W O R L D W I D E

wwPDB

PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Mar 19, 2024 – 12:37 pm GMT

PDB ID	:	8P4Q
Title	:	Structure of the IMP dehydrogenase related protein GUAB3 from Synechocystis PCC 6803
Authors	:	Hernandez-Gomez, A.; Fernandez-Justel, D.; Buey, R.M.
Deposited on	:	2023-05-23
Resolution	:	1.88 Å(reported)

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

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

1   Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.88 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Rfree		0.195
Clashscore		2
Ramachandran outliers		0
Sidechain outliers		0
RSRZ outliers		0.5%

Worse   *Better*

▮ Percentile relative to all X-ray structures

❏ Percentile relative to X-ray structures of similar resolution
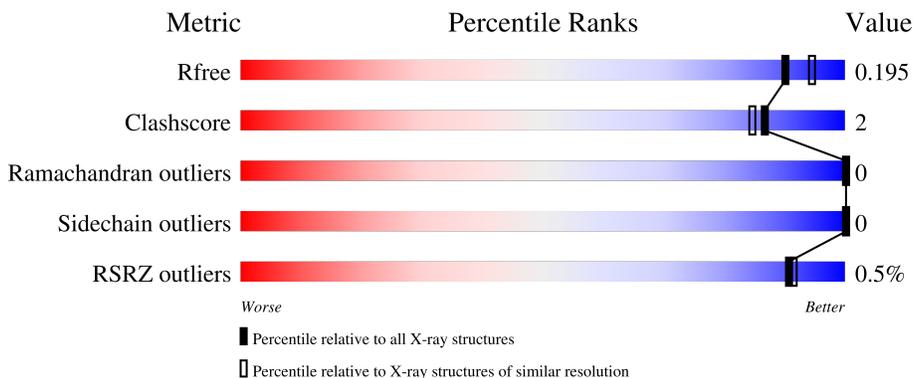
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	390	95% 5% •
1	B	390	94% 5% •
1	C	390	93% 7% •
1	D	390	95% 5% •
1	E	390	% 96% •

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Mol	Chain	Length	Quality of chain
1	F	390	94% 5%
1	G	390	94% 6%
1	H	390	96%
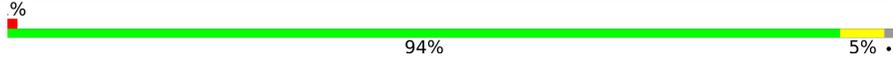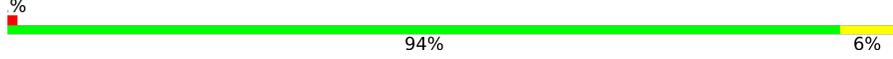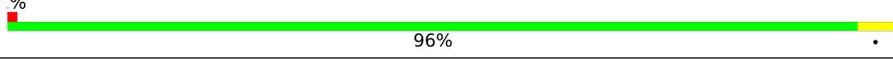
2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 46946 atoms, of which 22755 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 IMP dehydrogenase subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	388	Total	C	H	N	O	S	0	3	0
			5599	1745	2826	482	525	21			
1	B	388	Total	C	H	N	O	S	0	3	0
			5623	1749	2842	483	527	22			
1	C	388	Total	C	H	N	O	S	0	3	0
			5613	1747	2835	483	527	21			
1	D	388	Total	C	H	N	O	S	0	3	0
			5592	1743	2823	480	525	21			
1	E	390	Total	C	H	N	O	S	0	3	0
			5618	1750	2834	485	527	22			
1	F	388	Total	C	H	N	O	S	0	3	0
			5536	1731	2785	480	519	21			
1	G	389	Total	C	H	N	O	S	0	3	0
			5630	1752	2844	484	528	22			
1	H	390	Total	C	H	N	O	S	0	3	0
			5626	1752	2838	485	529	22			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P73853
A	-1	SER	-	expression tag	UNP P73853
A	0	HIS	-	expression tag	UNP P73853
B	-2	GLY	-	expression tag	UNP P73853
B	-1	SER	-	expression tag	UNP P73853
B	0	HIS	-	expression tag	UNP P73853
C	-2	GLY	-	expression tag	UNP P73853
C	-1	SER	-	expression tag	UNP P73853
C	0	HIS	-	expression tag	UNP P73853
D	-2	GLY	-	expression tag	UNP P73853
D	-1	SER	-	expression tag	UNP P73853
D	0	HIS	-	expression tag	UNP P73853
E	-2	GLY	-	expression tag	UNP P73853

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	SER	-	expression tag	UNP P73853
E	0	HIS	-	expression tag	UNP P73853
F	-2	GLY	-	expression tag	UNP P73853
F	-1	SER	-	expression tag	UNP P73853
F	0	HIS	-	expression tag	UNP P73853
G	-2	GLY	-	expression tag	UNP P73853
G	-1	SER	-	expression tag	UNP P73853
G	0	HIS	-	expression tag	UNP P73853
H	-2	GLY	-	expression tag	UNP P73853
H	-1	SER	-	expression tag	UNP P73853
H	0	HIS	-	expression tag	UNP P73853

- Molecule 2 is INOSINIC ACID (three-letter code: IMP) (formula: $C_{10}H_{13}N_4O_8P$).
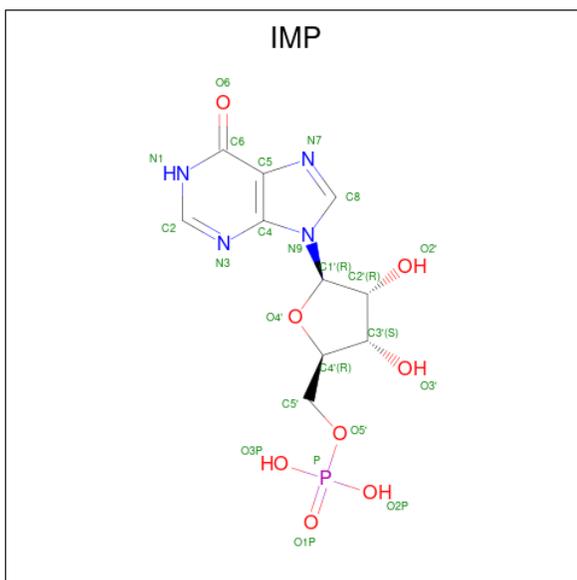
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	1
			31	10	8	4	8	1		
2	B	1	Total	C	H	N	O	P	0	1
			31	10	8	4	8	1		
2	C	1	Total	C	H	N	O	P	0	1
			31	10	8	4	8	1		
2	D	1	Total	C	H	N	O	P	0	1
			31	10	8	4	8	1		
2	E	1	Total	C	H	N	O	P	0	1
			31	10	8	4	8	1		
2	F	1	Total	C	H	N	O	P	0	1
			31	10	8	4	8	1		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	G	1	Total	C	H	N	O	P	0	1
			31	10	8	4	8	1		
2	H	1	Total	C	H	N	O	P	0	1
			31	10	8	4	8	1		

