



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 03:39 pm BST

PDB ID : 4ZT7  
Title : Trypanosoma brucei methionyl-tRNA synthetase in complex with inhibitor N-[(4R)-6,8-dichloro-1,2,3,4-tetrahydroquinolin-4-yl]-N'-(5-fluoro-3H-imidazo[4,5-b]pyridin-2-yl)propane-1,3-diamine (Chem 1717)  
Authors : Koh, C.-Y.; Hol, W.G.J.  
Deposited on : 2015-05-14  
Resolution : 2.40 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

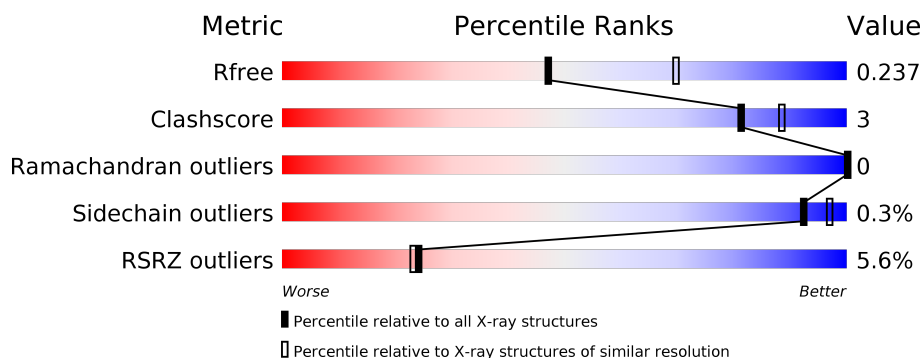
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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  $\geq 3$ , 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	<div> <div>5%</div> <div> <div></div> <div>90%</div> <div>6%</div> <div></div> </div> </div>
1	B	542	<div> <div>6%</div> <div> <div></div> <div>91%</div> <div>7%</div> <div></div> </div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8904 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.

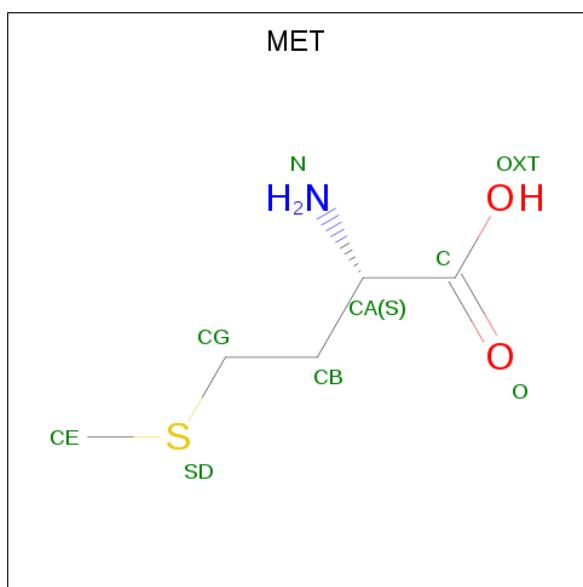
- Molecule 1 is a protein called Methionyl-tRNA synthetase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	520	Total	As	C	N	O	S	0	2	0
			4162	1	2680	699	770	12			
1	B	529	Total	As	C	N	O	S	0	0	0
			4177	1	2689	705	770	12			

There are 22 discrepancies between the modelled and reference sequences:

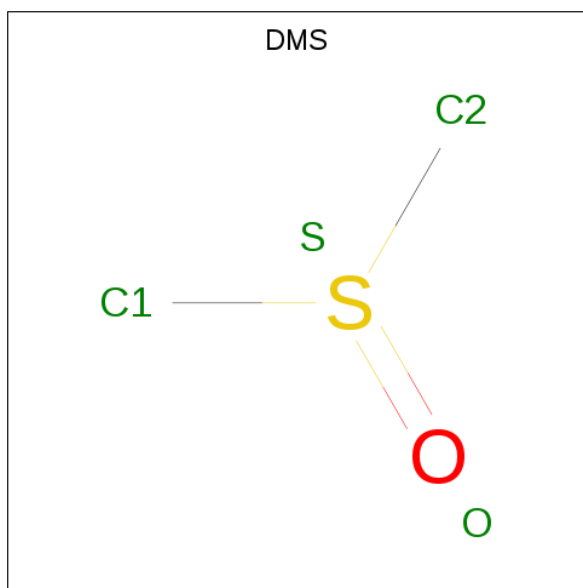
Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP Q38C91
A	-3	PRO	-	expression tag	UNP Q38C91
A	-2	GLY	-	expression tag	UNP Q38C91
A	-1	SER	-	expression tag	UNP Q38C91
A	0	MET	-	expression tag	UNP Q38C91
A	309	THR	ALA	conflict	UNP Q38C91
A	452	ALA	LYS	engineered mutation	UNP 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 METHIONINE (three-letter code: MET) (formula: C<sub>5</sub>H<sub>11</sub>NO<sub>2</sub>S).



