



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 01:55 PM UTC

PDB ID : 9HMP / pdb_00009hmp
Title : X-ray structure of *S. cerevisiae* threonylcarbamoyladenosine dehydratase 1 (residues 50-429) in complex with AMP
Authors : Hirschmann, J.; Huber, E.M.
Deposited on : 2024-12-09
Resolution : 4.00 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

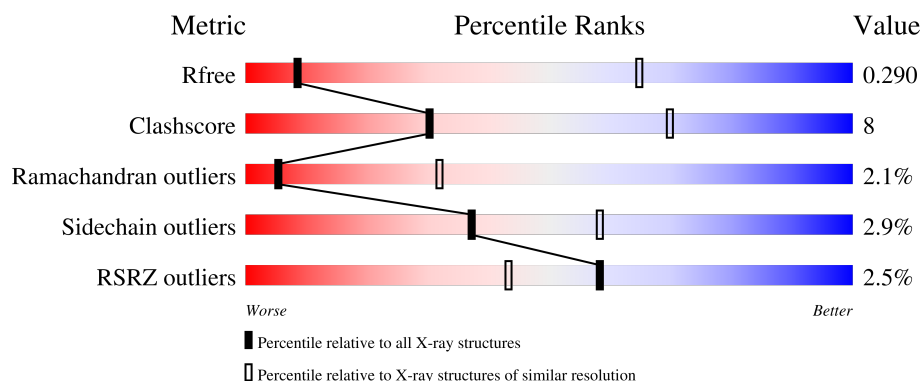
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

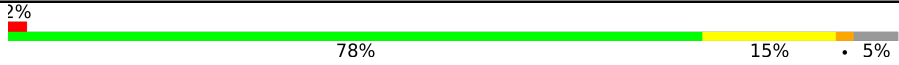



The reported resolution of this entry is 4.00 Å.

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	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)

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	382	
1	B	382	
1	C	382	
1	D	382	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11707 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.

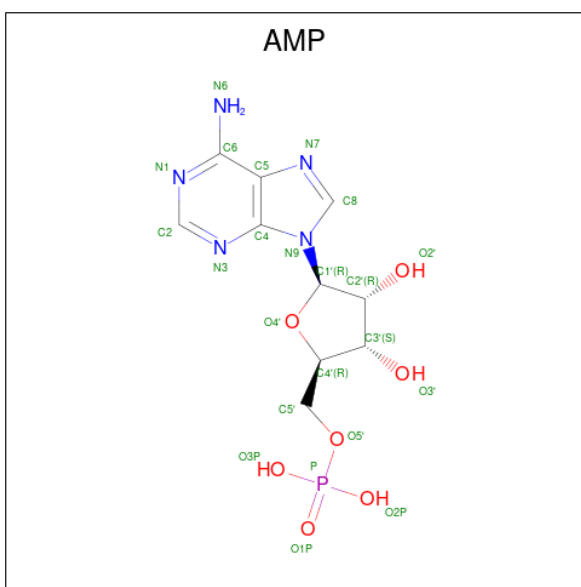
- Molecule 1 is a protein called tRNA threonylcarbamoyladenosine dehydratase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	363	Total	C	N	O	S	0	0	0
			2905	1838	494	555	18			
1	B	361	Total	C	N	O	S	0	0	0
			2882	1826	491	547	18			
1	C	362	Total	C	N	O	S	0	0	0
			2892	1831	490	553	18			
1	D	365	Total	C	N	O	S	0	0	0
			2914	1844	496	556	18			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	48	GLY	-	expression tag	UNP P38756
A	49	SER	-	expression tag	UNP P38756
B	48	GLY	-	expression tag	UNP P38756
B	49	SER	-	expression tag	UNP P38756
C	48	GLY	-	expression tag	UNP P38756
C	49	SER	-	expression tag	UNP P38756
D	48	GLY	-	expression tag	UNP P38756
D	49	SER	-	expression tag	UNP P38756

- Molecule 2 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: C₁₀H₁₄N₅O₇P) (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		
2	D	1	Total	C	N	O	P	0	0
			23	10	5	7	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	C	2	Total	Cl	0	0
			2	2		
3	D	1	Total	Cl	0	0
			1	1		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Na	0	0
			3	3		
4	B	3	Total	Na	0	0
			3	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Na	0	0
			1	1		
4	D	1	Total	Na	0	0
			1	1		

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



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

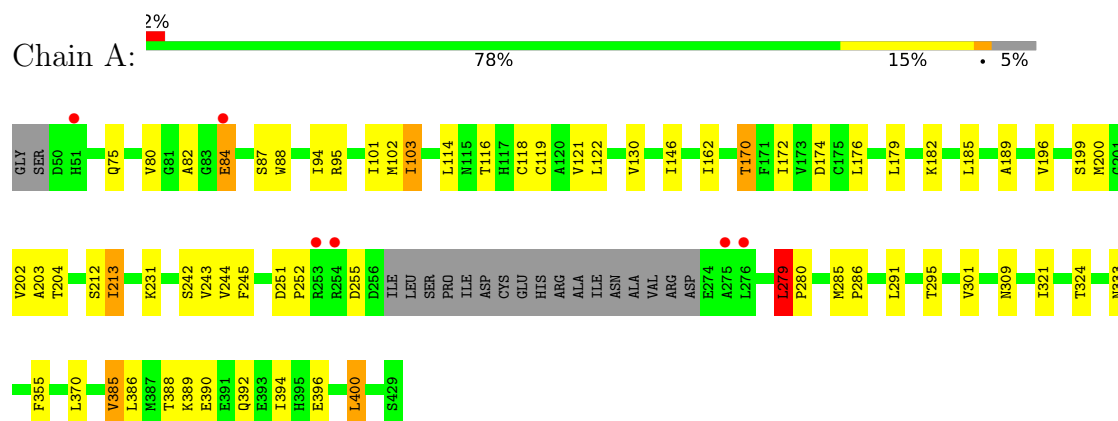
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total	O	0	0
			1	1		
6	D	2	Total	O	0	0
			2	2		

3 Residue-property plots

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

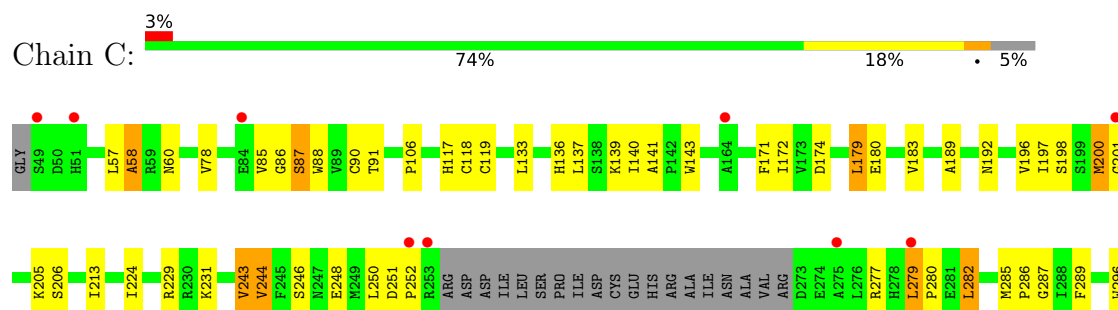
- Molecule 1: tRNA threonylcarbamoyladenosine dehydratase 1

