



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 01:43 pm BST

PDB ID : 1P3D
Title : Crystal Structure of UDP-N-acetylmuramic acid:L-alanine ligase (MurC) in Complex with UMA and ANP.
Authors : Mol, C.D.; Brooun, A.; Dougan, D.R.; Hilgers, M.T.; Tari, L.W.; Wijnands, R.A.; Knuth, M.W.; McRee, D.E.; Swanson, R.V.
Deposited on : 2003-04-17
Resolution : 1.70 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

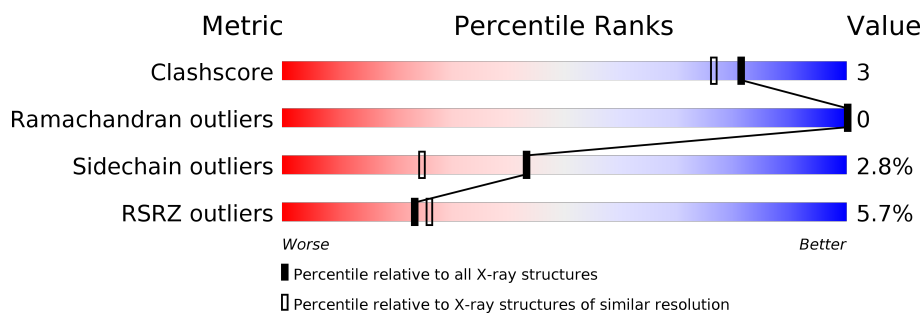
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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))
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	475	<div> <div>8%</div> <div>88%</div> <div>8%</div> <div>..</div> </div>
1	B	475	<div> <div>3%</div> <div>87%</div> <div>9%</div> <div>.</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8054 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 UDP-N-acetylmuramate--alanine ligase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	463	Total	C	N	O	S	Se	0	7	0
			3568	2250	623	678	3	14			
1	B	460	Total	C	N	O	S	Se	0	3	0
			3531	2223	617	674	3	14			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP P45066
A	15	MSE	MET	MODIFIED RESIDUE	UNP P45066
A	31	MSE	MET	MODIFIED RESIDUE	UNP P45066
A	110	MSE	MET	MODIFIED RESIDUE	UNP P45066
A	115	MSE	MET	MODIFIED RESIDUE	UNP P45066
A	135	MSE	MET	MODIFIED RESIDUE	UNP P45066
A	138	MSE	MET	MODIFIED RESIDUE	UNP P45066
A	187	MSE	MET	MODIFIED RESIDUE	UNP P45066
A	194	MSE	MET	MODIFIED RESIDUE	UNP P45066
A	199	MSE	MET	MODIFIED RESIDUE	UNP P45066
A	209	MSE	MET	MODIFIED RESIDUE	UNP P45066
A	228	MSE	MET	MODIFIED RESIDUE	UNP P45066
A	236	MSE	MET	MODIFIED RESIDUE	UNP P45066
A	371	MSE	MET	MODIFIED RESIDUE	UNP P45066
A	400	MSE	MET	MODIFIED RESIDUE	UNP P45066
B	1	MSE	MET	MODIFIED RESIDUE	UNP P45066
B	15	MSE	MET	MODIFIED RESIDUE	UNP P45066
B	31	MSE	MET	MODIFIED RESIDUE	UNP P45066
B	110	MSE	MET	MODIFIED RESIDUE	UNP P45066
B	115	MSE	MET	MODIFIED RESIDUE	UNP P45066
B	135	MSE	MET	MODIFIED RESIDUE	UNP P45066
B	138	MSE	MET	MODIFIED RESIDUE	UNP P45066
B	187	MSE	MET	MODIFIED RESIDUE	UNP P45066
B	194	MSE	MET	MODIFIED RESIDUE	UNP P45066
B	199	MSE	MET	MODIFIED RESIDUE	UNP P45066

Continued on next page...

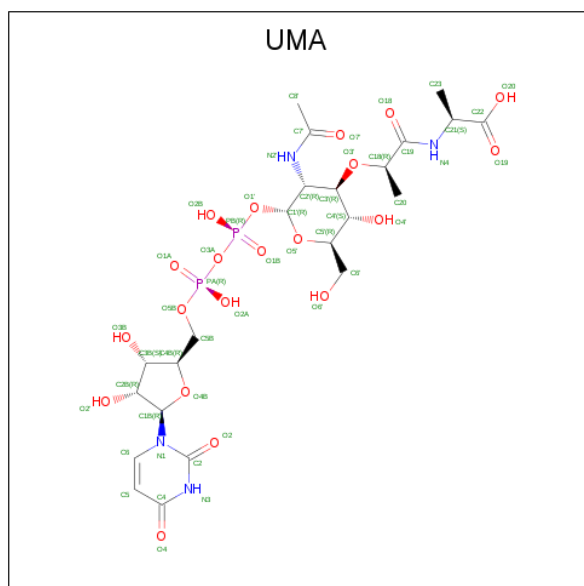
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	209	MSE	MET	MODIFIED RESIDUE	UNP P45066
B	228	MSE	MET	MODIFIED RESIDUE	UNP P45066
B	236	MSE	MET	MODIFIED RESIDUE	UNP P45066
B	371	MSE	MET	MODIFIED RESIDUE	UNP P45066
B	400	MSE	MET	MODIFIED RESIDUE	UNP P45066

