



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2020 – 05:28 PM BST

PDB ID : 4MW1  
Title : Trypanosoma brucei methionyl-tRNA synthetase in complex with inhibitor 1 -{3-[(3-chloro-5-methoxybenzyl)amino]propyl}-3-thiophen-3-ylurea (Chem 1444)  
Authors : Koh, C.Y.; Kim, J.E.; Wetzel, A.B.; de van der Schueren, W.J.; Shibata, S.; Liu, J.; Zhang, Z.; Fan, E.; Verlinde, C.L.M.J.; Hol, W.G.J.  
Deposited on : 2013-09-24  
Resolution : 2.49 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 : 2.14.4.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

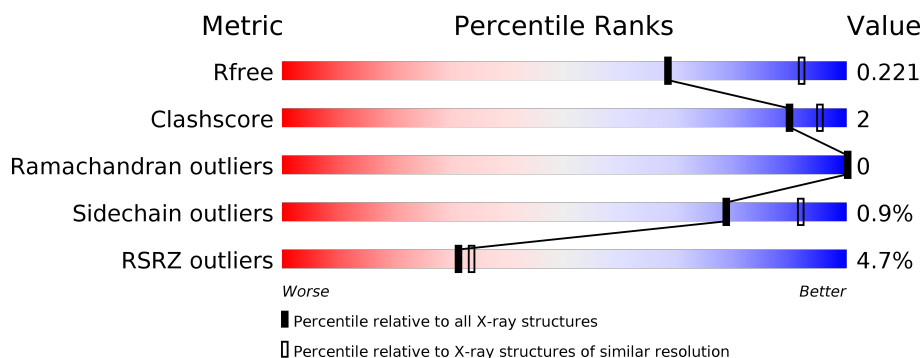
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.49 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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>4%</div> <div>94%</div> <div>5%</div> </div>
1	B	542	<div> <div>5%</div> <div>93%</div> <div>5%</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9063 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	530	Total	As	C	N	O	S	0	0	0
			4240	1	2730	716	782	11			
1	B	536	Total	As	C	N	O	S	0	2	0
			4288	1	2758	727	790	12			

There are 22 discrepancies between the modelled and reference sequences:

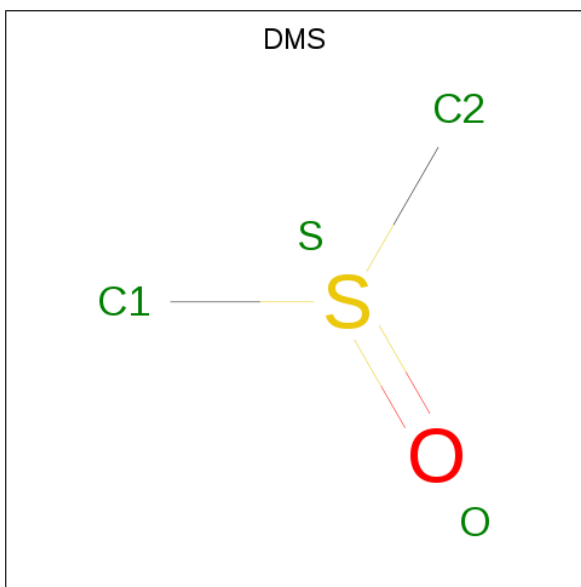
Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	EXPRESSION TAG	UNP Q38C91
A	-3	PRO	-	EXPRESSION TAG	UNP Q38C91
A	-2	GLY	-	EXPRESSION TAG	UNP Q38C91
A	-1	SER	-	EXPRESSION TAG	UNP Q38C91
A	0	MET	-	EXPRESSION TAG	UNP Q38C91
A	309	THR	ALA	CONFLICT	UNP Q38C91
A	452	ALA	LYS	ENGINEERED MUTATION	UNP 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 GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



