



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 09:04 am BST

PDB ID : 2Q5P  
Title : Crystal Structure of PPARgamma bound to partial agonist MRL24  
Authors : Bruning, J.B.; Nettles, K.W.  
Deposited on : 2007-06-01  
Resolution : 2.30 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](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 : 2.11  
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) : 2.11

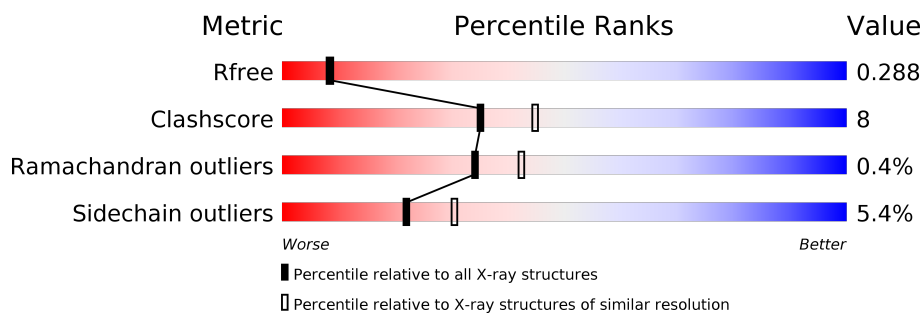
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	274	
1	B	274	



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.

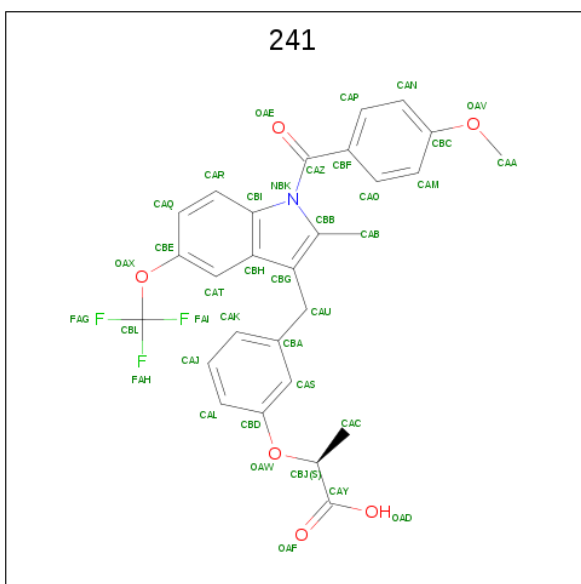
- Molecule 1 is a protein called Peroxisome Proliferator-Activated Receptor gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	256	Total 2087	C 1351	N 340	O 385	S 11	6	7	0
1	B	245	Total 1960	C 1270	N 322	O 359	S 9	0	2	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	204	SER	-	EXPRESSION TAG	UNP P37231
B	204	SER	-	EXPRESSION TAG	UNP P37231

- Molecule 2 is (2S)-2-(3-{[1-(4-METHOXYBENZOYL)-2-METHYL-5-(TRIFLUOROMETHOXY)-1H-INDOL-3-YL]METHYL}PHENOXY)PROPANOIC ACID (three-letter code: 241) (formula: C<sub>28</sub>H<sub>24</sub>F<sub>3</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			38	28	3	1	6		
2	B	1	Total	C	F	N	O	0	0
			38	28	3	1	6		

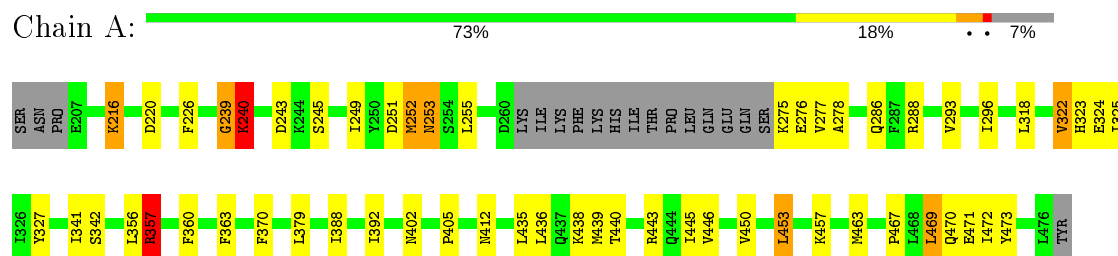
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	46	Total	O	0	0
			46	46		
3	B	54	Total	O	0	0
			54	54		

