



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:37 PM UTC

PDB ID : 8V4O / pdb_00008v4o
Title : Crystal structure of Acetyl-CoA synthetase 2 in complex with AMP from *Candida albicans*
Authors : Seattle Structural Genomics Center for Infectious Disease; Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2023-11-29
Resolution : 2.70 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 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

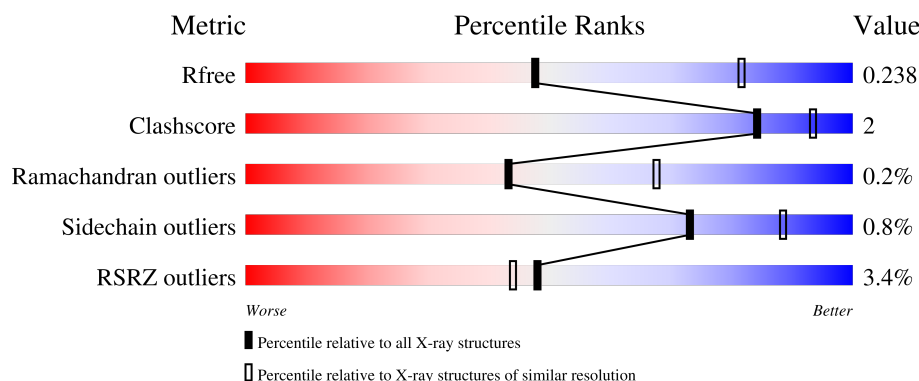
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	686	90% 6% .
1	B	686	5% 86% 6% 8%
1	C	686	3% 72% . 24%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14259 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 Acetyl-coenzyme A synthetase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	660	Total	C	N	O	S	0	0	0
			5085	3244	865	962	14			
1	B	628	Total	C	N	O	S	0	0	0
			4837	3098	815	911	13			
1	C	523	Total	C	N	O	S	0	0	0
			4038	2595	668	762	13			

There are 51 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q8NJJN3
A	2	HIS	-	expression tag	UNP Q8NJJN3
A	3	HIS	-	expression tag	UNP Q8NJJN3
A	4	HIS	-	expression tag	UNP Q8NJJN3
A	5	HIS	-	expression tag	UNP Q8NJJN3
A	6	HIS	-	expression tag	UNP Q8NJJN3
A	7	HIS	-	expression tag	UNP Q8NJJN3
A	8	HIS	-	expression tag	UNP Q8NJJN3
A	9	HIS	-	expression tag	UNP Q8NJJN3
A	10	GLU	-	expression tag	UNP Q8NJJN3
A	11	ASN	-	expression tag	UNP Q8NJJN3
A	12	LEU	-	expression tag	UNP Q8NJJN3
A	13	TYR	-	expression tag	UNP Q8NJJN3
A	14	PHE	-	expression tag	UNP Q8NJJN3
A	15	GLN	-	expression tag	UNP Q8NJJN3
A	16	GLY	-	expression tag	UNP Q8NJJN3
A	403	ALA	VAL	variant	UNP Q8NJJN3
B	1	MET	-	initiating methionine	UNP Q8NJJN3
B	2	HIS	-	expression tag	UNP Q8NJJN3
B	3	HIS	-	expression tag	UNP Q8NJJN3
B	4	HIS	-	expression tag	UNP Q8NJJN3
B	5	HIS	-	expression tag	UNP Q8NJJN3
B	6	HIS	-	expression tag	UNP Q8NJJN3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	7	HIS	-	expression tag	UNP Q8N3N3
B	8	HIS	-	expression tag	UNP Q8N3N3
B	9	HIS	-	expression tag	UNP Q8N3N3
B	10	GLU	-	expression tag	UNP Q8N3N3
B	11	ASN	-	expression tag	UNP Q8N3N3
B	12	LEU	-	expression tag	UNP Q8N3N3
B	13	TYR	-	expression tag	UNP Q8N3N3
B	14	PHE	-	expression tag	UNP Q8N3N3
B	15	GLN	-	expression tag	UNP Q8N3N3
B	16	GLY	-	expression tag	UNP Q8N3N3
B	403	ALA	VAL	variant	UNP Q8N3N3
C	1	MET	-	initiating methionine	UNP Q8N3N3
C	2	HIS	-	expression tag	UNP Q8N3N3
C	3	HIS	-	expression tag	UNP Q8N3N3
C	4	HIS	-	expression tag	UNP Q8N3N3
C	5	HIS	-	expression tag	UNP Q8N3N3
C	6	HIS	-	expression tag	UNP Q8N3N3
C	7	HIS	-	expression tag	UNP Q8N3N3
C	8	HIS	-	expression tag	UNP Q8N3N3
C	9	HIS	-	expression tag	UNP Q8N3N3
C	10	GLU	-	expression tag	UNP Q8N3N3
C	11	ASN	-	expression tag	UNP Q8N3N3
C	12	LEU	-	expression tag	UNP Q8N3N3
C	13	TYR	-	expression tag	UNP Q8N3N3
C	14	PHE	-	expression tag	UNP Q8N3N3
C	15	GLN	-	expression tag	UNP Q8N3N3
C	16	GLY	-	expression tag	UNP Q8N3N3
C	403	ALA	VAL	variant	UNP Q8N3N3

