]-5-carboxamide (three-letter code: I77) (formula:  $\rm C_{12}H_{11}N_5O_2)$ .



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
3	A	1	Total	_	Н	N	О	0	0	
	11	1	29	12	10	5	2	O		
3	В	1	Total	С	Η	N	О	0	0	
3	9 D	1	29	12	10	5	2	U		
3	С	C 1	Total	С	Н	N	О	0	0	
3	C	1	29	12	10	5	2	U	0	
2	3 D	1	Total	С	Н	N	О	0	0	
$\begin{vmatrix} 3 \end{vmatrix} = 1$	D		29	12	10	5	2	U	0	

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	4	Total O 4 4	0	0
4	В	1	Total O 1 1	0	0
4	С	2	Total O 2 2	0	0



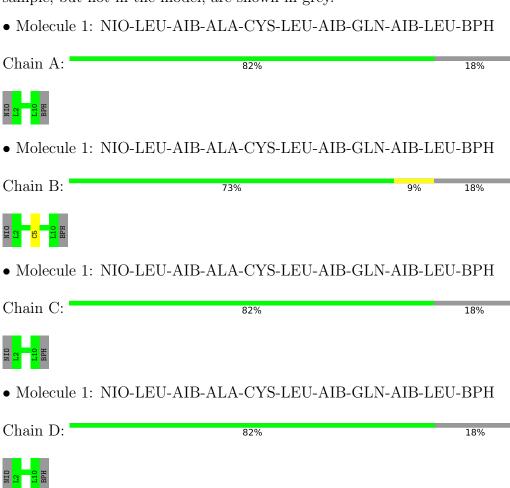
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	3	Total O 3 3	0	0



## 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. 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.





### 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	8.79Å 16.59Å 51.15Å	D
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$89.99^{\circ}$ $89.97^{\circ}$ $90.01^{\circ}$	Depositor
Resolution (Å)	16.59 - 1.04	Depositor
Resolution (A)	17.05  -  0.83	EDS
% Data completeness	79.7 (16.59-1.04)	Depositor
(in resolution range)	66.5 (17.05-0.83)	EDS
$R_{merge}$	0.05	Depositor
$\frac{R_{sym}}{\langle I/\sigma(I)\rangle^{-1}}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	5.82 (at 0.83Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
рρ.	0.206 , $0.231$	Depositor
$R, R_{free}$	0.206 , $0.231$	DCC
$R_{free}$ test set	1829 reflections (9.55%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	5.1	Xtriage
Anisotropy	0.940	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.77, 58.9	EDS
L-test for twinning <sup>2</sup>	$< L > = 0.45, < L^2> = 0.29$	Xtriage
	0.457 for h,-k,-l	
Estimated twinning fraction	0.438  for  -h,k,-l	Xtriage
	0.436  for -h,-k,l	
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	742	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	8.0	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 42.84 % 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 1.9241e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

<sup>&</sup>lt;sup>2</sup>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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

## 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: NIO, I77, AIB

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		
IVIOI		RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	A	0.39	0/49	0.77	0/65	
1	В	0.44	0/49	0.65	0/65	
1	С	0.36	0/49	0.71	0/65	
1	D	0.37	0/49	0.81	0/65	
All	All	0.39	0/196	0.74	0/260	

There are no bond length outliers.

There are no bond angle outliers.

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	68	74	75	0	0
1	В	68	74	75	0	0
1	С	68	74	75	0	0
1	D	68	74	75	0	0
2	A	8	4	4	0	0
2	В	8	4	4	0	0
2	С	8	4	4	0	0
2	D	8	4	4	0	0
3	A	19	10	0	0	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	В	19	10	0	0	0
3	С	19	10	0	0	0
3	D	19	10	0	0	0
4	A	4	0	0	0	0
4	В	1	0	0	0	0
4	С	2	0	0	0	0
4	D	3	0	0	0	0
All	All	390	352	316	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 0.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

### 5.3 Torsion angles (i)

#### 5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	A	5/11 (46%)	5 (100%)	0	0	100	100
1	В	5/11 (46%)	5 (100%)	0	0	100	100
1	C	5/11 (46%)	5 (100%)	0	0	100	100
1	D	5/11 (46%)	5 (100%)	0	0	100	100
All	All	20/44 (46%)	20 (100%)	0	0	100	100

There are no Ramachandran outliers to report.

