



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 9, 2017 – 10:54 am GMT

PDB ID : 5J59  
Title : Trypanosoma brucei methionyl-tRNA synthetase in complex with inhibitor (Chem 1893)  
Authors : Barros-Alvarez, X.; Hol, W.G.J.  
Deposited on : 2016-04-01  
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

<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 : recalc28906  
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) : recalc28906

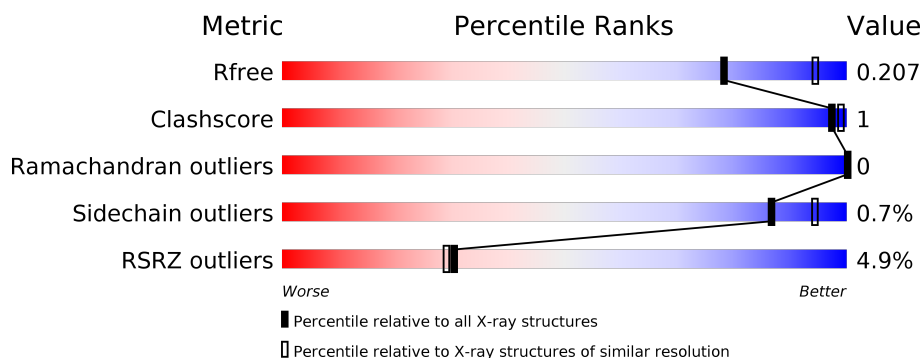
# 1 Overall quality at a glance

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))
$R_{free}$	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (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. 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> <div></div> <div>93%</div> <div>5%</div> </div> </div>
1	B	542	<div> <div>6%</div> <div> <div></div> <div>95%</div> <div></div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8815 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

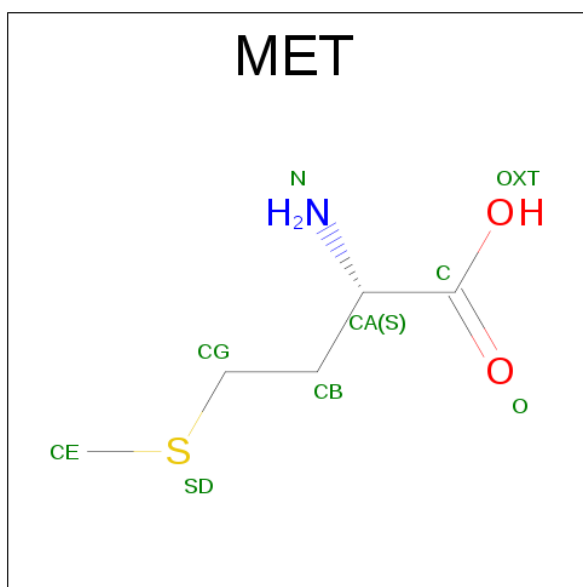
- Molecule 1 is a protein called Methionyl-tRNA synthetase, putative.

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

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	232	GLY	-	expression tag	UNP Q38C91
A	233	PRO	-	expression tag	UNP Q38C91
A	234	GLY	-	expression tag	UNP Q38C91
A	235	SER	-	expression tag	UNP Q38C91
A	236	MET	-	expression tag	UNP Q38C91
A	309	THR	ALA	engineered mutation	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	engineered mutation	UNP Q38C91
A	503	ASN	SER	engineered mutation	UNP Q38C91
B	232	GLY	-	expression tag	UNP Q38C91
B	233	PRO	-	expression tag	UNP Q38C91
B	234	GLY	-	expression tag	UNP Q38C91
B	235	SER	-	expression tag	UNP Q38C91
B	236	MET	-	expression tag	UNP Q38C91
B	309	THR	ALA	engineered mutation	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	engineered mutation	UNP Q38C91
B	503	ASN	SER	engineered mutation	UNP Q38C91

- Molecule 2 is METHIONINE (three-letter code: MET) (formula: C<sub>5</sub>H<sub>11</sub>NO<sub>2</sub>S).