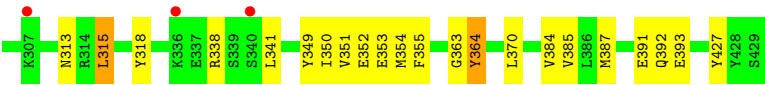


- Molecule 1: tRNA threonylcarbamoyladenosine dehydratase 1

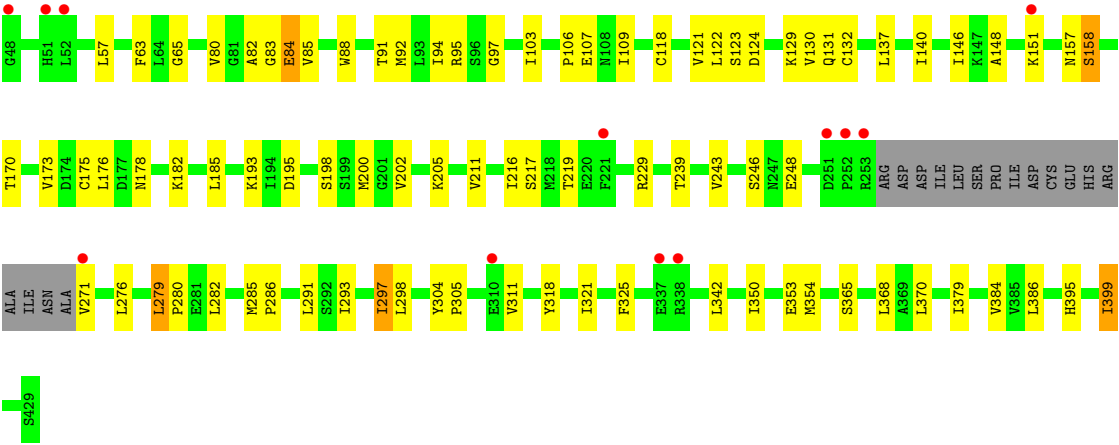
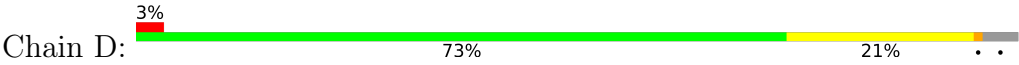


- Molecule 1: tRNA threonylcarbamoyladenosine dehydratase 1





● Molecule 1: tRNA threonylcarbamoyladenosine dehydratase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	259.44Å 259.44Å 236.11Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 4.00 30.00 – 4.00	Depositor EDS
% Data completeness (in resolution range)	98.5 (30.00-4.00) 98.5 (30.00-4.00)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 4.00Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.255 , 0.299 0.249 , 0.290	Depositor DCC
R_{free} test set	1979 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	116.4	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 108.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	11707	wwPDB-VP
Average B, all atoms (Å ²)	122.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.29% 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, CL, NA, 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	1.00	0/2954	1.44	0/3975
1	B	1.00	0/2930	1.47	0/3943
1	C	1.01	0/2941	1.46	2/3958 (0.1%)
1	D	1.00	0/2963	1.48	3/3987 (0.1%)
All	All	1.00	0/11788	1.47	5/15863 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	65	GLY	CA-C-O	-5.53	117.57	121.88
1	D	282	LEU	CA-C-N	5.23	125.78	119.98
1	D	282	LEU	C-N-CA	5.23	125.78	119.98
1	C	282	LEU	CA-C-N	5.03	125.67	120.03
1	C	282	LEU	C-N-CA	5.03	125.67	120.03

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	2905	0	2932	49	0
1	B	2882	0	2916	56	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2892	0	2918	52	0
1	D	2914	0	2945	48	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	C	2	0	0	0	0
3	D	1	0	0	0	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	B	6	0	8	0	0
6	C	1	0	0	0	0
6	D	2	0	0	0	0
All	All	11707	0	11767	195	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 8.

