WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Dec 18, 2023 – 08:35 am GMT

PDB ID	:	4A30
Title	:	CRYSTAL STRUCTURE OF LEISHMANIA MAJOR N-MYRISTOYLTR ANSFERASE (NMT) WITH BOUND MYRISTOYL-COA AND A PYRA- ZOLE SULPHONAMIDE LIGAND
Authors	:	Robinson, D.A.; Brand, S.; Fairlamb, A.H.; Ferguson, M.A.J.; Frearson, J.A.; Wyatt, P.G.
Deposited on	:	2011-09-29
Resolution	:	1.50 Å(reported)

The following versions of software and data (see references ①) were used in the production of this report:

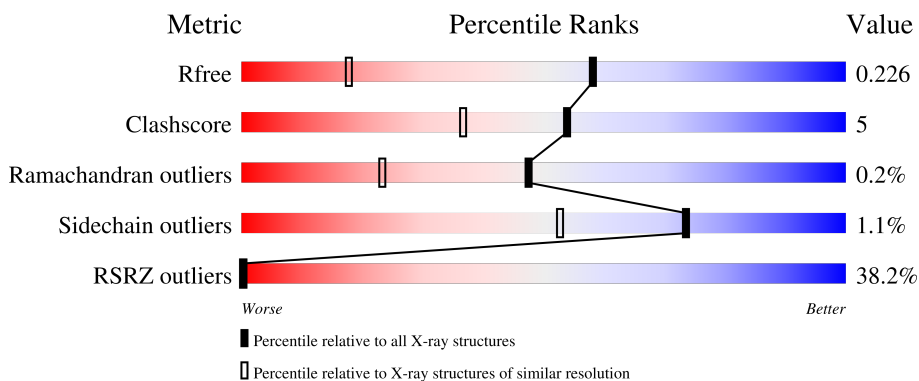|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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	Percentile Ranks	Value
Rfree		0.226
Clashscore		5
Ramachandran outliers		0.2%
Sidechain outliers		1.1%
RSRZ outliers		38.2%

Worse — *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=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	36% / 80% 13% · 6%

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 3342	C 2163	N 560	O 604	S 15	0	0	0

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 1	Cl 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 6	C 3	O 3	0	0

- Molecule 4 is 4-BROMO-2,6-DICHLORO-N-(1,3,5-TRIMETHYL-1H-PYRAZOL-4-YL)BE NZENESULFONAMIDE (three-letter code: QMI) (formula: $C_{12}H_{12}BrCl_2N_3O_2S$).
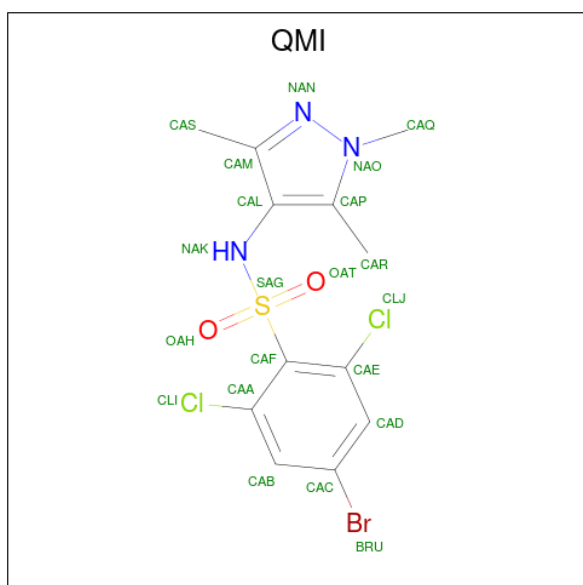
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
4	A	1	Total	Br	C	Cl	N	O	S	0	0
			21	1	12	2	3	2	1		

