



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 23, 2026 – 02:55 AM EDT

PDB ID : 1P4R / pdb_00001p4r
Title : Crystal Structure of Human ATIC in complex with folate-based inhibitor BW1540U88UD
Authors : Cheong, C.-G.; Greasley, S.E.; Horton, P.A.; Beardsley, G.P.; Wilson, I.A.
Deposited on : 2003-04-23
Resolution : 2.55 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 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

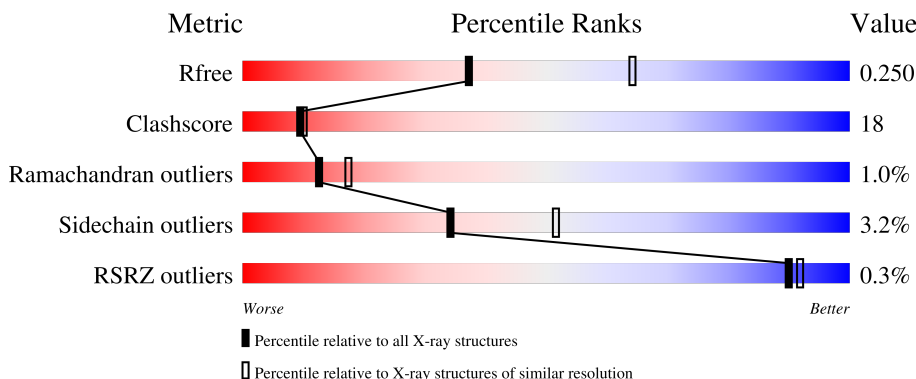
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

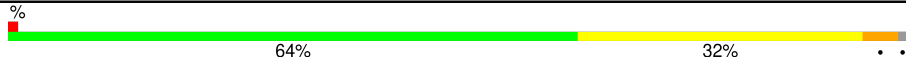
The reported resolution of this entry is 2.55 Å.

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}	180053	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	592	 64% 32% . .
1	B	592	 62% 34% . .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	354	A	1801	X	-	-	-
4	354	B	1802	X	-	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 9470 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.

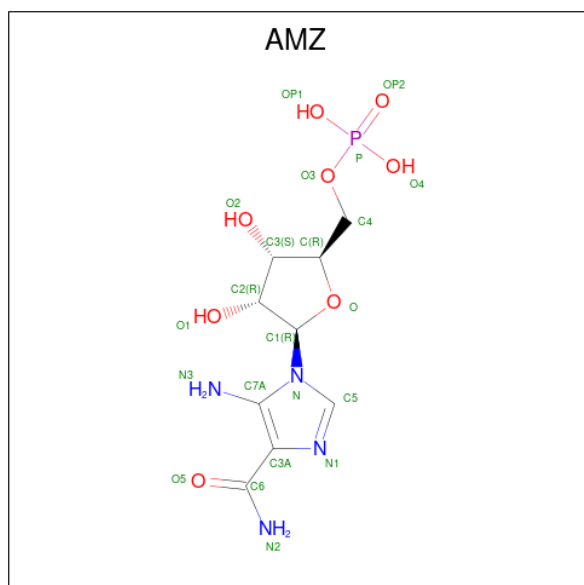
- Molecule 1 is a protein called Bifunctional purine biosynthesis protein PURH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	589	Total	C	N	O	S	0	0	0
			4453	2817	777	841	18			
1	B	588	Total	C	N	O	S	0	0	0
			4480	2831	778	853	18			

- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

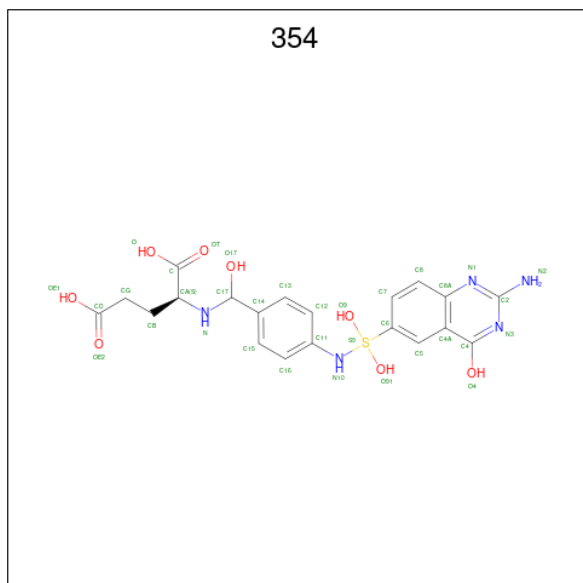
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	K	0	0
			1	1		
2	B	1	Total	K	0	0
			1	1		

- Molecule 3 is AMINOIMIDAZOLE 4-CARBOXAMIDE RIBONUCLEOTIDE (CCD ID: AMZ) (formula: C₉H₁₅N₄O₈P).