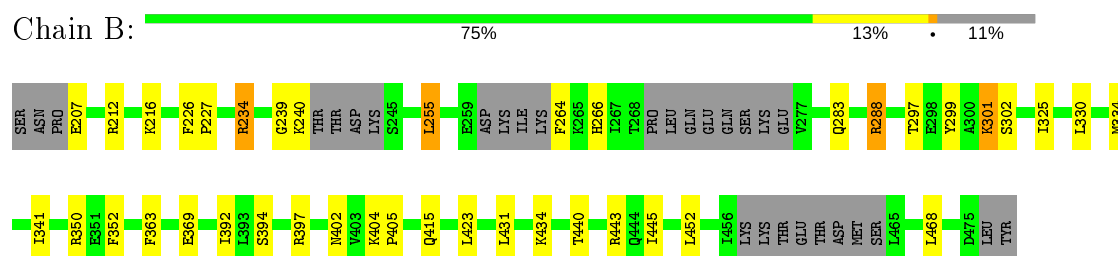
### 3 Residue-property plots

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.

- Molecule 1: Peroxisome Proliferator-Activated Receptor gamma



- Molecule 1: Peroxisome Proliferator-Activated Receptor gamma



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.36Å 61.45Å 117.95Å 90.00° 102.42° 90.00°	Depositor
Resolution (Å)	10.00 – 2.30 9.98 – 2.30	Depositor EDS
% Data completeness (in resolution range)	91.9 (10.00-2.30) 91.9 (9.98-2.30)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	9.33 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, $R_{free}$	0.206 , 0.247 0.264 , 0.288	Depositor DCC
$R_{free}$ test set	1273 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.2	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.46 , 58.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	4223	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.42% 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:  
241

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	0.96	7/2139 (0.3%)	0.91	8/2879 (0.3%)
1	B	0.66	3/1998 (0.2%)	0.61	0/2689
All	All	0.83	10/4137 (0.2%)	0.78	8/5568 (0.1%)

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
1	A	0	3

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	240[A]	LYS	N-CA	20.49	1.87	1.46
1	A	240[B]	LYS	N-CA	20.49	1.87	1.46
1	A	240[C]	LYS	N-CA	20.49	1.87	1.46
1	B	207	GLU	CD-OE2	12.66	1.39	1.25
1	B	240	LYS	C-O	10.92	1.44	1.23

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	240[A]	LYS	N-CA-CB	17.22	141.59	110.60
1	A	240[B]	LYS	N-CA-CB	17.22	141.59	110.60
1	A	240[C]	LYS	N-CA-CB	17.22	141.59	110.60
1	A	357	ARG	NE-CZ-NH1	-9.38	115.61	120.30
1	A	240[A]	LYS	N-CA-C	-8.35	88.44	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240[A]	LYS	Peptide
1	A	240[C]	LYS	Peptide
1	A	357	ARG	Sidechain

## 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	2087	0	2167	43	0
1	B	1960	0	2001	24	0
2	A	38	0	23	4	0
2	B	38	0	23	4	0
3	A	46	0	0	0	0
3	B	54	0	0	4	0
All	All	4223	0	4214	68	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 8.

The worst 5 of 68 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:288:ARG:NH2	2:A:5001:241:HAP	1.69	1.06
1:A:288:ARG:HH21	2:A:5001:241:HAP	1.10	1.05
1:A:288:ARG:HH21	2:A:5001:241:CAP	1.82	0.92
1:A:296[A]:ILE:HD12	1:A:325:ILE:HG21	1.55	0.88
1:A:323[B]:HIS:H	1:A:323[B]:HIS:CD2	1.92	0.83

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	260/274 (95%)	246 (95%)	13 (5%)	1 (0%)	34	42
1	B	237/274 (86%)	229 (97%)	7 (3%)	1 (0%)	34	42
All	All	497/548 (91%)	475 (96%)	20 (4%)	2 (0%)	34	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	239	GLY
1	B	239	GLY

### 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	235/247 (95%)	218 (93%)	17 (7%)	14	18
1	B	216/247 (87%)	207 (96%)	9 (4%)	30	42
All	All	451/494 (91%)	425 (94%)	26 (6%)	22	27

