wwPDB X-ray Structure Validation Summary Report (i)

Sep 13, 2020 – 09:46 PM BST

PDB ID	:	5NFH
Title	:	Trypanosoma brucei methionyl-tRNA synthetase in complex with a quinazolinone inhibitor
Authors	:	Robinson, D.A.; Eadsforth, T.C.; Shepherd, S.M.; Torrie, L.S.; De Rycker, M.; Gilbert, I.H.
Deposited on	:	2017-03-14
Resolution	:	2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

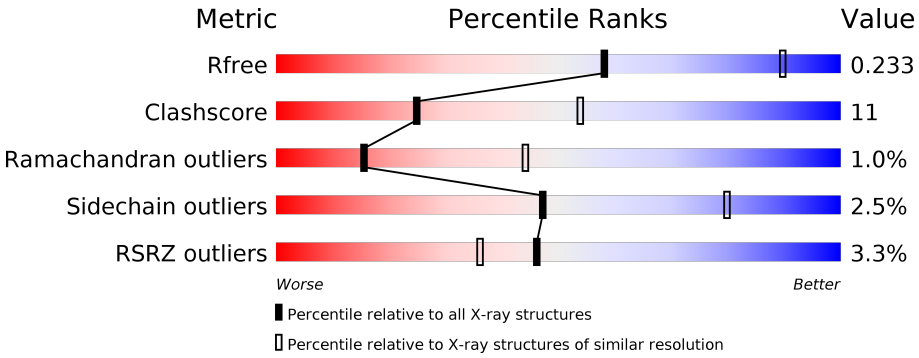
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.4.dev1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.4.dev1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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% 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	536	2% 77% 16%
1	B	536	4% 82% 15%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8701 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.

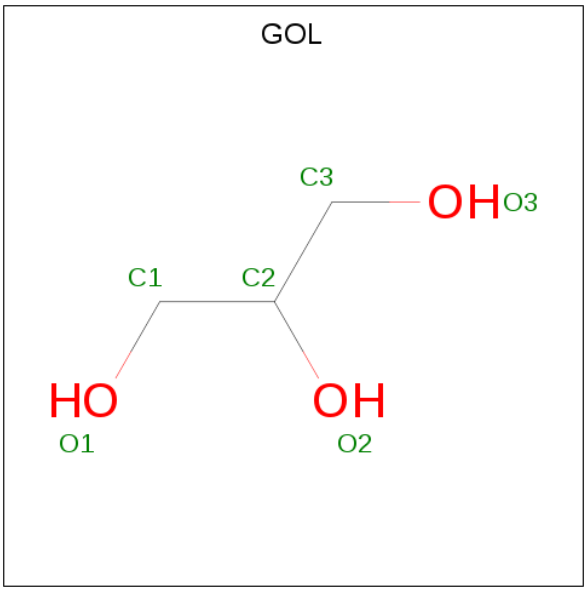
- Molecule 1 is a protein called Methionyl-tRNA synthetase, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	519	Total	C	N	O	S	0	0	0
			4152	2675	697	769	11			
1	B	527	Total	C	N	O	S	0	3	0
			4207	2711	711	773	12			

There are 22 discrepancies between the modelled and reference sequences:

