

Full wwPDB X-ray Structure Validation Report (i)

May 14, 2020 – 06:40 am BST

PDB ID : 2POB

Title : PPARgamma Ligand binding domain complexed with a farglitazar analogue

gw4709

Authors : Nolte, R.T. Deposited on : 2007-04-26

Resolution : 2.30 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 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 : 2.11

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)

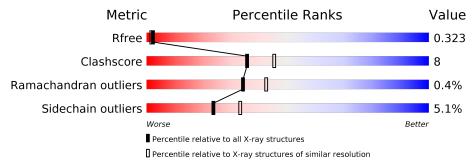
Validation Pipeline (wwPDB-VP) : 2.11

1 Overall quality at a glance (i)

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

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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{resolution range}(ext{Å}))$
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 >=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%

Mol	Chain	Length	Quality of chain					
1	A	272	75%	17%	•• 6%			
1	В	272	73%	18%	9%			



2 Entry composition (i)

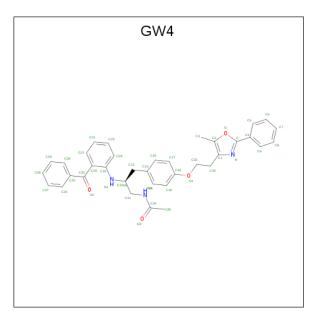
There are 4 unique types of molecules in this entry. The entry contains 4278 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	A	255	Total 2037	C 1312	N 332	O 384	S 9	0	2	0
1	В	247	Total 1971	C 1269	N 323	O 370	S 9	0	3	0

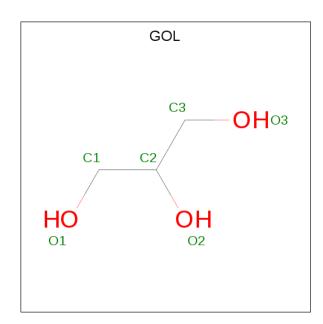
• Molecule 2 is N-[(2S)-2-[(2-BENZOYLPHENYL)AMINO]-3- $\{4-[2-(5-METHYL-2-PHENYL-1,3-OXAZOL-4-YL)ETHOXY]PHENYL\}PROPYL]ACETAMIDE (three-letter code: GW4) (formula: <math>C_{36}H_{35}N_3O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 43	C 36	N 3	O 4	0	0

• Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).





Mo	ol	Chain	Residues	Atoms		ZeroOcc	AltConf	
3		В	1	Total 6	C 3	O 3	0	0

• Molecule 4 is water.

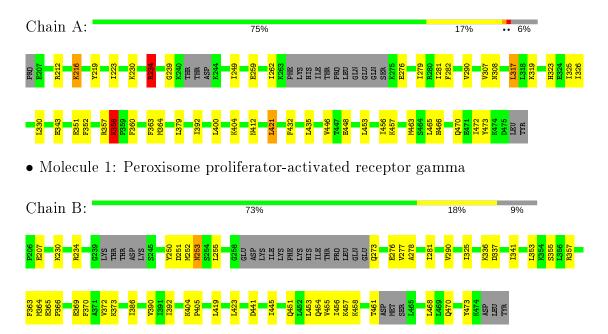
\mathbf{Mol}	Chain	Residues	${f Atoms}$	$\mathbf{ZeroOcc}$	AltConf
4	A	125	Total O 125 125	0	0
4	В	96	Total O 96 96	0	0



3 Residue-property plots (i)

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





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	92.92Å 62.01Å 118.17Å	Depositor
a, b, c, α , β , γ	90.00° 101.94° 90.00°	Depositor
Resolution (Å)	24.50 - 2.30	Depositor
resolution (11)	24.16 - 2.30	EDS
% Data completeness	$91.0 \ (24.50 - 2.30)$	Depositor
(in resolution range)	91.0 (24.16-2.30)	EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) > 1$	$1.60 \; ({\rm at} \; 2.31 {\rm \AA})$	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.225 , 0.273	Depositor
it, it free	0.279 , 0.323	DCC
R_{free} test set	875 reflections (3.27%)	wwPDB-VP
Wilson B-factor (\mathring{A}^2)	35.1	Xtriage
Anisotropy	0.348	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.36 , 71.0	EDS
L-test for twinning ²	$ < L > = 0.49, < L^2> = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o , F_c correlation	0.89	EDS
Total number of atoms	4278	wwPDB-VP
Average B, all atoms $(Å^2)$	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.39% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities 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: GOL, GW4