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

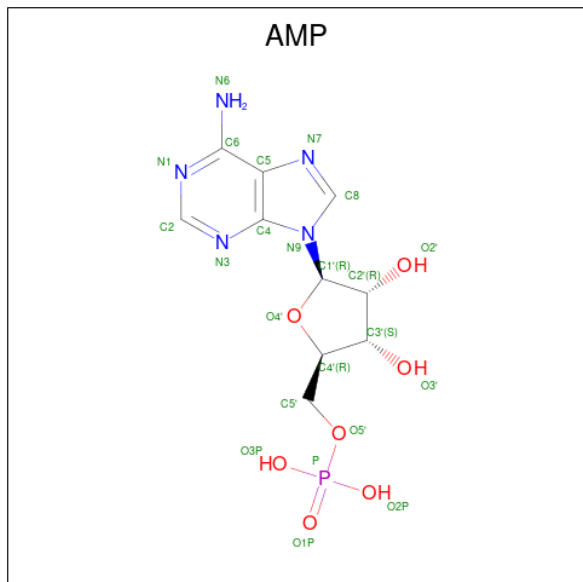


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 4 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	90	Total	O	0	0
			90	90		
5	B	70	Total	O	0	0
			70	70		
5	C	17	Total	O	0	0
			17	17		

GLN VAL ARG ARG THR THR GLY PRO PHE ALA ALA PRO PRO LYS SER VAL VAL ILE ILE VAL GLN ASP LEU LEU PRO PRO LYS THR ARG ARG SER GLY LYS ILE MET ARG ARG ILE LEU LEU ARG LYS VAL SER SER SER ASN ASN ALA ASP GLN LEU LEU GLY ILE ASP SER THR SER LEU LEU SER ASN ASN PRO GLN SER VAL VAL GLY ILE

ILE
SER
ALA
PHE
GLY
ALA
GLN
PHE
GLY
LYS
LYS

4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	139.46Å 139.46Å 544.99Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.68 – 2.70 49.68 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.68-2.70) 100.0 (49.68-2.70)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.21rc1_5162	Depositor
R, R_{free}	0.215 , 0.240 0.216 , 0.238	Depositor DCC
R_{free} test set	4340 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	61.9	Xtriage
Anisotropy	0.458	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 38.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14259	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.88% 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: CL, SO4, AMP

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	0.11	0/5214	0.29	0/7100
1	B	0.11	0/4961	0.29	0/6761
1	C	0.10	0/4157	0.26	0/5679
All	All	0.11	0/14332	0.28	0/19540

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	5085	0	4935	20	0
1	B	4837	0	4677	21	0
1	C	4038	0	3820	23	0
2	A	25	0	0	0	0
2	B	25	0	0	0	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
4	A	23	0	12	0	0
4	B	23	0	12	1	0
4	C	23	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	90	0	0	1	0
5	B	70	0	0	2	0
5	C	17	0	0	0	0
All	All	14259	0	13468	63	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.

