



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 19, 2020 – 09:18 AM BST

PDB ID : 6UKW  
Title : STING C-terminal Domain Complexed with Non-cyclic Dinucleotide Compound 10  
Authors : Lesburg, C.A.  
Deposited on : 2019-10-06  
Resolution : 1.97 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) 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 : 2.14.6  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.14.6

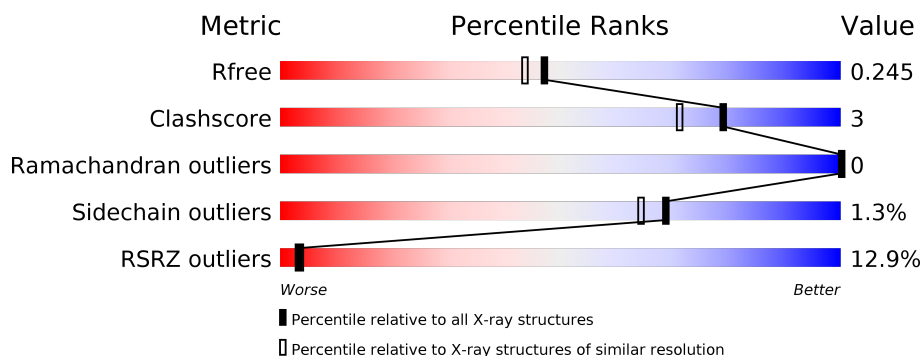
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.97 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	300	<div> <div>7%</div> <div>52%</div> <div>6%</div> <div>43%</div> </div>
1	B	300	<div> <div>8%</div> <div>54%</div> <div>5%</div> <div>41%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3180 atoms, of which 50 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 fusion protein of Ubiquitin-like protein SMT3 and Stimulator of interferon protein c-terminal domain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	172	Total	C	N	O	S	0	0	0
			1387	875	243	263	6			
1	B	176	Total	C	N	O	S	0	1	0
			1427	899	253	269	6			

There are 40 discrepancies between the modelled and reference sequences:

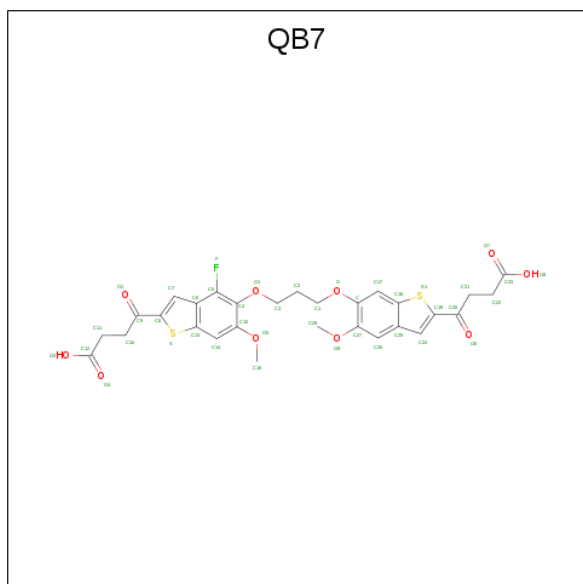
Chain	Residue	Modelled	Actual	Comment	Reference
A	42	MET	-	initiating methionine	UNP Q12306
A	43	ALA	-	expression tag	UNP Q12306
A	44	HIS	-	expression tag	UNP Q12306
A	45	HIS	-	expression tag	UNP Q12306
A	46	HIS	-	expression tag	UNP Q12306
A	47	HIS	-	expression tag	UNP Q12306
A	48	HIS	-	expression tag	UNP Q12306
A	49	HIS	-	expression tag	UNP Q12306
A	50	GLY	-	expression tag	UNP Q12306
A	113	THR	ARG	conflict	UNP Q12306
A	120	GLU	ARG	conflict	UNP Q12306
A	148	GLU	-	linker	UNP Q12306
A	149	ASN	-	linker	UNP Q12306
A	150	LEU	-	linker	UNP Q12306
A	151	TYR	-	linker	UNP Q12306
A	152	PHE	-	linker	UNP Q12306
A	153	GLN	-	linker	UNP Q12306
A	154	SER	-	linker	UNP Q12306
A	230	ALA	GLY	engineered mutation	UNP A0A2R3XZB7
A	293	GLN	ARG	engineered mutation	UNP A0A2R3XZB7
B	42	MET	-	initiating methionine	UNP Q12306
B	43	ALA	-	expression tag	UNP Q12306
B	44	HIS	-	expression tag	UNP Q12306
B	45	HIS	-	expression tag	UNP Q12306