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

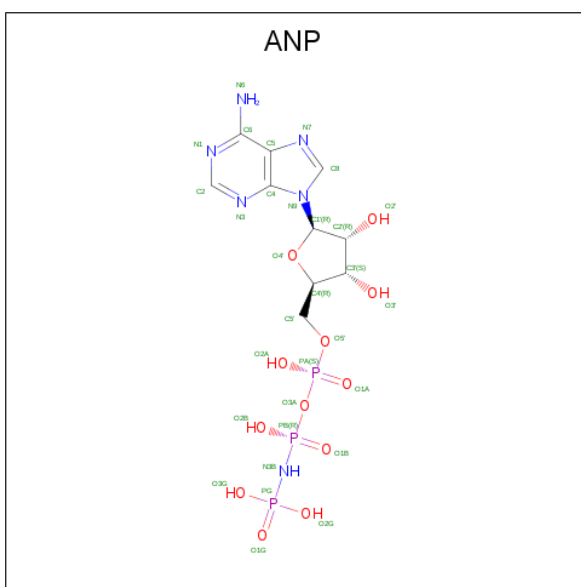
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	2	Total Mn 2 2	0	0
2	A	2	Total Mn 2 2	0	0

- Molecule 3 is URIDINE-5'-DIPHOSPHATE-N-ACETYLMURAMOYL-L-ALANINE (three-letter code: UMA) (formula: C₂₃H₃₆N₄O₂₀P₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 49 23 4 20 2	0	0
3	B	1	Total C N O P 49 23 4 20 2	0	0

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 31	C 10	N 6	O 12	P 3	0	0
4	B	1	Total 31	C 10	N 6	O 12	P 3	0	0

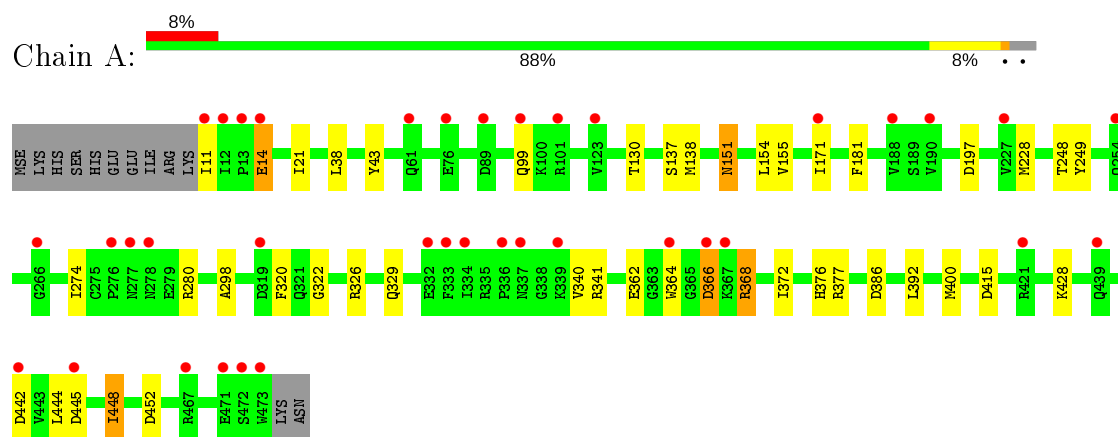
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	397	Total O 397 397	0	0
5	B	394	Total O 394 394	0	0

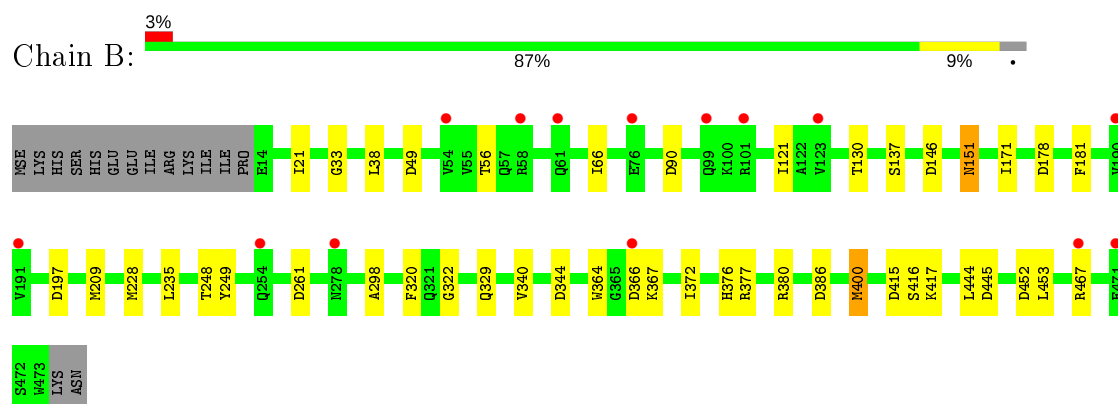
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: UDP-N-acetylmuramate--alanine ligase



- Molecule 1: UDP-N-acetylmuramate--alanine ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.92Å 87.33Å 86.11Å 90.00° 104.86° 90.00°	Depositor
Resolution (Å)	25.00 – 1.70 30.47 – 1.70	Depositor EDS
% Data completeness (in resolution range)	96.5 (25.00-1.70) 96.5 (30.47-1.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.15 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.168 , 0.194 0.170 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	22.0	Xtriage
Anisotropy	0.347	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 46.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8054	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.36% 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: UMA, MN, ANP

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	0.36	1/3649 (0.0%)	0.69	7/4917 (0.1%)
1	B	0.34	0/3592	0.70	10/4838 (0.2%)
All	All	0.35	1/7241 (0.0%)	0.70	17/9755 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	368	ARG	CZ-NH2	7.25	1.42	1.33