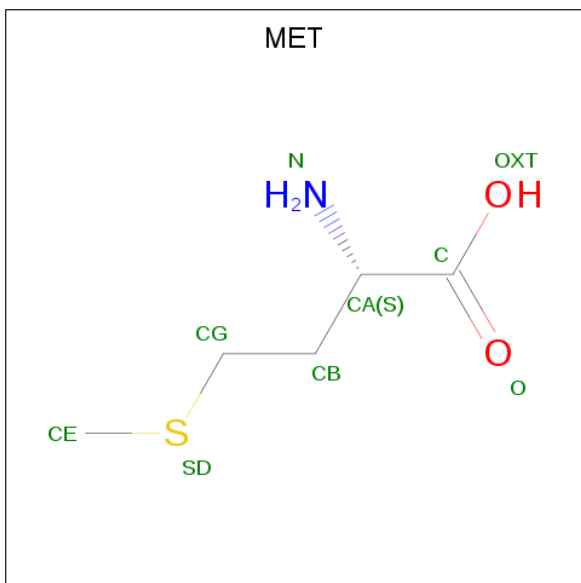
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		

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



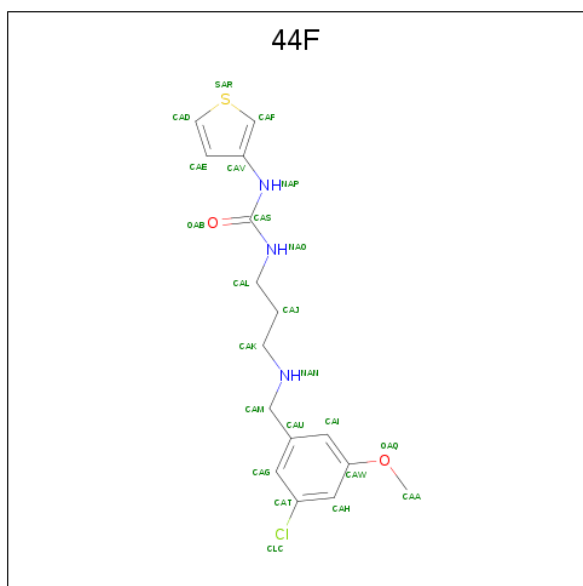
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	B	1	Total	C	O	S	0	0
			4	2	1	1		
3	B	1	Total	C	O	S	0	0
			4	2	1	1		

- 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	0	0
			9	5	1	2	1		

- Molecule 5 is 1-{3-[(3-chloro-5-methoxybenzyl)amino]propyl}-3-thiophen-3-ylurea (three-letter code: 44F) (formula: C<sub>16</sub>H<sub>20</sub>ClN<sub>3</sub>O<sub>2</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	Cl	N	O	S	0
			23	16	1	3	2	1	0

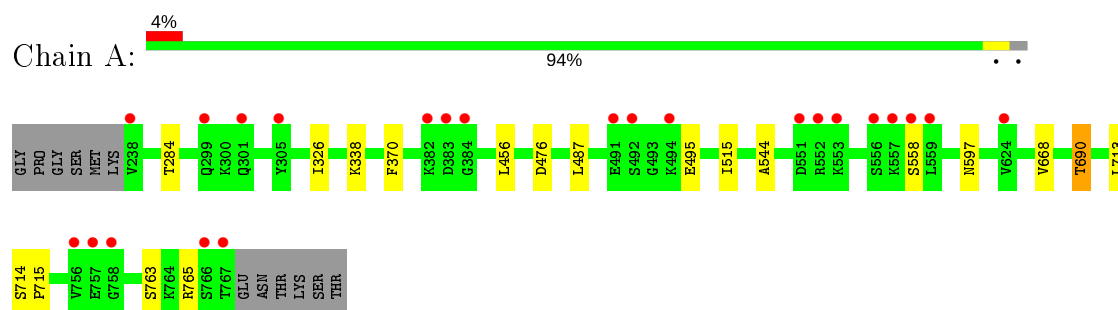
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	236	Total	O	0	0
			236	236		
6	B	191	Total	O	0	0
			191	191		