- Molecule 5 is TETRADECANOYL-COA (three-letter code: MYA) (formula: $C_{35}H_{62}N_7O_{17}P_3S$).
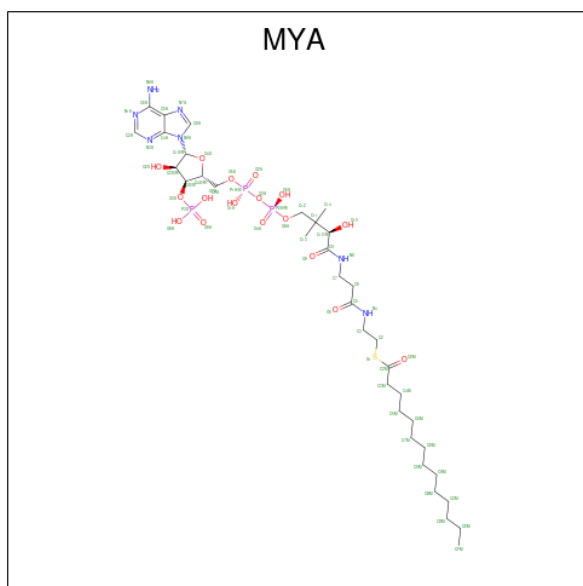
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	S	0	0
			63	35	7	17	3	1		

- 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, DNA and oligosaccharide 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: GLYCYLPEPTIDE N-TETRADECANOYLTRANSFERASE
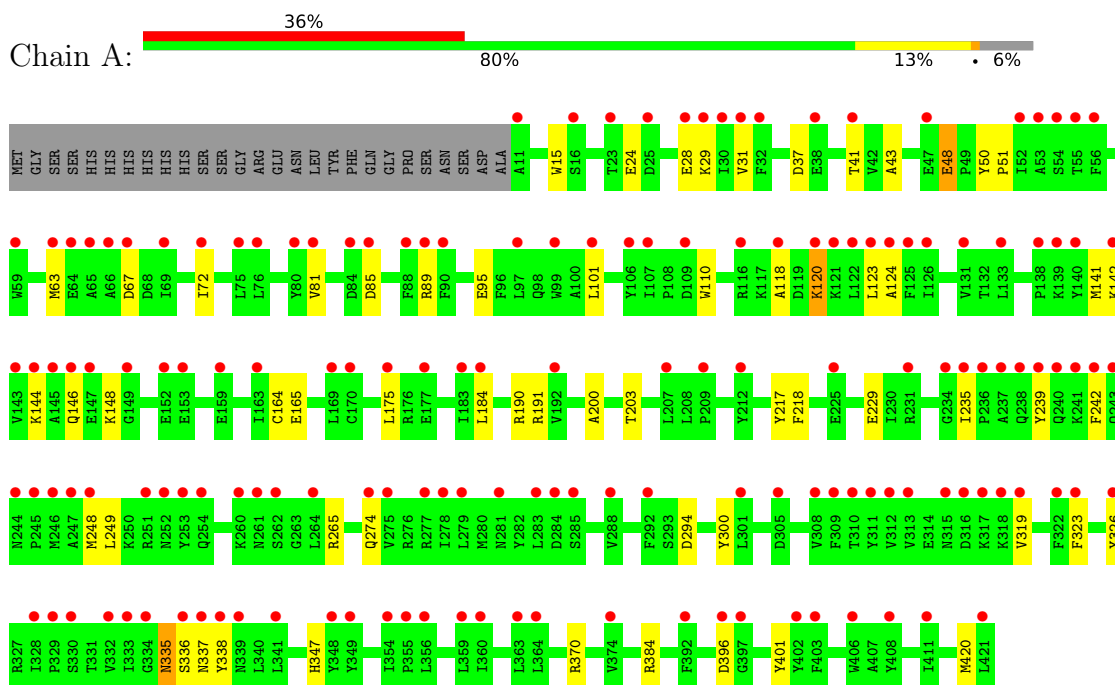
4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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 (7.32%)	wwPDB-VP
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
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.033 for h,-k,-h-l	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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: CL, GOL, MYA, QMI