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

- Molecule 3 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C<sub>2</sub>H<sub>6</sub>OS).



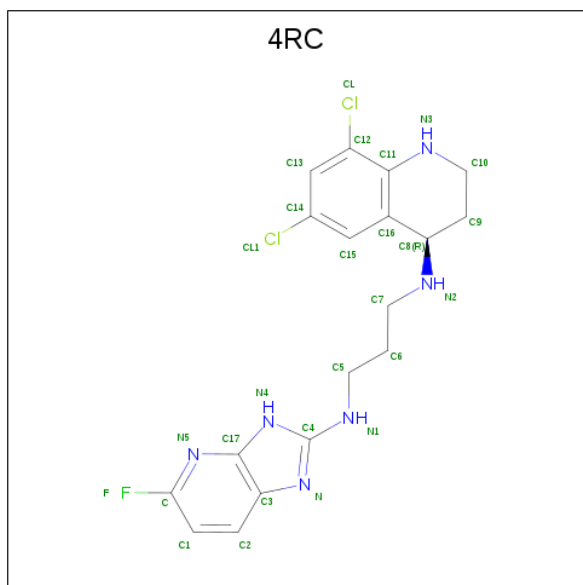
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	A	1	Total	C	O	S	0	0
			4	2	1	1		

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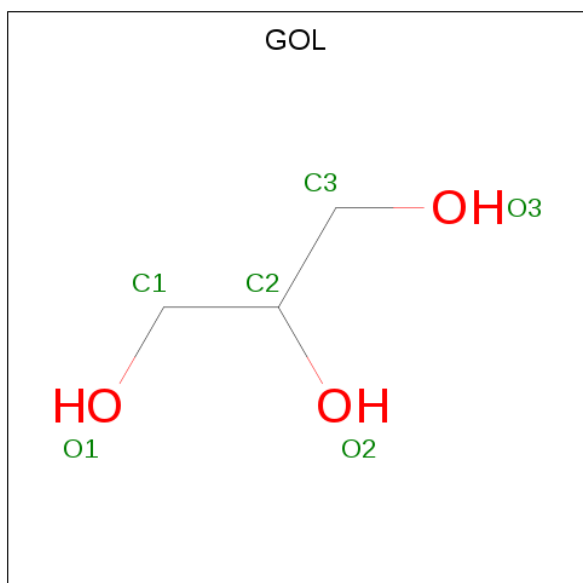
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 4 is N-[(4R)-6,8-dichloro-1,2,3,4-tetrahydroquinolin-4-yl]-N'-(5-fluoro-3H-imidazo[4,5-b]pyridin-2-yl)propane-1,3-diamine (three-letter code: 4RC) (formula: C<sub>18</sub>H<sub>19</sub>Cl<sub>2</sub>FN<sub>6</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	Cl	F	N	0	0
			27	18	2	1	6		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