- Molecule 3 is XANTHOSINE-5'-MONOPHOSPHATE (three-letter code: XMP) (formula: $C_{10}H_{14}N_4O_9P$).
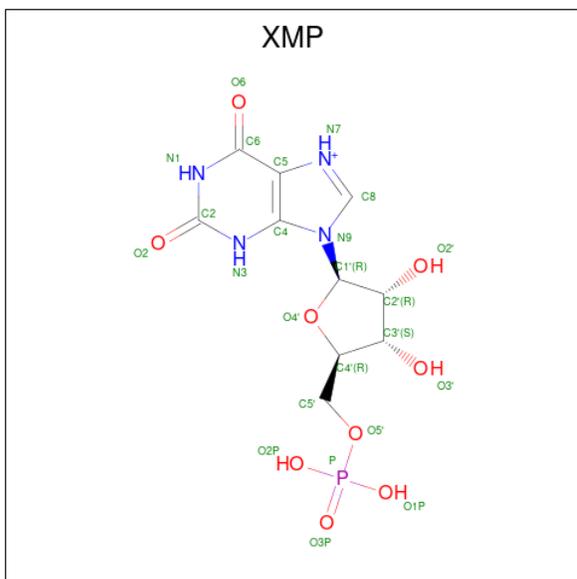
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	0	1
			32	10	8	4	9	1		
3	B	1	Total	C	H	N	O	P	0	1
			32	10	8	4	9	1		
3	C	1	Total	C	H	N	O	P	0	1
			32	10	8	4	9	1		
3	D	1	Total	C	H	N	O	P	0	1
			32	10	8	4	9	1		
3	E	1	Total	C	H	N	O	P	0	1
			32	10	8	4	9	1		
3	F	1	Total	C	H	N	O	P	0	1
			32	10	8	4	9	1		
3	G	1	Total	C	H	N	O	P	0	1
			32	10	8	4	9	1		
3	H	1	Total	C	H	N	O	P	0	1
			32	10	8	4	9	1		

- Molecule 4 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	231	Total 231	O 231	0	0
4	B	235	Total 235	O 235	0	0
4	C	194	Total 194	O 194	0	0
4	D	209	Total 209	O 209	0	0
4	E	206	Total 206	O 206	0	0
4	F	154	Total 154	O 154	0	0
4	G	184	Total 184	O 184	0	0
4	H	192	Total 192	O 192	0	0

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: IMP dehydrogenase subunit

Chain A:

- Molecule 1: IMP dehydrogenase subunit

Chain B:

- Molecule 1: IMP dehydrogenase subunit

Chain C:

- Molecule 1: IMP dehydrogenase subunit

Chain D:

- Molecule 1: IMP dehydrogenase subunit

Chain E:
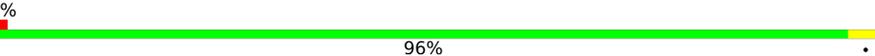
- Molecule 1: IMP dehydrogenase subunit

Chain F:

%

94%

5%

G-2 I3 A21 W38 I50 I80 P87 L91 S136 A150 F158 P171 E172 SER VAL E175 M186 P187 S201 M205 G217 P218 G219 C222 I270 M302 I344 L370 K387

• Molecule 1: IMP dehydrogenase subunit

Chain G:

%

94%

6%

G-2 S-1 H0 I3 A11 D18 I80 Y84 E85 V97 L105 K115 L118 S136 F158 P171 GLU S173 L192 A209 G217 P218 G219 C222 D240 M302 K332 K387

• Molecule 1: IMP dehydrogenase subunit

Chain H:

%

96%

G-2 M1 N2 I3 T4 A11 Y15 R27 V97 L105 V140 M186 L192 S201 M205 A209 G217 P218 G219 C222 I287 M302 I323 K387

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	123.98Å 131.68Å 182.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.04 – 1.88 49.04 – 1.88	Depositor EDS
% Data completeness (in resolution range)	90.4 (49.04-1.88) 90.4 (49.04-1.88)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.15 (at 1.88Å)	Xtriage
Refinement program	PHENIX 1.21rc1_4933	Depositor
R, R_{free}	0.178 , 0.197 0.178 , 0.195	Depositor DCC
R_{free} test set	11048 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	31.5	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 38.9	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	46946	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.12% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.
[2] Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.30	0/2821	0.54	0/3842
1	B	0.30	0/2829	0.54	0/3851
1	C	0.30	0/2826	0.54	0/3848
1	D	0.30	0/2816	0.55	0/3835
1	E	0.30	0/2833	0.53	0/3859
1	F	0.30	0/2799	0.54	0/3815
1	G	0.31	0/2834	0.55	0/3858
1	H	0.30	0/2837	0.56	0/3864
All	All	0.30	0/22595	0.54	0/30772

There are no bond length outliers.

There are no bond angle outliers.

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	2773	2826	2826	12	0
1	B	2781	2842	2842	12	0
1	C	2778	2835	2835	15	0
1	D	2769	2823	2823	12	0
1	E	2784	2834	2834	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2751	2785	2785	12	0
1	G	2786	2844	2844	15	0
1	H	2788	2838	2838	11	0
2	A	23	8	10	0	0
2	B	23	8	10	0	0
2	C	23	8	10	0	0
2	D	23	8	10	0	0
2	E	23	8	10	0	0
2	F	23	8	10	0	0
2	G	23	8	10	0	0
2	H	23	8	10	0	0
3	A	24	8	12	1	0
3	B	24	8	12	1	0
3	C	24	8	12	1	0
3	D	24	8	12	2	0
3	E	24	8	12	1	0
3	F	24	8	12	1	0
3	G	24	8	12	1	0
3	H	24	8	12	2	0
4	A	231	0	0	0	0
4	B	235	0	0	2	0
4	C	194	0	0	2	0
4	D	209	0	0	1	0
4	E	206	0	0	0	0
4	F	154	0	0	0	0
4	G	184	0	0	4	0
4	H	192	0	0	0	0
All	All	24191	22755	22803	96	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 2.

