



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:07 PM UTC

PDB ID : 2POB / pdb_00002pob
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

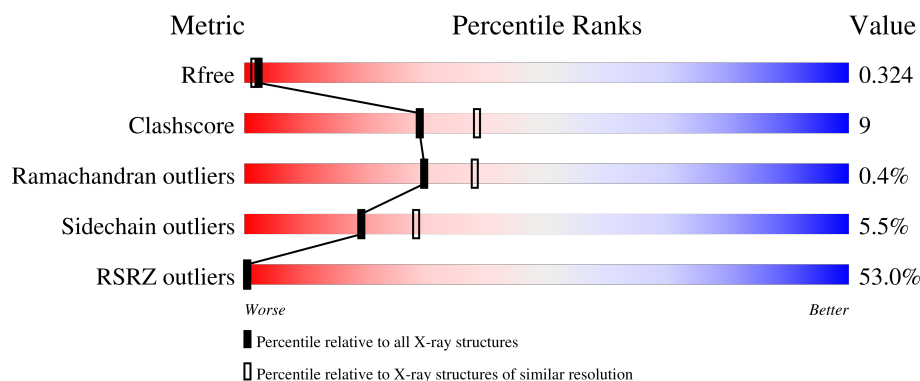
1 Overall quality at a glance

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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 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 $\leq 5\%$. 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	A	272	
1	B	272	

2 Entry composition [i](#)

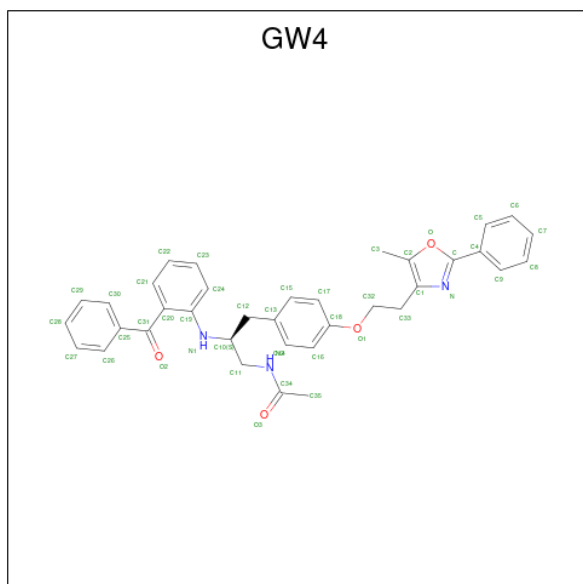
There are 4 unique types of molecules in this entry. The entry contains 4278 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- 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 (CCD ID: GW4) (formula: $C_{36}H_{35}N_3O_4$).



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

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		

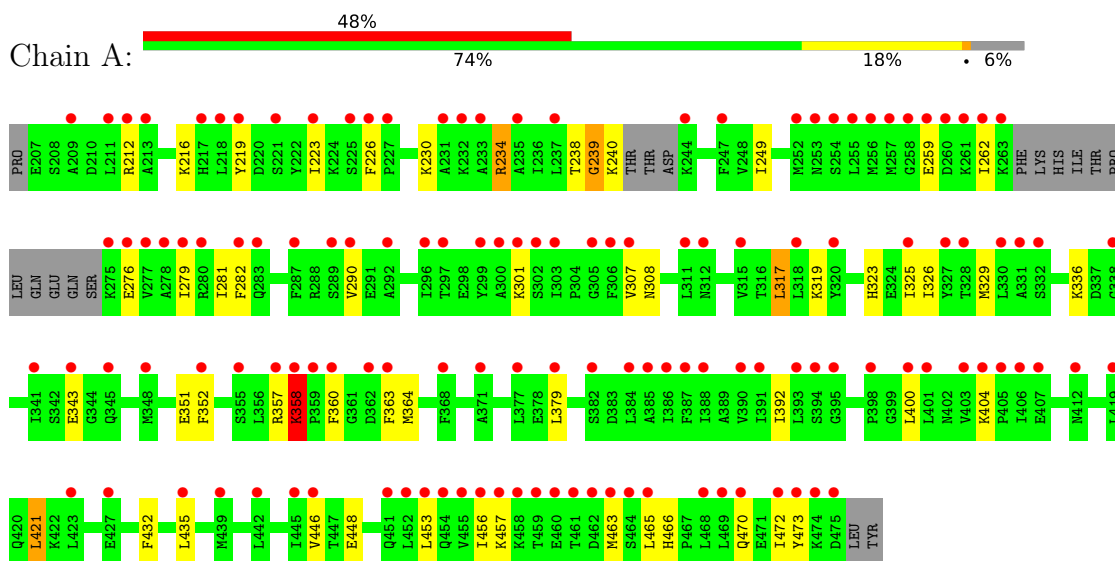
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	125	Total	O	0	0
			125	125		
4	B	96	Total	O	0	0
			96	96		