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	412	ASN
1	A	463	MET
1	B	440	THR
1	A	438	LYS

*Continued on next page...*

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Mol	Chain	Res	Type
1	A	453	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	449	HIS

### 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 carbohydrates 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	241	B	7001	-	35,41,41	1.28	4 (11%)	46,60,60	1.29	7 (15%)
2	241	A	5001	-	35,41,41	1.27	4 (11%)	46,60,60	1.44	6 (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
2	241	B	7001	-	-	6/19/27/27	0/4/4/4
2	241	A	5001	-	-	6/19/27/27	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	7001	241	CBF-CAZ	3.63	1.56	1.50
2	B	7001	241	CBI-NBK	-3.33	1.34	1.39
2	A	5001	241	CBI-NBK	-3.30	1.34	1.39
2	A	5001	241	CBF-CAZ	2.95	1.54	1.50
2	B	7001	241	OAX-CBL	2.83	1.47	1.31

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	5001	241	OAW-CBJ-CAC	4.31	114.31	105.53
2	A	5001	241	CBD-OAW-CBJ	4.08	123.90	118.57
2	B	7001	241	OAW-CBJ-CAC	3.56	112.77	105.53
2	A	5001	241	CBF-CAZ-NBK	3.37	121.89	117.95
2	A	5001	241	CAB-CBB-NBK	3.27	126.50	122.37

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	5001	241	CAS-CBD-OAW-CBJ
2	A	5001	241	CAL-CBD-OAW-CBJ
2	B	7001	241	CAC-CBJ-OAW-CBD
2	A	5001	241	CAC-CBJ-OAW-CBD
2	B	7001	241	CAS-CBD-OAW-CBJ

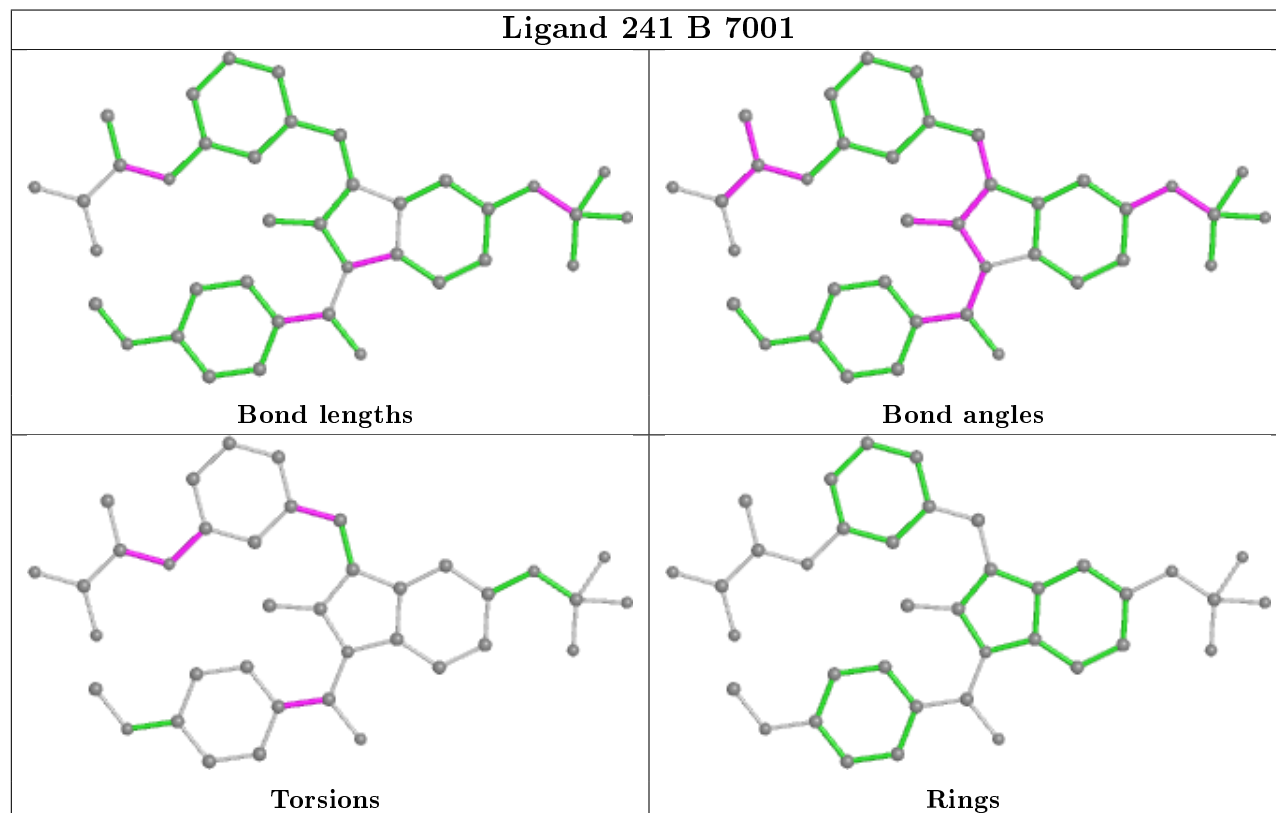
There are no ring outliers.