All (63) 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:B:222:ARG:NH1	5:B:802:HOH:O	2.20	0.73
1:C:172:MET:SD	1:C:337:VAL:HG23	2.32	0.70
1:A:633:VAL:HG11	1:A:675:ILE:HD13	1.77	0.66
1:C:180:MET:HE1	1:C:337:VAL:HG11	1.78	0.64
1:C:169:TYR:CZ	1:C:202:ILE:HD11	2.34	0.62
1:C:180:MET:CE	1:C:337:VAL:HG11	2.29	0.62
1:A:591:VAL:HG23	1:A:627:PRO:HA	1.84	0.60
1:B:591:VAL:HG23	1:B:627:PRO:HA	1.87	0.57
1:B:218:ASP:OD1	1:B:219:GLU:N	2.37	0.55
1:A:218:ASP:OD1	1:A:219:GLU:N	2.36	0.55
1:C:416:VAL:HG13	1:C:417:GLY:N	2.23	0.54
1:C:337:VAL:O	1:C:337:VAL:HG12	2.09	0.52
1:C:481:PRO:HG3	1:C:495:VAL:HG23	1.92	0.52
1:B:324:ASP:OD2	1:B:411:ARG:NH1	2.43	0.51
1:C:180:MET:SD	1:C:337:VAL:HG11	2.51	0.51
1:C:468:SER:OG	1:C:469:TYR:N	2.44	0.51
1:A:483:THR:OG1	1:A:485:VAL:HG22	2.10	0.50
1:A:102:LEU:HD22	1:B:118:PHE:CZ	2.47	0.50
1:B:40:PHE:CD2	1:B:411:ARG:HG2	2.47	0.49
1:B:597:LEU:O	5:B:801:HOH:O	2.20	0.48
1:B:169:TYR:CZ	1:B:202:ILE:HD11	2.50	0.47
1:A:639:THR:HG22	1:A:645:MET:HE2	1.96	0.47
1:C:416:VAL:HG13	1:C:417:GLY:H	1.80	0.46
1:A:222:ARG:NE	5:A:802:HOH:O	2.39	0.46
1:B:617:VAL:HG13	1:B:621:ILE:HD12	1.98	0.46
1:A:235:GLU:O	1:A:238:VAL:HG12	2.16	0.45
1:B:25:VAL:HG22	1:B:535:ALA:HB1	1.99	0.45
1:B:648:ILE:O	1:B:652:VAL:HG23	2.17	0.45
1:B:329:ASP:OD1	1:B:411:ARG:NH2	2.50	0.45
1:B:522:ASN:N	1:B:523:PRO:CD	2.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:552:VAL:HG11	1:B:591:VAL:CG1	2.47	0.44
1:C:53:VAL:O	1:C:53:VAL:HG22	2.17	0.44
1:C:420:ILE:O	1:C:420:ILE:HG23	2.18	0.44
1:A:169:TYR:CZ	1:A:202:ILE:HD11	2.53	0.43
1:C:144:LEU:O	1:C:148:VAL:HG23	2.19	0.43
1:A:420:ILE:O	1:A:420:ILE:HG23	2.18	0.43
1:A:505:MET:O	1:A:507:ARG:NH1	2.52	0.43
1:B:332:PHE:HB2	1:B:358:ILE:HD12	2.00	0.43
1:C:347:LEU:C	1:C:347:LEU:HD23	2.43	0.43
1:B:505:MET:O	1:B:507:ARG:NH1	2.52	0.42
1:A:203:LYS:NZ	1:A:239:ASP:OD2	2.52	0.42
1:A:332:PHE:HB2	1:A:358:ILE:HD12	2.01	0.42
1:B:544:ILE:HG21	4:B:707:AMP:C2	2.54	0.42
1:C:177:ILE:HA	1:C:180:MET:HE3	2.01	0.42
1:C:418:GLU:CB	1:C:419:PRO:CD	2.97	0.42
1:C:439:ILE:O	1:C:462:ASN:ND2	2.47	0.42
1:A:438:HIS:CD2	1:A:457:ALA:HA	2.54	0.42
1:A:347:LEU:C	1:A:347:LEU:HD23	2.45	0.42
1:B:386:VAL:HG22	1:B:387:ALA:N	2.34	0.42
1:C:456:LEU:HD12	1:C:456:LEU:N	2.35	0.42
1:A:522:ASN:N	1:A:523:PRO:CD	2.82	0.42
1:C:102:LEU:N	1:C:102:LEU:HD12	2.35	0.42
1:A:467:ALA:O	1:A:468:SER:OG	2.35	0.41
1:B:578:ALA:HB2	1:B:644:ILE:HD13	2.01	0.41
1:C:452:LEU:HD23	1:C:474:ILE:HG12	2.01	0.41
1:A:386:VAL:HG22	1:A:387:ALA:N	2.36	0.41
1:B:347:LEU:C	1:B:347:LEU:HD23	2.45	0.41
1:A:373:TRP:HB3	1:A:407:LEU:HD21	2.02	0.41
1:C:522:ASN:N	1:C:523:PRO:CD	2.83	0.41
1:A:615:LEU:HG	1:A:619:LYS:HE3	2.02	0.41
1:C:332:PHE:C	1:C:332:PHE:CD1	2.99	0.41
1:C:474:ILE:HD12	1:C:474:ILE:N	2.36	0.41
1:B:373:TRP:NE1	1:B:402:ILE:HG12	2.36	0.40

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	656/686 (96%)	637 (97%)	19 (3%)	0	100	100
1	B	618/686 (90%)	597 (97%)	21 (3%)	0	100	100
1	C	519/686 (76%)	486 (94%)	30 (6%)	3 (1%)	21	44
All	All	1793/2058 (87%)	1720 (96%)	70 (4%)	3 (0%)	43	68

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	417	GLY
1	C	468	SER
1	C	397	ALA

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	532/568 (94%)	528 (99%)	4 (1%)	73	88
1	B	504/568 (89%)	500 (99%)	4 (1%)	73	88
1	C	415/568 (73%)	412 (99%)	3 (1%)	76	90
All	All	1451/1704 (85%)	1440 (99%)	11 (1%)	73	88

