



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:37 AM UTC

PDB ID : 5V49 / pdb_00005v49
Title : Trypanosoma brucei methionyl-tRNA synthetase in complex with inhibitor (Chem 1917)
Authors : Barros-Alvarez, X.; Hol, W.G.J.
Deposited on : 2017-03-08
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

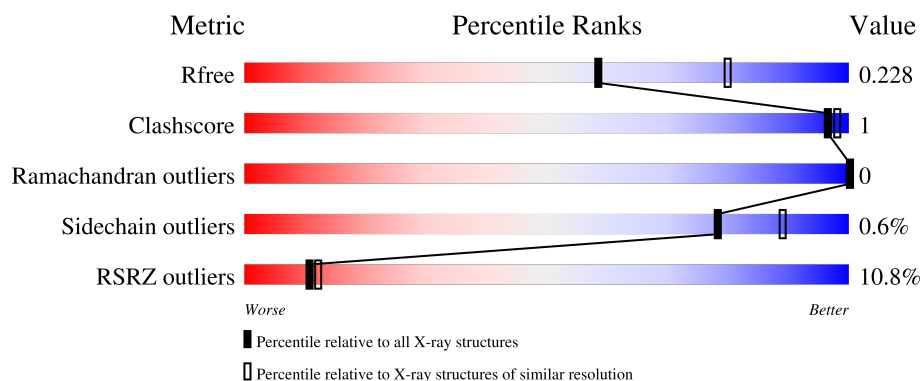
1 Overall quality at a glance

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	542	9% 92% 5%
1	B	542	12% 95% •

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8529 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 Methionyl-tRNA synthetase, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	517	Total	C	N	O	S	0	1	0
			4113	2655	691	756	11			
1	B	533	Total	C	N	O	S	0	1	0
			4204	2704	712	776	12			

There are 22 discrepancies between the modelled and reference sequences:

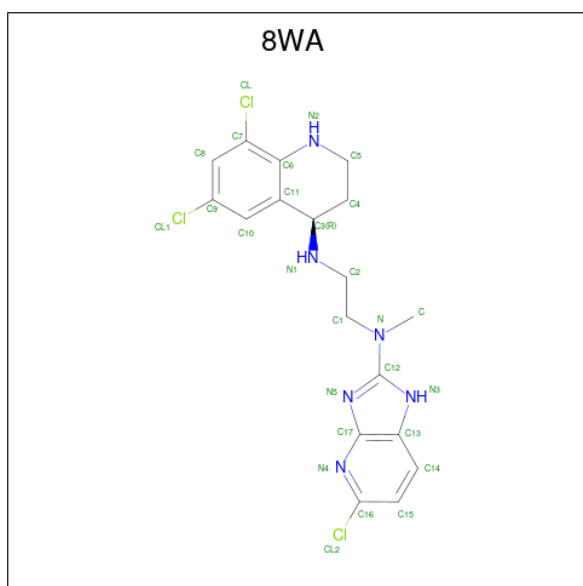
Chain	Residue	Modelled	Actual	Comment	Reference
A	232	GLY	-	expression tag	UNP Q38C91
A	233	PRO	-	expression tag	UNP Q38C91
A	234	GLY	-	expression tag	UNP Q38C91
A	235	SER	-	expression tag	UNP Q38C91
A	236	MET	-	expression tag	UNP Q38C91
A	309	THR	ALA	conflict	UNP Q38C91
A	452	ALA	LYS	conflict	UNP Q38C91
A	453	ARG	LYS	conflict	UNP Q38C91
A	454	ALA	GLU	conflict	UNP Q38C91
A	499	VAL	ALA	conflict	UNP Q38C91
A	503	ASN	SER	conflict	UNP Q38C91
B	232	GLY	-	expression tag	UNP Q38C91
B	233	PRO	-	expression tag	UNP Q38C91
B	234	GLY	-	expression tag	UNP Q38C91
B	235	SER	-	expression tag	UNP Q38C91
B	236	MET	-	expression tag	UNP Q38C91
B	309	THR	ALA	conflict	UNP Q38C91
B	452	ALA	LYS	conflict	UNP Q38C91
B	453	ARG	LYS	conflict	UNP Q38C91
B	454	ALA	GLU	conflict	UNP Q38C91
B	499	VAL	ALA	conflict	UNP Q38C91
B	503	ASN	SER	conflict	UNP Q38C91