The worst 5 of 96 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:C:97:VAL:HG11	1:C:105:LEU:HD22	1.70	0.71
1:G:-2:GLY:N	4:G:502:HOH:O	2.23	0.71
1:A:302:MET:H	3:A:402[B]:XMP:H7	1.43	0.66
1:G:85:GLU:OE1	1:G:118:LEU:HD21	1.95	0.66
1:G:332:LYS:CB	4:G:503:HOH:O	2.44	0.65

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	387/390 (99%)	381 (98%)	6 (2%)	0	100	100
1	B	387/390 (99%)	382 (99%)	5 (1%)	0	100	100
1	C	387/390 (99%)	382 (99%)	5 (1%)	0	100	100
1	D	387/390 (99%)	382 (99%)	5 (1%)	0	100	100
1	E	391/390 (100%)	385 (98%)	6 (2%)	0	100	100
1	F	387/390 (99%)	381 (98%)	6 (2%)	0	100	100
1	G	388/390 (100%)	382 (98%)	6 (2%)	0	100	100
1	H	391/390 (100%)	385 (98%)	6 (2%)	0	100	100
All	All	3105/3120 (100%)	3060 (99%)	45 (1%)	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	283/297 (95%)	283 (100%)	0	100	100
1	B	286/297 (96%)	286 (100%)	0	100	100
1	C	285/297 (96%)	285 (100%)	0	100	100
1	D	282/297 (95%)	282 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	284/297 (96%)	284 (100%)	0	100	100
1	F	277/297 (93%)	277 (100%)	0	100	100
1	G	286/297 (96%)	286 (100%)	0	100	100
1	H	285/297 (96%)	285 (100%)	0	100	100
All	All	2268/2376 (96%)	2268 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

16 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	$\#|Z| > 2$
3	XMP	D	402[B]	-	20,26,26	0.95	2 (10%)	27,40,40	2.43	7 (25%)
3	XMP	E	402[B]	-	20,26,26	0.93	2 (10%)	27,40,40	2.37	7 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	IMP	A	401[A]	1	21,25,25	0.98	3 (14%)	24,38,38	1.06	3 (12%)
3	XMP	F	402[B]	-	20,26,26	0.96	2 (10%)	27,40,40	2.38	7 (25%)
3	XMP	C	402[B]	-	20,26,26	0.89	1 (5%)	27,40,40	2.39	7 (25%)
2	IMP	D	401[A]	1	21,25,25	0.97	3 (14%)	24,38,38	1.08	3 (12%)
3	XMP	H	402[B]	-	20,26,26	0.96	2 (10%)	27,40,40	2.43	6 (22%)
2	IMP	G	401[A]	1	21,25,25	1.02	3 (14%)	24,38,38	1.07	3 (12%)
2	IMP	H	401[A]	1	21,25,25	1.04	3 (14%)	24,38,38	1.03	2 (8%)
2	IMP	B	401[A]	1	21,25,25	1.04	3 (14%)	24,38,38	1.06	3 (12%)
2	IMP	C	401[A]	1	21,25,25	0.95	3 (14%)	24,38,38	1.07	3 (12%)
2	IMP	E	401[A]	1	21,25,25	0.96	2 (9%)	24,38,38	1.08	3 (12%)
3	XMP	A	402[B]	-	20,26,26	0.85	1 (5%)	27,40,40	2.47	7 (25%)
2	IMP	F	401[A]	1	21,25,25	1.03	3 (14%)	24,38,38	1.05	3 (12%)
3	XMP	G	402[B]	-	20,26,26	0.97	2 (10%)	27,40,40	2.35	7 (25%)
3	XMP	B	402[B]	-	20,26,26	0.94	2 (10%)	27,40,40	2.45	7 (25%)

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
3	XMP	D	402[B]	-	-	0/6/26/26	0/3/3/3
3	XMP	E	402[B]	-	-	0/6/26/26	0/3/3/3
2	IMP	A	401[A]	1	-	0/6/26/26	0/3/3/3
3	XMP	F	402[B]	-	-	0/6/26/26	0/3/3/3
3	XMP	C	402[B]	-	-	0/6/26/26	0/3/3/3
2	IMP	D	401[A]	1	-	0/6/26/26	0/3/3/3
3	XMP	H	402[B]	-	-	0/6/26/26	0/3/3/3
2	IMP	G	401[A]	1	-	0/6/26/26	0/3/3/3
2	IMP	H	401[A]	1	-	0/6/26/26	0/3/3/3
2	IMP	B	401[A]	1	-	0/6/26/26	0/3/3/3
2	IMP	C	401[A]	1	-	0/6/26/26	0/3/3/3
2	IMP	E	401[A]	1	-	0/6/26/26	0/3/3/3
3	XMP	A	402[B]	-	-	0/6/26/26	0/3/3/3
2	IMP	F	401[A]	1	-	0/6/26/26	0/3/3/3
3	XMP	G	402[B]	-	-	0/6/26/26	0/3/3/3
3	XMP	B	402[B]	-	-	0/6/26/26	0/3/3/3

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401[A]	IMP	C2-N1	2.63	1.40	1.35
3	D	402[B]	XMP	C2-N3	2.56	1.41	1.36
2	H	401[A]	IMP	C2-N1	2.55	1.40	1.35
2	F	401[A]	IMP	C2-N1	2.52	1.40	1.35
2	G	401[A]	IMP	C2-N1	2.50	1.40	1.35

The worst 5 of 78 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	402[B]	XMP	N3-C2-N1	7.41	120.20	115.90
3	H	402[B]	XMP	N3-C2-N1	7.16	120.06	115.90
3	B	402[B]	XMP	N3-C2-N1	7.05	119.99	115.90
3	D	402[B]	XMP	N3-C2-N1	7.02	119.98	115.90
3	E	402[B]	XMP	N3-C2-N1	6.95	119.94	115.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	402[B]	XMP	2	0
3	E	402[B]	XMP	1	0
3	F	402[B]	XMP	1	0
3	C	402[B]	XMP	1	0
3	H	402[B]	XMP	2	0
3	A	402[B]	XMP	1	0
3	G	402[B]	XMP	1	0
3	B	402[B]	XMP	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand XMP D 402 (B)

Bond lengths

Bond angles

Torsions

Rings

Ligand XMP E 402 (B)

Bond lengths

Bond angles

Torsions

Rings

Ligand IMP A 401 (A)

Bond lengths

Bond angles

Torsions

Rings

Ligand XMP F 402 (B)

Bond lengths

Bond angles

Torsions

Rings

Ligand XMP C 402 (B)

Bond lengths

Bond angles

Torsions

Rings

Ligand IMP D 401 (A)

Bond lengths

Bond angles

Torsions

Rings

Ligand XMP H 402 (B)

Bond lengths

Bond angles

Torsions

Rings

Ligand IMP G 401 (A)

Bond lengths

Bond angles

Torsions

Rings

Ligand IMP H 401 (A)

Bond lengths

Bond angles

Torsions

Rings

Ligand IMP B 401 (A)

Bond lengths

Bond angles

Torsions

Rings

Ligand IMP C 401 (A)

Bond lengths

Bond angles

Torsions

Rings

Ligand IMP E 401 (A)