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	120	ASN
1	A	132	ASP
1	A	302	LYS
1	A	435	ASN
1	B	120	ASN
1	B	400	GLN
1	B	421	SER
1	B	653	SER
1	C	120	ASN
1	C	418	GLU
1	C	445	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	120	ASN
1	A	583	HIS
1	B	46	ASN
1	B	445	GLN
1	B	583	HIS
1	C	120	ASN
1	C	175	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 16 ligands modelled in this entry, 3 are monoatomic - leaving 13 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	AMP	A	708	-	25,25,25	1.41	4 (16%)	37,38,38	1.93	10 (27%)
2	SO4	A	702	-	4,4,4	0.71	0	6,6,6	0.06	0
4	AMP	C	701	-	25,25,25	1.41	4 (16%)	37,38,38	1.92	10 (27%)
2	SO4	B	704	-	4,4,4	0.72	0	6,6,6	0.04	0
2	SO4	A	701	-	4,4,4	0.70	0	6,6,6	0.08	0
2	SO4	B	705	-	4,4,4	0.70	0	6,6,6	0.11	0
2	SO4	B	701	-	4,4,4	0.68	0	6,6,6	0.09	0
2	SO4	A	704	-	4,4,4	0.69	0	6,6,6	0.13	0
2	SO4	A	705	-	4,4,4	0.69	0	6,6,6	0.13	0
4	AMP	B	707	-	25,25,25	1.39	4 (16%)	37,38,38	1.91	9 (24%)
2	SO4	B	703	-	4,4,4	0.67	0	6,6,6	0.06	0
2	SO4	B	702	-	4,4,4	0.70	0	6,6,6	0.11	0
2	SO4	A	703	-	4,4,4	0.71	0	6,6,6	0.08	0

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	AMP	B	707	-	-	1/10/26/26	0/3/3/3
4	AMP	A	708	-	-	5/10/26/26	0/3/3/3
4	AMP	C	701	-	-	5/10/26/26	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	701	AMP	C5-C4	4.71	1.47	1.39
4	B	707	AMP	C5-C4	4.70	1.47	1.39
4	A	708	AMP	C5-C4	4.54	1.47	1.39
4	C	701	AMP	C5-C6	2.76	1.48	1.41
4	B	707	AMP	C5-C6	2.74	1.48	1.41
4	A	708	AMP	C5-C6	2.71	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	708	AMP	C8-N7	2.50	1.36	1.31
4	B	707	AMP	C8-N7	2.49	1.36	1.31
4	C	701	AMP	C8-N7	2.42	1.36	1.31
4	C	701	AMP	C5-N7	-2.31	1.34	1.39
4	A	708	AMP	C5-N7	-2.20	1.35	1.39
4	B	707	AMP	C5-N7	-2.11	1.35	1.39

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	701	AMP	C5-C4-N3	-5.82	118.70	126.72
4	B	707	AMP	C5-C4-N3	-5.77	118.77	126.72
4	A	708	AMP	C5-C4-N3	-5.61	118.99	126.72
4	B	707	AMP	N3-C4-N9	4.57	134.93	127.17
4	C	701	AMP	N3-C4-N9	4.53	134.86	127.17
4	A	708	AMP	N3-C4-N9	4.37	134.59	127.17
4	A	708	AMP	C2-N3-C4	3.85	121.24	111.83
4	C	701	AMP	C2-N3-C4	3.80	121.12	111.83
4	B	707	AMP	C2-N3-C4	3.76	121.02	111.83
4	A	708	AMP	N3-C2-N1	-3.75	122.90	128.58
4	A	708	AMP	C4-C5-N7	-3.68	106.37	110.58
4	C	701	AMP	C4-C5-N7	-3.64	106.42	110.58
4	B	707	AMP	C4-C5-N7	-3.51	106.57	110.58
4	C	701	AMP	N3-C2-N1	-3.48	123.31	128.58
4	B	707	AMP	N3-C2-N1	-3.46	123.35	128.58
4	A	708	AMP	C4-N9-C8	3.06	108.95	105.74
4	B	707	AMP	C4-N9-C8	2.94	108.83	105.74
4	A	708	AMP	C5-N7-C8	2.81	107.87	103.45
4	B	707	AMP	C5-N7-C8	2.78	107.82	103.45
4	C	701	AMP	C5-N7-C8	2.76	107.79	103.45
4	C	701	AMP	C4-N9-C8	2.70	108.58	105.74
4	A	708	AMP	N9-C8-N7	-2.50	110.40	113.94
4	A	708	AMP	C6-C5-N7	2.46	136.83	132.09
4	B	707	AMP	N9-C8-N7	-2.44	110.48	113.94
4	C	701	AMP	C6-C5-N7	2.30	136.53	132.09
4	B	707	AMP	C6-C5-N7	2.28	136.49	132.09
4	C	701	AMP	N9-C8-N7	-2.23	110.77	113.94
4	A	708	AMP	C2-N1-C6	2.05	122.10	118.73
4	C	701	AMP	C2-N1-C6	2.01	122.04	118.73

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	708	AMP	C5'-O5'-P-O2P
4	A	708	AMP	C5'-O5'-P-O3P
4	A	708	AMP	C3'-C4'-C5'-O5'
4	C	701	AMP	C5'-O5'-P-O1P
4	C	701	AMP	C5'-O5'-P-O2P
4	C	701	AMP	C5'-O5'-P-O3P
4	C	701	AMP	C3'-C4'-C5'-O5'
4	A	708	AMP	O4'-C4'-C5'-O5'
4	C	701	AMP	O4'-C4'-C5'-O5'
4	A	708	AMP	C5'-O5'-P-O1P
4	B	707	AMP	C5'-O5'-P-O3P