- Molecule 2 is METHIONINE (CCD ID: MET) (formula: C₅H₁₁NO₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			9	5	1	2	1		

- Molecule 3 is N 1 -(5-chloro-1H-imidazo[4,5-b]pyridin-2-yl)-N 2 -[(4R)-6,8-dichloro-1,2,3,4-tetrahydroquinolin-4-yl]-N 1 -methylethane-1,2-diamine (CCD ID: 8WA) (formula: C₁₈H₁₉Cl₃N₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	Cl	N	0	0
			27	18	3	6		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

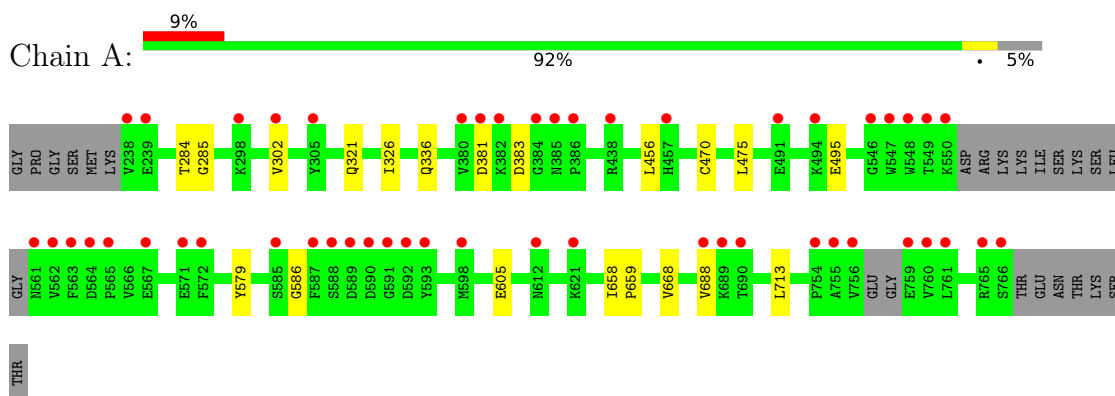
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	80	Total	O	0	0
			80	80		
5	B	90	Total	O	0	0
			90	90		

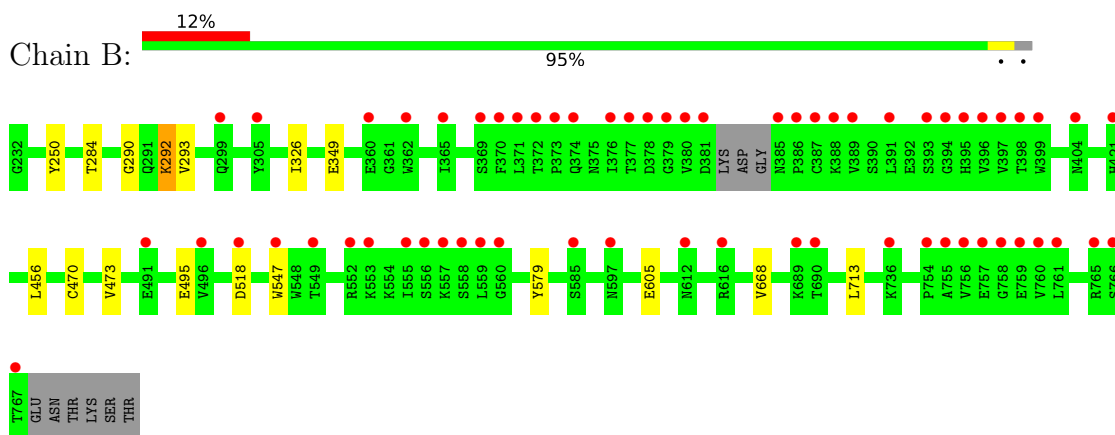
3 Residue-property plots

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: Methionyl-tRNA synthetase, putative