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	Boı	nd lengths	Bond angles		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z >5	
1	A	0.57	$2/2069 \ (0.1\%)$	0.63	1/2790 (0.0%)	
1	В	0.59	$2/2003 \ (0.1\%)$	0.65	1/2705 (0.0%)	
All	All	0.58	4/4072 (0.1%)	0.64	2/5495 (0.0%)	

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	Α	0	1		

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(ext{\AA})$
1	В	337	ASP	CG-OD2	7.51	1.42	1.25
1	В	336	LYS	CE-NZ	5.52	1.62	1.49
1	A	308	ASN	CG-ND2	5.33	1.46	1.32
1	A	308	ASN	CG-OD1	5.05	1.35	1.24

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^o)$
1	В	337	ASP	CB-CG-OD2	-5.84	113.04	118.30
1	A	234	ARG	NE-CZ-NH2	5.04	122.82	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	A	358	LYS	Peptide

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	2037	0	2059	37	0
1	В	1971	0	1972	30	0
2	A	43	0	35	7	0
3	В	6	0	8	1	0
4	A	125	0	0	1	0
4	В	96	0	0	0	0
All	All	4278	0	4074	66	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.

All (66) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
1:B:255:LEU:HD11	1:B:281:ILE:HD11	1.32	1.07
1:B:255:LEU:CD1	1:B:281:ILE:HD11	1.89	1.01
1:B:453:LEU:O	1:B:456:ILE:HG22	1.74	0.87
1:B:419:LEU:O	1:B:423:LEU:HD13	1.82	0.79
1:A:472:ILE:CD1	1:B:468:LEU:HD11	2.20	0.72
1:B:276:GLU:OE1	1:B:278:ALA:HB3	1.90	0.72
1:A:323:HIS:ND1	2:A:478:GW4:H352	2.09	0.68
1:B:250:TYR:CD2	1:B:251:ASP:HB2	2.29	0.68
1:A:219:TYR:O	1:A:223:ILE:HD12	1.94	0.67
1:A:453:LEU:HD11	1:A:473:TYR:CZ	2.31	0.66
1:B:370:PHE:HB2	1:B:445:ILE:HD11	1.77	0.66
1:B:325:ILE:HD11	1:B:392:ILE:HG13	1.77	0.65
1:B:455:VAL:O	1:B:455:VAL:HG12	1.99	0.61
1:A:465:LEU:HB3	1:A:470:GLN:HE21	1.65	0.60
1:A:319:LYS:HA	1:A:472:ILE:HD12	1.85	0.59
2:A:478:GW4:C30	2:A:478:GW4:H21	2.31	0.58
1:A:219:TYR:CE1	1:A:223:ILE:HD11	2.41	0.56

