

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

#### Sep 2, 2023 – 04:21 PM EDT

PDB ID	:	3R8A			
Title	:	X-ray crystal structure of the nuclear hormone receptor PPAR-gamma in a			
		complex with a compound with dual PPAR gamma agonism and Angiotensin			
		II Type I receptor antagonism activity			
Authors	:	Ohren, J.F.			
Deposited on	:	2011-03-23			
Resolution	:	2.41  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 (i)) were used in the production of this report:

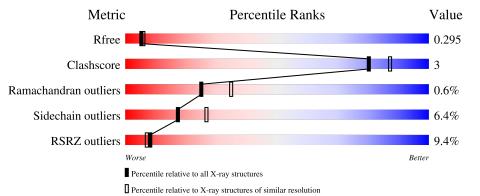
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.35
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

# 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 2.41 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	4647 (2.44-2.40)
Clashscore	141614	5161(2.44-2.40)
Ramachandran outliers	138981	5073(2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)
RSRZ outliers	127900	4543 (2.44-2.40)

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	А	282	10%	10% • 11%
1	В	282	7%	11% • 15%



# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4091 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.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Δ	251	Total	С	Ν	0	$\mathbf{S}$	0	2	0
	A	201	2014	1299	329	376	10	0	9	0
1	D	239	Total	С	Ν	0	S	0	2	0
	D	239	1918	1240	314	355	9	0		

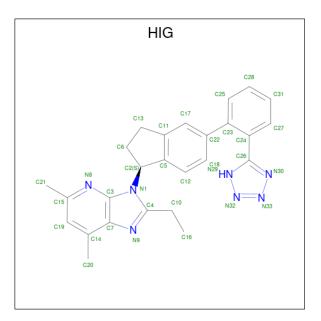
• Molecule 1 is a protein called Peroxisome proliferator-activated receptor gamma.

Chain	Residue	Modelled	Actual	Comment	Reference
А	196	MET	-	expression tag	UNP P37231
А	197	LYS	-	expression tag	UNP P37231
А	198	LYS	-	expression tag	UNP P37231
А	199	GLY	-	expression tag	UNP P37231
А	200	HIS	-	expression tag	UNP P37231
A	201	HIS	-	expression tag	UNP P37231
А	202	HIS	-	expression tag	UNP P37231
A	203	HIS	-	expression tag	UNP P37231
А	204	HIS	-	expression tag	UNP P37231
А	205	HIS	-	expression tag	UNP P37231
А	206	GLY	-	expression tag	UNP P37231
В	196	MET	-	expression tag	UNP P37231
В	197	LYS	-	expression tag	UNP P37231
В	198	LYS	-	expression tag	UNP P37231
В	199	GLY	-	expression tag	UNP P37231
В	200	HIS	-	expression tag	UNP P37231
В	201	HIS	-	expression tag	UNP P37231
В	202	HIS	-	expression tag	UNP P37231
В	203	HIS	-	expression tag	UNP P37231
В	204	HIS	-	expression tag	UNP P37231
В	205	HIS	-	expression tag	UNP P37231
В	206	GLY	-	expression tag	UNP P37231

There are 22 discrepancies between the modelled and reference sequences:

• Molecule 2 is 2-ethyl-5,7-dimethyl-3-{(1S)-5-[2-(1H-tetrazol-5-yl)phenyl]-2,3-dihydro-1H-ind en-1-yl}-3H-imidazo[4,5-b]pyridine (three-letter code: HIG) (formula:  $C_{26}H_{25}N_7$ ).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total         C         N           33         26         7	0	0
2	В	1	Total         C         N           33         26         7	0	0

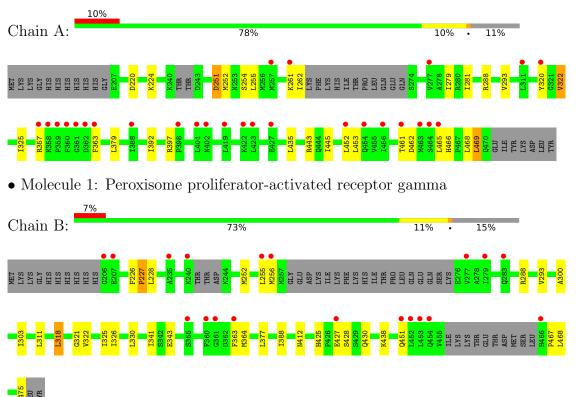
• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	59	Total O 59 59	0	0
3	В	34	Total O 34 34	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	C 1 2 1	Depositor
Cell constants	92.70Å 61.83Å 118.94Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $102.04^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	37.80 - 2.41	Depositor
Resolution (A)	36.32 - 2.41	EDS
% Data completeness	95.7 (37.80-2.41)	Depositor
(in resolution range)	95.7(36.32 - 2.41)	EDS
R <sub>merge</sub>	0.03	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$3.08 (at 2.42 \text{\AA})$	Xtriage
Refinement program	REFMAC 5, BUSTER 2.9.6	Depositor
D D.	0.230 , 0.281	Depositor
$R, R_{free}$	0.234 , $0.295$	DCC
$R_{free}$ test set	1287 reflections $(5.25\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	59.2	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.34,63.0	EDS
L-test for twinning <sup>2</sup>	$ \langle L  \rangle = 0.49, \langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4091	wwPDB-VP
Average B, all atoms $(Å^2)$	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.72% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<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: HIG