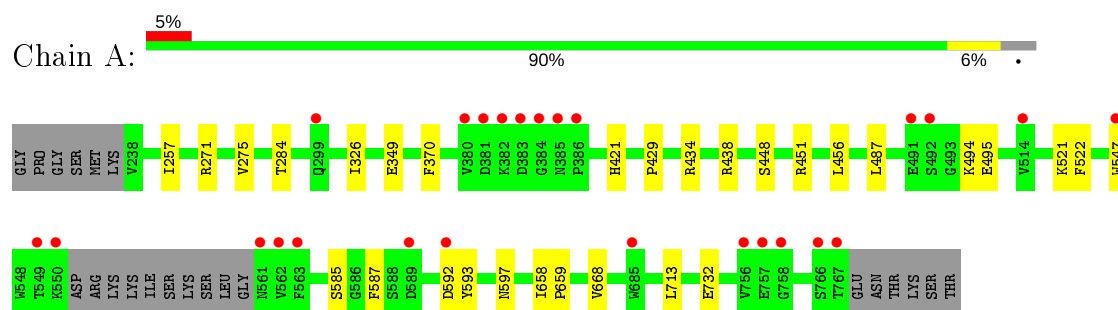
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	250	Total	O	0	0
			250	250		
6	B	257	Total	O	0	0
			257	257		

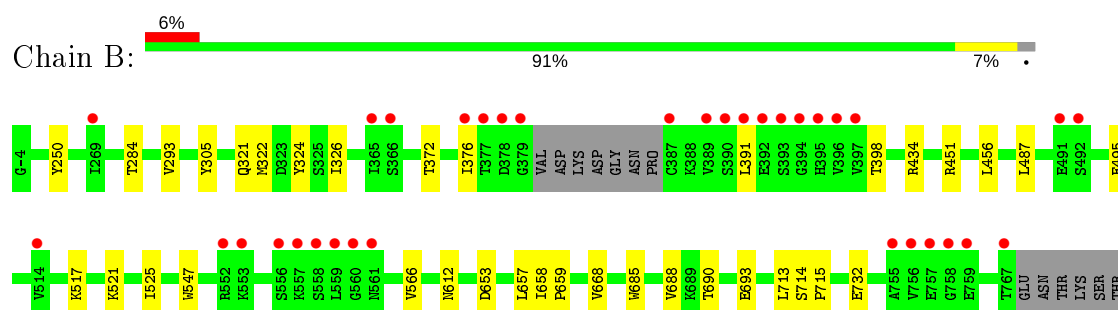
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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



#### • Molecule 1: Methionyl-tRNA synthetase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.63Å 105.84Å 207.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.80 – 2.40 37.80 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (37.80-2.40) 100.0 (37.80-2.40)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.34 (at 2.39Å)	Xtriage
Refinement program	REFMAC refmac_5.8.0073	Depositor
R, $R_{free}$	0.207 , 0.236 0.211 , 0.237	Depositor DCC
$R_{free}$ test set	3795 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.7	Xtriage
Anisotropy	0.520	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 41.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8904	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: CAS, GOL, 4RC, DMS

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	0.39	0/4261	0.59	0/5798
1	B	0.40	0/4276	0.58	0/5818
All	All	0.39	0/8537	0.59	0/11616

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	4162	0	4068	20	0
1	B	4177	0	4076	23	0
2	A	9	0	8	0	0
3	A	12	0	18	1	0
3	B	4	0	6	1	0
4	B	27	0	0	0	0
5	B	6	0	8	0	0
6	A	250	0	0	5	0
6	B	257	0	0	6	0
All	All	8904	0	8184	43	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 3.

