



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 04:56 pm BST

PDB ID : 3IU2
Title : Crystal Structure of human type-I N-myristoyltransferase with bound myristoyl-CoA and inhibitor DDD90096
Authors : Qiu, W.; Hutchinson, A.; Wernimont, A.; Lin, Y.-H.; Kania, A.; Ravichandran, M.; Kozieradzki, I.; Cossar, D.; Schapira, M.; Arrowsmith, C.H.; Bountra, C.; Weigelt, J.; Edwards, A.M.; Wyatt, P.G.; Ferguson, M.A.J.; Frearson, J.A.; Brand, S.Y.; Robinson, D.A.; Bochkarev, A.; Hui, R.; Structural Genomics Consortium (SGC)
Deposited on : 2009-08-29
Resolution : 1.73 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

<https://www.wwpdb.org/validation/2017/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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

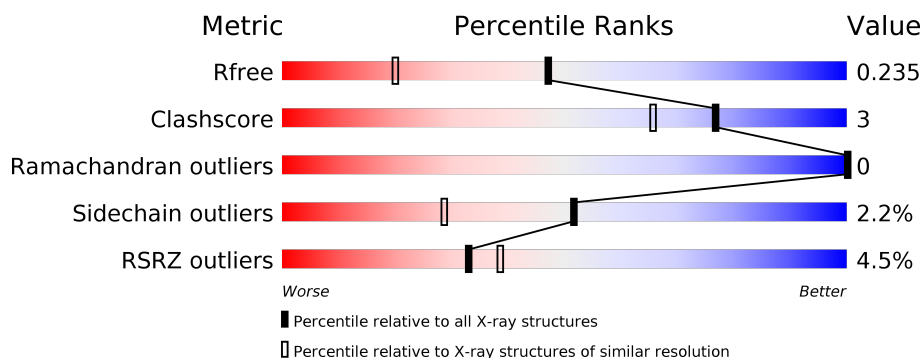
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.73 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}	130704	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

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 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 $\leq 5\%$. 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	383	<div> <div>5%</div> <div> <div></div> <div>93%</div> <div>6% •</div> </div> </div>
1	B	383	<div> <div>4%</div> <div> <div></div> <div>91%</div> <div>7% ••</div> </div> </div>

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
2	MYA	A	1001	X	-	-	-
2	MYA	B	2001	X	-	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7177 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.

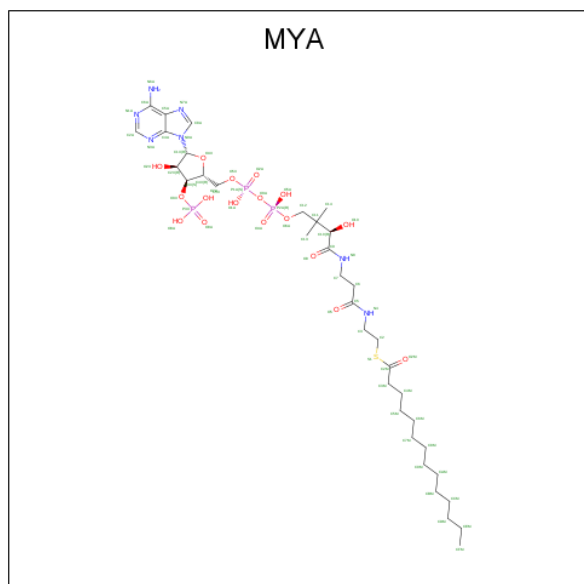
- Molecule 1 is a protein called Glycylpeptide N-tetradecanoyltransferase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	382	Total	C	N	O	S	0	5	0
			3157	2049	530	562	16			
1	B	379	Total	C	N	O	S	0	4	0
			3137	2036	533	552	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	114	GLY	-	EXPRESSION TAG	UNP P30419
B	114	GLY	-	EXPRESSION TAG	UNP P30419

- Molecule 2 is TETRADECANOYL-COA (three-letter code: MYA) (formula: $C_{35}H_{62}N_7O_{17}P_3S$).



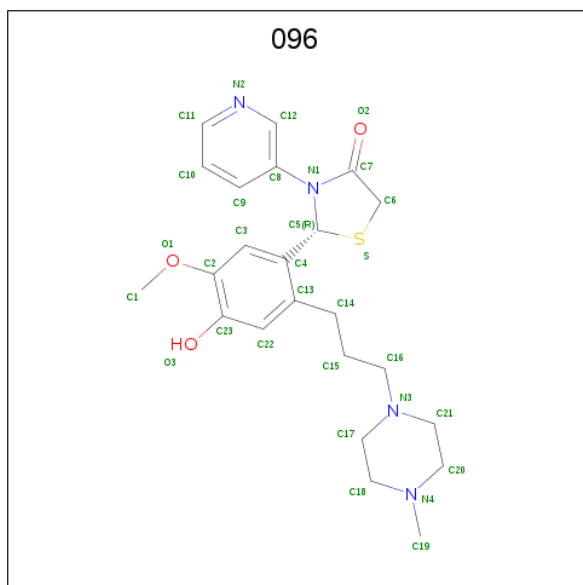
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			63	35	7	17	3		

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

- Molecule 3 is (2R)-2-{4-hydroxy-5-methoxy-2-[3-(4-methylpiperazin-1-yl)propyl]phenyl}-3-pyridin-3-yl-1,3-thiazolidin-4-one (three-letter code: 096) (formula: C₂₃H₃₀N₄O₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			31	23	4	3	1		
3	B	1	Total	C	N	O	S	0	0
			31	23	4	3	1		

