



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 08:32 PM UTC

PDB ID : 5BPH / pdb_00005bph
Title : Crystal structure of AMP complexed D-alanine-D-alanine ligase(DDL) from *Yersinia pestis*
Authors : Tran, H.T.; Kang, L.W.; Hong, M.K.
Deposited on : 2015-05-28
Resolution : 1.70 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

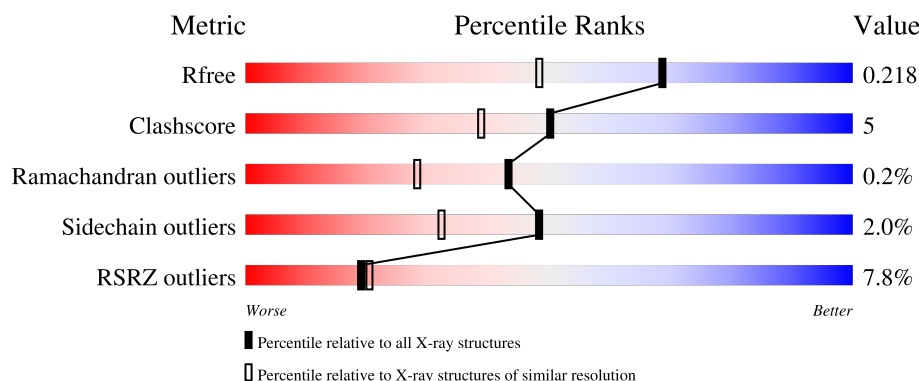
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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

Mol	Chain	Length	Quality of chain
1	A	306	2% 89% 10% .
1	B	306	6% 89% 11%
1	C	306	9% 89% 10% .
1	D	306	13% 82% 14% ...

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	ACT	D	406	-	-	X	-

2 Entry composition [i](#)

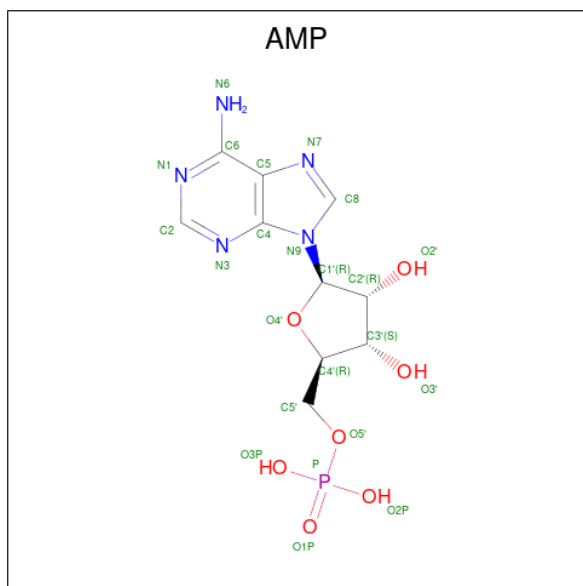
There are 6 unique types of molecules in this entry. The entry contains 10189 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 D-alanine–D-alanine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	306	Total	C	N	O	S	0	0	0
			2332	1487	384	450	11			
1	B	305	Total	C	N	O	S	0	0	0
			2324	1482	383	449	10			
1	C	306	Total	C	N	O	S	0	0	0
			2332	1487	384	450	11			
1	D	303	Total	C	N	O	S	0	0	0
			2308	1470	381	446	11			

- Molecule 2 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: C₁₀H₁₄N₅O₇P).



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		

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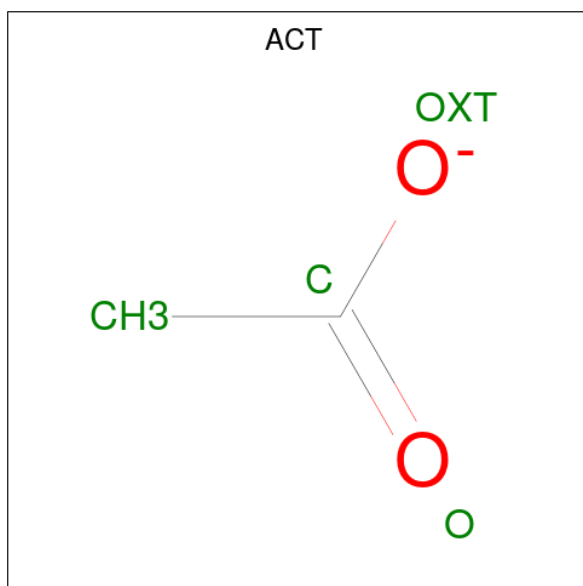
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	D	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Na	0	0
			2	2		
3	B	1	Total	Na	0	0
			1	1		
3	C	1	Total	Na	0	0
			1	1		
3	D	1	Total	Na	0	0
			1	1		

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	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	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		

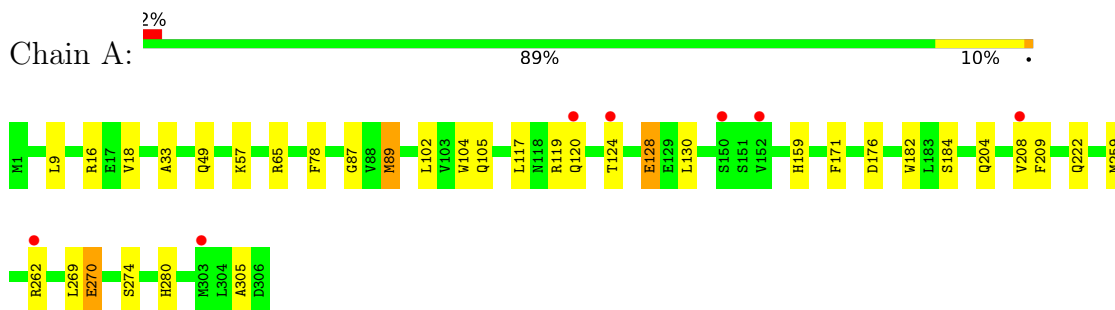
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	221	Total 221	O 221	0	0
6	B	216	Total 216	O 216	0	0
6	C	146	Total 146	O 146	0	0
6	D	147	Total 147	O 147	0	0

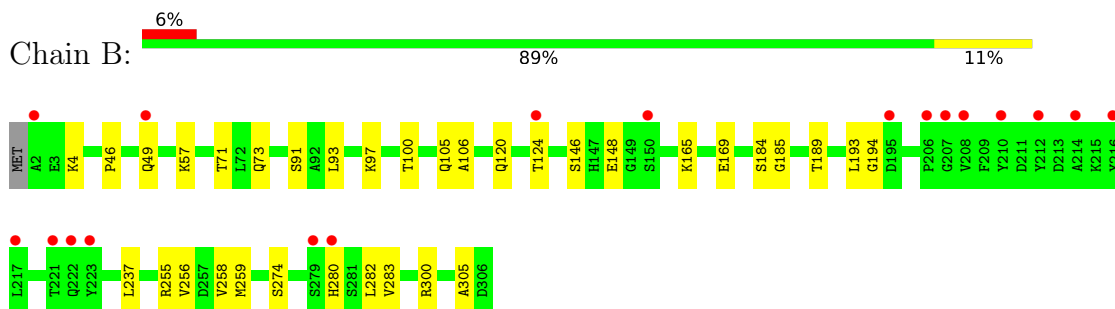
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

