



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 4, 2016 – 06:23 AM EDT

PDB ID : 4ZT6  
Title : Trypanosoma brucei methionyl-tRNA synthetase in complex with inhibitor N-[(4R)-6,8-dichloro-3,4-dihydro-2H-chromen-4-yl]-N'-(5-fluoro-1H-imidazo[4,5-b]pyridin-2-yl)propane-1,3-diamine (Chem 1709)  
Authors : Koh, C.-Y.; Hol, W.G.J.  
Deposited on : 2015-05-14  
Resolution : 2.25 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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027939  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : rb-20027939

i

## X-RAY DIFFRACTION

A.

 $R_{free}$ 1

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8997 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.

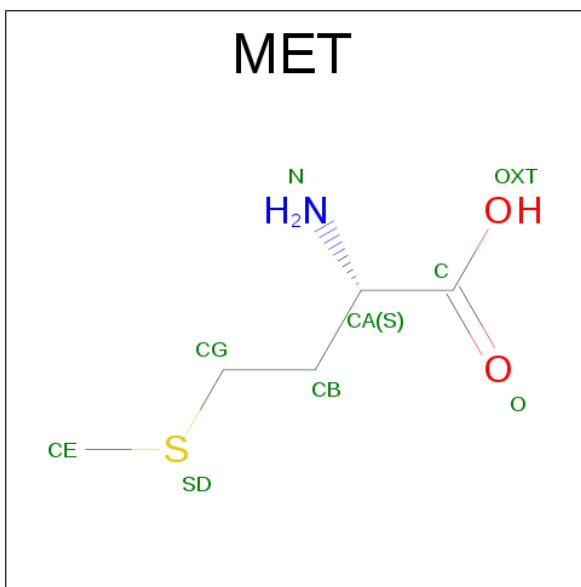
- Molecule 1 is a protein called Methionyl-tRNA synthetase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	526	Total	As	C	N	O	S	0	0	0
			4159	1	2678	697	772	11			
1	B	528	Total	As	C	N	O	S	0	0	0
			4170	1	2690	703	765	11			

There are 22 discrepancies between the modelled and reference sequences:

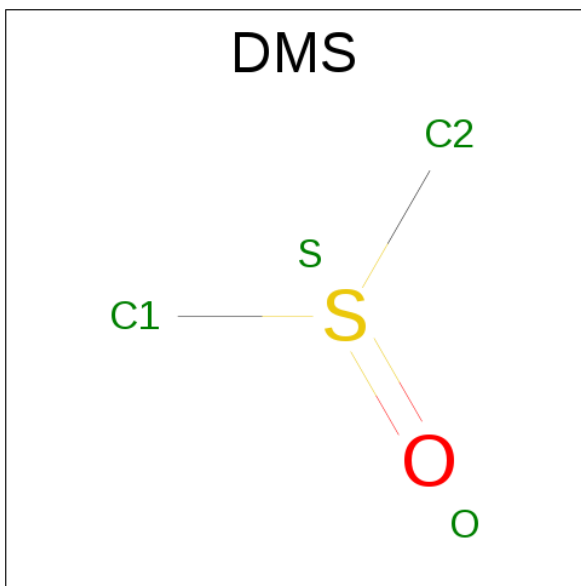
Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP Q38C91
A	-3	PRO	-	expression tag	UNP Q38C91
A	-2	GLY	-	expression tag	UNP Q38C91
A	-1	SER	-	expression tag	UNP Q38C91
A	0	MET	-	expression tag	UNP Q38C91
A	309	THR	ALA	conflict	UNP Q38C91
A	452	ALA	LYS	engineered mutation	UNP 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).



