



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 10:41 PM UTC

PDB ID : 1P3D / pdb_00001p3d
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)

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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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

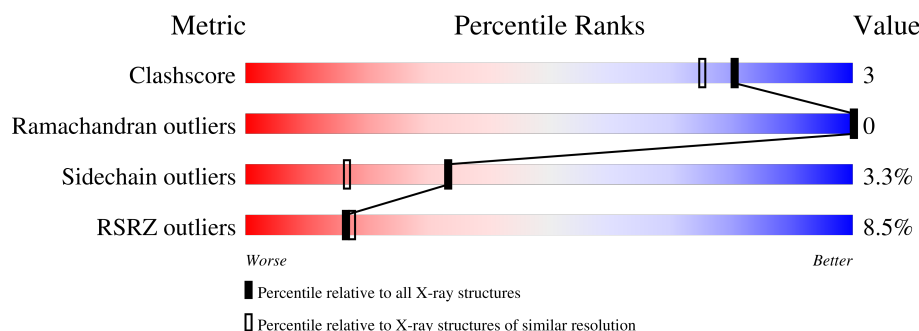
1 Overall quality at a glance

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	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (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 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 $\leq 5\%$. 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	9% 89% 7% ••
1	B	475	7% 89% 8% •

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

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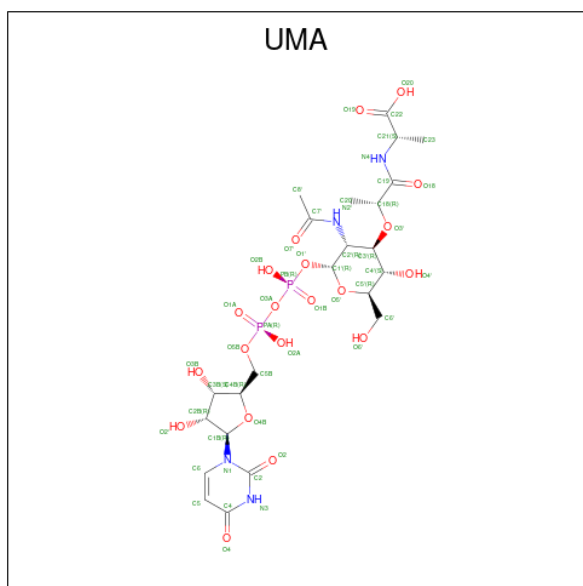
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Chain	Residue	Modelled	Actual	Comment	Reference
B	209	MSE	MET	modified residue	UNP P45066
B	228	MSE	MET	modified residue	UNP P45066
B	236	MSE	MET	modified residue	UNP P45066
B	371	MSE	MET	modified residue	UNP P45066
B	400	MSE	MET	modified residue	UNP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

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

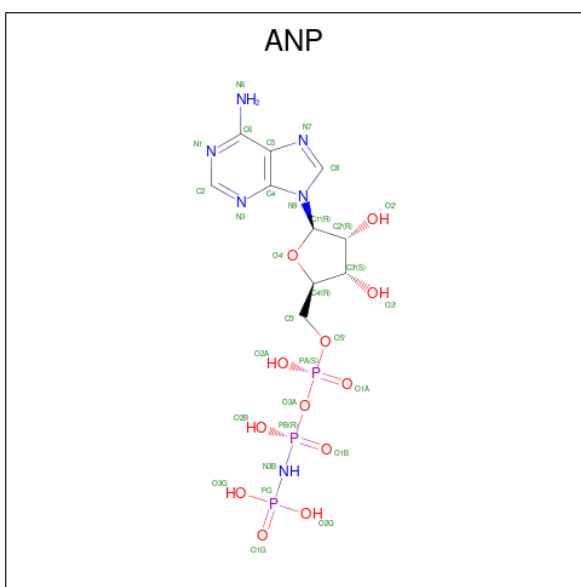
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Mn 2 2	0	0
2	B	2	Total Mn 2 2	0	0

- Molecule 3 is URIDINE-5'-DIPHOSPHATE-N-ACETYLMURAMOYL-L-ALANINE (CCD ID: 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 (CCD ID: 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

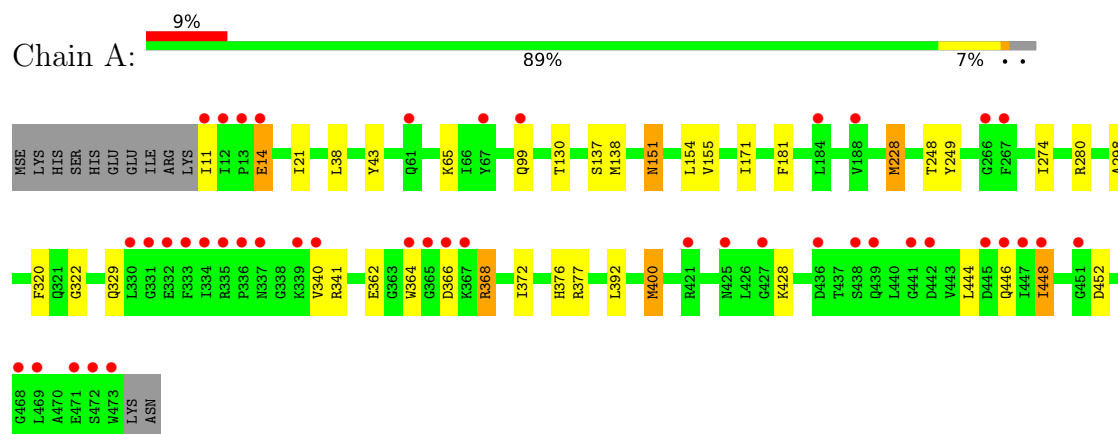
- Molecule 5 is water.

