



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:55 PM UTC

PDB ID : 4FGY / pdb_00004fgy
Title : Identification of a unique PPAR ligand with an unexpected binding mode and antibetic activity
Authors : Wang, R.; Li, Y.
Deposited on : 2012-06-05
Resolution : 2.84 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

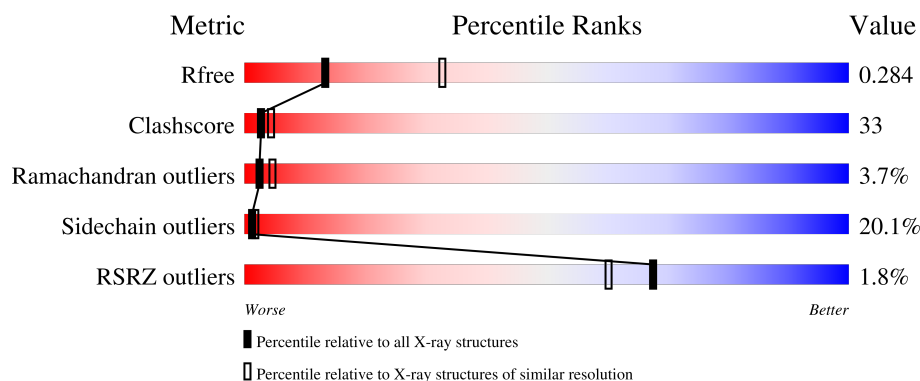
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.84 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	1520 (2.86-2.82)
Clashscore	190562	1559 (2.86-2.82)
Ramachandran outliers	187476	1517 (2.86-2.82)
Sidechain outliers	187428	1518 (2.86-2.82)
RSRZ outliers	180081	1521 (2.86-2.82)

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	270	2% 54% 34% 9% ..
2	B	11	18% 36% 36% 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	OW3	A	601	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2287 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.

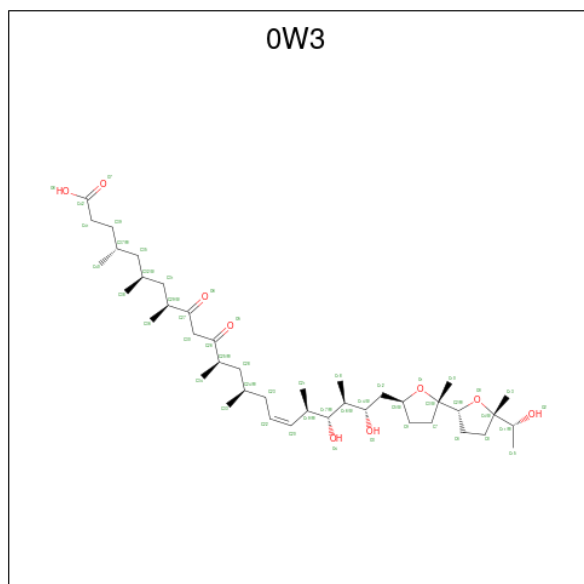
- Molecule 1 is a protein called Peroxisome proliferator-activated receptor gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	0	0	0
			2118	1364	345	399	10			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	11	Total	C	N	O	0	0	0
			101	64	23	14			

- Molecule 3 is (4R,6S,8S,12R,14R,16Z,18R,19R,20S,21S)-19,21-dihydroxy-22-[(2S,2'R,5S,5'S)-5'-[(1R)-1-hydroxyethyl]-2,5'-dimethyloctahydro-2,2'-bifuran-5-yl]-4,6,8,12,14,18,20-heptamethyl-9,11-dioxodocos-16-enoic acid (CCD ID: 0W3) (formula: C₄₁H₇₂O₉).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			50	41	9		