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Continued from prev		Interatomic	Clash	
Atom-1	Atom-2	${\rm distance} \ ({\rm \AA})$	$ m overlap~(\AA)$	
1:A:249:ILE:HD11	1:A:262:ILE:HD11	1.89	0.55	
1:A:472:ILE:HD13	1:B:468:LEU:HD11	1.87	0.55	
1:A:379:LEU:HD11	1:A:435:LEU:HD13	1.86	0.55	
1:A:472:ILE:HD11	1:B:468:LEU:HD11	1.89	0.55	
1:A:230:LYS:O	1:A:234:ARG:HG2	2.07	0.55	
1:A:421:LEU:HD23	1:A:432:PHE:HA	1.90	0.54	
1:B:451:GLN:O	1:B:455:VAL:HG23	2.07	0.53	
1:B:325:ILE:HD11	1:B:392:ILE:CG1	2.38	0.52	
1:A:323:HIS:NE2	1:A:472:ILE:HG22	2.24	0.51	
1:B:250:TYR:CE2	1:B:251:ASP:HB2	2.46	0.51	
1:A:330:LEU:HD21	1:A:364:MET:HE3	1.93	0.50	
1:A:323:HIS:HB3	1:A:446:VAL:HG22	1.93	0.50	
1:A:326:ILE:HD12	2:A:478:GW4:H353	1.93	0.50	
1:A:276:GLU:OE1	1:A:279:ILE:HD13	2.12	0.49	
2:A:478:GW4:C21	2:A:478:GW4:C30	2.90	0.49	
1:B:454:GLN:C	1:B:456:ILE:H	2.16	0.48	
1:A:453:LEU:HD11	1:A:473:TYR:CE2	2.48	0.48	
1:A:325:ILE:HD11	1:A:392:ILE:HG13	1.95	0.48	
1:A:456:ILE:HG22	1:A:457:LYS:N	2.29	0.48	
1:B:251:ASP:OD2	1:B:252:MET:N	2.46	0.48	
1:A:358:LYS:O	1:A:358:LYS:HG3	2.14	0.48	
1:B:253:ASN:ND2	1:B:253:ASN:O	2.44	0.48	
1:A:317:LEU:HD13	1:A:400:LEU:HD21	1.96	0.47	
1:A:276:GLU:HA	1:A:279:ILE:HD13	1.96	0.47	
1:B:457:LYS:O	1:B:461:THR:HG23	2.15	0.47	
1:A:363:PHE:CE2	2:A:478:GW4:H26	2.50	0.47	
1:A:290:VAL:HG21	1:A:466:HIS:CD2	2.50	0.47	
1:B:255:LEU:HD11	1:B:281:ILE:CD1	2.24	0.46	
1:B:252:MET:SD	1:B:277:VAL:HG21	2.56	0.46	
1:A:453:LEU:CD1	1:A:473:TYR:CZ	2.99	0.45	
1:A:282:PHE:HD2	2:A:478:GW4:C29	2.31	0.44	
1:A:358:LYS:O	1:A:358:LYS:CG	2.66	0.44	
1:B:290:VAL:HG21	1:B:473:TYR:CD1	2.53	0.43	
1:A:363:PHE:CE2	2:A:478:GW4:C26	3.02	0.43	
1:A:307:VAL:HG13	4:A:497:HOH:O	2.19	0.43	
1:A:319:LYS:HA	1:A:472:ILE:CD1	2.47	0.43	
1:A:281:ILE:HD11	1:A:352:PHE:HE2	1.84	0.42	
1:B:456:ILE:CG2	1:B:457:LYS:N	2.83	0.42	
1:B:404:LYS:N	1:B:405:PRO:HD2	2.35	0.42	
1:A:212:ARG:O	1:A:216:LYS:HD3	2.20	0.42	
1:B:386:ILE:O	1:B:390:VAL:HG23	2.20	0.42	

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Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	${f distance} \; ({f \AA})$	overlap (Å)
1:B:341:ILE:HB	3:B:478:GOL:H12	2.02	0.42
1:B:353:LEU:HD13	1:B:364:MET:HG3	2.01	0.42
1:A:290:VAL:HG21	1:A:466:HIS:CG	2.56	0.40
1:B:365:GLU:HB3	1:B:366:PRO:HD3	2.03	0.40
1:A:230:LYS:O	1:A:234:ARG:CG	2.69	0.40
1:A:360:PHE:CE1	1:A:456:ILE:HD11	2.56	0.40
1:B:230:LYS:O	1:B:234:ARG:HG2	2.21	0.40
1:B:369:GLU:O	1:B:372:VAL:HG12	2.22	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	$251/272 \ (92\%)$	240 (96%)	10 (4%)	1 (0%)	34	42	
1	В	242/272 (89%)	237 (98%)	4 (2%)	1 (0%)	34	42	
All	All	493/544 (91%)	477 (97%)	14 (3%)	2 (0%)	34	42	