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Chain	Residue	Modelled	Actual	Comment	Reference
B	46	HIS	-	expression tag	UNP Q12306
B	47	HIS	-	expression tag	UNP Q12306
B	48	HIS	-	expression tag	UNP Q12306
B	49	HIS	-	expression tag	UNP Q12306
B	50	GLY	-	expression tag	UNP Q12306
B	113	THR	ARG	conflict	UNP Q12306
B	120	GLU	ARG	conflict	UNP Q12306
B	148	GLU	-	linker	UNP Q12306
B	149	ASN	-	linker	UNP Q12306
B	150	LEU	-	linker	UNP Q12306
B	151	TYR	-	linker	UNP Q12306
B	152	PHE	-	linker	UNP Q12306
B	153	GLN	-	linker	UNP Q12306
B	154	SER	-	linker	UNP Q12306
B	230	ALA	GLY	engineered mutation	UNP A0A2R3XZB7
B	293	GLN	ARG	engineered mutation	UNP A0A2R3XZB7

- Molecule 2 is 4-[6-(3-{[2-(3-carboxypropanoyl)-4-fluoro-6-methoxy-1-benzothiophen-5-yl]oxy}propoxy)-5-methoxy-1-benzothiophen-2-yl]-4-oxobutanoic acid (three-letter code: QB7) (formula: C<sub>29</sub>H<sub>27</sub>FO<sub>10</sub>S<sub>2</sub>) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	H	O	S	0	1
			67	29	1	25	10	2		
2	B	1	Total	C	F	H	O	S	0	1
			67	29	1	25	10	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	121	Total 121	O 121	0	0
3	B	111	Total 111	O 111	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	36.44Å 109.52Å 59.32Å 90.00° 95.81° 90.00°	Depositor
Resolution (Å)	25.39 – 1.97 24.84 – 1.97	Depositor EDS
% Data completeness (in resolution range)	94.8 (25.39-1.97) 95.3 (24.84-1.97)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.72 (at 1.98Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, $R_{free}$	0.210 , 0.241 0.213 , 0.245	Depositor DCC
$R_{free}$ test set	1540 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.3	Xtriage
Anisotropy	0.262	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 45.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3180	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.09% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: QB7

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.52	0/1412	0.61	0/1911
1	B	0.51	0/1453	0.64	0/1968
All	All	0.52	0/2865	0.62	0/3879

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

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	1387	0	1360	11	0
1	B	1427	0	1406	7	0
2	A	42	25	0	0	0
2	B	42	25	0	0	0
3	A	121	0	0	2	0
3	B	111	0	0	0	0
All	All	3130	50	2766	16	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 3.