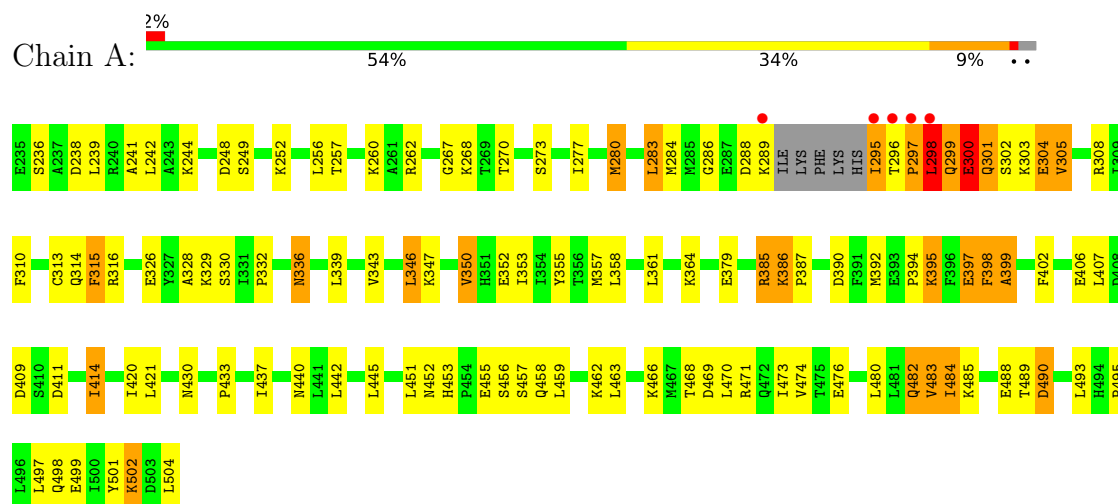
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	17	Total 17	O 17	0	0
4	B	1	Total 1	O 1	0	0

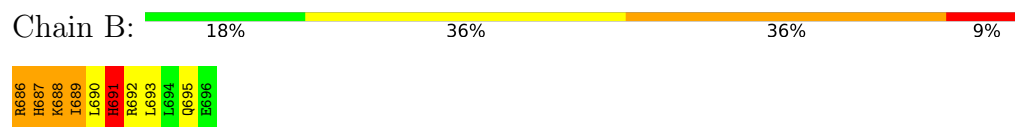
3 Residue-property plots

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 2: Nuclear receptor coactivator 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	57.36Å 86.53Å 122.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.36 – 2.84 35.36 – 2.84	Depositor EDS
% Data completeness (in resolution range)	93.8 (35.36-2.84) 93.8 (35.36-2.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.33 (at 2.85Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.219 , 0.285 0.219 , 0.284	Depositor DCC
R_{free} test set	366 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	48.1	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 27.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	2287	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.05% 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: 0W3

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	0.75	0/2152	1.10	6/2900 (0.2%)
2	B	1.23	1/102 (1.0%)	1.21	1/134 (0.7%)
All	All	0.78	1/2254 (0.0%)	1.10	7/3034 (0.2%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	687	HIS	CG-ND1	-5.81	1.31	1.38

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	268	LYS	N-CA-C	-7.35	105.49	114.75
1	A	399	ALA	N-CA-C	-7.07	103.64	112.90
1	A	397	GLU	N-CA-C	-6.66	99.97	109.96
1	A	504	LEU	N-CA-CB	-5.87	100.52	110.50
2	B	689	ILE	N-CA-C	5.81	115.99	110.53
1	A	302	SER	N-CA-C	-5.60	98.88	110.80
1	A	483	VAL	N-CA-C	-5.25	104.41	111.44

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	298	LEU	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	2118	0	2178	87	0
2	B	101	0	110	30	0
3	A	50	0	71	53	0
4	A	17	0	0	0	0
4	B	1	0	0	0	0
All	All	2287	0	2359	154	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 33.

