



# Full wwPDB X-ray Structure Validation Report ⓘ

May 5, 2025 – 12:40 PM EDT

PDB ID : 9O9N / pdb\_00009o9n  
Title : Crystal structure of PPARgamma ligand binding domain (LBD) in complex with NCoR1 corepressor peptide and inverse agonist FX-909  
Authors : Laughlin, Z.T.; Dong, J.; Harp, J.M.; Kojetin, D.J.  
Deposited on : 2025-04-18  
Resolution : 2.10 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0rc1  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

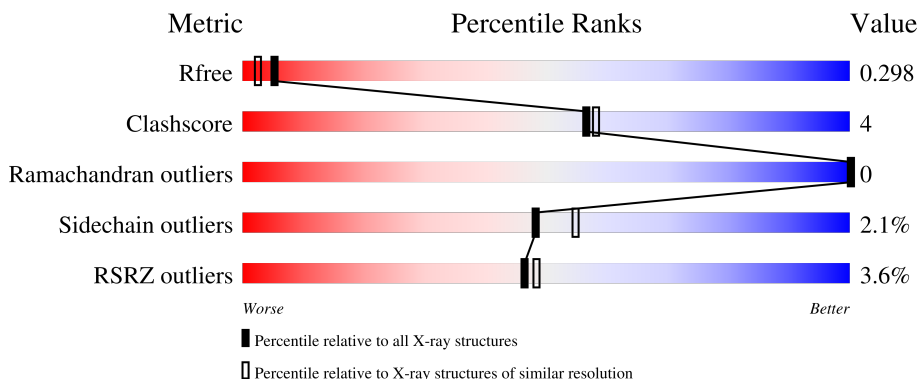
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

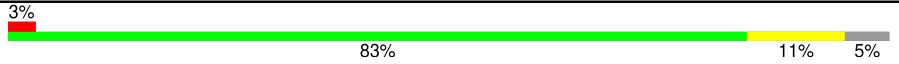
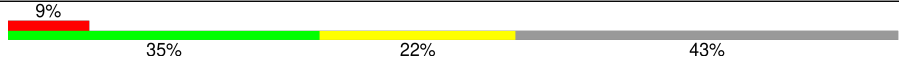
The reported resolution of this entry is 2.10 Å.

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))
$R_{free}$	164625	6234 (2.10-2.10)
Clashscore	180529	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)
RSRZ outliers	164620	6234 (2.10-2.10)

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  $\geq 3$ , 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	B	276	
2	D	23	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2250 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.

- Molecule 1 is a protein called Peroxisome proliferator-activated receptor gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	262	Total	C	N	O	S	0	0	0
			2086	1346	341	389	10			

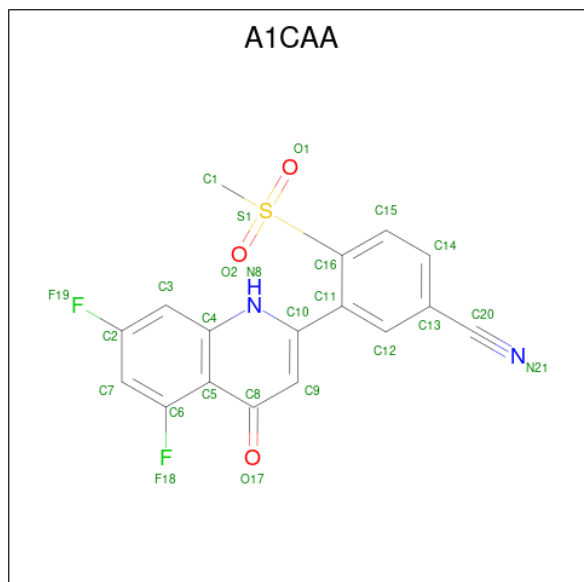
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	202	GLY	-	expression tag	UNP P37231

- Molecule 2 is a protein called Nuclear receptor corepressor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	13	Total	C	N	O	S	0	0	0
			102	65	18	18	1			

- Molecule 3 is (3P)-3-(5,7-difluoro-4-oxo-1,4-dihydroquinolin-2-yl)-4-(methanesulfonyl)benz onitrile (CCD ID: A1CAA) (formula: C<sub>17</sub>H<sub>10</sub>F<sub>2</sub>N<sub>2</sub>O<sub>3</sub>S) (labeled as "Ligand of Interest" by depositor).