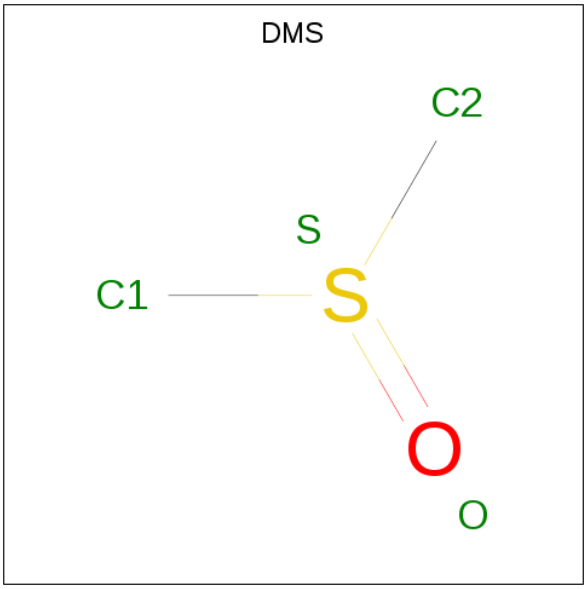
Chain	Residue	Modelled	Actual	Comment	Reference
A	232	GLY	-	expression tag	UNP Q38C91
A	233	PRO	-	expression tag	UNP Q38C91
A	234	GLY	-	expression tag	UNP Q38C91
A	235	SER	-	expression tag	UNP Q38C91
A	236	MET	-	expression tag	UNP Q38C91
A	309	THR	ALA	conflict	UNP Q38C91
A	452	ALA	LYS	engineered mutation	UNP Q38C91
A	453	ARG	LYS	engineered mutation	UNP Q38C91
A	454	ALA	GLU	engineered mutation	UNP Q38C91
A	499	VAL	ALA	conflict	UNP Q38C91
A	503	ASN	SER	conflict	UNP Q38C91
B	-4	GLY	-	expression tag	UNP Q38C91
B	-3	PRO	-	expression tag	UNP Q38C91
B	-2	GLY	-	expression tag	UNP Q38C91
B	-1	SER	-	expression tag	UNP Q38C91
B	0	MET	-	expression tag	UNP Q38C91
B	309	THR	ALA	conflict	UNP Q38C91
B	452	ALA	LYS	engineered mutation	UNP Q38C91
B	453	ARG	LYS	engineered mutation	UNP Q38C91
B	454	ALA	GLU	engineered mutation	UNP Q38C91
B	499	VAL	ALA	conflict	UNP Q38C91
B	503	ASN	SER	conflict	UNP Q38C91

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



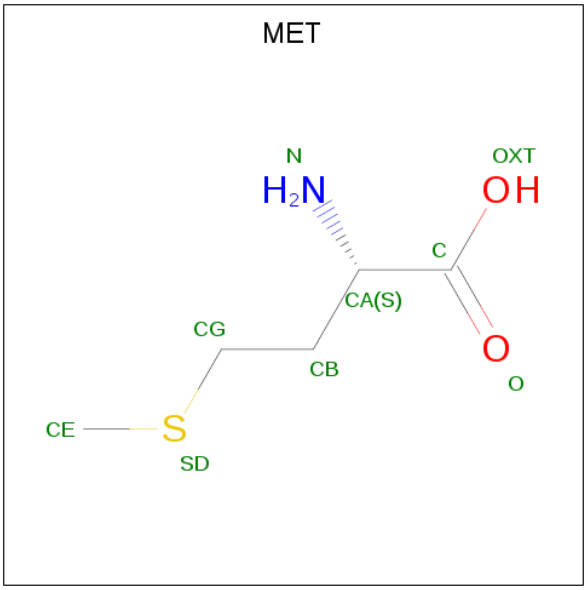
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0

- Molecule 3 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



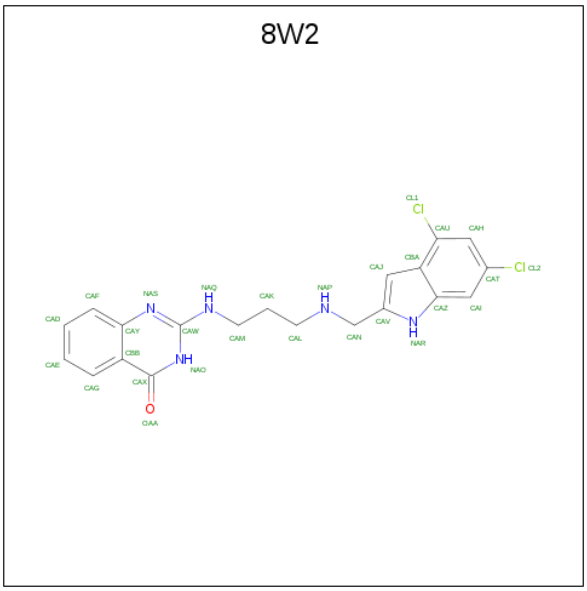
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O S 4 2 1 1	0	0
3	A	1	Total C O S 4 2 1 1	0	0
3	B	1	Total C O S 4 2 1 1	0	0

- Molecule 4 is METHIONINE (three-letter code: MET) (formula: $C_5H_{11}NO_2S$).



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

- Molecule 5 is 2-[3-[[4,6-bis(chloranyl)-1 {H}-indol-2-yl]methylamino]propylamino]-3 {H}-quinazolin-4-one (three-letter code: 8W2) (formula: $C_{20}H_{19}Cl_2N_5O$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	Cl	N	O	0	0
			28	20	2	5	1		

- Molecule 6 is water.

