



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:05 PM UTC

PDB ID : 8V4R / pdb_00008v4r
Title : Crystal structure of Acetyl-CoA synthetase 2 in complex with AMP and CoA 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

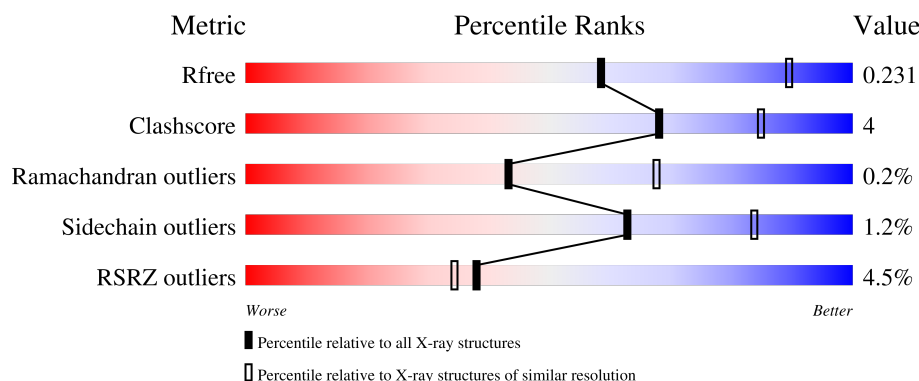
1 Overall quality at a glance

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	2% 87% 10% .
1	B	686	5% 78% 7% 14%
1	C	686	5% 80% 7% 13%

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	ACY	A	703	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14623 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	666	Total	C	N	O	S	0	0	0
			5157	3289	877	977	14			
1	B	589	Total	C	N	O	S	0	0	0
			4598	2948	775	862	13			
1	C	597	Total	C	N	O	S	0	0	0
			4632	2967	778	874	13			

There are 51 discrepancies between the modelled and reference sequences:

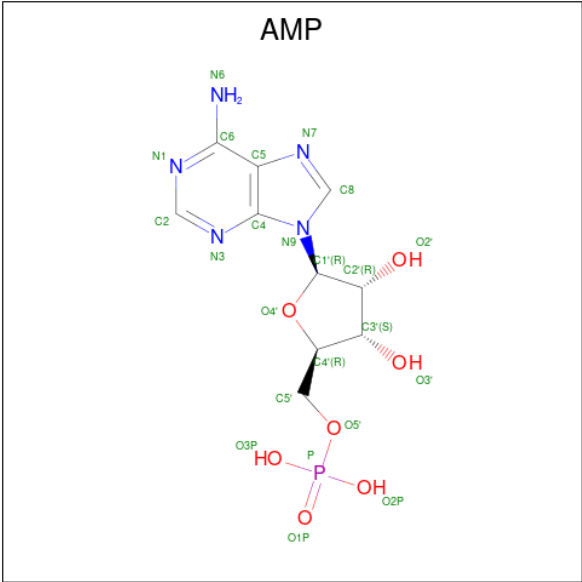
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q8NJJN3
A	2	HIS	-	expression tag	UNP Q8NJJN3
A	3	HIS	-	expression tag	UNP Q8NJJN3
A	4	HIS	-	expression tag	UNP Q8NJJN3
A	5	HIS	-	expression tag	UNP Q8NJJN3
A	6	HIS	-	expression tag	UNP Q8NJJN3
A	7	HIS	-	expression tag	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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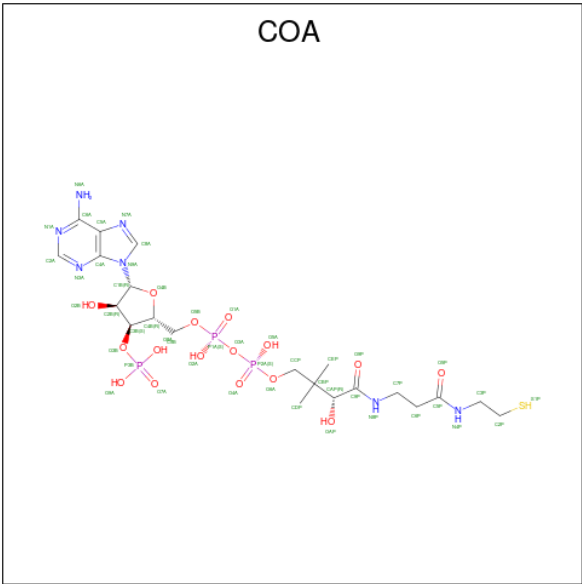
Chain	Residue	Modelled	Actual	Comment	Reference
B	7	HIS	-	expression tag	UNP Q8NJJ3
B	8	HIS	-	expression tag	UNP Q8NJJ3
B	9	HIS	-	expression tag	UNP Q8NJJ3
B	10	GLU	-	expression tag	UNP Q8NJJ3
B	11	ASN	-	expression tag	UNP Q8NJJ3
B	12	LEU	-	expression tag	UNP Q8NJJ3
B	13	TYR	-	expression tag	UNP Q8NJJ3
B	14	PHE	-	expression tag	UNP Q8NJJ3
B	15	GLN	-	expression tag	UNP Q8NJJ3
B	16	GLY	-	expression tag	UNP Q8NJJ3
B	403	ALA	VAL	variant	UNP Q8NJJ3
C	1	MET	-	initiating methionine	UNP Q8NJJ3
C	2	HIS	-	expression tag	UNP Q8NJJ3
C	3	HIS	-	expression tag	UNP Q8NJJ3
C	4	HIS	-	expression tag	UNP Q8NJJ3
C	5	HIS	-	expression tag	UNP Q8NJJ3
C	6	HIS	-	expression tag	UNP Q8NJJ3
C	7	HIS	-	expression tag	UNP Q8NJJ3
C	8	HIS	-	expression tag	UNP Q8NJJ3
C	9	HIS	-	expression tag	UNP Q8NJJ3
C	10	GLU	-	expression tag	UNP Q8NJJ3
C	11	ASN	-	expression tag	UNP Q8NJJ3
C	12	LEU	-	expression tag	UNP Q8NJJ3
C	13	TYR	-	expression tag	UNP Q8NJJ3
C	14	PHE	-	expression tag	UNP Q8NJJ3
C	15	GLN	-	expression tag	UNP Q8NJJ3
C	16	GLY	-	expression tag	UNP Q8NJJ3
C	403	ALA	VAL	variant	UNP Q8NJJ3

- Molecule 2 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$) (labeled as "Ligand of Interest" by depositor).



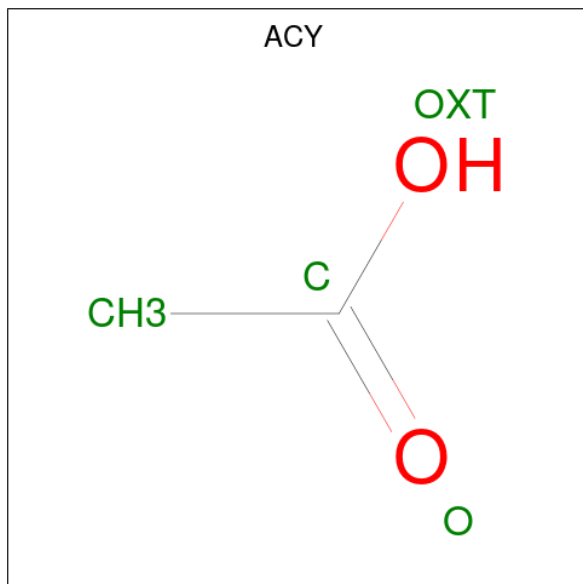
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 3 is COENZYME A (CCD ID: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S) (labeled as "Ligand of Interest" by depositor).