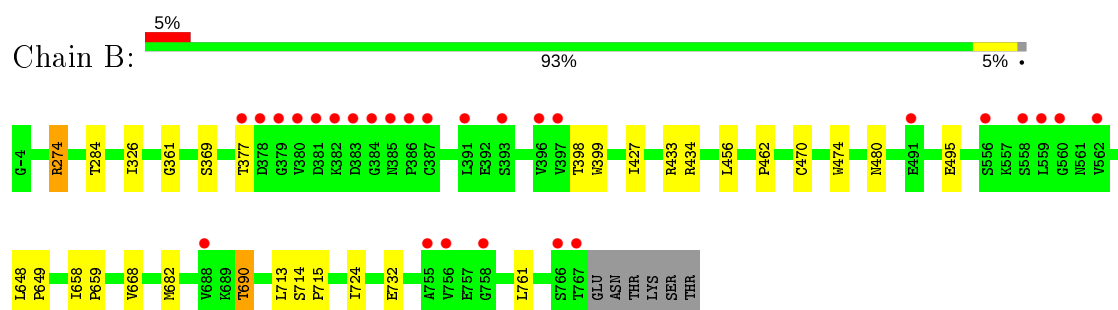
### 3 Residue-property plots

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



#### • 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, $\alpha$ , $\beta$ , $\gamma$	88.02Å 105.75Å 206.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.49 44.27 – 2.49	Depositor EDS
% Data completeness (in resolution range)	99.4 (30.00-2.49) 99.5 (44.27-2.49)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	0.16	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.41 (at 2.48Å)	Xtriage
Refinement program	REFMAC refmac_5.7.0032	Depositor
R, $R_{free}$	0.192 , 0.222 0.195 , 0.221	Depositor DCC
$R_{free}$ test set	3435 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.8	Xtriage
Anisotropy	0.516	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 33.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9063	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CAS, GOL, DMS, 44F

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	0.41	0/4340	0.59	1/5899 (0.0%)
1	B	0.41	0/4393	0.61	1/5971 (0.0%)
All	All	0.41	0/8733	0.60	2/11870 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	476	ASP	CB-CG-OD1	5.50	123.25	118.30
1	B	274	ARG	NE-CZ-NH2	-5.04	117.78	120.30

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	4240	0	4189	13	0
1	B	4288	0	4229	18	0
2	A	30	0	40	1	0
2	B	30	0	40	1	0
3	A	8	0	12	1	0
3	B	8	0	12	0	0
4	A	9	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	23	0	20	2	0
6	A	236	0	0	6	0
6	B	191	0	0	3	0
All	All	9063	0	8550	31	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 2.