All (43) 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)
6:A:983:HOH:O	1:B:434:ARG:HD3	1.95	0.66
1:B:487:LEU:HD22	1:B:495:GLU:HG3	1.78	0.65
1:A:487:LEU:HD22	1:A:495:GLU:HG3	1.79	0.65
1:B:284:THR:HG22	1:B:326:ILE:HG21	1.84	0.60
1:A:732:GLU:HG2	6:A:910:HOH:O	2.01	0.60
1:A:284:THR:HG22	1:A:326:ILE:HG21	1.87	0.57
1:B:322:MET:CE	1:B:566:VAL:HA	2.36	0.56
1:B:372:THR:O	1:B:376:ILE:HD12	2.09	0.52
1:A:668:VAL:HG11	1:A:713:LEU:HG	1.92	0.51
1:B:668:VAL:HG11	1:B:713:LEU:HG	1.93	0.51
1:A:585:SER:HB3	1:A:593:TYR:OH	2.11	0.50
1:A:658:ILE:N	1:A:659:PRO:HA	2.25	0.50
1:B:451:ARG:HB2	1:B:456:LEU:HD11	1.94	0.50
1:B:487:LEU:HD22	1:B:495:GLU:CG	2.42	0.50
1:A:434:ARG:HD3	6:B:912:HOH:O	2.11	0.50
1:B:322:MET:HE1	1:B:566:VAL:HA	1.94	0.49
1:B:658:ILE:N	1:B:659:PRO:HA	2.28	0.49
1:B:391:LEU:CB	6:B:1138:HOH:O	2.60	0.48
1:A:494:LYS:CB	6:A:1047:HOH:O	2.60	0.48
1:A:421:HIS:HB3	6:B:1046:HOH:O	2.13	0.48
1:A:487:LEU:HD22	1:A:495:GLU:CG	2.44	0.48
6:A:1145:HOH:O	1:B:690:THR:HG21	2.13	0.48
1:B:250:TYR:CZ	1:B:293:VAL:HG23	2.49	0.48
1:A:370:PHE:CZ	1:A:448:SER:HB3	2.50	0.47
1:A:592:ASP:OD2	1:A:597:ASN:HB2	2.16	0.46
1:B:517:LYS:HE2	1:B:547:TRP:CD1	2.50	0.46
1:A:257:ILE:HG13	1:A:547:TRP:HZ3	1.81	0.46
1:B:521:LYS:HG2	1:B:525:ILE:HD12	1.98	0.45
1:B:732:GLU:HG2	6:B:943:HOH:O	2.16	0.45
1:B:685:TRP:O	1:B:688:VAL:HG22	2.16	0.45
1:A:271:ARG:O	1:A:275:VAL:HG13	2.16	0.43
1:B:612:ASN:HB2	6:B:960:HOH:O	2.18	0.43
1:B:653:ASP:O	1:B:657:LEU:HD13	2.19	0.42
1:B:714:SER:N	1:B:715:PRO:CD	2.82	0.42
1:A:451:ARG:HB2	1:A:456:LEU:HD11	2.01	0.42
1:B:693:GLU:HB2	6:B:1061:HOH:O	2.18	0.42
1:A:349:GLU:HG3	3:A:804:DMS:H23	2.01	0.42
1:B:372:THR:O	1:B:376:ILE:CD1	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:LYS:HG3	1:A:522:PHE:N	2.36	0.41
1:A:429:PRO:HG3	1:A:587:PHE:HB3	2.02	0.41
1:A:438:ARG:NH1	6:A:917:HOH:O	2.54	0.41
1:A:456:LEU:N	1:A:456:LEU:HD12	2.36	0.41
1:B:324:TYR:HB2	3:B:803:DMS:H11	2.02	0.41

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	517/542 (95%)	507 (98%)	10 (2%)	0	100	100
1	B	524/542 (97%)	514 (98%)	10 (2%)	0	100	100
All	All	1041/1084 (96%)	1021 (98%)	20 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	444/468 (95%)	444 (100%)	0	100	100
1	B	441/468 (94%)	438 (99%)	3 (1%)	84	92
All	All	885/936 (95%)	882 (100%)	3 (0%)	92	97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	305	TYR
1	B	321	GLN
1	B	398	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	CAS	B	470	1	5,8,9	1.04	0	1,9,11	0.15	0
1	CAS	A	470	1	5,8,9	1.08	0	1,9,11	0.23	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
1	CAS	B	470	1	-	0/0/7/9	-
1	CAS	A	470	1	-	0/0/7/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

7 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	B	803	-	3,3,3	0.59	0	3,3,3	0.45	0
3	DMS	A	804	-	3,3,3	0.50	0	3,3,3	0.45	0
3	DMS	A	803	-	3,3,3	0.61	0	3,3,3	0.53	0
3	DMS	A	802	-	3,3,3	0.51	0	3,3,3	0.70	0
5	GOL	B	802	-	5,5,5	0.29	0	5,5,5	0.86	0
4	4RC	B	801	-	30,30,30	1.16	1 (3%)	30,42,42	1.77	1 (3%)

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	4RC	B	801	-	-	2/6/18/18	0/4/4/4
5	GOL	B	802	-	-	0/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	801	4RC	C-N5	5.34	1.40	1.32

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	801	4RC	C-N5-C17	-9.12	112.99	117.44

There are no chirality outliers.