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	368	ARG	NE-CZ-NH1	-7.67	116.47	120.30
1	B	344	ASP	CB-CG-OD2	6.79	124.41	118.30
1	A	386	ASP	CB-CG-OD2	6.29	123.96	118.30
1	A	415	ASP	CB-CG-OD2	6.11	123.80	118.30
1	B	366	ASP	CB-CG-OD2	5.85	123.57	118.30
1	A	445	ASP	CB-CG-OD2	5.82	123.54	118.30
1	B	445	ASP	CB-CG-OD2	5.79	123.51	118.30
1	B	386	ASP	CB-CG-OD2	5.77	123.49	118.30
1	B	415	ASP	CB-CG-OD2	5.72	123.44	118.30
1	B	90	ASP	CB-CG-OD2	5.54	123.28	118.30
1	A	366	ASP	CB-CG-OD2	5.32	123.08	118.30
1	A	442	ASP	CB-CG-OD2	5.12	122.91	118.30
1	B	146	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	197	ASP	CB-CG-OD2	5.09	122.88	118.30
1	B	178	ASP	CB-CG-OD2	5.06	122.86	118.30
1	B	49	ASP	CB-CG-OD2	5.06	122.86	118.30
1	B	261	ASP	CB-CG-OD2	5.06	122.86	118.30

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	3568	0	3562	16	0
1	B	3531	0	3513	20	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	49	0	33	0	0
3	B	49	0	33	1	0
4	A	31	0	13	0	0
4	B	31	0	13	0	0
5	A	397	0	0	0	0
5	B	394	0	0	3	0
All	All	8054	0	7167	37	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 (37) 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:137:SER:HA	1:A:171[B]:ILE:HD13	1.74	0.68
1:B:400:MSE:HG2	1:B:416:SER:HB3	1.78	0.66
1:A:21:ILE:HD13	1:A:38:LEU:HD13	1.82	0.62
1:B:130:THR:HA	1:B:151:ASN:HD21	1.65	0.61
1:B:121:ILE:HD12	1:B:171[A]:ILE:CD1	2.33	0.57
1:A:130:THR:HA	1:A:151:ASN:HD21	1.70	0.57
1:B:372:ILE:HD11	1:B:444:LEU:HD11	1.86	0.57
1:A:372:ILE:HD11	1:A:444:LEU:HD11	1.87	0.55
1:B:21:ILE:HD13	1:B:38:LEU:HD13	1.88	0.54
1:A:249:TYR:CZ	1:A:298:ALA:HB2	2.43	0.54
1:B:137:SER:HA	1:B:171[B]:ILE:HD13	1.90	0.54
1:A:138:MSE:HE3	1:A:155:VAL:HG11	1.93	0.50
1:B:249:TYR:CZ	1:B:298:ALA:HB2	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:VAL:HG12	1:B:452:ASP:HB2	1.96	0.48
1:A:274:ILE:HD12	1:A:280:ARG:HG2	1.96	0.48
1:B:400:MSE:HE3	1:B:400:MSE:HB2	1.72	0.48
1:B:467:ARG:HD3	5:B:890:HOH:O	2.15	0.46
1:A:340:VAL:HG12	1:A:452:ASP:HB2	1.97	0.46
1:B:364:TRP:CE2	1:B:453:LEU:HB2	2.51	0.45
1:A:137:SER:HA	1:A:171[B]:ILE:CD1	2.46	0.45
1:B:228:MSE:O	1:B:248:THR:HA	2.16	0.45
1:A:392:LEU:HD13	1:A:400:MSE:HE1	2.00	0.44
1:B:376:HIS:HD2	1:B:380:ARG:HH22	1.64	0.43
1:B:228:MSE:HE3	1:B:235:LEU:HB3	2.00	0.43
1:B:376:HIS:HE1	5:B:1215:HOH:O	2.01	0.43
3:B:1602:UMA:H2'	3:B:1602:UMA:H202	2.01	0.43
1:B:320:PHE:CE1	1:B:322:GLY:HA2	2.54	0.43
1:B:33:GLY:HA3	5:B:1198:HOH:O	2.17	0.42
1:A:320:PHE:CE1	1:A:322:GLY:HA2	2.55	0.42
1:B:376:HIS:CD2	1:B:377:ARG:HG3	2.55	0.41
1:B:56:THR:HB	1:B:66:ILE:HG21	2.01	0.41
1:A:376:HIS:O	1:A:377:ARG:HB2	2.20	0.41
1:B:197:ASP:O	1:B:209:MSE:HE1	2.21	0.41
1:A:228:MSE:O	1:A:248:THR:HA	2.21	0.41
1:A:14:GLU:HG3	1:A:43:TYR:CZ	2.56	0.41
1:A:340:VAL:HG11	1:A:448:ILE:HG12	2.04	0.40
1:A:228:MSE:HE2	1:A:228:MSE:HB3	1.94	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	468/475 (98%)	461 (98%)	7 (2%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	461/475 (97%)	454 (98%)	7 (2%)	0	100	100
All	All	929/950 (98%)	915 (98%)	14 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	382/372 (103%)	367 (96%)	15 (4%)	32	13
1	B	375/372 (101%)	369 (98%)	6 (2%)	62	48
All	All	757/744 (102%)	736 (97%)	21 (3%)	43	25

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ILE
1	A	14	GLU
1	A	99	GLN
1	A	151	ASN
1	A	154	LEU
1	A	181	PHE
1	A	326	ARG
1	A	329	GLN
1	A	341	ARG
1	A	362	GLU
1	A	364	TRP
1	A	366	ASP
1	A	368	ARG
1	A	428	LYS
1	A	448	ILE
1	B	151	ASN
1	B	181	PHE
1	B	329	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	367	LYS
1	B	400	MSE
1	B	417	LYS

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	142	GLN
1	A	151	ASN
1	A	282	ASN
1	B	20	GLN
1	B	61	GLN
1	B	151	ASN
1	B	282	ASN
1	B	376	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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	ANP	B	1603	2	29,33,33	1.34	4 (13%)	31,52,52	1.42	3 (9%)
3	UMA	B	1602	2	41,51,51	0.84	2 (4%)	53,76,76	0.92	1 (1%)
3	UMA	A	602	-	41,51,51	0.86	2 (4%)	53,76,76	1.03	2 (3%)
4	ANP	A	603	2	29,33,33	1.27	3 (10%)	31,52,52	1.44	3 (9%)