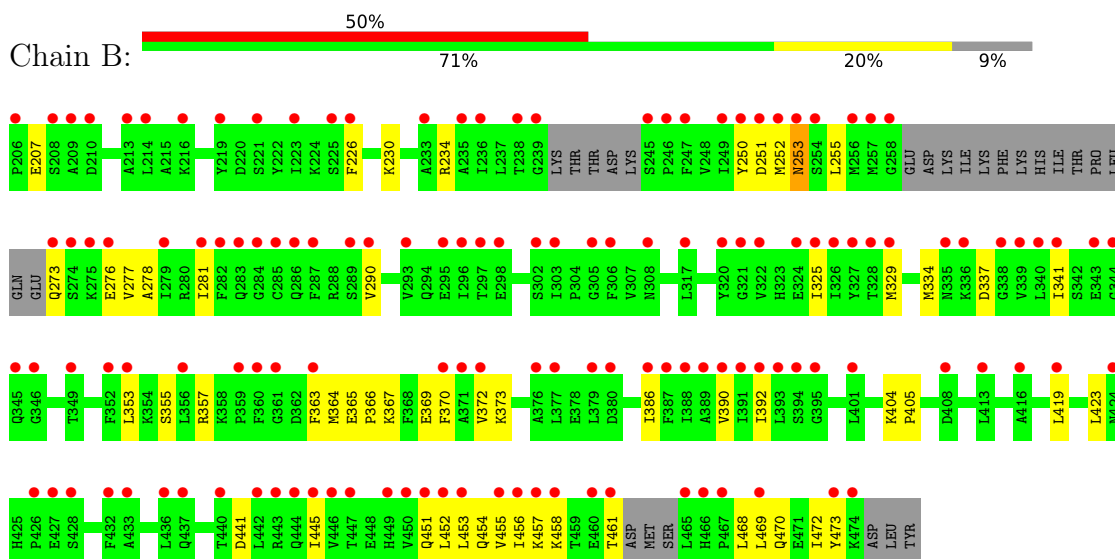
3 Residue-property plots

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



- 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, α , β , γ	92.92Å 62.01Å 118.17Å 90.00° 101.94° 90.00°	Depositor
Resolution (Å)	24.50 – 2.30 24.50 – 2.30	Depositor EDS
% Data completeness (in resolution range)	91.0 (24.50-2.30) 90.9 (24.50-2.30)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.225 , 0.273 0.279 , 0.324	Depositor DCC
R_{free} test set	875 reflections (2.97%)	wwPDB-VP
Wilson B-factor (Å ²)	35.1	Xtriage
Anisotropy	0.348	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 68.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: GW4, GOL

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	0.73	2/2069 (0.1%)	0.89	0/2790
1	B	0.74	1/2003 (0.0%)	0.90	0/2705
All	All	0.73	3/4072 (0.1%)	0.89	0/5495

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	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	337	ASP	CG-OD2	9.09	1.42	1.25
1	A	308	ASN	CG-ND2	6.15	1.46	1.33
1	A	308	ASN	CG-OD1	6.06	1.35	1.23

There are no bond angle outliers.