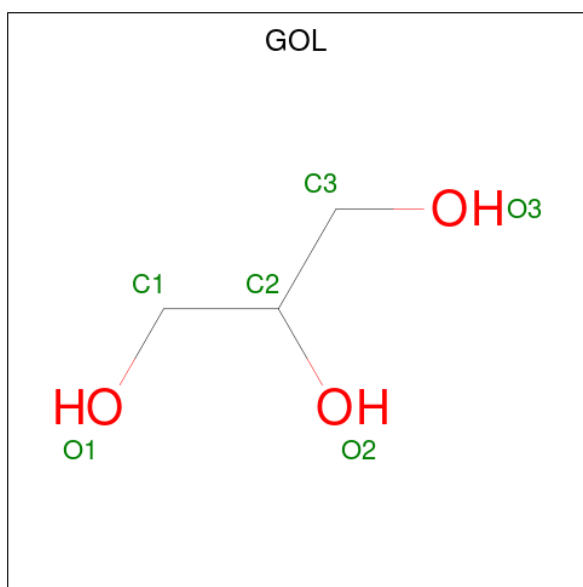
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	B	1	Total	C	N	O	P		0	0
			31	10	5	13	3			
3	C	1	Total	C	N	O	P		0	0
			31	10	5	13	3			

- Molecule 4 is ACETIC ACID (CCD ID: ACY) (formula: $C_2H_4O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

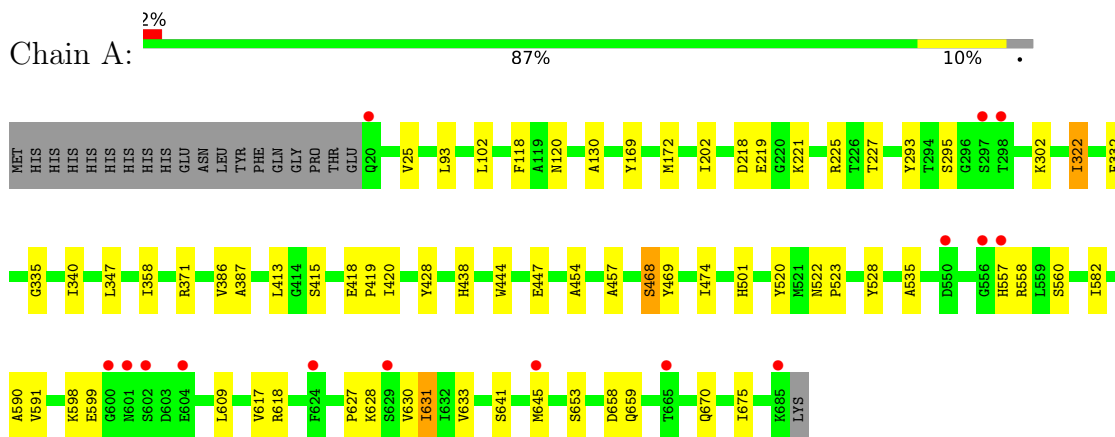
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	28	Total	O	0	0
			28	28		
6	B	12	Total	O	0	0
			12	12		
6	C	1	Total	O	0	0
			1	1		

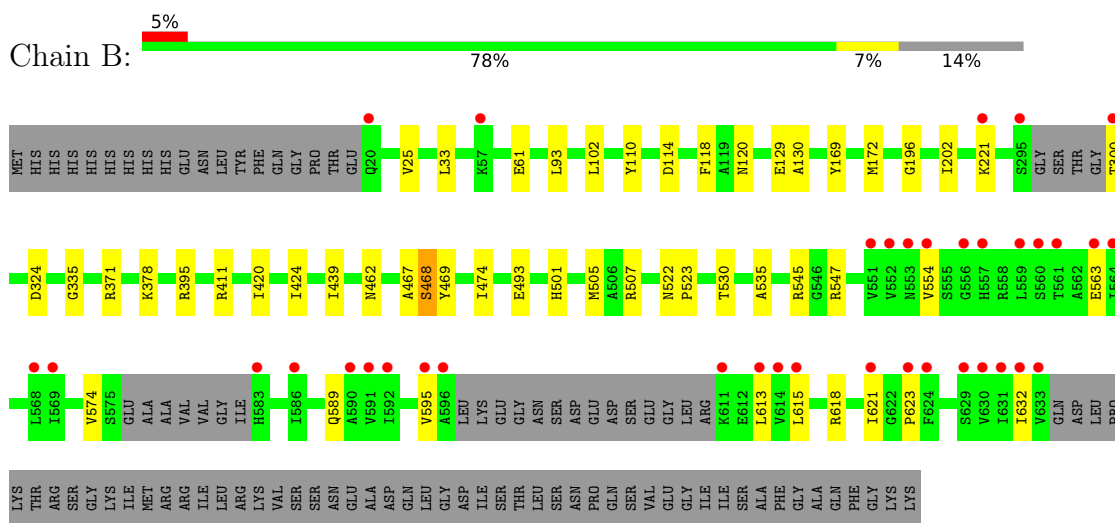
3 Residue-property plots [i](#)

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.

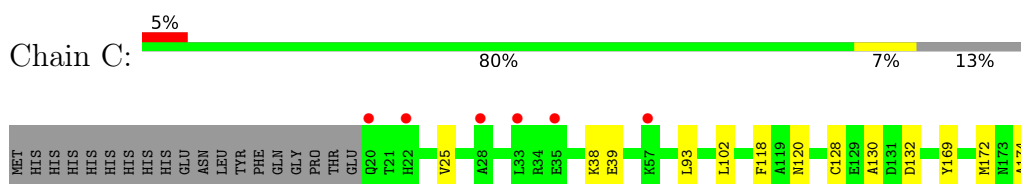
- Molecule 1: Acetyl-coenzyme A synthetase 2

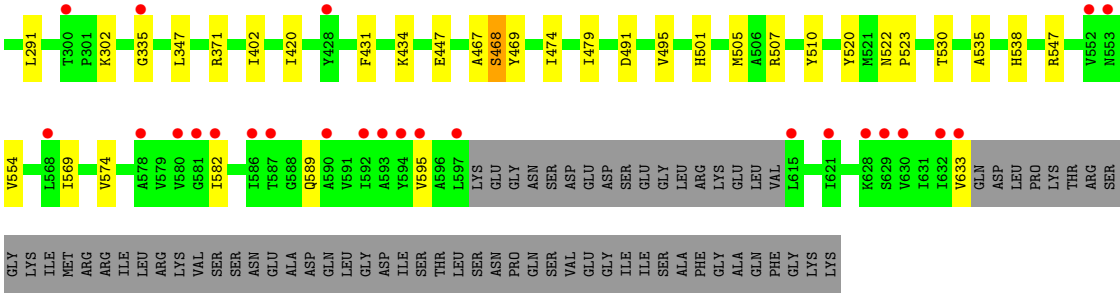


- Molecule 1: Acetyl-coenzyme A synthetase 2



- Molecule 1: Acetyl-coenzyme A synthetase 2





4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	139.41Å 139.41Å 542.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.46 – 2.70 49.46 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.46-2.70) 100.0 (49.46-2.70)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.21rc1_5162	Depositor
R, R_{free}	0.206 , 0.231 0.208 , 0.231	Depositor DCC
R_{free} test set	4354 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	63.1	Xtriage
Anisotropy	0.603	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 45.6	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	0.95	EDS
Total number of atoms	14623	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.78% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: AMP, COA, ACY, GOL

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	0.14	0/5287	0.34	0/7190
1	B	0.13	0/4721	0.32	0/6425
1	C	0.12	0/4756	0.29	0/6480
All	All	0.13	0/14764	0.32	0/20095

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 [i](#)

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	5157	0	5038	43	0
1	B	4598	0	4477	30	0
1	C	4632	0	4501	31	0
2	A	23	0	12	0	0
2	B	23	0	12	0	0
2	C	23	0	12	0	0
3	A	48	0	32	5	0
3	B	31	0	11	1	0
3	C	31	0	11	0	0
4	A	4	0	3	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	6	0	8	0	0
5	B	6	0	8	0	0
6	A	28	0	0	0	0
6	B	12	0	0	0	0
6	C	1	0	0	0	0
All	All	14623	0	14125	103	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 4.

