



Full wwPDB X-ray Structure Validation Report

Nov 21, 2014 – 12:29 AM EST

PDB ID : 4A30
Title : CRYSTAL STRUCTURE OF LEISHMANIA MAJOR N-MYRISTOYLTRANSFERASE(NMT) WITH BOUND MYRISTOYL-COA AND A PYRAZOLE SULPHONAMIDE LIGAND
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Deposited on : 2011-09-29
Resolution : 1.50 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

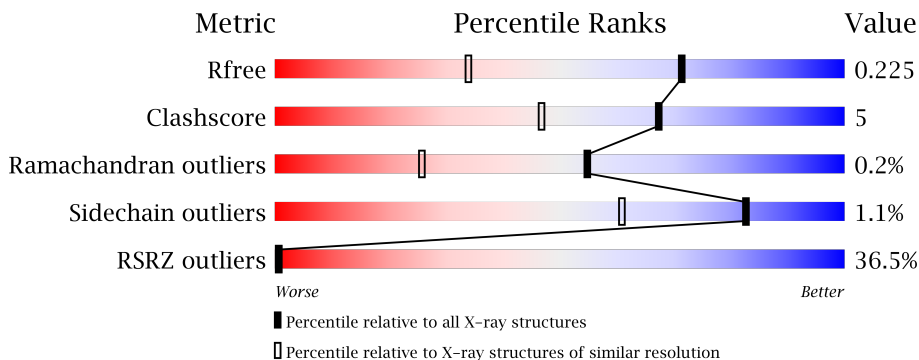
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : trunk24195
Percentile statistics : 23426
Refmac : 5.8.0049
CCP4 : 6.1.3
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk24195

1 Overall quality at a glance

The reported resolution of this entry is 1.50 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}	77520	1744 (1.50-1.50)
Clashscore	88313	1940 (1.50-1.50)
Ramachandran outliers	86584	1890 (1.50-1.50)
C α geometry	86677	1887 (1.50-1.50)
Sidechain outliers	86556	1888 (1.50-1.50)
RSRZ outliers	77580	1745 (1.50-1.50)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	438	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	QMI	A	1424	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3708 atoms, of which 0 are hydrogen and 0 are deuterium.

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	0	0
			3342	2163	560	604	15			

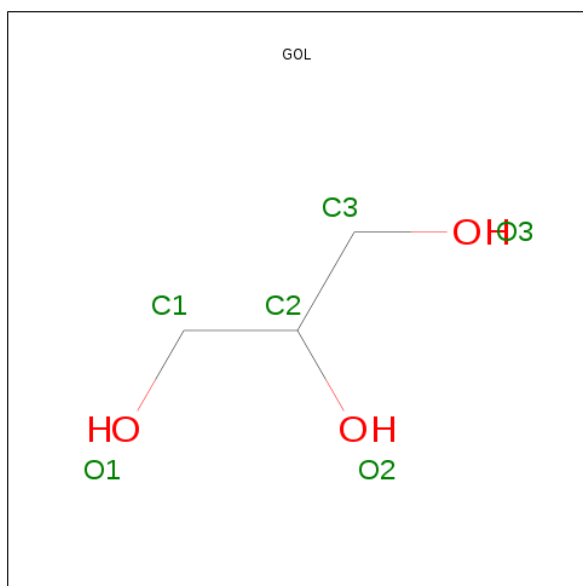
There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	MET	-	EXPRESSION TAG	UNP Q4Q5S8
A	-15	GLY	-	EXPRESSION TAG	UNP Q4Q5S8
A	-14	SER	-	EXPRESSION TAG	UNP Q4Q5S8
A	-13	SER	-	EXPRESSION TAG	UNP Q4Q5S8
A	-12	HIS	-	EXPRESSION TAG	UNP Q4Q5S8
A	-11	HIS	-	EXPRESSION TAG	UNP Q4Q5S8
A	-10	HIS	-	EXPRESSION TAG	UNP Q4Q5S8
A	-9	HIS	-	EXPRESSION TAG	UNP Q4Q5S8
A	-8	HIS	-	EXPRESSION TAG	UNP Q4Q5S8
A	-7	HIS	-	EXPRESSION TAG	UNP Q4Q5S8
A	-6	SER	-	EXPRESSION TAG	UNP Q4Q5S8
A	-5	SER	-	EXPRESSION TAG	UNP Q4Q5S8
A	-4	GLY	-	EXPRESSION TAG	UNP Q4Q5S8
A	-3	ARG	-	EXPRESSION TAG	UNP Q4Q5S8
A	-2	GLU	-	EXPRESSION TAG	UNP Q4Q5S8
A	-1	ASN	-	EXPRESSION TAG	UNP Q4Q5S8
A	0	LEU	-	EXPRESSION TAG	UNP Q4Q5S8
A	1	TYR	-	EXPRESSION TAG	UNP Q4Q5S8
A	2	PHE	-	EXPRESSION TAG	UNP Q4Q5S8
A	3	GLN	-	EXPRESSION TAG	UNP Q4Q5S8
A	4	GLY	-	EXPRESSION TAG	UNP Q4Q5S8