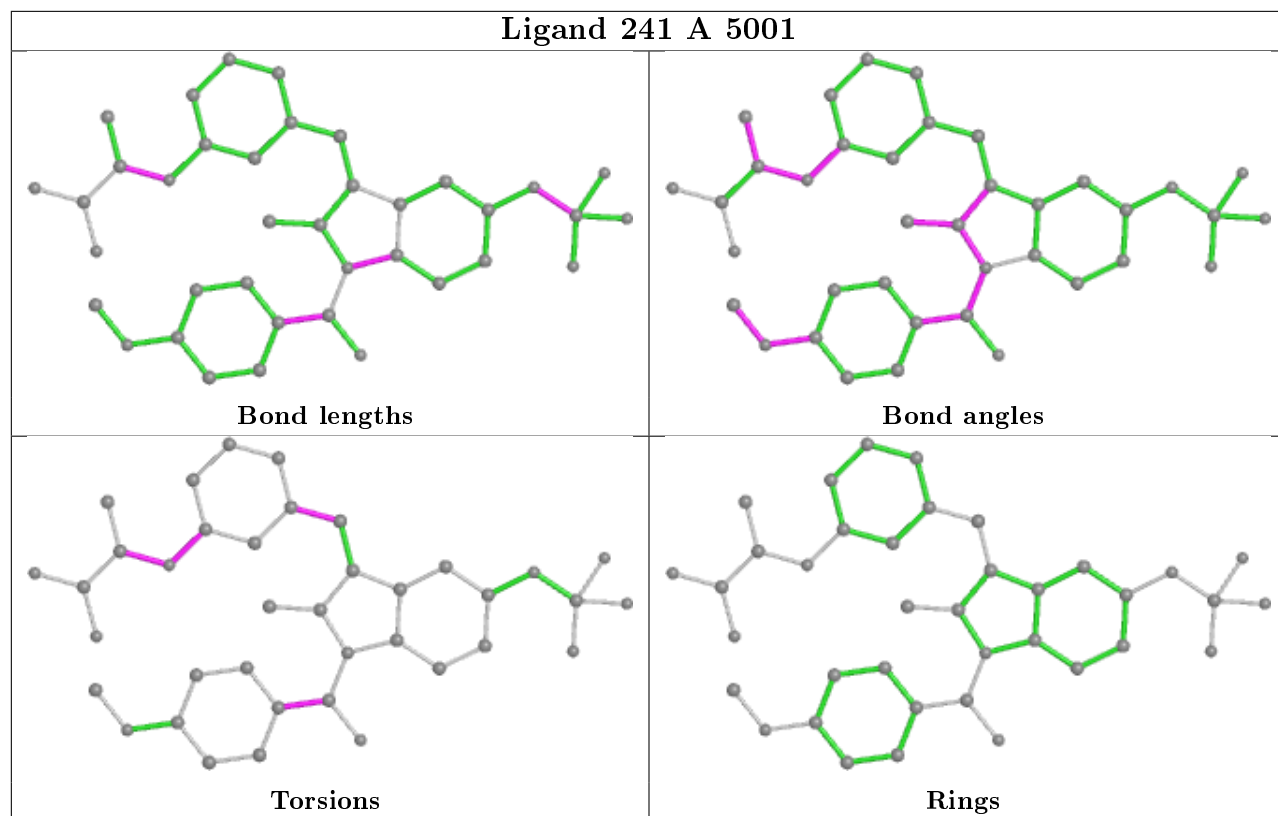
2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	7001	241	4	0
2	A	5001	241	4	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 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 ⓘ