#### 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	6/5~(120%)	6 (100%)	0	100 100
1	В	6/5 (120%)	4 (67%)	2 (33%)	0 0
1	С	6/5 (120%)	6 (100%)	0	100 100
1	D	6/5 (120%)	6 (100%)	0	100 100
All	All	24/20 (120%)	22 (92%)	2 (8%)	24 1

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	5[A]	CYS
1	В	5[B]	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

12 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).

Mal	Trme	Chain	Dag	Link	В	ond leng	$_{ m gths}$	Bond angles		
Mol	Type	Chain	Res	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2
1	AIB	С	7	1	1,5,6	1.02	0	2,7,9	0.27	0
1	AIB	D	9	1	1,5,6	1.09	0	2,7,9	0.47	0
1	AIB	С	3	1	1,5,6	0.77	0	2,7,9	0.52	0
1	AIB	С	9	1	1,5,6	1.22	0	2,7,9	0.47	0
1	AIB	A	7	1	1,5,6	1.22	0	2,7,9	0.81	0



Mol	Tuno	Chain	Res	Link	В	ond leng	$_{ m gths}$	В	ond ang	gles
MIOI	Type	Chain	nes	2   TIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
1	AIB	A	3	1	1,5,6	1.06	0	2,7,9	0.42	0
1	AIB	В	9	1	1,5,6	0.93	0	2,7,9	0.79	0
1	AIB	В	3	1	1,5,6	0.71	0	2,7,9	0.23	0
1	AIB	D	3	1	1,5,6	0.78	0	2,7,9	0.38	0
1	AIB	В	7	1	1,5,6	1.03	0	2,7,9	0.10	0
1	AIB	A	9	1	1,5,6	1.12	0	2,7,9	0.56	0
1	AIB	D	7	1	1,5,6	1.35	0	2,7,9	0.44	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
1	AIB	С	7	1	-	0/2/3/6	-
1	AIB	D	9	1	-	0/2/3/6	-
1	AIB	С	3	1	-	0/2/3/6	-
1	AIB	С	9	1	-	0/2/3/6	-
1	AIB	A	7	1	-	0/2/3/6	-
1	AIB	A	3	1	-	0/2/3/6	_
1	AIB	В	9	1	-	0/2/3/6	-
1	AIB	В	3	1	-	0/2/3/6	_
1	AIB	D	3	1	-	0/2/3/6	-
1	AIB	В	7	1	-	0/2/3/6	-
1	AIB	A	9	1	-	0/2/3/6	-
1	AIB	D	7	1	-	0/2/3/6	_

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

#### 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.



### 5.6 Ligand geometry (i)

8 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).

Mal	Trino	Chain	Dag	Link	Bo	ond leng	gths	В	ond ang	gles
Mol	Type	Chain	Res	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	I77	В	102	1	20,20,20	3.06	5 (25%)	27,27,27	1.95	13 (48%)
3	I77	A	102	1	20,20,20	3.32	5 (25%)	27,27,27	1.85	9 (33%)
3	I77	D	102	1	20,20,20	3.39	4 (20%)	27,27,27	1.72	8 (29%)
3	I77	С	102	1	20,20,20	3.08	5 (25%)	27,27,27	2.05	13 (48%)
2	NIO	С	101	1	8,8,9	0.32	0	9,9,11	0.44	0
2	NIO	A	101	1	8,8,9	0.28	0	9,9,11	0.59	0
2	NIO	D	101	1	8,8,9	0.23	0	9,9,11	0.56	0
2	NIO	В	101	1	8,8,9	0.27	0	9,9,11	0.44	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
3	I77	В	102	1	-	0/14/14/14	0/2/2/2
3	I77	A	102	1	-	0/14/14/14	0/2/2/2
3	I77	D	102	1	-	0/14/14/14	0/2/2/2
3	I77	С	102	1	-	0/14/14/14	0/2/2/2
2	NIO	С	101	1	-	2/2/2/4	0/1/1/1
2	NIO	A	101	1	-	2/2/2/4	0/1/1/1
2	NIO	D	101	1	-	2/2/2/4	0/1/1/1
2	NIO	В	101	1	-	2/2/2/4	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	${f Z}$	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\text{\AA})$
3	D	102	I77	C13-N14	12.44	1.46	1.33
3	A	102	I77	C13-N14	12.22	1.46	1.33