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			lengths	Bond angles	
	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.44	0/2061	0.63	0/2773
1	В	0.43	0/1959	0.64	0/2637
All	All	0.44	0/4020	0.63	0/5410

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	А	2014	0	2071	10	0
1	В	1918	0	1966	12	0
2	А	33	0	25	1	0
2	В	33	0	25	3	0
3	А	59	0	0	0	0
3	В	34	0	0	0	0
All	All	4091	0	4087	22	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 (22) 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:293:VAL:HG22	1:A:322:VAL:HG11	1.75	0.68
1:B:467:PRO:HB2	1:B:468:LEU:HA	1.79	0.63
1:A:261:LYS:H	1:A:262:ILE:HA	1.65	0.61
1:B:325:ILE:HD12	1:B:388:ILE:HG23	1.92	0.52
1:B:293:VAL:HG22	1:B:322:VAL:HG21	1.92	0.51
1:A:325:ILE:HD11	1:A:392:ILE:HG13	1.94	0.49
1:A:465:LEU:HB3	1:A:469:LEU:HB3	1.95	0.49
1:B:321:GLY:O	1:B:325:ILE:HG12	2.13	0.49
1:A:281:ILE:HG12	2:A:1:HIG:H25	1.97	0.47
1:B:300:ALA:HA	1:B:303:ILE:HD12	2.00	0.44
1:A:220:ASP:O	1:A:224:LYS:HG3	2.18	0.43
1:B:364:MET:CE	2:B:1:HIG:H6A	2.48	0.43
1:A:251:ASP:HB3	1:A:254:SER:H	1.84	0.43
1:B:318:LEU:HD12	1:B:318:LEU:HA	1.96	0.42
1:B:377:LEU:HD11	1:B:438:LYS:HD3	2.00	0.42
1:B:326:ILE:CG2	2:B:1:HIG:H19	2.50	0.41
1:A:320:TYR:HB2	1:A:397:ARG:HD2	2.02	0.41
1:B:226:PHE:HA	1:B:227:PRO:HD3	1.99	0.41
1:A:379:LEU:HD11	1:A:435:LEU:HD13	2.02	0.41
1:B:425:HIS:HB3	1:B:428:SER:HB3	2.03	0.41
1:A:466:HIS:CD2	1:A:468:LEU:H	2.39	0.40
1:B:288:ARG:HG3	2:B:1:HIG:H20B	2.03	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	А	248/282~(88%)	237~(96%)	9~(4%)	2(1%)	19 27
1	В	233/282~(83%)	225~(97%)	7 (3%)	1 (0%)	34 47
All	All	481/564~(85%)	462 (96%)	16 (3%)	3~(1%)	25 35



All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	462	ASP
1	А	461	THR
1	В	227	PRO

#### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Analysed Rotameric Outliers		Percentiles		
1	А	227/253~(90%)	214 (94%)	13~(6%)	20 32		
1	В	214/253~(85%)	199~(93%)	15 (7%)	15 23		
All	All	441/506~(87%)	413 (94%)	28~(6%)	17 27		

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	251	ASP
1	А	252	MET
1	А	255	LEU
1	А	279	ILE
1	А	288	ARG
1	А	322	VAL
1	А	357	ARG
1	А	363	PHE
1	А	443	ARG
1	А	445	ILE
1	А	452	LEU
1	А	453	LEU
1	А	469	LEU
1	В	228	LEU
1	В	252	MET
1	В	255	LEU
1	В	256	MET
1	В	311	LEU
1	В	318	LEU
1	В	330	LEU

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Contr	Continuea from previous page									
Mol	Chain	$\mathbf{Res}$	Type							
1	В	341	ILE							
1	В	343	GLU							
1	В	363	PHE							
1	В	412	ASN							
1	В	427	GLU							
1	В	430	GLN							
1	В	451	GLN							
1	В	475	ASP							

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Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	294	GLN
1	А	308	ASN
1	А	375	ASN
1	А	437	GLN
1	А	444	GLN
1	А	451	GLN
1	А	466	HIS
1	А	470	GLN
1	В	410	GLN
1	В	451	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)