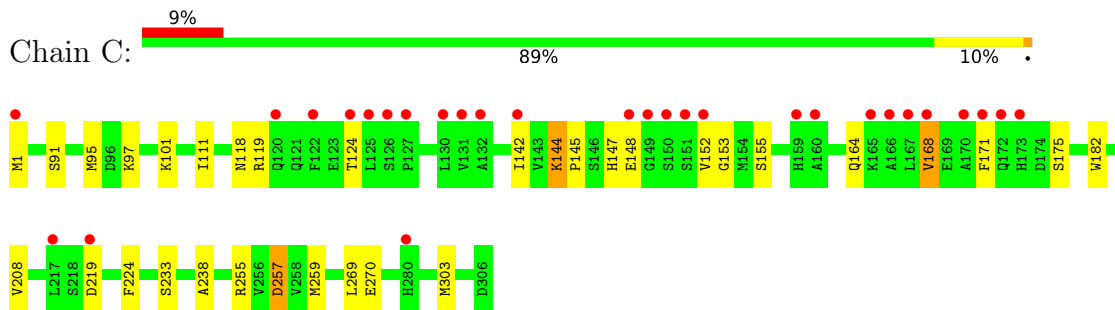
- Molecule 1: D-alanine–D-alanine ligase



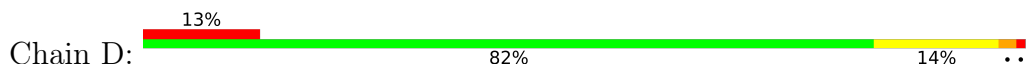
- Molecule 1: D-alanine–D-alanine ligase

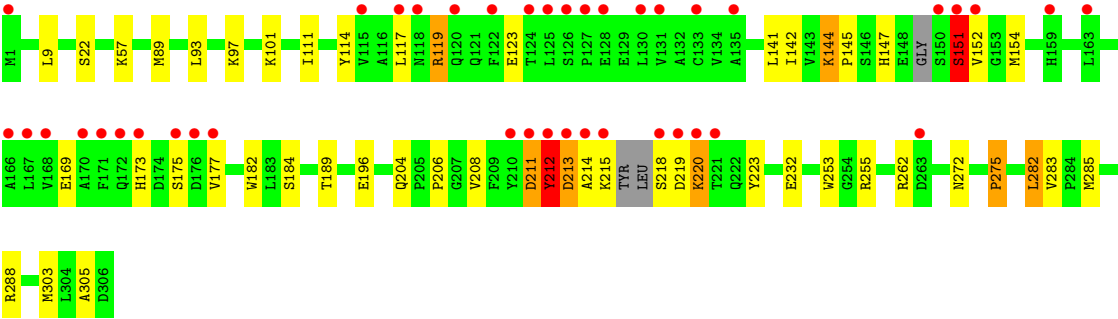


- Molecule 1: D-alanine–D-alanine ligase



- Molecule 1: D-alanine–D-alanine ligase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	62.59Å 106.07Å 210.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.96 – 1.70 34.96 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.6 (34.96-1.70) 99.6 (34.96-1.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.73 (at 1.71Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.177 , 0.209 0.188 , 0.218	Depositor DCC
R_{free} test set	7688 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	25.5	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 34.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10189	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.97% 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: GOL, NA, AMP, ACT

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	1.43	8/2379 (0.3%)	1.25	5/3226 (0.2%)
1	B	1.52	11/2371 (0.5%)	1.29	11/3216 (0.3%)
1	C	1.38	4/2379 (0.2%)	1.23	4/3226 (0.1%)
1	D	1.32	5/2352 (0.2%)	1.32	14/3186 (0.4%)
All	All	1.41	28/9481 (0.3%)	1.28	34/12854 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	185	GLY	N-CA	10.83	1.59	1.44
1	D	288	ARG	C-O	7.91	1.33	1.24
1	A	105	GLN	CD-NE2	7.31	1.48	1.33
1	B	105	GLN	CD-NE2	6.48	1.46	1.33
1	D	212	TYR	N-CA	6.37	1.54	1.46
1	A	274	SER	N-CA	6.35	1.53	1.46
1	B	194	GLY	C-O	-6.22	1.15	1.24
1	C	147	HIS	CA-C	-6.17	1.45	1.52
1	B	283	VAL	C-O	-6.16	1.19	1.24
1	B	97	LYS	N-CA	-6.16	1.39	1.46
1	C	224	PHE	N-CA	-6.15	1.39	1.46
1	A	102	LEU	N-CA	5.93	1.53	1.46
1	A	176	ASP	CA-C	5.87	1.59	1.52
1	C	257	ASP	N-CA	5.84	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	146	SER	N-CA	5.83	1.53	1.46
1	A	104	TRP	C-O	5.75	1.30	1.24
1	A	78	PHE	C-O	5.43	1.30	1.24
1	B	274	SER	N-CA	5.35	1.52	1.46
1	B	91	SER	CA-CB	5.34	1.61	1.53
1	A	33	ALA	C-O	-5.28	1.17	1.24
1	B	148	GLU	N-CA	5.22	1.52	1.46
1	D	275	PRO	C-O	5.20	1.29	1.23
1	A	87	GLY	C-O	5.11	1.28	1.23
1	B	256	VAL	CA-C	5.10	1.58	1.52
1	D	141	LEU	CA-C	-5.09	1.46	1.52
1	C	91	SER	C-O	5.08	1.29	1.24
1	D	303	MET	SD-CE	-5.08	1.66	1.79
1	B	106	ALA	CA-C	-5.01	1.46	1.52

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	89	MET	CG-SD-CE	-14.48	69.05	100.90
1	A	89	MET	CG-SD-CE	-14.05	69.98	100.90
1	D	303	MET	CG-SD-CE	-13.03	72.23	100.90
1	D	213	ASP	N-CA-C	-10.28	100.08	111.07
1	B	259	MET	CA-CB-CG	8.77	131.64	114.10
1	B	185	GLY	N-CA-C	-8.34	95.33	112.34
1	B	185	GLY	CA-C-N	-7.69	112.90	120.52
1	B	185	GLY	C-N-CA	-7.69	112.90	120.52
1	C	144	LYS	CA-C-N	7.44	127.42	119.76
1	C	144	LYS	C-N-CA	7.44	127.42	119.76
1	A	105	GLN	CA-CB-CG	6.74	127.58	114.10
1	D	211	ASP	N-CA-C	6.40	124.37	114.64
1	D	283	VAL	N-CA-CB	6.38	115.43	110.45
1	B	282	LEU	CA-C-N	-5.98	115.54	120.33
1	B	282	LEU	C-N-CA	-5.98	115.54	120.33
1	B	105	GLN	CA-CB-CG	5.85	125.79	114.10
1	D	22	SER	CA-C-N	5.81	126.39	119.94
1	D	22	SER	C-N-CA	5.81	126.39	119.94
1	A	18	VAL	CB-CA-C	-5.80	104.22	112.22
1	D	184	SER	N-CA-C	5.76	118.50	111.82
1	D	144	LYS	O-C-N	5.75	125.88	121.85
1	B	274	SER	O-C-N	5.66	125.98	121.17
1	D	204	GLN	CA-C-N	-5.45	114.77	120.38
1	D	204	GLN	C-N-CA	-5.45	114.77	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	282	LEU	CA-C-N	-5.41	116.00	120.33
1	D	282	LEU	C-N-CA	-5.41	116.00	120.33
1	B	100	THR	N-CA-CB	5.37	117.80	110.01
1	C	147	HIS	N-CA-C	5.25	118.38	109.76
1	A	105	GLN	N-CA-CB	-5.20	102.46	110.16
1	C	238	ALA	N-CA-C	-5.17	105.73	111.36
1	D	196	GLU	CA-CB-CG	5.17	124.43	114.10
1	A	16	ARG	N-CA-C	5.13	117.27	111.11
1	B	73	GLN	N-CA-C	-5.07	105.84	111.36
1	B	93	LEU	CA-C-O	-5.04	115.21	120.55

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	184	SER	Peptide

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	2332	0	2323	20	0
1	B	2324	0	2311	10	0
1	C	2332	0	2323	29	0
1	D	2308	0	2298	43	0
2	A	23	0	12	0	0
2	B	23	0	12	0	0
2	C	23	0	12	0	0
2	D	23	0	12	0	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	4	0	3	0	0
4	B	8	0	6	0	0
4	C	4	0	3	0	0
4	D	8	0	6	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	12	0	16	0	0
5	B	6	0	8	0	0
5	C	12	0	16	0	0
5	D	12	0	16	0	0
6	A	221	0	0	5	0
6	B	216	0	0	3	0
6	C	146	0	0	0	0
6	D	147	0	0	3	0
All	All	10189	0	9377	100	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 5.