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Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}( ext{\AA})$
3	С	102	I77	C13-N14	10.81	1.45	1.33
3	В	102	I77	C13-N14	10.56	1.44	1.33
3	В	102	I77	C02-N01	6.88	1.46	1.33
3	С	102	I77	C02-N01	6.82	1.46	1.33
3	D	102	I77	C02-N01	6.58	1.45	1.33
3	A	102	I77	C02-N01	6.39	1.45	1.33
3	В	102	I77	O19-C02	-3.17	1.18	1.24
3	С	102	I77	O19-C02	-3.04	1.18	1.24
3	D	102	I77	C03-C02	2.78	1.54	1.50
3	A	102	I77	O19-C02	-2.74	1.18	1.24
3	D	102	I77	O19-C02	-2.62	1.19	1.24
3	В	102	I77	O16-C13	-2.60	1.18	1.23
3	С	102	I77	C03-C02	2.50	1.54	1.50
3	В	102	I77	C03-C02	2.40	1.54	1.50
3	A	102	I77	C03-C02	2.35	1.54	1.50
3	A	102	I77	O16-C13	-2.15	1.18	1.23
3	С	102	I77	O16-C13	-2.15	1.18	1.23

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
3	С	102	I77	C12-C13-N14	-3.88	111.84	116.27
3	D	102	I77	C11-N10-C09	3.79	122.89	117.90
3	A	102	I77	C05-C04-C03	-3.71	116.46	120.78
3	A	102	I77	C11-N10-C09	3.59	122.62	117.90
3	A	102	I77	C12-C11-N10	-3.55	118.71	123.67
3	D	102	I77	C05-C04-C03	-3.51	116.69	120.78
3	В	102	I77	C12-C13-N14	-3.46	112.32	116.27
3	С	102	I77	C03-C06-N07	-3.28	119.08	123.67
3	A	102	I77	C04-C03-C06	3.25	121.32	117.63
3	С	102	I77	C06-N07-C08	3.20	122.12	117.90
3	С	102	I77	C17-C12-C11	3.15	121.20	117.63
3	В	102	I77	C03-C06-N07	-3.10	119.35	123.67
3	В	102	I77	C06-N07-C08	3.05	121.92	117.90
3	D	102	I77	C12-C11-N10	-3.04	119.43	123.67
3	С	102	I77	C18-C09-C08	-2.96	116.08	121.27
3	В	102	I77	C18-C09-C08	-2.91	116.17	121.27
3	С	102	I77	C12-C11-N10	-2.87	119.66	123.67
3	С	102	I77	C04-C03-C06	2.87	120.89	117.63
3	В	102	I77	C04-C03-C06	2.80	120.81	117.63
3	A	102	I77	C03-C06-N07	-2.79	119.77	123.67
3	С	102	I77	C05-C04-C03	-2.70	117.64	120.78