Bond lengths

Bond angles

Torsions

Rings

Ligand XMP A 402 (B)

Bond lengths

Bond angles

Torsions

Rings

Ligand IMP F 401 (A)

Bond lengths

Bond angles

Torsions

Rings

Ligand XMP G 402 (B)

Bond lengths

Bond angles

Torsions

Rings

Ligand XMP B 402 (B)

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	388/390 (99%)	-0.26	0	100	100	23, 30, 39, 48	0
1	B	388/390 (99%)	-0.17	0	100	100	24, 30, 41, 52	0
1	C	388/390 (99%)	-0.13	1 (0%)	94	94	25, 33, 44, 53	0
1	D	388/390 (99%)	-0.17	0	100	100	24, 32, 42, 55	0
1	E	390/390 (100%)	-0.04	2 (0%)	91	91	26, 35, 45, 51	0
1	F	388/390 (99%)	0.06	3 (0%)	86	87	27, 37, 51, 56	0
1	G	389/390 (99%)	-0.08	5 (1%)	77	79	25, 35, 50, 61	0
1	H	390/390 (100%)	-0.01	4 (1%)	82	83	26, 35, 52, 66	0
All	All	3109/3120 (99%)	-0.10	15 (0%)	91	91	23, 33, 47, 66	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	80	ILE	3.8
1	E	80	ILE	3.2
1	G	80	ILE	2.9
1	H	140	VAL	2.8
1	H	186	MET	2.4

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

WORLDWIDE
wwPDB
PROTEIN DATA BANK

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	IMP	F	401[A]	23/23	0.95	0.11	34,36,43,43	31
2	IMP	G	401[A]	23/23	0.95	0.11	32,36,42,42	31
3	XMP	G	402[B]	24/24	0.95	0.11	31,36,42,42	32
3	XMP	B	402[B]	24/24	0.96	0.11	26,29,34,36	32
3	XMP	E	402[B]	24/24	0.96	0.11	29,33,38,39	32
3	XMP	F	402[B]	24/24	0.96	0.10	34,36,42,43	32
2	IMP	H	401[A]	23/23	0.96	0.11	31,33,39,39	31
3	XMP	H	402[B]	24/24	0.96	0.10	31,33,39,39	32
3	XMP	A	402[B]	24/24	0.97	0.11	25,28,32,33	32
2	IMP	D	401[A]	23/23	0.97	0.11	26,29,34,35	31
3	XMP	C	402[B]	24/24	0.97	0.11	28,31,37,38	32
3	XMP	D	402[B]	24/24	0.97	0.11	26,29,34,36	32
2	IMP	E	401[A]	23/23	0.97	0.12	29,32,38,39	31
2	IMP	A	401[A]	23/23	0.97	0.12	25,28,32,34	31
2	IMP	B	401[A]	23/23	0.97	0.10	26,29,34,36	31
2	IMP	C	401[A]	23/23	0.97	0.11	28,31,37,37	31

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 IMP F 401 (A):

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
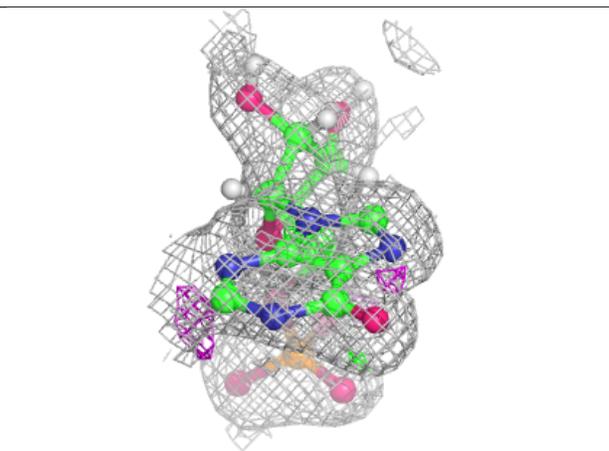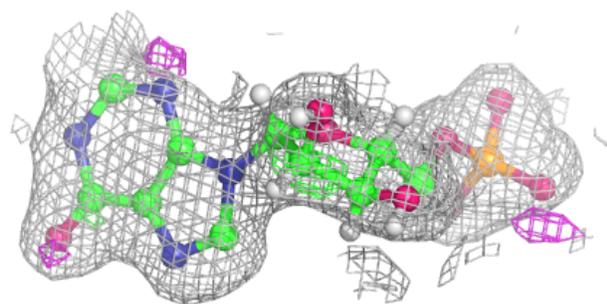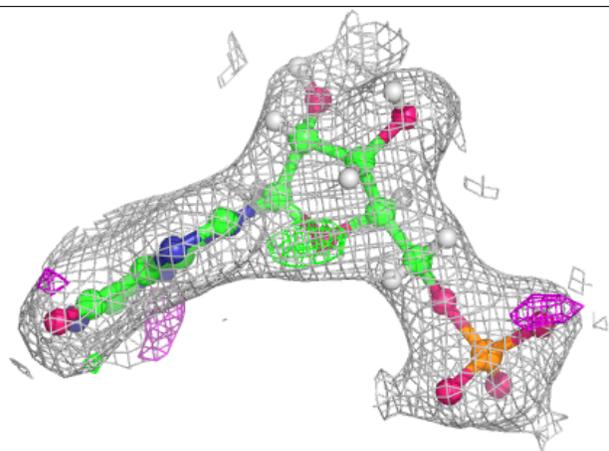
Electron density around IMP G 401 (A):