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

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

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

### 6.3 Carbohydrates ⓘ

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

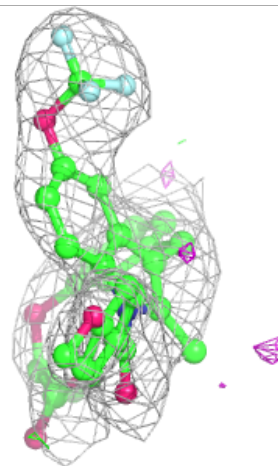
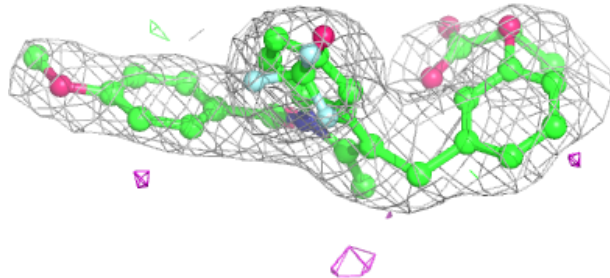
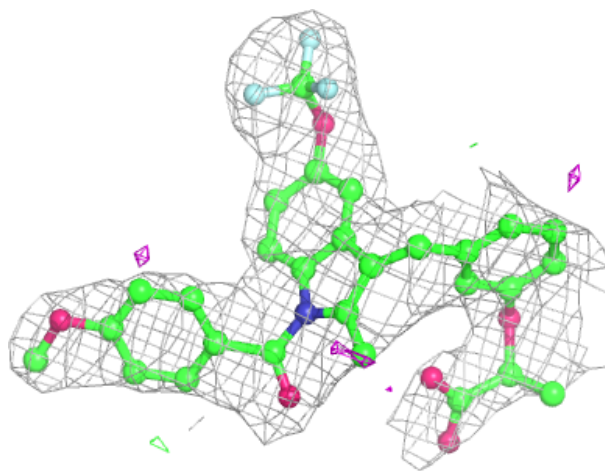
### 6.4 Ligands ⓘ

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.

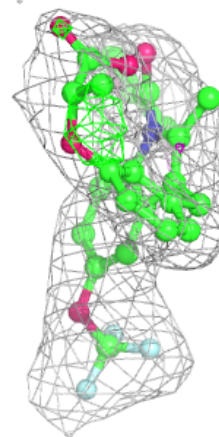
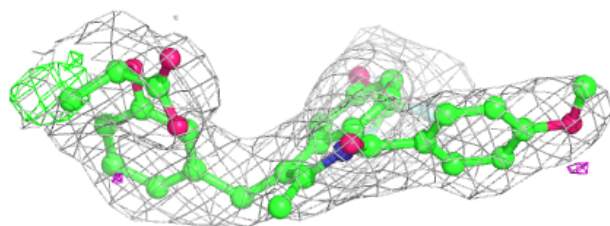
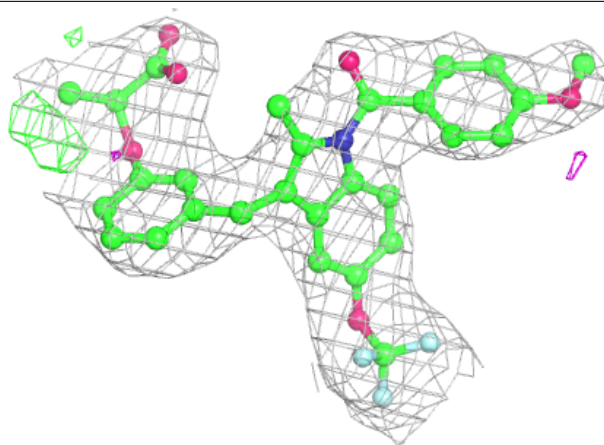
**Electron density around 241 B 7001:**

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



**Electron density around 241 A 5001:**

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



## 6.5 Other polymers [i](#)

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