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	ANP	B	1603	2	-	3/14/38/38	0/3/3/3
3	UMA	B	1602	2	-	10/36/79/79	0/3/3/3
3	UMA	A	602	-	-	10/36/79/79	0/3/3/3
4	ANP	A	603	2	-	4/14/38/38	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	603	ANP	C2-N3	4.08	1.38	1.32
4	B	1603	ANP	C2-N3	3.55	1.37	1.32
3	A	602	UMA	C7'-N2'	3.17	1.45	1.34
3	B	1602	UMA	C7'-N2'	3.03	1.44	1.34
4	B	1603	ANP	PB-O1B	2.97	1.50	1.46
4	A	603	ANP	C2-N1	2.50	1.38	1.33
3	B	1602	UMA	C2-N3	-2.30	1.33	1.38
3	A	602	UMA	C2-N3	-2.23	1.33	1.38
4	B	1603	ANP	C2-N1	2.22	1.38	1.33
4	B	1603	ANP	PG-O1G	2.10	1.49	1.46
4	A	603	ANP	PG-O1G	2.08	1.49	1.46

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	603	ANP	N3-C2-N1	-5.41	120.22	128.68
4	B	1603	ANP	N3-C2-N1	-4.66	121.39	128.68
3	A	602	UMA	C21-N4-C19	2.67	126.68	122.93
4	B	1603	ANP	O3G-PG-O1G	-2.43	107.33	113.45
4	B	1603	ANP	C1'-N9-C4	-2.34	122.53	126.64
3	A	602	UMA	O3'-C18-C20	2.21	113.94	107.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1602	UMA	C20-C18-C19	-2.18	105.73	111.11
4	A	603	ANP	C4-C5-N7	-2.05	107.26	109.40
4	A	603	ANP	O1G-PG-N3B	-2.05	108.75	111.77

There are no chirality outliers.

All (27) torsion outliers are listed below:

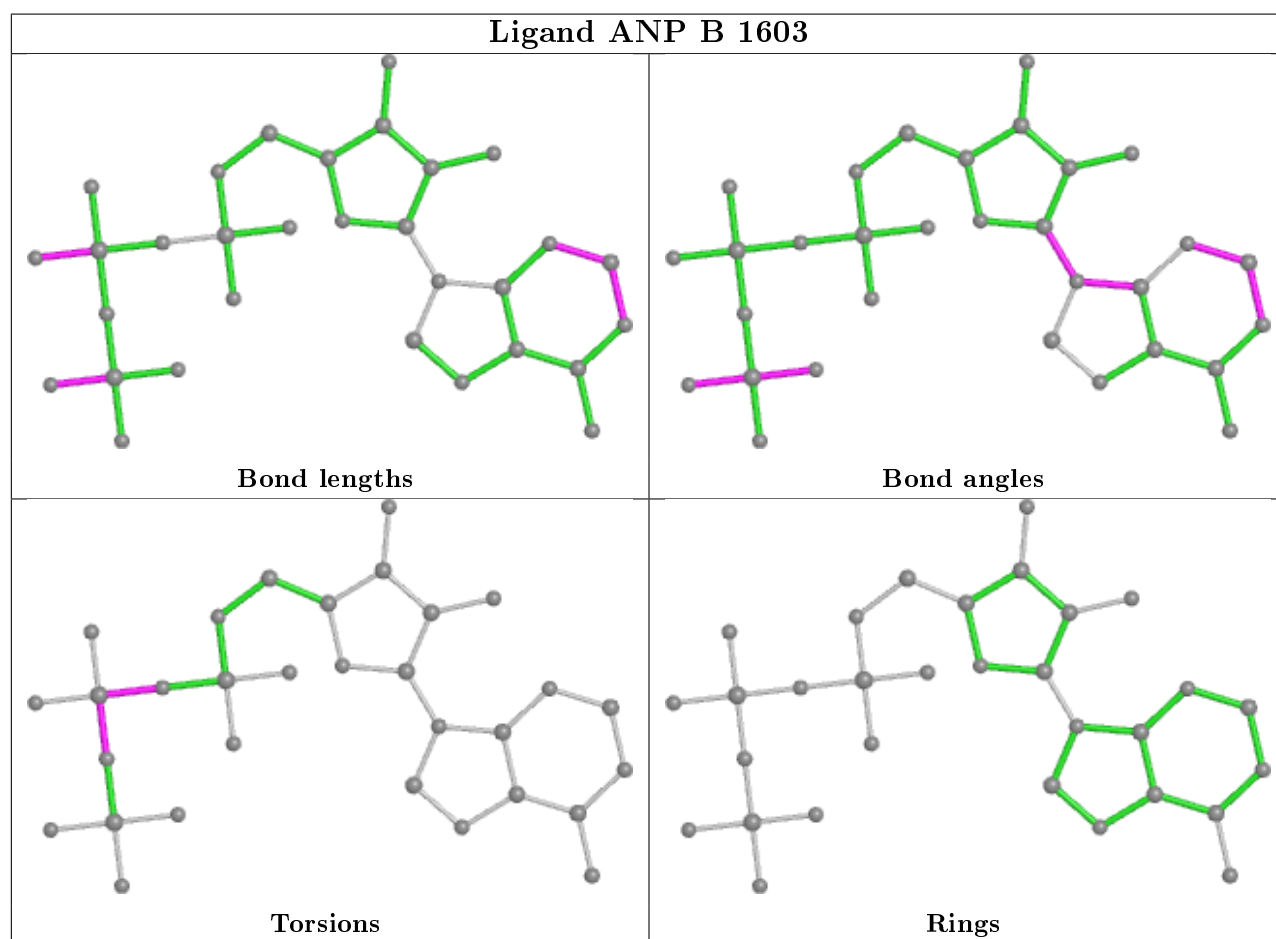
Mol	Chain	Res	Type	Atoms
4	B	1603	ANP	PG-N3B-PB-O1B
3	B	1602	UMA	C2B-C1B-N1-C6
3	B	1602	UMA	O4B-C1B-N1-C6
3	B	1602	UMA	C1'-O1'-PB-O2B
3	B	1602	UMA	O5'-C1'-O1'-PB
3	B	1602	UMA	C18-C19-N4-C21
4	A	603	ANP	PG-N3B-PB-O1B
4	A	603	ANP	PG-N3B-PB-O3A
3	A	602	UMA	C2B-C1B-N1-C6
3	A	602	UMA	O4B-C1B-N1-C6
3	A	602	UMA	C1'-O1'-PB-O2B
3	B	1602	UMA	O18-C19-N4-C21
3	A	602	UMA	C1'-O1'-PB-O3A
3	A	602	UMA	C20-C18-O3'-C3'
3	B	1602	UMA	C1'-O1'-PB-O3A
3	A	602	UMA	C23-C21-N4-C19
3	B	1602	UMA	PA-O3A-PB-O1'
3	A	602	UMA	PA-O3A-PB-O1'
3	A	602	UMA	C1'-O1'-PB-O1B
4	B	1603	ANP	PG-N3B-PB-O3A
3	A	602	UMA	O5'-C1'-O1'-PB
4	B	1603	ANP	PA-O3A-PB-O2B
4	A	603	ANP	PA-O3A-PB-O2B
3	B	1602	UMA	C4'-C3'-O3'-C18
3	B	1602	UMA	O4B-C4B-C5B-O5B
3	A	602	UMA	O4B-C4B-C5B-O5B
4	A	603	ANP	PB-N3B-PG-O1G