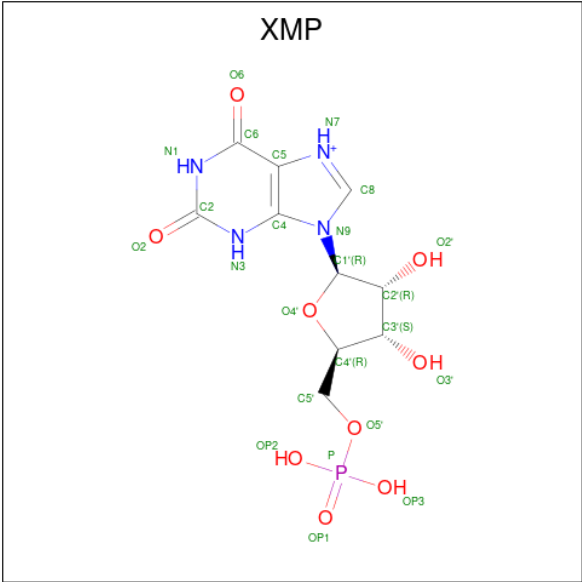
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			22	9	4	8	1		
3	B	1	Total	C	N	O	P	0	0
			22	9	4	8	1		

- Molecule 4 is N-[(S)-(4-{[(2-AMINO-4-HYDROXYQUINAZOLIN-6-YL)(DIHYDROXY)-LAMBDA 4 -SULFANYL]AMINO}PHENYL)(HYDROXY)METHYL]-L-GLUTAMIC ACID (CCD ID: 354) (formula: $C_{20}H_{23}N_5O_8S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			34	20	5	8	1		
4	B	1	Total	C	N	O	S	0	0
			34	20	5	8	1		

- Molecule 5 is XANTHOSINE-5'-MONOPHOSPHATE (CCD ID: XMP) (formula: $C_{10}H_{14}N_4O_9P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			24	10	4	9	1		

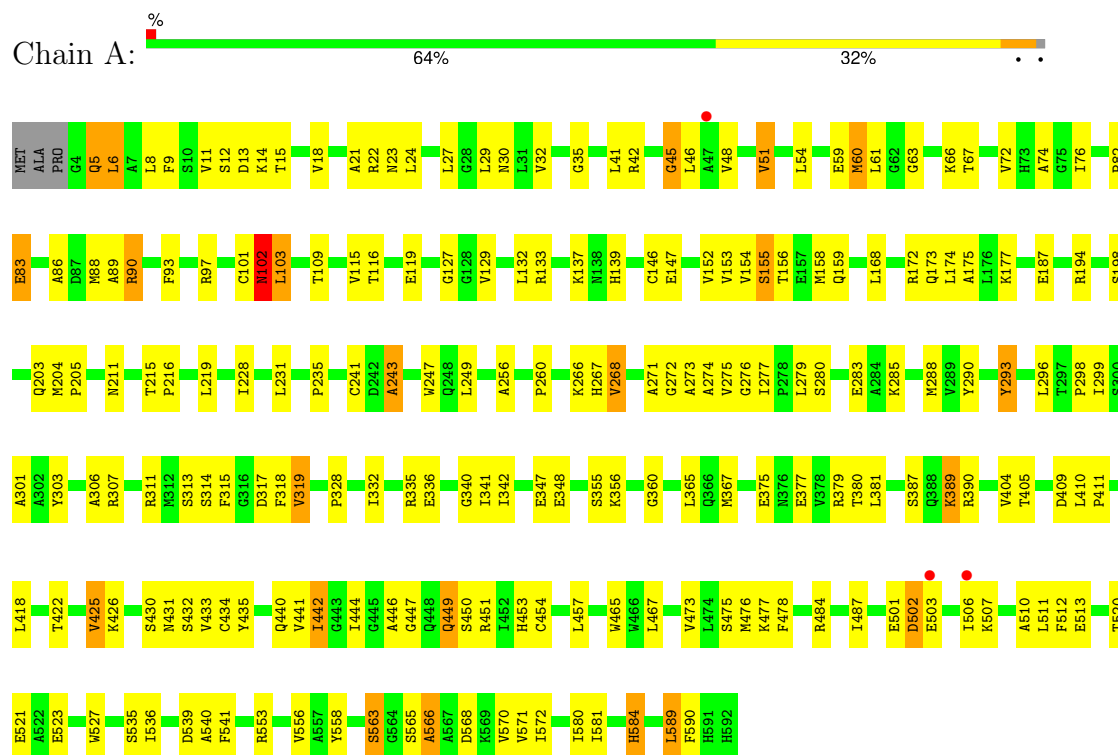
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	204	Total	O	0	0
			204	204		
6	B	195	Total	O	0	0
			195	195		

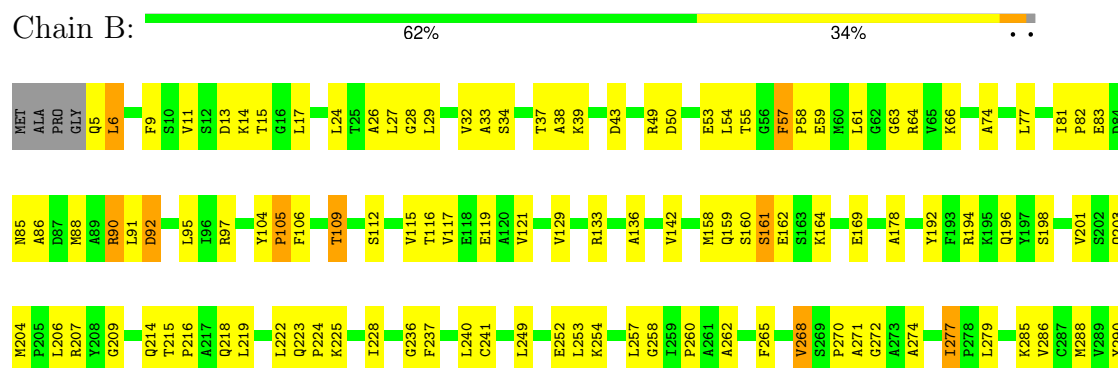
3 Residue-property plots

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: Bifunctional purine biosynthesis protein PURH