All (103) 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:574:VAL:HG13	1:B:595:VAL:HG13	1.67	0.76
1:A:582:ILE:HG21	1:A:653:SER:HB3	1.77	0.67
1:C:431:PHE:O	1:C:434:LYS:NZ	2.29	0.66
1:C:38:LYS:NZ	1:C:39:GLU:OE2	2.25	0.65
1:A:591:VAL:HG23	1:A:627:PRO:HA	1.79	0.64
1:B:25:VAL:HG22	1:B:535:ALA:HB1	1.81	0.63
1:A:172:MET:HE2	1:A:335:GLY:O	2.00	0.62
1:A:25:VAL:HG22	1:A:535:ALA:HB1	1.83	0.61
1:C:130:ALA:O	1:C:371:ARG:NH2	2.33	0.61
1:A:93:LEU:HD11	1:A:501:HIS:N	2.16	0.60
1:B:93:LEU:HD11	1:B:501:HIS:N	2.18	0.57
1:A:102:LEU:HD22	1:B:118:PHE:CZ	2.40	0.57
1:B:130:ALA:O	1:B:371:ARG:NH2	2.40	0.55
1:A:557:HIS:CE1	3:A:702:COA:H31	2.42	0.54
1:C:505:MET:O	1:C:507:ARG:NH1	2.40	0.54
1:C:93:LEU:HD11	1:C:501:HIS:N	2.22	0.54
1:B:172:MET:HE2	1:B:335:GLY:O	2.08	0.54
1:B:505:MET:O	1:B:507:ARG:NH1	2.41	0.54
1:C:25:VAL:HG22	1:C:535:ALA:HB1	1.89	0.54
1:C:169:TYR:CZ	1:C:202:ILE:HD11	2.43	0.53
1:C:569:ILE:HD13	1:C:574:VAL:HG12	1.91	0.52
1:A:444:TRP:CE2	4:A:703:ACY:H3	2.44	0.52
1:A:130:ALA:O	1:A:371:ARG:NH2	2.43	0.52
1:A:618:ARG:NH2	3:A:702:COA:O9A	2.42	0.51
1:A:93:LEU:HD12	1:A:93:LEU:N	2.26	0.50
1:B:493:GLU:OE1	1:B:545:ARG:NH1	2.42	0.50
1:B:110:TYR:CD1	1:B:114:ASP:HB2	2.47	0.50
1:C:93:LEU:HD12	1:C:93:LEU:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:TYR:CZ	1:B:202:ILE:HD11	2.47	0.50
1:B:554:VAL:HG13	1:B:589:GLN:O	2.11	0.49
1:B:613:LEU:HD12	1:B:632:ILE:HD11	1.95	0.48
1:A:93:LEU:HD23	1:A:528:TYR:HB2	1.95	0.48
1:A:169:TYR:CZ	1:A:202:ILE:HD11	2.49	0.48
1:C:172:MET:HE2	1:C:335:GLY:O	2.13	0.48
1:C:530:THR:O	1:C:547:ARG:NH2	2.47	0.47
1:B:563:GLU:O	1:B:621:ILE:HD11	2.14	0.47
1:B:615:LEU:HD23	1:B:618:ARG:HD3	1.95	0.47
1:C:468:SER:OG	1:C:469:TYR:N	2.48	0.47
1:C:291:LEU:HD21	1:C:510:TYR:CD1	2.51	0.46
1:A:322:ILE:HD13	1:A:454:ALA:HB3	1.97	0.46
1:A:658:ASP:O	1:A:659:GLN:HB2	2.16	0.46
1:C:554:VAL:HG13	1:C:589:GLN:O	2.15	0.46
1:B:93:LEU:N	1:B:93:LEU:HD12	2.30	0.46
1:A:522:ASN:N	1:A:523:PRO:CD	2.79	0.46
1:B:102:LEU:HD22	1:C:118:PHE:CZ	2.50	0.46
1:A:590:ALA:CB	1:A:628:LYS:HD2	2.46	0.46
1:A:670:GLN:OE1	1:A:670:GLN:N	2.39	0.46
1:C:633:VAL:HG23	1:C:633:VAL:O	2.15	0.46
1:A:658:ASP:O	1:A:659:GLN:CB	2.64	0.45
3:A:702:COA:O5P	3:A:702:COA:O9P	2.35	0.45
1:B:522:ASN:N	1:B:523:PRO:CD	2.80	0.45
1:B:439:ILE:O	1:B:462:ASN:ND2	2.37	0.45
1:A:218:ASP:OD1	1:A:219:GLU:N	2.45	0.45
1:A:420:ILE:O	1:A:420:ILE:HG23	2.16	0.44
1:C:420:ILE:O	1:C:420:ILE:HG23	2.18	0.44
1:C:479:ILE:HB	1:C:495:VAL:HG23	1.99	0.44
1:B:563:GLU:C	1:B:621:ILE:HD11	2.42	0.44
1:B:615:LEU:HA	1:B:618:ARG:HD3	2.00	0.44
1:C:128:CYS:SG	1:C:174:ALA:HB2	2.58	0.44
1:A:102:LEU:HD12	1:A:102:LEU:H	1.83	0.44
1:A:332:PHE:HB2	1:A:358:ILE:HD12	1.99	0.44
1:C:491:ASP:HB2	1:C:538:HIS:CE1	2.53	0.44
1:A:93:LEU:HD12	1:A:93:LEU:H	1.82	0.44
1:A:347:LEU:C	1:A:347:LEU:HD23	2.42	0.44
1:A:582:ILE:HG21	1:A:653:SER:CB	2.46	0.44
1:A:413:LEU:HB3	1:A:428:TYR:CZ	2.53	0.43
1:B:530:THR:O	1:B:547:ARG:NH2	2.51	0.43
1:A:295:SER:HB3	1:A:560:SER:HB2	2.00	0.43
1:B:395:ARG:HH11	1:B:424:ILE:HD13	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:PHE:CZ	1:C:102:LEU:HD22	2.54	0.42
1:A:418:GLU:HB2	1:A:419:PRO:HD2	2.01	0.42
1:B:324:ASP:O	1:B:411:ARG:NH2	2.52	0.42
1:A:447:GLU:HG2	1:A:520:TYR:CZ	2.53	0.42
1:C:447:GLU:HG2	1:C:520:TYR:CZ	2.54	0.42
1:C:522:ASN:N	1:C:523:PRO:CD	2.82	0.42
1:B:467:ALA:O	1:B:468:SER:OG	2.32	0.42
1:B:618:ARG:NH2	3:B:702:COA:O9A	2.40	0.42
1:C:347:LEU:C	1:C:347:LEU:HD23	2.44	0.42
1:A:386:VAL:HG22	1:A:387:ALA:N	2.33	0.42
1:C:93:LEU:HD12	1:C:93:LEU:H	1.84	0.42
1:A:293:TYR:HA	1:A:302:LYS:O	2.19	0.42
1:B:468:SER:OG	1:B:469:TYR:N	2.51	0.42
1:C:474:ILE:HD12	1:C:474:ILE:N	2.34	0.42
1:C:402:ILE:HG21	1:C:431:PHE:O	2.19	0.42
1:A:633:VAL:HG11	1:A:675:ILE:HD13	2.02	0.42
1:A:617:VAL:HG11	1:A:627:PRO:HD3	2.01	0.41
1:A:630:VAL:C	1:A:631:ILE:HD12	2.45	0.41
1:C:574:VAL:HG13	1:C:595:VAL:HG13	2.02	0.41
3:A:702:COA:O9P	3:A:702:COA:C6P	2.69	0.41
1:C:467:ALA:O	1:C:468:SER:OG	2.37	0.41
1:A:340:ILE:CG2	4:A:703:ACY:H2	2.50	0.41
1:C:302:LYS:NZ	1:C:520:TYR:OH	2.38	0.41
1:A:225:ARG:NH1	3:A:702:COA:O8A	2.52	0.41
1:A:438:HIS:CD2	1:A:457:ALA:HA	2.56	0.41
1:C:218:ASP:OD1	1:C:219:GLU:N	2.52	0.41
1:A:474:ILE:HD12	1:A:474:ILE:N	2.36	0.41
1:B:196:GLY:O	1:B:623:PRO:HD2	2.21	0.41
1:A:468:SER:OG	1:A:469:TYR:N	2.54	0.40
1:A:631:ILE:N	1:A:631:ILE:CD1	2.84	0.40
1:B:129:GLU:OE2	1:B:378:LYS:HE2	2.21	0.40
1:B:474:ILE:HD12	1:B:474:ILE:N	2.36	0.40
1:B:420:ILE:O	1:B:420:ILE:HG23	2.21	0.40
1:A:386:VAL:O	1:A:415:SER:HA	2.21	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	664/686 (97%)	639 (96%)	23 (4%)	2 (0%)	36	60
1	B	581/686 (85%)	564 (97%)	16 (3%)	1 (0%)	43	68
1	C	593/686 (86%)	575 (97%)	17 (3%)	1 (0%)	43	68
All	All	1838/2058 (89%)	1778 (97%)	56 (3%)	4 (0%)	43	68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	468	SER
1	C	468	SER
1	A	468	SER
1	A	599	GLU