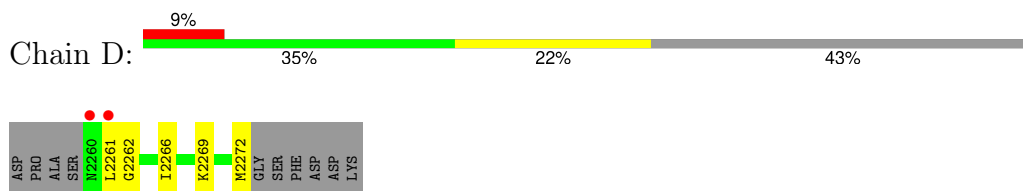
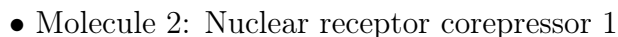
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	F	N	O	0	0
			21	16	2	2	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	39	Total	O	0	0
			39	39		
4	D	2	Total	O	0	0
			2	2		



- Molecule 1: Peroxisome proliferator-activated receptor gamma



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.04Å 62.04Å 166.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.89 – 2.10 20.89 – 2.10	Depositor EDS
% Data completeness (in resolution range)	77.7 (20.89-2.10) 77.6 (20.89-2.10)	Depositor EDS
$R_{merge}$	0.29	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.67 (at 2.09Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.239 , 0.297 0.239 , 0.298	Depositor DCC
$R_{free}$ test set	17958 reflections (10.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.4	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 36.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	2250	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.80% 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: A1CAA

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	B	0.36	0/2121	0.55	0/2859
2	D	0.22	0/101	0.44	0/133
All	All	0.35	0/2222	0.54	0/2992

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	B	2086	0	2131	17	1
2	D	102	0	113	3	0
3	B	21	0	0	0	0
4	B	39	0	0	3	0
4	D	2	0	0	0	0
All	All	2250	0	2244	20	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 4.

All (20) 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:B:259:GLU:HG3	1:B:468:LEU:HD11	1.56	0.87
1:B:325:ILE:HG23	1:B:388:ILE:HD12	1.80	0.62
1:B:373:LYS:HE3	1:B:373:LYS:HA	1.86	0.57
1:B:288:ARG:NH2	1:B:471:GLU:OE2	2.41	0.54
1:B:428:SER:HB3	1:B:431:LEU:HB2	1.91	0.52
1:B:434:LYS:O	1:B:438:LYS:HG2	2.11	0.51
2:D:2269:LYS:HA	2:D:2272:MET:HE3	1.94	0.50
1:B:286:GLN:HG3	4:B:637:HOH:O	2.11	0.49
1:B:357:ARG:HG2	4:B:622:HOH:O	2.12	0.49
1:B:277:VAL:HG11	1:B:463:MET:O	2.13	0.48
2:D:2262:GLY:O	2:D:2266:ILE:HD12	2.14	0.48
1:B:275:LYS:N	1:B:275:LYS:HD2	2.28	0.48
1:B:219:TYR:CE2	1:B:223:ILE:HD11	2.51	0.46
2:D:2261:LEU:HD12	2:D:2261:LEU:HA	1.87	0.43
1:B:379:LEU:HD11	1:B:435:LEU:CD1	2.47	0.43
1:B:289:SER:O	1:B:293:VAL:HG23	2.18	0.43
1:B:230:LYS:NZ	4:B:601:HOH:O	2.36	0.42
1:B:260:ASP:OD2	1:B:261:LYS:HD3	2.20	0.42
1:B:386:ILE:O	1:B:390:VAL:HG23	2.21	0.41
1:B:463:MET:HE3	1:B:463:MET:HB3	1.90	0.40

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:B:440:THR:OG1	1:B:440:THR:OG1[7_555]	2.11	0.09

## 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	B	258/276 (94%)	250 (97%)	8 (3%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	11/23 (48%)	11 (100%)	0	0	100	100
All	All	269/299 (90%)	261 (97%)	8 (3%)	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	B	231/248 (93%)	226 (98%)	5 (2%)	47	53
2	D	11/19 (58%)	11 (100%)	0	100	100
All	All	242/267 (91%)	237 (98%)	5 (2%)	48	55

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	261	LYS
1	B	281	ILE
1	B	310	ASP
1	B	401	LEU
1	B	447	THR

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

Mol	Chain	Res	Type
1	B	283	GLN
1	B	345	GLN
1	B	402	ASN
1	B	412	ASN
1	B	415	GLN
1	B	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 oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

1 ligand is 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	A1CAA	B	501	1	22,23,27	2.47	6 (27%)	30,33,41	1.97	8 (26%)