All (195) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:LEU:HB3	1:A:280:PRO:CD	1.99	0.92
1:D:279:LEU:HB3	1:D:280:PRO:HD3	1.63	0.81
1:C:189:ALA:HB1	1:C:196:VAL:HG11	1.66	0.76
1:A:95:ARG:NH2	1:B:120:ALA:O	2.20	0.75
1:C:279:LEU:HB3	1:C:280:PRO:CD	2.16	0.75
1:B:216:ILE:O	1:B:219:THR:HG22	1.86	0.75
1:A:279:LEU:HB3	1:A:280:PRO:HD3	1.70	0.73
1:A:213:ILE:HG23	1:A:244:VAL:HG12	1.70	0.73
1:A:189:ALA:HB1	1:A:196:VAL:HG21	1.76	0.67
1:A:87:SER:OG	1:A:118:CYS:SG	2.53	0.66
1:B:279:LEU:HB3	1:B:280:PRO:CD	2.24	0.66
1:C:279:LEU:HB3	1:C:280:PRO:HD3	1.76	0.66
1:D:279:LEU:CB	1:D:280:PRO:CD	2.75	0.65
1:B:89:VAL:O	1:B:93:LEU:HD12	1.99	0.63
1:B:341:LEU:C	1:B:341:LEU:HD22	2.24	0.63
1:C:88:TRP:CD1	1:C:287:GLY:HA2	2.34	0.63
1:A:75:GLN:CD	1:A:170:THR:HG21	2.24	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:LEU:HB3	1:A:280:PRO:HD2	1.79	0.61
1:D:94:ILE:HG13	1:D:137:LEU:HD23	1.82	0.61
1:D:279:LEU:HB3	1:D:280:PRO:CD	2.29	0.61
1:C:205:LYS:HD3	1:C:246:SER:HB3	1.82	0.60
1:B:279:LEU:CB	1:B:280:PRO:CD	2.81	0.59
1:A:251:ASP:N	1:A:252:PRO:CD	2.65	0.59
1:A:88:TRP:CZ3	1:A:118:CYS:HB3	2.38	0.58
1:B:77:ILE:HD13	1:B:93:LEU:HD22	1.84	0.58
1:B:88:TRP:CD1	1:B:287:GLY:HA2	2.38	0.58
1:C:285:MET:HB2	1:C:286:PRO:HD3	1.87	0.57
1:D:370:LEU:HD22	1:D:384:VAL:CG1	2.36	0.56
1:A:199:SER:HA	1:A:244:VAL:HG22	1.87	0.55
1:D:279:LEU:CB	1:D:280:PRO:HD3	2.34	0.55
1:A:279:LEU:HD12	1:A:280:PRO:HD3	1.87	0.55
1:D:205:LYS:HE3	1:D:246:SER:O	2.06	0.55
1:D:368:LEU:HD13	1:D:386:LEU:HD21	1.88	0.55
1:A:251:ASP:N	1:A:252:PRO:HD2	2.22	0.54
1:B:229:ARG:NE	1:B:353:GLU:OE1	2.39	0.54
1:B:200:MET:HA	1:B:200:MET:HE2	1.90	0.54
1:C:387:MET:HE2	1:C:391:GLU:HB3	1.90	0.54
1:B:53:PHE:CE2	1:B:57:LEU:HD22	2.43	0.53
1:A:80:VAL:HG12	1:A:176:LEU:HD21	1.90	0.53
1:A:396:GLU:HA	1:A:400:LEU:HD21	1.90	0.53
1:C:279:LEU:CB	1:C:280:PRO:HD3	2.39	0.53
1:C:315:LEU:HD22	1:C:315:LEU:C	2.33	0.53
1:D:109:ILE:HD11	1:D:124:ASP:O	2.08	0.53
1:B:80:VAL:HG12	1:B:176:LEU:HD21	1.91	0.53
1:B:299:THR:OG1	1:B:306:MET:HE3	2.09	0.53
1:D:82:ALA:HB2	1:D:103:ILE:CG2	2.39	0.52
1:D:239:THR:HG23	1:D:311:VAL:HG11	1.92	0.52
1:A:88:TRP:CH2	1:A:118:CYS:HB3	2.45	0.52
1:C:91:THR:HA	1:C:137:LEU:HD11	1.91	0.52
1:C:197:ILE:HD12	1:C:296:TRP:CE3	2.45	0.52
1:C:279:LEU:CB	1:C:280:PRO:CD	2.86	0.51
1:C:392:GLN:HG3	1:C:393:GLU:N	2.25	0.51
1:D:95:ARG:HH11	1:D:140:ILE:HD13	1.75	0.51
1:A:118:CYS:SG	1:A:119:CYS:N	2.84	0.51
1:B:370:LEU:HD22	1:B:384:VAL:HG22	1.92	0.51
1:A:172:ILE:HB	1:A:196:VAL:HG22	1.91	0.51
1:A:279:LEU:CB	1:A:280:PRO:HD3	2.38	0.51
1:C:285:MET:HA	1:C:285:MET:HE2	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:304:TYR:CD2	1:D:305:PRO:HD2	2.45	0.51
1:B:279:LEU:CB	1:B:280:PRO:HD2	2.41	0.51
1:C:313:ASN:O	1:C:318:TYR:CZ	2.65	0.50
1:B:279:LEU:HB3	1:B:280:PRO:HD3	1.93	0.50
1:D:370:LEU:HD22	1:D:384:VAL:HG12	1.94	0.50
1:C:251:ASP:N	1:C:252:PRO:CD	2.75	0.50
1:B:304:TYR:CG	1:B:305:PRO:HD2	2.46	0.50
1:C:251:ASP:N	1:C:252:PRO:HD3	2.27	0.50
1:A:102:MET:HE1	1:A:162:ILE:HA	1.94	0.49
1:B:279:LEU:HB3	1:B:280:PRO:HD2	1.94	0.49
1:C:229:ARG:NE	1:C:353:GLU:OE1	2.45	0.49
1:A:200:MET:HE3	1:A:243:VAL:HG21	1.94	0.49
1:B:137:LEU:HA	1:B:140:ILE:HG22	1.93	0.49
1:A:321:ILE:O	1:A:324:THR:OG1	2.25	0.49
1:D:107:GLU:O	1:D:129:LYS:HG3	2.12	0.49
1:D:130:VAL:HG22	1:D:148:ALA:HB1	1.95	0.48
1:A:279:LEU:CB	1:A:280:PRO:CD	2.80	0.48
1:B:211:VAL:HG13	1:B:211:VAL:O	2.13	0.48
1:A:95:ARG:NH1	1:B:117:HIS:O	2.46	0.48
1:B:396:GLU:O	1:B:400:LEU:HB2	2.14	0.48
1:A:82:ALA:HB2	1:A:103:ILE:CG2	2.44	0.48
1:D:216:ILE:HG22	1:D:243:VAL:HG11	1.95	0.48
1:B:237:ILE:HG23	1:B:237:ILE:O	2.14	0.48
1:C:338:ARG:HA	1:C:341:LEU:HD23	1.94	0.48
1:C:350:ILE:O	1:C:354:MET:HB2	2.14	0.48
1:D:173:VAL:HG12	1:D:175:CYS:SG	2.54	0.47
1:B:187:GLU:OE2	1:B:235:ARG:NH1	2.47	0.47
1:C:355:PHE:CE1	1:C:385:VAL:HG23	2.49	0.47
1:C:370:LEU:HD11	1:C:384:VAL:HG22	1.94	0.47
1:B:64:LEU:HD12	1:B:69:MET:CE	2.44	0.47
1:B:200:MET:HE1	1:B:228:VAL:HG11	1.95	0.47
1:C:174:ASP:OD1	1:C:198:SER:HA	2.14	0.47
1:A:75:GLN:NE2	1:A:170:THR:HG21	2.29	0.47
1:C:57:LEU:O	1:C:60:ASN:N	2.47	0.47
1:D:157:ASN:O	1:D:158:SER:C	2.58	0.47
1:C:205:LYS:HE2	1:C:224:ILE:HD13	1.95	0.47
1:A:84:GLU:HB2	1:A:116:THR:HG21	1.97	0.46
1:C:117:HIS:O	1:D:95:ARG:NH2	2.48	0.46
1:C:179:LEU:HD22	1:C:179:LEU:C	2.40	0.46
1:D:92:MET:HG3	1:D:291:LEU:CD2	2.46	0.46
1:B:64:LEU:HD12	1:B:69:MET:HE2	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:297:ILE:HG22	1:D:298:LEU:N	2.29	0.46