All (31) 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:474:TRP:HE3	5:B:808:44F:H1	1.63	0.62
1:A:487:LEU:HD22	1:A:495:GLU:HG3	1.83	0.60
1:B:732:GLU:HG2	6:B:919:HOH:O	2.02	0.60
1:A:668:VAL:HG11	1:A:713:LEU:HG	1.84	0.57
1:B:284:THR:HG22	1:B:326:ILE:HG21	1.88	0.55
1:A:284:THR:HG22	1:A:326:ILE:HG21	1.91	0.52
1:A:456:LEU:HD21	6:A:1020:HOH:O	2.10	0.51
1:B:668:VAL:HG11	1:B:713:LEU:HG	1.92	0.51
1:B:474:TRP:CE3	5:B:808:44F:H1	2.44	0.51
1:A:597:ASN:HB3	6:A:1076:HOH:O	2.10	0.51
6:A:984:HOH:O	1:B:682:MET:HE1	2.11	0.50
1:A:515:ILE:O	1:A:544:ALA:HA	2.12	0.49
1:B:724:ILE:HD11	1:B:761:LEU:HD21	1.95	0.49
1:B:361:GLY:HA2	1:B:399:TRP:CZ3	2.48	0.49
1:B:462:PRO:HA	1:B:470:CAS:AS	2.74	0.48
1:A:338:LYS:HE3	2:A:803:GOL:C3	2.44	0.47
1:A:690:THR:CG2	6:B:1073:HOH:O	2.63	0.46
1:A:714:SER:N	1:A:715:PRO:CD	2.80	0.45
1:B:648:LEU:HB3	1:B:649:PRO:HD3	1.99	0.43
1:A:487:LEU:HD22	1:A:495:GLU:CG	2.47	0.43
1:B:274:ARG:NH2	6:B:923:HOH:O	2.52	0.43
1:A:370:PHE:HB2	3:A:806:DMS:H22	1.99	0.43
1:A:338:LYS:NZ	6:A:1055:HOH:O	2.51	0.42
1:B:714:SER:N	1:B:715:PRO:CD	2.83	0.42
1:B:434:ARG:HD2	2:B:802:GOL:O2	2.20	0.41
1:B:427:ILE:HB	1:B:433:ARG:HG3	2.03	0.41
1:B:658:ILE:N	1:B:659:PRO:HA	2.36	0.41
1:B:456:LEU:HD12	1:B:470:CAS:HB3	2.02	0.41
6:A:1136:HOH:O	1:B:690:THR:HG21	2.21	0.41
6:A:1136:HOH:O	1:B:690:THR:CG2	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:763:SER:O	1:A:765:ARG:NH1	2.53	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	527/542 (97%)	516 (98%)	11 (2%)	0	100	100
1	B	535/542 (99%)	521 (97%)	14 (3%)	0	100	100
All	All	1062/1084 (98%)	1037 (98%)	25 (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	456/468 (97%)	454 (100%)	2 (0%)	91	97
1	B	460/468 (98%)	454 (99%)	6 (1%)	69	87
All	All	916/936 (98%)	908 (99%)	8 (1%)	78	92

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	558	SER
1	A	690	THR
1	B	369	SER
1	B	377	THR
1	B	398	THR
1	B	480	ASN
1	B	495	GLU
1	B	690	THR

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

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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	0.94	0	1,9,11	0.19	0
1	CAS	A	470	1	5,8,9	0.99	0	1,9,11	0.24	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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	470	CAS	2	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

16 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	807	-	3,3,3	0.47	0	3,3,3	0.62	0
2	GOL	B	805	-	5,5,5	0.27	0	5,5,5	0.27	0
2	GOL	A	803	-	5,5,5	0.51	0	5,5,5	0.51	0
2	GOL	B	801	-	5,5,5	0.20	0	5,5,5	0.44	0
3	DMS	B	806	-	3,3,3	0.44	0	3,3,3	0.80	0
3	DMS	A	806	-	3,3,3	0.51	0	3,3,3	0.80	0
4	MET	A	808	-	4,8,8	0.57	0	2,9,9	0.33	0
2	GOL	B	802	-	5,5,5	0.36	0	5,5,5	0.38	0
2	GOL	A	802	-	5,5,5	0.39	0	5,5,5	0.39	0
2	GOL	A	805	-	5,5,5	0.38	0	5,5,5	0.16	0
2	GOL	A	801	-	5,5,5	0.30	0	5,5,5	0.26	0
5	44F	B	808	-	23,24,24	0.93	1 (4%)	24,30,30	0.60	0
2	GOL	B	804	-	5,5,5	0.22	0	5,5,5	0.52	0
2	GOL	B	803	-	5,5,5	0.39	0	5,5,5	0.19	0
2	GOL	A	804	-	5,5,5	0.30	0	5,5,5	0.16	0
3	DMS	B	807	-	3,3,3	0.49	0	3,3,3	0.56	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
2	GOL	B	805	-	-	0/4/4/4	-
2	GOL	A	803	-	-	2/4/4/4	-
2	GOL	B	801	-	-	4/4/4/4	-
5	44F	B	808	-	-	0/13/15/15	0/2/2/2
4	MET	A	808	-	-	0/4/8/8	-
2	GOL	B	802	-	-	2/4/4/4	-
2	GOL	A	802	-	-	3/4/4/4	-
2	GOL	A	805	-	-	0/4/4/4	-
2	GOL	A	801	-	-	4/4/4/4	-
2	GOL	B	804	-	-	2/4/4/4	-
2	GOL	B	803	-	-	0/4/4/4	-
2	GOL	A	804	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	808	44F	CAE-CAV	4.21	1.43	1.39

There are no bond angle outliers.