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	Turne	Chain	Res	Link	Bo	ond leng	ths	B	ond ang	les
IVIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
2	HIG	В	1	-	31,38,38	1.85	9 (29%)	31,56,56	2.00	<mark>6 (19%)</mark>
2	HIG	А	1	-	31,38,38	2.12	8 (25%)	31,56,56	2.31	8 (25%)

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	HIG	В	1	-	-	2/2/23/23	0/6/6/6
2	HIG	А	1	-	-	2/2/23/23	0/6/6/6

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	А	1	HIG	C10-C4	7.90	1.54	1.49
2	В	1	HIG	C10-C4	6.41	1.53	1.49
2	А	1	HIG	C19-C14	3.80	1.43	1.37
2	В	1	HIG	C19-C14	3.25	1.42	1.37
2	В	1	HIG	C17-C11	2.92	1.42	1.37
2	В	1	HIG	C15-N8	2.87	1.39	1.33
2	А	1	HIG	C18-C12	2.86	1.42	1.36
2	В	1	HIG	C28-C25	2.79	1.43	1.36
2	А	1	HIG	C15-N8	2.74	1.38	1.33
2	А	1	HIG	C17-C11	2.66	1.42	1.37
2	А	1	HIG	C19-C15	2.54	1.43	1.38
2	А	1	HIG	C28-C25	2.51	1.42	1.36
2	В	1	HIG	C3-N8	2.17	1.39	1.35
2	А	1	HIG	C13-C11	2.15	1.54	1.51
2	В	1	HIG	C18-C12	2.09	1.41	1.36
2	В	1	HIG	C5-C2	-2.05	1.48	1.51
2	В	1	HIG	C19-C15	2.00	1.42	1.38

All (14) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	А	1	HIG	C4-N1-C2	8.72	132.50	125.50
2	В	1	HIG	C4-N1-C2	8.01	131.93	125.50
2	А	1	HIG	C2-N1-C3	-4.47	117.73	126.86
2	А	1	HIG	C3-C7-N9	-4.02	105.39	109.47
2	В	1	HIG	C2-N1-C3	-3.51	119.69	126.86
2	А	1	HIG	C20-C14-C7	3.43	123.36	120.03
2	В	1	HIG	C19-C15-N8	-3.16	118.83	122.57
2	А	1	HIG	C13-C6-C2	-2.56	103.26	105.91
2	А	1	HIG	C10-C4-N9	2.53	127.74	124.21
2	А	1	HIG	C27-C24-C23	2.49	122.01	118.54
2	В	1	HIG	C3-C7-N9	-2.39	107.05	109.47
2	В	1	HIG	C15-N8-C3	2.37	120.92	117.71
2	В	1	HIG	C18-C12-C5	-2.32	117.99	121.25
2	А	1	HIG	C18-C12-C5	-2.07	118.35	121.25

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	А	1	HIG	C16-C10-C4-N1
2	А	1	HIG	C16-C10-C4-N9
2	В	1	HIG	C16-C10-C4-N1
2	В	1	HIG	C16-C10-C4-N9

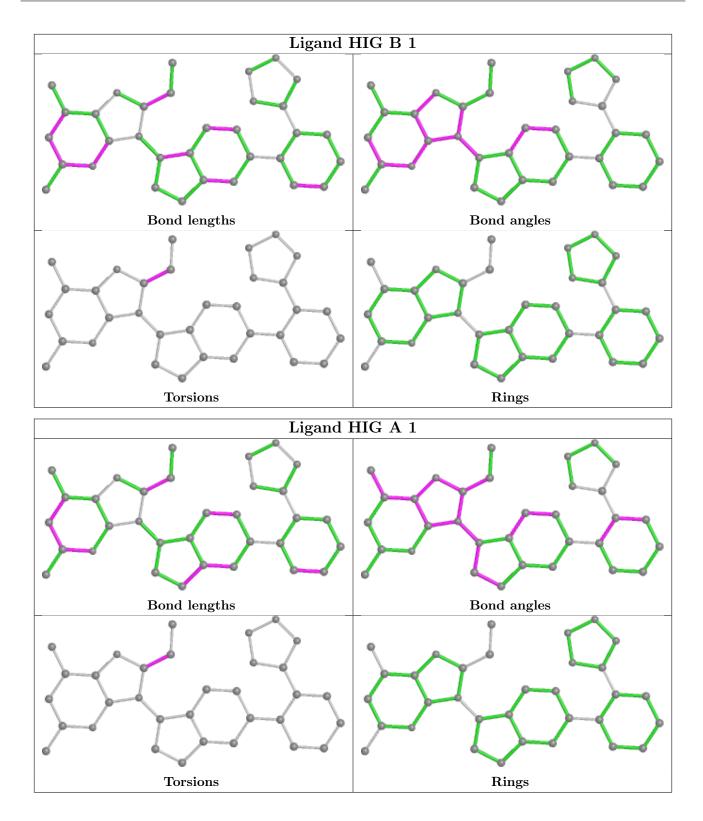
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	1	HIG	3	0
2	А	1	HIG	1	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 sufficient must be 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.