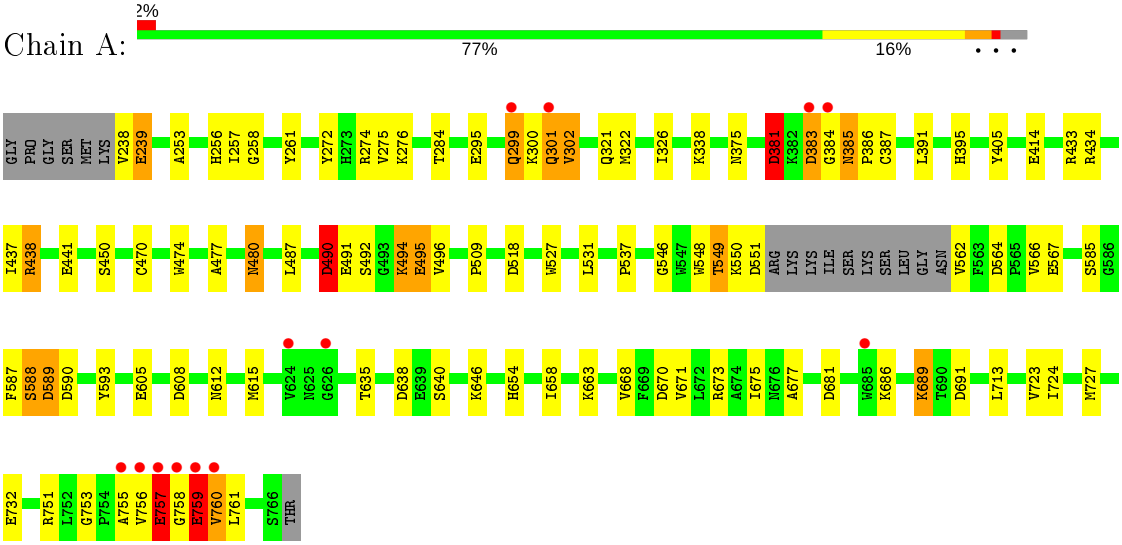
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	128	Total	O	0	0
			128	128		
6	B	135	Total	O	0	0
			135	135		

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.

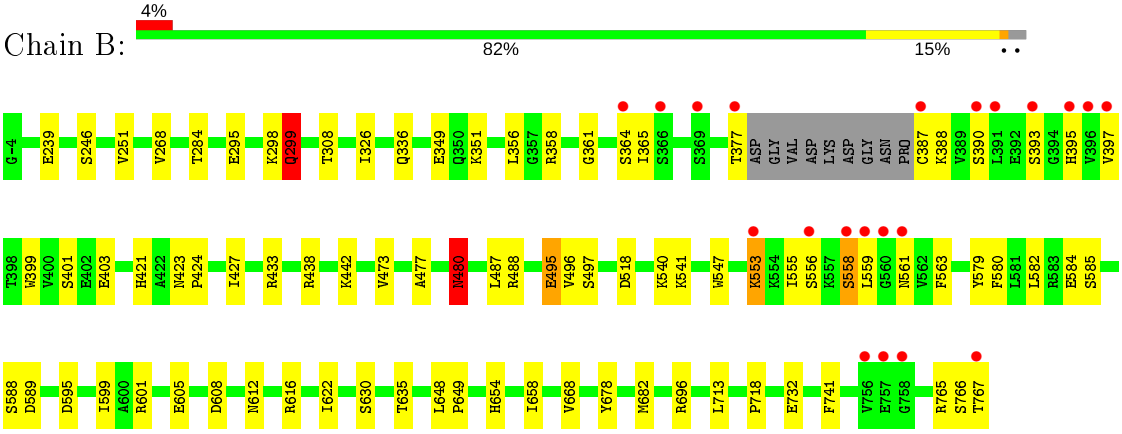
- Molecule 1: Methionyl-tRNA synthetase, putative

Chain A:



- Molecule 1: Methionyl-tRNA synthetase, putative

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	87.09Å 105.98Å 207.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 48.18 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.00-2.80) 99.7 (48.18-2.80)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.06 (at 2.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.195 , 0.230 0.198 , 0.233	Depositor DCC
R_{free} test set	2417 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	48.0	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 45.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8701	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical 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.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, DMS, 8W2

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	0.64	0/4261	0.65	2/5797 (0.0%)
1	B	0.58	0/4323	0.62	1/5878 (0.0%)
All	All	0.61	0/8584	0.63	3/11675 (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	A	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	385	ASN	C-N-CD	5.93	140.85	128.40
1	A	753	GLY	C-N-CD	5.22	139.35	128.40
1	B	299	GLN	CA-CB-CG	-5.09	102.21	113.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	562	VAL	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	4152	0	4083	92	0
1	B	4207	0	4149	91	0
2	A	24	0	32	2	0
2	B	6	0	8	0	0
3	A	8	0	12	0	0
3	B	4	0	6	0	0
4	A	9	0	8	2	0
5	B	28	0	0	1	0
6	A	128	0	0	32	0
6	B	135	0	0	34	0
All	All	8701	0	8298	181	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 11.