All (2) torsion outliers are listed below:

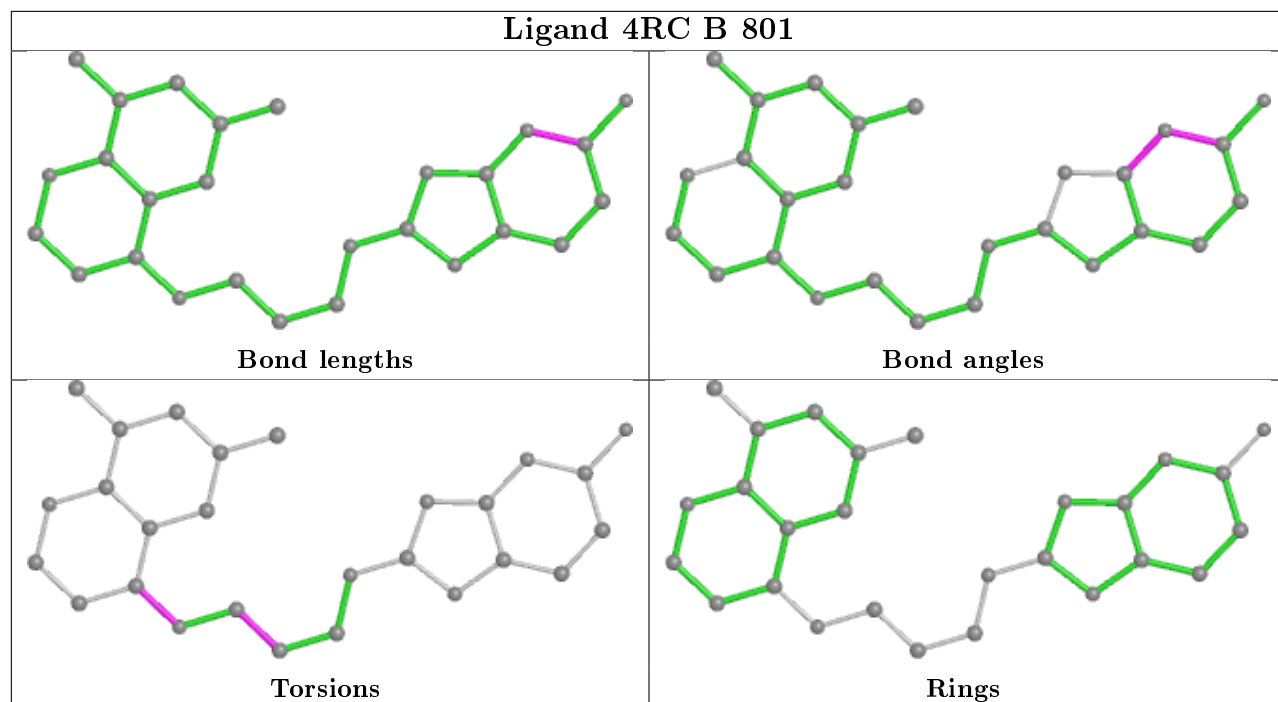
Mol	Chain	Res	Type	Atoms
4	B	801	4RC	C5-C6-C7-N2
4	B	801	4RC	C9-C8-N2-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	803	DMS	1	0
3	A	804	DMS	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	519/542 (95%)	-0.06	25 (4%) 30 29	20, 34, 75, 118	0
1	B	528/542 (97%)	0.02	34 (6%) 19 18	18, 35, 74, 114	0
All	All	1047/1084 (96%)	-0.02	59 (5%) 24 23	18, 35, 75, 118	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	383	ASP	6.5
1	A	562	VAL	6.3
1	B	558	SER	5.2
1	A	758	GLY	5.2
1	B	377	THR	5.2
1	A	767	THR	5.0
1	A	382	LYS	5.0
1	A	766	SER	4.9
1	B	758	GLY	4.4
1	B	394	GLY	4.3
1	A	589	ASP	4.1
1	B	387	CYS	4.0
1	A	561	ASN	4.0
1	B	757	GLU	4.0
1	B	767	THR	3.8
1	A	685	TRP	3.6
1	A	757	GLU	3.6
1	B	559	LEU	3.6
1	B	556	SER	3.5
1	B	376	ILE	3.5
1	B	378	ASP	3.4
1	A	384	GLY	3.4
1	B	366	SER	3.4
1	A	381	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	397	VAL	3.3
1	B	755	ALA	3.2
1	B	560	GLY	3.1
1	B	379	GLY	3.0
1	B	396	VAL	3.0
1	A	550	LYS	3.0
1	A	592	ASP	2.9
1	A	386	PRO	2.8
1	A	547	TRP	2.8
1	B	390	SER	2.7
1	A	563	PHE	2.7
1	A	380	VAL	2.7
1	B	395	HIS	2.7
1	B	365	ILE	2.6
1	B	391	LEU	2.6
1	B	492	SER	2.5
1	A	756	VAL	2.5
1	B	491	GLU	2.5
1	B	393	SER	2.5
1	B	392	GLU	2.4
1	B	552	ARG	2.4
1	A	549	THR	2.4
1	A	385	ASN	2.3
1	A	491	GLU	2.3
1	B	553	LYS	2.2
1	B	759	GLU	2.2
1	B	557	LYS	2.2
1	A	299	GLN	2.1
1	B	389	VAL	2.1
1	A	514	VAL	2.1
1	A	492	SER	2.1
1	B	514	VAL	2.0
1	B	756	VAL	2.0
1	B	269	ILE	2.0
1	B	561	ASN	2.0