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	543/568 (96%)	533 (98%)	10 (2%)	51	78
1	B	484/568 (85%)	479 (99%)	5 (1%)	68	86
1	C	486/568 (86%)	483 (99%)	3 (1%)	78	91
All	All	1513/1704 (89%)	1495 (99%)	18 (1%)	63	84

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	120	ASN
1	A	221	LYS
1	A	227	THR
1	A	322	ILE
1	A	558	ARG
1	A	598	LYS
1	A	609	LEU
1	A	631	ILE
1	A	641	SER
1	A	645	MET
1	B	33	LEU
1	B	61	GLU
1	B	120	ASN
1	B	221	LYS
1	B	300	THR
1	C	120	ASN
1	C	132	ASP
1	C	582	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	ASN
1	A	156	GLN
1	A	445	GLN
1	A	659	GLN
1	B	51	HIS
1	B	120	ASN
1	B	156	GLN
1	B	435	ASN
1	B	445	GLN
1	C	26	HIS
1	C	44	GLN
1	C	120	ASN
1	C	137	HIS
1	C	445	GLN

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](#)

9 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	COA	A	702	-	47,50,50	0.58	0	69,75,75	1.04	4 (5%)
2	AMP	A	701	-	25,25,25	1.40	4 (16%)	37,38,38	1.96	9 (24%)
3	COA	C	702	-	32,33,50	0.63	0	50,52,75	1.01	2 (4%)
5	GOL	A	704	-	5,5,5	0.32	0	5,5,5	0.29	0
3	COA	B	702	-	32,33,50	0.63	0	50,52,75	1.01	2 (4%)
2	AMP	B	701	-	25,25,25	1.39	3 (12%)	37,38,38	1.97	10 (27%)
5	GOL	B	703	-	5,5,5	0.31	0	5,5,5	0.38	0
2	AMP	C	701	-	25,25,25	1.40	4 (16%)	37,38,38	1.93	10 (27%)
4	ACY	A	703	-	3,3,3	1.15	0	3,3,3	1.27	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
3	COA	A	702	-	-	15/48/64/64	0/3/3/3
2	AMP	A	701	-	-	2/10/26/26	0/3/3/3
3	COA	C	702	-	-	1/21/37/64	0/3/3/3
5	GOL	A	704	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	COA	B	702	-	-	4/21/37/64	0/3/3/3
2	AMP	B	701	-	-	0/10/26/26	0/3/3/3
5	GOL	B	703	-	-	2/4/4/4	-
2	AMP	C	701	-	-	0/10/26/26	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	701	AMP	C5-C4	4.53	1.47	1.39
2	A	701	AMP	C5-C4	4.49	1.47	1.39
2	B	701	AMP	C5-C4	4.49	1.47	1.39
2	B	701	AMP	C5-C6	2.91	1.49	1.41
2	A	701	AMP	C5-C6	2.73	1.48	1.41
2	C	701	AMP	C5-C6	2.69	1.48	1.41
2	B	701	AMP	C8-N7	2.57	1.36	1.31
2	A	701	AMP	C8-N7	2.53	1.36	1.31
2	C	701	AMP	C8-N7	2.40	1.36	1.31
2	C	701	AMP	C5-N7	-2.31	1.34	1.39
2	A	701	AMP	C5-N7	-2.26	1.35	1.39

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	AMP	C5-C4-N3	-5.95	118.52	126.72
2	C	701	AMP	C5-C4-N3	-5.59	119.02	126.72
2	B	701	AMP	C5-C4-N3	-5.54	119.09	126.72
3	B	702	COA	P3B-O3B-C3B	-5.46	108.85	123.43
3	C	702	COA	P3B-O3B-C3B	-5.35	109.14	123.43
3	A	702	COA	P3B-O3B-C3B	-4.84	110.50	123.43
2	C	701	AMP	N3-C4-N9	4.53	134.88	127.17
2	A	701	AMP	N3-C4-N9	4.52	134.85	127.17
2	B	701	AMP	N3-C4-N9	4.17	134.26	127.17
2	A	701	AMP	C2-N3-C4	4.03	121.68	111.83
2	B	701	AMP	C2-N3-C4	3.89	121.33	111.83
2	C	701	AMP	C2-N3-C4	3.85	121.24	111.83
2	B	701	AMP	C4-C5-N7	-3.85	106.18	110.58
2	C	701	AMP	N3-C2-N1	-3.83	122.79	128.58
2	A	701	AMP	N3-C2-N1	-3.76	122.89	128.58
2	B	701	AMP	N3-C2-N1	-3.75	122.91	128.58
2	A	701	AMP	C4-C5-N7	-3.65	106.41	110.58
2	C	701	AMP	C4-C5-N7	-3.34	106.77	110.58
2	C	701	AMP	C4-N9-C8	3.04	108.93	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	AMP	C4-N9-C8	2.99	108.88	105.74
2	B	701	AMP	C5-N7-C8	2.90	108.02	103.45
2	A	701	AMP	C5-N7-C8	2.71	107.71	103.45
2	A	701	AMP	C4-N9-C8	2.70	108.57	105.74
2	B	701	AMP	C6-C5-N7	2.69	137.28	132.09
2	C	701	AMP	C5-N7-C8	2.65	107.62	103.45
2	B	701	AMP	N9-C8-N7	-2.58	110.27	113.94
3	A	702	COA	C7P-N8P-C9P	2.47	126.98	122.55
3	A	702	COA	C3P-N4P-C5P	2.44	127.36	122.82
2	A	701	AMP	C6-C5-N7	2.41	136.75	132.09
2	C	701	AMP	N9-C8-N7	-2.37	110.58	113.94
2	A	701	AMP	N9-C8-N7	-2.29	110.68	113.94
2	C	701	AMP	C6-C5-N7	2.25	136.44	132.09
3	A	702	COA	C6P-C5P-N4P	2.15	120.26	116.34
3	C	702	COA	O5A-P2A-O4A	2.12	119.09	110.83
2	C	701	AMP	C2-N1-C6	2.12	122.20	118.73
3	B	702	COA	O5A-P2A-O4A	2.05	118.83	110.83
2	B	701	AMP	C2-N1-C6	2.04	122.09	118.73

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	702	COA	O4B-C4B-C5B-O5B
3	A	702	COA	P1A-O3A-P2A-O6A
3	A	702	COA	CCP-O6A-P2A-O4A
3	A	702	COA	CDP-CBP-CCP-O6A
3	A	702	COA	CEP-CBP-CCP-O6A
3	A	702	COA	CAP-CBP-CCP-O6A
3	A	702	COA	O9P-C9P-CAP-CBP
3	A	702	COA	N8P-C9P-CAP-CBP
3	A	702	COA	N8P-C9P-CAP-OAP
3	B	702	COA	C5B-O5B-P1A-O2A
3	B	702	COA	C5B-O5B-P1A-O3A
5	A	704	GOL	O1-C1-C2-C3
5	B	703	GOL	O1-C1-C2-C3
3	A	702	COA	C6P-C7P-N8P-C9P
3	A	702	COA	C6P-C5P-N4P-C3P
3	A	702	COA	O5P-C5P-N4P-C3P
5	A	704	GOL	O1-C1-C2-O2
5	B	703	GOL	O1-C1-C2-O2
3	A	702	COA	C3B-C4B-C5B-O5B

