



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 9, 2017 – 11:24 AM EST

PDB ID : 5G20  
Title : Leishmania major N-myristoyltransferase in complex with a quinoline inhibitor (compound 19).  
Authors : Goncalves, V.; Brannigan, J.A.; Laporte, A.; Bell, A.S.; Roberts, S.M.; Wilkinson, A.J.; Leatherbarrow, R.J.; Tate, E.W.  
Deposited on : 2016-04-06  
Resolution : 1.52 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-20028442  
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-20028442

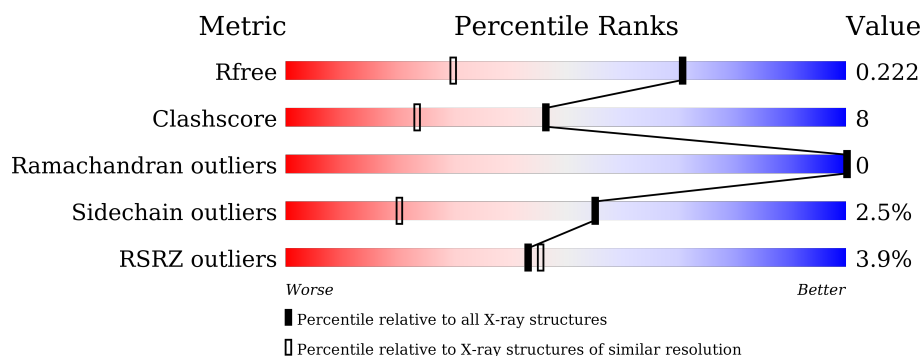
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.52 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))
$R_{free}$	91344	2658 (1.54-1.50)
Clashscore	102246	2887 (1.54-1.50)
Ramachandran outliers	100387	2818 (1.54-1.50)
Sidechain outliers	100360	2816 (1.54-1.50)
RSRZ outliers	91569	2660 (1.54-1.50)

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. 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	411	<div> <div>4%</div> <div>82%</div> <div>17%</div> <div>.</div> </div>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 3990 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.

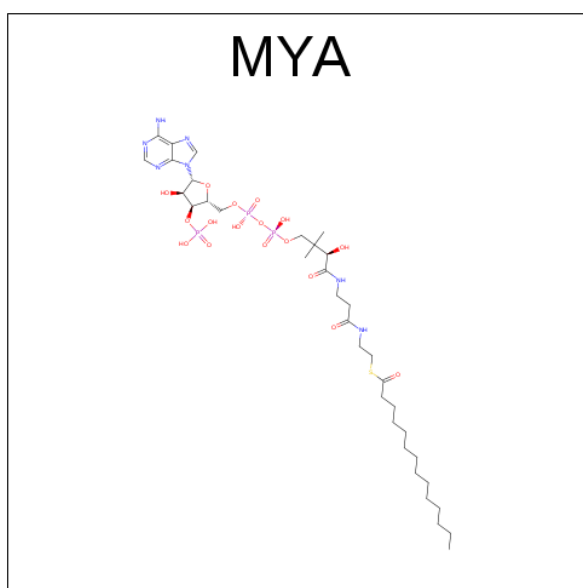
- Molecule 1 is a protein called GLYCYLPEPTIDE N-TETRADECANOYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	411	Total	C	N	O	S	0	31	0
			3512	2283	580	631	18			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

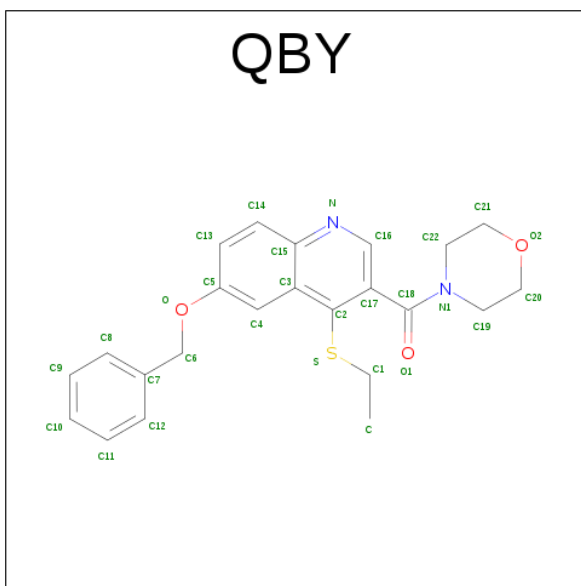
- Molecule 3 is TETRADECANOYL-COA (three-letter code: MYA) (formula: C<sub>35</sub>H<sub>62</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			63	35	7	17	3	1		