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

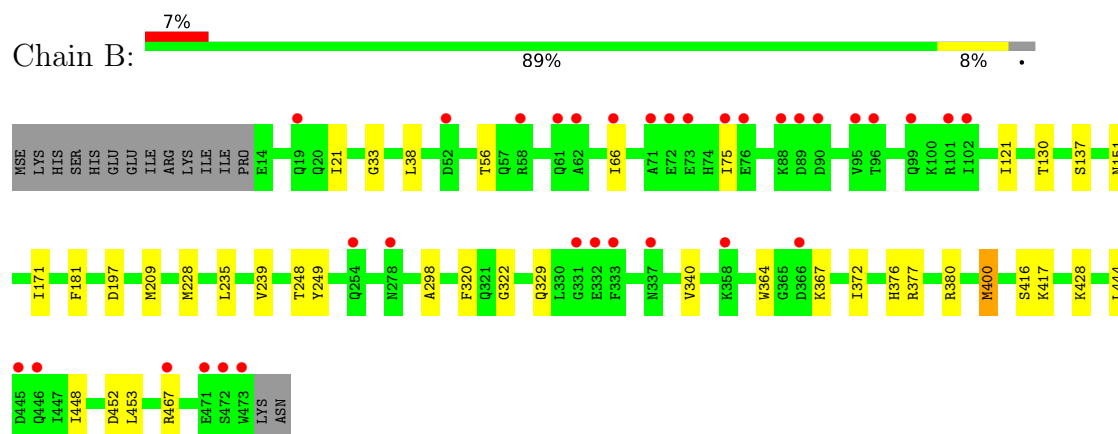
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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: 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 25.00 – 1.70	Depositor EDS
% Data completeness (in resolution range)	96.5 (25.00-1.70) 96.5 (25.00-1.70)	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)	0.39 , 44.0	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	0.94	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MN, UMA, 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	0.46	2/3649 (0.1%)	0.78	1/4917 (0.0%)
1	B	0.43	1/3592 (0.0%)	0.78	0/4838
All	All	0.45	3/7241 (0.0%)	0.78	1/9755 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	228	MSE	SE-CE	-7.16	1.74	1.95
1	A	368	ARG	CZ-NH2	6.94	1.42	1.33
1	B	239	VAL	CA-CB	5.45	1.56	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	368	ARG	NE-CZ-NH1	-5.03	116.47	121.50

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:PHE:CE1	1:B:322:GLY:HA2	2.54	0.43
3:B:1602:UMA:H2'	3:B:1602:UMA:H202	2.01	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:56:THR:HB	1:B:66:ILE:HG21	2.01	0.41
1:B:376:HIS:CD2	1:B:377:ARG:HG3	2.55	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:HB3	1:A:228:MSE:HE2	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
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 [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	382/372 (103%)	365 (96%)	17 (4%)	24	9
1	B	375/372 (101%)	367 (98%)	8 (2%)	47	30
All	All	757/744 (102%)	732 (97%)	25 (3%)	33	17

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ILE
1	A	14	GLU
1	A	65	LYS
1	A	99	GLN
1	A	151	ASN
1	A	154	LEU
1	A	181	PHE
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	400	MSE
1	A	428	LYS
1	A	446	GLN
1	A	448	ILE
1	B	75	ILE
1	B	181	PHE
1	B	329	GLN
1	B	367	LYS
1	B	400	MSE
1	B	417	LYS
1	B	428	LYS
1	B	448	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	142	GLN
1	A	151	ASN

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Mol	Chain	Res	Type
1	A	185	GLN
1	A	268	GLN
1	A	282	ASN
1	B	19	GLN
1	B	20	GLN
1	B	40	ASN
1	B	61	GLN
1	B	106	GLN
1	B	151	ASN
1	B	163	HIS
1	B	185	GLN
1	B	268	GLN
1	B	278	ASN
1	B	286	ASN
1	B	376	HIS
1	B	394	GLN

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 oligosaccharides 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	A	603	2	33,33,33	1.19	4 (12%)	45,52,52	1.80	9 (20%)
4	ANP	B	1603	2	33,33,33	1.37	6 (18%)	45,52,52	1.71	7 (15%)
3	UMA	B	1602	2	50,51,51	1.13	5 (10%)	70,76,76	1.25	5 (7%)
3	UMA	A	602	-	50,51,51	1.16	7 (14%)	70,76,76	1.32	6 (8%)