All (100) 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:142:ILE:HD11	1:C:182:TRP:CZ3	1.75	1.21
1:C:142:ILE:HD11	1:C:182:TRP:CE3	1.81	1.15
1:A:280:HIS:HE1	6:A:615:HOH:O	1.56	0.87
1:C:142:ILE:CD1	1:C:182:TRP:CE3	2.58	0.86
1:A:280:HIS:CE1	6:A:615:HOH:O	2.30	0.84
1:C:182:TRP:CH2	1:C:208:VAL:HG13	2.11	0.84
1:C:142:ILE:HD11	1:C:182:TRP:HZ3	1.42	0.84
1:B:280:HIS:CD2	6:B:509:HOH:O	2.43	0.71
1:C:142:ILE:CD1	1:C:182:TRP:HE3	2.03	0.71
1:A:49:GLN:HG2	6:A:650:HOH:O	1.91	0.70
1:D:211:ASP:O	1:D:212:TYR:CD2	2.44	0.70
1:D:262:ARG:NH2	6:D:501:HOH:O	2.23	0.69
1:C:142:ILE:CD1	1:C:182:TRP:CZ3	2.66	0.69
1:A:117:LEU:HD11	1:A:130:LEU:HD22	1.75	0.69
1:D:182:TRP:CH2	1:D:208:VAL:HG13	2.29	0.68
1:A:159:HIS:HD2	6:A:695:HOH:O	1.75	0.68
1:B:120:GLN:O	1:B:124:THR:HG22	1.94	0.67
1:D:152:VAL:HG21	1:D:173:HIS:CD2	2.30	0.66
1:D:212:TYR:HA	1:D:215:LYS:HB2	1.78	0.65
1:D:144:LYS:HB3	1:D:154:MET:HE3	1.80	0.64
1:C:142:ILE:CG1	1:C:182:TRP:HE3	2.11	0.62
1:D:151:SER:HA	1:D:212:TYR:HE2	1.64	0.62
1:D:101:LYS:HE3	1:D:111:ILE:HD12	1.82	0.61
1:D:223:TYR:HD2	1:D:285:MET:HE1	1.66	0.61
1:D:211:ASP:O	1:D:212:TYR:CG	2.53	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:ARG:NH2	6:B:501:HOH:O	2.33	0.61
1:C:182:TRP:HH2	1:C:208:VAL:HG13	1.61	0.61
1:D:218:SER:OG	1:D:220:LYS:N	2.23	0.61
1:B:189:THR:OG1	1:B:255:ARG:HG2	2.01	0.60
1:D:144:LYS:CB	1:D:154:MET:HE3	2.32	0.59
1:D:152:VAL:HG21	1:D:173:HIS:NE2	2.18	0.59
1:C:142:ILE:CG1	1:C:182:TRP:CE3	2.85	0.58
1:D:212:TYR:HD1	1:D:213:ASP:H	1.52	0.57
1:D:119:ARG:O	1:D:123:GLU:HG2	2.04	0.57
1:C:164:GLN:O	1:C:168:VAL:HG13	2.04	0.57
1:C:259:MET:HG3	1:C:269:LEU:HD11	1.87	0.56
1:D:182:TRP:HH2	1:D:208:VAL:HG13	1.70	0.56
1:C:182:TRP:CH2	1:C:208:VAL:CG1	2.88	0.55
1:D:144:LYS:HB3	1:D:154:MET:CE	2.36	0.55
1:D:212:TYR:HD1	1:D:213:ASP:N	2.05	0.55
1:B:71:THR:HG21	6:B:612:HOH:O	2.06	0.54
1:A:204:GLN:NE2	1:A:222:GLN:OE1	2.41	0.53
1:B:237:LEU:HD11	1:B:258:VAL:HG21	1.91	0.53
1:C:255:ARG:NH1	1:C:257:ASP:OD1	2.41	0.53
1:D:142:ILE:HD11	1:D:154:MET:HE2	1.89	0.53
1:D:97:LYS:O	1:D:101:LYS:HG3	2.08	0.52
1:A:208:VAL:HG23	1:A:209:PHE:CD2	2.44	0.52
1:C:119:ARG:NH2	1:C:171:PHE:O	2.43	0.52
1:C:142:ILE:CD1	1:C:182:TRP:HZ3	2.17	0.52
1:C:142:ILE:HG12	1:C:182:TRP:HE3	1.73	0.52
1:D:151:SER:HA	1:D:212:TYR:CE2	2.45	0.51
1:A:119:ARG:NH1	1:A:171:PHE:O	2.42	0.51
1:D:189:THR:OG1	1:D:255:ARG:HG2	2.12	0.50
1:C:97:LYS:O	1:C:101:LYS:HG3	2.11	0.50
1:D:218:SER:OG	1:D:219:ASP:N	2.45	0.50
1:A:262:ARG:NH1	6:A:505:HOH:O	2.44	0.49
1:C:118:ASN:HA	1:C:175:SER:O	2.12	0.49
1:D:101:LYS:HG3	6:D:610:HOH:O	2.12	0.49
1:C:95:MET:HE3	1:C:148:GLU:HB3	1.94	0.49
1:D:57:LYS:HE3	1:D:305:ALA:O	2.13	0.49
1:A:159:HIS:HE1	1:C:233:SER:OG	1.96	0.48
1:A:128:GLU:H	1:A:128:GLU:CD	2.21	0.48
1:A:259:MET:HG3	1:A:269:LEU:HD11	1.95	0.48
1:D:144:LYS:HE2	1:D:154:MET:HE1	1.96	0.48
1:A:269:LEU:C	1:A:270:GLU:HG3	2.39	0.48
1:D:144:LYS:HE2	1:D:154:MET:CE	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:152:VAL:HG22	1:C:153:GLY:N	2.29	0.47
1:B:165:LYS:O	1:B:169:GLU:HG3	2.14	0.47
1:D:211:ASP:H	1:D:214:ALA:HB3	1.79	0.47
1:D:142:ILE:HD11	1:D:154:MET:CE	2.45	0.47
1:D:255:ARG:HH22	4:D:406:ACT:H3	1.80	0.47
1:D:169:GLU:HA	1:D:169:GLU:OE1	2.16	0.46
1:A:57:LYS:HE2	1:A:305:ALA:O	2.15	0.46
1:C:303:MET:HE3	1:C:303:MET:HB3	1.78	0.46
1:A:182:TRP:CH2	1:A:184:SER:HA	2.51	0.46
1:D:213:ASP:O	1:D:218:SER:N	2.49	0.46
1:A:9:LEU:C	1:A:9:LEU:HD12	2.42	0.45
1:A:89:MET:HE2	1:D:93:LEU:HA	1.97	0.45
1:D:101:LYS:HG2	6:D:586:HOH:O	2.17	0.45
1:D:253:TRP:CH2	1:D:275:PRO:HD2	2.52	0.44
1:D:255:ARG:HH22	4:D:406:ACT:CH3	2.30	0.44
1:B:46:PRO:HG2	1:B:49:GLN:CD	2.43	0.44
1:D:189:THR:HG21	1:D:282:LEU:HD13	1.99	0.44
1:D:101:LYS:HE2	1:D:114:TYR:CG	2.52	0.44
1:C:182:TRP:HH2	1:C:208:VAL:CG1	2.27	0.44
1:A:117:LEU:HD11	1:A:130:LEU:CD2	2.46	0.44
1:D:212:TYR:CD1	1:D:213:ASP:N	2.83	0.43
1:C:142:ILE:HA	1:C:142:ILE:HD13	1.69	0.43
1:D:206:PRO:HB3	1:D:220:LYS:HB3	2.01	0.42
1:A:57:LYS:NZ	1:A:305:ALA:O	2.50	0.42
1:D:9:LEU:C	1:D:9:LEU:HD12	2.44	0.41
1:C:142:ILE:HD12	1:C:142:ILE:HG23	1.76	0.41
1:B:189:THR:OG1	1:B:255:ARG:CG	2.69	0.41
1:D:152:VAL:CG2	1:D:173:HIS:CD2	3.03	0.41
1:B:57:LYS:HE2	1:B:305:ALA:HB3	2.02	0.41
1:C:1:MET:HE2	1:C:1:MET:HA	2.03	0.41
1:D:145:PRO:HB2	1:D:147:HIS:O	2.21	0.40
1:A:57:LYS:CE	1:A:305:ALA:O	2.69	0.40
1:C:101:LYS:HE3	1:C:111:ILE:HD12	2.02	0.40
1:C:144:LYS:HA	1:C:145:PRO:HD3	1.89	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	304/306 (99%)	299 (98%)	5 (2%)	0	100	100
1	B	303/306 (99%)	295 (97%)	8 (3%)	0	100	100
1	C	304/306 (99%)	298 (98%)	6 (2%)	0	100	100
1	D	297/306 (97%)	288 (97%)	7 (2%)	2 (1%)	18	7
All	All	1208/1224 (99%)	1180 (98%)	26 (2%)	2 (0%)	43	28