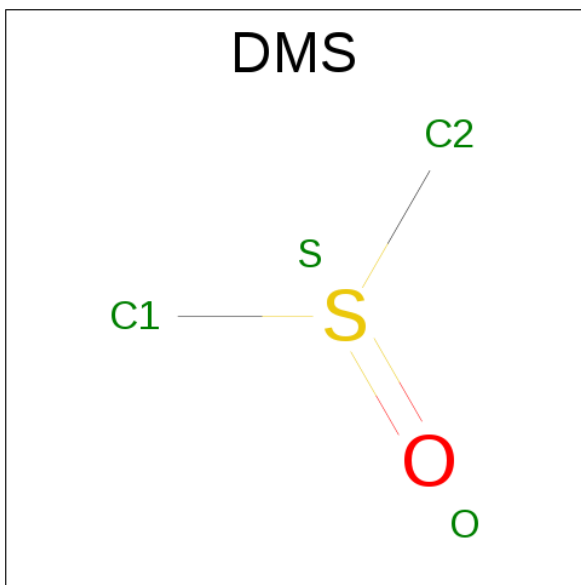
- Molecule 4 is 6-(BENZYLOXY)-4-(ETHYLSULFANYL)-3-[(MORPHOLIN-4-YL)

(three-letter code: QBY) (formula:  $C_{23}H_{24}N_2O_3S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			29	23	2	3	1		

- Molecule 5 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula:  $C_2H_6OS$ ).



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

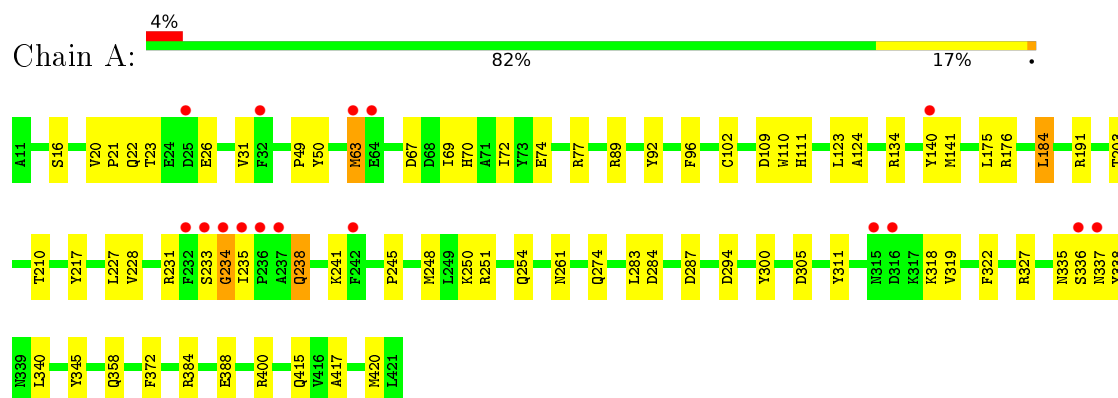
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	381	Total 381	O 381	0	0