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

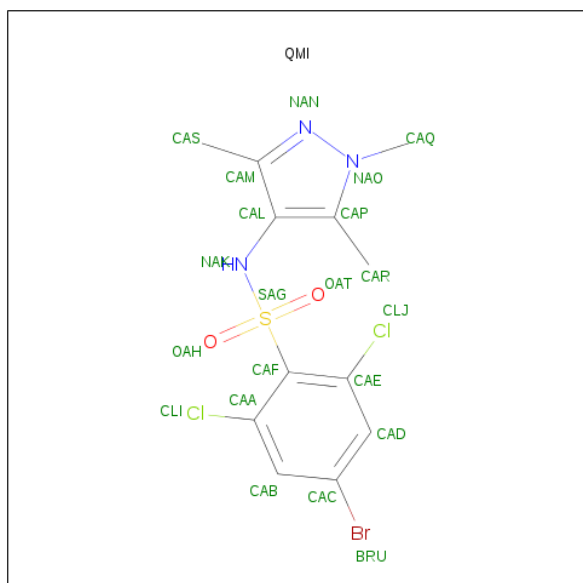
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		

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



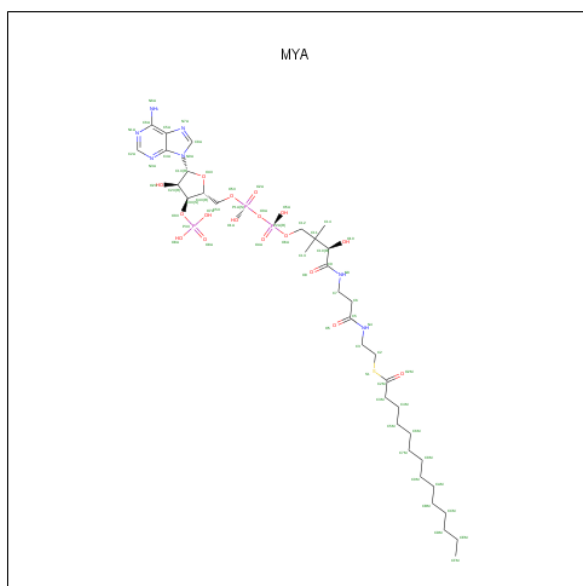
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is 4-BROMO-2,6-DICHLORO-N-(1,3,5-TRIMETHYL-1H-PYRAZOL-4-YL)BENZENESULFONAMIDE (three-letter code: QMI) (formula: $C_{12}H_{12}BrCl_2N_3O_2S$).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
4	A	1	Total	Br	C	Cl	N	O	S	0	0
			21	1	12	2	3	2	1		

- Molecule 5 is TETRADECANOYL-COA (three-letter code: MYA) (formula: $C_{35}H_{62}N_7O_{17}P_3S$).



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

- Molecule 6 is water.