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
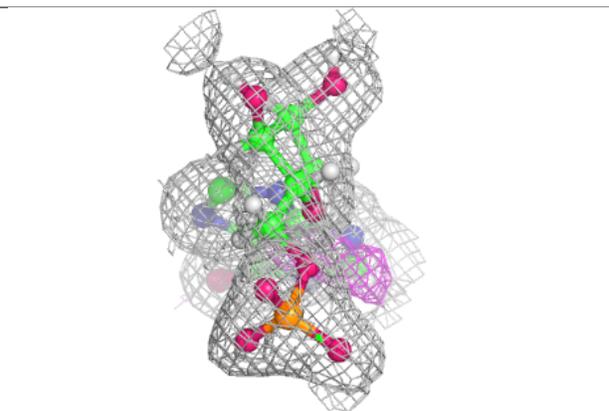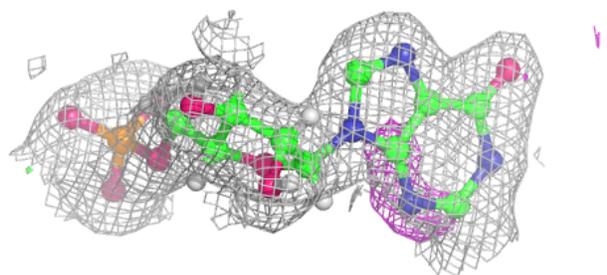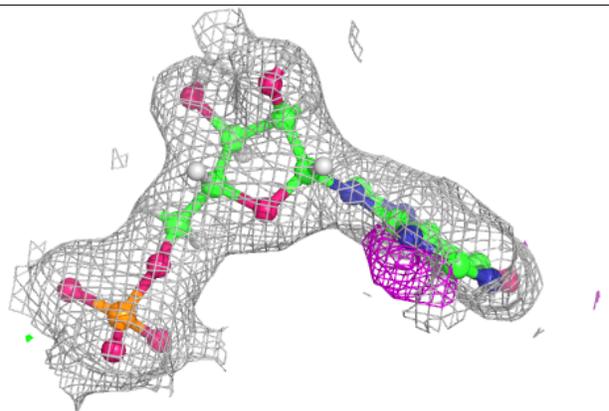
Electron density around XMP G 402 (B):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
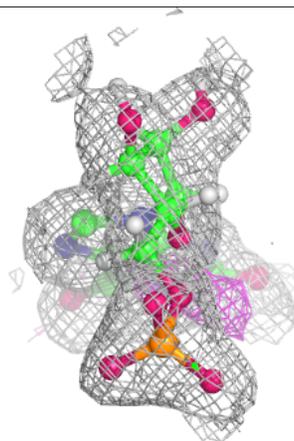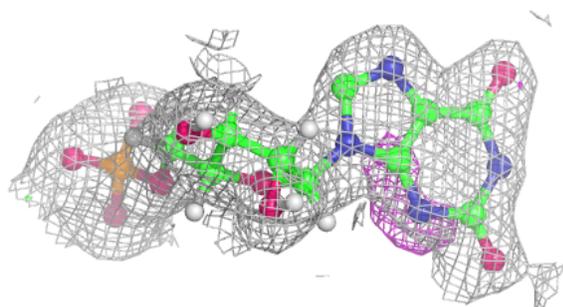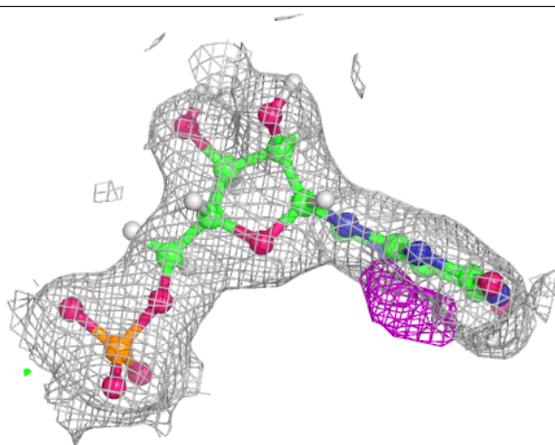
Electron density around XMP B 402 (B):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
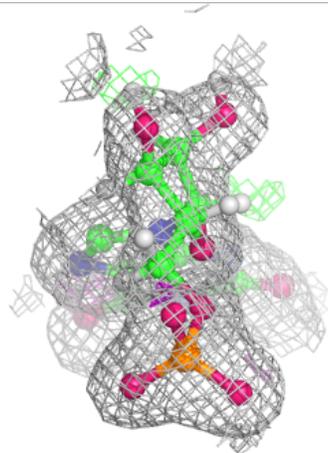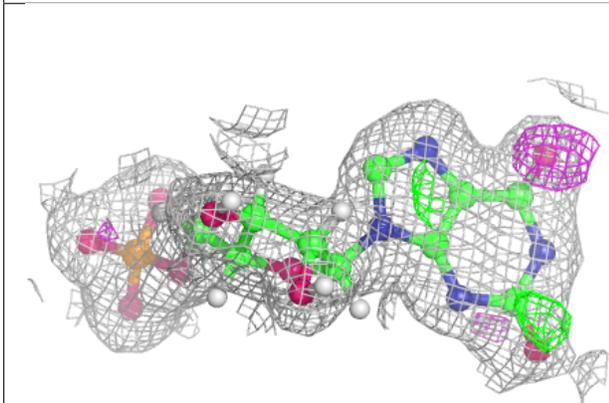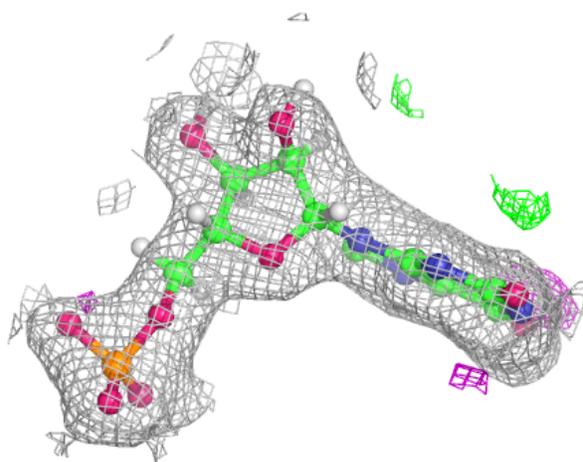
Electron density around XMP E 402 (B):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
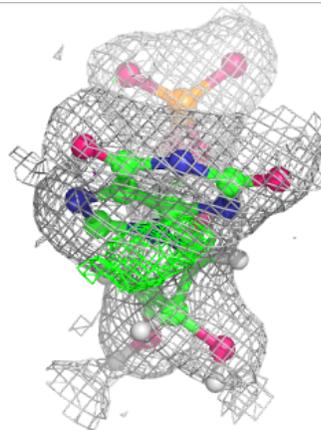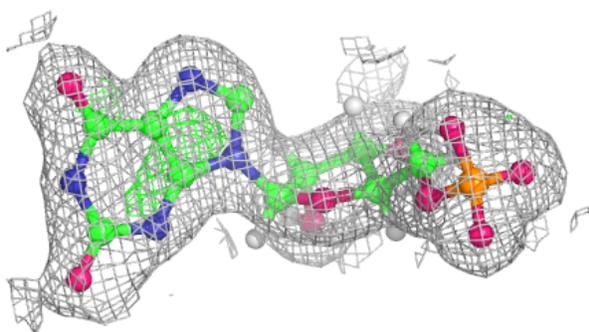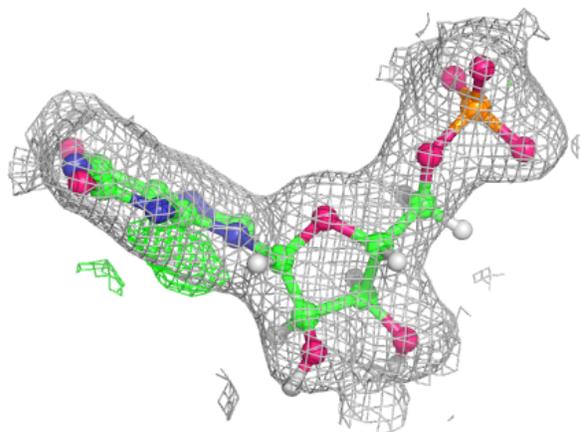
Electron density around XMP F 402 (B):