1:B:92:MET:HG3	1:B:291:LEU:HD23	1.96	0.46
1:D:395:HIS:CE1	1:D:399:ILE:HG21	2.51	0.46
1:A:114:LEU:HD12	1:B:140:ILE:CD1	2.46	0.46
1:C:140:ILE:HD13	1:D:121:VAL:HA	1.98	0.45
1:A:321:ILE:CG2	1:A:370:LEU:HD23	2.46	0.45
1:B:60:ASN:ND2	1:B:96:SER:OG	2.50	0.45
1:A:202:VAL:HG22	1:A:202:VAL:O	2.15	0.45
1:B:190:HIS:CG	1:B:237:ILE:HD11	2.51	0.45
1:D:80:VAL:HG12	1:D:176:LEU:HD21	1.98	0.45
1:B:232:LEU:HG	1:B:237:ILE:HG23	1.98	0.45
1:C:179:LEU:HD22	1:C:180:GLU:N	2.31	0.45
1:D:88:TRP:CD2	1:D:118:CYS:HB3	2.52	0.45
1:A:203:ALA:O	1:A:204:THR:OG1	2.32	0.45
1:C:349:TYR:O	1:C:353:GLU:HB2	2.17	0.45
1:A:94:ILE:HD11	1:A:101:ILE:HG12	1.98	0.45
1:D:83:GLY:O	1:D:84:GLU:C	2.59	0.45
1:A:390:GLU:O	1:A:394:ILE:HG12	2.17	0.45
1:B:157:ASN:O	1:B:158:SER:C	2.59	0.45
1:D:202:VAL:HG12	1:D:202:VAL:O	2.16	0.45
1:A:75:GLN:NE2	1:A:301:VAL:HG13	2.32	0.44
1:A:103:ILE:HD11	1:A:146:ILE:CG2	2.48	0.44
1:B:190:HIS:CG	1:B:237:ILE:CD1	3.00	0.44
1:C:206:SER:N	1:C:248:GLU:OE1	2.49	0.44
1:B:201:GLY:HA3	1:B:224:ILE:HG21	1.98	0.44
1:C:139:LYS:O	1:D:122:LEU:HG	2.16	0.44
1:C:200:MET:HE3	1:C:243:VAL:HG21	2.00	0.44
1:A:212:SER:O	1:A:244:VAL:HA	2.17	0.44
1:D:92:MET:HG3	1:D:291:LEU:HD23	1.99	0.44
1:C:277:ARG:NH2	1:C:427:TYR:OH	2.50	0.44
1:C:318:TYR:OH	1:C:352:GLU:HG3	2.17	0.44
1:C:172:ILE:HB	1:C:196:VAL:HG12	1.99	0.43
1:C:213:ILE:HG12	1:C:244:VAL:HG12	1.99	0.43
1:D:325:PHE:CE1	1:D:342:LEU:HD12	2.53	0.43
1:B:109:ILE:HD13	1:B:129:LYS:HG2	2.00	0.43
1:D:200:MET:CE	1:D:243:VAL:HG11	2.47	0.43
1:A:174:ASP:HB2	1:A:185:LEU:HD23	2.00	0.43
1:C:183:VAL:HG21	1:C:231:LYS:HB3	1.99	0.43
1:C:118:CYS:SG	1:C:119:CYS:N	2.91	0.43
1:B:106:PRO:HA	1:B:150:ALA:O	2.18	0.43
1:C:285:MET:O	1:C:286:PRO:C	2.62	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:318:TYR:HA	1:D:321:ILE:HG22	2.01	0.43
1:A:295:THR:HG21	1:B:208:PRO:HG3	2.00	0.43
1:B:177:ASP:N	1:B:177:ASP:OD1	2.51	0.43
1:C:57:LEU:O	1:C:58:ALA:C	2.62	0.43
1:A:285:MET:HB2	1:A:286:PRO:HD3	2.00	0.43
1:A:179:LEU:HD21	1:A:231:LYS:HD3	2.01	0.42
1:D:182:LYS:O	1:D:185:LEU:HB3	2.19	0.42
1:D:217:SER:HB3	1:D:311:VAL:CG1	2.48	0.42
1:B:285:MET:O	1:B:286:PRO:C	2.62	0.42
1:C:363:GLY:O	1:C:364:TYR:C	2.62	0.42
1:A:355:PHE:CE1	1:A:385:VAL:HG23	2.54	0.42
1:B:197:ILE:HD13	1:B:198:SER:H	1.83	0.42
1:D:122:LEU:C	1:D:122:LEU:HD12	2.44	0.42
1:D:229:ARG:NE	1:D:353:GLU:OE1	2.50	0.42
1:C:201:GLY:HA3	1:C:224:ILE:HG21	2.02	0.42
1:C:282:LEU:HB2	1:D:63:PHE:CE1	2.53	0.42
1:D:198:SER:HB3	1:D:243:VAL:HG12	2.02	0.42
1:D:219:THR:OG1	1:D:229:ARG:NH1	2.52	0.42
1:D:304:TYR:CG	1:D:305:PRO:HD2	2.55	0.42
1:C:141:ALA:HB1	1:C:143:TRP:NE1	2.35	0.42
1:A:88:TRP:CE3	1:A:118:CYS:HB3	2.55	0.42
1:B:342:LEU:HD23	1:B:342:LEU:HA	1.91	0.42
1:D:103:ILE:HB	1:D:130:VAL:HG23	2.00	0.42
1:A:103:ILE:HG22	1:A:130:VAL:HG12	2.01	0.42
1:B:153:TRP:CH2	1:B:185:LEU:HA	2.55	0.42
1:C:90:CYS:SG	1:C:133:LEU:HD23	2.60	0.41
1:D:350:ILE:HG12	1:D:354:MET:HE2	2.02	0.41
1:B:304:TYR:CD2	1:B:305:PRO:HD2	2.56	0.41
1:A:176:LEU:HB2	1:A:182:LYS:HG2	2.01	0.41
1:B:147:LYS:HD3	1:B:147:LYS:HA	1.94	0.41
1:C:86:GLY:O	1:C:87:SER:C	2.63	0.41
1:C:244:VAL:HG23	1:C:289:PHE:CD1	2.56	0.41
1:C:119:CYS:HB3	1:C:136:HIS:CG	2.56	0.41
1:D:131:GLN:O	1:D:132:CYS:C	2.63	0.41
1:B:202:VAL:CG1	1:B:285:MET:HB3	2.50	0.41
1:B:224:ILE:N	1:B:224:ILE:HD12	2.36	0.41
1:A:121:VAL:O	1:A:122:LEU:C	2.63	0.41
1:A:291:LEU:HD22	1:B:291:LEU:HD12	2.01	0.41
1:A:388:THR:O	1:A:389:LYS:C	2.63	0.41
1:B:88:TRP:CG	1:B:287:GLY:HA2	2.55	0.41
1:B:186:LEU:HD21	1:B:198:SER:HB2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:ILE:HG21	1:B:370:LEU:HD21	2.03	0.41
1:D:84:GLU:HG2	1:D:85:VAL:H	1.85	0.41
1:D:285:MET:HB2	1:D:286:PRO:HD3	2.03	0.41
1:D:350:ILE:O	1:D:354:MET:HB2	2.21	0.41
1:A:242:SER:HB3	1:A:309:ASN:ND2	2.37	0.40
1:C:355:PHE:CZ	1:C:385:VAL:HG23	2.56	0.40
1:A:88:TRP:HZ3	1:B:88:TRP:HZ3	1.69	0.40
1:B:370:LEU:HD22	1:B:384:VAL:CG2	2.51	0.40
1:B:130:VAL:HB	1:B:148:ALA:HB1	2.02	0.40
1:C:88:TRP:CH2	1:C:118:CYS:HA	2.57	0.40
1:B:88:TRP:CE3	1:B:118:CYS:HB2	2.57	0.40
1:B:202:VAL:O	1:B:202:VAL:HG12	2.21	0.40
1:C:224:ILE:HD12	1:C:224:ILE:H	1.86	0.40
1:D:365:SER:HA	1:D:368:LEU:HD11	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	359/382 (94%)	305 (85%)	51 (14%)	3 (1%)	16	52
1	B	355/382 (93%)	285 (80%)	61 (17%)	9 (2%)	4	29
1	C	358/382 (94%)	302 (84%)	49 (14%)	7 (2%)	6	33
1	D	361/382 (94%)	302 (84%)	48 (13%)	11 (3%)	3	26
All	All	1433/1528 (94%)	1194 (83%)	209 (15%)	30 (2%)	5	32