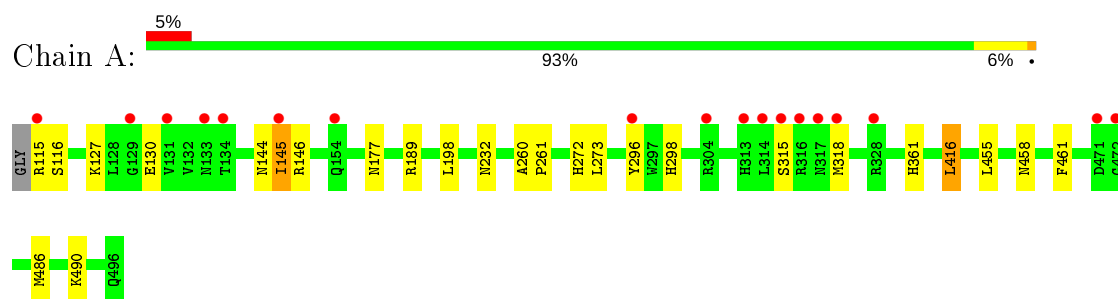
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	339	Total	O	0	0
			339	339		
4	B	356	Total	O	0	0
			356	356		

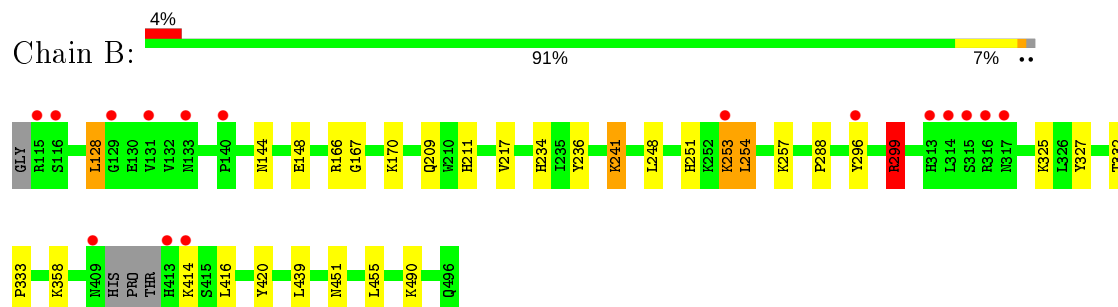
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 1



- Molecule 1: Glycylpeptide N-tetradecanoyltransferase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.57Å 77.74Å 179.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.60 – 1.73 19.60 – 1.73	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.60-1.73) 98.1 (19.60-1.73)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 1.73Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.207 , 0.235 0.207 , 0.235	Depositor DCC
R_{free} test set	4214 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	18.3	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7177	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.93% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MYA, 096

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	0.46	0/3262	0.56	1/4434 (0.0%)
1	B	0.46	1/3236 (0.0%)	0.57	2/4391 (0.0%)
All	All	0.46	1/6498 (0.0%)	0.57	3/8825 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	217	VAL	CB-CG2	-5.64	1.41	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	416	LEU	CA-CB-CG	8.68	135.26	115.30
1	B	299	ARG	NE-CZ-NH2	-5.43	117.59	120.30
1	B	144	ASN	N-CA-C	-5.34	96.58	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3157	0	3149	21	0
1	B	3137	0	3150	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	63	0	58	0	0
2	B	63	0	58	0	0
3	A	31	0	30	1	0
3	B	31	0	30	1	0
4	A	339	0	0	0	0
4	B	356	0	0	4	0
All	All	7177	0	6475	39	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 3.

All (39) 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:115:ARG:N	1:A:116:SER:HA	1.73	1.04
1:B:296[B]:TYR:CE1	1:B:451:ASN:HB3	2.15	0.81
1:B:296[B]:TYR:HH	1:B:420:TYR:HD1	1.28	0.80
1:B:296[B]:TYR:HE1	1:B:451:ASN:HB3	1.45	0.79
1:A:296[B]:TYR:HD1	1:A:298:HIS:CE1	2.03	0.76
1:A:115:ARG:N	1:A:116:SER:CA	2.55	0.67
1:B:166:ARG:HG3	1:B:170:LYS:HE2	1.79	0.64
1:A:296[B]:TYR:CD1	1:A:298:HIS:CE1	2.84	0.64
1:A:361:HIS:CD2	1:A:490:LYS:HD2	2.32	0.63
1:A:145[A]:ILE:HD13	1:A:273:LEU:HG	1.81	0.62
1:A:315:SER:HB3	1:A:318:MET:HB2	1.82	0.62
1:A:296[B]:TYR:CD1	1:A:298:HIS:HE1	2.18	0.60
1:B:234:HIS:CE1	1:B:236:TYR:O	2.55	0.59
1:B:296[B]:TYR:OH	1:B:420:TYR:HD1	1.87	0.58
1:A:486:MET:HB2	1:A:490:LYS:HE2	1.88	0.55
1:B:209[A]:GLN:HG3	4:B:520:HOH:O	2.07	0.54
1:A:232:ASN:HD21	1:B:241:LYS:NZ	2.05	0.54
1:B:148:GLU:HG2	4:B:628:HOH:O	2.08	0.52
1:B:251:HIS:CE1	1:B:253:LYS:HD2	2.45	0.52
1:A:145[A]:ILE:HG12	1:A:146:ARG:N	2.25	0.51
1:B:299:ARG:HG2	1:B:439:LEU:HD22	1.93	0.50
1:A:145[A]:ILE:CD1	1:A:273:LEU:HG	2.43	0.48
1:A:232:ASN:ND2	1:B:241:LYS:HZ1	2.12	0.47
1:B:167:GLY:HA2	1:B:170:LYS:HE3	1.98	0.45
1:B:254:LEU:HD23	1:B:257:LYS:HD2	1.98	0.45
1:A:127:LYS:O	1:A:130:GLU:HG2	2.17	0.45
3:B:2002:096:H3	3:B:2002:096:C8	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:ASN:HA	1:A:461:PHE:CE2	2.52	0.44
1:A:177:ASN:O	1:A:189:ARG:HD2	2.18	0.44
1:B:299:ARG:NH2	1:B:327:TYR:O	2.51	0.44
1:B:358:LYS:HE2	4:B:823:HOH:O	2.18	0.43
1:A:296[A]:TYR:CE2	3:A:1002:096:H15A	2.54	0.43
1:B:128:LEU:HD13	1:B:288:PRO:HA	1.99	0.43
1:B:211:HIS:HD2	4:B:658:HOH:O	2.02	0.42
1:A:145[B]:ILE:HD12	1:A:272:HIS:HB3	2.01	0.41
1:B:332:THR:HG22	1:B:333:PRO:HD2	2.01	0.41
1:A:232:ASN:HD21	1:B:241:LYS:HZ1	1.67	0.41
1:A:260:ALA:HB3	1:A:261:PRO:HD3	2.03	0.41