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
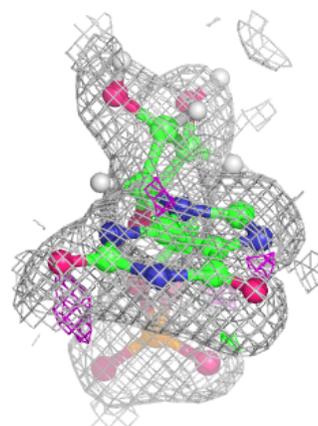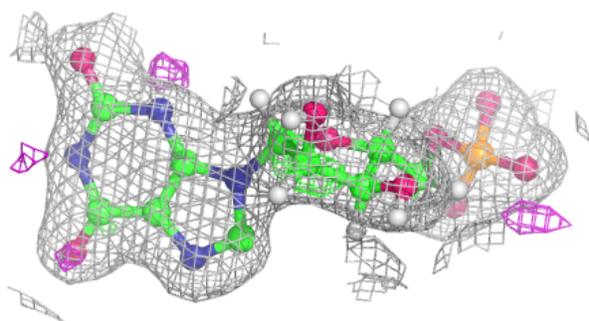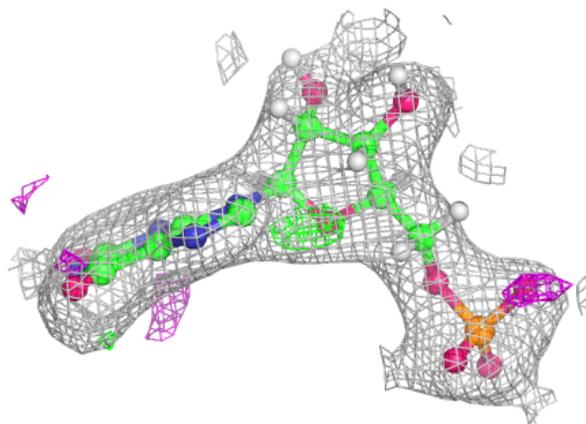
Electron density around IMP H 401 (A):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
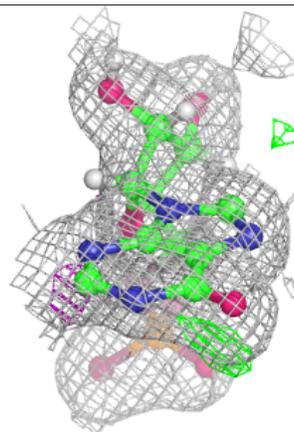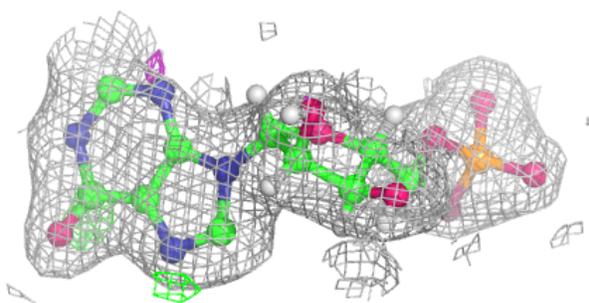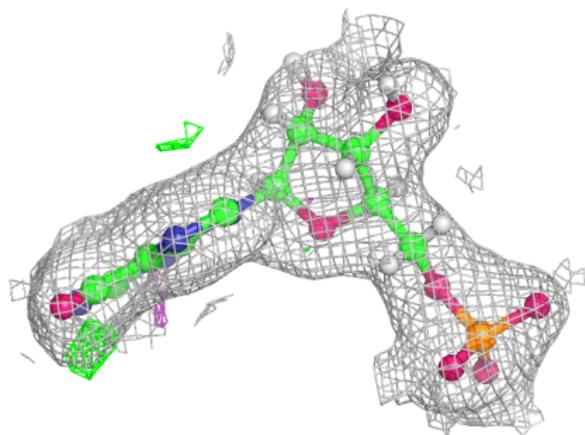
Electron density around XMP H 402 (B):

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
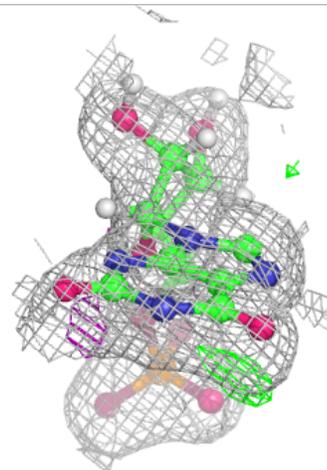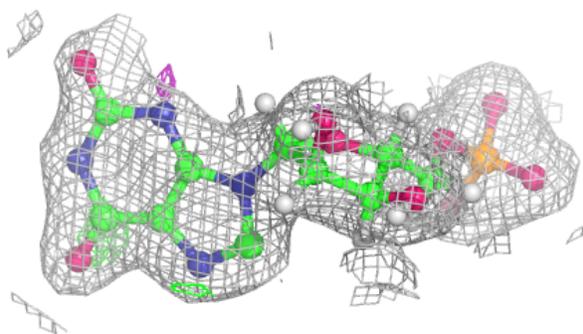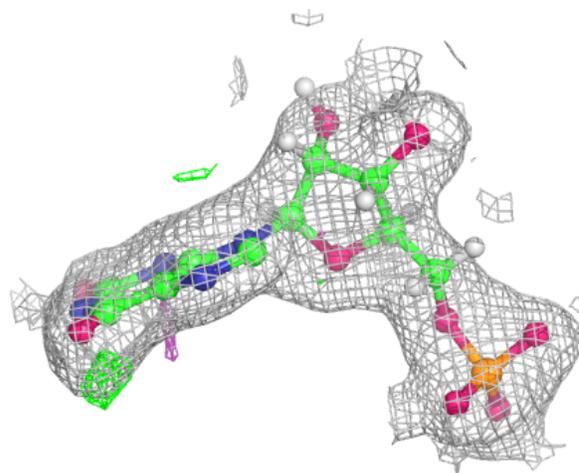
Electron density around XMP A 402 (B):