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	A	603	2	-	5/18/38/38	0/3/3/3
4	ANP	B	1603	2	-	4/18/38/38	0/3/3/3
3	UMA	B	1602	2	-	9/42/79/79	0/3/3/3
3	UMA	A	602	-	-	8/42/79/79	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	UMA	C7'-N2'	3.38	1.45	1.34
3	B	1602	UMA	C7'-N2'	3.23	1.44	1.34
4	B	1603	ANP	PB-O1B	3.09	1.50	1.46
4	B	1603	ANP	C6-N6	-2.92	1.26	1.34
3	A	602	UMA	C4-N3	-2.71	1.34	1.38
4	A	603	ANP	C2-N3	2.67	1.38	1.33
4	A	603	ANP	C2-N1	2.61	1.38	1.33
3	A	602	UMA	PA-O3A	2.59	1.62	1.59
3	B	1602	UMA	PB-O3A	2.58	1.62	1.59
3	B	1602	UMA	C2-N3	-2.50	1.33	1.38
3	A	602	UMA	C2-N3	-2.42	1.33	1.38
3	B	1602	UMA	PA-O3A	2.39	1.62	1.59
3	B	1602	UMA	C4-N3	-2.39	1.34	1.38
4	B	1603	ANP	PA-O3A	2.36	1.62	1.59
3	A	602	UMA	PB-O3A	2.35	1.62	1.59
4	B	1603	ANP	C2-N1	2.31	1.38	1.33
4	B	1603	ANP	C2-N3	2.19	1.37	1.33
4	B	1603	ANP	PG-O1G	2.18	1.49	1.46
4	A	603	ANP	PG-O1G	2.15	1.49	1.46
3	A	602	UMA	C6-C5	2.12	1.40	1.35
4	A	603	ANP	C8-N7	2.02	1.35	1.31
3	A	602	UMA	C2-N1	2.02	1.41	1.38

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	603	ANP	N3-C2-N1	-5.52	120.22	128.58
4	B	1603	ANP	N3-C2-N1	-4.75	121.39	128.58
3	A	602	UMA	C4-N3-C2	-4.27	121.31	126.61
3	B	1602	UMA	C4-N3-C2	-4.17	121.43	126.61
3	B	1602	UMA	C5-C4-N3	4.16	120.63	114.80
4	A	603	ANP	N9-C8-N7	-4.07	108.17	113.94
4	A	603	ANP	C5-C4-N3	-4.07	121.12	126.72
3	A	602	UMA	C5-C4-N3	4.04	120.46	114.80
4	B	1603	ANP	N9-C8-N7	-3.94	108.35	113.94
3	A	602	UMA	N3-C2-N1	3.79	119.83	114.89
4	A	603	ANP	C5-N7-C8	3.69	109.24	103.45
4	B	1603	ANP	C5-C4-N3	-3.59	121.78	126.72
4	B	1603	ANP	C5-N7-C8	3.50	108.94	103.45
3	B	1602	UMA	N3-C2-N1	3.36	119.26	114.89
4	A	603	ANP	C2-N3-C4	3.20	119.66	111.83
3	B	1602	UMA	O4-C4-C5	-2.99	120.01	125.16
4	A	603	ANP	C4-C5-N7	-2.90	107.26	110.58
4	B	1603	ANP	C4-C5-N7	-2.83	107.34	110.58
4	B	1603	ANP	C2-N3-C4	2.73	118.50	111.83
3	A	602	UMA	C21-N4-C19	2.55	126.68	121.32
3	A	602	UMA	O4-C4-C5	-2.53	120.80	125.16
4	B	1603	ANP	O3G-PG-O1G	-2.44	107.33	113.45
4	A	603	ANP	N3-C4-N9	2.34	131.14	127.17
3	A	602	UMA	O3'-C18-C20	2.30	113.94	107.54
4	A	603	ANP	O4'-C1'-N9	-2.24	103.79	108.09
3	B	1602	UMA	C20-C18-C19	-2.16	105.73	111.11
4	A	603	ANP	O1G-PG-N3B	-2.05	108.75	111.77

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	UMA	C1'-O1'-PB-O3A
3	A	602	UMA	C1'-O1'-PB-O2B
3	B	1602	UMA	C1'-O1'-PB-O3A
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
4	B	1603	ANP	PG-N3B-PB-O1B