### 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 ( $RSRZ > 2$ ). 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: GLYCYLPEPTIDE N-TETRADECANOYLTRANSFERASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	47.72Å 90.65Å 52.91Å 90.00° 112.72° 90.00°	Depositor
Resolution (Å)	48.81 – 1.52 48.81 – 1.52	Depositor EDS
% Data completeness (in resolution range)	98.8 (48.81-1.52) 98.8 (48.81-1.52)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.74 (at 1.52Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.174 , 0.219 0.174 , 0.222	Depositor DCC
$R_{free}$ test set	3118 reflections (5.21%)	DCC
Wilson B-factor (Å <sup>2</sup> )	18.8	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 39.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	3990	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.61% 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: MYA, QBY, MG, 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	1.25	6/3705 (0.2%)	1.29	27/5031 (0.5%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	217	TYR	CE1-CZ	-6.95	1.29	1.38
1	A	110	TRP	CG-CD1	6.72	1.46	1.36
1	A	140	TYR	CG-CD1	6.62	1.47	1.39
1	A	191	ARG	CZ-NH1	5.86	1.40	1.33
1	A	284[A]	ASP	CB-CG	5.27	1.62	1.51
1	A	284[B]	ASP	CB-CG	5.27	1.62	1.51

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	89	ARG	NE-CZ-NH2	-11.72	114.44	120.30
1	A	134	ARG	NE-CZ-NH2	-11.31	114.64	120.30
1	A	400	ARG	NE-CZ-NH2	-10.45	115.08	120.30
1	A	191	ARG	NE-CZ-NH2	-8.54	116.03	120.30
1	A	96	PHE	CB-CG-CD2	-8.21	115.05	120.80
1	A	345	TYR	CB-CG-CD2	-8.00	116.20	121.00
1	A	294	ASP	CB-CG-OD1	7.66	125.20	118.30
1	A	284[A]	ASP	CB-CG-OD1	7.57	125.11	118.30
1	A	284[B]	ASP	CB-CG-OD1	7.57	125.11	118.30
1	A	89	ARG	NE-CZ-NH1	7.35	123.98	120.30
1	A	311	TYR	CB-CG-CD2	-6.64	117.02	121.00
1	A	234	GLY	N-CA-C	-6.41	97.09	113.10
1	A	327	ARG	NE-CZ-NH2	-6.39	117.11	120.30
1	A	191	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	A	50	TYR	CB-CG-CD2	-6.05	117.37	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	372	PHE	CB-CG-CD2	-6.03	116.58	120.80
1	A	92	TYR	CB-CG-CD2	-5.91	117.46	121.00
1	A	184[A]	LEU	CB-CG-CD1	-5.86	101.04	111.00
1	A	184[B]	LEU	CB-CG-CD1	-5.86	101.04	111.00
1	A	176	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	A	92	TYR	CB-CG-CD1	5.67	124.40	121.00
1	A	322	PHE	CB-CG-CD2	-5.59	116.89	120.80
1	A	384	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	A	77	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	327	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	A	294	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	A	300	TYR	CB-CG-CD2	-5.17	117.90	121.00

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	3512	0	3537	55	0
2	A	1	0	0	0	0
3	A	63	0	58	0	0
4	A	29	0	0	0	0
5	A	4	0	6	0	0
6	A	381	0	0	4	0
All	All	3990	0	3601	55	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 8.