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	279	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	279	LEU
1	C	279	LEU
1	D	279	LEU
1	B	98	CYS
1	C	200	MET
1	D	178	ASN
1	C	364	TYR
1	D	106	PRO
1	D	158	SER
1	B	89	VAL
1	B	109	ILE
1	B	151	LYS
1	D	248	GLU
1	A	245	PHE
1	A	255	ASP
1	C	58	ALA
1	C	87	SER
1	C	106	PRO
1	D	97	GLY
1	D	151	LYS
1	D	193	LYS
1	D	195	ASP
1	D	84	GLU
1	D	211	VAL
1	B	283	GLY
1	B	237	ILE
1	B	303	GLY
1	C	351	VAL
1	B	106	PRO

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	325/341 (95%)	315 (97%)	10 (3%)	35 56
1	B	322/341 (94%)	315 (98%)	7 (2%)	45 65

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	324/341 (95%)	315 (97%)	9 (3%)	38	60
1	D	326/341 (96%)	315 (97%)	11 (3%)	32	55
All	All	1297/1364 (95%)	1260 (97%)	37 (3%)	37	58

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	GLU
1	A	103	ILE
1	A	170	THR
1	A	213	ILE
1	A	279	LEU
1	A	333	ASN
1	A	385	VAL
1	A	386	LEU
1	A	392	GLN
1	A	400	LEU
1	B	94	ILE
1	B	154	THR
1	B	171	PHE
1	B	197	ILE
1	B	315	LEU
1	B	341	LEU
1	B	346	GLU
1	C	78	VAL
1	C	85	VAL
1	C	171	PHE
1	C	179	LEU
1	C	192	ASN
1	C	243	VAL
1	C	244	VAL
1	C	250	LEU
1	C	315	LEU
1	D	57	LEU
1	D	91	THR
1	D	123	SER
1	D	146	ILE
1	D	170	THR
1	D	271	VAL
1	D	276	LEU
1	D	293	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	297	ILE
1	D	379	ILE
1	D	399	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	ASN
1	A	117	HIS
1	B	51	HIS
1	B	117	HIS
1	D	56	GLN
1	D	192	ASN
1	D	313	ASN

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 18 ligands modelled in this entry, 13 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	AMP	B	501	-	25,25,25	0.36	0	37,38,38	0.45	0
2	AMP	C	501	-	25,25,25	0.36	0	37,38,38	0.51	0
5	GOL	B	502	-	5,5,5	0.10	0	5,5,5	0.25	0
2	AMP	A	501	-	25,25,25	0.35	0	37,38,38	0.42	0
2	AMP	D	501	-	25,25,25	0.34	0	37,38,38	0.46	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
2	AMP	B	501	-	-	1/10/26/26	0/3/3/3
2	AMP	C	501	-	-	6/10/26/26	0/3/3/3
5	GOL	B	502	-	-	2/4/4/4	-
2	AMP	A	501	-	-	5/10/26/26	0/3/3/3
2	AMP	D	501	-	-	7/10/26/26	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	501	AMP	C5'-O5'-P-O2P
2	C	501	AMP	C5'-O5'-P-O3P
2	C	501	AMP	C2'-C1'-N9-C8
2	D	501	AMP	C5'-O5'-P-O2P
5	B	502	GOL	O1-C1-C2-O2
5	B	502	GOL	O1-C1-C2-C3
2	A	501	AMP	O4'-C4'-C5'-O5'
2	C	501	AMP	C2'-C1'-N9-C4
2	A	501	AMP	C3'-C4'-C5'-O5'
2	D	501	AMP	C3'-C4'-C5'-O5'
2	D	501	AMP	O4'-C4'-C5'-O5'
2	C	501	AMP	C5'-O5'-P-O1P
2	D	501	AMP	C5'-O5'-P-O1P
2	D	501	AMP	C5'-O5'-P-O3P
2	A	501	AMP	C2'-C1'-N9-C8
2	D	501	AMP	C2'-C1'-N9-C8

Continued on next page...

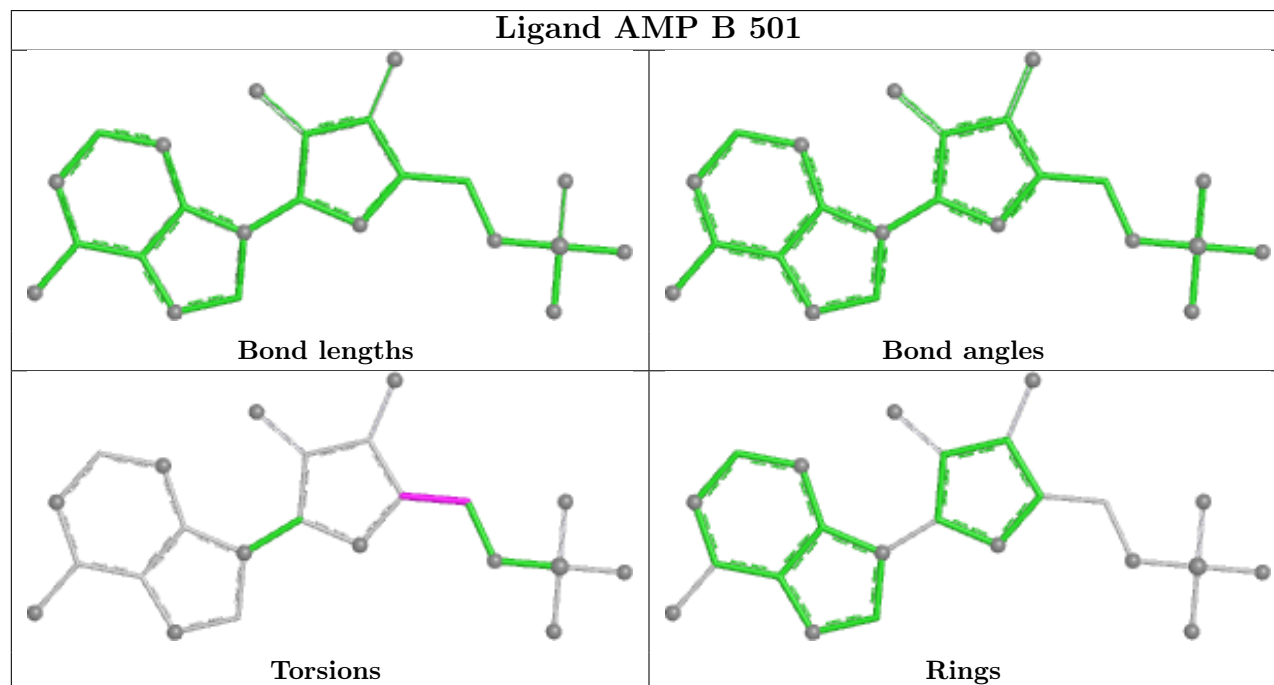
Continued from previous page...