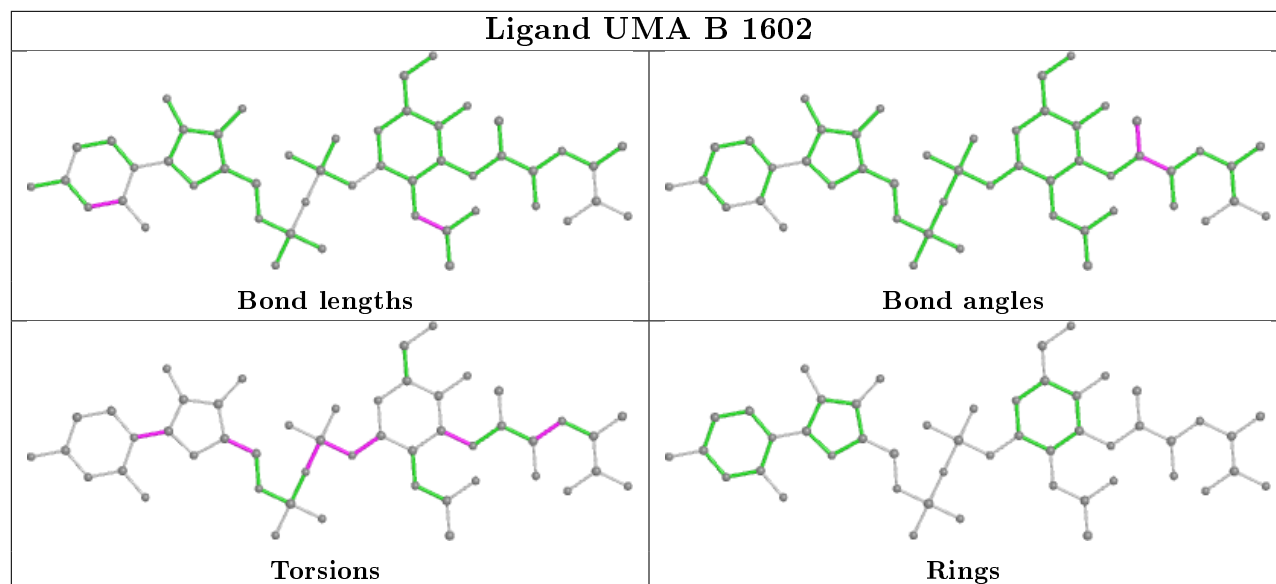
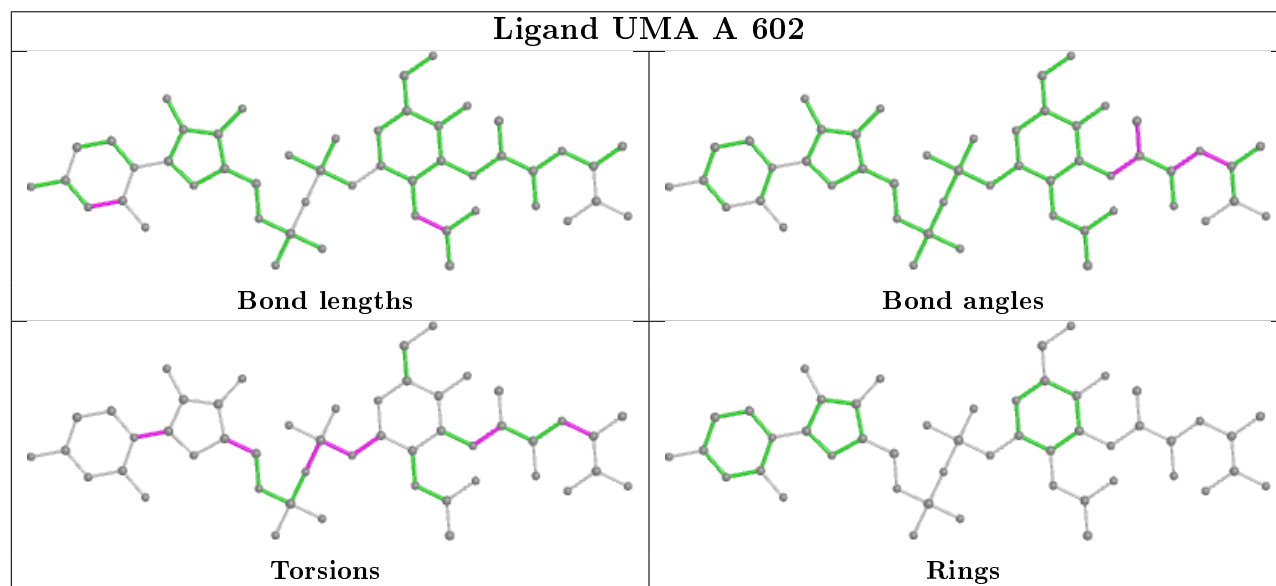
There are no ring outliers.