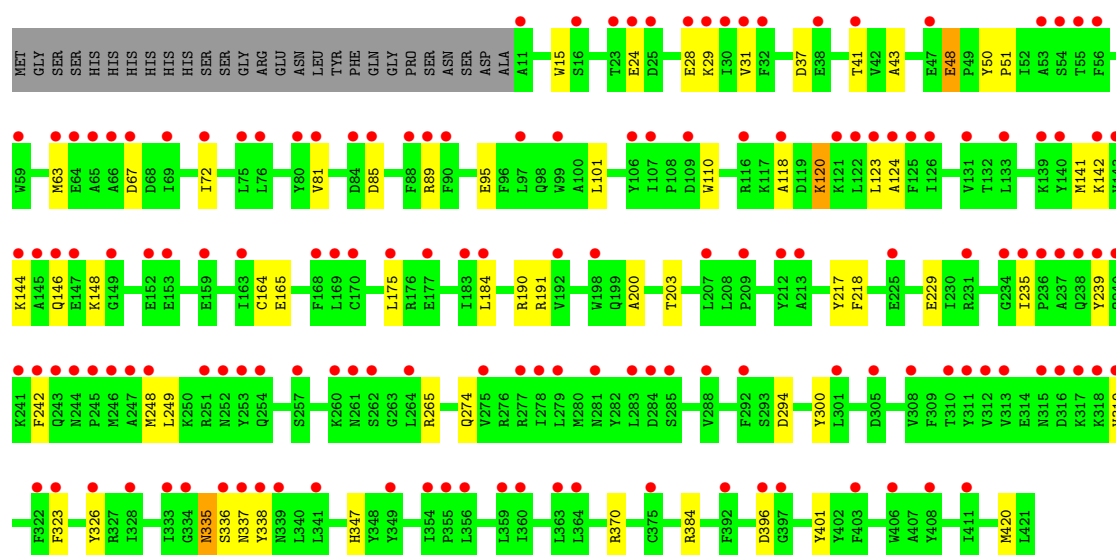
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	275	Total	O	0	0
			275	275		

3 Residue-property plots

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

Chain A: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	48.64Å 90.68Å 53.51Å 90.00° 114.02° 90.00°	Depositor
Resolution (Å)	19.95 – 1.50 19.95 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.2 (19.95-1.50) 95.0 (19.95-2.30)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.08 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.187 , 0.221 0.223 , 0.225	Depositor DCC
R_{free} test set	1312 reflections (7.32%)	DCC
Wilson B-factor (Å ²)	25.4	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 29.6	EDS
Estimated twinning fraction	0.033 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 17929 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	3708	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: QMI, GOL, CL, MYA

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	1.38	15/3441 (0.4%)	1.34	22/4684 (0.5%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	85	ASP	CG-OD1	10.17	1.48	1.25
1	A	85	ASP	CB-CG	8.98	1.70	1.51
1	A	89	ARG	CZ-NH2	-7.93	1.22	1.33
1	A	85	ASP	CG-OD2	-6.24	1.11	1.25
1	A	336	SER	CA-CB	6.15	1.62	1.52
1	A	323	PHE	CE1-CZ	6.13	1.49	1.37
1	A	15	TRP	CE3-CZ3	6.06	1.48	1.38
1	A	67	ASP	CB-CG	5.96	1.64	1.51
1	A	81	VAL	CB-CG2	5.93	1.65	1.52
1	A	48	GLU	CG-CD	5.79	1.60	1.51
1	A	217	TYR	CD2-CE2	5.53	1.47	1.39
1	A	110	TRP	CE3-CZ3	-5.33	1.29	1.38
1	A	165	GLU	CG-CD	5.25	1.59	1.51
1	A	326	TYR	CE2-CZ	-5.24	1.31	1.38
1	A	401	TYR	CB-CG	5.00	1.59	1.51