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
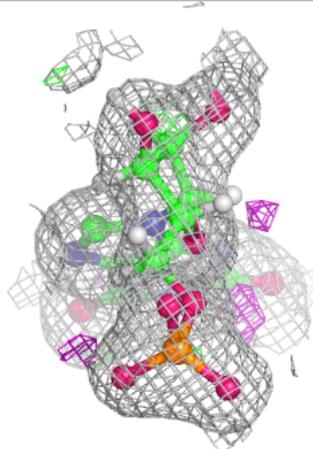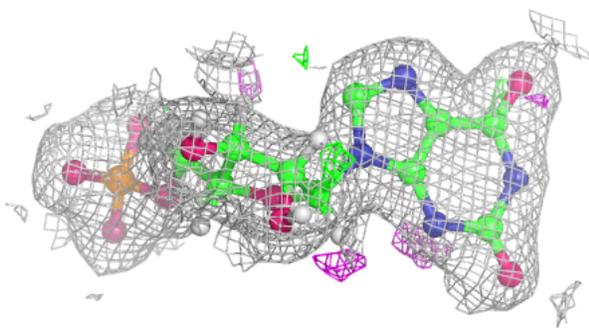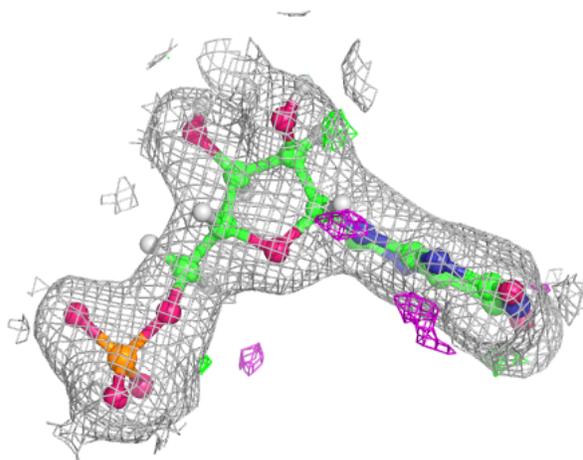
Electron density around IMP D 401 (A):

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
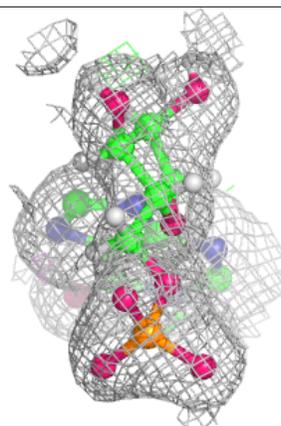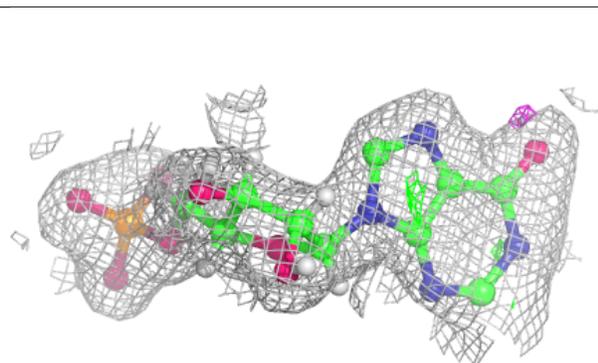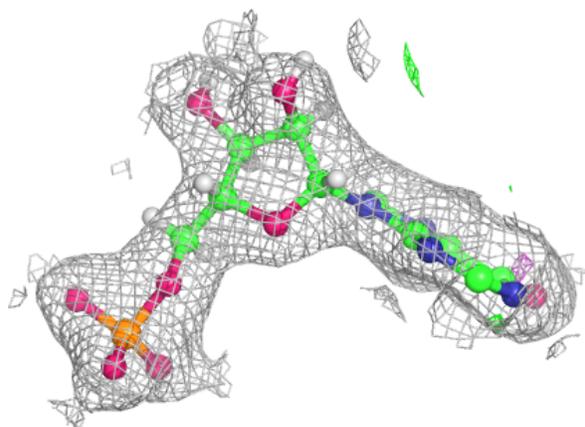
Electron density around XMP C 402 (B):

