



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:38 PM GMT

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 X-ray Structure 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/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

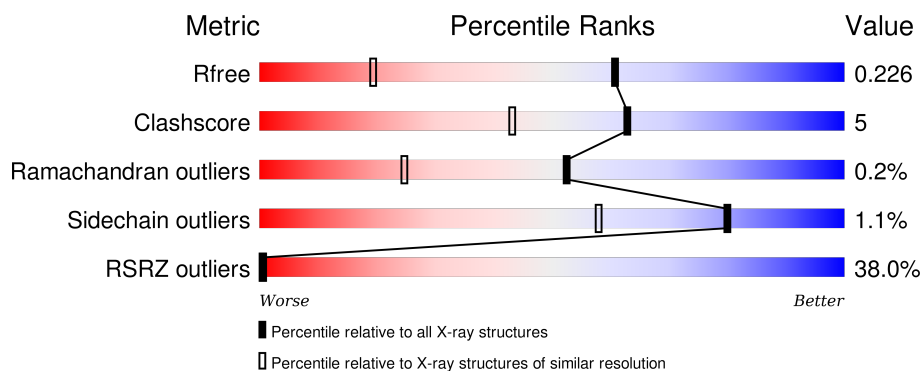
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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}	91344	2072 (1.50-1.50)
Clashscore	102246	2274 (1.50-1.50)
Ramachandran outliers	100387	2218 (1.50-1.50)
Sidechain outliers	100360	2216 (1.50-1.50)
RSRZ outliers	91569	2075 (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. 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	438	

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
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 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	0	0
			3342	2163	560	604	15			

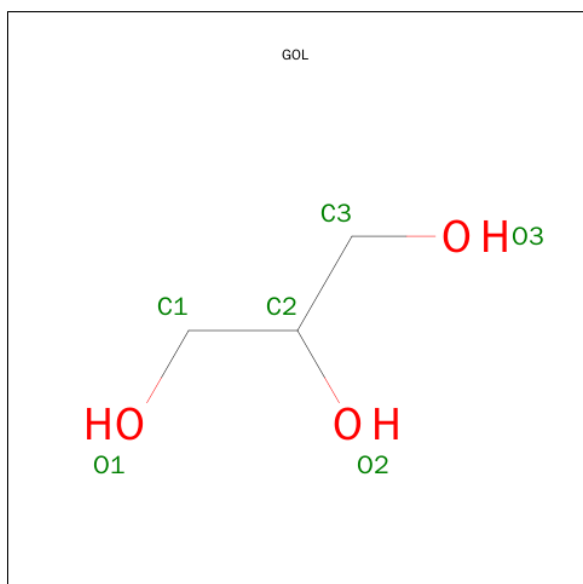
There are 21 discrepancies between the modelled and reference sequences:

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).

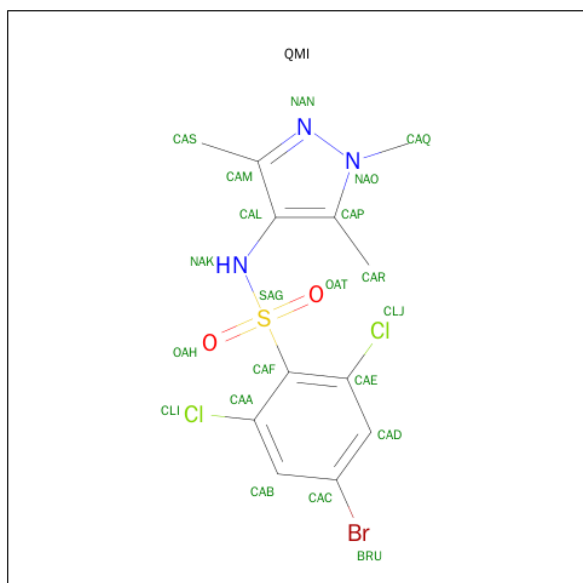
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C1 1 1	0	0