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Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
3	В	102	I77	C05-C04-C03	-2.69	117.64	120.78
3	В	102	I77	C08-C09-N10	2.62	121.41	116.77
3	С	102	I77	C08-C09-N10	2.57	121.32	116.77
3	A	102	I77	C17-C12-C11	2.57	120.54	117.63
3	С	102	I77	C18-C17-C12	-2.56	117.80	120.78
3	В	102	I77	C17-C12-C11	2.55	120.52	117.63
3	D	102	I77	C04-C03-C06	2.49	120.45	117.63
3	D	102	I77	C06-N07-C08	2.47	121.16	117.90
3	A	102	I77	C09-C08-N07	2.47	121.15	116.77
3	A	102	I77	C05-C08-C09	-2.46	116.96	121.27
3	В	102	I77	C18-C17-C12	-2.41	117.98	120.78
3	D	102	I77	C09-C08-N07	2.37	120.97	116.77
3	В	102	I77	C12-C11-N10	-2.29	120.47	123.67
3	D	102	I77	C03-C06-N07	-2.28	120.48	123.67
3	С	102	I77	O19-C02-C03	2.28	122.36	119.63
3	A	102	I77	C06-N07-C08	2.28	120.90	117.90
3	В	102	I77	O19-C02-C03	2.17	122.23	119.63
3	С	102	I77	O16-C13-C12	2.14	124.75	120.94
3	С	102	I77	C11-N10-C09	2.09	120.66	117.90
3	В	102	I77	O16-C13-C12	2.07	124.63	120.94
3	В	102	I77	C09-C08-N07	2.02	120.35	116.77
3	D	102	I77	C05-C08-C09	-2.02	117.73	121.27

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	101	NIO	C1-C2-C6-O1
2	D	101	NIO	C1-C2-C6-O1
2	A	101	NIO	C3-C2-C6-O1
2	В	101	NIO	C3-C2-C6-O1
2	С	101	NIO	C3-C2-C6-O1
2	D	101	NIO	C3-C2-C6-O1
2	В	101	NIO	C1-C2-C6-O1
2	С	101	NIO	C1-C2-C6-O1

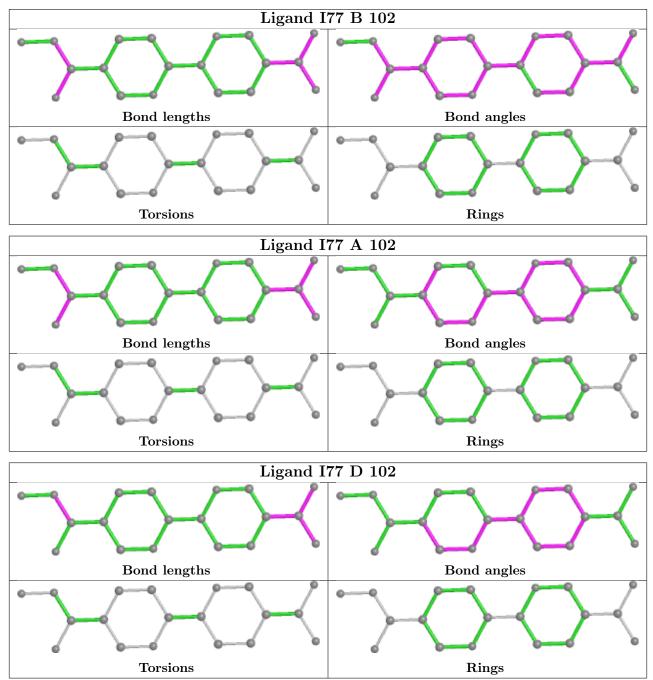
There are no ring outliers.

No monomer is involved in short contacts.

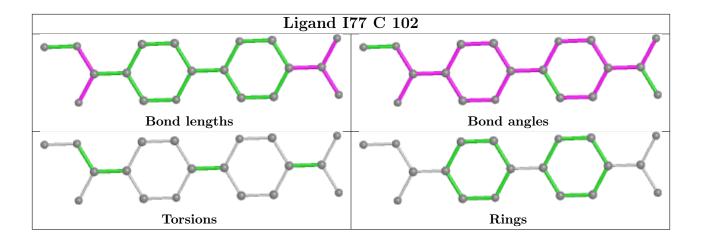
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will



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.