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
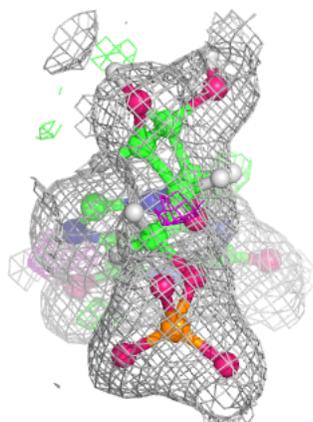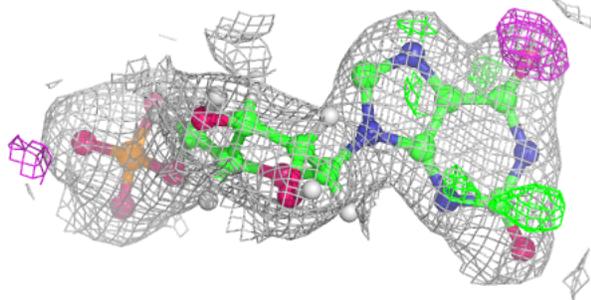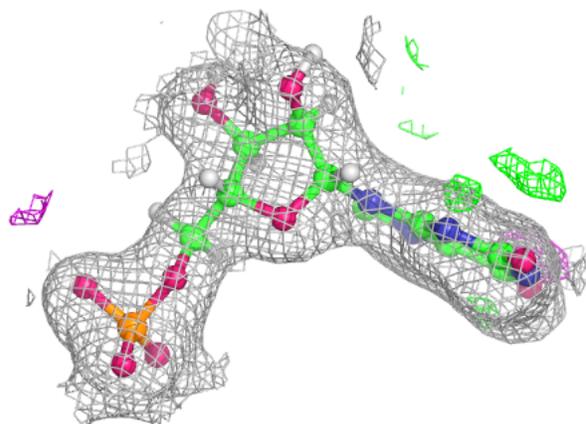
Electron density around XMP D 402 (B):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
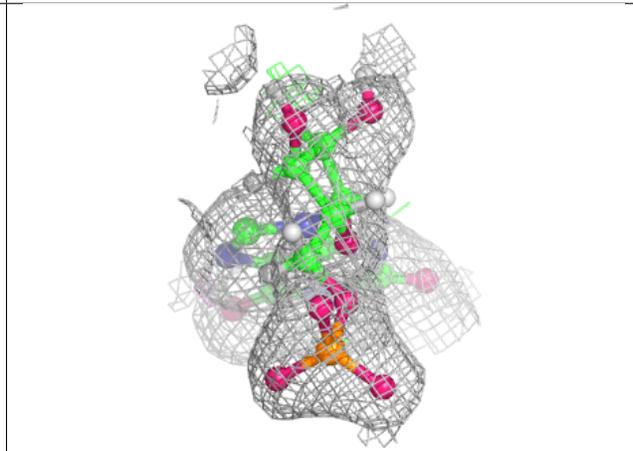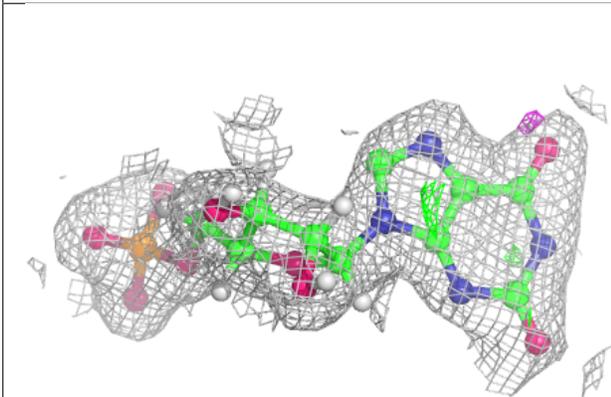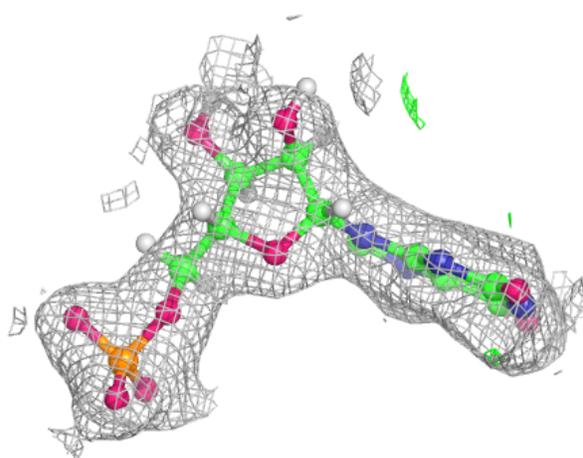
Electron density around IMP E 401 (A):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
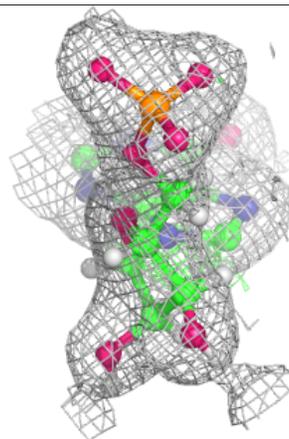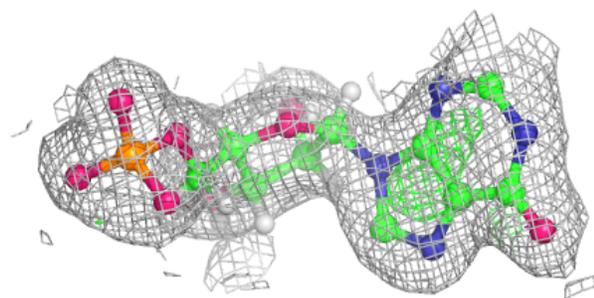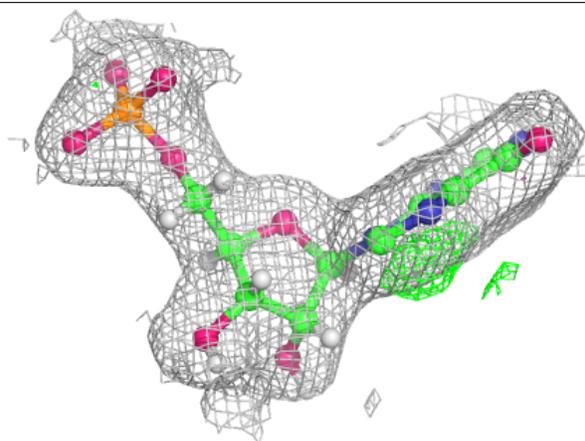
Electron density around IMP A 401 (A):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
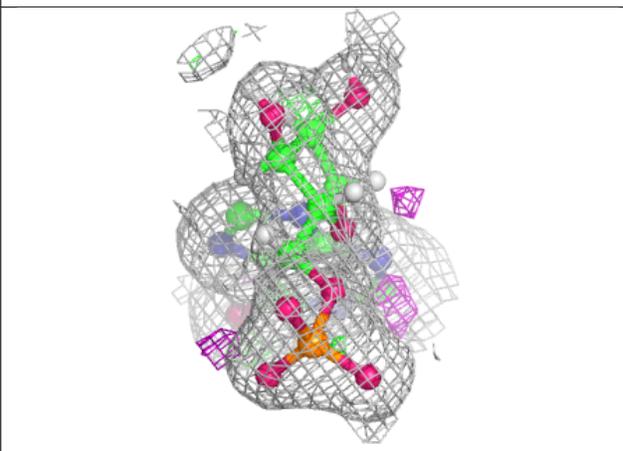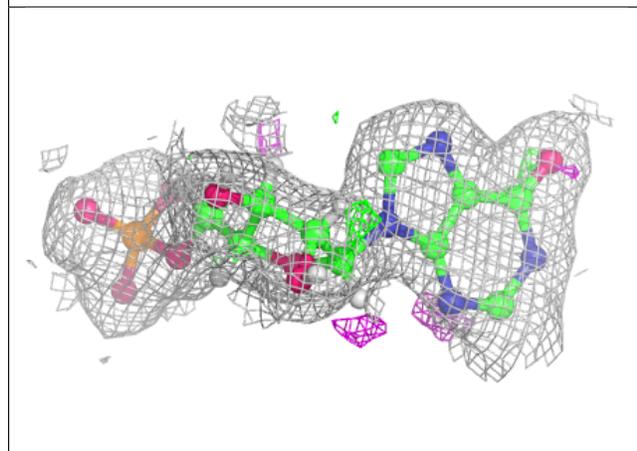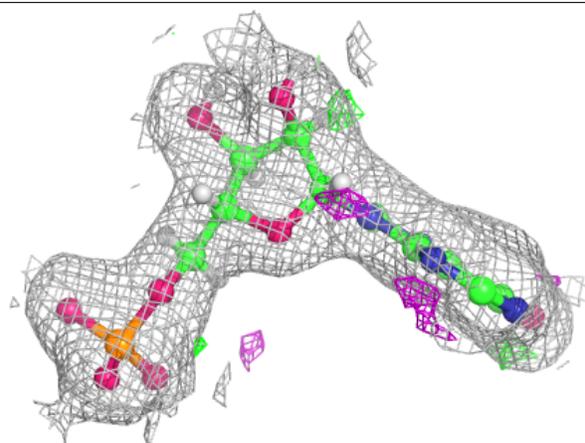
Electron density around IMP B 401 (A):

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

Electron density around IMP C 401 (A):

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

6.5   Other polymers ⓘ

There are no such residues in this entry.