All (55) 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:388[B]:GLU:OE2	6:A:2358:HOH:O	1.54	1.25
1:A:388[A]:GLU:OE1	6:A:2351:HOH:O	1.61	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63[A]:MET:CE	1:A:72:ILE:CD1	2.31	1.08
1:A:63[A]:MET:HE1	1:A:72:ILE:CD1	1.88	1.04
1:A:63[A]:MET:HE1	1:A:72:ILE:HD13	1.42	0.98
1:A:63[A]:MET:CE	1:A:72:ILE:HD12	1.95	0.96
1:A:63[A]:MET:HE3	1:A:72:ILE:HD12	1.51	0.87
1:A:63[A]:MET:HE3	1:A:72:ILE:CD1	2.01	0.87
1:A:63[A]:MET:HB3	1:A:102:CYS:SG	2.15	0.87
1:A:238:GLN:H	1:A:238:GLN:HE21	1.23	0.84
1:A:287:ASP:OD2	1:A:415[B]:GLN:NE2	2.11	0.81
1:A:335:ASN:HD22	1:A:338:TYR:H	1.34	0.72
1:A:250:LYS:O	1:A:254[B]:GLN:HG2	1.90	0.71
1:A:124:ALA:HB1	1:A:184[A]:LEU:HD11	1.73	0.69
1:A:63[B]:MET:HB3	1:A:102:CYS:SG	2.34	0.68
1:A:63[B]:MET:CB	1:A:102:CYS:SG	2.84	0.66
1:A:31:VAL:HA	1:A:141:MET:HE2	1.78	0.65
1:A:31:VAL:HB	1:A:141:MET:CE	2.27	0.64
1:A:261:ASN:ND2	1:A:358:GLN:HE21	1.99	0.61
1:A:20:VAL:HB	1:A:21:PRO:HD2	1.82	0.61
1:A:305:ASP:HB3	6:A:2308:HOH:O	2.00	0.60
1:A:16:SER:HA	1:A:22:GLN:HE22	1.66	0.59
1:A:109[A]:ASP:OD1	6:A:2154:HOH:O	2.17	0.59
1:A:238:GLN:H	1:A:238:GLN:NE2	1.99	0.58
1:A:31:VAL:HG12	1:A:141:MET:HE1	1.87	0.56
1:A:21:PRO:HG2	1:A:210:THR:HB	1.88	0.54
1:A:261:ASN:HD21	1:A:358:GLN:HE21	1.54	0.54
1:A:31:VAL:CA	1:A:141:MET:HE2	2.37	0.53
1:A:248:MET:HE2	1:A:251[B]:ARG:HD3	1.90	0.53
1:A:248:MET:CE	1:A:251[B]:ARG:HD3	2.40	0.51
1:A:63[B]:MET:HB2	1:A:102:CYS:SG	2.52	0.49
1:A:31:VAL:CB	1:A:141:MET:CE	2.90	0.49
1:A:31:VAL:HA	1:A:141:MET:CE	2.43	0.49
1:A:16:SER:HA	1:A:22:GLN:NE2	2.29	0.46
1:A:248:MET:CE	1:A:248:MET:HA	2.46	0.46
1:A:228:VAL:HG13	1:A:234:GLY:C	2.36	0.46
1:A:235:ILE:HD13	1:A:245:PRO:HB2	1.96	0.46
1:A:227:LEU:O	1:A:231[B]:ARG:HB2	2.17	0.45
1:A:335:ASN:ND2	1:A:338:TYR:H	2.10	0.45
1:A:63[B]:MET:HG2	1:A:111:HIS:ND1	2.32	0.45
1:A:283:LEU:HD22	1:A:417:ALA:HB1	1.98	0.44
1:A:123:LEU:HD13	1:A:175:LEU:HD11	1.99	0.44
1:A:31:VAL:CG1	1:A:141:MET:HE1	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:GLN:N	1:A:238:GLN:HE21	2.04	0.44
1:A:63[B]:MET:HG3	1:A:111:HIS:CE1	2.53	0.44
1:A:63[A]:MET:HE3	1:A:72:ILE:HD11	1.97	0.43
1:A:335:ASN:ND2	1:A:337:ASN:H	2.15	0.43
1:A:248:MET:HA	1:A:248:MET:HE2	2.00	0.42
1:A:203:THR:CG2	1:A:420:MET:HG3	2.49	0.42
1:A:31:VAL:CB	1:A:141:MET:HE1	2.48	0.41
1:A:70:HIS:NE2	1:A:74:GLU:OE2	2.53	0.41
1:A:274:GLN:NE2	1:A:319:VAL:H	2.18	0.41
1:A:23:THR:O	1:A:26[B]:GLU:HB2	2.21	0.40
1:A:31:VAL:HB	1:A:141:MET:HE1	2.04	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	440/411 (107%)	424 (96%)	16 (4%)	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	393/362 (109%)	383 (98%)	10 (2%)	55 20

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

Mol	Chain	Res	Type
1	A	49	PRO
1	A	63[A]	MET
1	A	63[B]	MET
1	A	67	ASP
1	A	233	SER
1	A	238	GLN
1	A	241	LYS
1	A	318	LYS
1	A	336	SER
1	A	340	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	91	ASN
1	A	238	GLN
1	A	252	ASN
1	A	261	ASN
1	A	274	GLN
1	A	335	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 for Mogul analysis.