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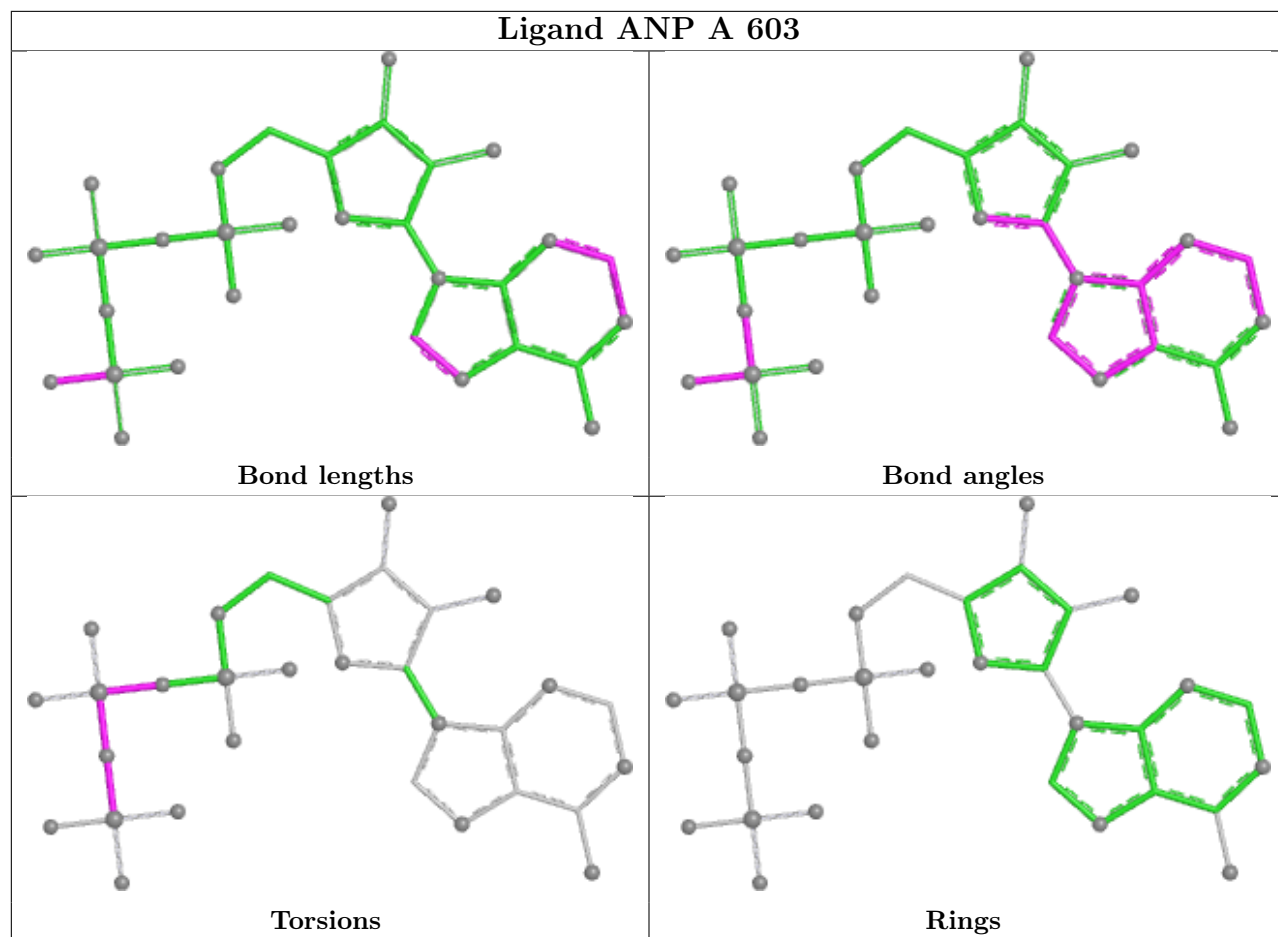
Mol	Chain	Res	Type	Atoms
3	B	1602	UMA	O18-C19-N4-C21
3	A	602	UMA	C20-C18-O3'-C3'
3	A	602	UMA	PA-O3A-PB-O1'
3	B	1602	UMA	PA-O3A-PB-O1'
3	B	1602	UMA	C1'-O1'-PB-O1B
4	B	1603	ANP	PG-N3B-PB-O3A
3	A	602	UMA	C23-C21-N4-C19
3	A	602	UMA	O5'-C1'-O1'-PB
4	A	603	ANP	PA-O3A-PB-O2B
4	B	1603	ANP	PA-O3A-PB-O2B
4	A	603	ANP	PA-O3A-PB-O1B
4	B	1603	ANP	PA-O3A-PB-O1B
4	A	603	ANP	PB-N3B-PG-O1G
3	A	602	UMA	PA-O3A-PB-O2B
3	B	1602	UMA	PB-O3A-PA-O2A
3	A	602	UMA	O4B-C4B-C5B-O5B
3	B	1602	UMA	O4B-C4B-C5B-O5B

There are no ring outliers.