- Molecule 1: Methionyl-tRNA synthetase, putative



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	87.19Å 106.20Å 207.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	103.76 – 2.30 103.76 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (103.76-2.30) 100.0 (103.76-2.30)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.63 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.205 , 0.228 0.209 , 0.228	Depositor DCC
R_{free} test set	4288 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	35.0	Xtriage
Anisotropy	0.718	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 30.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8529	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 3.22% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 8WA

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	0.69	0/4225	0.88	5/5752 (0.1%)
1	B	0.69	0/4314	0.86	1/5875 (0.0%)
All	All	0.69	0/8539	0.87	6/11627 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	688	VAL	CB-CA-C	-5.68	104.70	111.97
1	B	290	GLY	N-CA-C	5.37	117.52	112.04
1	A	586	GLY	N-CA-C	-5.32	105.00	112.13
1	A	285	GLY	N-CA-C	5.20	117.20	110.45
1	A	475	LEU	CA-C-N	5.02	127.31	120.54
1	A	475	LEU	C-N-CA	5.02	127.31	120.54

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	A	4113	0	4028	7	0
1	B	4204	0	4093	9	0
2	A	9	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	27	0	0	1	0
4	B	6	0	8	0	0
5	A	80	0	0	0	0
5	B	90	0	0	2	0
All	All	8529	0	8137	16	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 1.

All (16) 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:292:LYS:HG3	5:B:982:HOH:O	1.85	0.77
1:A:381:ASP:OD1	1:A:383:ASP:N	2.37	0.57
1:B:250:TYR:CZ	1:B:293:VAL:HG23	2.42	0.55
1:B:579:TYR:OH	1:B:605:GLU:OE1	2.24	0.55
1:A:579:TYR:OH	1:A:605:GLU:OE2	2.26	0.53
1:A:668:VAL:HG11	1:A:713:LEU:HG	1.90	0.53
1:B:668:VAL:HG11	1:B:713:LEU:HG	1.91	0.52
1:B:284:THR:HG22	1:B:326:ILE:HG21	1.92	0.52
1:A:284:THR:HG22	1:A:326:ILE:HG21	1.96	0.47
1:B:292:LYS:CG	5:B:982:HOH:O	2.54	0.46
1:A:456:LEU:HD12	1:A:470:CYS:HB2	1.98	0.46
1:A:336:GLN:NE2	1:A:495:GLU:OE2	2.49	0.43
1:B:518:ASP:CG	1:B:547:TRP:HZ2	2.27	0.42
1:B:456:LEU:HD12	1:B:470:CYS:HB2	2.03	0.41
1:A:658:ILE:N	1:A:659:PRO:HA	2.35	0.40
1:B:473:VAL:HG23	3:B:801:8WA:C13	2.52	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	512/542 (94%)	504 (98%)	8 (2%)	0	100	100
1	B	530/542 (98%)	518 (98%)	12 (2%)	0	100	100
All	All	1042/1084 (96%)	1022 (98%)	20 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	439/469 (94%)	437 (100%)	2 (0%)	81	90
1	B	445/469 (95%)	442 (99%)	3 (1%)	76	87
All	All	884/938 (94%)	879 (99%)	5 (1%)	78	89

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	302	VAL
1	A	321	GLN
1	B	292	LYS
1	B	349	GLU
1	B	495	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	480	ASN
1	A	503	ASN
1	A	643	GLN
1	B	291	GLN
1	B	375	ASN
1	B	503	ASN
1	B	643	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	$\# Z > 2$
4	GOL	B	802	-	5,5,5	0.23	0	5,5,5	0.96	0
2	MET	A	800	-	7,8,8	0.97	1 (14%)	5,9,9	0.93	0
3	8WA	B	801	-	30,30,30	0.89	3 (10%)	33,43,43	1.00	3 (9%)

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
4	GOL	B	802	-	-	0/4/4/4	-
2	MET	A	800	-	-	0/8/8/8	-
3	8WA	B	801	-	-	1/9/20/20	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	801	8WA	C13-C17	-2.96	1.37	1.40
3	B	801	8WA	C12-N3	-2.53	1.31	1.36
2	A	800	MET	OXT-C	-2.33	1.23	1.30
3	B	801	8WA	C12-N5	2.28	1.35	1.32

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	801	8WA	C2-N1-C3	2.81	118.48	113.98
3	B	801	8WA	C17-C13-N3	2.71	110.14	105.47
3	B	801	8WA	C13-C17-N5	-2.32	105.82	109.96

There are no chirality outliers.