All (154) 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)
2:B:686:ARG:HD3	2:B:691:HIS:CE1	1.71	1.25
1:A:386:LYS:HB3	1:A:387:PRO:CD	1.72	1.19
2:B:690:LEU:O	2:B:691:HIS:HB2	1.40	1.18
3:A:601:OW3:C18	3:A:601:OW3:H36	1.78	1.13
3:A:601:OW3:H21A	3:A:601:OW3:H18	1.12	1.12
3:A:601:OW3:H36	3:A:601:OW3:C16	1.78	1.12
2:B:686:ARG:HH11	2:B:686:ARG:HG2	0.98	1.11
3:A:601:OW3:C27	3:A:601:OW3:H38B	1.81	1.10
3:A:601:OW3:H36	3:A:601:OW3:H16	1.32	1.08
2:B:688:LYS:HE3	2:B:688:LYS:H	1.18	1.06
1:A:386:LYS:HB3	1:A:387:PRO:HD2	1.32	1.06
3:A:601:OW3:H18	3:A:601:OW3:C21	1.86	1.04
2:B:686:ARG:CD	2:B:691:HIS:HE1	1.72	1.01
3:A:601:OW3:H21	3:A:601:OW3:H24	1.43	0.99
2:B:686:ARG:N	2:B:687:HIS:HB2	1.78	0.98
3:A:601:OW3:C27	3:A:601:OW3:C38	2.43	0.96
2:B:686:ARG:N	2:B:686:ARG:CZ	2.29	0.95
1:A:397:GLU:O	1:A:398:PHE:HB3	1.65	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:686:ARG:HG2	2:B:686:ARG:NH1	1.72	0.91
2:B:686:ARG:HD3	2:B:691:HIS:HE1	1.11	0.89
3:A:601:OW3:C18	3:A:601:OW3:H21A	2.02	0.89
1:A:295:ILE:N	1:A:315:PHE:CE2	2.40	0.89
3:A:601:OW3:C21	3:A:601:OW3:H24	2.04	0.86
1:A:385:ARG:HE	1:A:386:LYS:HB2	1.40	0.85
3:A:601:OW3:H16	3:A:601:OW3:C36	2.08	0.83
3:A:601:OW3:H21A	3:A:601:OW3:H36B	1.60	0.82
1:A:353:ILE:O	1:A:357:MET:HG3	1.80	0.81
1:A:298:LEU:C	1:A:300:GLU:H	1.87	0.81
1:A:336:ASN:H	1:A:336:ASN:HD22	1.25	0.80
1:A:386:LYS:CB	1:A:387:PRO:CD	2.58	0.80
2:B:686:ARG:N	2:B:686:ARG:NE	2.29	0.80
3:A:601:OW3:C18	3:A:601:OW3:C36	2.60	0.79
3:A:601:OW3:H21A	3:A:601:OW3:C36	2.11	0.79
1:A:295:ILE:HD12	1:A:296:THR:H	1.48	0.78
2:B:686:ARG:CD	2:B:691:HIS:CE1	2.53	0.78
1:A:386:LYS:CB	1:A:387:PRO:HD2	2.12	0.78
3:A:601:OW3:C18	3:A:601:OW3:C21	2.60	0.78
3:A:601:OW3:H36	3:A:601:OW3:H18	1.66	0.76
1:A:336:ASN:HD22	1:A:336:ASN:N	1.84	0.75
3:A:601:OW3:H6	3:A:601:OW3:H15	1.68	0.75
3:A:601:OW3:C38	3:A:601:OW3:O6	2.35	0.74
3:A:601:OW3:H18	3:A:601:OW3:C36	2.17	0.74
3:A:601:OW3:H15B	3:A:601:OW3:O1	1.88	0.73
1:A:386:LYS:HB3	1:A:387:PRO:HD3	1.67	0.73
3:A:601:OW3:H21	3:A:601:OW3:C24	2.18	0.73
1:A:489:THR:O	1:A:490:ASP:HB3	1.89	0.72
2:B:688:LYS:HE3	2:B:688:LYS:N	2.01	0.72
1:A:329:LYS:NZ	2:B:693:LEU:O	2.23	0.72
1:A:315:PHE:C	1:A:315:PHE:CD1	2.69	0.70
3:A:601:OW3:H38B	3:A:601:OW3:O6	1.92	0.69
2:B:686:ARG:CA	2:B:687:HIS:HB2	2.22	0.69
2:B:686:ARG:HH11	2:B:686:ARG:CG	1.88	0.68