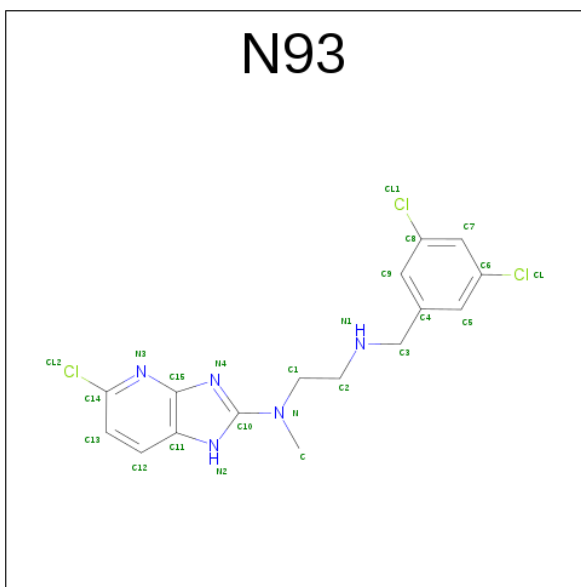
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			9	5	1	2	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 4 is 5-chloro-N-(2-([(3,5-dichlorophenyl)methyl]amino)ethyl)-N-methyl-3H-imidazo[4,5-b]pyridin-2-amine (three-letter code: N93) (formula:  $C_{16}H_{16}Cl_3N_5$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	Cl	N	0	0
			24	16	3	5		

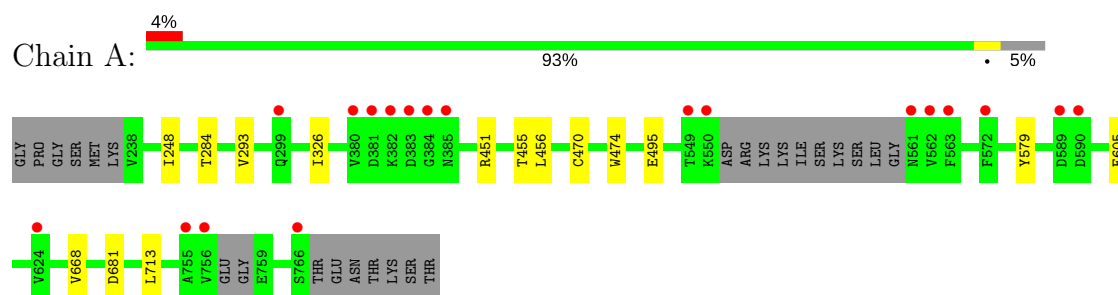
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	217	Total	O	0	0
			217	217		
5	B	242	Total	O	0	0
			242	242		

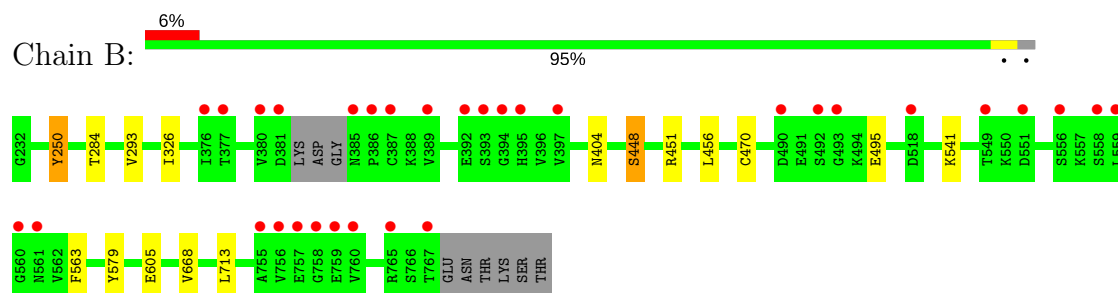
### 3 Residue-property plots [i](#)

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, putative



- Molecule 1: Methionyl-tRNA synthetase, putative



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.31Å 106.40Å 207.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	103.96 – 2.40 40.25 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.6 (103.96-2.40) 98.6 (40.25-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.28 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.192 , 0.207 0.193 , 0.207	Depositor DCC
$R_{free}$ test set	3708 reflections (5.17%)	DCC
Wilson B-factor (Å <sup>2</sup> )	41.5	Xtriage
Anisotropy	0.443	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 34.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8815	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% 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: GOL, N93

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	0/4225	0.65	0/5752
1	B	0.42	0/4314	0.64	1/5875 (0.0%)
All	All	0.42	0/8539	0.64	1/11627 (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	B	563	PHE	CB-CG-CD1	5.17	124.42	120.80