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



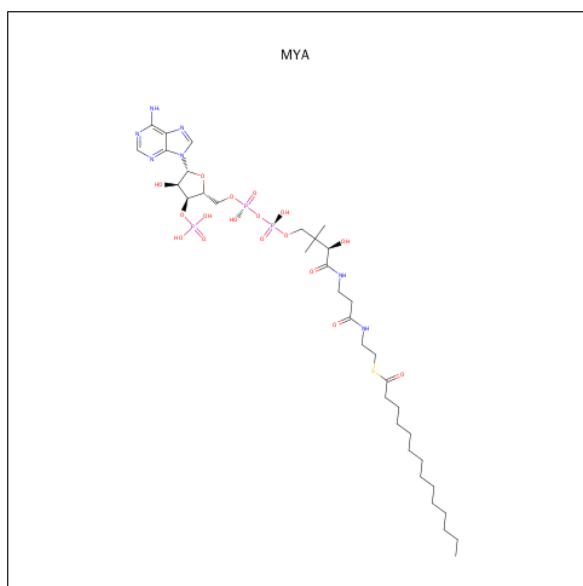
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0

- 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
			Total	Br	C	Cl	N	O	S		
4	A	1	21	1	12	2	3	2	1	0	0

- 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
			Total	C	N	O	P	S		
5	A	1	63	35	7	17	3	1	0	0

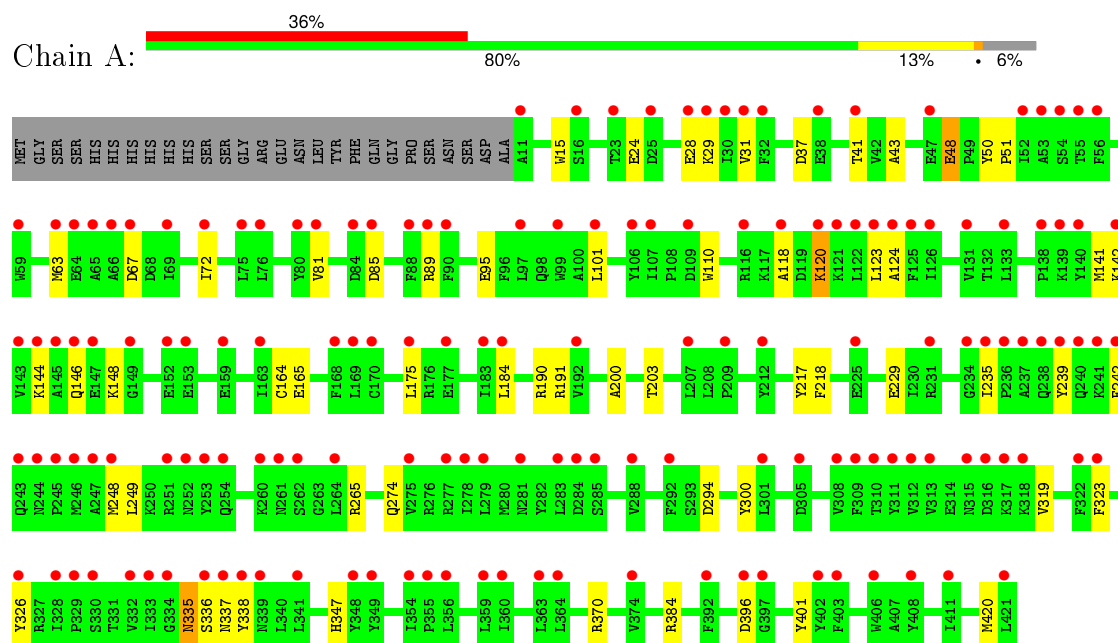
- Molecule 6 is water.

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

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, 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 0.225 , 0.226	Depositor DCC
R_{free} test set	1312 reflections (7.90%)	DCC
Wilson B-factor (Å ²)	25.4	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 46.9	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	0.92	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 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	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

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 5.

All (36) 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: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:63:MET:HE2	1:A:101:LEU:CD1	2.48	0.44
1:A:120:LYS:HD3	6:A:2049:HOH:O	2.16	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 [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	409/438 (93%)	397 (97%)	11 (3%)	1 (0%)	52 25

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	118	ALA

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	357/385 (93%)	353 (99%)	4 (1%)	80 58

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

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Mol	Chain	Res	Type
1	A	91	ASN
1	A	162	HIS
1	A	193	ASN
1	A	274	GLN
1	A	315	ASN
1	A	335	ASN
1	A	347	HIS

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 [i](#)

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	0.84	0	5,5,5	1.27	1 (20%)
4	QMI	A	1424	-	20,22,22	1.80	4 (20%)	27,34,34	2.70	13 (48%)
5	MYA	A	1425	-	53,65,65	1.19	4 (7%)	65,91,91	2.06	12 (18%)