2:B:690:LEU:O	2:B:691:HIS:CB	2.28	0.67
1:A:298:LEU:C	1:A:300:GLU:N	2.53	0.67
1:A:295:ILE:HD13	1:A:297:PRO:HD3	1.77	0.66
1:A:242:LEU:HD13	1:A:332:PRO:HG2	1.76	0.66
1:A:244:LYS:HE2	1:A:248:ASP:OD1	1.97	0.65
1:A:411:ASP:OD2	1:A:453:HIS:HE1	1.79	0.65
1:A:314:GLN:HE21	1:A:497:LEU:HD12	1.62	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:GLU:HG3	1:A:301:GLN:H	1.63	0.64
1:A:469:ASP:O	1:A:473:ILE:HD13	1.98	0.63
1:A:295:ILE:N	1:A:315:PHE:CD2	2.66	0.63
1:A:397:GLU:O	1:A:398:PHE:CB	2.40	0.63
1:A:456:SER:O	1:A:458:GLN:N	2.32	0.63
1:A:314:GLN:NE2	1:A:497:LEU:HD12	2.13	0.62
1:A:385:ARG:HE	1:A:386:LYS:CB	2.12	0.61
1:A:361:LEU:CD1	3:A:601:OW3:H11	2.31	0.61
2:B:688:LYS:H	2:B:688:LYS:CE	2.04	0.60
3:A:601:OW3:C16	3:A:601:OW3:C36	2.66	0.60
3:A:601:OW3:O1	3:A:601:OW3:C15	2.49	0.60
2:B:686:ARG:HA	2:B:687:HIS:C	2.26	0.60
3:A:601:OW3:H15	3:A:601:OW3:C6	2.32	0.59
3:A:601:OW3:H21	3:A:601:OW3:C23	2.31	0.59
2:B:686:ARG:NH1	2:B:686:ARG:CG	2.54	0.58
2:B:691:HIS:HD2	2:B:695:GLN:HE22	1.52	0.58
3:A:601:OW3:O6	3:A:601:OW3:H38A	2.02	0.58
1:A:421:LEU:HG	1:A:437:ILE:CG2	2.33	0.57
1:A:502:LYS:NZ	1:A:502:LYS:HB2	2.17	0.57
1:A:343:VAL:CG1	2:B:687:HIS:HD2	2.17	0.57
1:A:394:PRO:O	1:A:397:GLU:O	2.22	0.57
1:A:295:ILE:CD1	1:A:297:PRO:HD3	2.34	0.57
1:A:336:ASN:N	1:A:336:ASN:ND2	2.47	0.56
1:A:499:GLU:OE2	2:B:689:ILE:HG13	2.05	0.56
1:A:421:LEU:HG	1:A:437:ILE:HG22	1.88	0.55
1:A:295:ILE:HD12	1:A:296:THR:N	2.20	0.55
3:A:601:OW3:H24	3:A:601:OW3:C19	2.36	0.55
3:A:601:OW3:H15B	3:A:601:OW3:C3	2.37	0.54
2:B:687:HIS:N	2:B:687:HIS:HD1	2.06	0.53
1:A:430:ASN:O	1:A:433:PRO:HD2	2.07	0.53
1:A:310:PHE:CD1	3:A:601:OW3:H33A	2.43	0.53
1:A:385:ARG:NE	1:A:386:LYS:HG3	2.24	0.52
3:A:601:OW3:H33B	3:A:601:OW3:C20	2.40	0.52
1:A:347:LYS:NZ	1:A:502:LYS:O	2.38	0.52
1:A:482:GLN:NE2	1:A:501:TYR:OH	2.43	0.51
2:B:688:LYS:O	2:B:692:ARG:HG2	2.10	0.51
2:B:691:HIS:CD2	2:B:695:GLN:HE22	2.28	0.51
3:A:601:OW3:C15	3:A:601:OW3:C2	2.89	0.51
1:A:392:MET:HE2	3:A:601:OW3:H35	1.93	0.50
1:A:300:GLU:CG	1:A:301:GLN:H	2.24	0.50
3:A:601:OW3:H18	3:A:601:OW3:H36B	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:ASP:HA	1:A:241:ALA:HB3	1.94	0.50
1:A:358:LEU:HB2	3:A:601:0W3:H15A	1.94	0.50
3:A:601:0W3:C15	3:A:601:0W3:C6	2.91	0.49
1:A:490:ASP:C	1:A:490:ASP:OD1	2.56	0.48
1:A:343:VAL:CG1	2:B:687:HIS:CD2	2.95	0.48