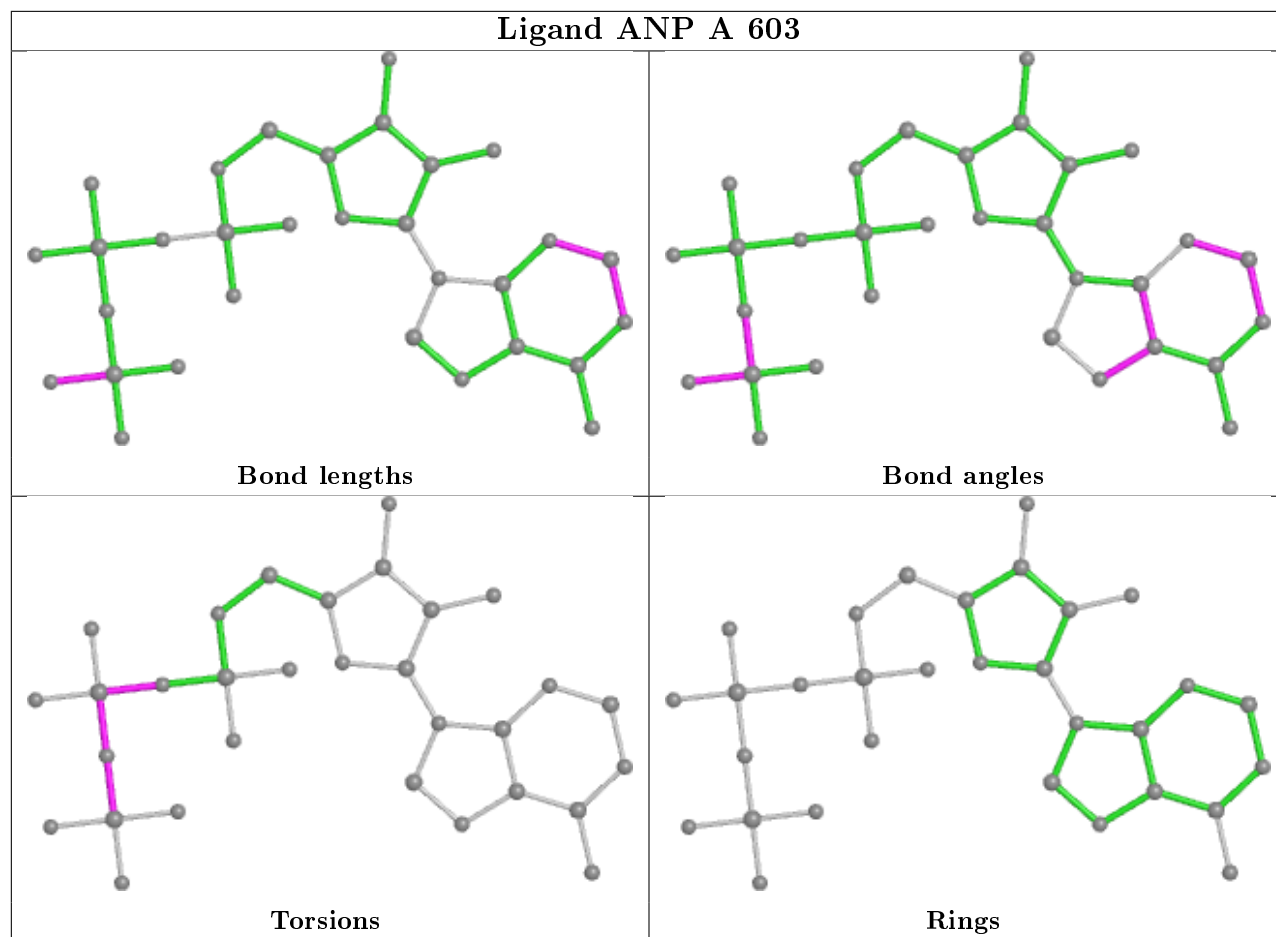
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1602	UMA	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 UMA B 1602**Ligand UMA A 602**



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	449/475 (94%)	0.35	37 (8%) 11 13	6, 11, 17, 31	0
1	B	446/475 (93%)	0.03	14 (3%) 49 53	5, 10, 17, 24	0
All	All	895/950 (94%)	0.20	51 (5%) 23 26	5, 11, 17, 31	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	11	ILE	10.1
1	A	364	TRP	10.0
1	A	12	ILE	7.7
1	A	13	PRO	5.5
1	A	471	GLU	4.8
1	B	58	ARG	4.6
1	A	473	TRP	4.2
1	A	366	ASP	4.0
1	B	61	GLN	3.9
1	A	334	ILE	3.8
1	A	333	PHE	3.8
1	B	366	ASP	3.6
1	B	101	ARG	3.5
1	B	467	ARG	3.4
1	A	99	GLN	3.4
1	B	471	GLU	3.3
1	A	336	PRO	3.1
1	A	467	ARG	3.1
1	A	367	LYS	3.0
1	A	339	LYS	2.9
1	A	421	ARG	2.9
1	A	101	ARG	2.8
1	B	190	VAL	2.8
1	A	89	ASP	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	76	GLU	2.7
1	A	277	ASN	2.7
1	A	266	GLY	2.7
1	B	99	GLN	2.7
1	A	332	GLU	2.7
1	A	472	SER	2.7
1	A	188	VAL	2.6
1	A	227	VAL	2.6
1	A	254	GLN	2.6
1	B	54	VAL	2.5
1	A	278	ASN	2.5
1	A	123	VAL	2.5
1	A	190	VAL	2.5
1	A	439	GLN	2.5
1	A	14	GLU	2.4
1	A	61	GLN	2.4
1	B	254	GLN	2.3
1	A	442	ASP	2.3
1	A	171[A]	ILE	2.3
1	B	278	ASN	2.2
1	B	191	VAL	2.2
1	A	445	ASP	2.2
1	A	76	GLU	2.2
1	A	276	PRO	2.1
1	A	319	ASP	2.1
1	B	123	VAL	2.1
1	A	337	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.