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	801	GOL	O1-C1-C2-C3
2	B	801	GOL	C1-C2-C3-O3
2	A	802	GOL	O1-C1-C2-C3
2	A	801	GOL	C1-C2-C3-O3
2	A	804	GOL	O1-C1-C2-C3
2	B	801	GOL	O1-C1-C2-O2
2	A	803	GOL	C1-C2-C3-O3
2	B	802	GOL	C1-C2-C3-O3
2	A	801	GOL	O1-C1-C2-C3
2	B	804	GOL	O1-C1-C2-C3
2	B	802	GOL	O2-C2-C3-O3
2	A	802	GOL	O1-C1-C2-O2
2	A	801	GOL	O2-C2-C3-O3

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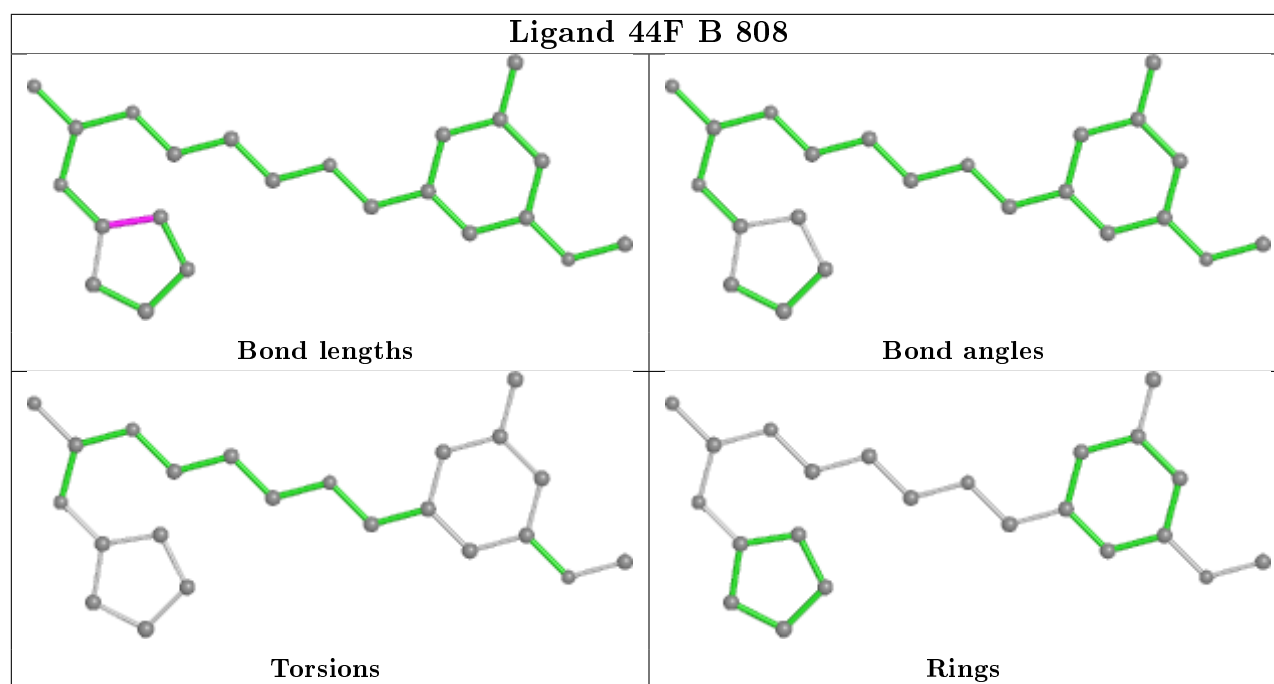
Mol	Chain	Res	Type	Atoms
2	A	804	GOL	O1-C1-C2-O2
2	B	801	GOL	O2-C2-C3-O3
2	A	803	GOL	O2-C2-C3-O3
2	B	804	GOL	O1-C1-C2-O2
2	A	802	GOL	C1-C2-C3-O3
2	A	801	GOL	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	803	GOL	1	0
3	A	806	DMS	1	0
2	B	802	GOL	1	0
5	B	808	44F	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 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	529/542 (97%)	-0.17	23 (4%) 35 38	20, 30, 69, 108	0
1	B	535/542 (98%)	-0.13	27 (5%) 28 30	19, 30, 81, 127	0
All	All	1064/1084 (98%)	-0.15	50 (4%) 31 33	19, 30, 76, 127	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	382	LYS	8.1