1:A:280:MET:SD	1:A:305:VAL:HG21	2.54	0.48
1:A:361:LEU:HD11	3:A:601:0W3:H11	1.96	0.48
1:A:313:CYS:SG	3:A:601:0W3:H32	2.54	0.47
1:A:392:MET:HA	1:A:395:LYS:HD2	1.96	0.47
1:A:328:ALA:C	1:A:330:SER:H	2.23	0.47
1:A:347:LYS:HD2	2:B:687:HIS:NE2	2.30	0.47
3:A:601:0W3:C21	3:A:601:0W3:C36	2.90	0.47
1:A:414:ILE:HB	1:A:445:LEU:HD13	1.97	0.46
1:A:495:PRO:HA	1:A:498:GLN:HB2	1.96	0.46
3:A:601:0W3:H25	3:A:601:0W3:H33	1.43	0.46
1:A:283:LEU:HD13	1:A:308:ARG:NH2	2.31	0.46
3:A:601:0W3:H33B	3:A:601:0W3:H19	1.97	0.45
1:A:310:PHE:HD1	3:A:601:0W3:H33A	1.79	0.45
1:A:355:TYR:OH	3:A:601:0W3:H18B	2.17	0.45
1:A:286:GLY:O	1:A:289:LYS:HD3	2.16	0.45
3:A:601:0W3:O3	3:A:601:0W3:C7	2.64	0.45
3:A:601:0W3:C24	3:A:601:0W3:C19	2.94	0.45
1:A:314:GLN:NE2	1:A:497:LEU:CD1	2.80	0.44
1:A:316:ARG:HB3	3:A:601:0W3:H2	1.98	0.44
3:A:601:0W3:H30	3:A:601:0W3:H36A	1.67	0.44
2:B:687:HIS:O	2:B:690:LEU:O	2.34	0.44
1:A:298:LEU:HA	1:A:300:GLU:HG2	1.99	0.44
2:B:686:ARG:CD	2:B:686:ARG:N	2.79	0.44
1:A:280:MET:SD	1:A:305:VAL:CG2	3.05	0.44
1:A:402:PHE:HD1	1:A:466:LYS:HG3	1.82	0.44
1:A:352:GLU:OE2	1:A:471:ARG:HG2	2.18	0.44
3:A:601:0W3:H19	3:A:601:0W3:C33	2.48	0.43
1:A:473:ILE:O	1:A:476:GLU:HB2	2.18	0.43
1:A:328:ALA:C	1:A:330:SER:N	2.76	0.43
1:A:304:GLU:OE2	1:A:385:ARG:NH1	2.52	0.43
1:A:502:LYS:HB2	1:A:502:LYS:HZ2	1.80	0.42
1:A:257:THR:HB	1:A:409:ASP:OD1	2.20	0.42
1:A:353:ILE:HD11	1:A:420:ILE:HG13	2.01	0.42
1:A:484:ILE:HA	1:A:488:GLU:HB2	2.01	0.42
2:B:687:HIS:N	2:B:687:HIS:ND1	2.67	0.42
1:A:297:PRO:C	1:A:299:GLN:N	2.78	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:GLU:HG3	1:A:474:VAL:HG21	2.02	0.41
1:A:470:LEU:O	1:A:474:VAL:HG23	2.20	0.41
3:A:601:OW3:H15B	3:A:601:OW3:C2	2.51	0.41
1:A:301:GLN:O	1:A:303:LYS:N	2.53	0.41
1:A:395:LYS:O	1:A:399:ALA:HB2	2.20	0.41
3:A:601:OW3:H36B	3:A:601:OW3:H30A	1.66	0.41
1:A:361:LEU:HD12	3:A:601:OW3:H11	2.02	0.41
1:A:385:ARG:NH2	1:A:386:LYS:HD2	2.35	0.40
1:A:421:LEU:HG	1:A:437:ILE:HG21	2.01	0.40
1:A:313:CYS:HB3	3:A:601:OW3:O4	2.21	0.40
1:A:490:ASP:OD1	1:A:490:ASP:O	2.38	0.40
1:A:236:SER:HA	1:A:239:LEU:HB2	2.04	0.40
1:A:346:LEU:O	1:A:350:VAL:HB	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	261/270 (97%)	233 (89%)	19 (7%)	9 (3%)	3	6
2	B	9/11 (82%)	7 (78%)	1 (11%)	1 (11%)	0	0
All	All	270/281 (96%)	240 (89%)	20 (7%)	10 (4%)	2	4