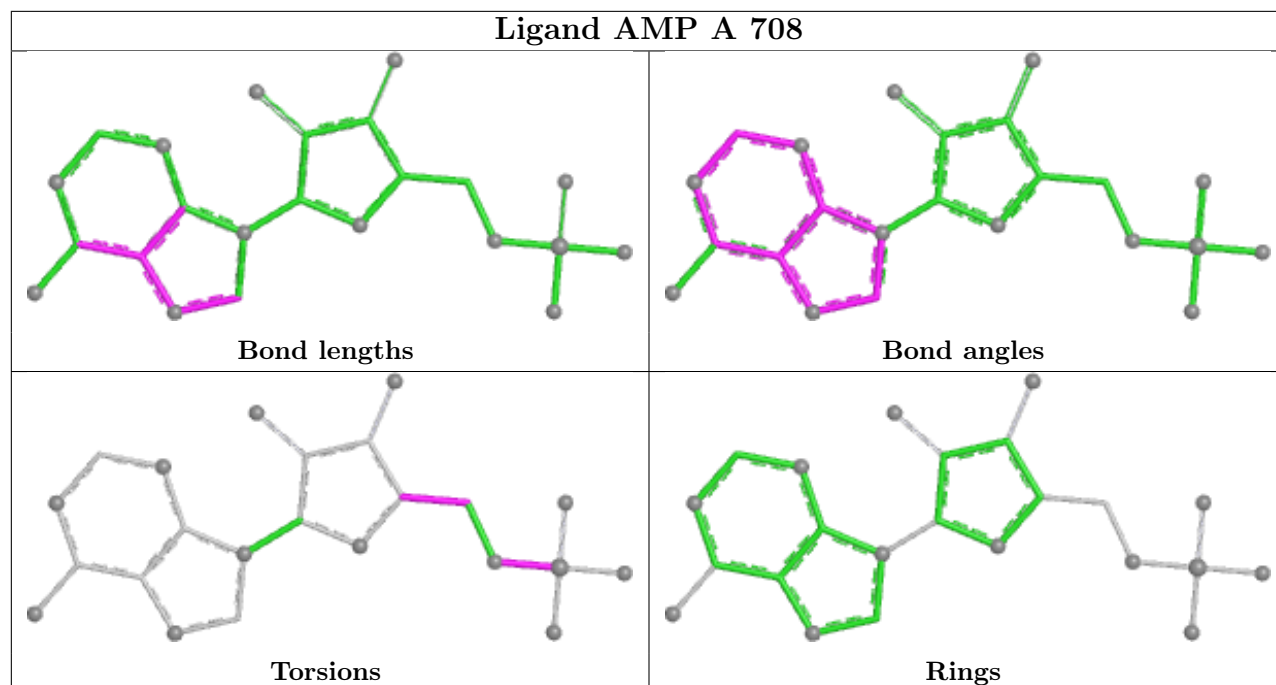
There are no ring outliers.

1 monomer is involved in 1 short contact:

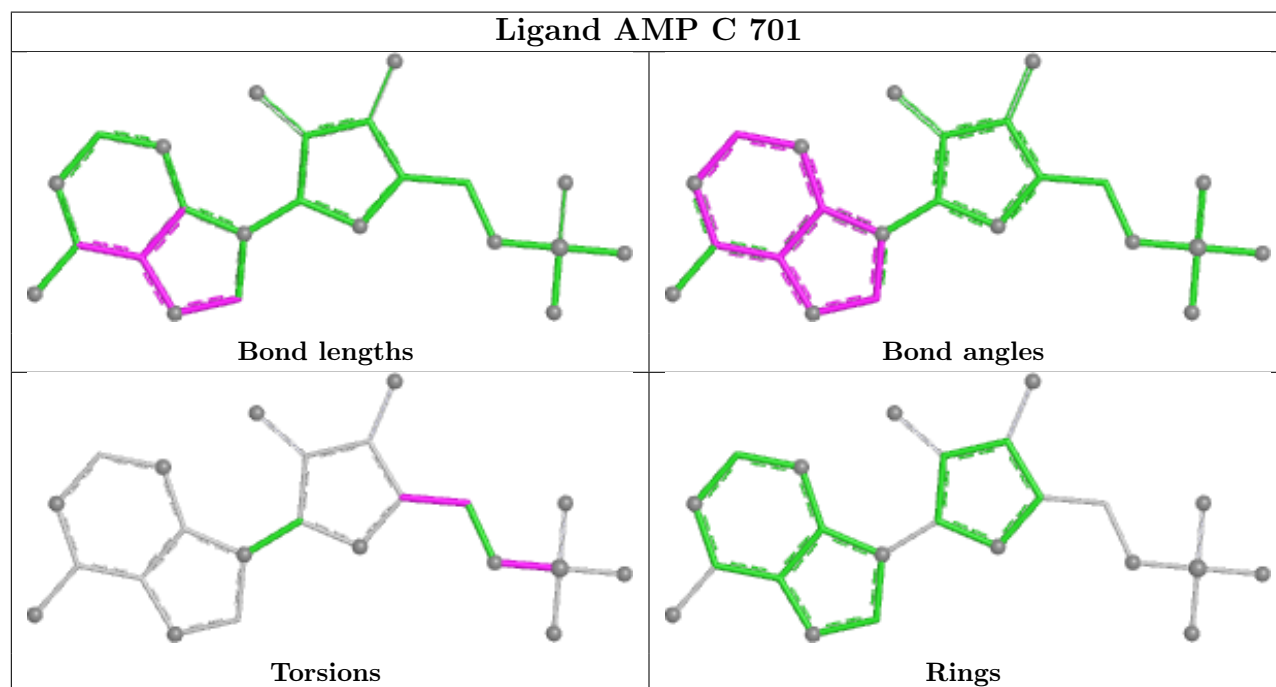
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	707	AMP	1	0

