

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

#### Feb 11, 2024 – 03:56 AM EST

PDB ID : 3BC5

Title: X-ray crystal structure of human ppar gamma with 2-(5-(3-(2-(5-methyl-2-ph

enyloxazol-4-yl)ethoxy)benzyl)-2-phenyl-2h-1,2,3-triazol-4-yl)acetic acid

Authors : Muckelbauer, J.K.

Deposited on : 2007-11-12

Resolution : 2.27 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)

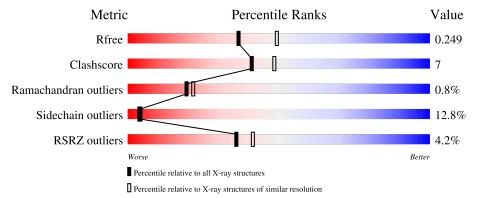
Validation Pipeline (wwPDB-VP) : 2.36

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY\ DIFFRACTION$ 

The reported resolution of this entry is 2.27 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},{\rm resolution\ range}(\mathring{\rm A})) \end{array}$
$R_{free}$	130704	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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% 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	Α.	200	4%			
I	A	296	69%	15%	5%	11%



# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2264 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.

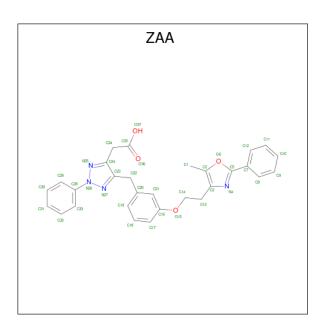
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	٨	263	Total	С	N	О	S	1.4	0	0
1	A	203	2072	1341	339	382	10	14	U	

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	182	MET	-	expression tag	UNP P37231
A	183	GLY	-	expression tag	UNP P37231
A	184	SER	-	expression tag	UNP P37231
A	185	SER	-	expression tag	UNP P37231
A	186	HIS	-	expression tag	UNP P37231
A	187	HIS	-	expression tag	UNP P37231
A	188	HIS	-	expression tag	UNP P37231
A	189	HIS	-	expression tag	UNP P37231
A	190	HIS	-	expression tag	UNP P37231
A	191	HIS	-	expression tag	UNP P37231
A	192	SER	-	expression tag	UNP P37231
A	193	SER	-	expression tag	UNP P37231
A	194	GLY	-	expression tag	UNP P37231
A	195	LEU	-	expression tag	UNP P37231
A	196	VAL	-	expression tag	UNP P37231
A	197	PRO	-	expression tag	UNP P37231
A	198	ARG	-	expression tag	UNP P37231
A	199	GLY	-	expression tag	UNP P37231
A	200	SER	-	expression tag	UNP P37231
A	201	HIS		expression tag	UNP P37231
A	202	MET	-	expression tag	UNP P37231

• Molecule 2 is  $(5-\{3-[2-(5-methyl-2-phenyl-1,3-oxazol-4-yl)ethoxy]benzyl\}-2-phenyl-2H-1,2,3-triazol-4-yl)acetic acid (three-letter code: ZAA) (formula: <math>C_{29}H_{26}N_4O_4$ ).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 37	C 29	N 4	O 4	0	0

#### • Molecule 3 is water.

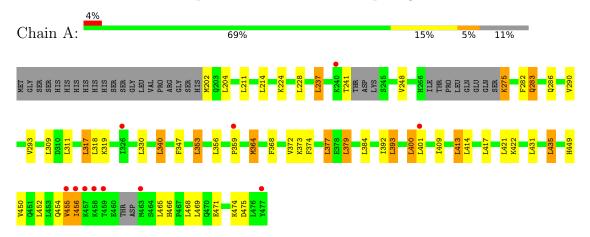
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	155	Total O 155 155	0	0



# 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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants	66.30Å 66.30Å 156.30Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 - 2.27	Depositor
resolution (A)	34.85 - 2.27	EDS
% Data completeness	95.0 (50.00-2.27)	Depositor
(in resolution range)	95.1 (34.85-2.27)	EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	8.76 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
P. P.	0.210 , 0.249	Depositor
$R, R_{free}$	0.209 , 0.249	DCC
$R_{free}$ test set	632  reflections  (3.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.9	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.34, 45.8	EDS
L-test for twinning <sup>2</sup>	$ < L >=0.50, < L^2>=0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	2264	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.10% of the height of the origin peak. No significant pseudotranslation is detected.

<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: ZAA

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).