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	385/383 (100%)	377 (98%)	8 (2%)	0	100	100
1	B	379/383 (99%)	372 (98%)	7 (2%)	0	100	100
All	All	764/766 (100%)	749 (98%)	15 (2%)	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	351/348 (101%)	346 (99%)	5 (1%)	67	50
1	B	348/348 (100%)	336 (97%)	12 (3%)	37	13
All	All	699/696 (100%)	682 (98%)	17 (2%)	52	26

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	145[A]	ILE
1	A	145[B]	ILE
1	A	198	LEU
1	A	416	LEU
1	A	455	LEU
1	B	128	LEU
1	B	241	LYS
1	B	248	LEU
1	B	253	LYS
1	B	254	LEU
1	B	299	ARG
1	B	325	LYS
1	B	414	LYS
1	B	416	LEU
1	B	455	LEU
1	B	490[A]	LYS
1	B	490[B]	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	GLN
1	A	232	ASN
1	A	234	HIS
1	A	317	ASN
1	A	413	HIS
1	A	475	GLN
1	A	496	GLN
1	B	154	GLN
1	B	211	HIS
1	B	234	HIS
1	B	361	HIS
1	B	409	ASN
1	B	428	GLN

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Mol	Chain	Res	Type
1	B	458	ASN

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](#)

4 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	MYA	A	1001	-	54,65,65	1.16	5 (9%)	67,91,91	1.71	10 (14%)
3	096	A	1002	-	34,34,34	1.33	3 (8%)	45,47,47	2.84	17 (37%)
2	MYA	B	2001	-	54,65,65	1.18	4 (7%)	67,91,91	1.63	8 (11%)
3	096	B	2002	-	34,34,34	1.22	2 (5%)	45,47,47	2.80	18 (40%)

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	MYA	A	1001	-	1/1/12/14	14/59/80/80	0/3/3/3
3	096	A	1002	-	-	5/16/39/39	0/4/4/4
2	MYA	B	2001	-	1/1/12/14	16/59/80/80	0/3/3/3
3	096	B	2002	-	-	5/16/39/39	1/4/4/4

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1002	096	C5-S	-6.36	1.76	1.84
3	B	2002	096	C5-S	-5.78	1.77	1.84
2	A	1001	MYA	O4X-C1X	3.85	1.46	1.41
2	B	2001	MYA	P3X-O9A	3.55	1.62	1.50
2	B	2001	MYA	O4X-C1X	3.20	1.45	1.41
2	B	2001	MYA	P2A-O4A	3.17	1.62	1.50
2	B	2001	MYA	P1A-O2A	3.12	1.62	1.50
2	A	1001	MYA	P2A-O4A	3.09	1.61	1.50
2	A	1001	MYA	P1A-O2A	2.91	1.61	1.50
2	A	1001	MYA	P3X-O9A	2.73	1.59	1.50
3	B	2002	096	C6-S	-2.41	1.75	1.80
3	A	1002	096	C6-S	-2.41	1.75	1.80
2	A	1001	MYA	C6-C5	2.11	1.55	1.51
3	A	1002	096	C7-N1	-2.07	1.35	1.37