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	151	SER
1	D	212	TYR

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	251/251 (100%)	246 (98%)	5 (2%)	48	32
1	B	250/251 (100%)	248 (99%)	2 (1%)	73	65
1	C	251/251 (100%)	246 (98%)	5 (2%)	48	32
1	D	249/251 (99%)	241 (97%)	8 (3%)	34	17
All	All	1001/1004 (100%)	981 (98%)	20 (2%)	48	32

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	ARG
1	A	120	GLN
1	A	124	THR
1	A	128	GLU
1	A	270	GLU
1	B	4	LYS
1	B	193	LEU
1	C	124	THR
1	C	155	SER
1	C	168	VAL
1	C	219	ASP
1	C	270	GLU
1	D	117	LEU
1	D	119	ARG
1	D	151	SER
1	D	175	SER
1	D	177	VAL
1	D	220	LYS
1	D	232	GLU
1	D	272	ASN

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

Mol	Chain	Res	Type
1	A	159	HIS
1	A	173	HIS
1	A	204	GLN
1	B	24	GLN
1	B	120	GLN
1	B	164	GLN
1	B	173	HIS
1	B	243	GLN
1	B	265	HIS
1	B	280	HIS
1	C	105	GLN
1	C	159	HIS
1	C	204	GLN
1	D	80	GLN
1	D	105	GLN
1	D	120	GLN
1	D	204	GLN
1	D	272	ASN
1	D	280	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 22 ligands modelled in this entry, 5 are monoatomic - leaving 17 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	ACT	D	406	-	3,3,3	1.67	1 (33%)	3,3,3	0.74	0
4	ACT	D	403	-	3,3,3	0.60	0	3,3,3	1.67	1 (33%)
4	ACT	A	403	-	3,3,3	1.10	0	3,3,3	0.88	0
4	ACT	B	403	-	3,3,3	0.63	0	3,3,3	1.79	1 (33%)
4	ACT	C	403	-	3,3,3	1.12	0	3,3,3	1.36	0
5	GOL	B	405	-	5,5,5	0.92	0	5,5,5	0.74	0
5	GOL	C	404	-	5,5,5	0.12	0	5,5,5	0.64	0
5	GOL	D	404	-	5,5,5	0.24	0	5,5,5	1.24	0
5	GOL	D	405	-	5,5,5	0.20	0	5,5,5	1.25	0
5	GOL	C	405	-	5,5,5	0.88	0	5,5,5	1.50	1 (20%)
5	GOL	A	404	-	5,5,5	0.50	0	5,5,5	0.79	0
5	GOL	A	405	-	5,5,5	0.36	0	5,5,5	0.71	0
2	AMP	D	401	-	25,25,25	1.15	2 (8%)	37,38,38	1.82	9 (24%)
2	AMP	B	401	-	25,25,25	1.51	4 (16%)	37,38,38	1.56	5 (13%)
2	AMP	C	401	-	25,25,25	1.25	2 (8%)	37,38,38	2.05	7 (18%)
2	AMP	A	401	-	25,25,25	1.70	4 (16%)	37,38,38	2.03	7 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ACT	B	404	-	3,3,3	1.65	1 (33%)	3,3,3	1.14	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
5	GOL	C	404	-	-	0/4/4/4	-
5	GOL	D	404	-	-	2/4/4/4	-
5	GOL	B	405	-	-	0/4/4/4	-
5	GOL	D	405	-	-	0/4/4/4	-
5	GOL	C	405	-	-	1/4/4/4	-
5	GOL	A	404	-	-	4/4/4/4	-
5	GOL	A	405	-	-	4/4/4/4	-
2	AMP	D	401	-	-	0/10/26/26	0/3/3/3
2	AMP	B	401	-	-	0/10/26/26	0/3/3/3
2	AMP	C	401	-	-	2/10/26/26	0/3/3/3
2	AMP	A	401	-	-	0/10/26/26	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	AMP	C5-C4	5.27	1.48	1.39
2	B	401	AMP	C5-C4	4.18	1.46	1.39
2	B	401	AMP	C8-N7	3.39	1.38	1.31
2	C	401	AMP	C5-C4	2.98	1.44	1.39
2	A	401	AMP	C8-N7	2.92	1.37	1.31
2	B	401	AMP	P-O5'	2.74	1.69	1.60
4	D	406	ACT	O-C	2.53	1.33	1.22
2	A	401	AMP	C4-N9	-2.49	1.32	1.37
2	C	401	AMP	C4-N9	-2.43	1.32	1.37
4	B	404	ACT	O-C	2.36	1.32	1.22
2	D	401	AMP	P-O2P	-2.25	1.46	1.54
2	B	401	AMP	C2-N3	2.20	1.37	1.33
2	D	401	AMP	C5-C4	2.04	1.42	1.39
2	A	401	AMP	C2'-C3'	-2.03	1.47	1.53