All (1) torsion outliers are listed below:

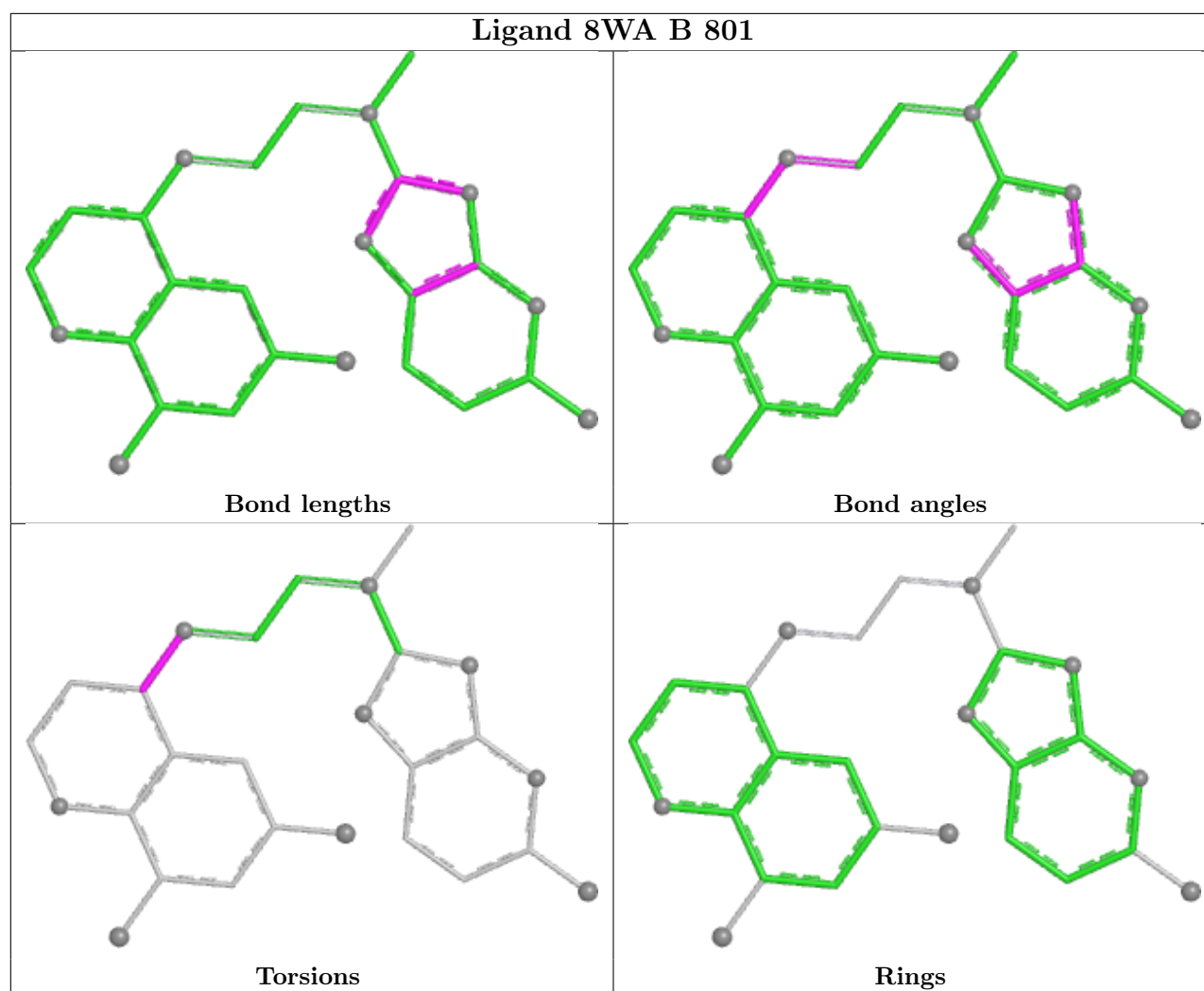
Mol	Chain	Res	Type	Atoms
3	B	801	8WA	C4-C3-N1-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	801	8WA	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 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	517/542 (95%)	0.48	50 (9%)	13 15	25, 39, 81, 115	1 (0%)
1	B	533/542 (98%)	0.47	63 (11%)	9 10	25, 40, 83, 125	1 (0%)
All	All	1050/1084 (96%)	0.48	113 (10%)	11 12	25, 40, 83, 125	2 (0%)