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2002	096	C20-N4-C18	8.93	122.01	109.52
3	A	1002	096	C20-N4-C18	8.11	120.86	109.52
2	A	1001	MYA	O2M-C2M-C3M	6.97	121.43	109.02
2	B	2001	MYA	O2M-C2M-C3M	6.57	120.72	109.02
3	A	1002	096	C19-N4-C18	5.97	119.59	110.66
3	A	1002	096	C19-N4-C20	5.94	119.55	110.66
3	B	2002	096	C19-N4-C18	5.79	119.32	110.66
3	A	1002	096	C7-C6-S	-5.74	102.69	107.60
3	B	2002	096	C21-N3-C17	5.64	121.53	108.83
3	A	1002	096	C6-C7-N1	5.52	115.92	112.14
3	A	1002	096	C21-N3-C17	5.46	121.13	108.83
3	B	2002	096	C19-N4-C20	5.35	118.67	110.66
3	B	2002	096	C7-C6-S	-4.80	103.49	107.60
3	B	2002	096	C6-C7-N1	4.77	115.41	112.14
2	B	2001	MYA	C14-C11-C10	4.75	117.06	108.82
2	A	1001	MYA	C14-C11-C10	4.60	116.80	108.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2001	MYA	N3A-C2A-N1A	-4.48	121.67	128.68
2	A	1001	MYA	N3A-C2A-N1A	-4.45	121.72	128.68
2	A	1001	MYA	C13-C11-C10	-3.94	101.99	108.82
2	B	2001	MYA	C10-C9-N8	-3.94	108.74	116.58
3	A	1002	096	C16-N3-C21	3.91	121.23	111.23
2	A	1001	MYA	C10-C9-N8	-3.90	108.81	116.58
3	B	2002	096	C6-S-C5	3.76	98.83	93.14
3	A	1002	096	C6-S-C5	3.75	98.82	93.14
3	A	1002	096	C17-C18-N4	-3.66	106.67	110.80
3	B	2002	096	O1-C2-C23	3.66	119.86	114.57
3	A	1002	096	C8-N1-C5	3.58	123.41	118.91
3	B	2002	096	C16-N3-C21	3.51	120.22	111.23
3	A	1002	096	O1-C2-C23	3.46	119.58	114.57
3	B	2002	096	C15-C16-N3	-3.26	105.63	113.84
2	B	2001	MYA	O10-C10-C11	3.26	117.92	110.25
2	A	1001	MYA	O10-C10-C11	3.16	117.69	110.25
2	B	2001	MYA	C13-C11-C10	-3.12	103.41	108.82
3	B	2002	096	C21-C20-N4	-3.02	107.40	110.80
3	B	2002	096	C1-O1-C2	3.00	122.06	117.53
3	B	2002	096	C8-N1-C5	2.97	122.64	118.91
2	A	1001	MYA	C6-C7-N8	-2.82	106.21	111.90
3	A	1002	096	C15-C16-N3	-2.81	106.76	113.84
2	B	2001	MYA	P2A-O3A-P1A	-2.81	123.19	132.83
3	B	2002	096	C16-N3-C17	2.74	118.25	111.23
3	B	2002	096	C17-C18-N4	-2.68	107.78	110.80
3	A	1002	096	C21-C20-N4	-2.65	107.81	110.80
3	A	1002	096	C11-N2-C12	2.64	121.42	116.85
2	A	1001	MYA	P2A-O3A-P1A	-2.57	123.99	132.83
3	B	2002	096	C11-N2-C12	2.53	121.22	116.85
3	A	1002	096	C16-N3-C17	2.50	117.64	111.23
3	A	1002	096	C1-O1-C2	2.50	121.30	117.53
3	A	1002	096	C15-C14-C13	-2.48	106.62	114.10
2	B	2001	MYA	C6-C7-N8	-2.41	107.04	111.90
3	B	2002	096	C15-C14-C13	-2.12	107.70	114.10
3	B	2002	096	O1-C2-C3	-2.10	120.50	124.12
2	A	1001	MYA	C4A-C5A-N7A	-2.04	107.27	109.40
2	A	1001	MYA	O4X-C1X-C2X	-2.02	103.97	106.93

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1001	MYA	C10

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Mol	Chain	Res	Type	Atom
2	B	2001	MYA	C10

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	MYA	O10-C10-C9-O9
2	A	1001	MYA	C9-C10-C11-C14
2	A	1001	MYA	O10-C10-C11-C12
2	A	1001	MYA	O10-C10-C11-C13
2	A	1001	MYA	O10-C10-C11-C14
2	A	1001	MYA	S1-C2M-C3M-C4M
3	A	1002	096	C13-C14-C15-C16
2	B	2001	MYA	O10-C10-C9-O9
2	B	2001	MYA	C9-C10-C11-C12
2	B	2001	MYA	C9-C10-C11-C13
2	B	2001	MYA	C9-C10-C11-C14
2	B	2001	MYA	O10-C10-C11-C12
2	B	2001	MYA	O10-C10-C11-C13
2	B	2001	MYA	O10-C10-C11-C14
3	B	2002	096	C3-C2-O1-C1
3	B	2002	096	C23-C2-O1-C1
3	A	1002	096	C23-C2-O1-C1
3	A	1002	096	C3-C2-O1-C1
3	A	1002	096	C15-C16-N3-C17
3	B	2002	096	C15-C16-N3-C17
3	A	1002	096	C14-C15-C16-N3
3	B	2002	096	C13-C14-C15-C16
2	B	2001	MYA	C5-C6-C7-N8
3	B	2002	096	C14-C15-C16-N3
2	B	2001	MYA	C11-C10-C9-N8
2	A	1001	MYA	O10-C10-C9-N8
2	B	2001	MYA	O10-C10-C9-N8
2	A	1001	MYA	C9-C10-C11-C13
2	B	2001	MYA	C3X-O3X-P3X-O8A
2	B	2001	MYA	C8M-C9M-CAM-CBM
2	A	1001	MYA	C11-C10-C9-O9
2	B	2001	MYA	C11-C10-C9-O9
2	A	1001	MYA	C8M-C9M-CAM-CBM
2	A	1001	MYA	C11-C10-C9-N8
2	A	1001	MYA	C5-C6-C7-N8
2	B	2001	MYA	CAM-CBM-CCM-CDM
2	B	2001	MYA	P2A-O3A-P1A-O1A