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(^{o})	Ideal(^{o})
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 ⓘ

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%)	47	23

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%)	73	53

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

Sometimes 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 ⓘ

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 monosaccharides 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	#$|Z| > 2$
4	QMI	A	1424	-	17,22,22	1.95	2 (11%)	24,34,34	2.80	12 (50%)
3	GOL	A	1423	-	5,5,5	0.87	0	5,5,5	1.33	1 (20%)
5	MYA	A	1425	-	57,65,65	1.29	6 (10%)	68,91,91	1.32	10 (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
4	QMI	A	1424	-	-	0/9/11/11	0/2/2/2
3	GOL	A	1423	-	-	0/4/4/4	-
5	MYA	A	1425	-	-	1/60/80/80	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	-6.63	1.68	1.79
5	A	1425	MYA	C2A-N3A	3.39	1.37	1.32
5	A	1425	MYA	C3M-C2M	3.16	1.54	1.50
5	A	1425	MYA	P2A-O5A	-3.11	1.40	1.55
5	A	1425	MYA	O4X-C1X	-3.08	1.36	1.41
5	A	1425	MYA	C3X-C4X	-2.70	1.45	1.52
5	A	1425	MYA	P3X-O3X	2.69	1.64	1.59
4	A	1424	QMI	CAL-NAK	-2.22	1.39	1.43

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1424	QMI	CAD-CAE-CAF	5.88	127.29	121.37
4	A	1424	QMI	OAT-SAG-OAH	-5.49	112.80	119.55
5	A	1425	MYA	N3A-C2A-N1A	-4.98	120.90	128.68
4	A	1424	QMI	CAD-CAE-CLJ	-4.47	111.28	118.49
4	A	1424	QMI	CAM-NAN-NAO	4.02	107.80	104.35
4	A	1424	QMI	CAP-CAL-CAM	3.95	110.82	107.29
4	A	1424	QMI	CAA-CAF-SAG	3.82	125.79	123.27
4	A	1424	QMI	CAB-CAA-CLI	-3.41	112.99	118.49
4	A	1424	QMI	CAR-CAP-CAL	3.03	132.97	129.07
4	A	1424	QMI	BRU-CAC-CAD	-2.77	115.42	119.27
5	A	1425	MYA	C3X-C2X-C1X	-2.45	94.46	99.89
4	A	1424	QMI	CAB-CAA-CAF	2.34	123.72	121.37
5	A	1425	MYA	C2X-C3X-C4X	2.33	107.36	103.22
5	A	1425	MYA	O6A-C12-C11	-2.32	106.82	110.55
3	A	1423	GOL	O2-C2-C3	-2.26	99.18	109.12
5	A	1425	MYA	C2A-N1A-C6A	2.23	122.57	118.75
5	A	1425	MYA	O2M-C2M-C3M	-2.20	121.39	123.99
5	A	1425	MYA	C5A-C6A-N6A	2.15	123.61	120.35
5	A	1425	MYA	O5-C5-N4	-2.13	118.99	123.01
4	A	1424	QMI	OAH-SAG-NAK	2.12	112.05	106.73
5	A	1425	MYA	C4M-C3M-C2M	-2.05	107.78	112.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1424	QMI	CAB-CAC-CAD	2.01	124.48	121.51
5	A	1425	MYA	O5A-P2A-O4A	2.01	122.17	112.24