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	85	ASP	CB-CG-OD2	-21.69	98.78	118.30
1	A	89	ARG	NE-CZ-NH2	-19.59	110.50	120.30
1	A	85	ASP	CB-CG-OD1	18.65	135.09	118.30
1	A	89	ARG	NE-CZ-NH1	17.94	129.27	120.30
1	A	218	PHE	CB-CG-CD2	-8.20	115.06	120.80
1	A	384	ARG	NE-CZ-NH2	-7.31	116.64	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	294	ASP	CB-CG-OD1	6.61	124.24	118.30
1	A	396	ASP	CB-CG-OD1	-6.55	112.41	118.30
1	A	190	ARG	NE-CZ-NH1	-6.50	117.05	120.30
1	A	384	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	A	191	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	A	300	TYR	CG-CD2-CE2	-5.57	116.84	121.30
1	A	50	TYR	CB-CG-CD2	-5.50	117.70	121.00
1	A	95	GLU	CG-CD-OE1	5.49	129.28	118.30
1	A	300	TYR	CB-CG-CD2	-5.48	117.71	121.00
1	A	265	ARG	NE-CZ-NH1	-5.36	117.62	120.30
1	A	37	ASP	CB-CG-OD1	5.35	123.12	118.30
1	A	249	LEU	CB-CG-CD2	-5.33	101.93	111.00
1	A	67	ASP	CB-CG-OD2	5.25	123.02	118.30
1	A	217	TYR	CD1-CE1-CZ	-5.25	115.08	119.80
1	A	89	ARG	CD-NE-CZ	5.16	130.82	123.60
1	A	370	ARG	NE-CZ-NH2	-5.13	117.73	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3342	0	3255	36	0
2	A	1	0	0	0	0
3	A	6	0	7	0	0
4	A	21	0	12	0	0
5	A	63	0	58	0	0
6	A	275	0	0	6	0
All	All	3708	0	3332	36	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (36) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:63:MET:SD	1:A:72:ILE:HD12	1.61	1.39
1:A:63:MET:SD	1:A:72:ILE:CD1	2.27	1.21
1:A:31:VAL:HA	1:A:141:MET:HE2	1.72	0.70
1:A:124:ALA:HB1	1:A:184:LEU:HD11	1.73	0.69
1:A:274:GLN:NE2	1:A:319:VAL:H	1.91	0.67
1:A:41:THR:HG22	1:A:43:ALA:H	1.60	0.67
1:A:229:GLU:HG2	1:A:338:TYR:HE2	1.61	0.65
1:A:63:MET:SD	1:A:72:ILE:HD11	2.34	0.65
1:A:63:MET:HE2	1:A:101:LEU:HD12	1.79	0.65
1:A:274:GLN:HE22	1:A:319:VAL:H	1.45	0.63
1:A:347:HIS:HE1	6:A:2234:HOH:O	1.84	0.60
1:A:141:MET:SD	1:A:144:LYS:HD2	2.41	0.60
1:A:142:LYS:NZ	6:A:2120:HOH:O	2.36	0.57
1:A:146:GLN:HG2	6:A:2124:HOH:O	2.04	0.57
1:A:63:MET:CE	1:A:101:LEU:HD12	2.35	0.56
1:A:24:GLU:O	1:A:28:GLU:HG3	2.07	0.55
1:A:123:LEU:HD13	1:A:175:LEU:HD21	1.88	0.55
1:A:31:VAL:CA	1:A:141:MET:HE2	2.35	0.55
1:A:63:MET:CE	1:A:72:ILE:HD12	2.36	0.51
1:A:203:THR:CG2	1:A:420:MET:HG3	2.41	0.50
1:A:48:GLU:HG2	6:A:2035:HOH:O	2.11	0.50
1:A:335:ASN:HD21	1:A:337:ASN:HB2	1.77	0.49
1:A:203:THR:HG21	1:A:420:MET:HG3	1.94	0.49
1:A:63:MET:CE	1:A:101:LEU:CD1	2.91	0.48
1:A:235:ILE:HG22	1:A:239:TYR:HB2	1.96	0.48
1:A:31:VAL:HG12	1:A:141:MET:HE1	1.99	0.44
1:A:120:LYS:HD3	6:A:2049:HOH:O	2.16	0.44
1:A:63:MET:HE2	1:A:101:LEU:CD1	2.48	0.44
1:A:235:ILE:CG2	1:A:239:TYR:HB2	2.48	0.44
1:A:148:LYS:NZ	6:A:2129:HOH:O	2.52	0.42
1:A:123:LEU:HB3	1:A:175:LEU:HD22	2.00	0.42
1:A:31:VAL:HA	1:A:141:MET:CE	2.46	0.41
1:A:335:ASN:ND2	1:A:337:ASN:H	2.19	0.41
1:A:164:CYS:O	1:A:200:ALA:HA	2.20	0.41
1:A:242:PHE:CD2	1:A:248:MET:HG3	2.56	0.40
1:A:31:VAL:HB	1:A:141:MET:CE	2.51	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	409/438 (93%)	397 (97%)	11 (3%)	1 (0%)	55 26

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	118	ALA

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	357/385 (93%)	353 (99%)	4 (1%)	83 61

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

Mol	Chain	Res	Type
1	A	29	LYS
1	A	51	PRO
1	A	120	LYS
1	A	335	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	91	ASN
1	A	162	HIS

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Mol	Chain	Res	Type
1	A	193	ASN
1	A	274	GLN
1	A	315	ASN
1	A	335	ASN
1	A	347	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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	GOL	A	1423	-	5,5,5	0.83	0	5,5,5	1.32	0
4	QMI	A	1424	-	22,22,22	2.26	5 (22%)	32,34,34	2.56	13 (40%)
5	MYA	A	1425	-	65,65,65	1.41	8 (12%)	91,91,91	1.85	13 (14%)