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	756	VAL	13.3
1	A	548	TRP	9.5
1	A	549	THR	8.5
1	B	386	PRO	7.8
1	A	562	VAL	7.3
1	B	305	TYR	6.8
1	A	238	VAL	6.6
1	B	757	GLU	6.5
1	A	547	TRP	6.4
1	A	382	LYS	6.3
1	B	547	TRP	5.9
1	B	559	LEU	5.8
1	B	380	VAL	5.7
1	B	758	GLY	5.3
1	A	563	PHE	5.3
1	A	755	ALA	5.3
1	A	766	SER	5.2
1	A	590	ASP	5.2
1	B	756	VAL	5.1
1	A	760	VAL	4.8
1	A	386	PRO	4.8
1	A	759	GLU	4.5
1	B	760	VAL	4.5
1	B	767	THR	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	550	LYS	4.4
1	B	398	THR	4.3
1	B	377	THR	4.2
1	B	491	GLU	4.2
1	B	391	LEU	4.2
1	A	588	SER	4.0
1	B	755	ALA	3.9
1	A	491	GLU	3.9
1	A	689	LYS	3.9
1	A	565	PRO	3.9
1	B	365	ILE	3.8
1	B	396	VAL	3.8
1	B	395	HIS	3.7
1	B	381	ASP	3.7
1	B	557	LYS	3.7
1	A	591	GLY	3.6
1	A	385	ASN	3.6
1	A	561	ASN	3.6
1	A	589	ASP	3.5
1	B	560	GLY	3.5
1	B	370	PHE	3.4
1	A	593	TYR	3.4
1	B	385	ASN	3.3
1	B	388	LYS	3.3
1	B	397	VAL	3.3
1	A	690	THR	3.2
1	A	302	VAL	3.2
1	A	612	ASN	3.2
1	B	759	GLU	3.1
1	B	360	GLU	3.1
1	A	546	GLY	3.1
1	B	616	ARG	3.1
1	B	556	SER	3.1
1	B	555	ILE	3.0
1	B	612	ASN	3.0
1	B	389	VAL	3.0
1	B	496	VAL	3.0
1	A	688	VAL	2.9
1	A	384	GLY	2.9
1	B	376	ILE	2.9
1	B	597[A]	ASN	2.9
1	A	765	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	387	CYS	2.9
1	B	585	SER	2.9
1	A	587	PHE	2.9
1	A	438	ARG	2.8
1	B	393	SER	2.7
1	B	761	LEU	2.7
1	A	380	VAL	2.6
1	A	298	LYS	2.6
1	A	567	GLU	2.6
1	B	372	THR	2.6
1	B	394	GLY	2.6
1	B	369	SER	2.6
1	A	381	ASP	2.5
1	B	379	GLY	2.5
1	A	572	PHE	2.5
1	B	765	ARG	2.4
1	B	689	LYS	2.4
1	A	564	ASP	2.4
1	A	621	LYS	2.4
1	B	766	SER	2.4
1	B	374	GLN	2.4
1	B	754	PRO	2.3
1	A	585	SER	2.3
1	B	421	HIS	2.3
1	B	558	SER	2.3
1	A	571	GLU	2.3
1	B	299	GLN	2.3
1	B	518	ASP	2.2
1	B	373	PRO	2.2
1	B	549	THR	2.2
1	B	690	THR	2.2
1	B	736	LYS	2.2
1	B	362	TRP	2.2
1	A	754	PRO	2.2
1	A	305	TYR	2.1
1	B	371	LEU	2.1
1	B	404	ASN	2.1
1	A	592	ASP	2.1
1	B	378	ASP	2.1
1	B	552	ARG	2.1
1	A	239	GLU	2.1
1	A	494	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	553	LYS	2.0
1	A	598	MET	2.0
1	A	457	HIS	2.0
1	A	761	LEU	2.0
1	B	399	TRP	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](#)