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1425	MYA	C6-C7-N8-C9

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand QMI A 1424

Bond lengths

Bond angles

Torsions

Rings

Ligand MYA A 1425

Bond lengths

Bond angles

Torsions

Rings
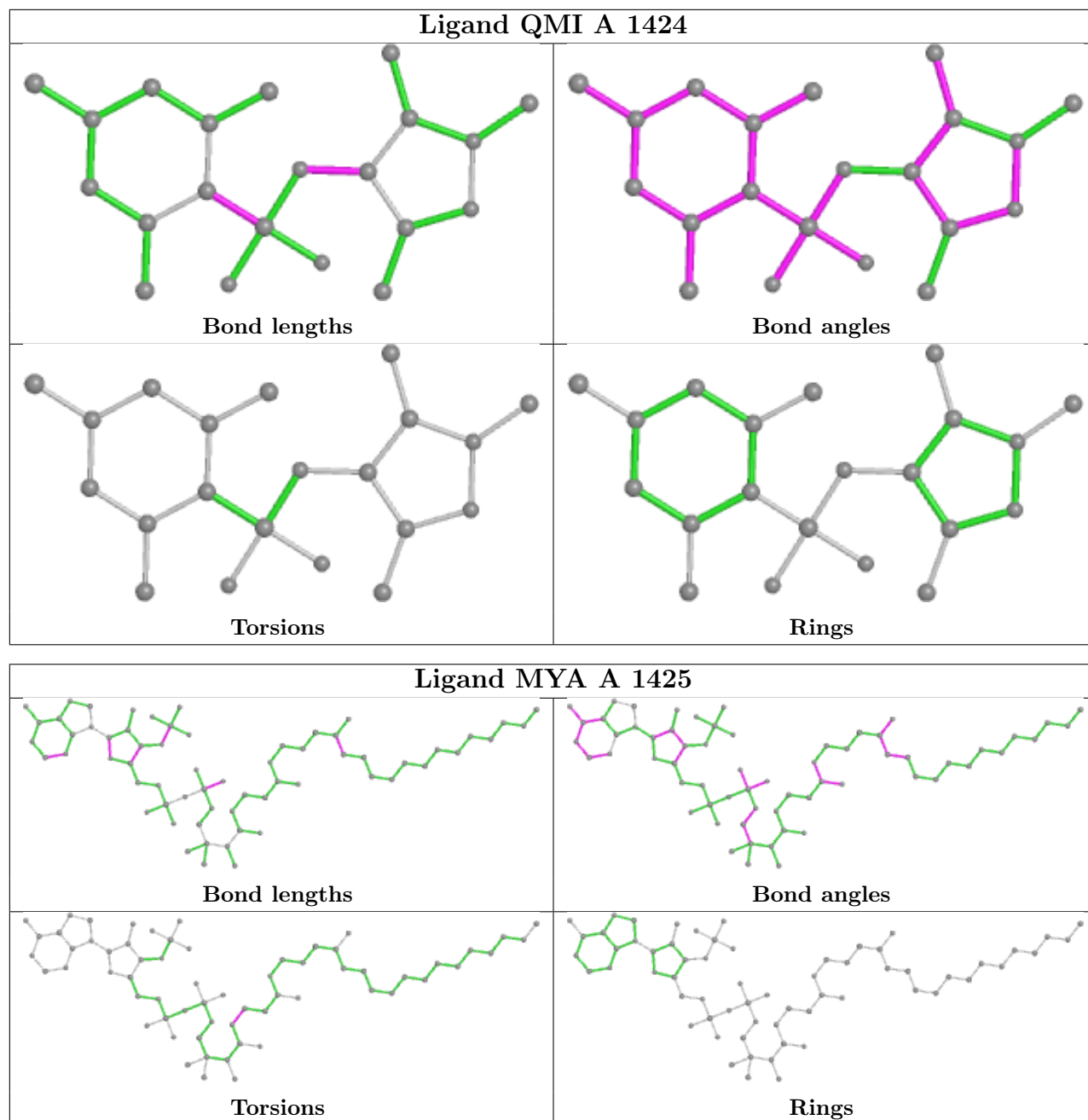
5.7 Other polymers ⓘ

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%)	1.91	157 (38%)	0	0	11, 18, 38, 50	2 (0%)