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Mol	Chain	Res	Type	Atoms
2	A	1001	MYA	C5X-O5X-P1A-O2A
2	A	1001	MYA	C9-C10-C11-C12
2	B	2001	MYA	C5M-C6M-C7M-C8M

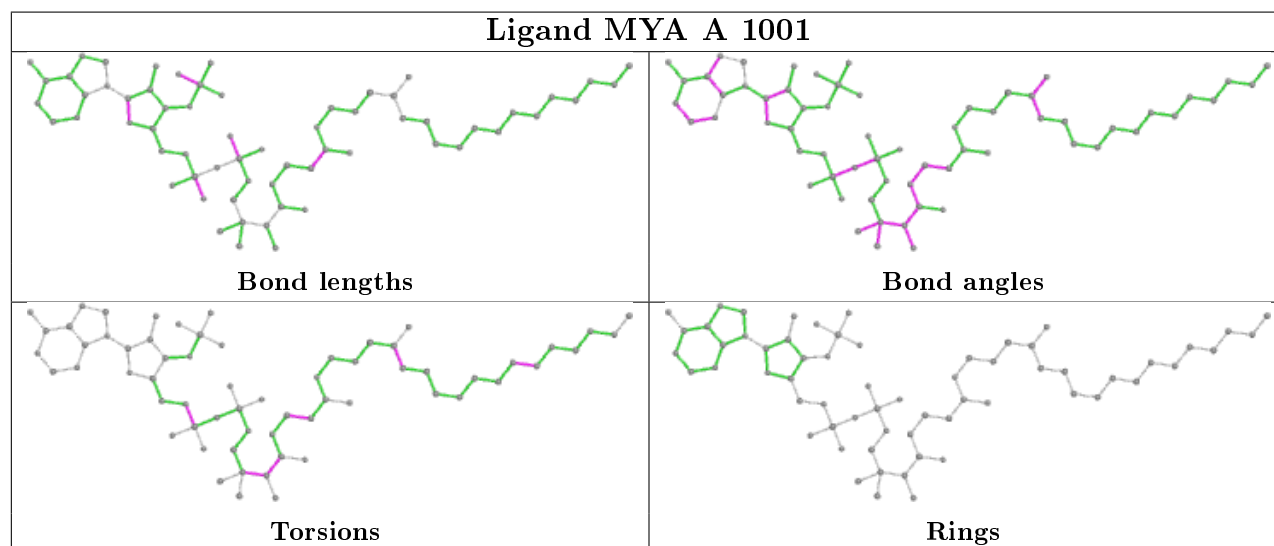
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2002	096	C17-C18-C20-C21-N3-N4

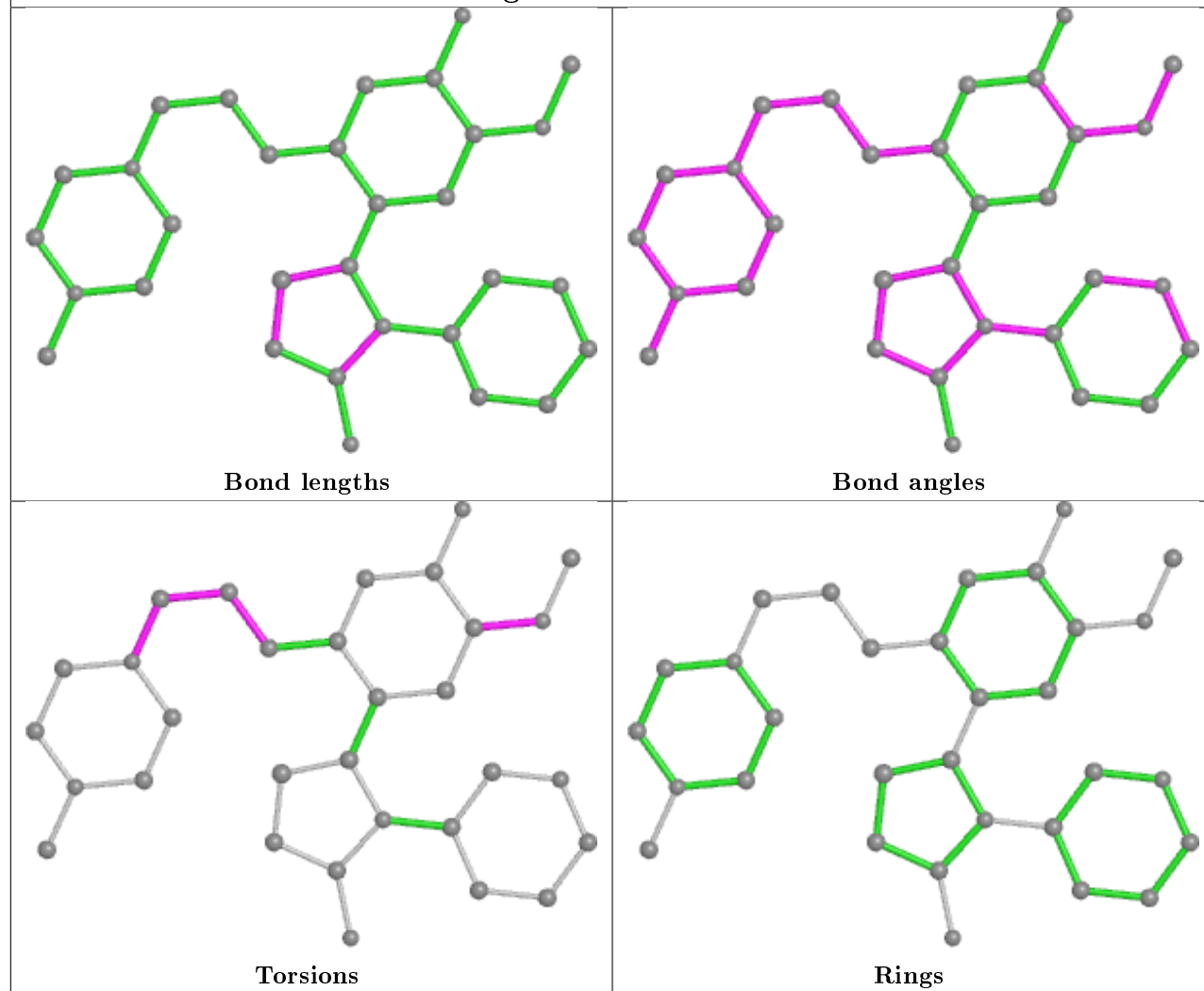
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1002	096	1	0
3	B	2002	096	1	0