- Molecule 1: Bifunctional purine biosynthesis protein PURH



D291	L292	Y293	K294	A301	R305	A306	R311	M312	S313	S314	F315	G316	D317	F318	V319	A320	D326	V327	P328	T329	I332	E336	I341	I342	A343	P344	G345	Y346	K357	Y362	L365	Q366	M367	E377	T380	L381	K389	D396	K397	S398	V403	V404	T405	K406
N407	K408	D409	R416	D417	L418	I419	V420	A421	T422	V425	K426	S430	N431	C434	Y435	Q440	I444	G447	Q448	Q449	S450	R451	I452	H453	C454	L457	K461	W465	W466	H469	V473	R484	D492	T496	I499	E503	D504	I505	I506	K507	W508			
F512	E513	E514	V515	T520	E523	V534	S535	I536	A540	F541	F542	P543	F544	R545	R553	V556	A557	S565	A566	A567	D568	K569	V570	W571	I572	C575	I580	I581	L582	N586	L587	R588	L589	F590	H591	H592								

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.59Å 93.03Å 164.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.55 30.00 – 2.55	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.55) 93.9 (30.00-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.12 (at 2.54Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.189 , 0.257 0.183 , 0.250	Depositor DCC
R_{free} test set	2131 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	25.6	Xtriage
Anisotropy	0.680	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9470	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% 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: XMP, 354, K, AMZ

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	0.52	0/4536	1.02	21/6166 (0.3%)
1	B	0.51	0/4563	1.02	23/6197 (0.4%)
All	All	0.52	0/9099	1.02	44/12363 (0.4%)

There are no bond length outliers.

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	566	ALA	N-CA-C	-8.34	102.56	112.89
1	B	513	GLU	N-CA-C	-7.68	102.84	112.90
1	A	271	ALA	N-CA-C	-7.64	102.60	112.23
1	B	142	VAL	N-CA-C	7.16	118.89	108.58
1	B	406	LYS	N-CA-C	-7.10	99.52	110.10

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	4453	0	4420	169	0
1	B	4480	0	4467	170	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	22	0	13	0	0
3	B	22	0	13	1	0
4	A	34	0	19	4	0
4	B	34	0	19	2	0
5	A	24	0	12	2	0
6	A	204	0	0	12	0
6	B	195	0	0	7	0
All	All	9470	0	8963	322	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 18.

The worst 5 of 322 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:503:GLU:O	1:A:506:ILE:HG22	1.61	0.98
1:B:409:ASP:HA	6:B:1833:HOH:O	1.70	0.92
1:B:194:ARG:HG2	1:B:203:GLN:HB2	1.56	0.87
1:B:13:ASP:OD1	1:B:15:THR:HG22	1.74	0.87
1:A:41:LEU:O	1:A:46:LEU:HB2	1.75	0.86

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	587/592 (99%)	552 (94%)	29 (5%)	6 (1%)	12 17
1	B	586/592 (99%)	542 (92%)	38 (6%)	6 (1%)	12 17
All	All	1173/1184 (99%)	1094 (93%)	67 (6%)	12 (1%)	12 17

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	502	ASP
1	A	45	GLY
1	A	511	LEU
1	B	160	SER
1	B	293	TYR

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	465/488 (95%)	451 (97%)	14 (3%)	36	53
1	B	475/488 (97%)	459 (97%)	16 (3%)	32	48
All	All	940/976 (96%)	910 (97%)	30 (3%)	34	51

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	6	LEU
1	B	513	GLU
1	B	109	THR
1	B	553	ARG
1	B	397	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	245	ASN
1	A	453	HIS
1	B	472	GLN
1	B	196	GLN
1	B	438	ASN

5.3.3 RNA ⓘ

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 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	354	B	1802	-	31,36,36	3.32	18 (58%)	43,52,52	2.79	16 (37%)
5	XMP	A	1901	-	26,26,26	2.15	7 (26%)	34,40,40	1.73	10 (29%)
3	AMZ	B	1702	-	22,23,23	2.38	5 (22%)	32,35,35	2.61	8 (25%)
3	AMZ	A	1701	-	22,23,23	2.23	4 (18%)	32,35,35	2.68	7 (21%)
4	354	A	1801	-	31,36,36	3.25	18 (58%)	43,52,52	2.92	15 (34%)

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	354	B	1802	-	1/1/5/7	4/21/28/28	0/3/3/3
5	XMP	A	1901	-	-	5/10/26/26	0/3/3/3
3	AMZ	B	1702	-	-	0/14/30/30	0/2/2/2
3	AMZ	A	1701	-	-	0/14/30/30	0/2/2/2
4	354	A	1801	-	1/1/5/7	3/21/28/28	0/3/3/3