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	MYA	A	1423	2	53,65,65	1.18	4 (7%)	64,91,91	1.58	8 (12%)
4	QBY	A	1424	-	32,32,32	1.87	9 (28%)	37,43,43	1.99	10 (27%)
5	DMS	A	1425	-	3,3,3	0.65	0	3,3,3	1.16	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
3	MYA	A	1423	2	-	0/59/80/80	0/3/3/3
4	QBY	A	1424	-	-	0/16/24/24	0/4/4/4
5	DMS	A	1425	-	-	0/0/0/0	0/0/0/0

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1424	QBY	C2-S	-3.39	1.73	1.77
4	A	1424	QBY	O1-C18	-2.33	1.17	1.22
3	A	1423	MYA	P1A-O2A	-2.27	1.43	1.51
4	A	1424	QBY	C19-N1	2.02	1.50	1.47
3	A	1423	MYA	C2A-N3A	2.05	1.35	1.32
4	A	1424	QBY	C17-C2	2.10	1.44	1.41
4	A	1424	QBY	C16-N	2.26	1.35	1.31
4	A	1424	QBY	C12-C7	2.43	1.44	1.38
3	A	1423	MYA	C7-C6	2.66	1.59	1.51
4	A	1424	QBY	C4-C5	2.72	1.42	1.37
3	A	1423	MYA	C2-S1	4.00	1.87	1.81
4	A	1424	QBY	C2-C3	4.15	1.48	1.43
4	A	1424	QBY	C3-C15	5.07	1.50	1.42

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1423	MYA	N3A-C2A-N1A	-5.12	124.85	128.87
3	A	1423	MYA	C4X-O4X-C1X	-4.48	104.90	109.64
3	A	1423	MYA	C1X-N9A-C4A	-3.98	122.37	126.81
4	A	1424	QBY	O2-C20-C19	-3.39	104.00	111.83
4	A	1424	QBY	C17-C16-N	-2.76	122.43	125.52
3	A	1423	MYA	C6-C5-N4	-2.55	112.03	116.46
3	A	1423	MYA	C7-N8-C9	-2.22	118.17	122.62
4	A	1424	QBY	C22-N1-C18	-2.20	116.27	122.86
3	A	1423	MYA	C3-C2-S1	-2.08	107.45	113.84
4	A	1424	QBY	C6-C7-C8	2.00	125.44	120.66
3	A	1423	MYA	C2X-C3X-C4X	2.03	107.15	103.25
4	A	1424	QBY	C19-N1-C22	2.28	116.75	112.57
4	A	1424	QBY	C17-C18-N1	2.54	121.13	118.27
4	A	1424	QBY	C9-C8-C7	3.03	125.24	120.65
4	A	1424	QBY	C16-N-C15	3.39	121.37	116.96
4	A	1424	QBY	C10-C11-C12	3.79	125.47	120.20
3	A	1423	MYA	O2M-C2M-C3M	5.99	120.12	109.26
4	A	1424	QBY	C1-S-C2	6.30	110.14	103.33

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	411/411 (100%)	-0.03	16 (3%)	43 45	11, 19, 46, 89	1 (0%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	234	GLY	11.8
1	A	232	PHE	10.6
1	A	233	SER	9.4
1	A	235	ILE	5.1
1	A	336	SER	4.1
1	A	316	ASP	3.9
1	A	64	GLU	3.7
1	A	237	ALA	3.5
1	A	236	PRO	3.2
1	A	315	ASN	3.2
1	A	337	ASN	3.1
1	A	140	TYR	2.7
1	A	63[A]	MET	2.6
1	A	32	PHE	2.5
1	A	242	PHE	2.4
1	A	25	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

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
5	DMS	A	1425	4/4	0.96	0.09	1.83	34,35,36,38	0
4	QBY	A	1424	29/29	0.95	0.10	0.39	18,24,35,35	0
3	MYA	A	1423	63/63	0.98	0.06	-0.52	11,15,19,21	0
2	MG	A	1422	1/1	0.98	0.06	-0.66	27,27,27,27	0

## 6.5 Other polymers

There are no such residues in this entry.