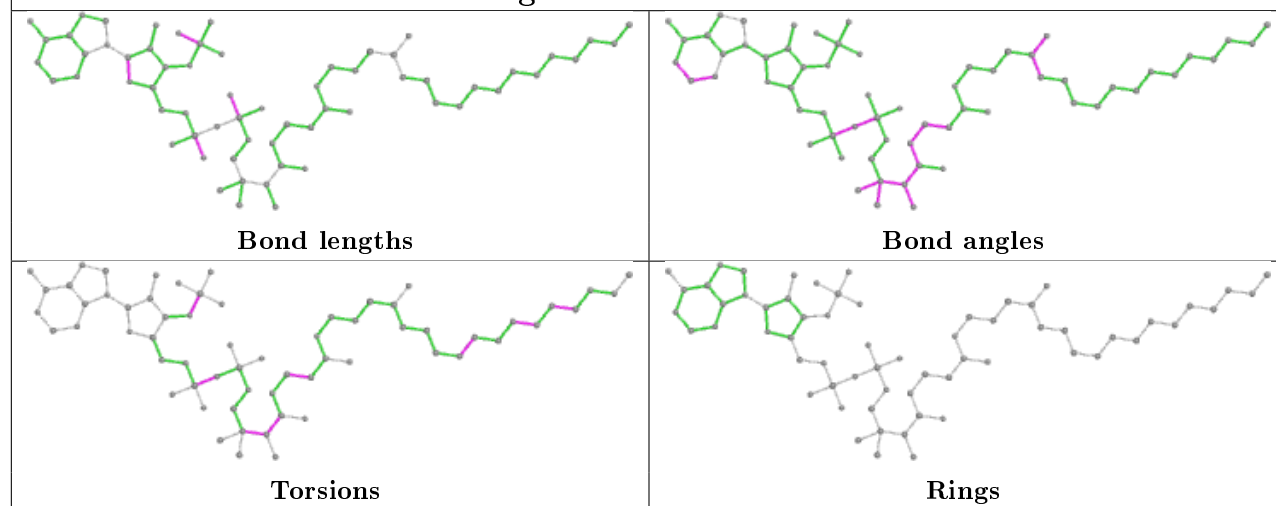
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.