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	299	GLN
1	A	301	GLN
1	A	386	LYS
1	A	457	SER
2	B	691	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	300	GLU
1	A	297	PRO
1	A	398	PHE
1	A	267	GLY
1	A	305	VAL

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	A	238/243 (98%)	191 (80%)	47 (20%)	1	2
2	B	11/11 (100%)	8 (73%)	3 (27%)	0	0
All	All	249/254 (98%)	199 (80%)	50 (20%)	1	2

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	249	SER
1	A	252	LYS
1	A	256	LEU
1	A	260	LYS
1	A	262	ARG
1	A	270	THR
1	A	273	SER
1	A	277	ILE
1	A	280	MET
1	A	283	LEU
1	A	284	MET
1	A	288	ASP
1	A	295	ILE
1	A	298	LEU
1	A	300	GLU
1	A	304	GLU
1	A	315	PHE
1	A	326	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	336	ASN
1	A	339	LEU
1	A	346	LEU
1	A	350	VAL
1	A	364	LYS
1	A	379	GLU
1	A	385	ARG
1	A	390	ASP
1	A	395	LYS
1	A	406	GLU
1	A	407	LEU
1	A	414	ILE
1	A	440	ASN
1	A	442	LEU
1	A	451	LEU
1	A	452	ASN
1	A	455	GLU
1	A	459	LEU
1	A	462	LYS
1	A	463	LEU
1	A	468	THR
1	A	480	LEU
1	A	482	GLN
1	A	483	VAL
1	A	484	ILE
1	A	485	LYS
1	A	490	ASP
1	A	493	LEU
1	A	502	LYS
2	B	686	ARG
2	B	688	LYS
2	B	691	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	314	GLN
1	A	336	ASN
1	A	403	ASN
1	A	452	ASN
1	A	453	HIS
1	A	465	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	482	GLN
2	B	691	HIS
2	B	695	GLN

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	OW3	A	601	-	50,51,51	1.40	3 (6%)	67,73,73	1.90	13 (19%)

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	OW3	A	601	-	-	27/63/85/85	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	OW3	O5-C26	7.80	1.34	1.21
3	A	601	OW3	C29-C27	-2.77	1.49	1.52
3	A	601	OW3	C30-C26	-2.57	1.35	1.51

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	OW3	O1-C3-C2	6.14	116.27	106.47
3	A	601	OW3	O0-C4-C11	-5.41	101.37	106.22
3	A	601	OW3	C36-C29-C27	-4.52	99.03	109.58
3	A	601	OW3	C10-C3-C2	-4.24	103.69	111.08
3	A	601	OW3	C31-C29-C27	4.11	119.39	110.96
3	A	601	OW3	O0-C4-C13	3.84	115.17	108.05
3	A	601	OW3	C7-C3-C2	-3.32	106.96	113.47
3	A	601	OW3	C41-C39-C37	-3.15	109.18	115.29
3	A	601	OW3	C37-C35-C32	-3.07	105.68	115.80
3	A	601	OW3	C34-C25-C26	-2.98	102.62	109.58
3	A	601	OW3	O0-C2-C6	2.36	108.60	104.24
3	A	601	OW3	C28-C24-C23	2.27	117.95	111.17
3	A	601	OW3	C13-C4-C8	-2.13	108.71	113.09

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	OW3	C14-C12-C5-C9
3	A	601	OW3	C5-C12-C14-O3
3	A	601	OW3	C5-C12-C14-C16
3	A	601	OW3	O3-C14-C16-C17
3	A	601	OW3	C12-C14-C16-C17
3	A	601	OW3	C33-C24-C28-C25
3	A	601	OW3	C27-C29-C31-C32
3	A	601	OW3	C29-C31-C32-C38
3	A	601	OW3	C31-C32-C35-C37
3	A	601	OW3	C20-C22-C23-C24
3	A	601	OW3	C21-C19-C20-C22
3	A	601	OW3	C36-C29-C31-C32
3	A	601	OW3	C37-C39-C41-C42
3	A	601	OW3	C17-C19-C20-C22
3	A	601	OW3	O3-C14-C16-C18
3	A	601	OW3	C26-C25-C28-C24

Continued on next page...

Continued from previous page...

