



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 03:33 pm GMT

PDB ID : 4MWC  
Title : Trypanosoma brucei methionyl-tRNA synthetase in complex with inhibitor 1-(3-[[[(2-methyl-1-benzothiophen-3-yl)methyl]amino]propyl]-3-thiophen-3-yl]urea (Chem 1540)  
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 : 2.65 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

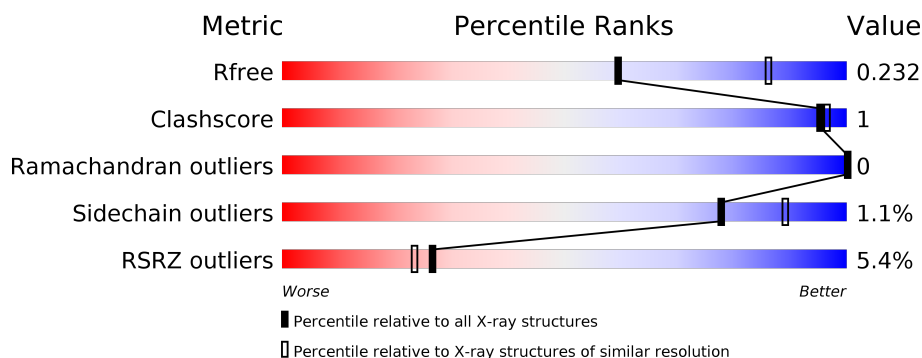
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 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))
$R_{free}$	100719	1044 (2.66-2.62)
Clashscore	112137	1092 (2.66-2.62)
Ramachandran outliers	110173	1077 (2.66-2.62)
Sidechain outliers	110143	1077 (2.66-2.62)
RSRZ outliers	101464	1047 (2.66-2.62)

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. 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>93%</div> <div>5%</div> </div> </div>
1	B	542	<div> <div>6%</div> <div> <div></div> <div>93%</div> <div>5%</div> </div> </div>

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
2	GOL	A	802	-	-	-	X
2	GOL	B	802	-	-	-	X
3	DMS	A	805	-	-	-	X
4	SO4	A	806	-	-	-	X
4	SO4	B	804	-	-	-	X
4	SO4	B	805	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8928 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	531	Total	As	C	N	O	S	0	0	0
			4249	1	2735	717	785	11			
1	B	533	Total	As	C	N	O	S	0	1	0
			4260	1	2744	721	782	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>).



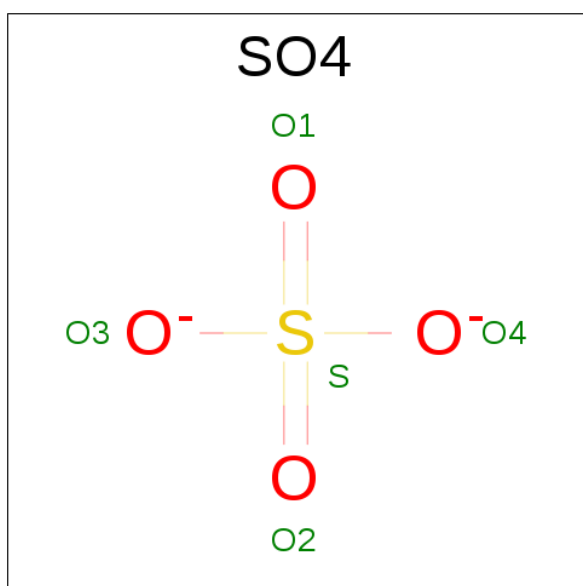
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		

- 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	B	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



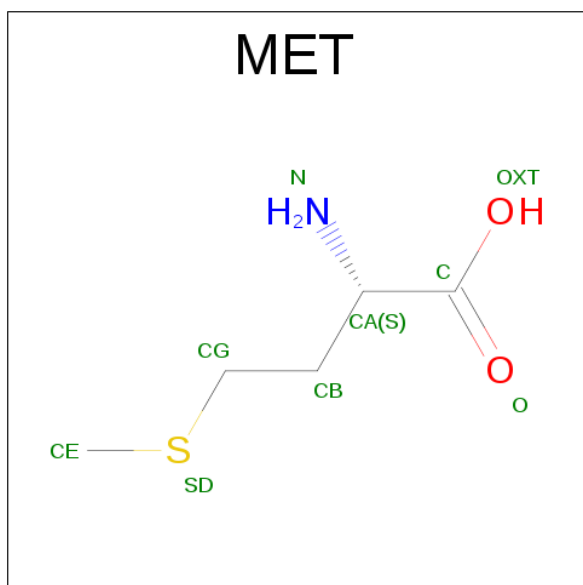
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