The worst 5 of 181 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:349:GLU:HG3	6:B:936:HOH:O	1.34	1.27
1:B:767:THR:HG21	6:B:993:HOH:O	1.36	1.26
1:B:616:ARG:HG2	6:B:1025:HOH:O	1.38	1.21
1:B:616:ARG:HB3	6:B:1000:HOH:O	1.36	1.21
1:B:299:GLN:HB3	6:B:942:HOH:O	1.40	1.17

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	515/536 (96%)	482 (94%)	24 (5%)	9 (2%)	9 29
1	B	525/536 (98%)	508 (97%)	16 (3%)	1 (0%)	47 78
All	All	1040/1072 (97%)	990 (95%)	40 (4%)	10 (1%)	15 44

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	490	ASP
1	A	549	THR
1	A	757	GLU
1	A	759	GLU
1	A	381	ASP

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	447/463 (96%)	432 (97%)	15 (3%)	37 71
1	B	451/463 (97%)	444 (98%)	7 (2%)	62 88
All	All	898/926 (97%)	876 (98%)	22 (2%)	47 81

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	491	GLU
1	A	689	LYS
1	B	553	LYS
1	A	494	LYS
1	A	495	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	336	GLN
1	B	395	HIS
1	B	561	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry

10 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	DMS	A	805	-	3,3,3	0.27	0	3,3,3	1.12	0
4	MET	A	807	-	4,8,8	0.27	0	2,9,9	0.46	0
2	GOL	A	801	-	5,5,5	0.29	0	5,5,5	0.86	0
2	GOL	A	804	-	5,5,5	0.51	0	5,5,5	0.63	0
5	8W2	B	803	-	28,31,31	2.37	7 (25%)	35,43,43	2.30	7 (20%)
2	GOL	A	803	-	5,5,5	0.15	0	5,5,5	0.59	0
2	GOL	B	801	-	5,5,5	0.26	0	5,5,5	0.85	0
3	DMS	B	802	-	3,3,3	0.27	0	3,3,3	0.68	0
3	DMS	A	806	-	3,3,3	0.36	0	3,3,3	0.44	0
2	GOL	A	802	-	5,5,5	0.44	0	5,5,5	0.57	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
4	MET	A	807	-	-	0/4/8/8	-
2	GOL	A	801	-	-	4/4/4/4	-
2	GOL	A	804	-	-	3/4/4/4	-
5	8W2	B	803	-	-	1/7/9/9	0/4/4/4
2	GOL	A	803	-	-	2/4/4/4	-
2	GOL	B	801	-	-	4/4/4/4	-
2	GOL	A	802	-	-	4/4/4/4	-

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	803	8W2	CAT-CL2	-6.12	1.61	1.74
5	B	803	8W2	CAU-CBA	-5.86	1.31	1.42
5	B	803	8W2	CAI-CAZ	-4.75	1.34	1.41
5	B	803	8W2	CAX-NAO	4.28	1.40	1.33
5	B	803	8W2	CAJ-CAV	-3.42	1.35	1.39

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	803	8W2	CBB-CAX-NAO	-9.05	118.09	124.40
5	B	803	8W2	CBB-CAY-NAS	-5.22	120.77	123.60
5	B	803	8W2	CAN-CAV-CAJ	-3.57	124.68	129.54
5	B	803	8W2	CAW-NAS-CAY	3.41	121.15	115.60
5	B	803	8W2	NAS-CAW-NAO	-3.28	121.05	126.23

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	GOL	O1-C1-C2-C3
2	A	801	GOL	C1-C2-C3-O3
2	A	804	GOL	C1-C2-C3-O3
2	A	803	GOL	O1-C1-C2-C3
2	B	801	GOL	C1-C2-C3-O3