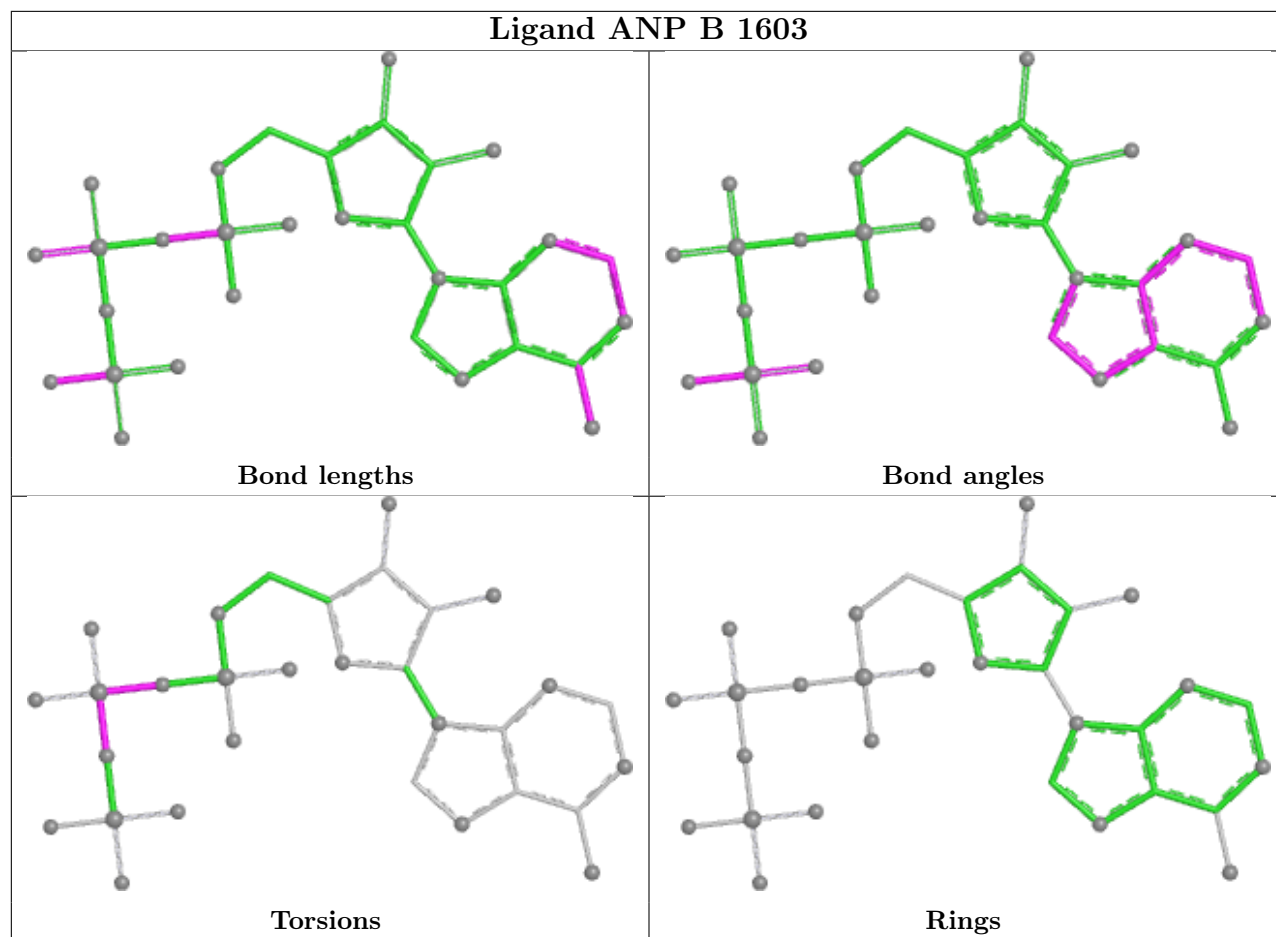
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1602	UMA	1	0

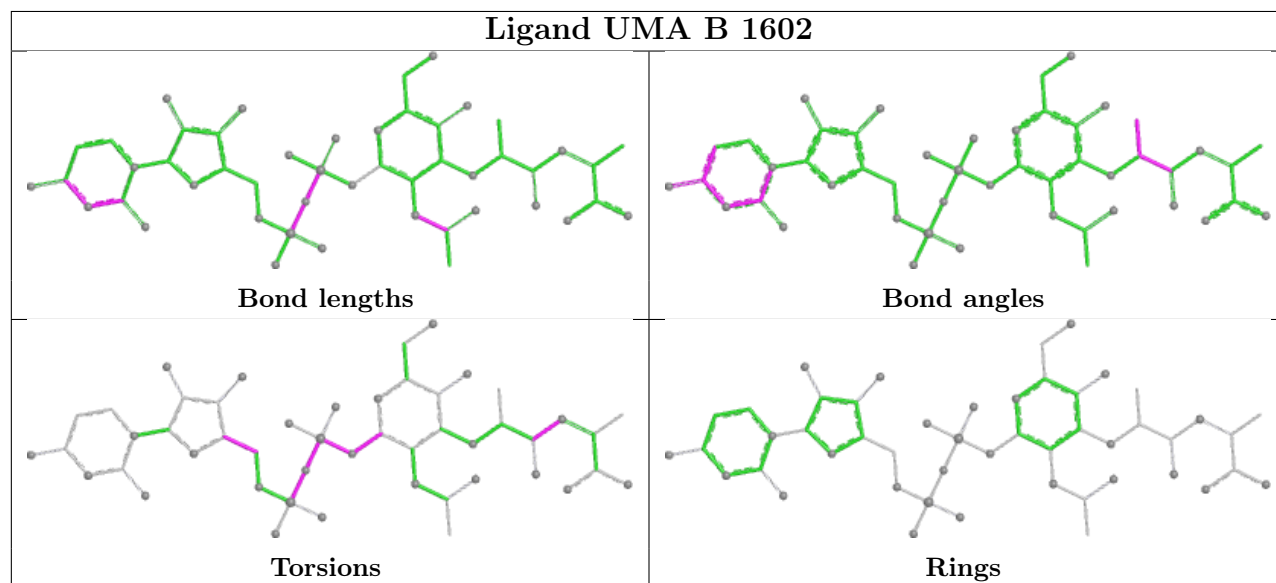
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