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 ⓘ

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	40	0
1	B	1971	0	1972	33	0
2	A	43	0	35	8	0
3	B	6	0	8	1	0
4	A	125	0	0	1	0
4	B	96	0	0	0	0
All	All	4278	0	4074	71	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 9.

All (71) 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: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:HG12	1:B:455:VAL:O	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:454:GLN:C	1:B:456:ILE:H	2.16	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: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:B:334:MET:HE1	1:B:367:LYS:HB2	1.94	0.50
1:A:276:GLU:OE1	1:A:279:ILE:HD13	2.12	0.49
2:A:478:GW4:C30	2:A:478:GW4:C21	2.90	0.49
1:B:226:PHE:CE1	1:B:329:MET:HE1	2.47	0.49
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:HG3	1:A:358:LYS:O	2.14	0.48
1:B:253:ASN:O	1:B:253:ASN:ND2	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:252:MET:SD	1:B:277:VAL:HG21	2.56	0.46
1:B:255:LEU:HD11	1:B:281:ILE:CD1	2.24	0.46
1:A:301:LYS:NZ	1:B:472:ILE:O	2.43	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
1:B:341:ILE:HB	3:B:478:GOL:H12	2.02	0.42
1:A:364:MET:HE1	2:A:478:GW4:H16	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:353:LEU:HD13	1:B:364:MET:HG3	2.01	0.42
1:A:238:THR:O	1:A:239:GLY:C	2.63	0.41
1:A:226:PHE:CG	1:A:329:MET:HE1	2.56	0.40
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%)	30	38
1	B	242/272 (89%)	237 (98%)	4 (2%)	1 (0%)	30	38
All	All	493/544 (91%)	477 (97%)	14 (3%)	2 (0%)	30	38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	239	GLY
1	B	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	Rotameric	Outliers	Percentiles	
1	A	224/245 (91%)	211 (94%)	13 (6%)	18	26
1	B	215/245 (88%)	203 (94%)	12 (6%)	19	28
All	All	439/490 (90%)	414 (94%)	25 (6%)	19	27

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	234	ARG
1	A	240	LYS
1	A	259	GLU
1	A	317	LEU
1	A	336	LYS
1	A	343	GLU
1	A	351	GLU
1	A	357	ARG
1	A	358	LYS
1	A	404	LYS
1	A	421	LEU
1	A	448	GLU
1	A	463	MET
1	B	207[A]	GLU
1	B	207[B]	GLU
1	B	253	ASN
1	B	273	GLN
1	B	355	SER
1	B	357	ARG
1	B	363	PHE
1	B	373	LYS
1	B	441	ASP
1	B	452	LEU
1	B	469	LEU
1	B	470	GLN

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	314	GLN
1	A	410	GLN

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Mol	Chain	Res	Type
1	A	470	GLN
1	B	294	GLN
1	B	308	ASN

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 oligosaccharides 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GOL	B	478	-	5,5,5	0.37	0	5,5,5	0.30	0
2	GW4	A	478	-	46,47,47	0.88	1 (2%)	60,63,63	1.31	7 (11%)

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	GOL	B	478	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GW4	A	478	-	-	1/31/31/31	0/5/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	478	GW4	C19-N1	2.36	1.42	1.37

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	478	GW4	C19-N1-C10	-5.46	115.63	124.60
2	A	478	GW4	C24-C19-C20	-2.72	115.82	119.37
2	A	478	GW4	C21-C20-C19	2.66	121.80	118.81
2	A	478	GW4	C35-C34-N2	-2.43	111.97	116.12
2	A	478	GW4	C32-O1-C18	-2.42	111.64	117.93
2	A	478	GW4	C19-C20-C31	-2.14	120.56	121.96
2	A	478	GW4	O-C-C4	-2.09	115.08	118.73