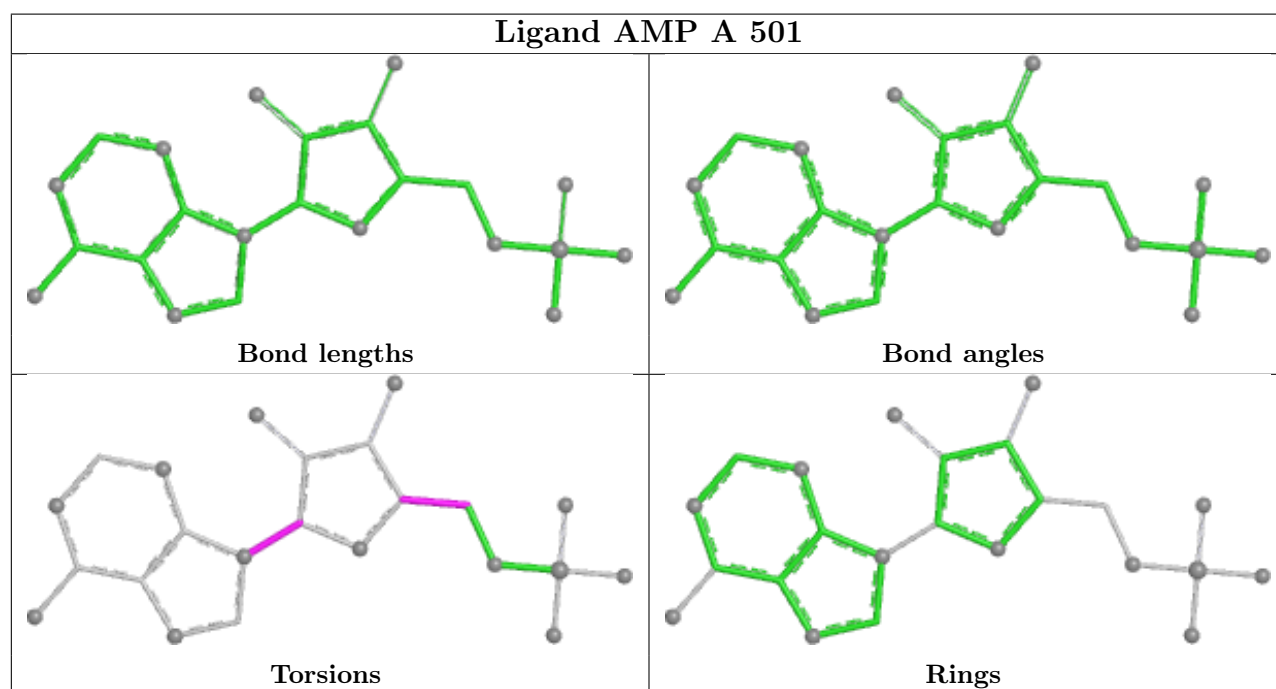
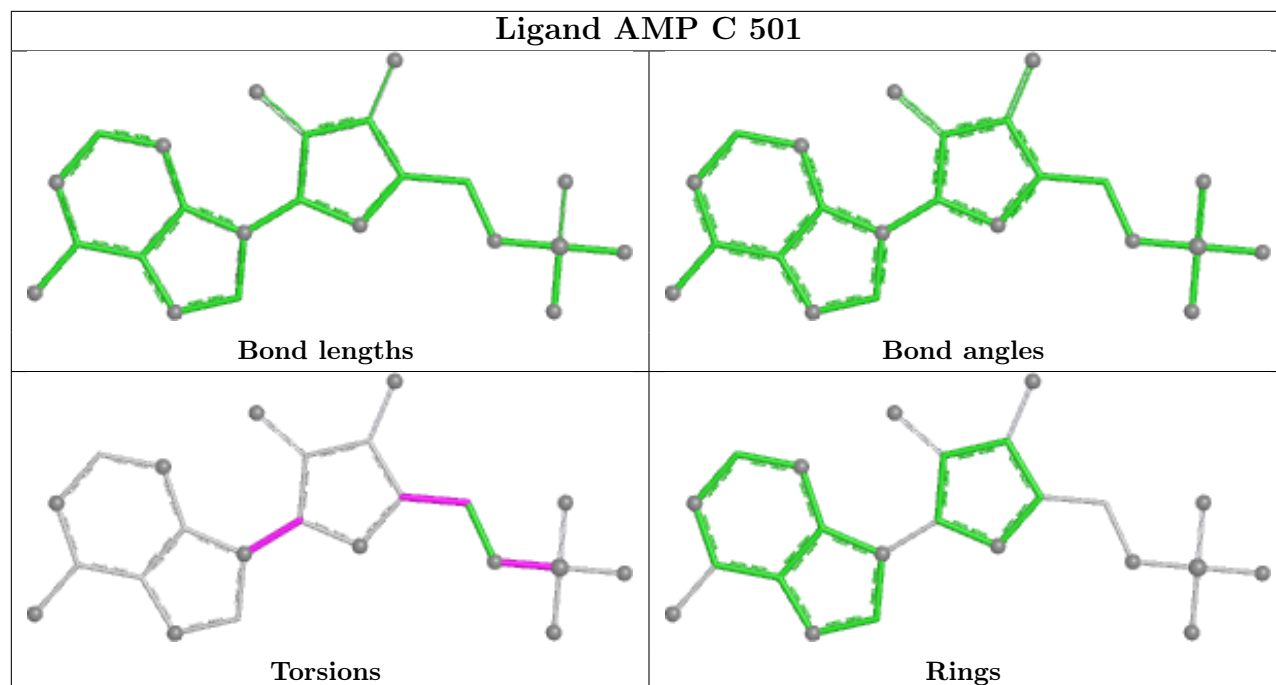
Mol	Chain	Res	Type	Atoms
2	C	501	AMP	O4'-C4'-C5'-O5'
2	A	501	AMP	O4'-C1'-N9-C8
2	D	501	AMP	O4'-C1'-N9-C8
2	A	501	AMP	C2'-C1'-N9-C4
2	B	501	AMP	O4'-C4'-C5'-O5'