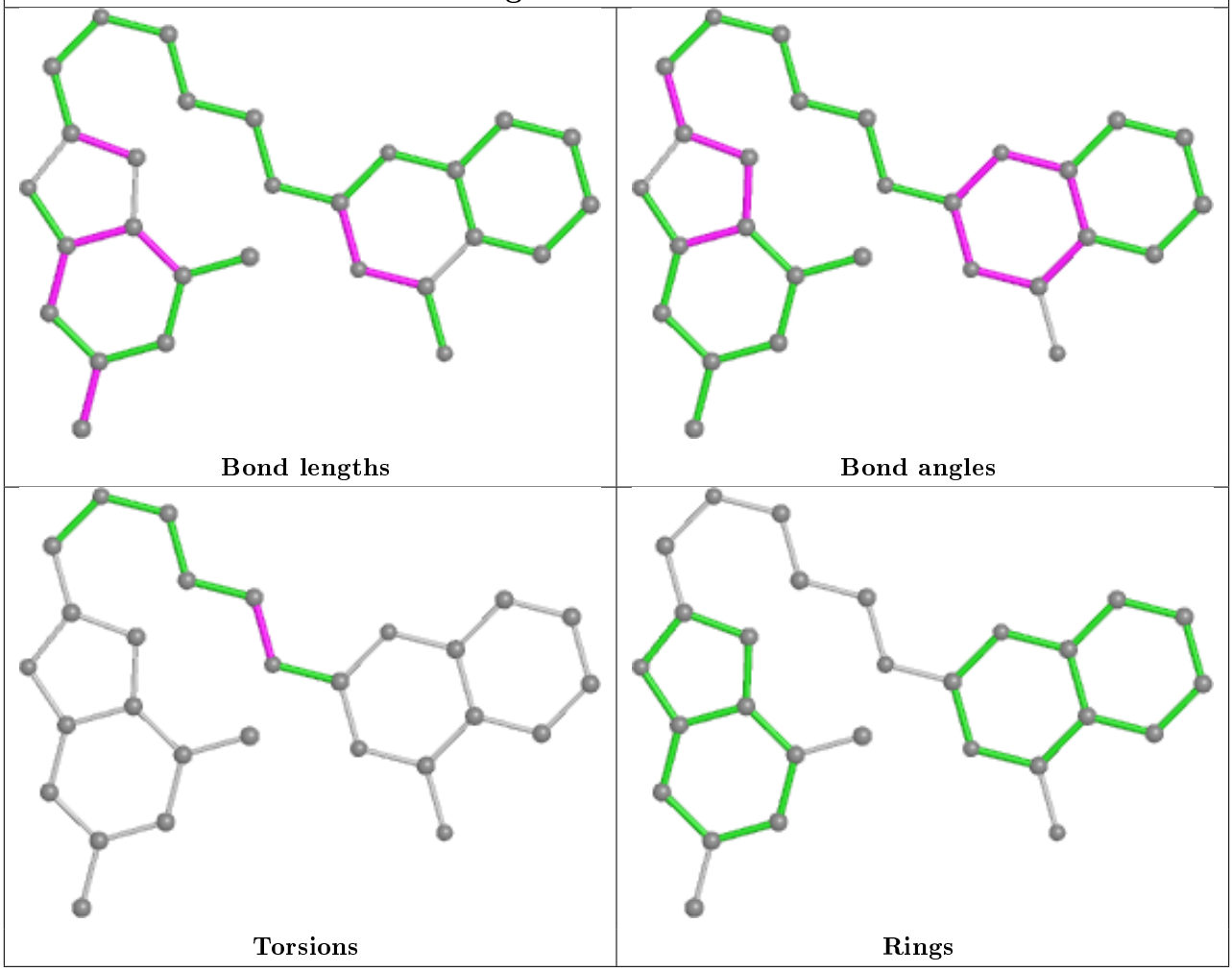
There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	807	MET	2	0
5	B	803	8W2	1	0
2	A	802	GOL	2	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.