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	GOL	A	1423	-	-	0/4/4/4	0/0/0/0
4	QMI	A	1424	-	-	0/9/11/11	0/2/2/2
5	MYA	A	1425	-	-	0/63/80/80	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1424	QMI	CAL-CAP	6.73	1.44	1.38
4	A	1424	QMI	CAF-SAG	-5.76	1.68	1.79
5	A	1425	MYA	O2M-C2M	-4.26	1.24	1.42
5	A	1425	MYA	C2M-S1	-4.13	1.72	1.81
5	A	1425	MYA	O4X-C1X	-3.50	1.36	1.41
5	A	1425	MYA	P1A-O3A	3.32	1.65	1.59
5	A	1425	MYA	P2A-O5A	-3.27	1.40	1.55
5	A	1425	MYA	C2A-N3A	3.09	1.37	1.32
4	A	1424	QMI	CAA-CAF	2.72	1.44	1.40
5	A	1425	MYA	C3X-C4X	-2.46	1.45	1.52
5	A	1425	MYA	C8A-N9A	-2.08	1.33	1.36
4	A	1424	QMI	CAL-NAK	-2.04	1.39	1.43
4	A	1424	QMI	CAL-CAM	-2.03	1.37	1.38

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1425	MYA	N3A-C2A-N1A	-9.08	120.90	128.89
5	A	1425	MYA	O2M-C2M-C3M	6.76	121.39	109.10
4	A	1424	QMI	OAT-SAG-OAH	-5.11	112.80	119.55
5	A	1425	MYA	O2M-C2M-S1	4.82	123.66	110.04
4	A	1424	QMI	CAD-CAE-CAF	4.76	127.29	121.26
4	A	1424	QMI	CAP-CAL-CAM	4.75	110.82	107.52
5	A	1425	MYA	C5A-C4A-N3A	-4.65	121.44	125.98
4	A	1424	QMI	CAD-CAE-CLJ	-4.64	111.28	118.55
4	A	1424	QMI	CAM-NAN-NAO	4.02	107.80	104.35
4	A	1424	QMI	CAL-CAP-NAO	-4.01	102.08	106.87
5	A	1425	MYA	C4X-O4X-C1X	-3.83	105.51	109.72
4	A	1424	QMI	CAA-CAF-SAG	3.64	125.79	123.41
4	A	1424	QMI	CAB-CAA-CLI	-3.55	112.99	118.55
4	A	1424	QMI	CAA-CAF-CAE	-3.08	111.62	116.65
5	A	1425	MYA	N3A-C4A-N9A	2.92	130.40	125.39
4	A	1424	QMI	BRU-CAC-CAD	-2.62	115.42	119.29
5	A	1425	MYA	O6A-C12-C11	-2.32	106.82	110.55
5	A	1425	MYA	C3X-C2X-C1X	-2.29	94.46	99.96
5	A	1425	MYA	C4M-C3M-C2M	-2.15	107.78	113.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1425	MYA	C2A-N1A-C6A	2.14	122.57	118.76
5	A	1425	MYA	C2X-C3X-C4X	2.12	107.36	103.18
4	A	1424	QMI	OAH-SAG-NAK	2.12	112.05	106.73
4	A	1424	QMI	CAE-CAF-SAG	-2.10	122.03	123.41
5	A	1425	MYA	C4A-C5A-N7A	-2.07	107.41	109.41
4	A	1424	QMI	CAR-CAP-CAL	2.03	132.97	130.09
5	A	1425	MYA	O5-C5-N4	-2.00	118.99	122.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95th 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 ²)	Q<0.9
1	A	411/438 (93%)	1.80	150 (36%) 1 1	11, 18, 38, 51	2 (0%)