Mol	Chain	Analysed	$\langle RSRZ \rangle$	#RSRZ>2	$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q<0.9
1	А	251/282 (89%)	0.57	27 (10%) 5 4	48, 72, 115, 141	0
1	В	239/282~(84%)	0.39	19 (7%) 12 11	43, 67, 112, 131	0
All	All	490/564~(86%)	0.48	46 (9%) 8 7	43, 69, 113, 141	0

All (46) RSRZ outliers are listed below:

Mol			Type	RSRZ
1	А	465	LEU	6.2
1	В	466	HIS	5.9
1	В	360	PHE	5.9
1	В	277	VAL	5.6
1	А	456	ILE	4.9
1	А	402[A]	ASN	4.8
1	А	360	PHE	4.6
1	А	398	PRO	4.2
1	В	206	GLY	4.1
1	А	357	ARG	4.0
1	В	361	GLY	4.0
1	В	451	GLN	3.9
1	А	257	MET	3.7
1	В	363	PHE	3.7
1	А	464	SER	3.6
1	В	240	LYS	3.5
1	А	261	LYS	3.4
1	В	283[A]	GLN	3.3
1	В	454	GLN	3.3
1	В	256	MET	3.3
1	А	401	LEU	3.2
1	А	362	ASP	3.2
1	А	463	MET	3.1
1	А	423	LEU	3.1

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3R8A
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Mol	Chain	Res	Type	RSRZ
1	А	454	GLN	3.1
1	В	235	ALA	2.9
1	В	207	GLU	2.8
1	В	453	LEU	2.8
1	А	452	LEU	2.8
1	В	279	ILE	2.7
1	А	277	VAL	2.6
1	В	427	GLU	2.6
1	А	311	LEU	2.5
1	А	358	LYS	2.4
1	А	388	ILE	2.4
1	В	255	LEU	2.4
1	А	359	PRO	2.3
1	А	422	LYS	2.3
1	А	320	TYR	2.3
1	В	355	SER	2.3
1	А	461	THR	2.2
1	А	427[A]	GLU	2.1
1	А	361	GLY	2.1
1	В	452	LEU	2.1
1	А	363	PHE	2.0
1	А	419	LEU	2.0

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### 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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
2	HIG	В	1	33/33	0.88	0.18	75,87,102,103	0

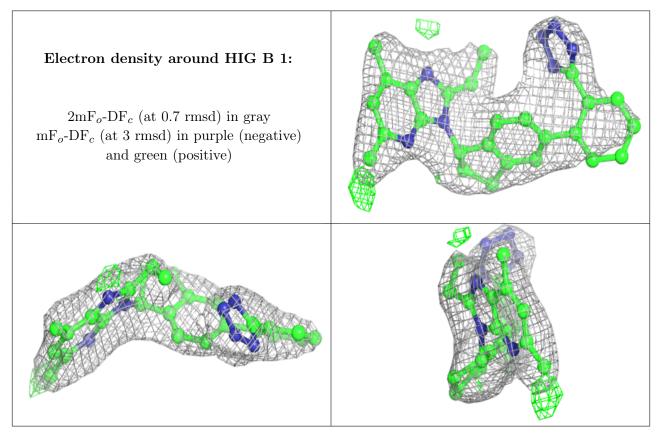
Continued on next page...



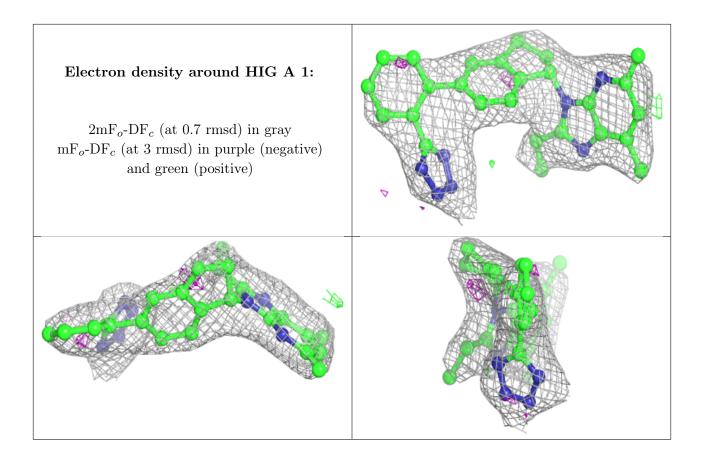
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
2	HIG	А	1	33/33	0.91	0.18	62,70,79,79	0

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.