All (16) close contacts within the same asymmetric unit are listed below, sorted by their clash



magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:TYR:HD2	1:A:312:ILE:HD11	1.63	0.64
1:B:199:TYR:HD2	1:B:312:ILE:HD11	1.66	0.60
1:A:261:TYR:HB2	1:B:233:ALA:HB1	1.89	0.54
1:A:233:ALA:HB1	1:B:261:TYR:HB2	1.91	0.53
1:A:241:SER:HB2	3:A:597:HOH:O	2.08	0.52
1:B:176:GLN:HG3	1:B:308:ASN:HD21	1.77	0.50
1:B:229:THR:HG22	1:B:239:VAL:HG22	1.95	0.49
1:A:279:PHE:CE1	1:A:287:GLN:HG3	2.49	0.47
1:A:279:PHE:HE1	1:A:287:GLN:HG3	1.79	0.47
1:A:229:THR:HG22	1:A:239:VAL:HG22	1.97	0.46
1:B:272:SER:HB2	1:B:281:ARG:HA	1.97	0.44
1:A:202:LEU:HB2	1:A:313:ALA:HA	1.99	0.44
1:A:284:ARG:HD2	3:A:503:HOH:O	2.19	0.42
1:B:202:LEU:HB2	1:B:313:ALA:HA	2.01	0.41
1:A:222:LEU:HB2	1:A:246:GLU:HG3	2.03	0.41
1:A:299:LEU:O	1:A:306:GLN:HB2	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	166/300 (55%)	162 (98%)	4 (2%)	0	100	100
1	B	173/300 (58%)	169 (98%)	4 (2%)	0	100	100
All	All	339/600 (56%)	331 (98%)	8 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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	149/264 (56%)	148 (99%)	1 (1%)	84	83
1	B	154/264 (58%)	151 (98%)	3 (2%)	57	50
All	All	303/528 (57%)	299 (99%)	4 (1%)	69	64

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	236	LYS
1	B	223	ASP
1	B	236	LYS
1	B	253	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	196	GLN
1	A	218	ASN
1	A	306	GLN
1	B	196	GLN
1	B	218	ASN
1	B	308	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

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	$\# Z  > 2$
2	QB7	B	401[B]	-	30,45,45	0.91	2 (6%)	38,63,63	0.55	0
2	QB7	A	401[A]	-	30,45,45	0.84	2 (6%)	38,63,63	0.54	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	QB7	B	401[B]	-	-	10/18/30/30	0/4/4/4
2	QB7	A	401[A]	-	-	9/18/30/30	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401[B]	QB7	C8-S	2.90	1.75	1.72
2	B	401[B]	QB7	C19-S1	2.81	1.75	1.72
2	A	401[A]	QB7	C19-S1	2.60	1.75	1.72
2	A	401[A]	QB7	C8-S	2.32	1.75	1.72

There are no bond angle outliers.

There are no chirality outliers.