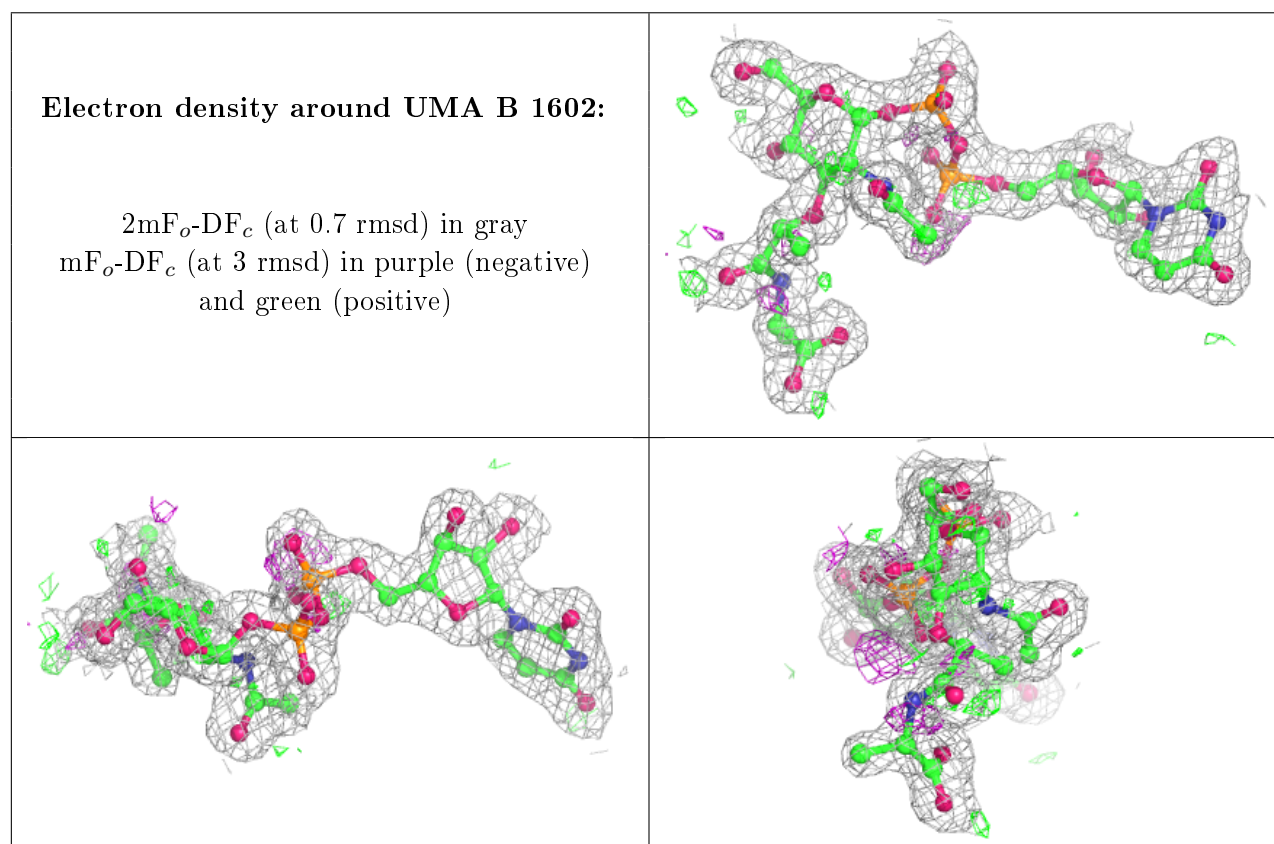
6.4 Ligands [i](#)

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.