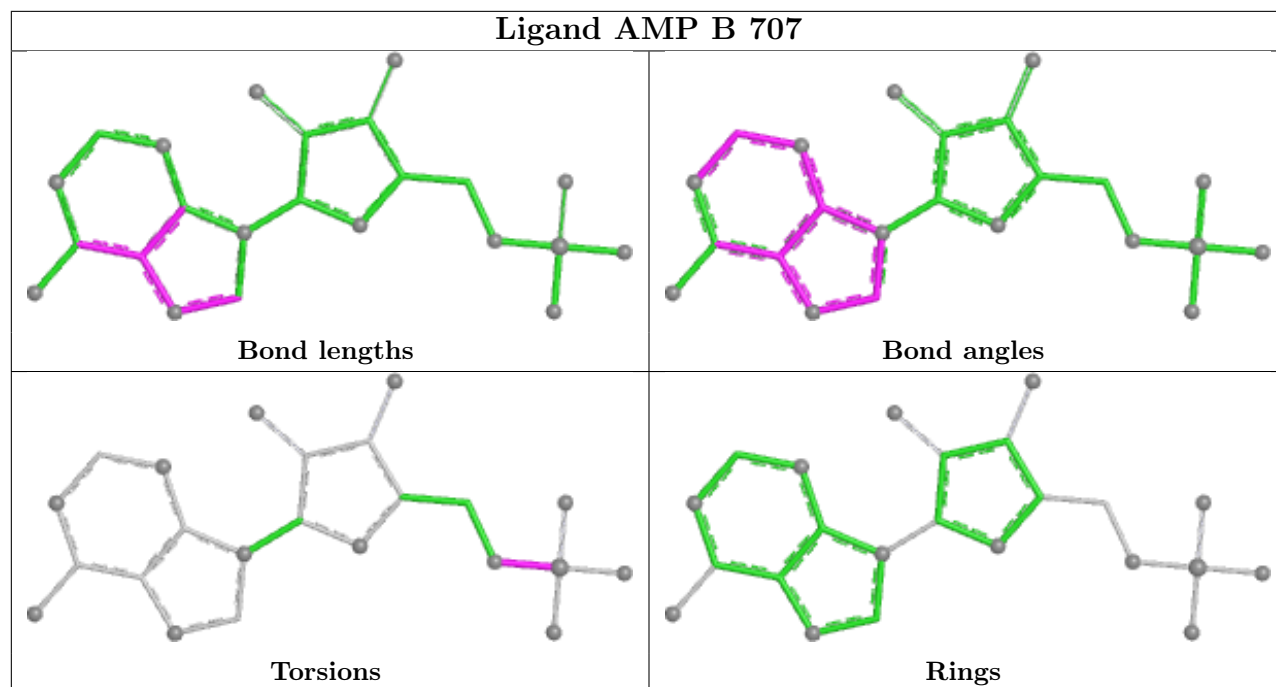
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 AMP A 708