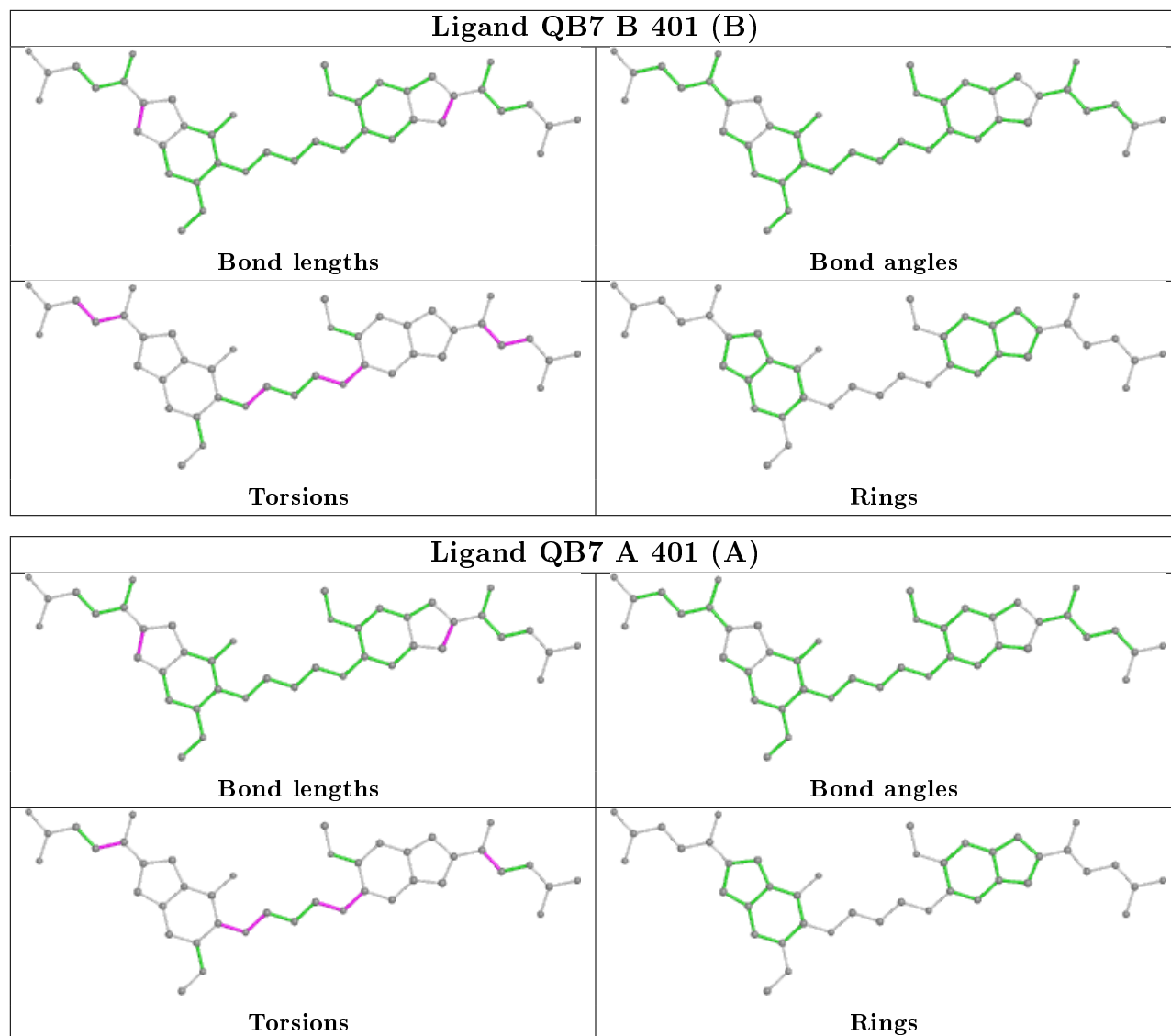
All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401[A]	QB7	C19-C20-C21-C22
2	B	401[B]	QB7	O6-C20-C21-C22
2	A	401[A]	QB7	O6-C20-C21-C22
2	A	401[A]	QB7	C11-C10-C9-O2
2	B	401[B]	QB7	C19-C20-C21-C22
2	A	401[A]	QB7	C11-C10-C9-C8
2	B	401[B]	QB7	C11-C10-C9-C8
2	B	401[B]	QB7	C11-C10-C9-O2
2	A	401[A]	QB7	C2-C3-O1-C4
2	B	401[B]	QB7	C2-C3-O1-C4
2	B	401[B]	QB7	C2-C1-O-C
2	A	401[A]	QB7	C2-C1-O-C
2	B	401[B]	QB7	C27-C-O-C1
2	A	401[A]	QB7	C27-C-O-C1
2	B	401[B]	QB7	C17-C-O-C1
2	A	401[A]	QB7	C15-C4-O1-C3
2	A	401[A]	QB7	C17-C-O-C1
2	B	401[B]	QB7	C9-C10-C11-C12
2	B	401[B]	QB7	C20-C21-C22-C23

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 than 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