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	AMP	C5-C4-N3	-6.93	117.18	126.72
2	C	401	AMP	O5'-P-O1P	-6.37	89.21	106.44
2	D	401	AMP	C5-C4-N3	-5.54	119.09	126.72
2	C	401	AMP	O3P-P-O2P	5.47	128.33	107.80
2	B	401	AMP	C5-C4-N3	-5.40	119.29	126.72
2	A	401	AMP	N3-C4-N9	5.38	136.32	127.17
2	A	401	AMP	C2-N3-C4	4.24	122.19	111.83
2	C	401	AMP	O2P-P-O5'	4.20	117.63	106.67
2	B	401	AMP	N3-C4-N9	4.04	134.05	127.17
2	C	401	AMP	C5-C4-N3	-3.86	121.40	126.72
2	C	401	AMP	C4-C5-N7	-3.46	106.63	110.58
2	D	401	AMP	C6-C5-C4	3.39	121.80	117.18
2	D	401	AMP	N3-C4-N9	3.31	132.79	127.17
2	D	401	AMP	O2P-P-O5'	3.26	115.18	106.67
2	A	401	AMP	C4-N9-C8	3.10	108.99	105.74
2	D	401	AMP	N3-C2-N1	3.10	133.27	128.58
2	D	401	AMP	O3P-P-O5'	-3.04	98.74	106.67
2	A	401	AMP	C4-C5-N7	-2.91	107.25	110.58
2	D	401	AMP	O3P-P-O2P	2.90	118.66	107.80
2	C	401	AMP	O3P-P-O5'	-2.65	99.77	106.67
2	B	401	AMP	C4-N9-C8	2.62	108.49	105.74
2	B	401	AMP	C2-N3-C4	2.61	118.20	111.83
2	A	401	AMP	N3-C2-N1	-2.58	124.68	128.58
4	B	403	ACT	OXT-C-CH3	2.48	125.45	115.05
5	C	405	GOL	O3-C3-C2	2.47	121.51	110.38
2	D	401	AMP	C4-C5-N7	-2.41	107.83	110.58
2	C	401	AMP	N3-C4-N9	2.33	131.12	127.17
2	B	401	AMP	C4-C5-N7	-2.24	108.03	110.58
2	A	401	AMP	C6-C5-N7	2.23	136.39	132.09
4	D	403	ACT	O-C-CH3	-2.20	113.52	122.53
2	D	401	AMP	C5-C4-N9	2.09	108.09	105.81

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	405	GOL	O1-C1-C2-C3
5	A	405	GOL	C1-C2-C3-O3
5	D	404	GOL	O1-C1-C2-C3
5	A	405	GOL	O2-C2-C3-O3
5	D	404	GOL	O1-C1-C2-O2
5	A	404	GOL	C1-C2-C3-O3
5	A	404	GOL	O2-C2-C3-O3

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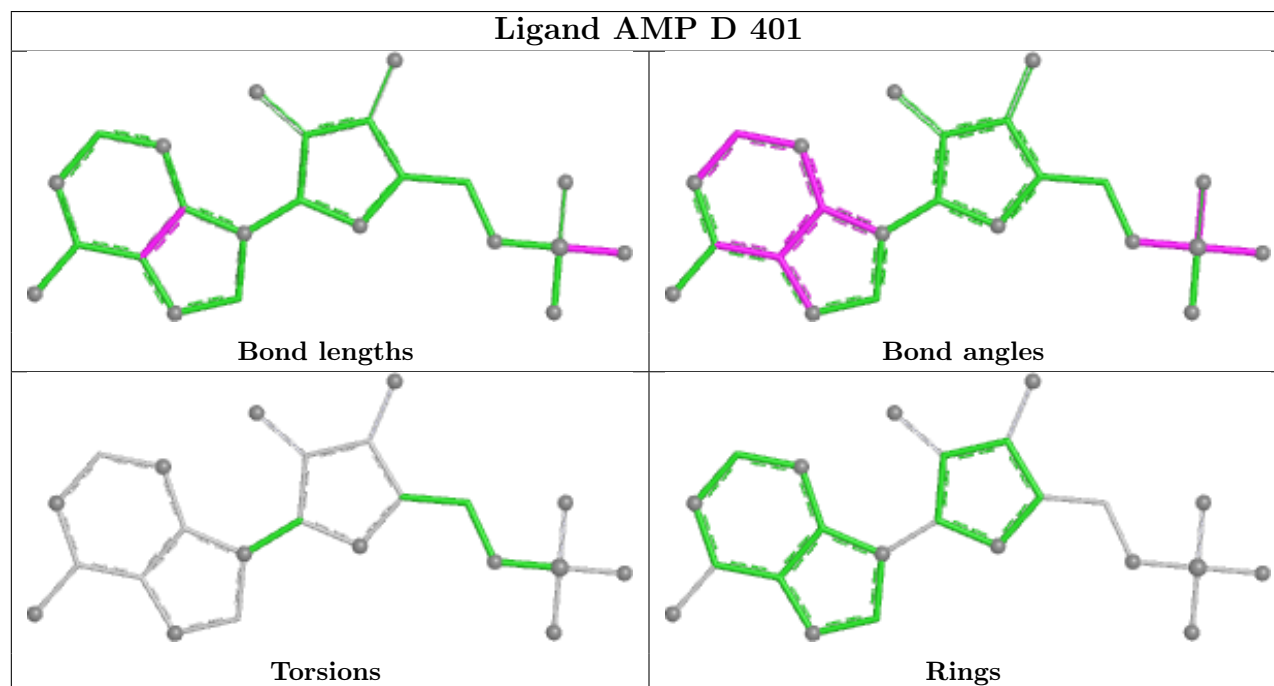
Mol	Chain	Res	Type	Atoms
5	A	405	GOL	O1-C1-C2-O2
2	C	401	AMP	C5'-O5'-P-O3P
5	A	404	GOL	O1-C1-C2-C3
5	A	404	GOL	O1-C1-C2-O2
2	C	401	AMP	C5'-O5'-P-O1P
5	C	405	GOL	O1-C1-C2-O2