The worst 5 of 52 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1802	354	OT-C	7.54	1.44	1.22
3	B	1702	AMZ	C7A-N3	7.35	1.50	1.34
4	A	1801	354	OT-C	7.01	1.42	1.22
4	B	1802	354	C2-N3	6.13	1.46	1.35
3	A	1701	AMZ	C7A-N3	6.07	1.47	1.34

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1701	AMZ	C3A-C7A-N	11.38	110.41	105.75
4	A	1801	354	O17-C17-C14	10.88	120.97	109.87
4	B	1802	354	O17-C17-C14	10.29	120.37	109.87
3	B	1702	AMZ	C3A-C7A-N	9.65	109.70	105.75
4	A	1801	354	C17-N-CA	8.44	130.01	115.07

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	1801	354	C17
4	B	1802	354	C17

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1901	XMP	C5'-O5'-P-OP3
5	A	1901	XMP	C5'-O5'-P-OP2
5	A	1901	XMP	C5'-O5'-P-OP1
5	A	1901	XMP	O4'-C4'-C5'-O5'
5	A	1901	XMP	C3'-C4'-C5'-O5'

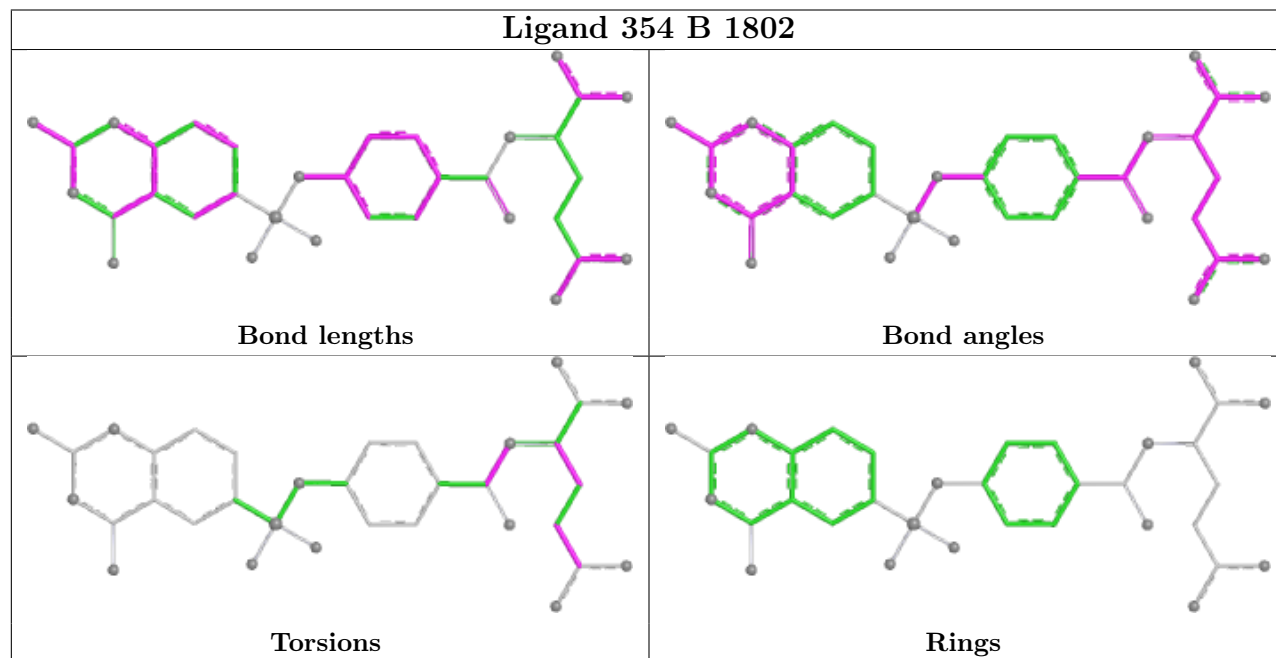
There are no ring outliers.