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	172/300 (57%)	0.73	20 (11%) 4 5	13, 26, 49, 91	0
1	B	176/300 (58%)	0.88	25 (14%) 2 2	13, 30, 57, 78	0
All	All	348/600 (58%)	0.81	45 (12%) 3 3	13, 28, 54, 91	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	250	ASN	6.1
1	B	186	TYR	5.9
1	B	252	GLN	4.6
1	B	304	GLU	4.5
1	B	214	MET	4.4
1	A	185	HIS	4.3
1	A	186	TYR	4.2
1	A	304	GLU	4.0
1	B	215	ALA	4.0
1	A	214	MET	3.7
1	A	184	GLN	3.7
1	A	192	GLY	3.7
1	A	303	PRO	3.4
1	B	257	CYS	3.4
1	B	219	ILE	3.3
1	B	154	SER	3.3
1	B	259	LEU	3.3
1	B	185	HIS	3.2
1	A	323	PHE	3.1
1	A	215	ALA	3.0
1	B	258	VAL	2.8
1	B	303	PRO	2.8
1	A	335	GLN	2.8
1	B	323	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	225	LEU	2.6
1	A	250	ASN	2.6
1	A	193	ALA	2.6
1	B	188	ASN	2.5
1	B	251	GLY	2.5
1	A	201	LEU	2.5
1	A	336	GLU	2.5
1	B	220	ARG	2.5
1	B	335	GLN	2.5
1	B	217	PRO	2.4
1	A	173	PRO	2.4
1	A	180	ARG	2.3
1	A	200	ILE	2.3
1	B	208	VAL	2.2
1	B	253	ARG	2.2
1	B	325	LEU	2.1
1	A	198	LEU	2.1
1	A	265	LEU	2.1
1	B	173	PRO	2.0
1	B	235	ILE	2.0
1	B	307	ASN	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

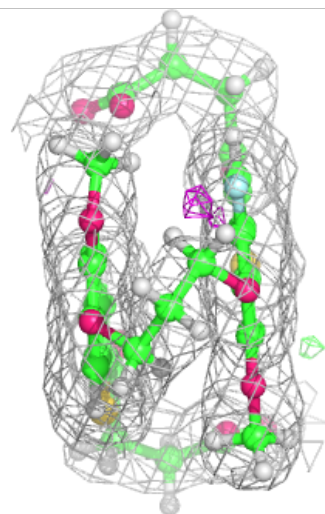
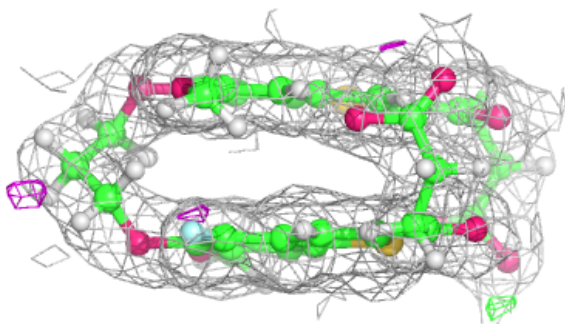
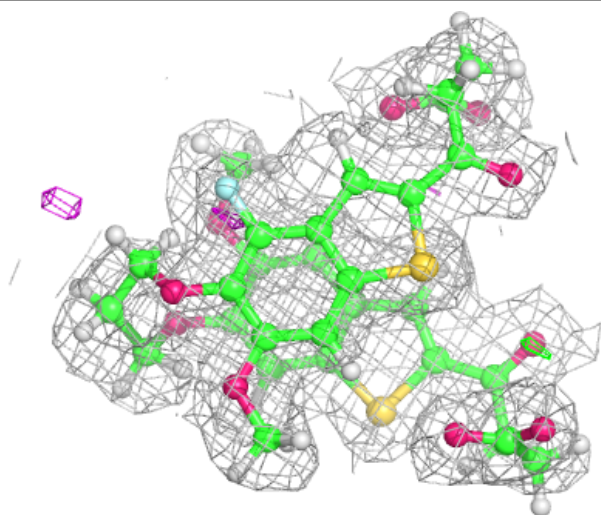
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	QB7	B	401[B]	42/42	0.96	0.12	9,16,20,21	67
2	QB7	A	401[A]	42/42	0.96	0.13	8,15,23,25	67