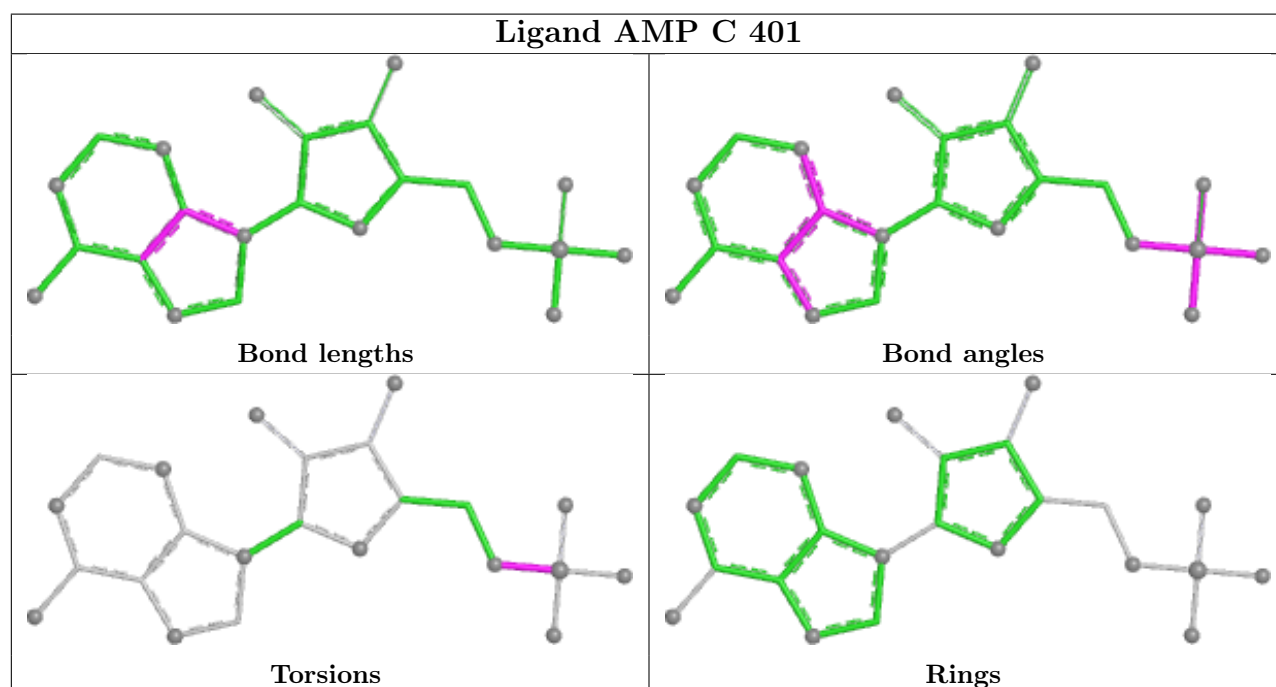
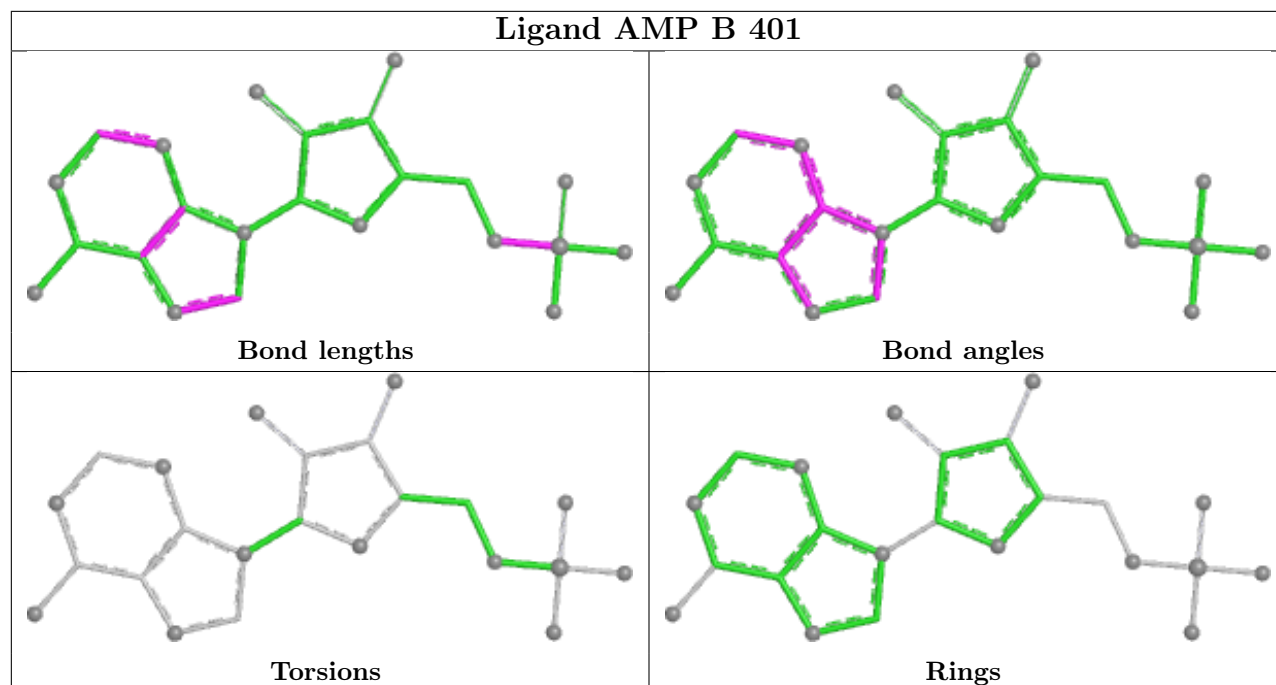
There are no ring outliers.

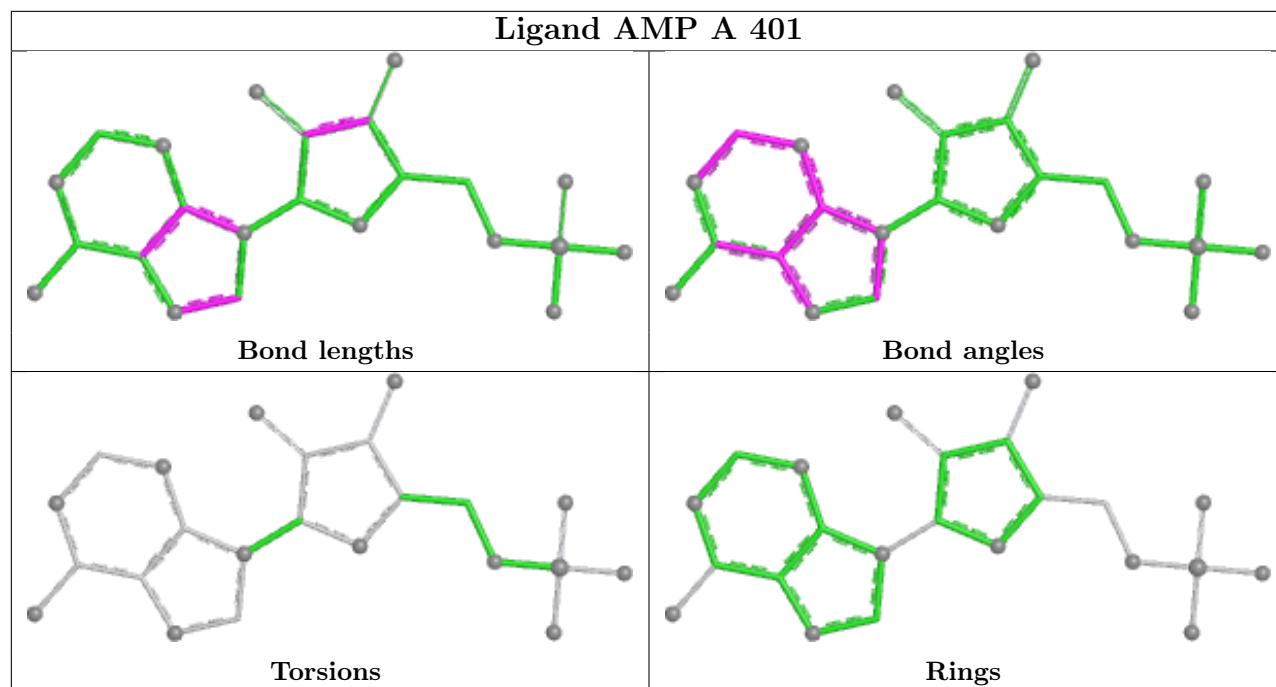
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	406	ACT	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	306/306 (100%)	0.02	7 (2%) 61 65	16, 24, 41, 62	0
1	B	305/306 (99%)	0.19	18 (5%) 28 31	16, 25, 45, 70	0
1	C	306/306 (100%)	0.36	29 (9%) 14 14	16, 26, 58, 79	0
1	D	303/306 (99%)	0.78	41 (13%) 7 6	17, 32, 61, 93	0
All	All	1220/1224 (99%)	0.34	95 (7%) 19 20	16, 27, 54, 93	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	212	TYR	6.6
1	D	168	VAL	5.3
1	C	149	GLY	4.7
1	D	214	ALA	4.3
1	C	168	VAL	4.1
1	D	152	VAL	4.0
1	D	118	ASN	3.9
1	B	214	ALA	3.8
1	D	170	ALA	3.8
1	B	207	GLY	3.7
1	C	152	VAL	3.7
1	D	131	VAL	3.7
1	B	2	ALA	3.7
1	B	216	TYR	3.6
1	C	124	THR	3.5
1	D	124	THR	3.5
1	B	212	TYR	3.4
1	C	150	SER	3.3
1	D	213	ASP	3.3
1	C	280	HIS	3.3
1	B	280	HIS	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	1	MET	3.2
1	D	175	SER	3.2
1	D	122	PHE	3.1
1	D	117	LEU	3.1
1	B	206	PRO	3.0
1	C	171	PHE	3.0
1	D	166	ALA	3.0
1	C	148	GLU	3.0
1	B	221	THR	2.9
1	D	125	LEU	2.9
1	D	215	LYS	2.9
1	D	220	LYS	2.9
1	D	126	SER	2.9
1	D	171	PHE	2.8
1	D	1	MET	2.8
1	B	124	THR	2.8
1	D	221	THR	2.8
1	D	173	HIS	2.8
1	D	130	LEU	2.7
1	D	133	CYS	2.7
1	C	217	LEU	2.7
1	A	124	THR	2.7
1	D	150	SER	2.7
1	C	132	ALA	2.7
1	C	125	LEU	2.6
1	D	127	PRO	2.6
1	D	176	ASP	2.6
1	C	127	PRO	2.6
1	A	262	ARG	2.6
1	D	172	GLN	2.5
1	C	120	GLN	2.5
1	C	172	GLN	2.5
1	B	279	SER	2.5
1	D	151	SER	2.5
1	D	218	SER	2.5
1	B	217	LEU	2.4
1	A	120	GLN	2.4
1	D	120	GLN	2.4
1	D	219	ASP	2.4
1	D	163	LEU	2.4
1	D	263	ASP	2.4
1	D	167	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	142	ILE	2.4
1	C	131	VAL	2.4
1	D	177	VAL	2.3
1	D	135	ALA	2.3
1	C	159	HIS	2.3
1	C	122	PHE	2.3
1	B	208	VAL	2.3
1	B	49	GLN	2.3
1	C	160	ALA	2.3
1	D	211	ASP	2.3
1	C	167	LEU	2.2
1	D	210	TYR	2.2
1	A	208	VAL	2.2
1	C	170	ALA	2.2
1	C	219	ASP	2.2
1	C	130	LEU	2.2
1	B	222	GLN	2.2
1	D	159	HIS	2.2
1	C	165	LYS	2.2
1	D	115	VAL	2.2
1	A	150	SER	2.2
1	B	210	TYR	2.2
1	B	223	TYR	2.2
1	C	166	ALA	2.1
1	B	195	ASP	2.1
1	C	126	SER	2.1
1	A	152	VAL	2.1
1	D	128	GLU	2.1
1	B	150	SER	2.0
1	C	173	HIS	2.0
1	A	303	MET	2.0
1	C	151	SER	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 ⓘ