1	B	383	ASP	6.9
1	B	384	GLY	6.9
1	B	386	PRO	6.3
1	B	380	VAL	5.2
1	B	385	ASN	5.1
1	A	767	THR	4.7
1	A	757	GLU	4.7
1	A	558	SER	4.5
1	B	381	ASP	4.5
1	B	387	CYS	4.3
1	A	383	ASP	4.2
1	A	756	VAL	4.2
1	B	559	LEU	3.8
1	A	491	GLU	3.7
1	A	557	LYS	3.7
1	B	767	THR	3.4
1	B	391	LEU	3.3
1	B	378	ASP	3.3
1	A	552	ARG	3.3
1	B	377	THR	3.3
1	B	491	GLU	3.2
1	B	758	GLY	3.2
1	A	766	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	238	VAL	3.1
1	B	562	VAL	3.1
1	A	551	ASP	2.8
1	A	301	GLN	2.7
1	A	299	GLN	2.6
1	A	556	SER	2.6
1	B	560	GLY	2.6
1	B	397	VAL	2.5
1	A	758	GLY	2.4
1	A	382	LYS	2.4
1	A	559	LEU	2.4
1	B	396	VAL	2.4
1	B	379	GLY	2.3
1	B	558	SER	2.3
1	B	766	SER	2.3
1	B	688	VAL	2.3
1	B	756	VAL	2.3
1	A	624	VAL	2.2
1	A	384	GLY	2.2
1	A	494	LYS	2.2
1	B	556	SER	2.2
1	B	393	SER	2.2
1	A	305	TYR	2.1
1	B	755	ALA	2.1
1	A	492	SER	2.1
1	A	553	LYS	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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(Å <sup>2</sup> )	Q<0.9
1	CAS	B	470	9/10	0.95	0.13	26,28,29,29	3
1	CAS	A	470	9/10	0.98	0.10	26,28,29,29	3