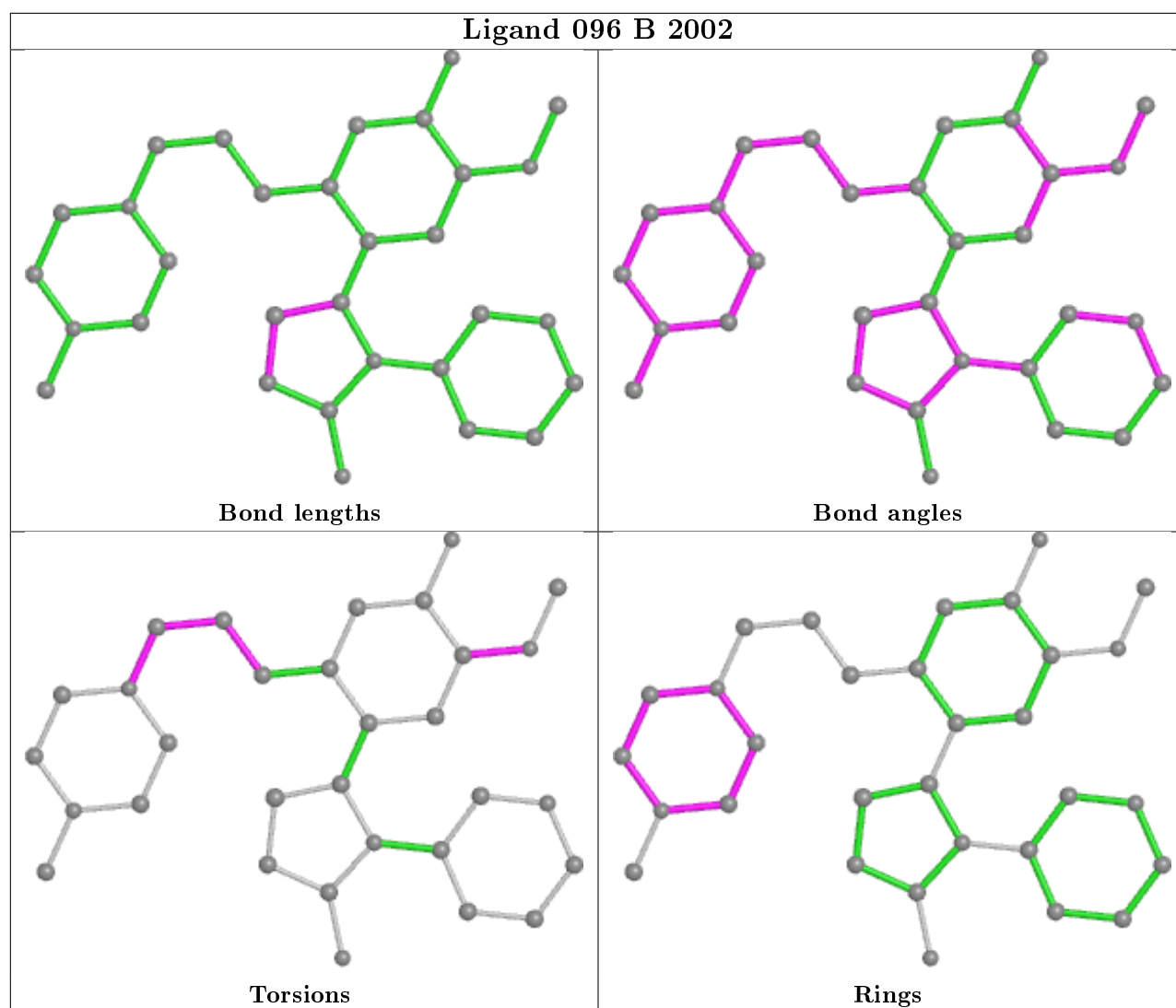


Ligand 096 A 1002



Ligand MYA B 2001





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	382/383 (99%)	0.34	18 (4%) 31 36	10, 16, 29, 40	0
1	B	379/383 (98%)	0.30	16 (4%) 36 41	10, 16, 27, 38	0
All	All	761/766 (99%)	0.32	34 (4%) 33 38	10, 16, 29, 40	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	316	ARG	5.7
1	B	316	ARG	4.8
1	B	115	ARG	4.7
1	A	115	ARG	4.0
1	B	133	ASN	3.9
1	A	315	SER	3.9
1	B	131	VAL	3.8
1	B	313	HIS	3.8
1	B	413	HIS	3.7
1	A	129	GLY	3.4
1	A	314	LEU	3.4
1	A	313	HIS	3.4
1	B	296[A]	TYR	3.3
1	B	315	SER	3.2
1	A	317	ASN	3.1
1	B	409	ASN	3.0
1	A	131	VAL	2.9
1	A	133	ASN	2.9
1	A	328	ARG	2.8
1	A	154	GLN	2.8
1	B	314	LEU	2.8
1	B	116	SER	2.7
1	A	304	ARG	2.6
1	A	296[A]	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	472	GLY	2.5
1	A	134	THR	2.5
1	B	253	LYS	2.4
1	A	318	MET	2.2
1	A	145[A]	ILE	2.2
1	B	129	GLY	2.2
1	B	414	LYS	2.1
1	B	140	PRO	2.1
1	A	471	ASP	2.1
1	B	317	ASN	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](#)

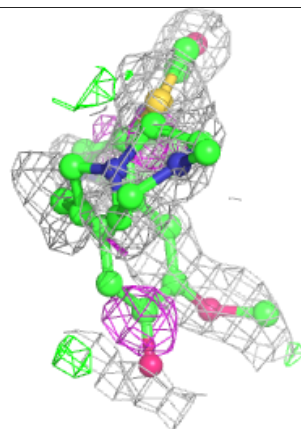
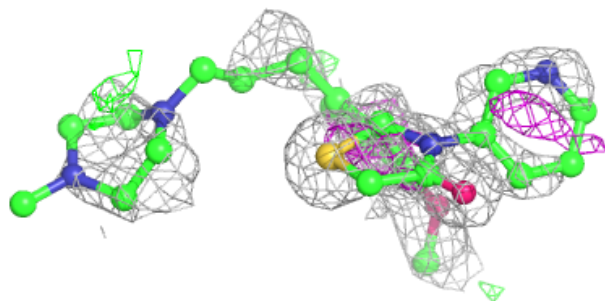
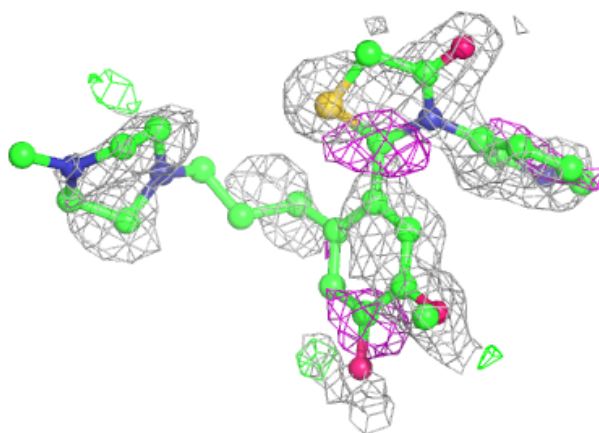
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	096	B	2002	31/31	0.63	0.34	39,44,49,49	0
3	096	A	1002	31/31	0.87	0.18	19,27,34,34	0
2	MYA	B	2001	63/63	0.94	0.09	6,18,20,20	0
2	MYA	A	1001	63/63	0.94	0.09	7,16,19,21	0