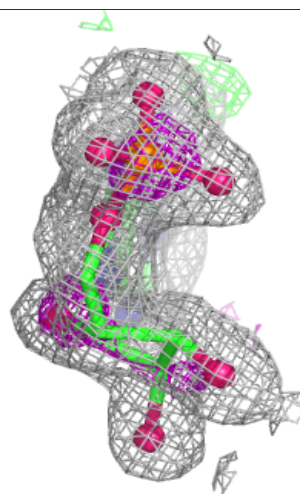
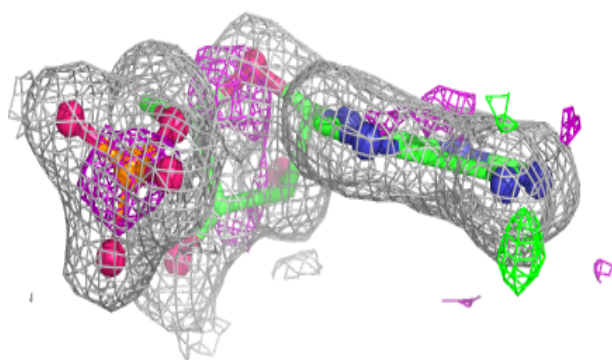
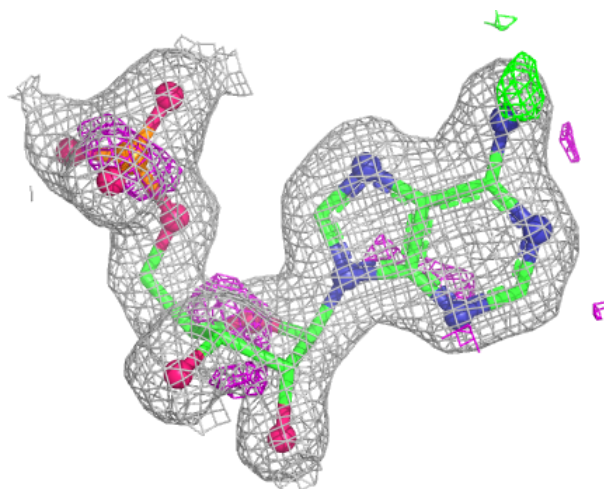
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	ACT	D	406	4/4	0.77	0.16	36,40,43,49	0
5	GOL	A	404	6/6	0.82	0.18	32,53,56,62	0
4	ACT	B	403	4/4	0.83	0.16	32,37,38,42	0
5	GOL	C	404	6/6	0.83	0.15	30,45,46,55	0
5	GOL	D	404	6/6	0.84	0.14	32,43,48,49	0
5	GOL	D	405	6/6	0.84	0.14	33,47,50,51	0
5	GOL	A	405	6/6	0.86	0.13	36,45,53,55	0
5	GOL	C	405	6/6	0.87	0.14	28,42,45,46	0
5	GOL	B	405	6/6	0.87	0.11	36,46,47,49	0
3	NA	A	406	1/1	0.87	0.10	29,29,29,29	0
4	ACT	C	403	4/4	0.88	0.15	33,41,42,42	0
4	ACT	D	403	4/4	0.88	0.14	38,41,41,42	0
4	ACT	B	404	4/4	0.94	0.09	27,29,31,31	0
2	AMP	B	401	23/23	0.95	0.08	21,25,29,32	0
2	AMP	D	401	23/23	0.96	0.07	22,30,40,45	0
4	ACT	A	403	4/4	0.96	0.10	25,26,27,30	0
2	AMP	C	401	23/23	0.97	0.06	23,26,35,42	0
3	NA	C	402	1/1	0.98	0.03	18,18,18,18	0
3	NA	D	402	1/1	0.98	0.07	20,20,20,20	0
2	AMP	A	401	23/23	0.98	0.06	20,23,27,29	0
3	NA	B	402	1/1	0.99	0.03	18,18,18,18	0
3	NA	A	402	1/1	0.99	0.06	17,17,17,17	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.