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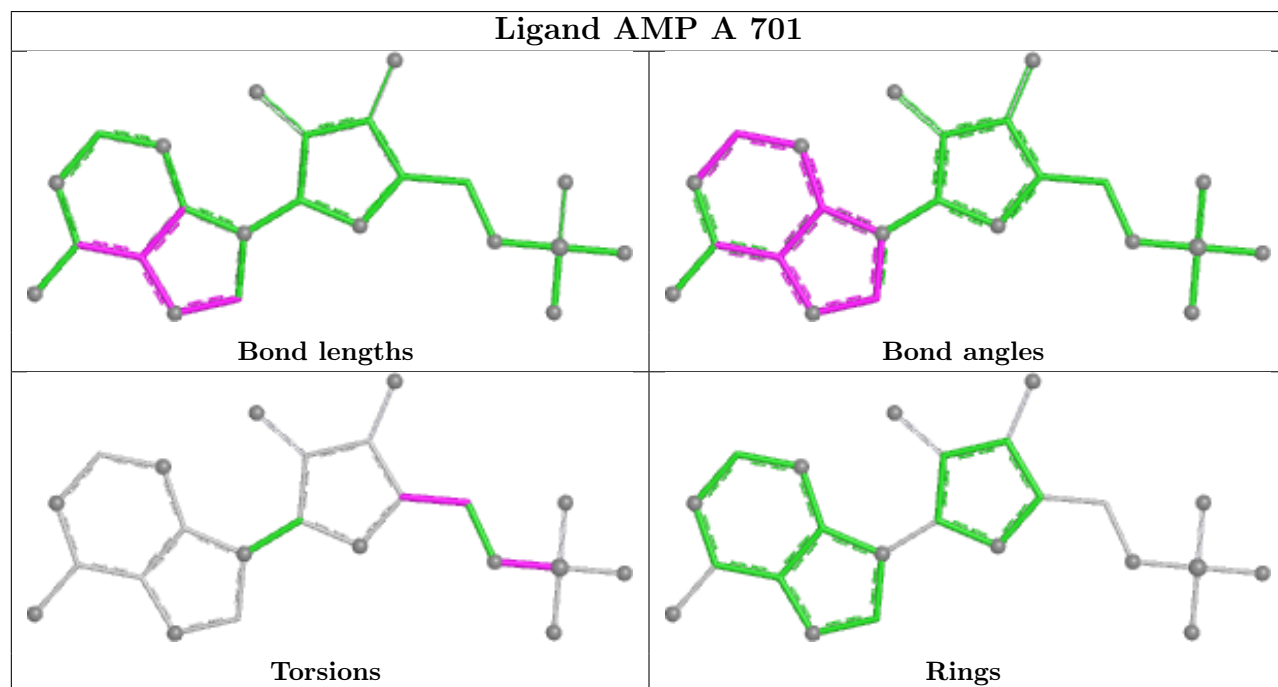
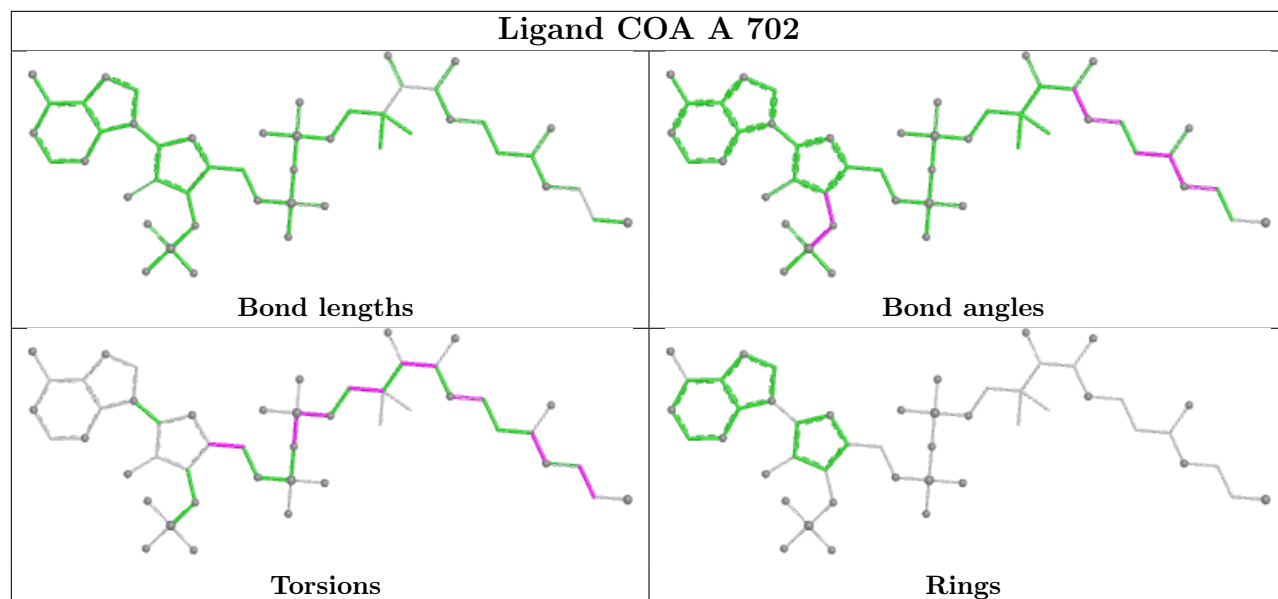
Mol	Chain	Res	Type	Atoms
3	B	702	COA	O4B-C4B-C5B-O5B
3	A	702	COA	O9P-C9P-CAP-OAP
2	A	701	AMP	C5'-O5'-P-O1P
3	A	702	COA	S1P-C2P-C3P-N4P
3	C	702	COA	C5B-O5B-P1A-O1A
3	B	702	COA	C3B-C4B-C5B-O5B
2	A	701	AMP	C3'-C4'-C5'-O5'

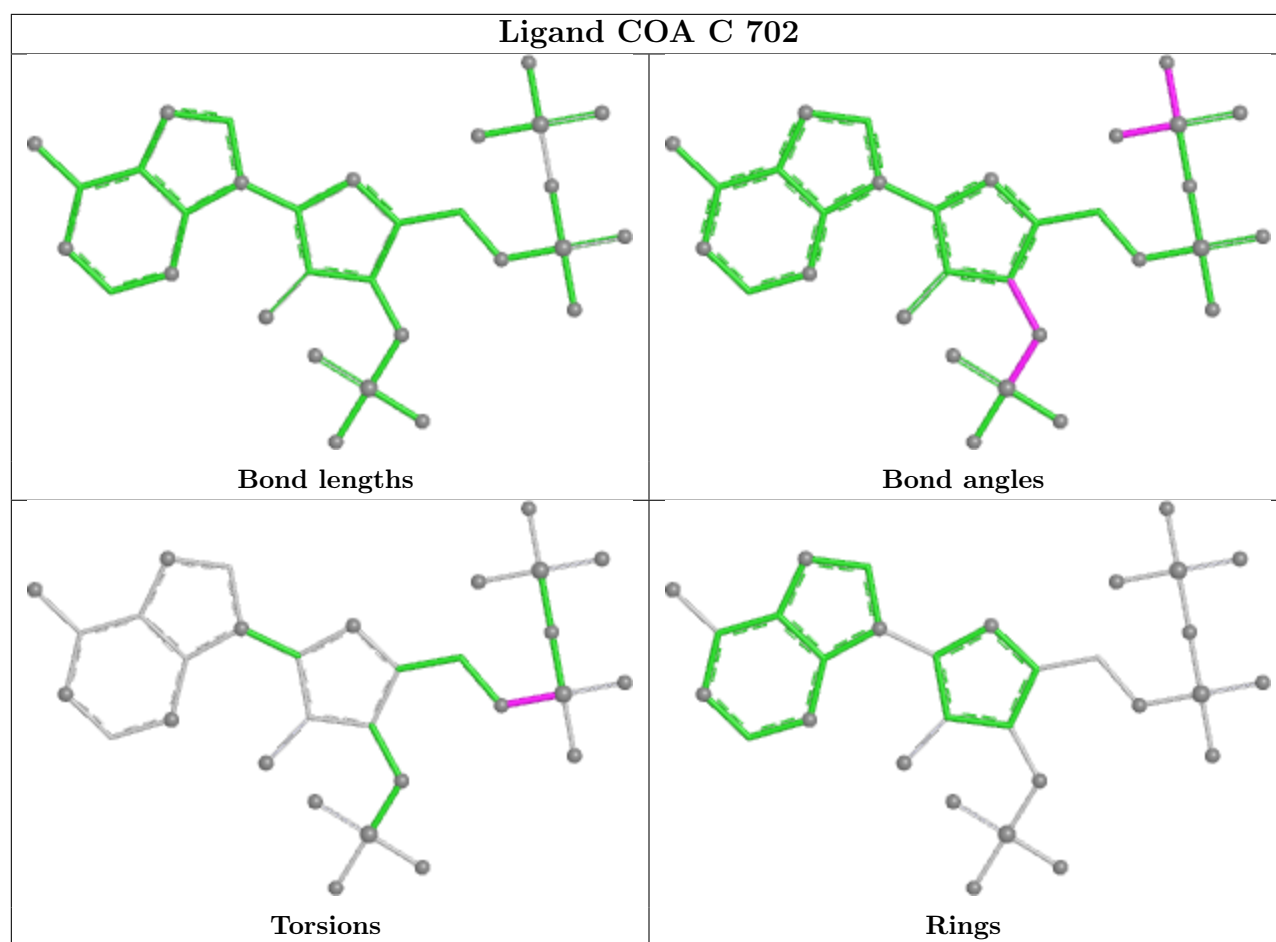
There are no ring outliers.