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

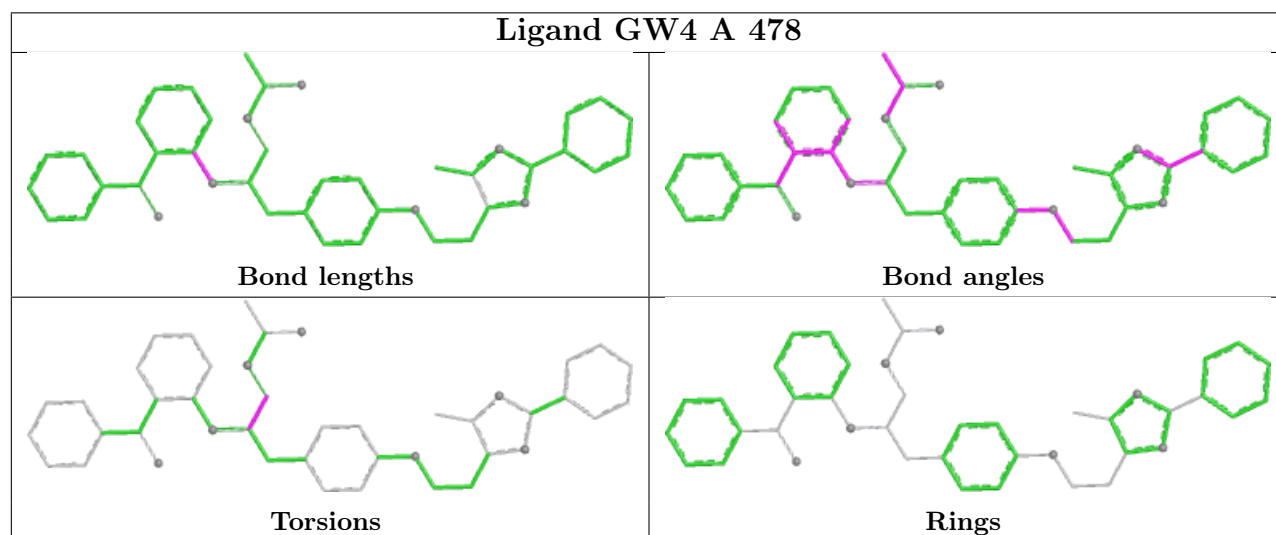
There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	478	GOL	1	0
2	A	478	GW4	8	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

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, 95th 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 ²)	Q<0.9
1	A	255/272 (93%)	2.16	131 (51%) 0 0	34, 73, 88, 100	2 (0%)
1	B	247/272 (90%)	2.23	135 (54%) 0 0	37, 74, 93, 107	3 (1%)
All	All	502/544 (92%)	2.19	266 (52%) 0 0	34, 74, 90, 107	5 (0%)