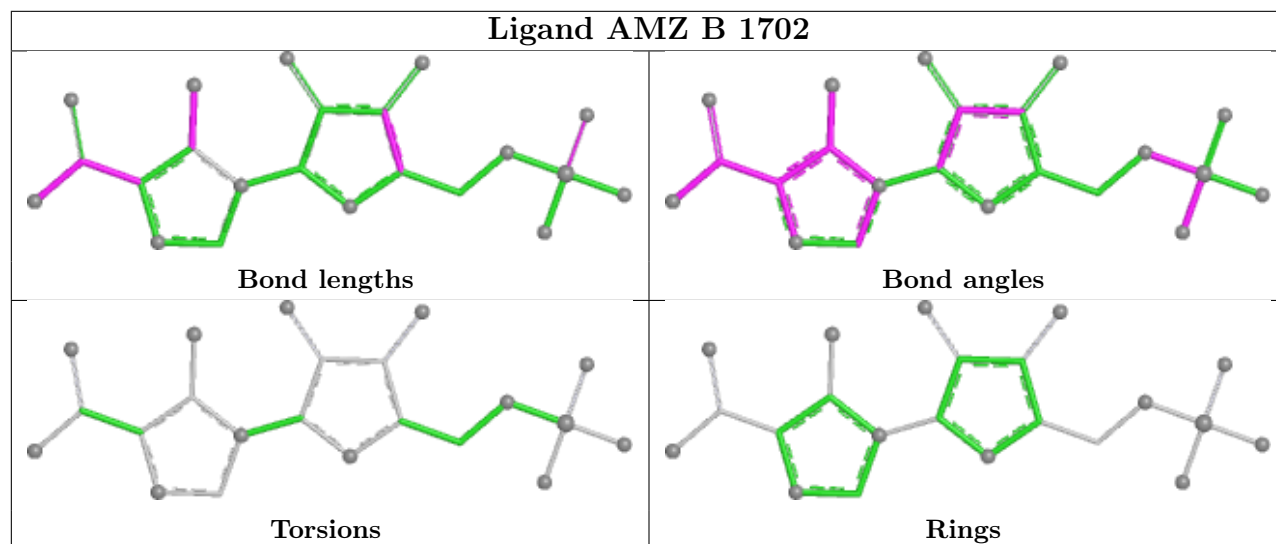
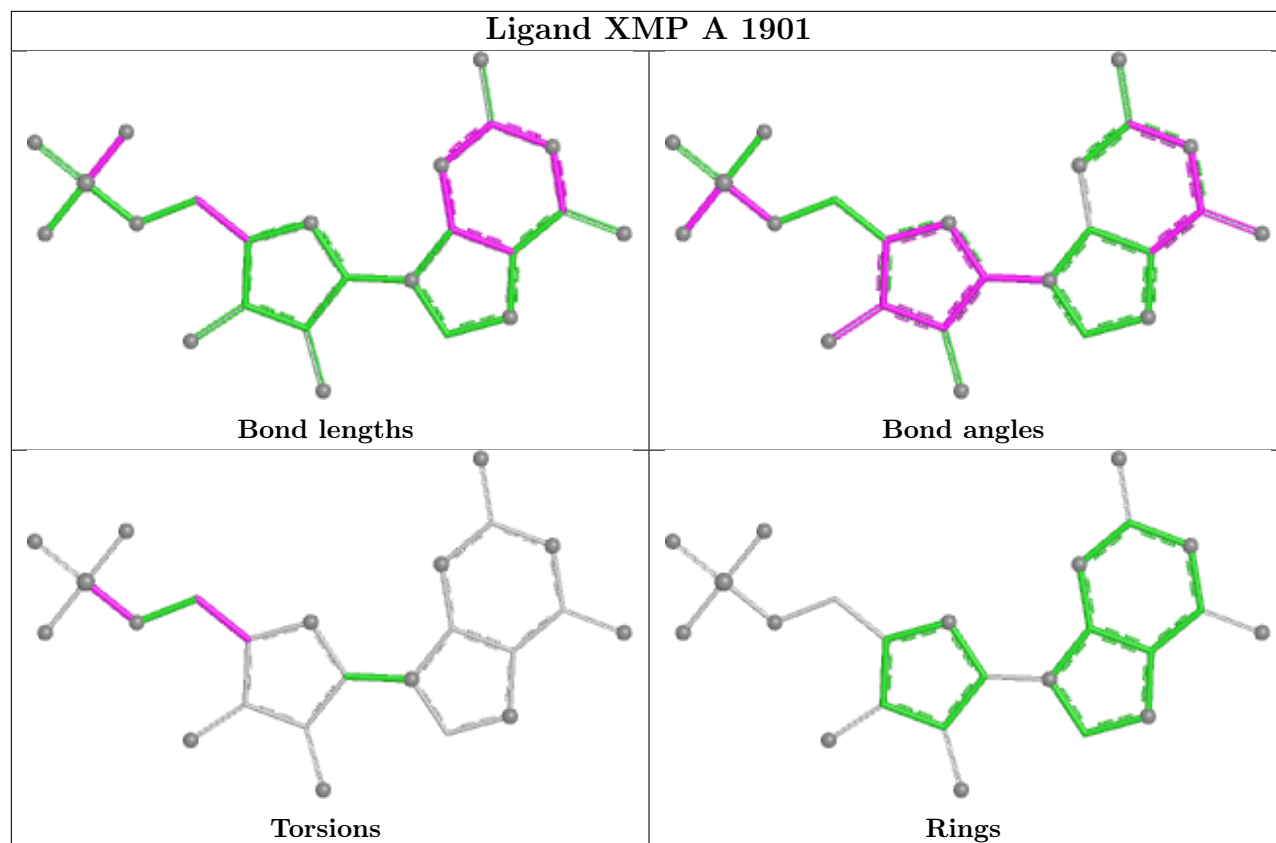
4 monomers are involved in 9 short contacts:

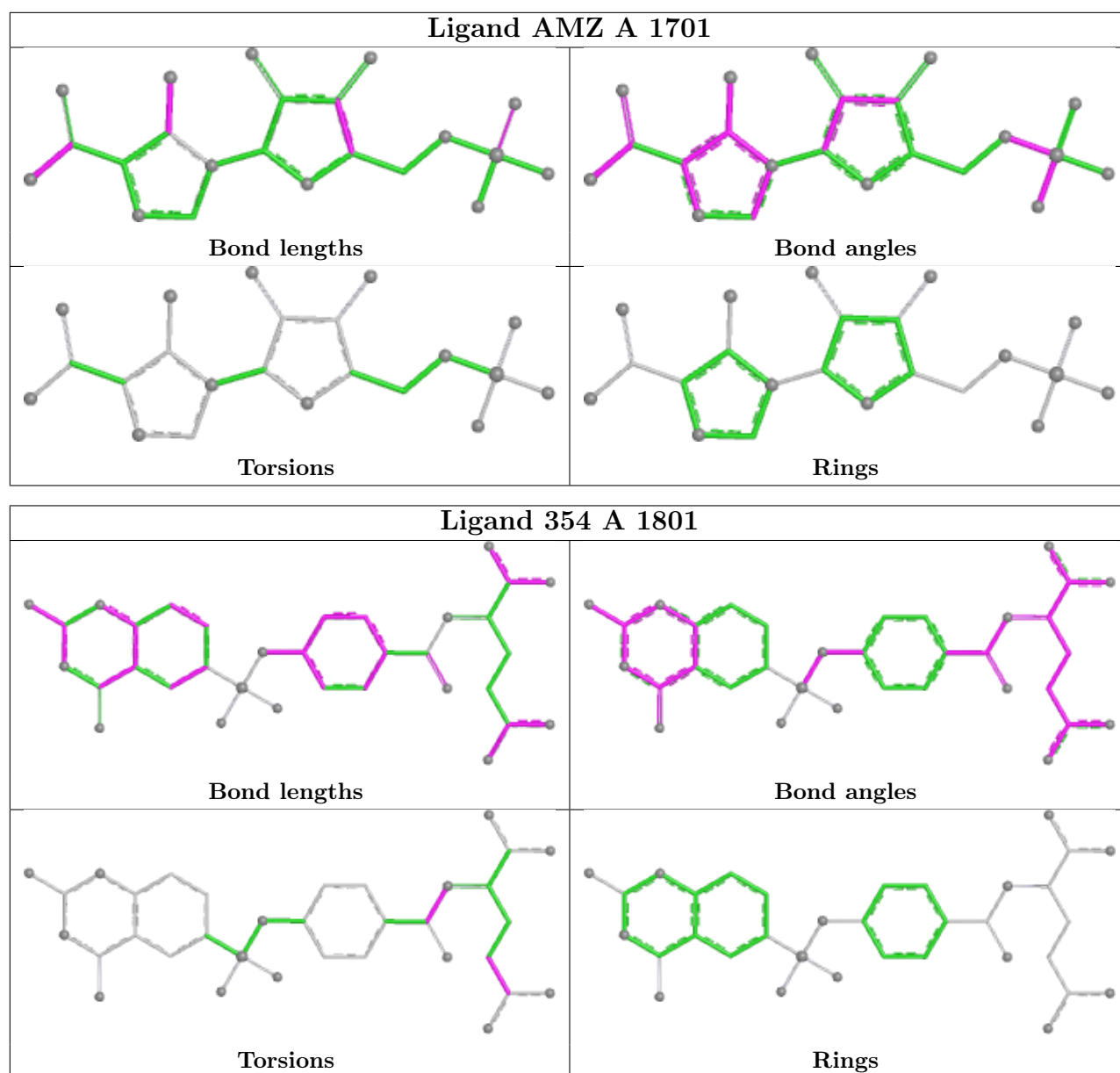
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1802	354	2	0
5	A	1901	XMP	2	0
3	B	1702	AMZ	1	0
4	A	1801	354	4	0

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.







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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	589/592 (99%)	-0.26	3 (0%) 87 89	10, 27, 54, 67	0
1	B	588/592 (99%)	-0.18	0 100 100	11, 29, 50, 70	0
All	All	1177/1184 (99%)	-0.22	3 (0%) 90 92	10, 28, 52, 70	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	503	GLU	2.3
1	A	47	ALA	2.3
1	A	506	ILE	2.2

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(Å ²)	Q<0.9
4	354	B	1802	34/34	0.92	0.10	32,40,48,50	0
3	AMZ	B	1702	22/22	0.94	0.09	27,31,37,38	0