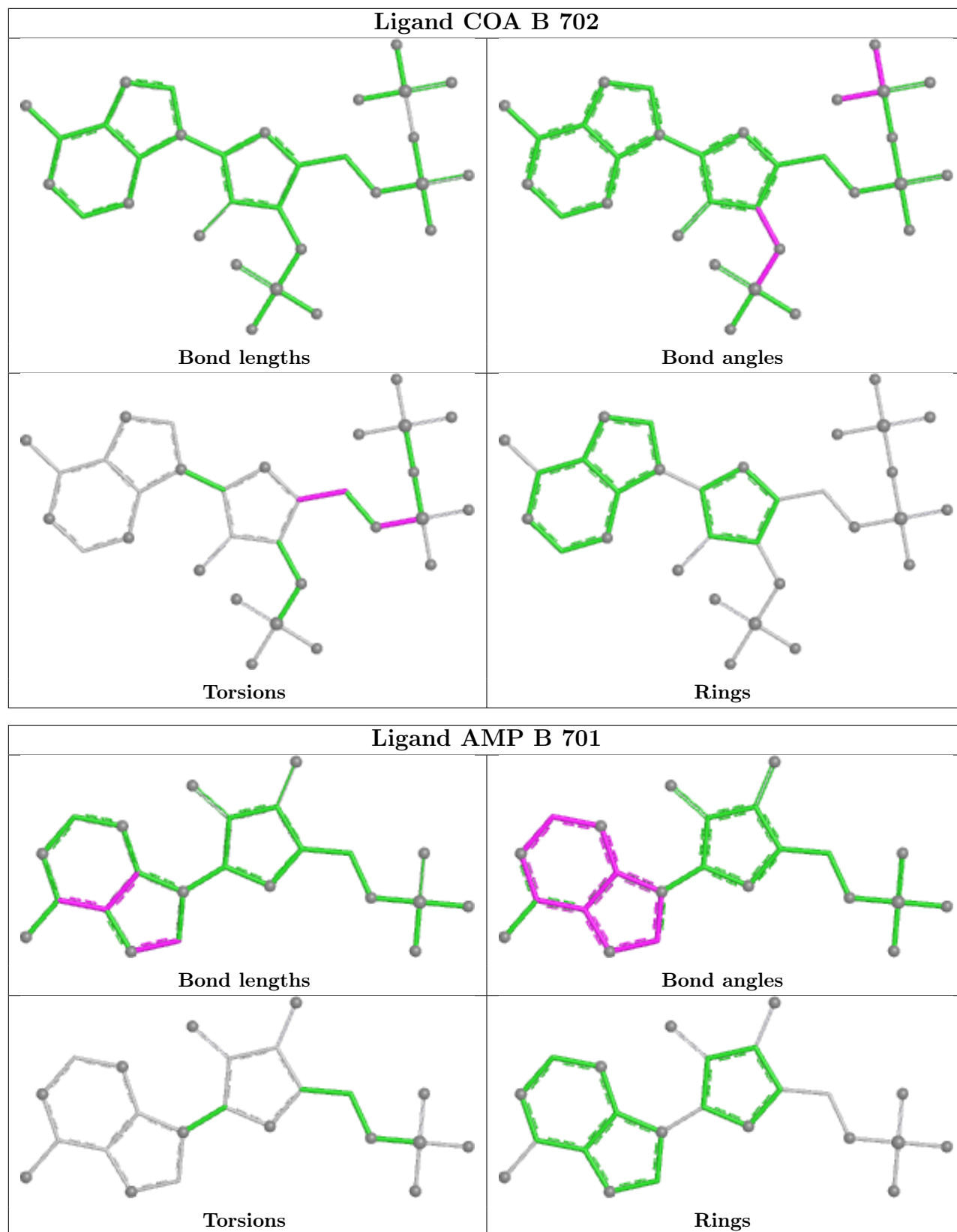
3 monomers are involved in 8 short contacts:

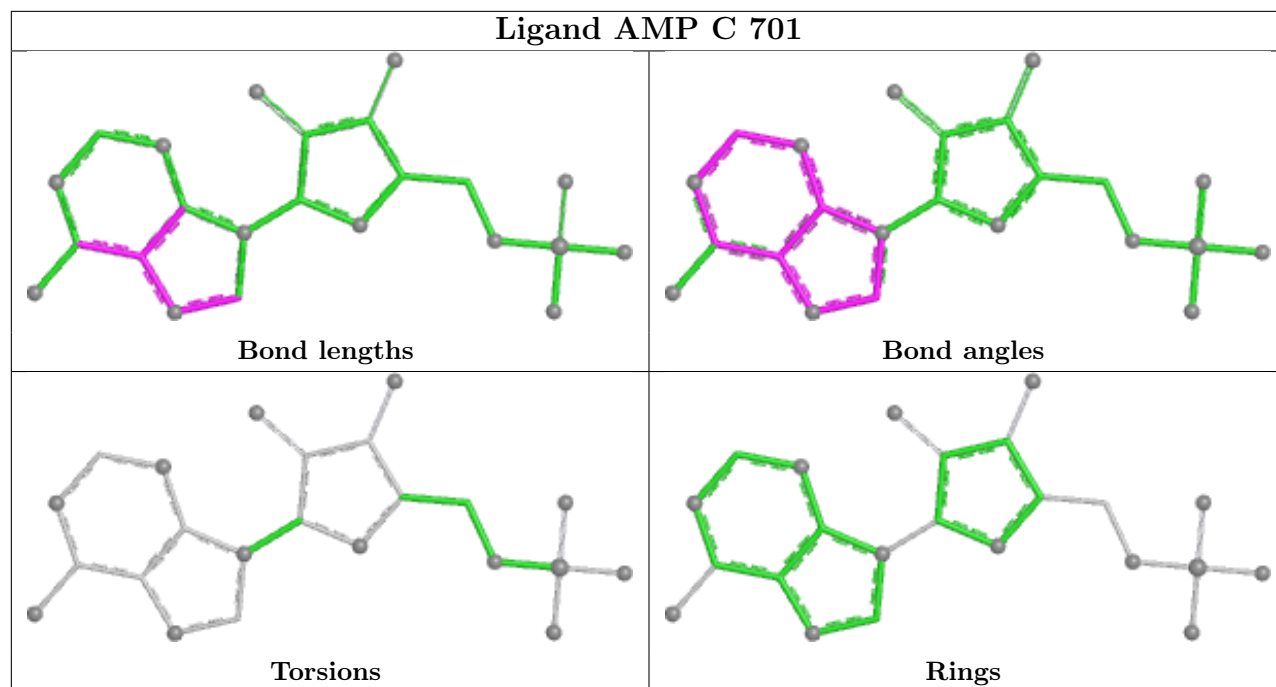
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	702	COA	5	0
3	B	702	COA	1	0
4	A	703	ACY	2	0