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	-	-	0/59/80/80	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1424	QMI	CAF-SAG	-5.71	1.68	1.79
5	A	1425	MYA	O4X-C1X	-3.50	1.36	1.41
5	A	1425	MYA	P2A-O5A	-3.34	1.40	1.54
5	A	1425	MYA	C3X-C4X	-2.49	1.45	1.52
4	A	1424	QMI	CAL-NAK	-2.15	1.39	1.43
4	A	1424	QMI	CAQ-NAO	2.36	1.49	1.46
4	A	1424	QMI	CAA-CAF	2.67	1.44	1.40
5	A	1425	MYA	C2A-N3A	3.04	1.37	1.32

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1425	MYA	N3A-C2A-N1A	-10.44	120.90	128.89
4	A	1424	QMI	OAT-SAG-OAH	-5.08	112.80	119.54
4	A	1424	QMI	CAD-CAE-CLJ	-4.68	111.28	118.50
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	CAB-CAA-CLI	-3.58	112.99	118.50
5	A	1425	MYA	C2X-C1X-N9A	-3.28	109.28	114.29
4	A	1424	QMI	BRU-CAC-CAD	-2.65	115.42	119.28
5	A	1425	MYA	C1X-N9A-C4A	-2.39	123.34	126.94
5	A	1425	MYA	O6A-C12-C11	-2.32	106.82	110.55
5	A	1425	MYA	C3X-C2X-C1X	-2.30	94.46	99.98
5	A	1425	MYA	C4A-C5A-N7A	-2.25	107.41	109.48
5	A	1425	MYA	C4M-C3M-C2M	-2.15	107.78	113.97
4	A	1424	QMI	CAE-CAF-SAG	-2.07	122.03	123.30
3	A	1423	GOL	O2-C2-C3	-2.06	99.18	108.65
4	A	1424	QMI	CAR-CAP-CAL	2.03	132.97	130.09
5	A	1425	MYA	O5A-P2A-O3A	2.07	114.49	105.09
4	A	1424	QMI	OAH-SAG-NAK	2.11	112.05	106.69
5	A	1425	MYA	C2A-N1A-C6A	2.13	122.57	118.77
5	A	1425	MYA	C2X-C3X-C4X	2.16	107.36	103.29
4	A	1424	QMI	CAF-CAA-CLI	2.23	123.20	121.55

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	A	1424	QMI	CAM-NAN-NAO	3.89	107.80	104.34
4	A	1424	QMI	CAA-CAF-SAG	4.07	125.79	123.30
4	A	1424	QMI	CAP-CAL-CAM	4.75	110.82	107.52
4	A	1424	QMI	CAD-CAE-CAF	4.88	127.29	121.36
5	A	1425	MYA	O2M-C2M-C3M	6.75	121.39	109.05

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, 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%)	1.90	156 (37%) 0 0	11, 18, 38, 51	2 (0%)