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 QB7 B 401 (B):**

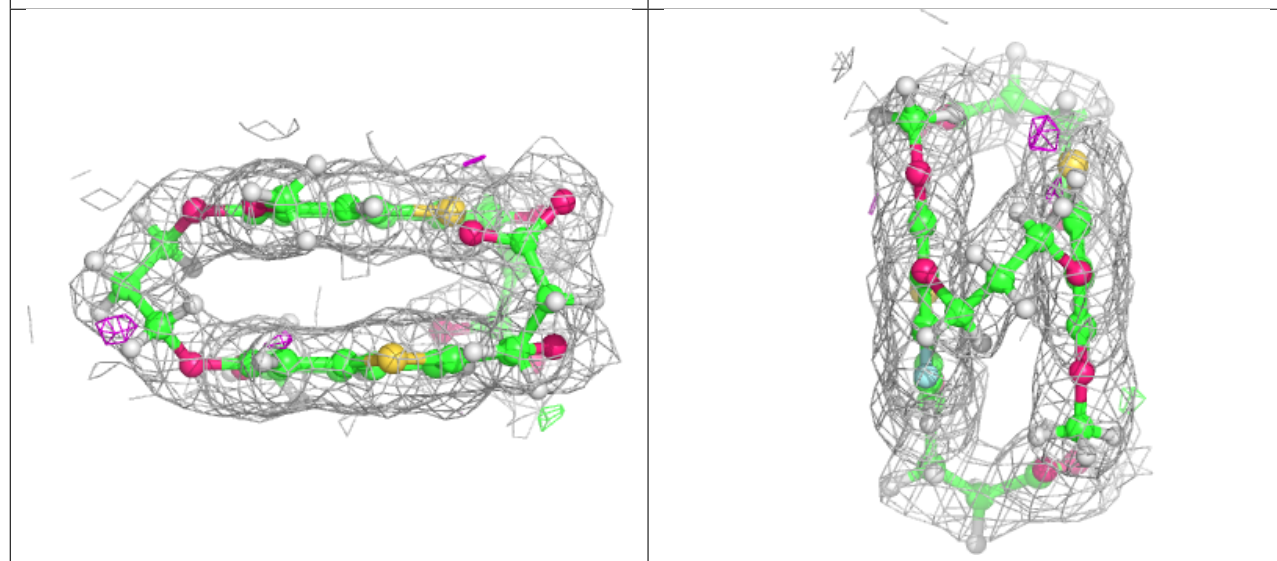
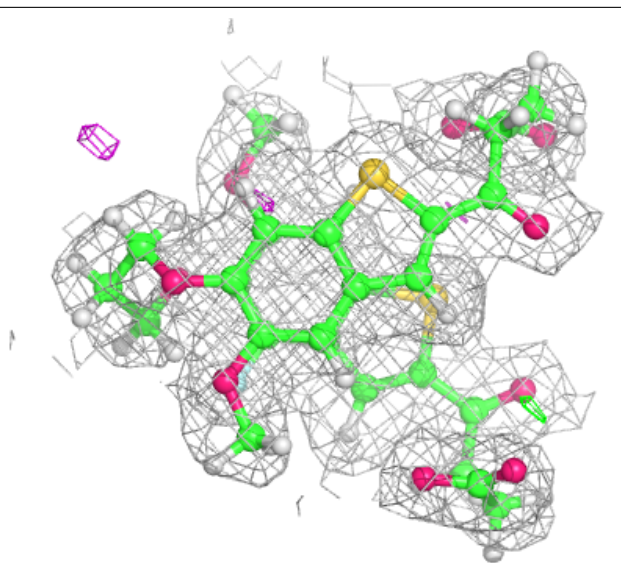
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around QB7 A 401 (A):**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.