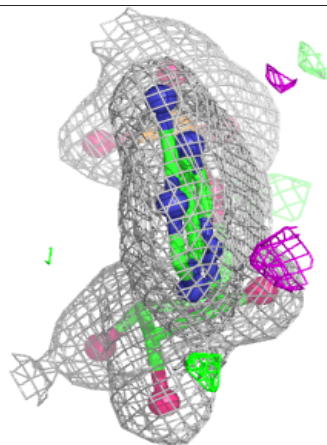
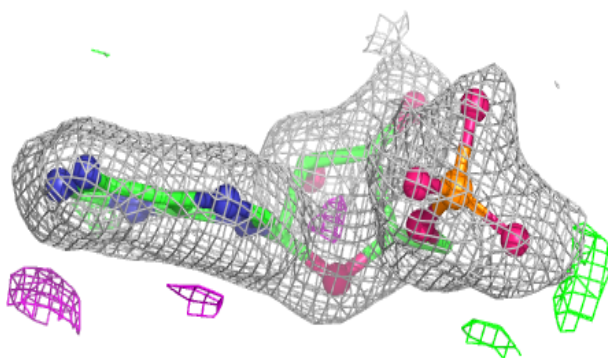
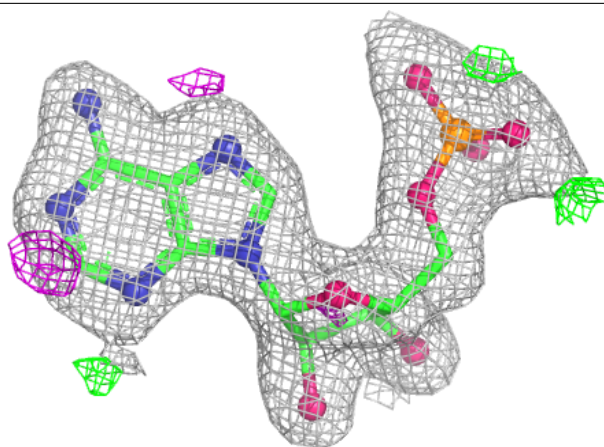
Electron density around AMP B 401:

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



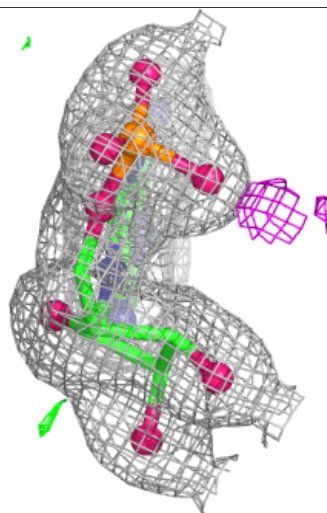
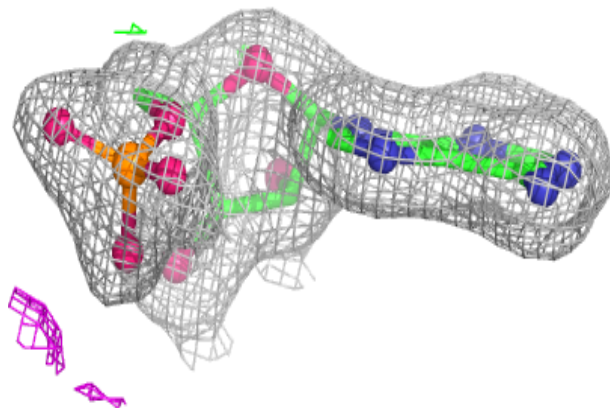
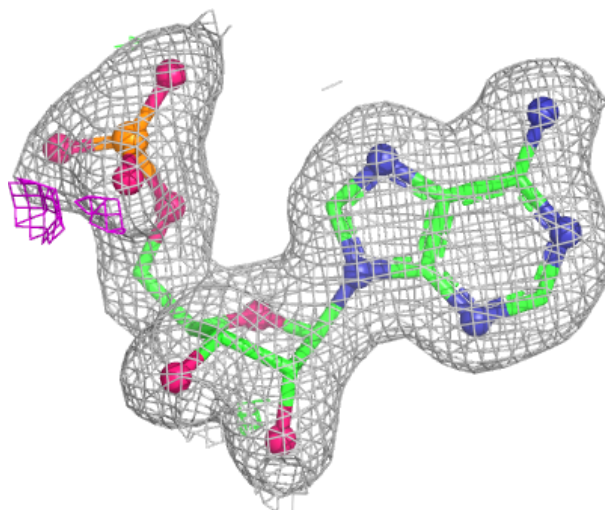
Electron density around AMP D 401:

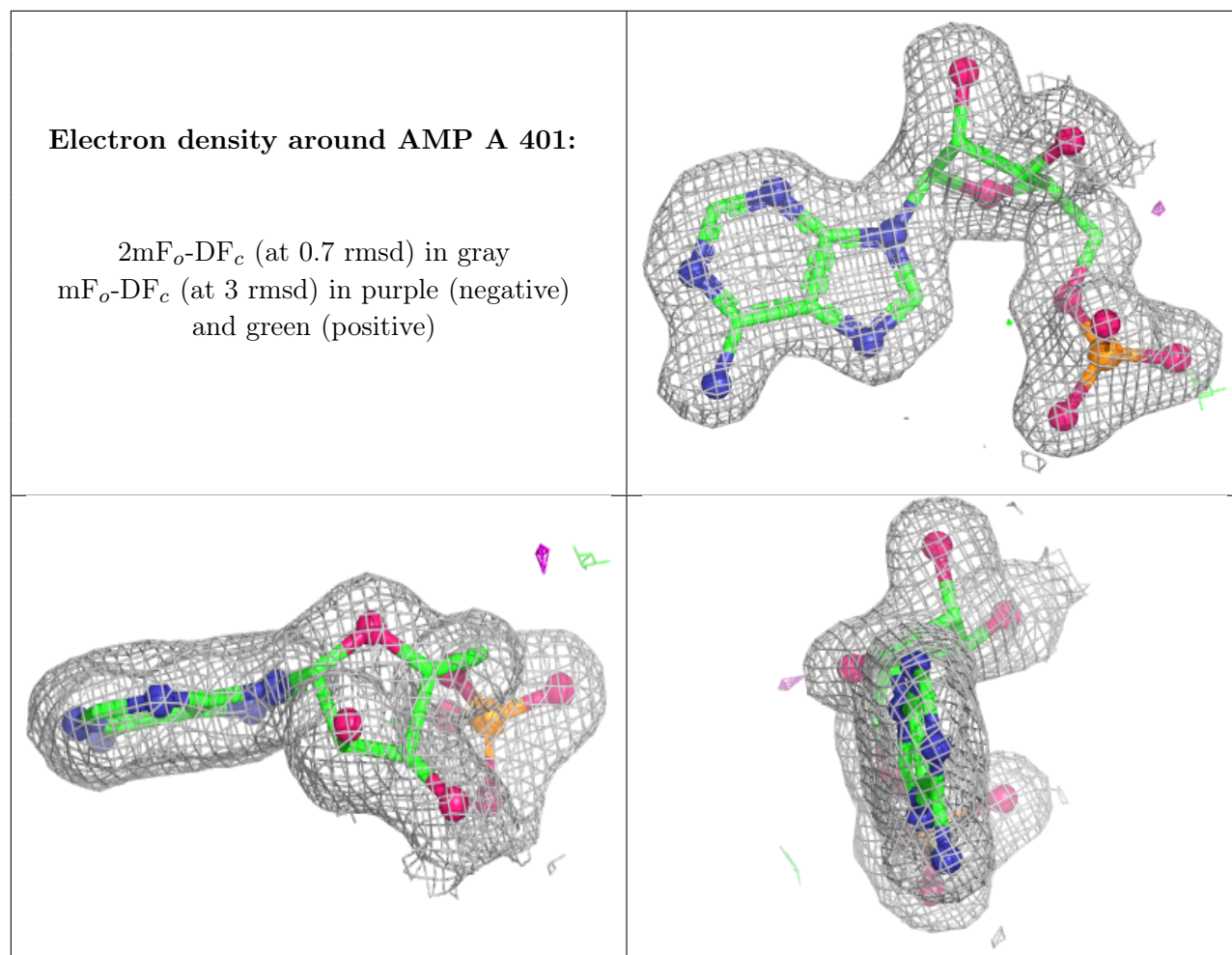
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around AMP C 401:

$2mF_o-DF_c$ (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.