All (156) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	242	PHE	13.3
1	A	243	GLN	7.5
1	A	241	LYS	6.6
1	A	63	MET	6.2
1	A	236	PRO	6.1
1	A	147	GLU	6.0
1	A	237	ALA	5.7
1	A	338	TYR	5.5
1	A	315	ASN	5.4
1	A	140	TYR	5.3
1	A	143	VAL	5.3
1	A	245	PRO	5.2
1	A	244	ASN	5.2
1	A	65	ALA	5.2
1	A	29	LYS	5.2
1	A	30	ILE	5.1
1	A	11	ALA	5.1
1	A	322	PHE	5.0
1	A	337	ASN	4.9
1	A	64	GLU	4.9
1	A	25	ASP	4.8
1	A	239	TYR	4.5
1	A	240	GLN	4.4
1	A	316	ASP	4.4
1	A	28	GLU	4.4
1	A	56	PHE	4.4
1	A	251	ARG	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	235	ILE	4.2
1	A	90	PHE	4.2
1	A	125	PHE	4.2
1	A	122	LEU	4.2
1	A	312	VAL	4.1
1	A	275	VAL	4.1
1	A	408	TYR	4.1
1	A	85	ASP	4.1
1	A	262	SER	4.1
1	A	32	PHE	4.0
1	A	323	PHE	4.0
1	A	336	SER	3.9
1	A	339	ASN	3.8
1	A	341	LEU	3.8
1	A	144	LYS	3.8
1	A	288	VAL	3.8
1	A	146	GLN	3.8
1	A	359	LEU	3.7
1	A	118	ALA	3.7
1	A	301	LEU	3.7
1	A	126	ILE	3.6
1	A	81	VAL	3.6
1	A	334	GLY	3.6
1	A	246	MET	3.5
1	A	31	VAL	3.5
1	A	318	LYS	3.5
1	A	124	ALA	3.4
1	A	159	GLU	3.4
1	A	311	TYR	3.3
1	A	69	ILE	3.3
1	A	41	THR	3.2
1	A	234	GLY	3.2
1	A	247	ALA	3.2
1	A	76	LEU	3.2
1	A	47	GLU	3.2
1	A	284	ASP	3.2
1	A	53	ALA	3.1
1	A	88	PHE	3.1
1	A	72	ILE	3.1
1	A	292	PHE	3.1
1	A	360	ILE	3.1
1	A	279	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	403	PHE	3.1
1	A	310	THR	3.0
1	A	411	ILE	3.0
1	A	55	THR	3.0
1	A	328	ILE	3.0
1	A	252	ASN	3.0
1	A	38	GLU	3.0
1	A	66	ALA	3.0
1	A	123	LEU	2.9
1	A	333	ILE	2.9
1	A	106	TYR	2.9
1	A	139	LYS	2.9
1	A	231	ARG	2.9
1	A	153	GLU	2.9
1	A	305	ASP	2.8
1	A	169	LEU	2.8
1	A	184	LEU	2.8
1	A	349	TYR	2.8
1	A	238	GLN	2.7
1	A	354	ILE	2.7
1	A	308	VAL	2.7
1	A	80	TYR	2.7
1	A	253	TYR	2.7
1	A	67	ASP	2.7
1	A	212	TYR	2.7
1	A	175	LEU	2.7
1	A	116	ARG	2.6
1	A	225	GLU	2.6
1	A	248	MET	2.6
1	A	207	LEU	2.6
1	A	54	SER	2.6
1	A	99	TRP	2.6
1	A	326	TYR	2.6
1	A	145	ALA	2.6
1	A	278	ILE	2.6
1	A	283	LEU	2.6
1	A	363	LEU	2.6
1	A	23	THR	2.6
1	A	163	ILE	2.6
1	A	261	ASN	2.5
1	A	133	LEU	2.5
1	A	84	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	317	LYS	2.5
1	A	131	VAL	2.4
1	A	97	LEU	2.4
1	A	152	GLU	2.4
1	A	406	TRP	2.4
1	A	209	PRO	2.4
1	A	107	ILE	2.4
1	A	332	VAL	2.4
1	A	89	ARG	2.4
1	A	59	TRP	2.4
1	A	177	GLU	2.4
1	A	170	CYS	2.3
1	A	313	VAL	2.3
1	A	355	PRO	2.3
1	A	264	LEU	2.3
1	A	149	GLY	2.3
1	A	120	LYS	2.3
1	A	281	ASN	2.3
1	A	421	LEU	2.3
1	A	348	TYR	2.2
1	A	75	LEU	2.2
1	A	356	LEU	2.2
1	A	364	LEU	2.2
1	A	397	GLY	2.2
1	A	396	ASP	2.2
1	A	254	GLN	2.2
1	A	277	ARG	2.2
1	A	402	TYR	2.2
1	A	109	ASP	2.2
1	A	260	LYS	2.2
1	A	192	VAL	2.1
1	A	121	LYS	2.1
1	A	101	LEU	2.1
1	A	392	PHE	2.1
1	A	285	SER	2.1
1	A	330	SER	2.1
1	A	183	ILE	2.1
1	A	142	LYS	2.0
1	A	168	PHE	2.0
1	A	309	PHE	2.0
1	A	374	VAL	2.0
1	A	16	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	138	PRO	2.0
1	A	329	PRO	2.0
1	A	52	ILE	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, 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	QMI	A	1424	21/21	0.61	0.32	3.52	14,17,23,34	1
3	GOL	A	1423	6/6	0.83	0.17	0.98	20,27,29,31	0
5	MYA	A	1425	63/63	0.94	0.13	-0.42	9,15,20,23	0
2	CL	A	1422	1/1	0.75	0.22	-	53,53,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.