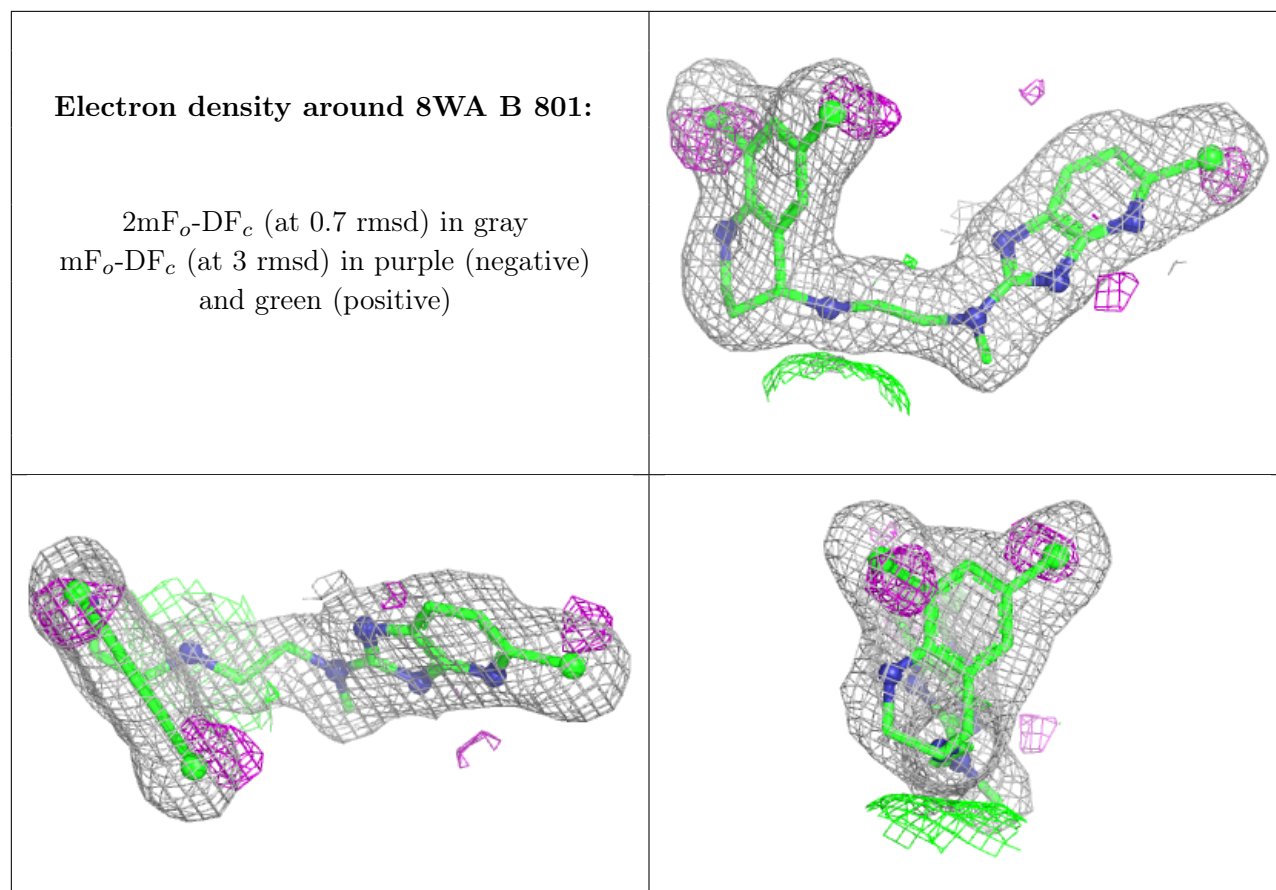
There are no oligosaccharides in this entry.

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
4	GOL	B	802	6/6	0.84	0.22	54,56,60,60	0
3	8WA	B	801	27/27	0.96	0.08	29,32,35,41	0
2	MET	A	800	9/9	0.97	0.08	30,32,34,35	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 ⓘ

There are no such residues in this entry.