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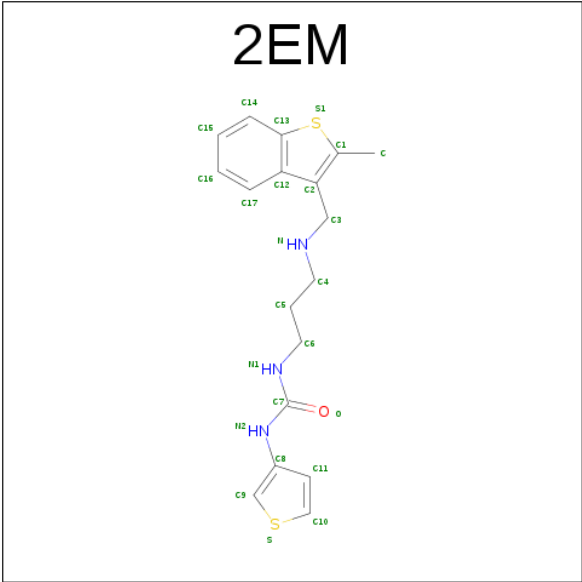
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is METHIONINE (three-letter code: MET) (formula:  $C_5H_{11}NO_2S$ ).



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

- Molecule 6 is 1-(3-[(2-METHYL-1-BENZOTHIOPHEN-3-YL)METHYL]AMINO}PROPYL)-3-THIOPHEN-3-YLUREA (three-letter code: 2EM) (formula:  $C_{18}H_{21}N_3OS_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	S	0	0
			24	18	3	1	2		

- Molecule 7 is water.

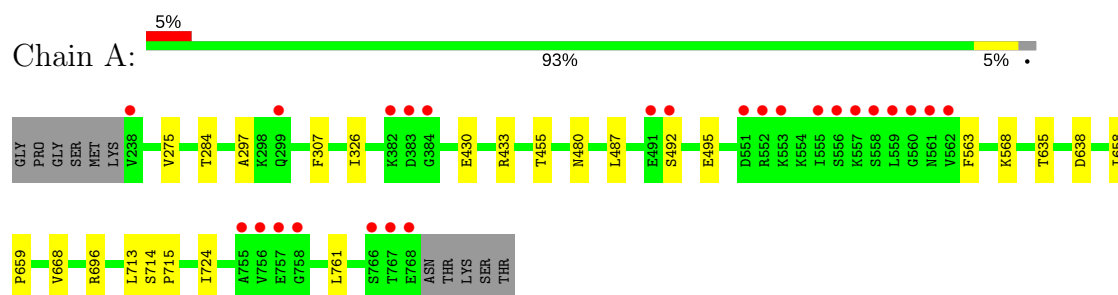
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	171	Total	O	0	0
			171	171		
7	B	151	Total	O	0	0
			151	151		



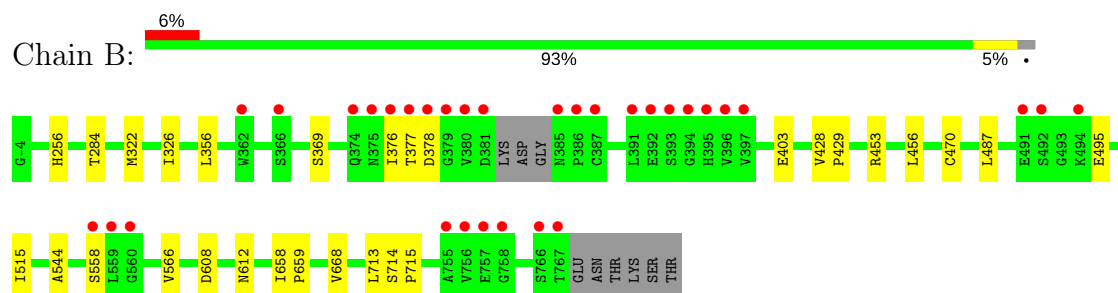
### 3 Residue-property plots [i](#)

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, $\alpha$ , $\beta$ , $\gamma$	87.74Å 105.74Å 206.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.55 – 2.65 29.54 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.3 (29.55-2.65) 99.4 (29.54-2.65)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.37 (at 2.64Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.215 , 0.255 0.196 , 0.232	Depositor DCC
$R_{free}$ test set	2858 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.2	Xtriage
Anisotropy	0.542	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 36.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8928	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% 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, SO4, 2EM