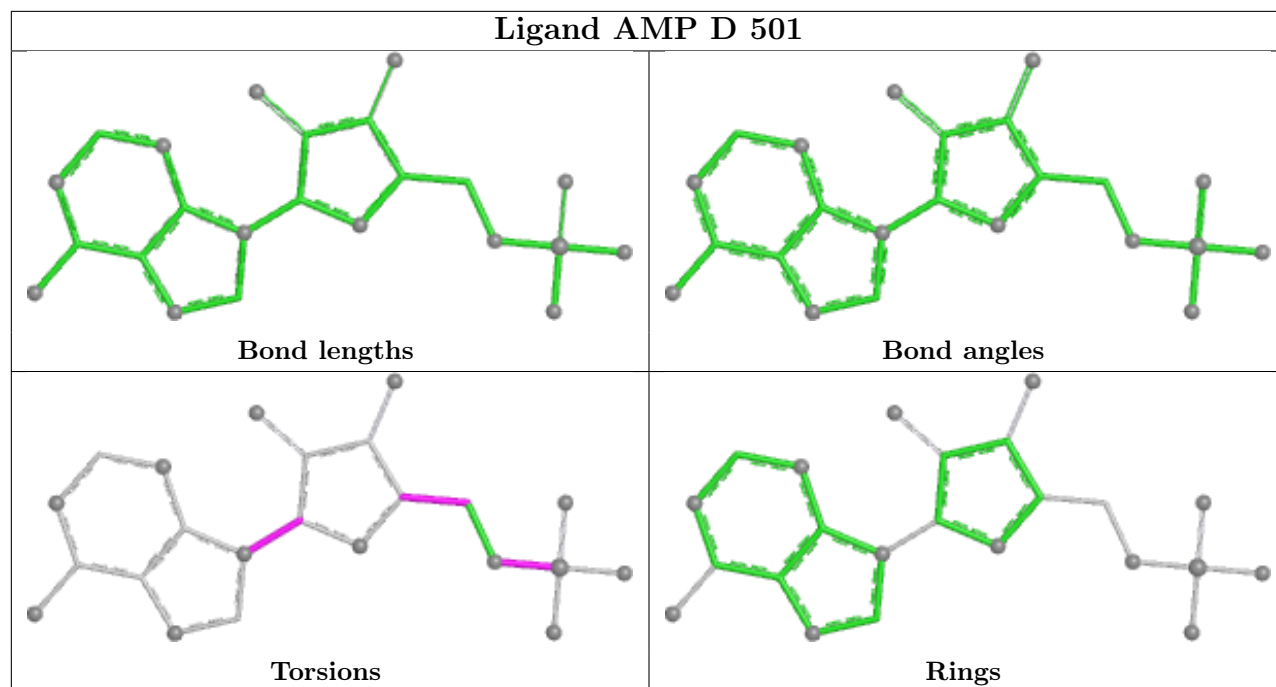
There are no ring outliers.

No monomer is involved in short contacts.

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	363/382 (95%)	0.22	6 (1%) 69 51	73, 122, 180, 245	0
1	B	361/382 (94%)	0.11	7 (1%) 66 49	67, 110, 166, 235	0
1	C	362/382 (94%)	0.17	12 (3%) 49 36	71, 118, 183, 216	0
1	D	365/382 (95%)	0.20	12 (3%) 49 36	64, 116, 187, 267	0
All	All	1451/1528 (94%)	0.18	37 (2%) 58 43	64, 116, 182, 267	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	271	VAL	3.6
1	C	164	ALA	3.6
1	B	254	ARG	3.4
1	C	336	LYS	3.4
1	D	252	PRO	3.1
1	A	51	HIS	3.0
1	D	338	ARG	2.8
1	B	270	ALA	2.8
1	B	252	PRO	2.6
1	D	52	LEU	2.6
1	D	337	GLU	2.6
1	C	51	HIS	2.5
1	A	84	GLU	2.5
1	C	252	PRO	2.5
1	C	201	GLY	2.5
1	C	275	ALA	2.5
1	D	151	LYS	2.5
1	C	49	SER	2.5
1	B	310	GLU	2.5
1	D	48	GLY	2.5
1	D	51	HIS	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	279	LEU	2.4
1	C	307	LYS	2.4
1	C	253	ARG	2.4
1	B	307	LYS	2.4
1	D	221	PHE	2.3
1	D	251	ASP	2.3
1	A	253	ARG	2.3
1	A	275	ALA	2.2
1	A	276	LEU	2.2
1	D	310	GLU	2.2
1	A	254	ARG	2.2
1	B	271	VAL	2.1
1	C	340	SER	2.1
1	B	49	SER	2.1
1	C	84	GLU	2.0
1	D	253	ARG	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
5	GOL	B	502	6/6	0.78	0.37	127,133,134,135	0
2	AMP	B	501	23/23	0.83	0.23	174,201,228,233	0
2	AMP	D	501	23/23	0.86	0.20	159,181,196,198	0
4	NA	A	504	1/1	0.86	0.41	80,80,80,80	0
2	AMP	A	501	23/23	0.86	0.17	135,154,163,164	0
2	AMP	C	501	23/23	0.88	0.18	161,174,181,189	0
4	NA	B	503	1/1	0.89	0.17	46,46,46,46	0

Continued on next page...

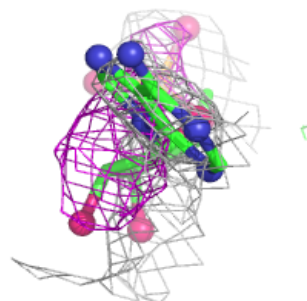
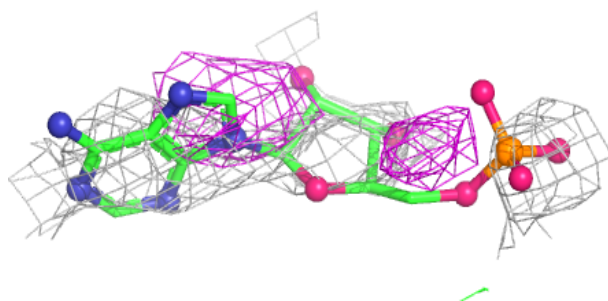
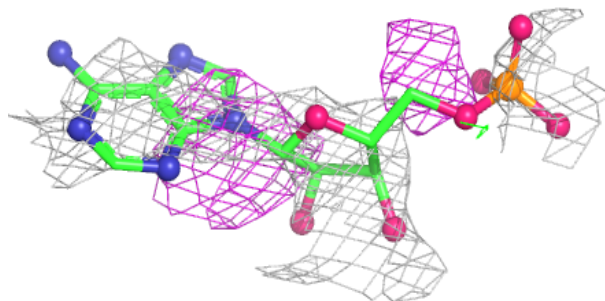
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	CL	C	503	1/1	0.91	0.07	106,106,106,106	0
3	CL	A	502	1/1	0.91	0.09	84,84,84,84	0
4	NA	D	503	1/1	0.92	0.41	70,70,70,70	0
4	NA	A	506	1/1	0.92	0.24	70,70,70,70	0
4	NA	B	504	1/1	0.93	0.38	68,68,68,68	0
3	CL	D	502	1/1	0.93	0.10	97,97,97,97	0
3	CL	A	503	1/1	0.93	0.07	73,73,73,73	0
3	CL	C	502	1/1	0.95	0.07	55,55,55,55	0
4	NA	C	504	1/1	0.95	0.13	59,59,59,59	0
4	NA	B	505	1/1	0.96	0.11	52,52,52,52	0
4	NA	A	505	1/1	0.98	0.07	70,70,70,70	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.