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	A1CAA	B	501	1	-	2/6/6/12	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	A1CAA	O17-C8	7.25	1.40	1.24
3	B	501	A1CAA	C4-N8	5.99	1.50	1.39
3	B	501	A1CAA	C13-C20	3.48	1.52	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	A1CAA	C11-C10	2.84	1.51	1.47
3	B	501	A1CAA	C5-C6	2.07	1.42	1.39
3	B	501	A1CAA	C3-C4	-2.06	1.36	1.39

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	A1CAA	C12-C11-C10	-5.37	112.14	120.43
3	B	501	A1CAA	C16-C11-C10	3.92	126.75	120.81
3	B	501	A1CAA	C12-C13-C20	-3.70	114.56	119.55
3	B	501	A1CAA	C7-C6-C5	-3.52	120.59	123.96
3	B	501	A1CAA	C14-C13-C20	3.15	125.11	119.97
3	B	501	A1CAA	C11-C10-N8	-2.66	113.35	116.76
3	B	501	A1CAA	O17-C8-C9	-2.43	117.99	121.88
3	B	501	A1CAA	C9-C10-N8	2.03	121.62	118.98

There are no chirality outliers.

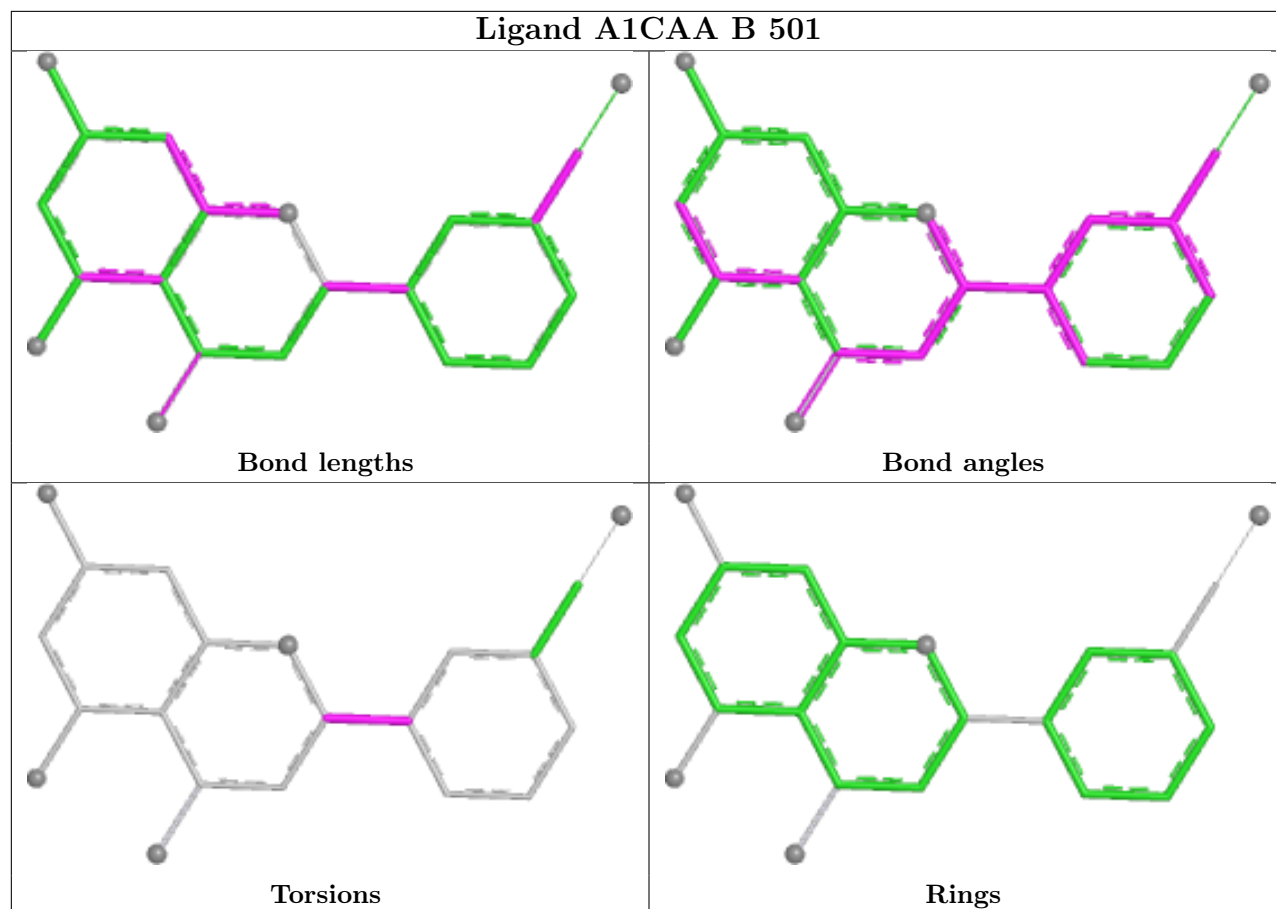
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	501	A1CAA	C9-C10-C11-C16
3	B	501	A1CAA	N8-C10-C11-C16