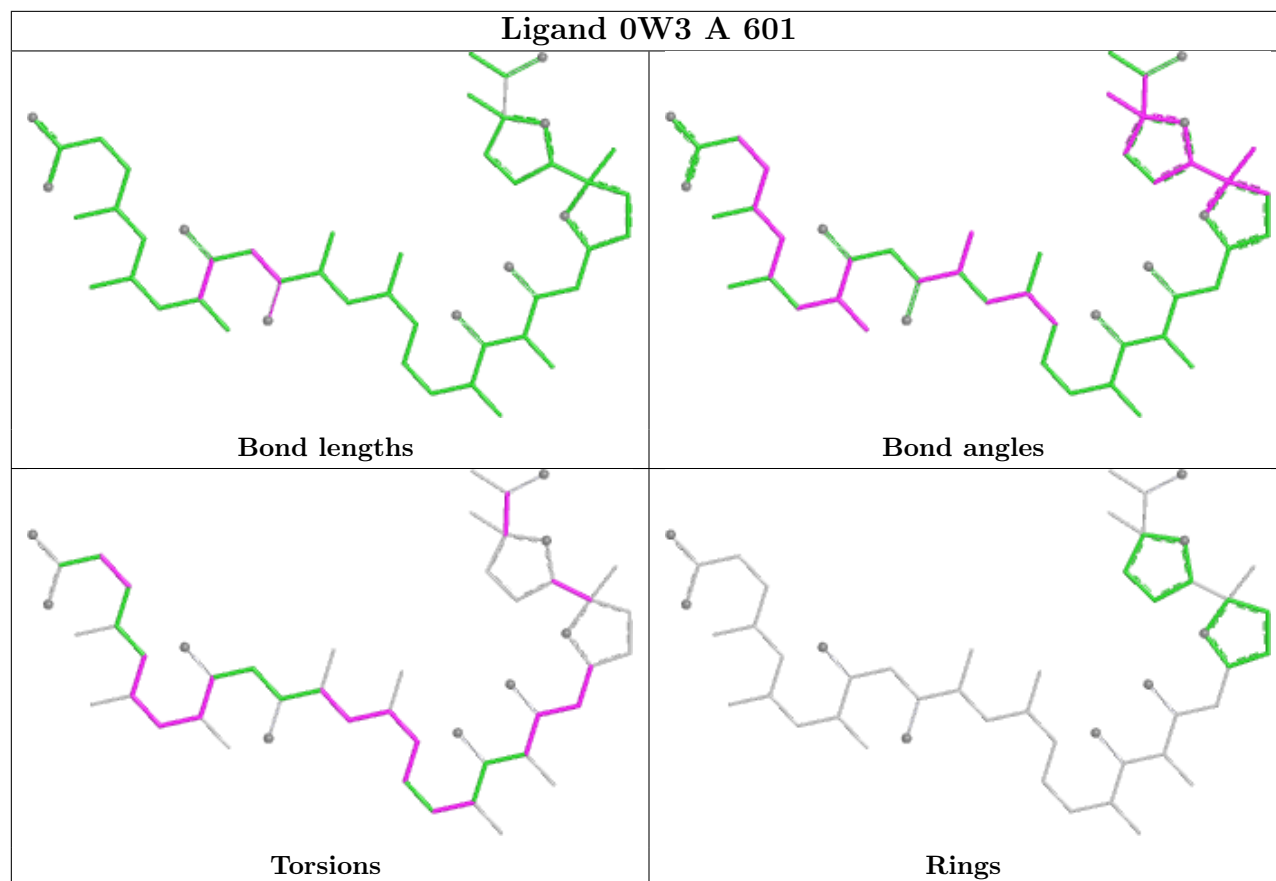
Mol	Chain	Res	Type	Atoms
3	A	601	0W3	C12-C14-C16-C18
3	A	601	0W3	O6-C27-C29-C36
3	A	601	0W3	C38-C32-C35-C37
3	A	601	0W3	O0-C2-C3-C10
3	A	601	0W3	C30-C27-C29-C36
3	A	601	0W3	O0-C2-C3-C7
3	A	601	0W3	O0-C2-C3-O1
3	A	601	0W3	C29-C31-C32-C35
3	A	601	0W3	O2-C11-C4-O0
3	A	601	0W3	C34-C25-C28-C24
3	A	601	0W3	C22-C23-C24-C33

There are no ring outliers.