All (266) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	258	GLY	5.4
1	B	363	PHE	5.3
1	B	253	ASN	5.2
1	B	456	ILE	5.1
1	B	442	LEU	4.9
1	B	445	ILE	4.7
1	B	239	GLY	4.6
1	A	260	ASP	4.4
1	B	251	ASP	4.4
1	A	235	ALA	4.3
1	B	457	LYS	4.3
1	A	300	ALA	4.3
1	A	261	LYS	4.2
1	A	256	MET	4.1
1	A	461	THR	4.1
1	A	456	ILE	4.1
1	B	455	VAL	4.1
1	A	451	GLN	4.0
1	B	274	SER	4.0
1	B	352	PHE	4.0
1	B	302	SER	4.0
1	B	450	VAL	3.9
1	A	290	VAL	3.9
1	A	296	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	473	TYR	3.8
1	A	453	LEU	3.8
1	B	252	MET	3.8
1	B	335	ASN	3.7
1	A	325	ILE	3.7
1	B	388	ILE	3.7
1	B	473	TYR	3.7
1	A	282	PHE	3.7
1	A	223	ILE	3.7
1	A	459	THR	3.7
1	B	376	ALA	3.6
1	A	394	SER	3.6
1	A	464	SER	3.6
1	B	391	ILE	3.6
1	A	442	LEU	3.6
1	B	276	GLU	3.6
1	B	221	SER	3.5
1	B	256	MET	3.5
1	A	279	ILE	3.5
1	A	244	LYS	3.5
1	B	461	THR	3.5
1	A	343	GLU	3.5
1	A	463	MET	3.5
1	B	341	ILE	3.5
1	A	439	MET	3.5
1	A	460	GLU	3.4
1	A	311	LEU	3.4
1	B	344	GLY	3.4
1	B	469	LEU	3.4
1	A	379	LEU	3.3
1	A	231	ALA	3.3
1	B	446	VAL	3.3
1	A	275	LYS	3.3
1	A	318	LEU	3.3
1	A	355	SER	3.3
1	B	209	ALA	3.3
1	A	257	MET	3.3
1	B	257	MET	3.3
1	A	412	ASN	3.3
1	A	287	PHE	3.3
1	A	259	GLU	3.2
1	B	247	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	371	ALA	3.2
1	B	305	GLY	3.2
1	A	400	LEU	3.2
1	A	362	ASP	3.2
1	A	384	LEU	3.2
1	A	345	GLN	3.2
1	B	361	GLY	3.2
1	A	469	LEU	3.1
1	A	359	PRO	3.1
1	B	379	LEU	3.1
1	A	263	LYS	3.1
1	B	452	LEU	3.1
1	B	296	ILE	3.1
1	B	466	HIS	3.1
1	A	390	VAL	3.1
1	A	237	LEU	3.1
1	B	327	TYR	3.0
1	B	249	ILE	3.0
1	A	474	LYS	3.0
1	B	346	GLY	3.0
1	A	278	ALA	3.0
1	A	303	ILE	3.0
1	B	297	THR	3.0
1	B	275	LYS	3.0
1	B	359	PRO	3.0
1	B	340	LEU	3.0
1	B	390	VAL	3.0
1	B	447	THR	3.0
1	B	254	SER	3.0
1	A	462	ASP	3.0
1	A	209	ALA	2.9
1	A	233	ALA	2.9
1	A	221	SER	2.9
1	B	225	SER	2.9
1	A	348	MET	2.9
1	B	401	LEU	2.9
1	A	277	VAL	2.9
1	A	289	SER	2.9
1	B	210	ASP	2.9
1	B	321	GLY	2.9
1	A	454	GLN	2.9
1	A	386	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	407	GLU	2.9
1	B	474	LYS	2.9
1	B	287	PHE	2.9
1	B	328	THR	2.9
1	A	395	GLY	2.8
1	B	395	GLY	2.8
1	A	306	PHE	2.8
1	B	238	THR	2.8
1	A	258	GLY	2.8
1	A	358	LYS	2.8
1	B	386	ILE	2.8
1	B	356	LEU	2.8
1	A	360	PHE	2.8
1	A	253	ASN	2.8
1	B	426	PRO	2.8
1	B	236	ILE	2.7
1	A	404	LYS	2.7
1	B	389	ALA	2.7
1	B	289	SER	2.7
1	A	227	PRO	2.7
1	B	295	GLU	2.7
1	B	453	LEU	2.7
1	A	371	ALA	2.7
1	A	403	VAL	2.7
1	A	297	THR	2.7