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

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<sup>th</sup> 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
1	CAS	A	470	9/10	0.95	0.12	29,33,51,52	3
1	CAS	B	470	9/10	0.96	0.12	31,36,50,50	3

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

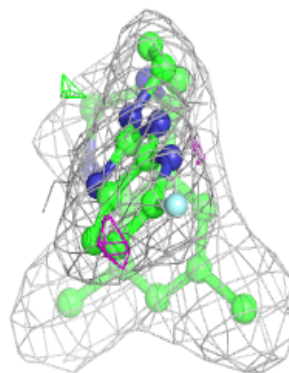
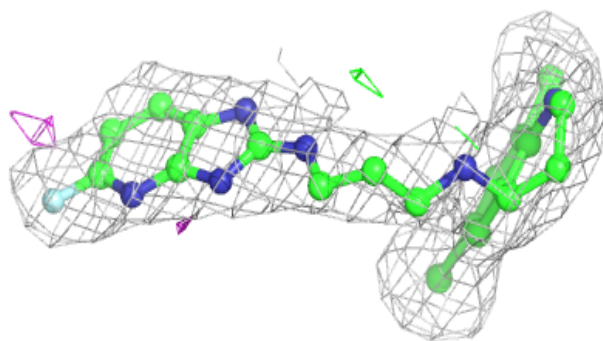
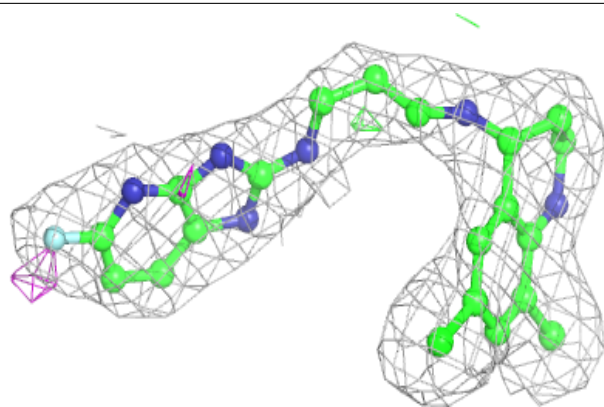
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	DMS	A	803	4/4	0.84	0.26	66,70,72,75	0
5	GOL	B	802	6/6	0.88	0.16	41,42,42,44	0
3	DMS	A	802	4/4	0.91	0.20	70,70,72,75	0
3	DMS	B	803	4/4	0.94	0.15	47,52,52,56	0
4	4RC	B	801	27/27	0.95	0.11	29,32,34,34	0
3	DMS	A	804	4/4	0.96	0.14	61,62,63,64	0
2	MET	A	801	9/9	0.97	0.22	22,24,24,25	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.

**Electron density around 4RC B 801:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.