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	239	GLY
1	В	458	LYS

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	${f Rotameric}$	Outliers	Percentiles		
1	A	$224/245 \ (91\%)$	211 (94%)	13 (6%)	20 27		
1	В	215/245~(88%)	205~(95%)	10 (5%)	26 37		
All	All	439/490 (90%)	416 (95%)	23 (5%)	24 32		

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	216	LYS
1	A	234	ARG
1	A	259	GLU
1	A	317	LEU
1	A	343	GLU
1	A	351	GLU
1	A	357	ARG
1	A	358	LYS
1	A	404	LYS
1	A	412	ASN
1	A	421	LEU
1	A	448	GLU
1	A	463	MET
1	В	207[A]	GLU
1	В	207[B]	GLU
1	В	253	ASN
1	В	273	GLN
1	В	355	SER
1	В	357	ARG
1	В	363	PHE
1	В	373	LYS
1	В	441	ASP
1	В	470	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	${f Res}$	\mathbf{Type}
1	A	412	ASN
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 carbohydrates 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	ol Type Chain Res Link		Link	Bond lengths			Bond angles			
10101	туре	Chain	nes	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GW4	A	478	-	43,47,47	0.84	1 (2%)	52,63,63	1.46	7 (13%)
3	GOL	В	478	_	5,5,5	0.36	0	5,5,5	0.29	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	GW4	A	478	_	_	1/28/31/31	0/5/5/5
3	GOL	В	478	_	-	0/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(ext{\AA})$
2	A	478	GW4	C19-N1	2.26	1.42	1.37



All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^o)$
2	A	478	GW4	C19-N1-C10	-5.27	115.63	124.69
2	A	478	GW4	C4-C-N	4.58	129.71	123.56
2	A	478	GW4	C24-C19-C20	-2.71	115.82	119.38
2	A	478	GW4	C21-C20-C19	2.64	121.80	118.81
2	A	478	GW4	C32-O1-C18	-2.40	111.64	117.93
2	A	478	GW4	C35-C34-N2	-2.32	111.97	116.09
2	A	478	GW4	C19-C20-C31	-2.14	120.56	121.96

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	Α	478	GW4	N1-C10-C11-N2

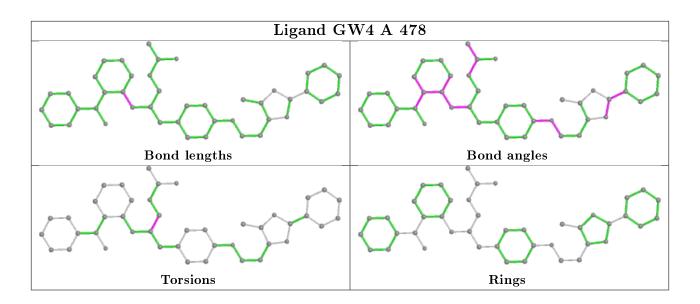
There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	478	GW4	7	0
3	В	478	GOL	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 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)

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

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

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

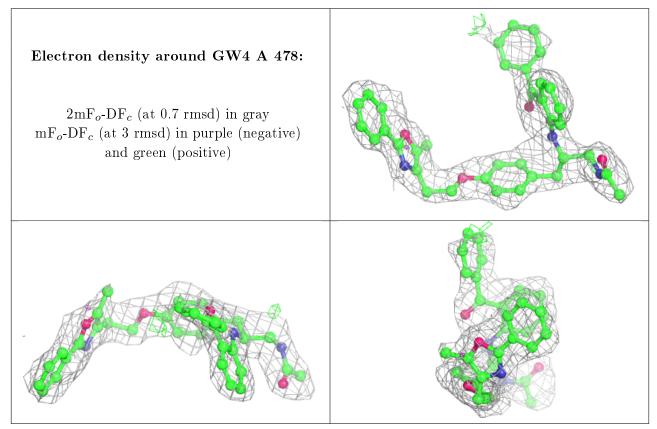
6.3 Carbohydrates (i)

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

6.4 Ligands (i)

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.





6.5 Other polymers (i)

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