Mal	Chain	Boı	nd lengths	Bo	nd angles
Mol   Chain		RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	A	1.92	4/2105~(0.2%)	1.05	8/2836 (0.3%)

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 maintain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	Observed(A)	$\operatorname{Ideal}( ext{\AA})$
1	A	283	GLN	CD-NE2	61.48	2.86	1.32
1	A	275	LYS	CA-CB	55.61	2.76	1.53
1	A	373	LYS	CE-NZ	10.48	1.75	1.49
1	A	224	LYS	CD-CE	6.29	1.67	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	275	LYS	N-CA-CB	-30.85	55.07	110.60
1	A	275	LYS	CB-CA-C	-19.16	72.07	110.40
1	A	373	LYS	CD-CE-NZ	-11.26	85.80	111.70
1	A	283	GLN	OE1-CD-NE2	-6.88	106.08	121.90
1	A	393	LEU	CA-CB-CG	-6.63	100.05	115.30
1	A	353	LEU	CA-CB-CG	5.22	127.30	115.30
1	A	283	GLN	CG-CD-OE1	-5.15	111.29	121.60
1	A	237	LEU	CA-CB-CG	5.09	127.00	115.30



All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	275	LYS	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group	
1	A	283	GLN	Sidechain	

# 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	2072	0	2106	30	0
2	A	37	0	25	2	0
3	A	155	0	0	2	0
All	All	2264	0	2131	30	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 7.

All (30) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance}  (\mathring{\rm A}) \end{array}$	Clash overlap (Å)
1:A:275:LYS:HA	3:A:519:HOH:O	1.66	0.96
1:A:286:GLN:HE22	1:A:465:LEU:HD23	1.43	0.83
1:A:319:LYS:HE2	1:A:475:ASP:HB2	1.74	0.69
1:A:359:PRO:CG	1:A:456:ILE:HG12	2.23	0.68
1:A:364:MET:HA	1:A:364:MET:CE	2.30	0.62
1:A:286:GLN:NE2	1:A:465:LEU:HD23	2.15	0.61
1:A:359:PRO:HG2	1:A:456:ILE:HG12	1.86	0.57
1:A:466:HIS:HD2	1:A:468:LEU:H	1.54	0.55
1:A:452:LEU:O	1:A:456:ILE:HD12	2.06	0.54
1:A:450:VAL:O	1:A:454:GLN:HG2	2.08	0.54
1:A:202:MET:HE3	1:A:422:LYS:HD3	1.90	0.53
1:A:466:HIS:CD2	1:A:468:LEU:H	2.29	0.50
1:A:379:LEU:HD21	1:A:435:LEU:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	${f distance}({ m \AA})$	overlap (Å)
1:A:409:ILE:HG22	1:A:413:LEU:HD22	1.95	0.48
1:A:290:VAL:HA	1:A:293:VAL:HG22	1.94	0.48
1:A:359:PRO:HG3	1:A:456:ILE:HG12	1.96	0.46
1:A:202:MET:CE	1:A:422:LYS:HD3	2.47	0.45
1:A:290:VAL:O	1:A:293:VAL:HG22	2.16	0.45
1:A:449:HIS:NE2	2:A:1:ZAA:O37	2.48	0.45
1:A:455:VAL:O	1:A:456:ILE:HG13	2.17	0.45
1:A:374:PHE:O	1:A:377:LEU:HB2	2.17	0.44
1:A:317:LEU:HG	1:A:392:ILE:O	2.17	0.44
1:A:340:LEU:HD13	1:A:347:PHE:HD2	1.83	0.44
1:A:364:MET:HA	1:A:364:MET:HE3	2.00	0.43
1:A:282:PHE:HD1	2:A:1:ZAA:H29	1.83	0.43
1:A:435:LEU:HD12	1:A:435:LEU:HA	1.91	0.42
1:A:471:GLU:O	1:A:474:LYS:HG2	2.21	0.41
1:A:317:LEU:HD13	1:A:400:LEU:HD11	2.03	0.40
1:A:372:VAL:HG22	3:A:524:HOH:O	2.21	0.40
1:A:368:PHE:O	1:A:372:VAL:HG13	2.21	0.40

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	Percentiles
1	A	255/296~(86%)	248 (97%)	5 (2%)	2 (1%)	19 22

#### All (2) Ramachandran outliers are listed below:

$\mathbf{Mol}$	Chain	$\operatorname{Res}$	Type
1	A	455	VAL
1	A	456	ILE



#### 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	226/266~(85%)	197 (87%)	29 (13%)	4 4

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	204	LEU
1	A	211	LEU
1	A	214	LEU
1	A	228	LEU
1	A	237	LEU
1	A	241	THR
1	A	248	VAL
1	A	309	LEU
1	A	311	LEU
1	A	317	LEU
1	A	318	LEU
1	A A	330	LEU
1	A	340	LEU
1	A	353	LEU
1	A	356	LEU
1	A	364	MET
1	A	377	LEU
1	A	379	LEU
1	A	384	LEU
1	A	393	LEU
1	A	400	LEU
1	A	401	LEU
1	A	413	LEU
1	A	414	LEU
1	A	417	LEU
1	A	421	LEU
1	A	431	LEU
1	A	435	LEU
1	A	469	LEU



Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	410	GLN
1	A	424	ASN
1	A	451	GLN
1	A	466	HIS
1	A	470	GLN

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

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	Tuno	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Res	Link	Bo	ond leng	ths	В	ond ang	gles
MIOI	туре		nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2							
2	ZAA	A	1	-	32,41,41	1.04	1 (3%)	31,56,56	2.29	11 (35%)							

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	ZAA	A	1	-	-	2/12/22/22	0/5/5/5

#### All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	Observed(A)	$\operatorname{Ideal}( ext{\AA})$
2	A	1	ZAA	C1-C2	2.70	1.52	1.48

#### All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}(^{o})$
2	A	1	ZAA	C30-C29-C28	-5.02	118.41	121.25
2	A	1	ZAA	C16-C21-C20	4.97	125.20	119.73
2	A	1	ZAA	C13-C3-C2	4.49	133.79	127.06
2	A	1	ZAA	C32-C33-C28	-4.43	118.74	121.25
2	A	1	ZAA	C33-C28-C29	3.81	121.98	116.27
2	A	1	ZAA	C12-C7-C8	3.12	121.42	118.65
2	A	1	ZAA	C34-C24-C23	2.94	134.22	127.17
2	A	1	ZAA	C17-C16-C21	-2.53	117.05	120.53
2	A	1	ZAA	O37-C35-O36	-2.50	117.08	123.30
2	A	1	ZAA	C19-C20-C21	-2.40	115.18	118.54
2	A	1	ZAA	O37-C35-C34	2.13	122.11	114.02

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	ZAA	C24-C34-C35-O36
2	A	1	ZAA	C24-C34-C35-O37

There are no ring outliers.

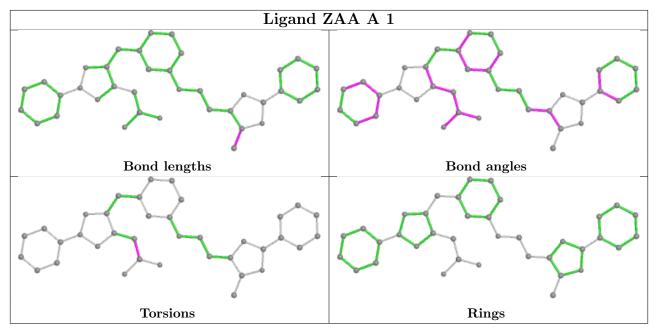
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	ZAA	2	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 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)

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,  $95^{th}$  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.

Mo	Chain	Analysed	<RSRZ $>$	# RSRZ > 2		$\mathrm{OWAB}(\mathrm{\AA}^2)$	Q < 0.9	
1	A	263/296 (88%)	0.07	11 (4%)	36	41	23, 36, 64, 88	5 (1%)

All (11) RSRZ outliers are listed below:

Mol	Chain	$\operatorname{Res}$	Type	RSRZ
1	A	455	VAL	5.3
1	A	458	LYS	3.9
1	A	456	ILE	3.9
1	A	459	THR	3.2
1	A	477	TYR	2.9
1	A	401	LEU	2.5
1	A	463	MET	2.5
1	A	359	PRO	2.3
1	A	240	LYS	2.2
1	A	457	LYS	2.1
1	A	326	ILE	2.0

# 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)

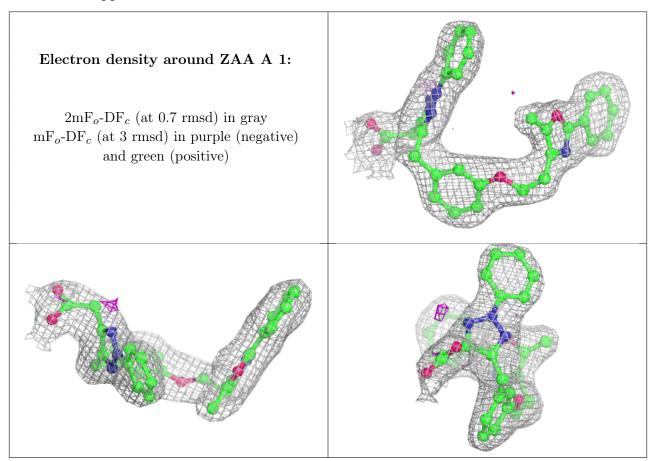
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,



median,  $95^{th}$  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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
2	ZAA	A	1	37/37	0.91	0.14	32,38,46,47	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.