1	A	391	ILE	2.7
1	B	246	PRO	2.7
1	A	211	LEU	2.7
1	B	465	LEU	2.7
1	A	327	TYR	2.7
1	A	472	ILE	2.7
1	B	317	LEU	2.7
1	B	283	GLN	2.6
1	A	435	LEU	2.6
1	B	419	LEU	2.6
1	B	436	LEU	2.6
1	B	273	GLN	2.6
1	A	331	ALA	2.6
1	A	357	ARG	2.6
1	B	443	ARG	2.6
1	B	216	LYS	2.6
1	B	416	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	387	PHE	2.6
1	B	440	THR	2.6
1	B	353	LEU	2.6
1	B	308	ASN	2.6
1	A	405	PRO	2.6
1	A	382	SER	2.6
1	A	406	ILE	2.6
1	B	223	ILE	2.6
1	B	303	ILE	2.6
1	A	401	LEU	2.5
1	B	281	ILE	2.5
1	A	218	LEU	2.5
1	A	225	SER	2.5
1	A	262	ILE	2.5
1	A	385	ALA	2.5
1	A	217	HIS	2.5
1	B	245	SER	2.5
1	B	432	PHE	2.5
1	A	452	LEU	2.5
1	A	468	LEU	2.5
1	B	380	ASP	2.5
1	A	213	ALA	2.5
1	B	284	GLY	2.5
1	A	388	ILE	2.4
1	A	377	LEU	2.4
1	A	252	MET	2.4
1	A	292	ALA	2.4
1	A	305	GLY	2.4
1	B	338	GLY	2.4
1	A	226	PHE	2.4
1	B	290	VAL	2.4
1	A	299	TYR	2.4
1	A	363	PHE	2.4
1	B	393	LEU	2.4
1	A	455	VAL	2.4
1	B	282	PHE	2.4
1	B	293	VAL	2.4
1	B	326	ILE	2.4
1	A	283	GLN	2.4
1	A	470	GLN	2.4
1	B	427	GLU	2.4
1	A	475	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	394	SER	2.3
1	B	286[A]	GLN	2.3
1	A	457	LYS	2.3
1	B	306	PHE	2.3
1	B	214	LEU	2.3
1	B	424	ASN	2.3
1	B	449	HIS	2.3
1	A	307	VAL	2.3
1	A	419	LEU	2.2
1	B	322	VAL	2.3
1	B	298	GLU	2.2
1	B	320	TYR	2.2
1	B	349	THR	2.2
1	A	302	SER	2.2
1	A	458	LYS	2.2
1	B	458	LYS	2.2
1	B	226	PHE	2.2
1	A	280	ARG	2.2
1	B	329	MET	2.2
1	B	467	PRO	2.2
1	B	208	SER	2.2
1	B	219	TYR	2.2
1	B	279	ILE	2.2
1	A	255	LEU	2.2
1	B	339	VAL	2.2
1	B	408	ASP	2.2
1	B	437	GLN	2.2
1	B	233	ALA	2.2
1	A	219	TYR	2.2
1	A	320	TYR	2.2
1	A	212	ARG	2.2
1	B	377	LEU	2.2
1	A	315	VAL	2.2
1	A	446	VAL	2.2
1	B	372	VAL	2.2
1	B	370	PHE	2.2
1	B	345	GLN	2.2
1	B	387	PHE	2.1
1	B	460	GLU	2.1
1	B	451	GLN	2.1
1	A	328	THR	2.1
1	A	332	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	250	TYR	2.1
1	A	301	LYS	2.1
1	A	393	LEU	2.1
1	B	336	LYS	2.1
1	A	368	PHE	2.1
1	A	398	PRO	2.1
1	A	330	LEU	2.1
1	B	413	LEU	2.1
1	A	312	ASN	2.1
1	B	206	PRO	2.1
1	A	247	PHE	2.1
1	B	360	PHE	2.1
1	B	428	SER	2.1
1	B	235	ALA	2.1
1	A	427	GLU	2.1
1	A	445	ILE	2.1
1	B	392	ILE	2.1
1	B	444	GLN	2.1
1	A	232	LYS	2.0
1	A	254	SER	2.0
1	B	213	ALA	2.0
1	B	285	CYS	2.0
1	B	343	GLU	2.0
1	A	423	LEU	2.0
1	A	341	ILE	2.0
1	A	338	GLY	2.0
1	A	352	PHE	2.0
1	A	276	GLU	2.0
1	B	324	GLU	2.0
1	B	433	ALA	2.0
1	A	465	LEU	2.0
1	B	325	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](#)