Ligand AMP C 701





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	660/686 (96%)	-0.04	8 (1%) 76 75	44, 59, 86, 148	0
1	B	628/686 (91%)	0.13	33 (5%) 32 28	46, 62, 130, 175	0
1	C	523/686 (76%)	0.43	20 (3%) 44 40	59, 89, 134, 158	0
All	All	1811/2058 (87%)	0.15	61 (3%) 48 44	44, 66, 126, 175	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	666	LEU	6.1
1	A	684	GLY	5.1
1	B	647	ARG	4.3
1	A	605	ASP	4.2
1	B	672	VAL	4.2
1	B	629	SER	3.8
1	B	551	VAL	3.8
1	A	641	SER	3.8
1	B	608	GLY	3.8
1	C	294	THR	3.5
1	B	676	ILE	3.4
1	C	23	ASN	3.4
1	B	550	ASP	3.3
1	C	548	VAL	3.3
1	C	435	ASN	3.2
1	B	675	ILE	3.2
1	C	21	THR	3.1
1	B	588	GLY	3.1
1	B	549	ASP	3.0
1	C	36	THR	3.0
1	C	53	VAL	3.0
1	B	586	ILE	3.0
1	B	681	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	669	PRO	2.9
1	C	35	GLU	2.9
1	B	655	ASN	2.8
1	B	582	ILE	2.8
1	B	654	SER	2.7
1	C	51	HIS	2.7
1	B	294	THR	2.7
1	B	635	ASP	2.7
1	B	576	GLU	2.6
1	B	572	LYS	2.6
1	C	300	THR	2.6
1	C	33	LEU	2.5
1	A	369	TYR	2.5
1	A	298	THR	2.4
1	C	134	LYS	2.4
1	B	645	MET	2.4
1	B	589	GLN	2.4
1	B	21	THR	2.3
1	C	221	LYS	2.3
1	C	482	VAL	2.3
1	B	556	GLY	2.2
1	A	582	ILE	2.2
1	C	483	THR	2.2
1	C	256	GLU	2.1
1	B	419	PRO	2.1
1	C	54	ASN	2.1
1	B	651	LYS	2.1
1	B	648	ILE	2.1
1	B	610	ARG	2.0
1	B	646	ARG	2.0
1	B	628	LYS	2.0
1	C	391	LEU	2.0
1	B	644	ILE	2.0
1	C	30	GLY	2.0
1	A	618	ARG	2.0
1	A	654	SER	2.0
1	B	667	SER	2.0
1	C	225	ARG	2.0

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 oligosaccharides in this entry.

6.4 Ligands ⓘ

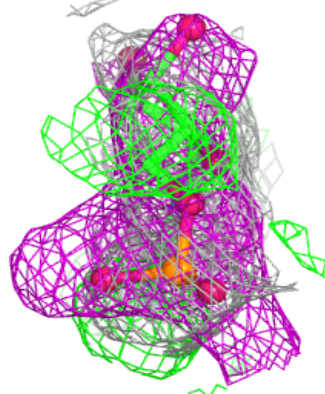
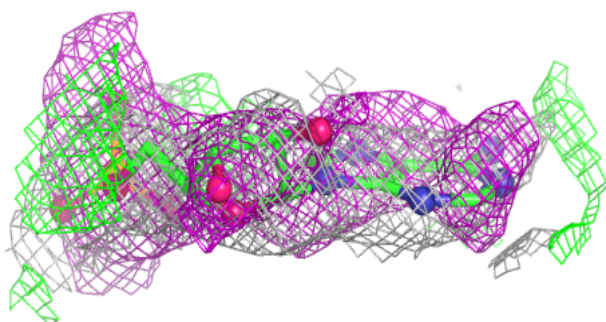
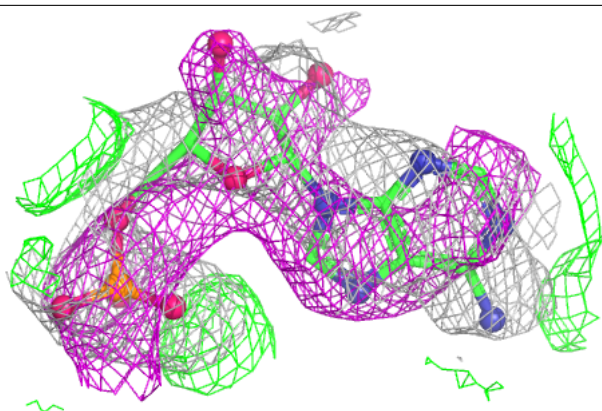
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	AMP	B	707	23/23	0.46	0.22	70,78,89,93	0
2	SO4	B	705	5/5	0.71	0.18	75,75,86,94	0
2	SO4	B	701	5/5	0.73	0.11	111,117,119,122	0
2	SO4	B	704	5/5	0.73	0.28	74,74,80,98	0
2	SO4	A	702	5/5	0.74	0.25	77,77,91,92	0
2	SO4	A	705	5/5	0.74	0.24	82,82,85,98	0
2	SO4	B	703	5/5	0.81	0.28	85,87,89,92	0
2	SO4	B	702	5/5	0.82	0.37	70,78,87,104	0
2	SO4	A	704	5/5	0.83	0.22	74,75,84,90	0
2	SO4	A	703	5/5	0.84	0.26	59,62,77,81	0
4	AMP	C	701	23/23	0.87	0.11	99,109,113,115	0
2	SO4	A	701	5/5	0.88	0.18	73,73,75,76	0
3	CL	A	707	1/1	0.91	0.24	75,75,75,75	0
3	CL	B	706	1/1	0.93	0.20	98,98,98,98	0
4	AMP	A	708	23/23	0.95	0.09	50,51,53,55	0
3	CL	A	706	1/1	0.97	0.13	71,71,71,71	0