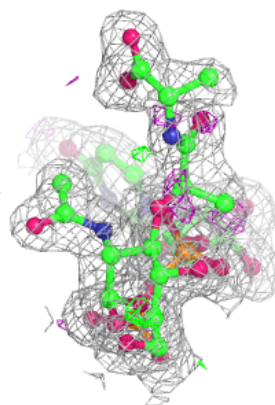
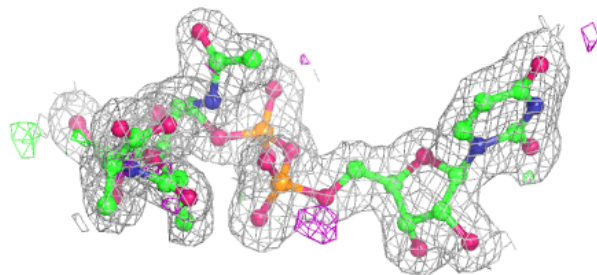
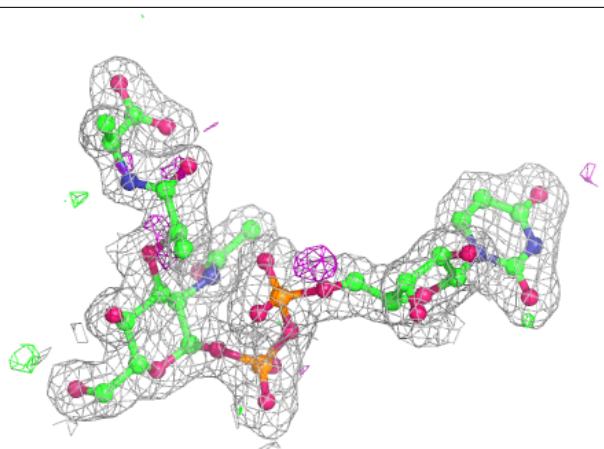
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	UMA	B	1602	49/49	0.96	0.09	18,24,26,28	0
3	UMA	A	602	49/49	0.96	0.09	21,26,31,33	0
4	ANP	A	603	31/31	0.98	0.10	19,22,23,24	0
4	ANP	B	1603	31/31	0.98	0.09	15,18,19,20	0
2	MN	B	1604	1/1	0.99	0.05	17,17,17,17	0
2	MN	A	605	1/1	1.00	0.02	22,22,22,22	0
2	MN	A	604	1/1	1.00	0.04	20,20,20,20	0
2	MN	B	1605	1/1	1.00	0.03	19,19,19,19	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.



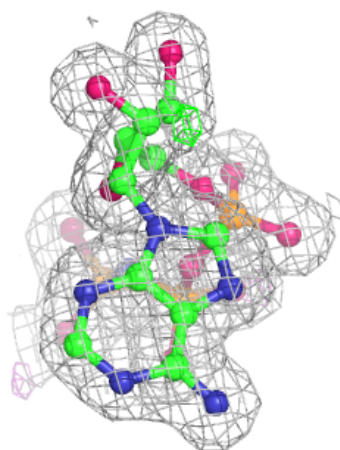
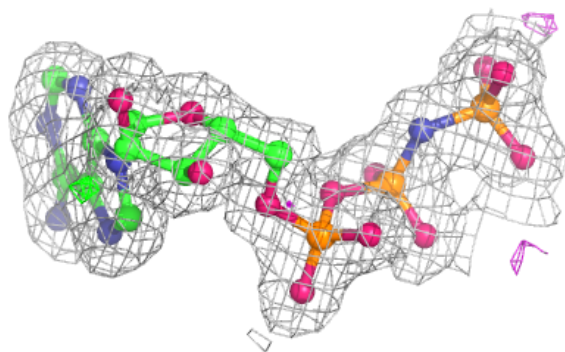
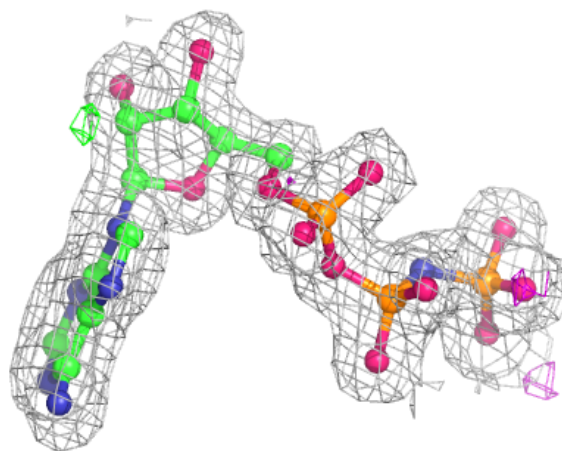
Electron density around UMA A 602:

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



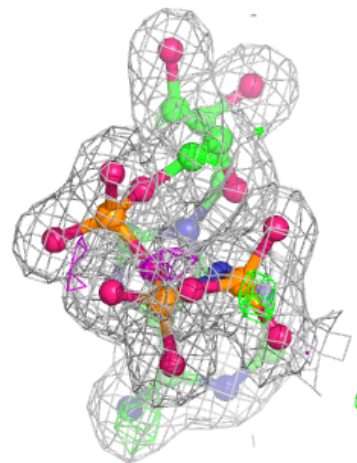
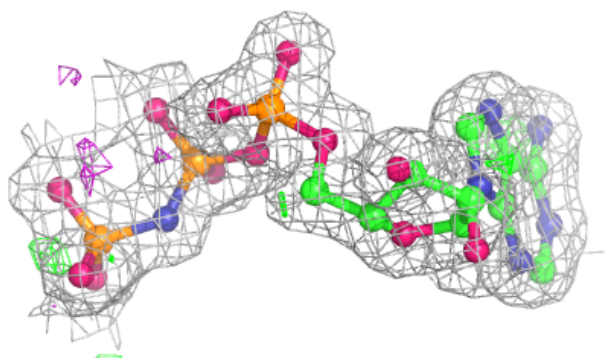
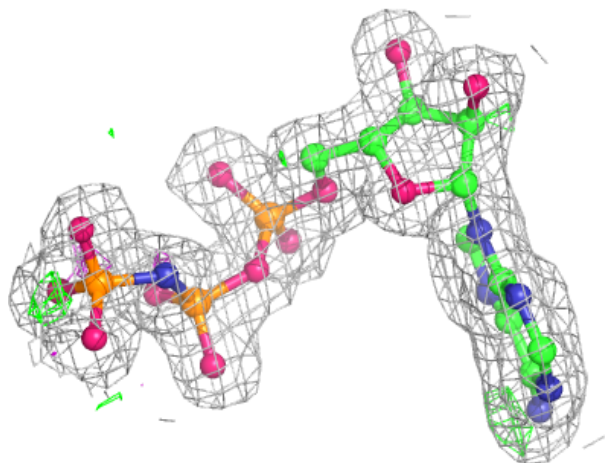
Electron density around ANP A 603:

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



Electron density around ANP B 1603:

$2mF_o-DF_c$ (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.