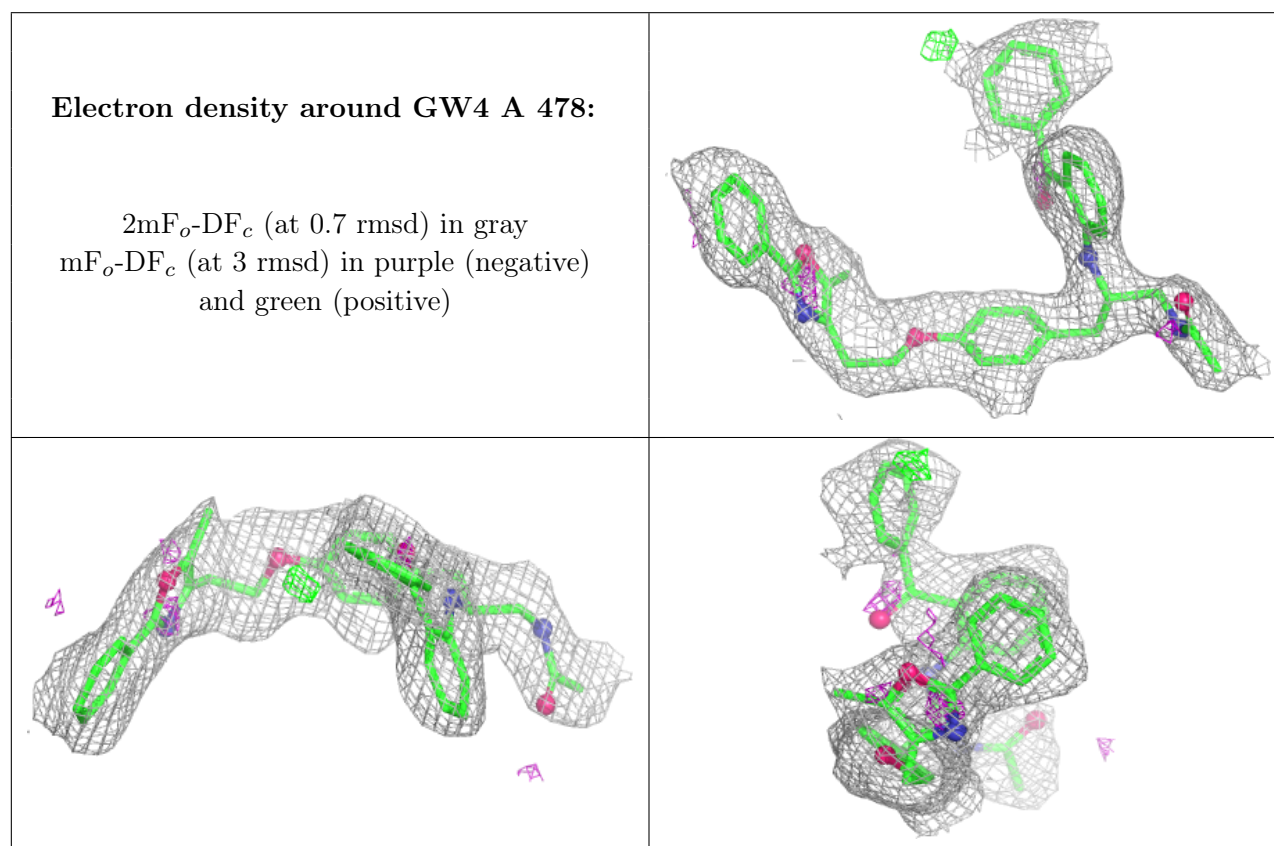
There are no oligosaccharides in this entry.

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, 95th 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(Å ²)	Q<0.9
3	GOL	B	478	6/6	0.85	0.16	56,61,62,62	0
2	GW4	A	478	43/43	0.86	0.14	61,71,80,81	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.