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4113	0	4028	10	0
1	B	4204	0	4093	7	0
2	A	9	0	8	2	0
3	B	6	0	8	0	0
4	B	24	0	0	0	0
5	A	217	0	0	3	0
5	B	242	0	0	1	0
All	All	8815	0	8137	17	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 (17) 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:470:CYS:SG	5:A:1060:HOH:O	2.44	0.76
1:B:284:THR:HG22	1:B:326:ILE:HG21	1.82	0.61
1:B:250:TYR:CZ	1:B:293:VAL:HG23	2.38	0.59
1:A:284:THR:HG22	1:A:326:ILE:HG21	1.84	0.58
1:B:668:VAL:HG11	1:B:713:LEU:HG	1.94	0.50
1:A:668:VAL:HG11	1:A:713:LEU:HG	1.93	0.49
1:A:451:ARG:NH2	1:A:455:THR:HG21	2.31	0.46
1:A:293:VAL:HG13	5:A:971:HOH:O	2.17	0.44
1:B:579:TYR:OH	1:B:605:GLU:OE1	2.26	0.43
1:A:456:LEU:HD12	1:A:470:CYS:HB2	1.99	0.43
1:A:474:TRP:CZ3	2:A:800:MET:HG2	2.54	0.43
1:B:541:LYS:NZ	5:B:903:HOH:O	2.45	0.42
1:A:579:TYR:OH	1:A:605:GLU:OE2	2.26	0.41
1:A:248:ILE:O	2:A:800:MET:HB2	2.20	0.41
1:B:456:LEU:HD12	1:B:470:CYS:HB2	2.03	0.41
1:A:293:VAL:HG22	5:A:971:HOH:O	2.21	0.41
1:B:448:SER:OG	1:B:451:ARG:NH1	2.54	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	512/542 (94%)	505 (99%)	7 (1%)	0	100	100
1	B	530/542 (98%)	522 (98%)	8 (2%)	0	100	100
All	All	1042/1084 (96%)	1027 (99%)	15 (1%)	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	439/469 (94%)	437 (100%)	2 (0%)	91	96
1	B	445/469 (95%)	441 (99%)	4 (1%)	82	92
All	All	884/938 (94%)	878 (99%)	6 (1%)	87	94

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	495	GLU
1	A	681	ASP
1	B	250	TYR
1	B	404	ASN
1	B	448	SER
1	B	495	GLU

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](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	MET	A	800	-	3,8,8	0.16	0	3,9,9	0.24	0
3	GOL	B	801	-	5,5,5	0.20	0	5,5,5	0.40	0
4	N93	B	802	-	26,26,26	1.09	2 (7%)	27,36,36	0.87	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
2	MET	A	800	-	-	0/4/8/8	0/0/0/0
3	GOL	B	801	-	-	0/4/4/4	0/0/0/0
4	N93	B	802	-	-	0/7/11/11	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	802	N93	C11-C15	-3.33	1.33	1.40
4	B	802	N93	C10-N2	-2.20	1.31	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	802	N93	C11-C15-N4	-2.61	105.96	109.11

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
2	A	800	MET	2	0

## 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	517/542 (95%)	-0.05	19 (3%) 42 41	31, 45, 86, 118	0
1	B	533/542 (98%)	0.03	32 (6%) 23 21	31, 45, 81, 126	0
All	All	1050/1084 (96%)	-0.01	51 (4%) 30 29	31, 45, 82, 126	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	380	VAL	6.8
1	B	758	GLY	5.8
1	B	757	GLU	5.2
1	A	562	VAL	4.8
1	A	382	LYS	4.7
1	B	767	THR	4.6
1	B	560	GLY	4.3
1	A	383	ASP	4.3
1	B	558	SER	4.2
1	A	381	ASP	4.0
1	B	492	SER	4.0
1	A	549	THR	3.9
1	A	766	SER	3.9
1	B	377	THR	3.9
1	B	385	ASN	3.8
1	B	376	ILE	3.8
1	B	386	PRO	3.7
1	B	559	LEU	3.6
1	A	756	VAL	3.6
1	B	381	ASP	3.5
1	A	561	ASN	3.5
1	A	380	VAL	3.5
1	A	755	ALA	3.4
1	A	384	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	756	VAL	3.4
1	B	755	ALA	3.3
1	A	563	PHE	3.1
1	B	387	CYS	3.0
1	B	556	SER	2.9
1	A	299	GLN	2.7
1	B	493	GLY	2.7
1	A	590	ASP	2.6
1	B	518	ASP	2.5
1	B	393	SER	2.4
1	B	765	ARG	2.3
1	B	490	ASP	2.3
1	B	392	GLU	2.3
1	B	549	THR	2.3
1	B	394	GLY	2.2
1	B	561	ASN	2.2
1	B	760	VAL	2.2
1	A	572	PHE	2.2
1	B	389	VAL	2.1
1	B	397	VAL	2.1
1	B	551	ASP	2.1
1	B	395	HIS	2.1
1	B	759	GLU	2.1
1	A	550	LYS	2.0
1	A	624	VAL	2.0
1	A	385	ASN	2.0
1	A	589	ASP	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no 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(Å <sup>2</sup> )	Q<0.9
2	MET	A	800	9/9	0.96	0.19	-0.25	38,40,46,47	0
4	N93	B	802	24/24	0.96	0.12	-0.97	37,42,62,69	0
3	GOL	B	801	6/6	0.89	0.14	-	68,69,71,71	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.