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 ⓘ

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	666/686 (97%)	-0.11	15 (2%) 61 58	48, 64, 99, 157	0
1	B	589/686 (85%)	0.10	37 (6%) 26 23	49, 69, 163, 202	0
1	C	597/686 (87%)	0.33	31 (5%) 33 29	60, 96, 165, 198	0
All	All	1852/2058 (89%)	0.10	83 (4%) 38 34	48, 73, 156, 202	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	564	ILE	5.3
1	B	621	ILE	5.2
1	C	20	GLN	4.8
1	B	57	LYS	4.4
1	B	551	VAL	4.3
1	B	632	ILE	4.3
1	B	568	LEU	4.1
1	B	596	ALA	4.0
1	B	20	GLN	4.0
1	C	615	LEU	4.0
1	B	591	VAL	4.0
1	B	590	ALA	4.0
1	B	559	LEU	3.9
1	B	613	LEU	3.8
1	B	624	PHE	3.7
1	B	552	VAL	3.6
1	B	560	SER	3.6
1	C	580	VAL	3.5
1	B	295	SER	3.5
1	A	602	SER	3.4
1	A	20	GLN	3.3
1	C	633	VAL	3.3
1	C	621	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	300	THR	3.2
1	B	631	ILE	3.2
1	B	563	GLU	3.1
1	B	557	HIS	3.0
1	C	57	LYS	3.0
1	C	632	ILE	3.0
1	C	593	ALA	3.0
1	B	592	ILE	3.0
1	C	578	ALA	2.9
1	C	582	ILE	2.8
1	A	557	HIS	2.8
1	A	298	THR	2.8
1	B	630	VAL	2.8
1	B	633	VAL	2.8
1	B	553	ASN	2.7
1	C	597	LEU	2.7
1	C	568	LEU	2.7
1	A	550	ASP	2.7
1	B	629	SER	2.6
1	B	586	ILE	2.6
1	C	630	VAL	2.6
1	A	601	ASN	2.6
1	B	569	ILE	2.5
1	B	554	VAL	2.5
1	C	587	THR	2.5
1	A	685	LYS	2.5
1	B	623	PRO	2.5
1	C	590	ALA	2.5
1	B	611	LYS	2.4
1	C	552	VAL	2.4
1	A	556	GLY	2.4
1	C	428	TYR	2.4
1	C	581	GLY	2.4
1	B	615	LEU	2.4
1	C	586	ILE	2.4
1	A	297	SER	2.4
1	A	629	SER	2.3
1	C	35	GLU	2.3
1	B	595	VAL	2.3
1	C	22	HIS	2.3
1	A	665	THR	2.3
1	B	556	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	614	VAL	2.3
1	C	592	ILE	2.3
1	B	300	THR	2.2
1	C	594	TYR	2.2
1	C	629	SER	2.2
1	B	561	THR	2.2
1	A	600	GLY	2.2
1	C	33	LEU	2.2
1	C	595	VAL	2.1
1	A	624	PHE	2.1
1	B	583	HIS	2.1
1	C	335	GLY	2.1
1	C	628	LYS	2.1
1	A	645	MET	2.1
1	C	553	ASN	2.1
1	C	28	ALA	2.0
1	A	604	GLU	2.0
1	B	221	LYS	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(Å ²)	Q<0.9
3	COA	B	702	31/48	0.55	0.13	106,145,153,156	0
3	COA	C	702	31/48	0.66	0.12	127,149,156,159	0
3	COA	A	702	48/48	0.68	0.18	75,97,105,110	0
5	GOL	B	703	6/6	0.77	0.21	70,80,88,92	0
5	GOL	A	704	6/6	0.81	0.16	67,81,85,88	0

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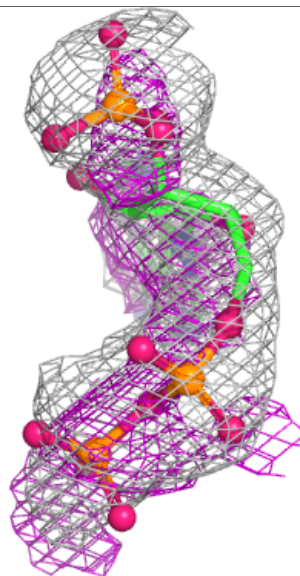
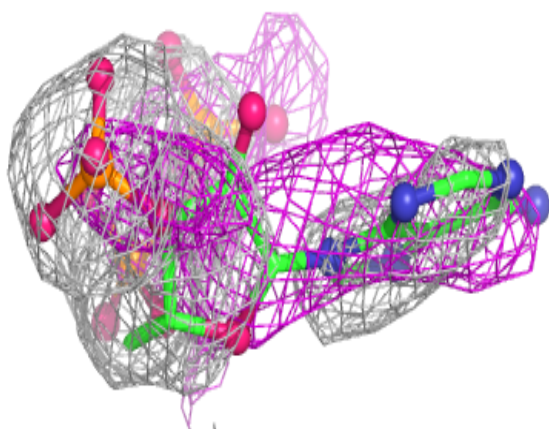
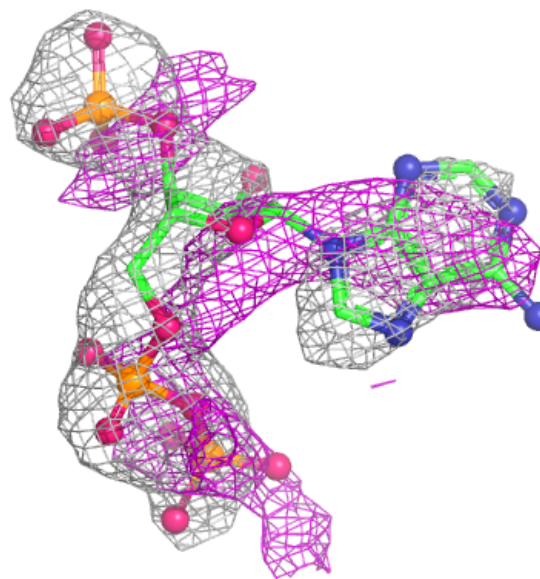
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ACY	A	703	4/4	0.84	0.28	65,66,72,77	0
2	AMP	B	701	23/23	0.86	0.11	72,91,115,133	0
2	AMP	C	701	23/23	0.88	0.10	100,108,120,121	0
2	AMP	A	701	23/23	0.91	0.10	52,57,66,74	0

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.

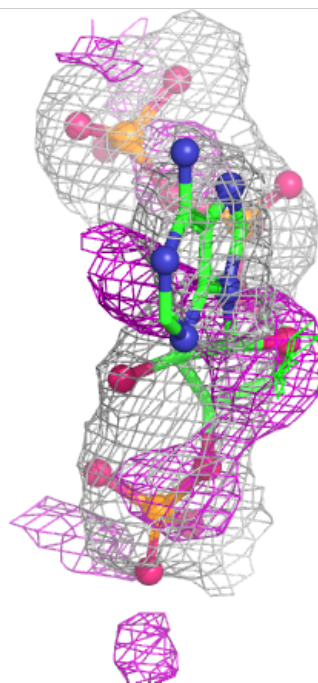
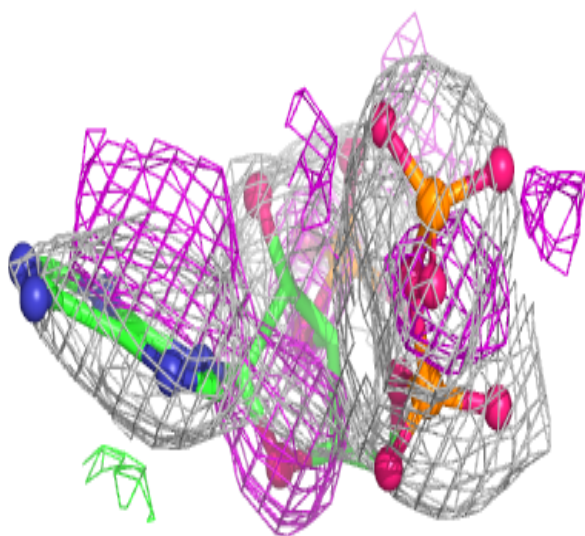
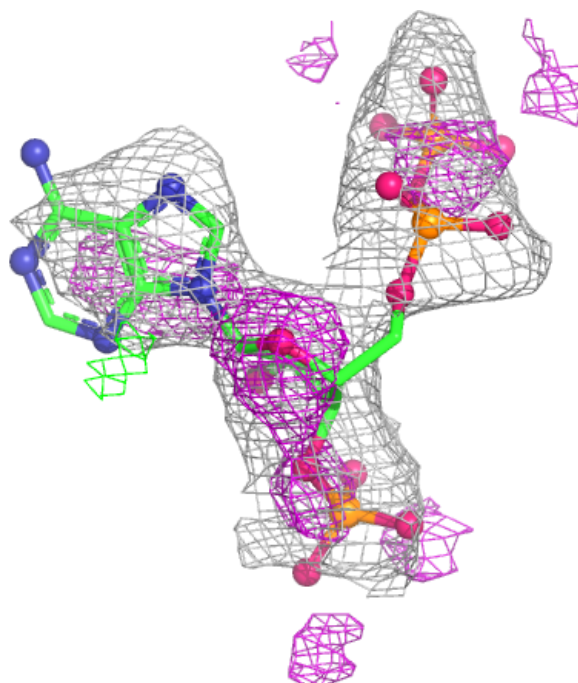
Electron density around COA B 702:

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



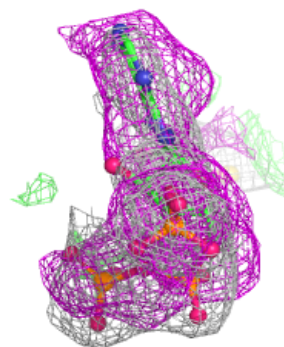
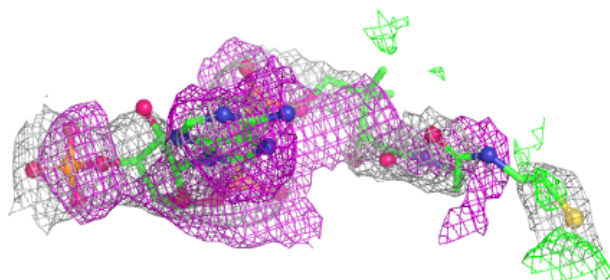
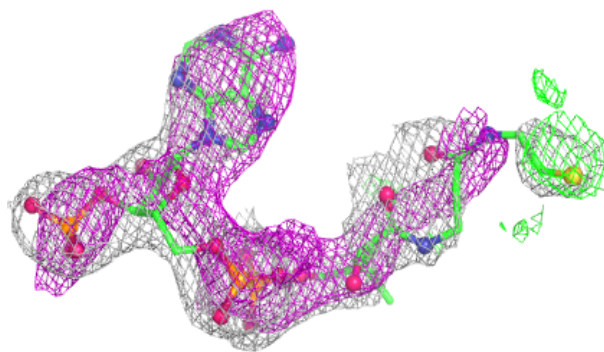
Electron density around COA C 702:

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

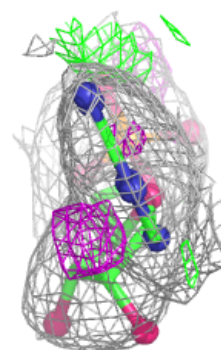
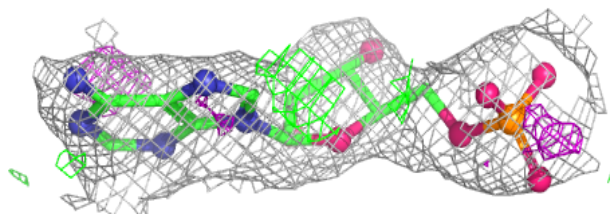
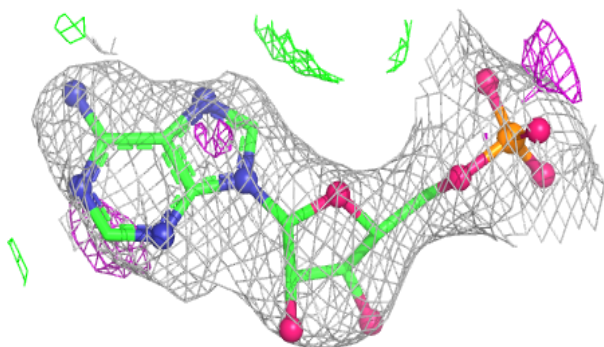


Electron density around COA A 702:

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

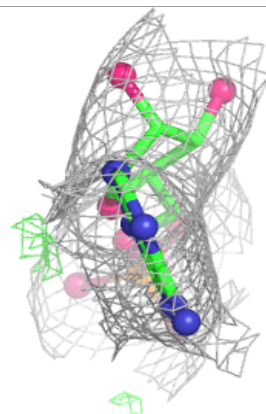
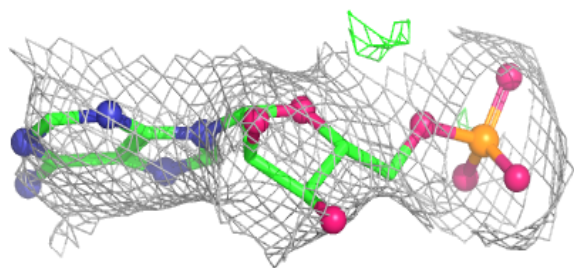
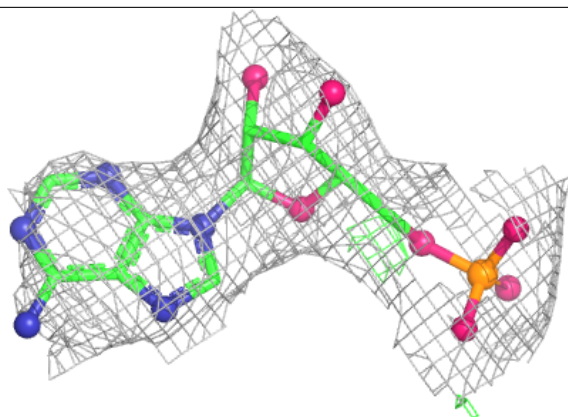
**Electron density around AMP B 701:**

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

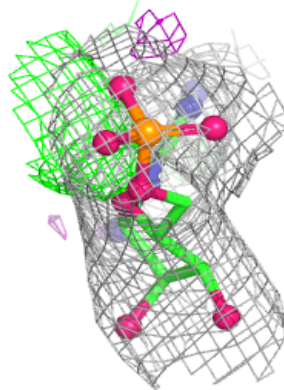
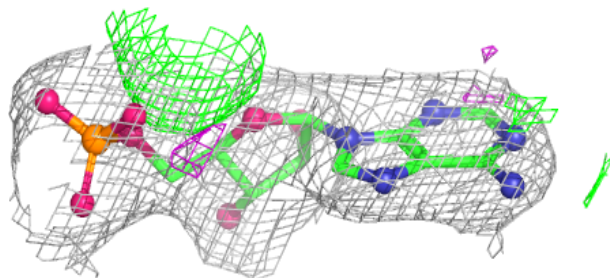
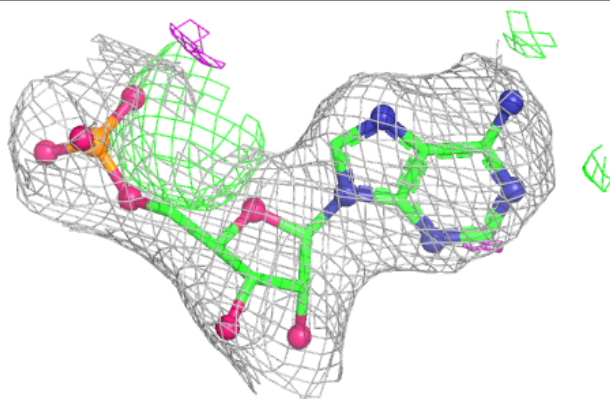


Electron density around AMP C 701:

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

**Electron density around AMP A 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.