All (157) 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	5.9
1	A	237	ALA	5.8
1	A	338	TYR	5.6
1	A	315	ASN	5.4
1	A	143	VAL	5.4
1	A	140	TYR	5.3
1	A	245	PRO	5.3
1	A	65	ALA	5.2
1	A	29	LYS	5.2
1	A	244	ASN	5.1
1	A	30	ILE	5.1
1	A	11	ALA	5.1
1	A	322	PHE	4.9
1	A	337	ASN	4.9
1	A	25	ASP	4.9
1	A	64	GLU	4.9
1	A	239	TYR	4.5
1	A	240	GLN	4.5
1	A	316	ASP	4.4
1	A	28	GLU	4.4
1	A	251	ARG	4.4
1	A	56	PHE	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	235	ILE	4.3
1	A	125	PHE	4.2
1	A	275	VAL	4.2
1	A	312	VAL	4.2
1	A	408	TYR	4.2
1	A	122	LEU	4.2
1	A	90	PHE	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	144	LYS	3.8
1	A	341	LEU	3.8
1	A	288	VAL	3.8
1	A	339	ASN	3.8
1	A	146	GLN	3.8
1	A	118	ALA	3.7
1	A	359	LEU	3.7
1	A	301	LEU	3.7
1	A	126	ILE	3.6
1	A	334	GLY	3.6
1	A	81	VAL	3.6
1	A	246	MET	3.6
1	A	318	LYS	3.5
1	A	31	VAL	3.5
1	A	124	ALA	3.4
1	A	159	GLU	3.4
1	A	69	ILE	3.4
1	A	311	TYR	3.4
1	A	41	THR	3.3
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	234	GLY	3.2
1	A	53	ALA	3.2
1	A	88	PHE	3.1
1	A	72	ILE	3.1
1	A	360	ILE	3.1
1	A	310	THR	3.1
1	A	279	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	292	PHE	3.1
1	A	403	PHE	3.0
1	A	55	THR	3.0
1	A	411	ILE	3.0
1	A	38	GLU	3.0
1	A	252	ASN	3.0
1	A	328	ILE	3.0
1	A	66	ALA	2.9
1	A	123	LEU	2.9
1	A	231	ARG	2.9
1	A	139	LYS	2.9
1	A	106	TYR	2.9
1	A	153	GLU	2.9
1	A	333	ILE	2.9
1	A	169	LEU	2.8
1	A	305	ASP	2.8
1	A	184	LEU	2.8
1	A	238	GLN	2.8
1	A	349	TYR	2.8
1	A	67	ASP	2.8
1	A	308	VAL	2.7
1	A	80	TYR	2.7
1	A	212	TYR	2.7
1	A	354	ILE	2.7
1	A	54	SER	2.7
1	A	253	TYR	2.7
1	A	116	ARG	2.7
1	A	175	LEU	2.7
1	A	225	GLU	2.7
1	A	145	ALA	2.7
1	A	248	MET	2.7
1	A	23	THR	2.6
1	A	99	TRP	2.6
1	A	278	ILE	2.6
1	A	326	TYR	2.6
1	A	207	LEU	2.6
1	A	283	LEU	2.6
1	A	363	LEU	2.6
1	A	163	ILE	2.6
1	A	133	LEU	2.6
1	A	261	ASN	2.6
1	A	84	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	406	TRP	2.5
1	A	317	LYS	2.5
1	A	209	PRO	2.5
1	A	131	VAL	2.5
1	A	152	GLU	2.4
1	A	97	LEU	2.4
1	A	332	VAL	2.4
1	A	89	ARG	2.4
1	A	107	ILE	2.4
1	A	59	TRP	2.4
1	A	149	GLY	2.4
1	A	120	LYS	2.3
1	A	313	VAL	2.3
1	A	355	PRO	2.3
1	A	264	LEU	2.3
1	A	177	GLU	2.3
1	A	170	CYS	2.3
1	A	281	ASN	2.3
1	A	397	GLY	2.3
1	A	75	LEU	2.3
1	A	421	LEU	2.3
1	A	348	TYR	2.3
1	A	277	ARG	2.2
1	A	356	LEU	2.2
1	A	396	ASP	2.2
1	A	402	TYR	2.2
1	A	260	LYS	2.2
1	A	254	GLN	2.2
1	A	364	LEU	2.2
1	A	109	ASP	2.2
1	A	192	VAL	2.2
1	A	121	LYS	2.2
1	A	101	LEU	2.1
1	A	142	LYS	2.1
1	A	285	SER	2.1
1	A	330	SER	2.1
1	A	392	PHE	2.1
1	A	183	ILE	2.1
1	A	329	PRO	2.0
1	A	319	VAL	2.0
1	A	138	PRO	2.0
1	A	309	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	274	GLN	2.0
1	A	52	ILE	2.0
1	A	374	VAL	2.0
1	A	16	SER	2.0