1 monomer is involved in 53 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	0W3	53	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 [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, 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	265/270 (98%)	-0.14	5 (1%) 66 59	22, 39, 77, 141	0
2	B	11/11 (100%)	0.20	0 100 100	40, 54, 77, 94	0
All	All	276/281 (98%)	-0.13	5 (1%) 67 60	22, 40, 77, 141	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	297	PRO	3.2
1	A	296	THR	3.1
1	A	298	LEU	2.9
1	A	295	ILE	2.1
1	A	289	LYS	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](#)

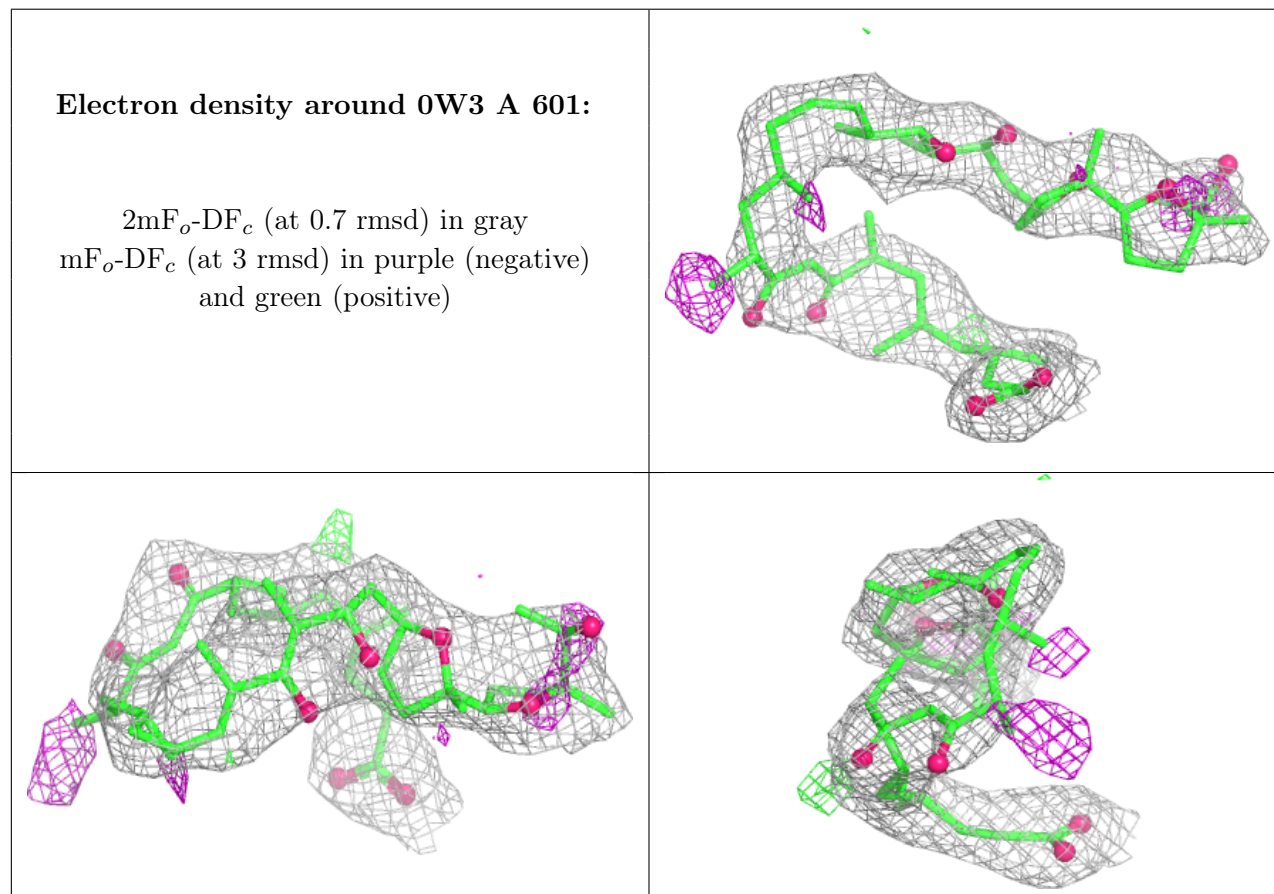
There are no oligosaccharides in this entry.

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($\text{\AA}^2$)	Q<0.9
3	OW3	A	601	50/50	0.85	0.13	27,31,34,35	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.