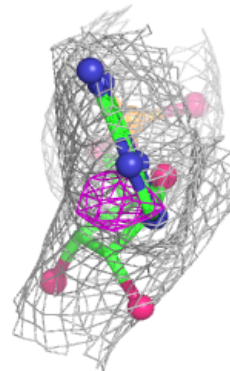
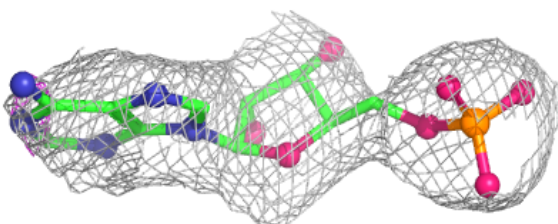
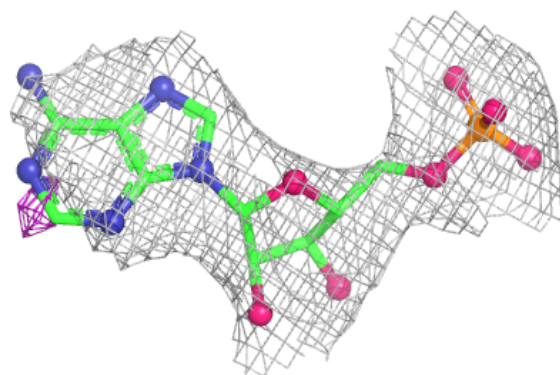
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

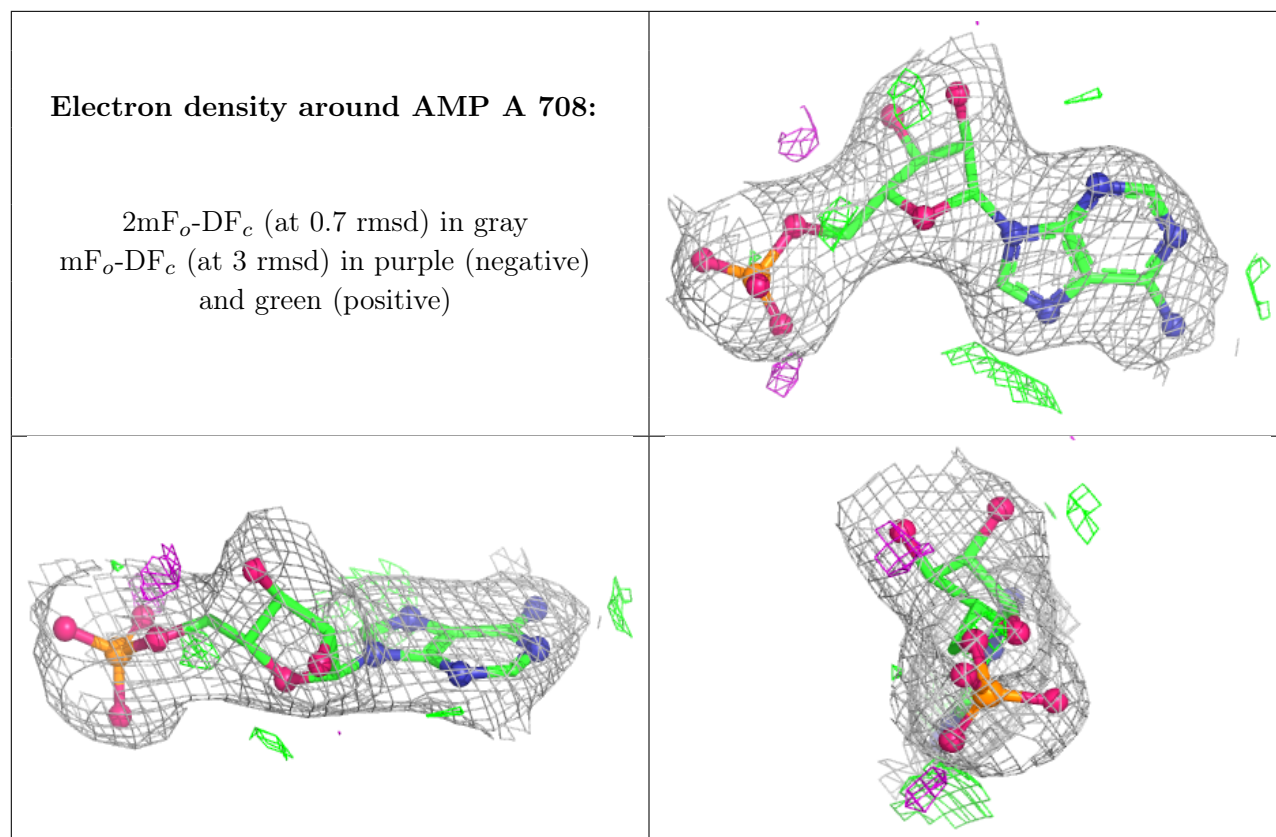
Electron density around AMP B 707:

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

**Electron density around AMP C 701:**

$2mF_o-DF_c$ (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.