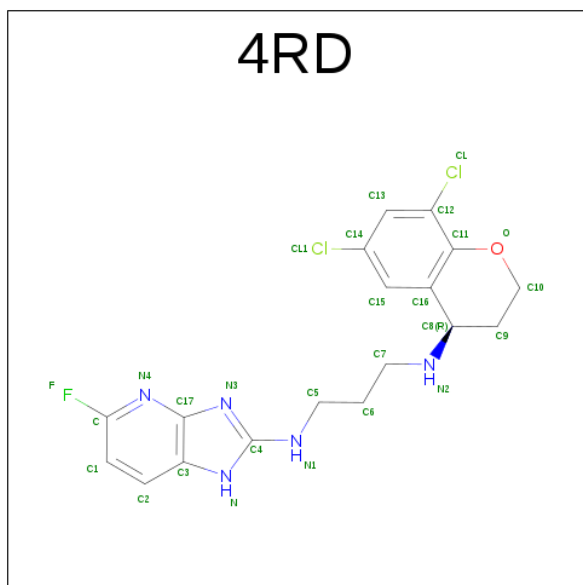
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	A	1	Total	C	O	S	0	0
			4	2	1	1		

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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-3,4-dihydro-2H-chromen-4-yl]-N'-(5-fluoro-1H-imidazo[4,5-b]pyridin-2-yl)propane-1,3-diamine (three-letter code: 4RD) (formula: C<sub>18</sub>H<sub>18</sub>Cl<sub>2</sub>FN<sub>5</sub>O).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	B	1	Total	C	Cl	F	N	O	0	0
			27	18	2	1	5	1		

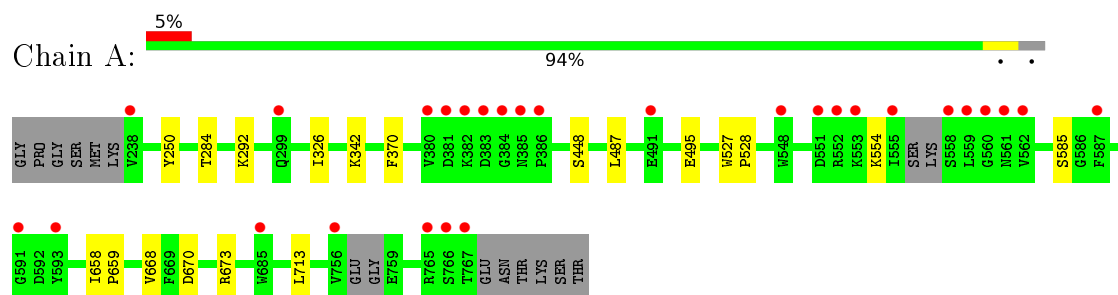
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	298	Total	O	0	0
			298	298		
5	B	318	Total	O	0	0
			318	318		

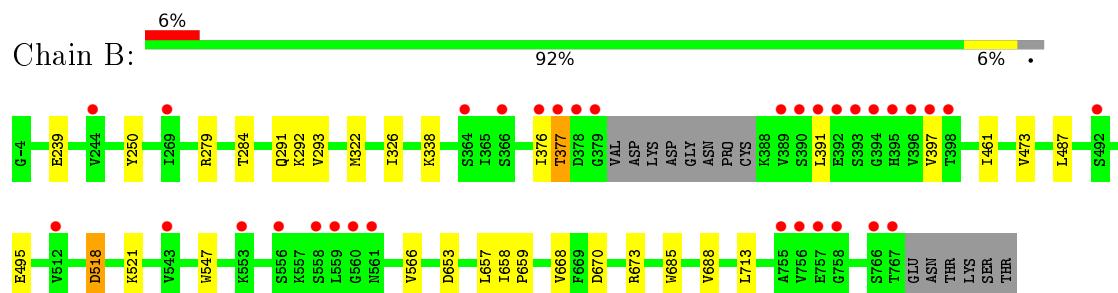
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ( $\text{RSRZ} > 2$ ). 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, $\alpha$ , $\beta$ , $\gamma$	87.08Å 106.23Å 206.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.87 – 2.25 37.87 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.5 (37.87-2.25) 99.6 (37.87-2.25)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.40 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.208 , 0.233 0.211 , 0.234	Depositor DCC
$R_{free}$ test set	4584 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.2	Xtriage
Anisotropy	0.560	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 41.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8997	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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, DMS, 4RD

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	0.38	0/4257	0.58	0/5798
1	B	0.40	0/4269	0.59	0/5808
All	All	0.39	0/8526	0.58	0/11606