All (150) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	242	PHE	11.7
1	A	243	GLN	7.4
1	A	241	LYS	7.1
1	A	63	MET	6.4
1	A	236	PRO	5.8
1	A	143	VAL	5.8
1	A	237	ALA	5.7
1	A	147	GLU	5.5
1	A	315	ASN	5.5
1	A	29	LYS	5.2
1	A	140	TYR	5.1
1	A	245	PRO	5.1
1	A	244	ASN	5.0
1	A	11	ALA	5.0
1	A	338	TYR	4.9
1	A	30	ILE	4.7
1	A	64	GLU	4.7
1	A	322	PHE	4.7
1	A	65	ALA	4.5
1	A	28	GLU	4.4
1	A	122	LEU	4.4
1	A	25	ASP	4.4
1	A	240	GLN	4.4
1	A	251	ARG	4.3
1	A	275	VAL	4.3
1	A	239	TYR	4.2
1	A	262	SER	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	337	ASN	4.1
1	A	316	ASP	3.9
1	A	56	PHE	3.8
1	A	144	LYS	3.8
1	A	339	ASN	3.8
1	A	235	ILE	3.8
1	A	146	GLN	3.7
1	A	312	VAL	3.7
1	A	90	PHE	3.7
1	A	125	PHE	3.7
1	A	336	SER	3.7
1	A	32	PHE	3.6
1	A	85	ASP	3.6
1	A	408	TYR	3.6
1	A	159	GLU	3.5
1	A	246	MET	3.5
1	A	359	LEU	3.5
1	A	124	ALA	3.4
1	A	318	LYS	3.3
1	A	126	ILE	3.3
1	A	334	GLY	3.3
1	A	31	VAL	3.3
1	A	323	PHE	3.2
1	A	53	ALA	3.2
1	A	288	VAL	3.2
1	A	301	LEU	3.2
1	A	76	LEU	3.1
1	A	66	ALA	3.1
1	A	118	ALA	3.1
1	A	81	VAL	3.0
1	A	279	LEU	3.0
1	A	247	ALA	3.0
1	A	69	ILE	3.0
1	A	341	LEU	3.0
1	A	333	ILE	3.0
1	A	231	ARG	2.9
1	A	252	ASN	2.9
1	A	123	LEU	2.9
1	A	411	ILE	2.9
1	A	47	GLU	2.9
1	A	55	THR	2.9
1	A	169	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	284	ASP	2.9
1	A	139	LYS	2.8
1	A	72	ILE	2.8
1	A	212	TYR	2.8
1	A	163	ILE	2.8
1	A	80	TYR	2.7
1	A	106	TYR	2.7
1	A	88	PHE	2.7
1	A	38	GLU	2.7
1	A	311	TYR	2.7
1	A	116	ARG	2.7
1	A	403	PHE	2.7
1	A	248	MET	2.7
1	A	67	ASP	2.7
1	A	360	ILE	2.7
1	A	234	GLY	2.7
1	A	328	ILE	2.6
1	A	184	LEU	2.6
1	A	23	THR	2.6
1	A	41	THR	2.6
1	A	153	GLU	2.6
1	A	278	ILE	2.6
1	A	253	TYR	2.6
1	A	97	LEU	2.6
1	A	305	ASP	2.6
1	A	99	TRP	2.6
1	A	326	TYR	2.5
1	A	59	TRP	2.5
1	A	292	PHE	2.5
1	A	145	ALA	2.5
1	A	54	SER	2.5
1	A	349	TYR	2.5
1	A	363	LEU	2.5
1	A	317	LYS	2.4
1	A	261	ASN	2.4
1	A	225	GLU	2.4
1	A	107	ILE	2.4
1	A	133	LEU	2.4
1	A	152	GLU	2.4
1	A	397	GLY	2.4
1	A	84	ASP	2.4
1	A	75	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	177	GLU	2.4
1	A	175	LEU	2.4
1	A	310	THR	2.4
1	A	238	GLN	2.3
1	A	285	SER	2.3
1	A	170	CYS	2.3
1	A	308	VAL	2.3
1	A	319	VAL	2.3
1	A	396	ASP	2.3
1	A	354	ILE	2.2
1	A	209	PRO	2.2
1	A	183	ILE	2.2
1	A	207	LEU	2.2
1	A	254	GLN	2.2
1	A	89	ARG	2.2
1	A	260	LYS	2.2
1	A	283	LEU	2.2
1	A	198	TRP	2.2
1	A	406	TRP	2.2
1	A	16	SER	2.2
1	A	131	VAL	2.2
1	A	192	VAL	2.2
1	A	313	VAL	2.2
1	A	257	SER	2.1
1	A	264	LEU	2.1
1	A	149	GLY	2.1
1	A	277	ARG	2.1
1	A	121	LYS	2.1
1	A	142	LYS	2.1
1	A	356	LEU	2.1
1	A	375	CYS	2.1
1	A	355	PRO	2.1
1	A	364	LEU	2.1
1	A	109	ASP	2.1
1	A	24	GLU	2.1
1	A	213	ALA	2.1
1	A	281	ASN	2.1
1	A	168	PHE	2.1
1	A	392	PHE	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

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, 95th 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	QMI	A	1424	21/21	0.32	3.72	14,17,23,34	1
3	GOL	A	1423	6/6	0.15	0.76	20,27,29,31	0
2	CL	A	1422	1/1	0.17	0.50	53,53,53,53	0
5	MYA	A	1425	63/63	0.13	-0.33	9,15,20,23	0

6.5 Other polymers ⓘ

There are no such residues in this entry.