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	0/4349	0.59	1/5911 (0.0%)
1	B	0.41	0/4364	0.60	0/5930
All	All	0.41	0/8713	0.60	1/11841 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	696	ARG	NE-CZ-NH1	5.14	122.87	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	4249	0	4195	10	0
1	B	4260	0	4214	14	0
2	A	24	0	32	0	0
2	B	12	0	16	0	0
3	A	4	0	6	0	0
3	B	4	0	6	0	0
4	A	10	0	0	0	0
4	B	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	9	0	8	0	0
6	B	24	0	21	0	0
7	A	171	0	0	0	0
7	B	151	0	0	0	0
All	All	8928	0	8498	24	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 (24) 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:A:668:VAL:HG11	1:A:713:LEU:HG	1.78	0.66
1:B:487:LEU:HD22	1:B:495:GLU:HG3	1.82	0.61
1:A:284:THR:HG22	1:A:326:ILE:HG21	1.88	0.55
1:B:284:THR:HG22	1:B:326:ILE:HG21	1.89	0.54
1:A:487:LEU:HD22	1:A:495:GLU:HG3	1.91	0.53
1:A:563:PHE:CE1	1:A:568:LYS:HG3	2.45	0.51
1:B:453:ARG:HA	1:B:470:CAS:SG	2.52	0.49
1:B:322:MET:HE3	1:B:566:VAL:HG22	1.97	0.47
1:B:487:LEU:HD22	1:B:495:GLU:CG	2.45	0.46
1:B:658:ILE:N	1:B:659:PRO:HA	2.30	0.46
1:B:456:LEU:HD12	1:B:470:CAS:HB3	1.96	0.46
1:B:668:VAL:HG11	1:B:713:LEU:HG	1.97	0.46
1:B:714:SER:N	1:B:715:PRO:CD	2.79	0.46
1:A:635:THR:O	1:A:638:ASP:HB2	2.16	0.46
1:B:515:ILE:O	1:B:544:ALA:HA	2.15	0.46
1:A:658:ILE:N	1:A:659:PRO:HA	2.31	0.45
1:B:356:LEU:HD11	1:B:403:GLU:HB3	2.00	0.44
1:A:297:ALA:HB2	1:A:307:PHE:CD2	2.53	0.43
1:A:724:ILE:HG12	1:A:761:LEU:HD11	2.00	0.43
1:A:714:SER:N	1:A:715:PRO:CD	2.81	0.43
1:B:428:VAL:HG13	1:B:429:PRO:HA	2.00	0.42
1:A:430:GLU:OE2	1:A:433:ARG:NH1	2.54	0.41
1:B:456:LEU:HD12	1:B:470:CAS:CB	2.51	0.41
1:B:608:ASP:O	1:B:612:ASN:HB3	2.20	0.40

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	528/542 (97%)	518 (98%)	10 (2%)	0	100	100
1	B	529/542 (98%)	515 (97%)	14 (3%)	0	100	100
All	All	1057/1084 (98%)	1033 (98%)	24 (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	457/468 (98%)	453 (99%)	4 (1%)	82	91
1	B	458/468 (98%)	452 (99%)	6 (1%)	73	87
All	All	915/936 (98%)	905 (99%)	10 (1%)	78	89

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	275	VAL
1	A	455	THR
1	A	480	ASN
1	A	492	SER
1	B	256	HIS
1	B	369	SER
1	B	376	ILE
1	B	377	THR

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Mol	Chain	Res	Type
1	B	378	ASP
1	B	558	SER

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	A	470	1	6,8,9	0.94	0	2,9,11	1.21	0
1	CAS	B	470	1	6,8,9	0.97	0	2,9,11	1.01	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	A	470	1	-	0/0/7/9	0/0/0/0
1	CAS	B	470	1	-	0/0/7/9	0/0/0/0

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 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	470	CAS	3	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

14 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	$\# Z  > 2$
2	GOL	A	801	-	5,5,5	0.24	0	5,5,5	0.55	0
2	GOL	A	802	-	5,5,5	0.23	0	5,5,5	0.30	0
2	GOL	A	803	-	5,5,5	0.23	0	5,5,5	0.33	0
2	GOL	A	804	-	5,5,5	0.63	0	5,5,5	0.59	0
3	DMS	A	805	-	3,3,3	0.42	0	3,3,3	0.87	0
4	SO4	A	806	-	4,4,4	0.49	0	6,6,6	0.27	0
4	SO4	A	807	-	4,4,4	0.48	0	6,6,6	0.22	0
5	MET	A	808	-	3,8,8	0.31	0	3,9,9	0.82	0
2	GOL	B	801	-	5,5,5	0.24	0	5,5,5	0.65	0
2	GOL	B	802	-	5,5,5	0.21	0	5,5,5	0.29	0
3	DMS	B	803	-	3,3,3	0.47	0	3,3,3	0.60	0
4	SO4	B	804	-	4,4,4	0.43	0	6,6,6	0.35	0
4	SO4	B	805	-	4,4,4	0.52	0	6,6,6	0.29	0
6	2EM	B	806	-	19,26,26	1.18	1 (5%)	17,34,34	0.98	2 (11%)