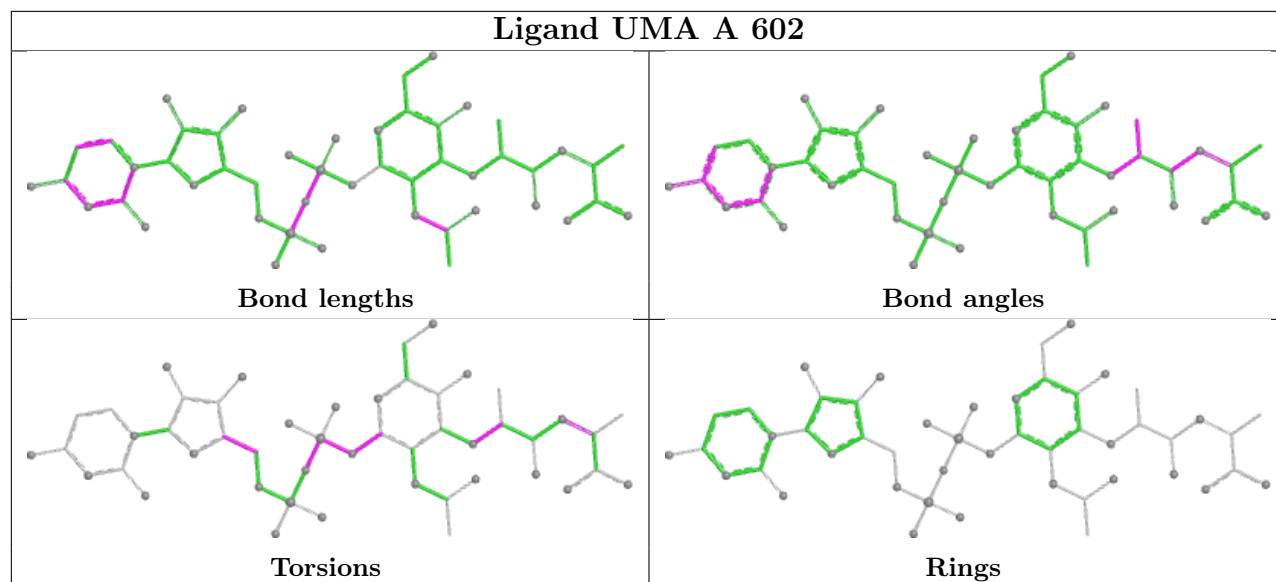


Ligand ANP B 1603



Ligand UMA B 1602





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%)	0.70	43 (9%) 13 14	6, 10, 17, 31	7 (1%)
1	B	446/475 (93%)	0.51	33 (7%) 20 22	5, 10, 17, 24	3 (0%)
All	All	895/950 (94%)	0.61	76 (8%) 16 17	5, 10, 17, 31	10 (1%)

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	12	ILE	6.2
1	A	364	TRP	5.7
1	A	11	ILE	4.8
1	A	333	PHE	4.6
1	B	72	GLU	4.3
1	B	101	ARG	4.3
1	A	471	GLU	4.2
1	A	336	PRO	4.1
1	A	331	GLY	3.9
1	B	471	GLU	3.9
1	A	13	PRO	3.9
1	A	473	TRP	3.9
1	A	445	ASP	3.8
1	B	76	GLU	3.8
1	A	442	ASP	3.7
1	A	448	ILE	3.5
1	B	61	GLN	3.5
1	A	366	ASP	3.4
1	B	366	ASP	3.4
1	B	99	GLN	3.4
1	A	468	GLY	3.4
1	A	451	GLY	3.3
1	B	58	ARG	3.3
1	A	337	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	334	ILE	3.2
1	A	332	GLU	3.1
1	B	331	GLY	3.1
1	B	467	ARG	3.0
1	B	90	ASP	3.0
1	A	365	GLY	2.9
1	A	425	ASN	2.9
1	B	71	ALA	2.8
1	A	421	ARG	2.7
1	B	66	ILE	2.7
1	B	472	SER	2.6
1	A	367	LYS	2.6
1	A	447	ILE	2.5
1	B	75	ILE	2.5
1	A	330	LEU	2.5
1	B	95	VAL	2.5
1	B	102	ILE	2.5
1	B	332	GLU	2.4
1	B	337	ASN	2.4
1	A	339	LYS	2.4
1	A	184	LEU	2.4
1	B	62	ALA	2.4
1	B	333	PHE	2.4
1	A	67	TYR	2.4
1	A	188	VAL	2.4
1	B	73	GLU	2.3
1	B	445	ASP	2.3
1	A	99	GLN	2.3
1	A	446	GLN	2.3
1	B	96	THR	2.3
1	A	441	GLY	2.3
1	A	335	ARG	2.3
1	A	427	GLY	2.3
1	B	446	GLN	2.2
1	B	278	ASN	2.2
1	B	52	ASP	2.2
1	A	438	SER	2.2
1	A	439	GLN	2.2
1	B	88	LYS	2.2
1	B	473	TRP	2.2
1	A	469	LEU	2.2
1	A	472	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	14	GLU	2.1
1	A	266	GLY	2.1
1	B	89	ASP	2.1
1	A	340	VAL	2.1
1	A	436	ASP	2.1
1	A	267	PHE	2.1
1	B	358	LYS	2.0
1	A	61	GLN	2.0
1	B	19	GLN	2.0
1	B	254	GLN	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