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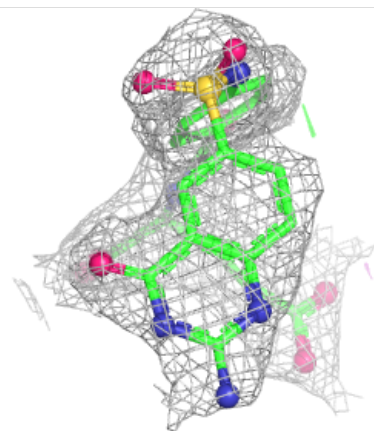
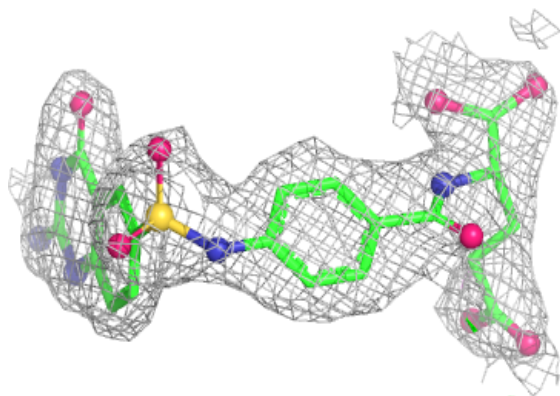
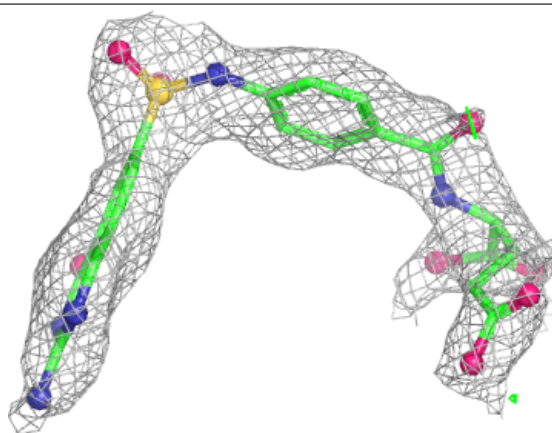
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	354	A	1801	34/34	0.95	0.08	20,26,37,38	0
5	XMP	A	1901	24/24	0.95	0.07	30,34,39,40	0
3	AMZ	A	1701	22/22	0.97	0.07	15,17,21,22	0
2	K	B	1002	1/1	0.99	0.02	19,19,19,19	0
2	K	A	1001	1/1	0.99	0.02	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.

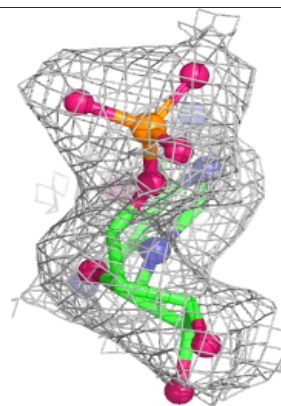
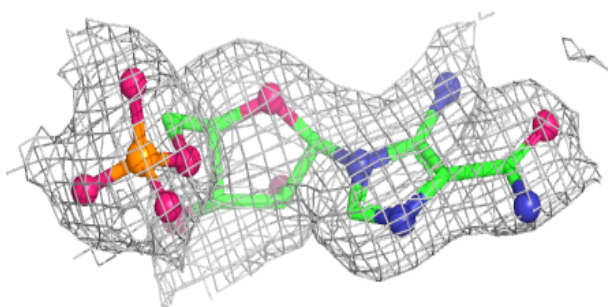
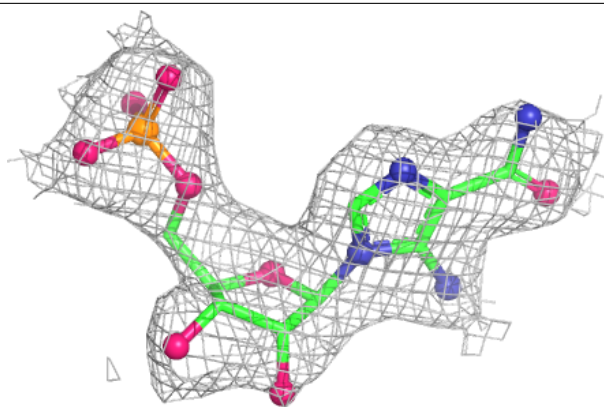
Electron density around 354 B 1802:

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



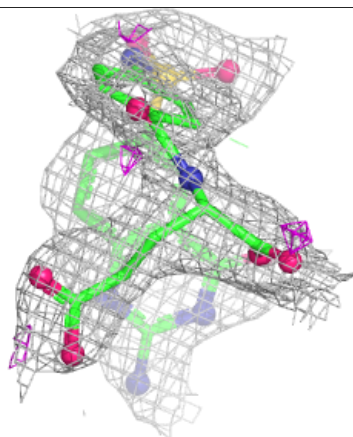
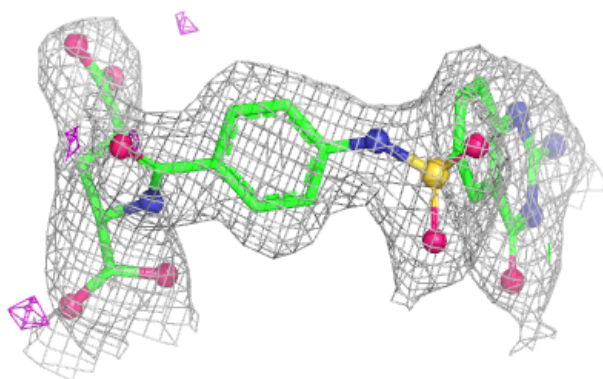
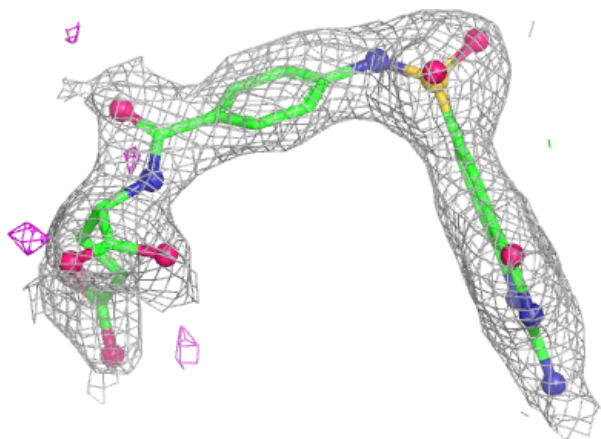
Electron density around AMZ B 1702:

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



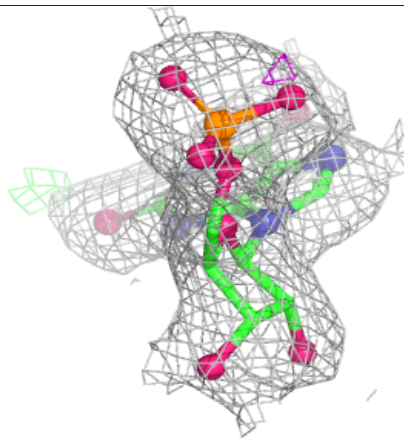
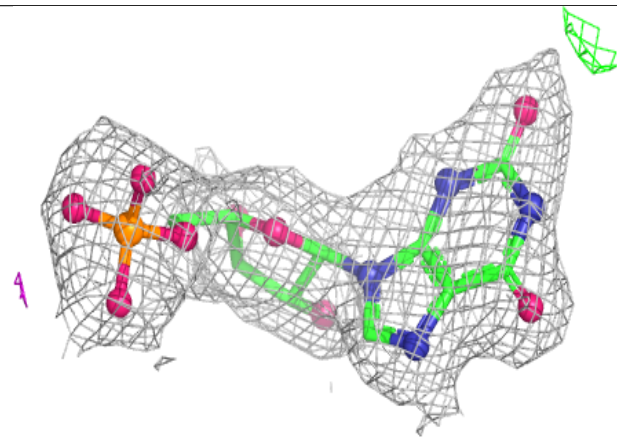
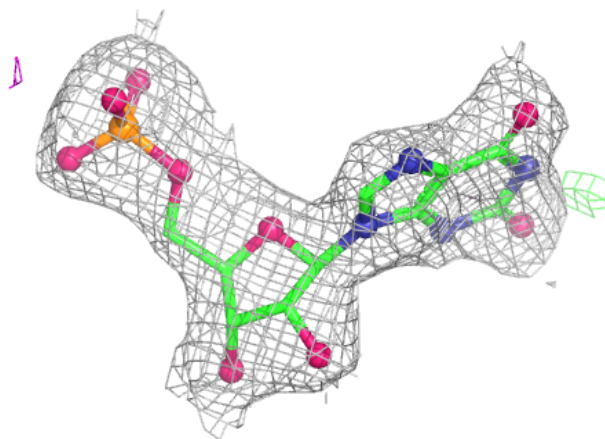
Electron density around 354 A 1801:

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



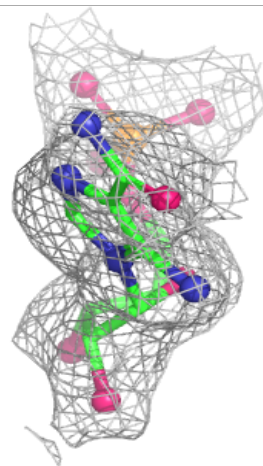
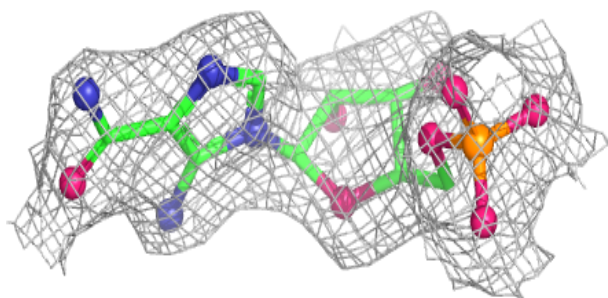
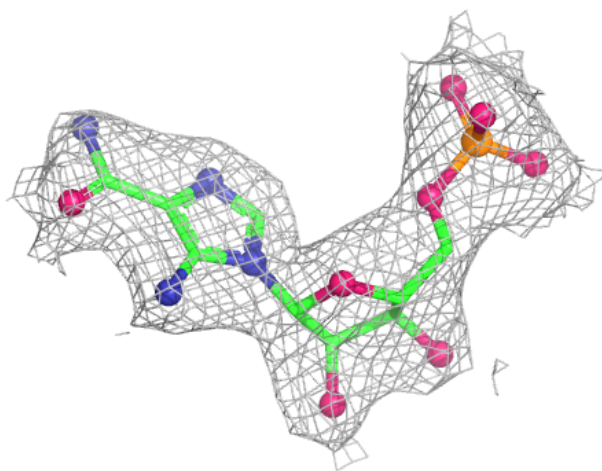
Electron density around XMP A 1901:

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



Electron density around AMZ A 1701:

$2mF_o-DF_c$ (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.