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	4159	0	4035	11	0
1	B	4170	0	4090	21	0
2	A	9	0	8	0	0
3	A	12	0	18	0	0
3	B	4	0	6	0	0
4	B	27	0	0	1	0
5	A	298	0	0	2	0
5	B	318	0	0	2	0
All	All	8997	0	8157	32	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 (32) 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:487:LEU:HD22	1:A:495:GLU:HG3	1.71	0.73
1:B:487:LEU:HD22	1:B:495:GLU:HG3	1.72	0.71
1:B:284:THR:HG22	1:B:326:ILE:HG21	1.81	0.62
1:A:585:SER:HB3	5:A:1096:HOH:O	2.00	0.61
1:B:685:TRP:O	1:B:688:VAL:HG22	2.01	0.60
1:A:284:THR:HG22	1:A:326:ILE:HG21	1.85	0.57
1:B:322:MET:CE	1:B:566:VAL:HA	2.35	0.57
1:B:338:LYS:HG2	1:B:461:ILE:HG12	1.85	0.57
1:A:668:VAL:HG11	1:A:713:LEU:HG	1.86	0.56
1:B:668:VAL:HG11	1:B:713:LEU:HG	1.88	0.56
1:A:487:LEU:HD22	1:A:495:GLU:CG	2.38	0.54
1:A:342:LYS:HE2	5:A:1127:HOH:O	2.08	0.52
1:B:376:ILE:HG13	1:B:397:VAL:HG21	1.92	0.51
1:A:658:ILE:N	1:A:659:PRO:HA	2.26	0.50
1:B:473:VAL:HG23	4:B:802:4RD:N	2.27	0.49
1:B:487:LEU:HD22	1:B:495:GLU:CG	2.39	0.49
1:B:291:GLN:NE2	5:B:904:HOH:O	2.46	0.48
1:B:653:ASP:O	1:B:657:LEU:HD13	2.14	0.48
1:B:658:ILE:N	1:B:659:PRO:HA	2.29	0.48
1:B:322:MET:HE1	1:B:566:VAL:HA	1.96	0.47
1:B:322:MET:HE2	1:B:566:VAL:HG22	1.96	0.47
1:B:250:TYR:CZ	1:B:293:VAL:HG23	2.49	0.47
1:B:322:MET:CE	1:B:566:VAL:HG22	2.48	0.44
1:A:250:TYR:CD2	1:A:292:LYS:HE2	2.53	0.44
1:B:239:GLU:O	1:B:279:ARG:NH2	2.49	0.43
1:B:670:ASP:OD1	1:B:673:ARG:NH2	2.50	0.43
1:B:377:THR:OG1	1:B:391:LEU:HG	2.19	0.42
1:A:370:PHE:CZ	1:A:448:SER:HB3	2.55	0.42
1:A:527:TRP:HB3	1:A:528:PRO:CD	2.50	0.42
1:A:670:ASP:OD1	1:A:673:ARG:NH2	2.50	0.42
1:B:518:ASP:HB2	1:B:547:TRP:HZ2	1.85	0.41
1:B:292:LYS:NZ	5:B:905:HOH:O	2.47	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	519/542 (96%)	511 (98%)	8 (2%)	0	100	100
1	B	523/542 (96%)	514 (98%)	9 (2%)	0	100	100
All	All	1042/1084 (96%)	1025 (98%)	17 (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	440/468 (94%)	439 (100%)	1 (0%)	95	98
1	B	441/468 (94%)	438 (99%)	3 (1%)	88	93
All	All	881/936 (94%)	877 (100%)	4 (0%)	92	95

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	554	LYS
1	B	377	THR
1	B	518	ASP
1	B	521	LYS

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	4,8,9	0.97	0	2,9,11	1.38	0
1	CAS	B	470	1	4,8,9	0.81	0	2,9,11	1.09	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.