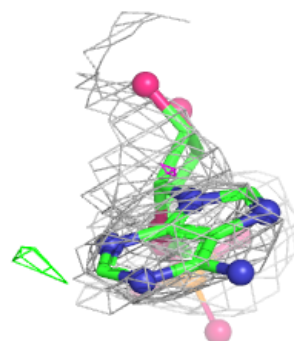
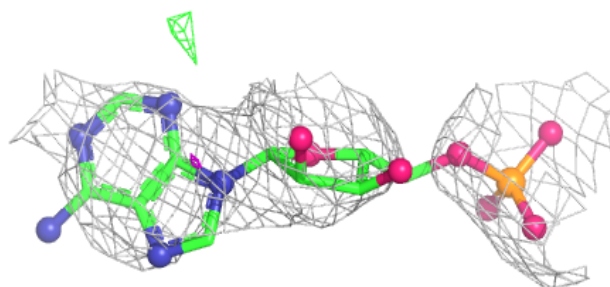
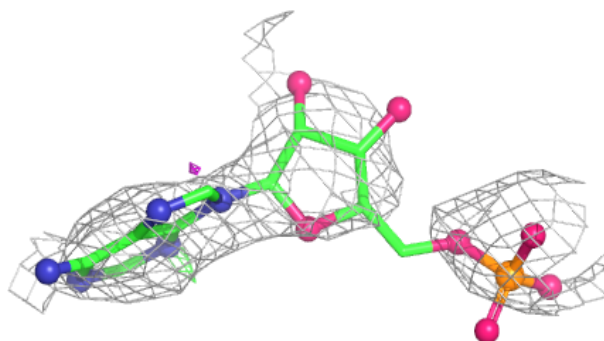
Electron density around AMP B 501:

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

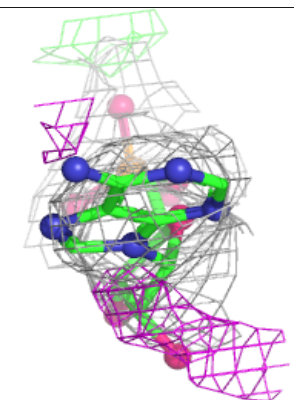
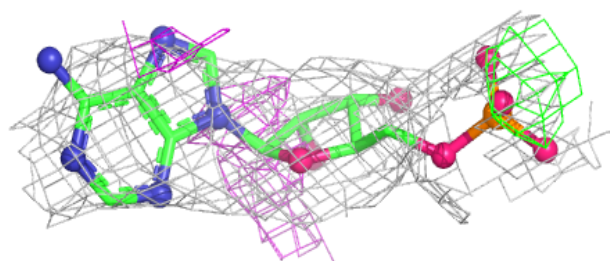
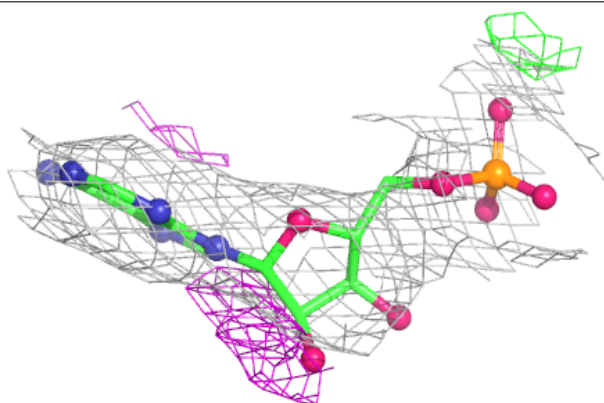


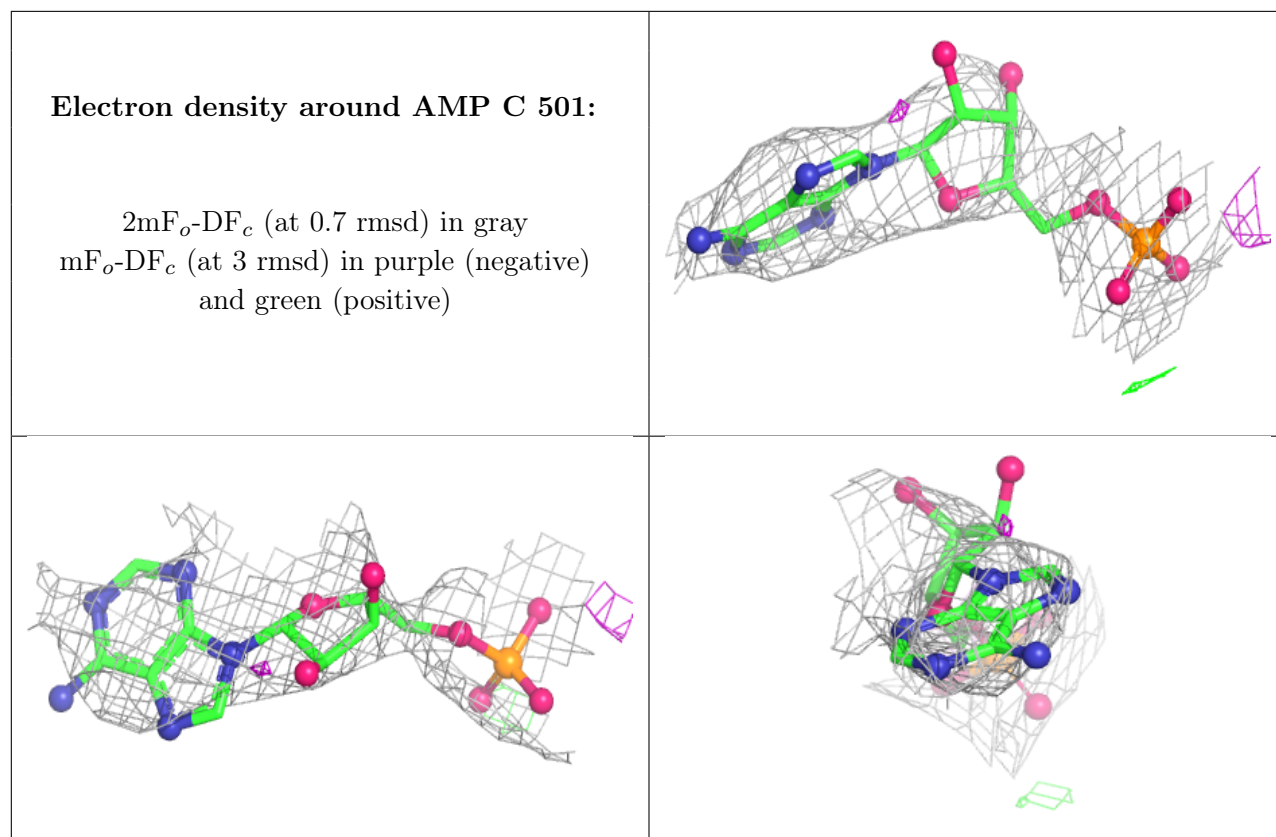
Electron density around AMP D 501:

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

**Electron density around AMP A 501:**

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





6.5 Other polymers ⓘ

There are no such residues in this entry.