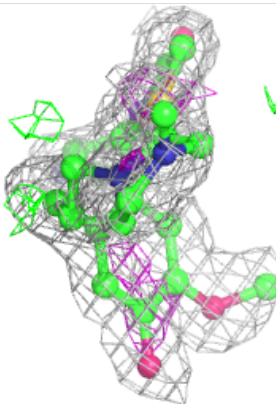
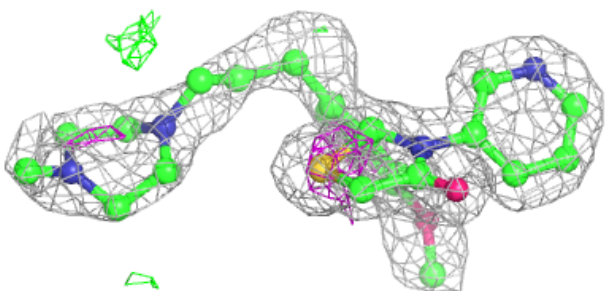
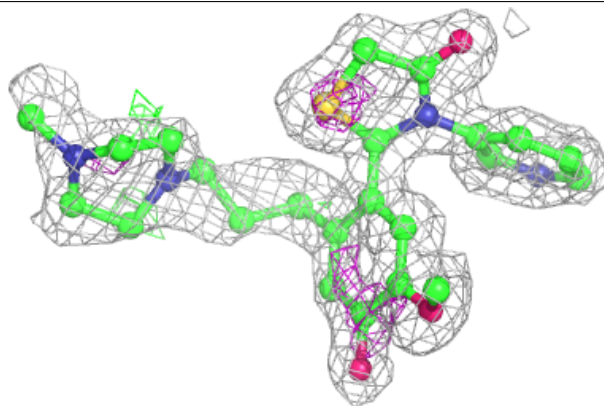
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 096 B 2002:

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

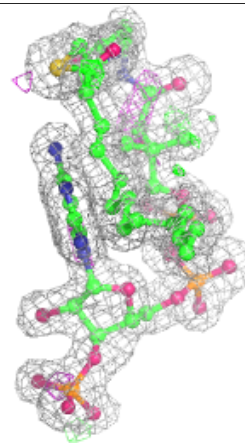
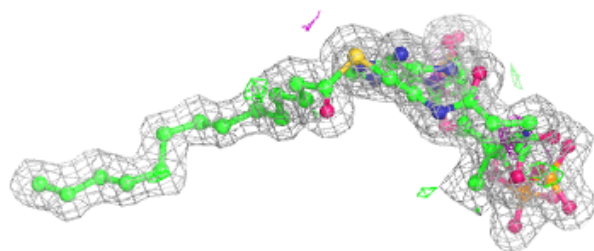
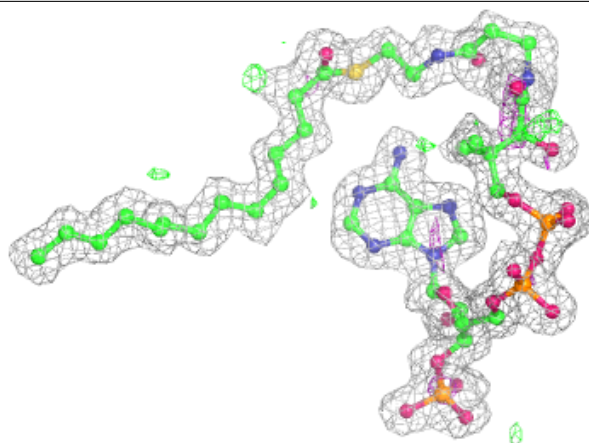
**Electron density around 096 A 1002:**

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



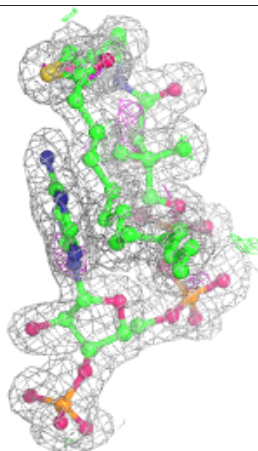
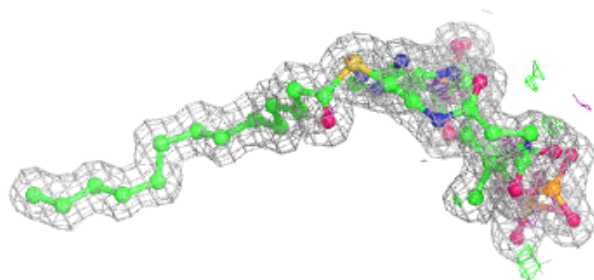
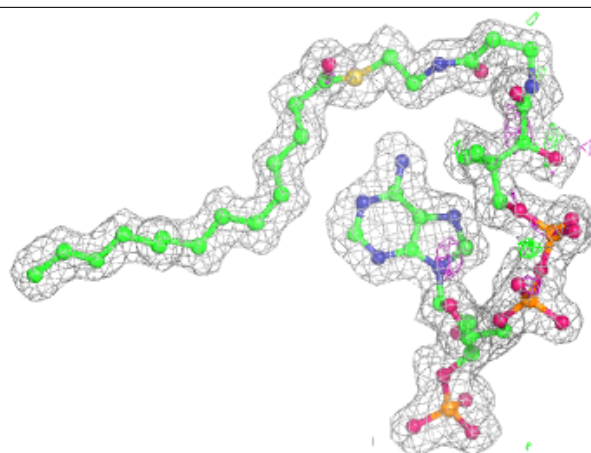
Electron density around MYA B 2001:

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



Electron density around MYA A 1001:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.