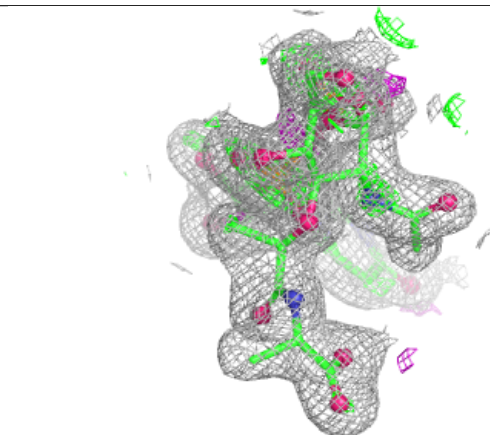
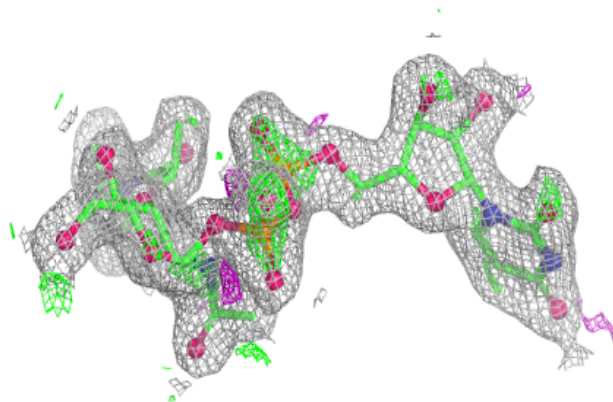
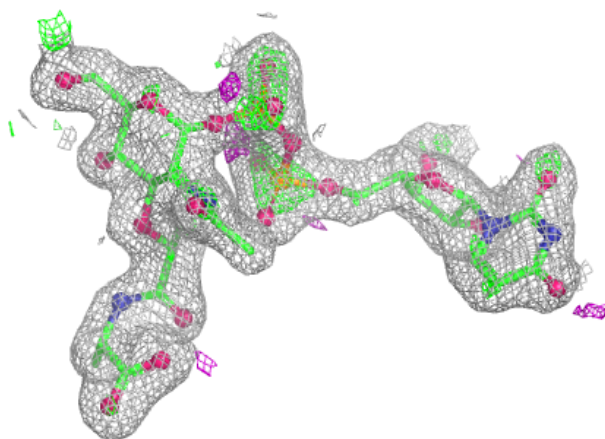
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	UMA	A	602	49/49	0.92	0.14	21,26,31,33	0
3	UMA	B	1602	49/49	0.93	0.14	18,24,26,28	0
4	ANP	A	603	31/31	0.94	0.12	19,22,23,24	0
4	ANP	B	1603	31/31	0.95	0.11	15,18,19,20	0
2	MN	A	605	1/1	0.99	0.09	22,22,22,22	0
2	MN	B	1604	1/1	0.99	0.15	17,17,17,17	0
2	MN	A	604	1/1	0.99	0.13	20,20,20,20	0
2	MN	B	1605	1/1	1.00	0.10	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.

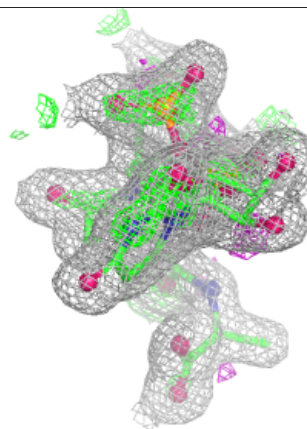
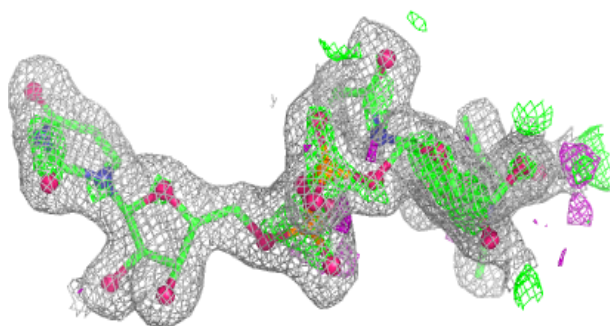
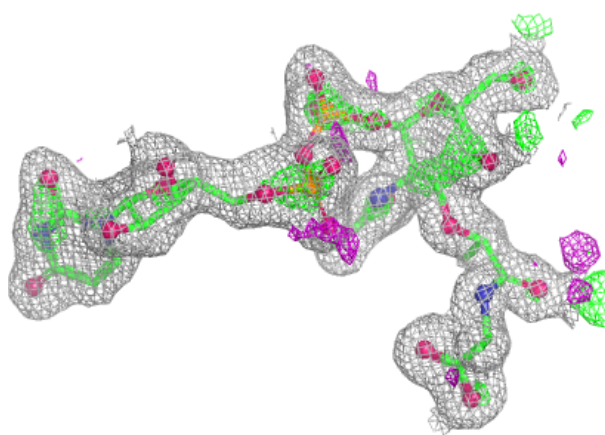
Electron density around UMA A 602:

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



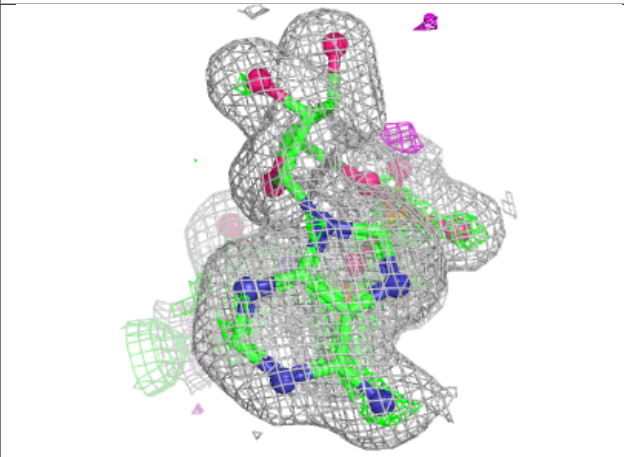
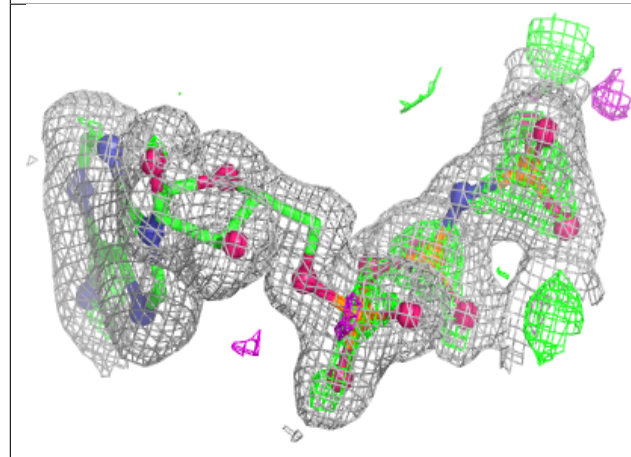
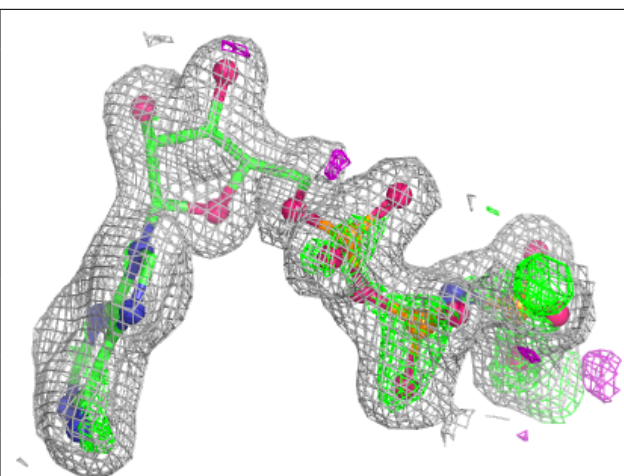
Electron density around UMA B 1602:

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



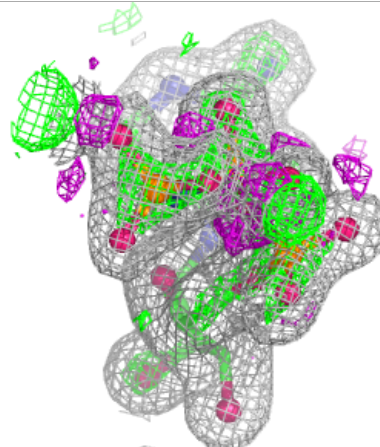
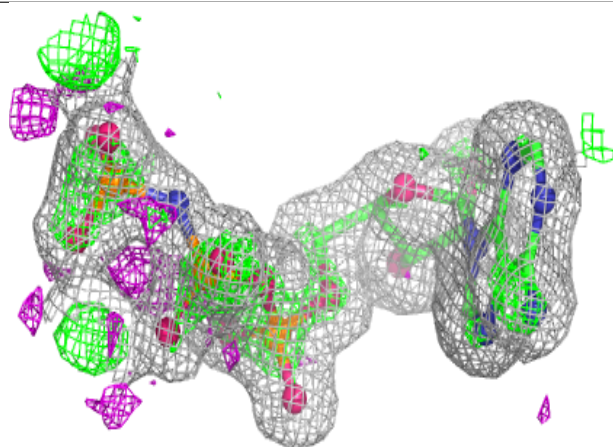
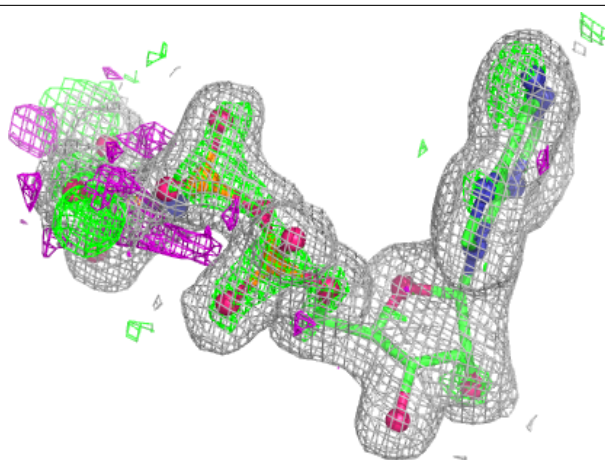
Electron density around ANP A 603:

$2mF_o-DF_c$ (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.