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	A	801	-	-	0/4/4/4	0/0/0/0
2	GOL	A	802	-	-	0/4/4/4	0/0/0/0
2	GOL	A	803	-	-	0/4/4/4	0/0/0/0
2	GOL	A	804	-	-	0/4/4/4	0/0/0/0
3	DMS	A	805	-	-	0/0/0/0	0/0/0/0
4	SO4	A	806	-	-	0/0/0/0	0/0/0/0
4	SO4	A	807	-	-	0/0/0/0	0/0/0/0
5	MET	A	808	-	-	0/4/8/8	0/0/0/0
2	GOL	B	801	-	-	0/4/4/4	0/0/0/0
2	GOL	B	802	-	-	0/4/4/4	0/0/0/0
3	DMS	B	803	-	-	0/0/0/0	0/0/0/0
4	SO4	B	804	-	-	0/0/0/0	0/0/0/0
4	SO4	B	805	-	-	0/0/0/0	0/0/0/0
6	2EM	B	806	-	-	0/9/13/13	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	806	2EM	C11-C8	4.52	1.43	1.39

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	806	2EM	C3-C2-C1	-2.06	123.29	127.66
6	B	806	2EM	C2-C3-N	2.49	116.23	111.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	530/542 (97%)	-0.32	25 (4%)	32 28	19, 31, 76, 117	0
1	B	532/542 (98%)	-0.26	32 (6%)	23 19	20, 32, 82, 131	0
All	All	1062/1084 (97%)	-0.29	57 (5%)	26 23	19, 32, 80, 131	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	380	VAL	5.8
1	A	768	GLU	5.5
1	A	558	SER	5.3
1	A	556	SER	5.1
1	B	385	ASN	4.9
1	A	552	ARG	4.7
1	B	391	LEU	4.7
1	A	767	THR	4.7
1	B	386	PRO	4.5
1	B	756	VAL	4.3
1	A	559	LEU	4.2
1	B	559	LEU	4.2
1	B	387	CYS	4.1
1	A	557	LYS	4.0
1	B	767	THR	4.0
1	A	756	VAL	3.9
1	B	757	GLU	3.8
1	A	757	GLU	3.8
1	B	758	GLY	3.8
1	B	377	THR	3.7
1	B	379	GLY	3.6
1	B	375	ASN	3.6
1	A	384	GLY	3.5
1	B	381	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	383	ASP	3.3
1	A	491	GLU	3.2
1	B	558	SER	3.2
1	B	395	HIS	3.2
1	B	374	GLN	3.1
1	A	766	SER	3.0
1	B	394	GLY	2.9
1	A	561	ASN	2.9
1	B	755	ALA	2.8
1	B	376	ILE	2.7
1	A	492	SER	2.7
1	B	491	GLU	2.6
1	A	758	GLY	2.6
1	B	397	VAL	2.6
1	A	238	VAL	2.6
1	A	560	GLY	2.5
1	B	766	SER	2.5
1	B	396	VAL	2.4
1	B	393	SER	2.4
1	A	551	ASP	2.4
1	A	562	VAL	2.4
1	B	560	GLY	2.4
1	A	299	GLN	2.3
1	B	392	GLU	2.3
1	B	492	SER	2.3
1	B	366	SER	2.3
1	B	378	ASP	2.2
1	B	494	LYS	2.2
1	B	362	TRP	2.2
1	A	555	ILE	2.1
1	A	755	ALA	2.1
1	A	382	LYS	2.0
1	A	553	LYS	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	CAS	A	470	9/10	0.97	0.12	-	27,30,47,48	3
1	CAS	B	470	9/10	0.95	0.14	-	30,33,45,46	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SO4	B	805	5/5	0.91	0.45	12.37	59,63,65,69	0
2	GOL	A	802	6/6	0.85	0.28	6.72	59,59,60,62	0
2	GOL	B	802	6/6	0.78	0.33	6.28	46,49,51,51	0
3	DMS	A	805	4/4	0.83	0.25	5.48	69,69,74,76	0
4	SO4	B	804	5/5	0.95	0.24	4.84	59,61,67,68	0
4	SO4	A	806	5/5	0.93	0.24	3.69	64,64,70,72	0
3	DMS	B	803	4/4	0.89	0.21	1.39	84,87,89,92	0
5	MET	A	808	9/9	0.97	0.14	-0.33	21,23,23,23	0
6	2EM	B	806	24/24	0.98	0.14	-0.41	23,26,28,28	0
2	GOL	A	804	6/6	0.78	0.25	-	50,54,57,57	0
2	GOL	A	801	6/6	0.89	0.17	-	43,43,45,45	0
2	GOL	B	801	6/6	0.88	0.15	-	42,43,44,45	0
4	SO4	A	807	5/5	0.91	0.35	-	64,72,75,75	0
2	GOL	A	803	6/6	0.90	0.28	-	52,56,57,59	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.