## 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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

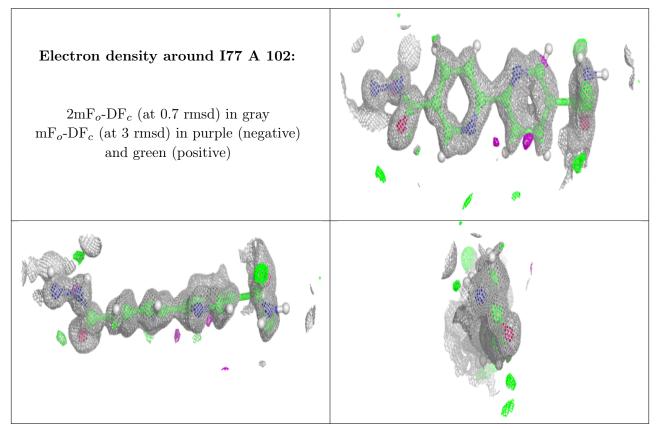
### 6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

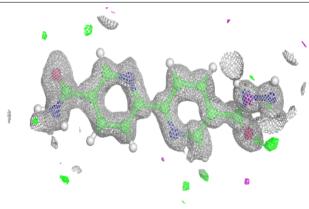
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

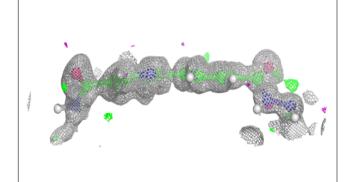


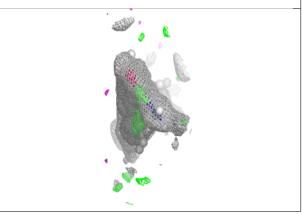


#### Electron density around I77 B 102:

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

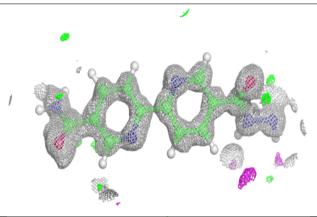


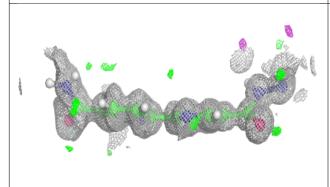


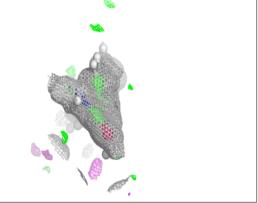


#### Electron density around I77 C 102:

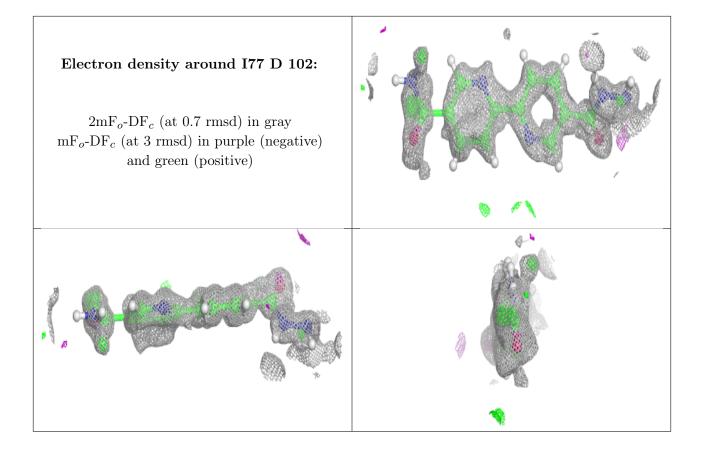
 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$  (at 0.7 rmsd) in gray  $\mathrm{mF}_o\text{-}\mathrm{DF}_c$  (at 3 rmsd) in purple (negative) and green (positive)











### 6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