Ligand 8W2 B 803



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, 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	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	519/536 (96%)	-0.27	13 (2%)	57	47	27, 38, 81, 139	0
1	B	527/536 (98%)	-0.17	21 (3%)	38	28	24, 41, 101, 132	0
All	All	1046/1072 (97%)	-0.22	34 (3%)	46	36	24, 39, 92, 139	0

The worst 5 of 34 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	384	GLY	5.3
1	B	757	GLU	4.9
1	A	757	GLU	4.6
1	A	760	VAL	4.5
1	B	758	GLY	4.3

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

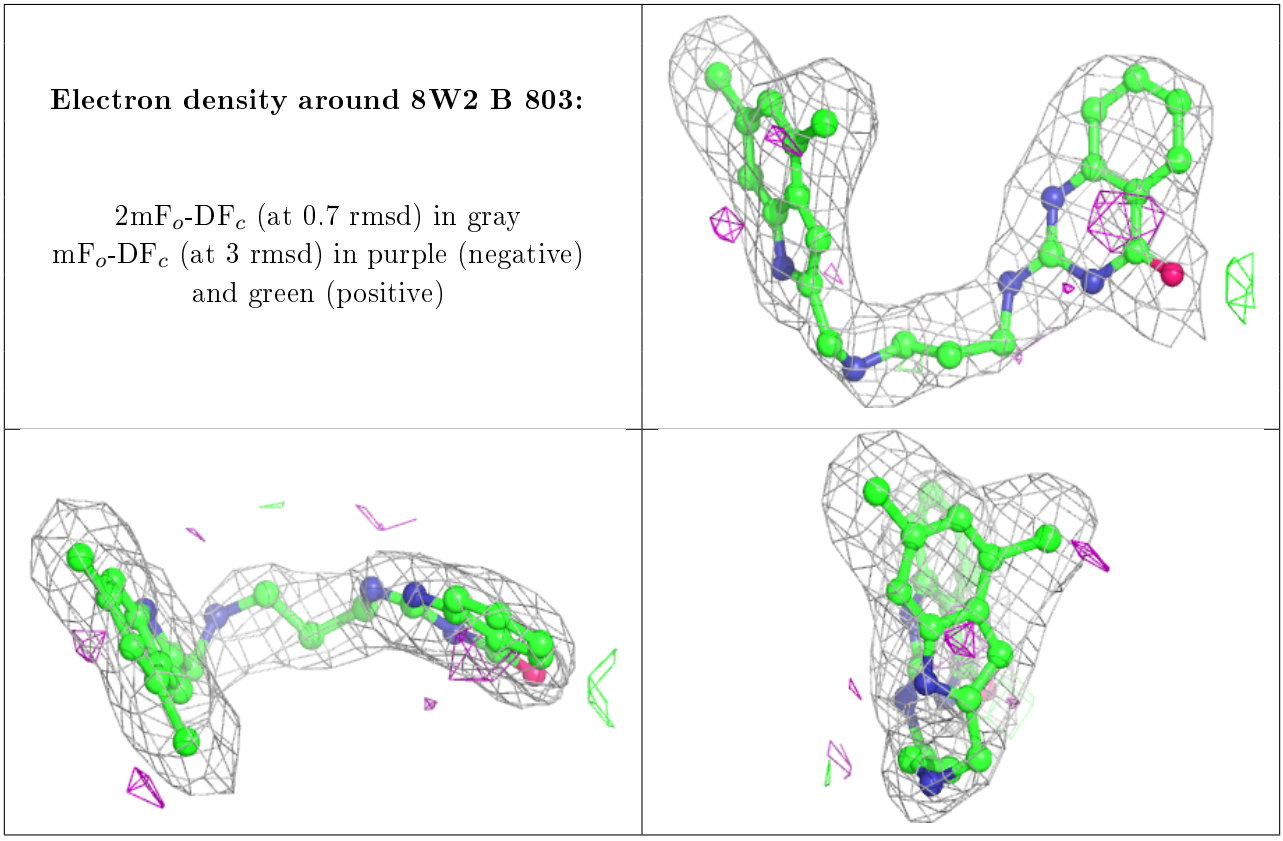
There are no monosaccharides in this entry.

6.4 Ligands

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	B-factors(Å^2)	Q<0.9
3	DMS	A	805	4/4	0.83	0.23	79,94,96,106	0
2	GOL	A	804	6/6	0.86	0.24	52,56,63,68	0
2	GOL	A	802	6/6	0.91	0.19	45,48,52,56	0
2	GOL	A	803	6/6	0.92	0.29	63,71,77,87	0
3	DMS	B	802	4/4	0.93	0.19	55,61,62,62	0
5	8W2	B	803	28/28	0.94	0.19	43,53,58,61	0
2	GOL	A	801	6/6	0.95	0.17	45,46,47,47	0
3	DMS	A	806	4/4	0.96	0.15	68,77,78,80	0
2	GOL	B	801	6/6	0.96	0.18	46,49,50,50	0
4	MET	A	807	9/9	0.99	0.17	31,35,37,41	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.