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	B	262/276 (94%)	0.19	8 (3%) 51 53	11, 19, 46, 79	0
2	D	13/23 (56%)	0.90	2 (15%) 6 7	23, 29, 64, 74	0
All	All	275/299 (91%)	0.23	10 (3%) 46 48	11, 19, 48, 79	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	2261	LEU	3.9
1	B	460	GLU	3.6
1	B	461	THR	3.4
1	B	459	THR	3.2
1	B	228	LEU	3.0
2	D	2260	ASN	3.0
1	B	243	ASP	2.8
1	B	454	GLN	2.8
1	B	458	LYS	2.6
1	B	287	PHE	2.3

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

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

### 6.3 Carbohydrates [i](#)

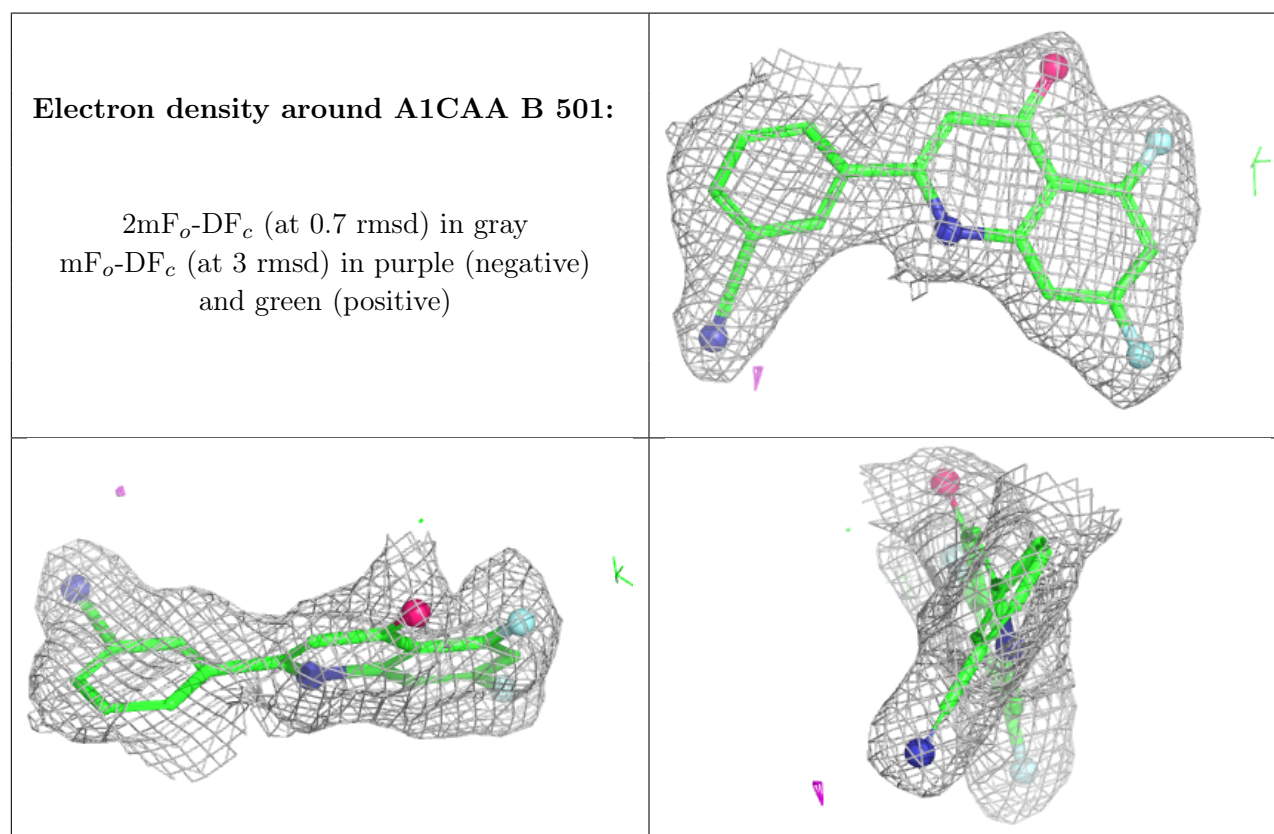
There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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
3	A1CAA	B	501	21/25	0.91	0.08	15,18,22,23	0

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.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.