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 ⓘ

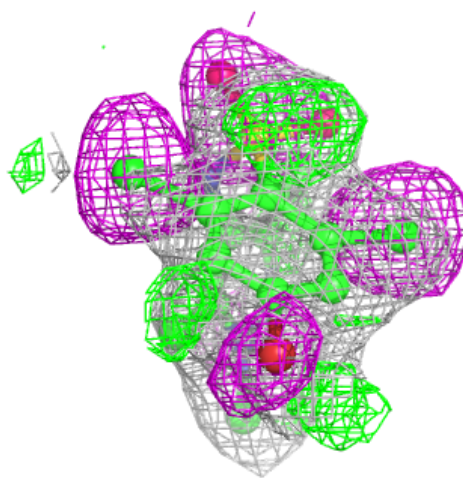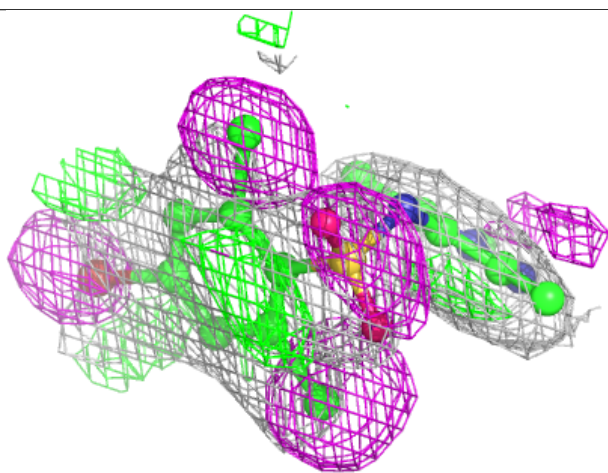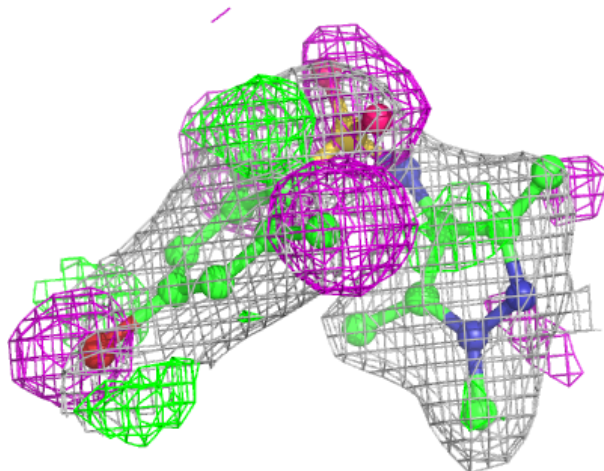There are no monosaccharides in this entry.