## 6.3 Carbohydrates [i](#)

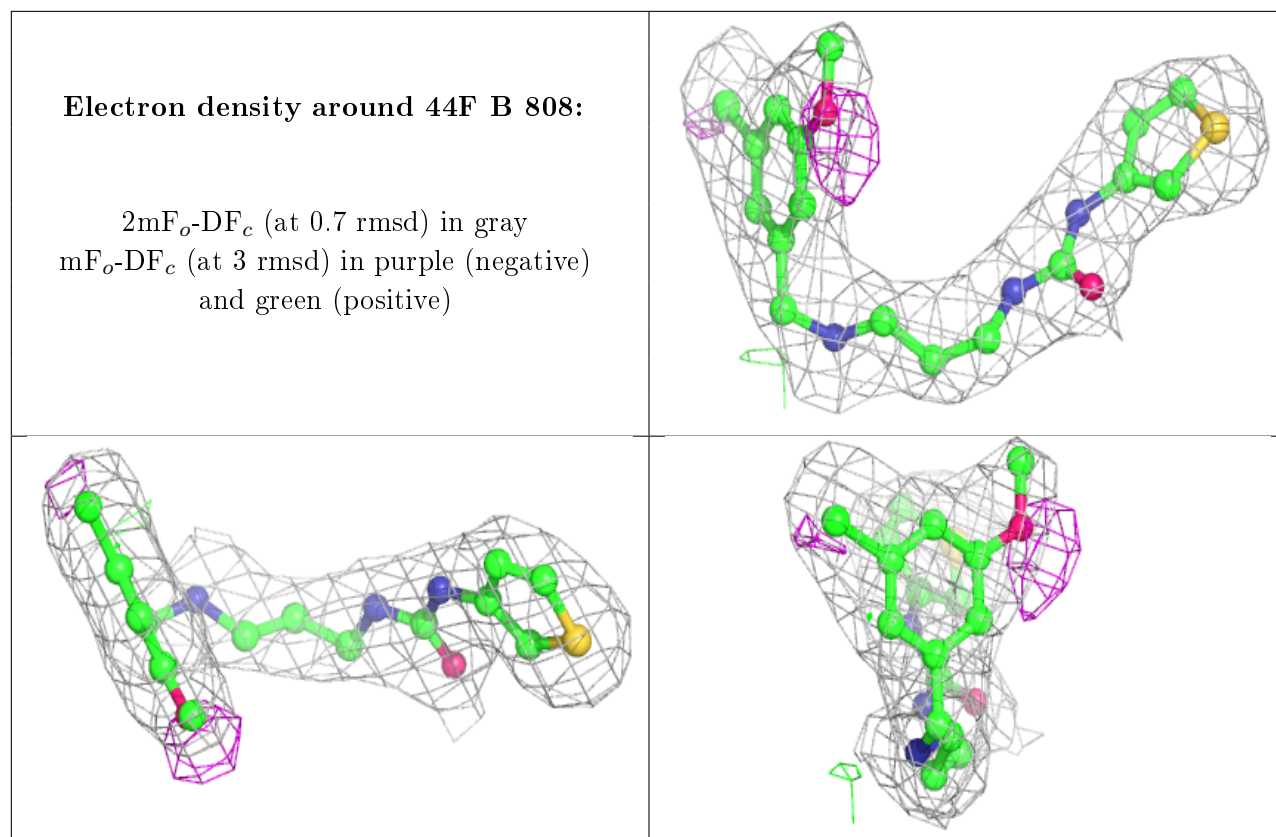
There are no monosaccharides in this entry.

## 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<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(Å <sup>2</sup> )	Q<0.9
2	GOL	A	805	6/6	0.78	0.23	55,59,59,59	0
3	DMS	A	806	4/4	0.81	0.26	65,71,73,78	0
2	GOL	B	805	6/6	0.82	0.21	60,67,67,68	0
2	GOL	B	801	6/6	0.82	0.26	49,52,55,57	0
2	GOL	B	802	6/6	0.84	0.25	47,52,52,53	0
2	GOL	A	803	6/6	0.84	0.27	55,58,62,65	0
3	DMS	B	807	4/4	0.84	0.32	84,89,93,94	0
3	DMS	A	807	4/4	0.86	0.26	82,84,86,90	0
2	GOL	A	801	6/6	0.87	0.23	46,48,50,51	0
2	GOL	A	804	6/6	0.87	0.16	56,60,64,65	0
2	GOL	B	803	6/6	0.89	0.23	49,54,55,60	0
2	GOL	A	802	6/6	0.92	0.16	41,43,44,45	0
3	DMS	B	806	4/4	0.92	0.20	57,64,67,69	0
2	GOL	B	804	6/6	0.95	0.16	41,43,45,45	0
5	44F	B	808	23/23	0.97	0.14	26,28,31,40	0
4	MET	A	808	9/9	0.98	0.16	21,21,22,23	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.