No monomer is involved in short contacts.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

6 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	801	-	5,8,8	0.23	0	3,9,9	0.27	0
3	DMS	A	802	-	3,3,3	0.48	0	3,3,3	0.57	0
3	DMS	A	803	-	3,3,3	0.55	0	3,3,3	0.26	0
3	DMS	A	804	-	3,3,3	0.48	0	3,3,3	0.57	0
3	DMS	B	801	-	3,3,3	0.44	0	3,3,3	0.63	0
4	4RD	B	802	-	30,30,30	0.89	1 (3%)	29,42,42	1.10	3 (10%)

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	801	-	-	0/4/8/8	0/0/0/0
3	DMS	A	802	-	-	0/0/0/0	0/0/0/0
3	DMS	A	803	-	-	0/0/0/0	0/0/0/0
3	DMS	A	804	-	-	0/0/0/0	0/0/0/0
3	DMS	B	801	-	-	0/0/0/0	0/0/0/0
4	4RD	B	802	-	-	0/6/18/18	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	802	4RD	C-N4	3.62	1.38	1.32

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	802	4RD	C4-N-C3	-2.47	103.15	106.64
4	B	802	4RD	C10-O-C11	2.48	120.92	114.10
4	B	802	4RD	C7-N2-C8	2.64	117.91	113.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	802	4RD	1	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	525/542 (96%)	0.01	28 (5%)	30 33	24, 38, 82, 117	0
1	B	527/542 (97%)	0.04	33 (6%)	23 25	25, 38, 77, 114	0
All	All	1052/1084 (97%)	0.03	61 (5%)	26 29	24, 38, 80, 117	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	383	ASP	7.3
1	B	377	THR	6.5
1	A	766	SER	6.1
1	A	756	VAL	5.8
1	A	767	THR	5.7
1	A	562	VAL	5.6
1	B	767	THR	5.2
1	B	396	VAL	4.9
1	A	593	TYR	4.3
1	B	391	LEU	4.2
1	B	394	GLY	4.2
1	A	382	LYS	4.0
1	B	559	LEU	4.0
1	A	551	ASP	4.0
1	B	558	SER	3.9
1	B	379	GLY	3.6
1	A	560	GLY	3.6
1	A	238	VAL	3.5
1	A	587	PHE	3.5
1	A	559	LEU	3.5
1	B	378	ASP	3.4
1	B	366	SER	3.3
1	B	757	GLU	3.3
1	A	384	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	766	SER	3.1
1	A	380	VAL	3.1
1	B	389	VAL	3.1
1	B	398	THR	3.0
1	A	555	ILE	3.0
1	B	390	SER	3.0
1	A	381	ASP	3.0
1	B	756	VAL	2.9
1	B	376	ILE	2.9
1	B	556	SER	2.9
1	B	492	SER	2.9
1	A	591	GLY	2.9
1	A	548	TRP	2.9
1	B	560	GLY	2.8
1	B	395	HIS	2.8
1	A	561	ASN	2.8
1	A	386	PRO	2.8
1	A	685	TRP	2.6
1	B	397	VAL	2.6
1	B	758	GLY	2.6
1	B	392	GLU	2.5
1	B	364	SER	2.4
1	A	491	GLU	2.4
1	A	552	ARG	2.4
1	B	269	ILE	2.3
1	A	558	SER	2.3
1	B	393	SER	2.2
1	B	512	VAL	2.2
1	A	553	LYS	2.1
1	A	299	GLN	2.1
1	B	244	VAL	2.1
1	A	385	ASN	2.1
1	B	553	LYS	2.1
1	B	755	ALA	2.1
1	B	561	ASN	2.1
1	B	543	VAL	2.1
1	A	765	ARG	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(Å <sup>2</sup> )	Q<0.9
1	CAS	A	470	9/10	0.96	0.11	-	31,35,50,51	3
1	CAS	B	470	9/10	0.98	0.09	-	33,37,52,52	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(Å <sup>2</sup> )	Q<0.9
3	DMS	A	804	4/4	0.93	0.14	1.57	79,87,90,91	0
2	MET	A	801	9/9	0.97	0.21	0.80	27,28,30,31	0
3	DMS	A	803	4/4	0.94	0.17	0.10	73,74,74,76	0
3	DMS	A	802	4/4	0.93	0.15	-0.07	85,89,91,92	0
4	4RD	B	802	27/27	0.95	0.10	-1.01	33,37,38,47	0
3	DMS	B	801	4/4	0.96	0.10	-	61,66,67,69	0

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

There are no such residues in this entry.