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. 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.
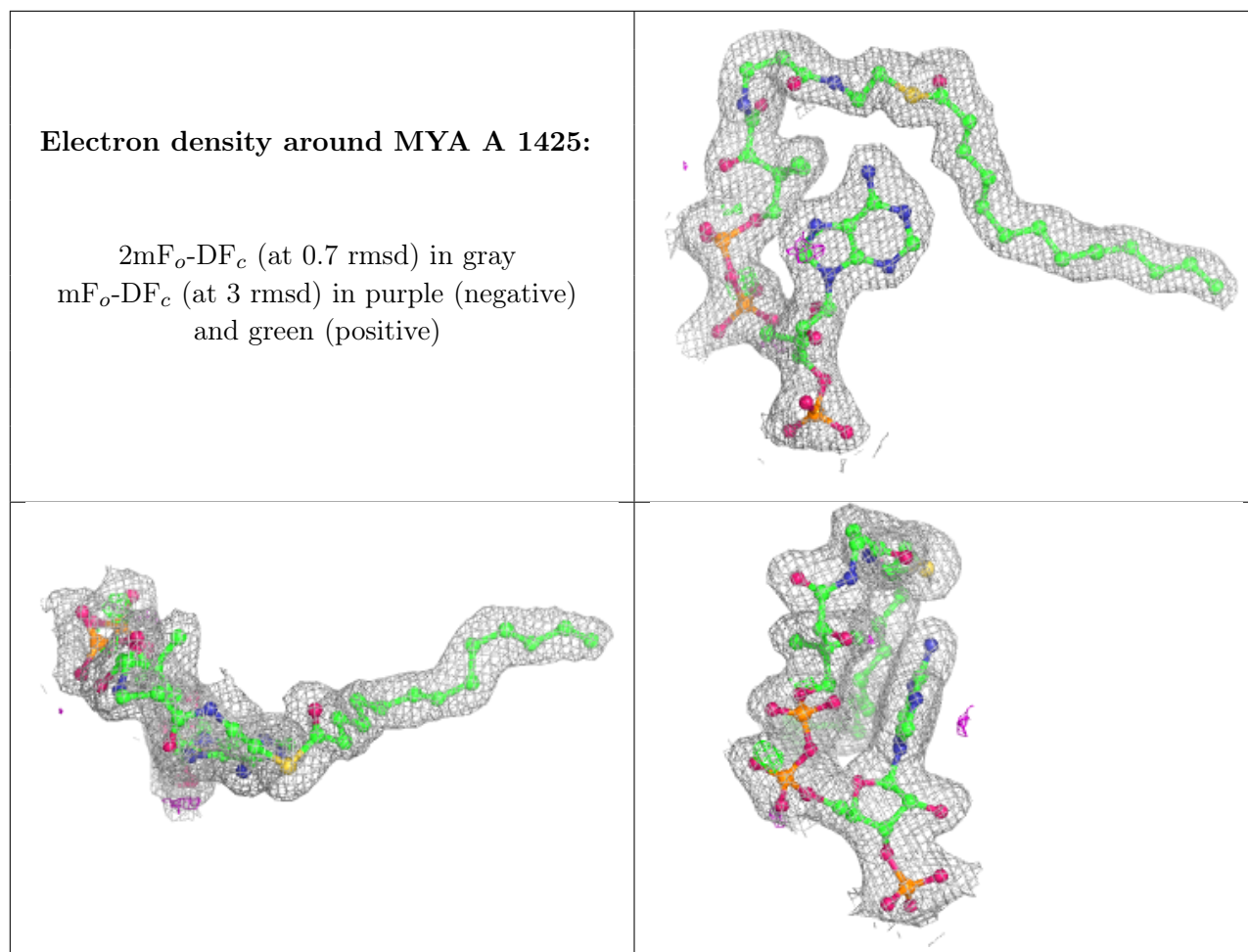
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	QMI	A	1424	21/21	0.60	0.32	14,17,23,34	1
2	CL	A	1422	1/1	0.74	0.23	53,53,53,53	0
3	GOL	A	1423	6/6	0.83	0.17	20,27,29,31	0
5	MYA	A	1425	63/63	0.94	0.13	9,15,20,23	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around QMI A 1424:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around MYA A 1425:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

6.5 Other polymers ⓘ

There are no such residues in this entry.