



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:50 PM UTC

PDB ID : 4MX2 / pdb\_00004mx2  
Title : Crystal Structure of adenylosuccinate lyase from Leishmania donovani  
Authors : Wernimont, A.K.; Loppnau, P.; Dong, A.; Krojer, T.; Bradley, A.; Bushell, S.; von Delft, F.; Robinson, D.; Gilbert, I.; Bountra, C.; Arrowsmith, C.H.; Edwards, A.M.; Hui, R.; Mottaghi, K.; Structural Genomics Consortium (SGC)  
Deposited on : 2013-09-25  
Resolution : 1.90 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](mailto:validation@mail.wwpdb.org)

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<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>.

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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

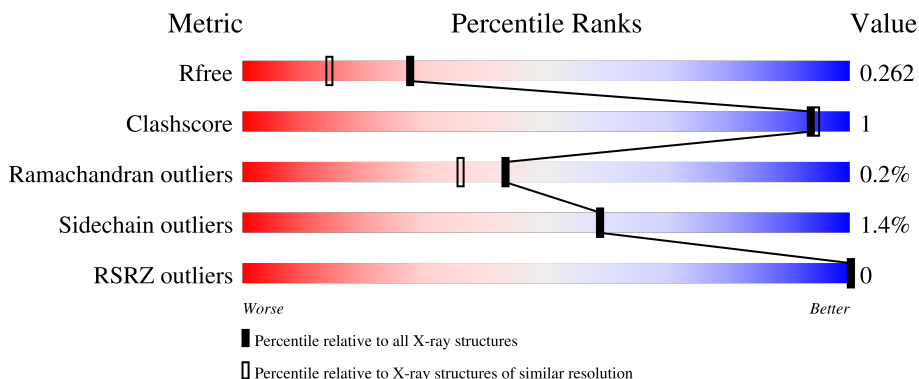
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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  $\geq 3$ , 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	480	 84% 5% 12%
1	B	480	 85% 6% 9%
1	C	480	 83% 6% 11%
1	D	480	 86% 5% 9%

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Mol	Chain	Length	Quality of chain		
1	E	480		84%	5% 11%
1	F	480		84%	6% 10%
1	G	480		84%	5% 11%
1	H	480		85%	7% 9%

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	GOL	E	501	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 29460 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.

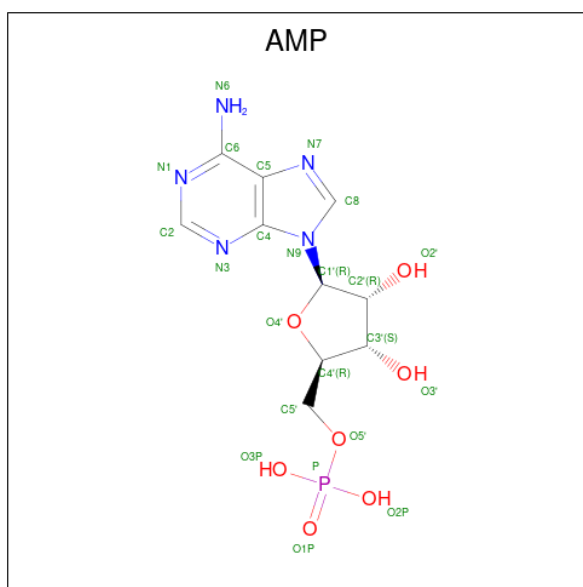
- Molecule 1 is a protein called Adenylosuccinate lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	424	3333	2145	557	617	14	0	8	0
1	B	439	3522	2261	595	652	14	0	15	0
1	C	426	3367	2167	568	618	14	0	8	0
1	D	439	3487	2239	588	647	13	0	9	0
1	E	425	3347	2154	560	619	14	0	9	0
1	F	431	3450	2222	577	637	14	0	12	0
1	G	427	3375	2174	567	620	14	0	9	0
1	H	438	3490	2247	584	644	15	0	14	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP A7LBL3
B	0	GLY	-	expression tag	UNP A7LBL3
C	0	GLY	-	expression tag	UNP A7LBL3
D	0	GLY	-	expression tag	UNP A7LBL3
E	0	GLY	-	expression tag	UNP A7LBL3
F	0	GLY	-	expression tag	UNP A7LBL3
G	0	GLY	-	expression tag	UNP A7LBL3
H	0	GLY	-	expression tag	UNP A7LBL3

- Molecule 2 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>7</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
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		
2	E	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	F	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	G	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	H	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total C O 6 3 3	0	0


- Molecule 5 is water.

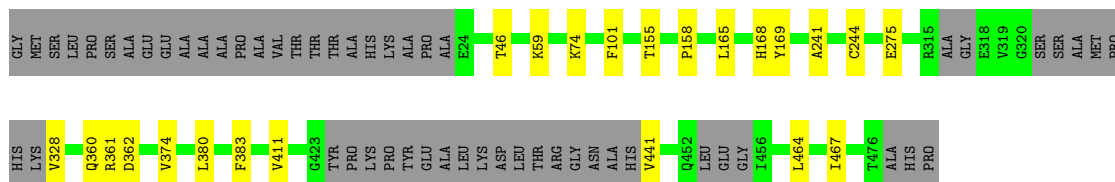
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	232	Total O 233 233	0	1
5	B	244	Total O 244 244	0	0
5	C	212	Total O 212 212	0	0
5	D	264	Total O 265 265	0	1
5	E	215	Total O 215 215	0	0
5	F	239	Total O 239 239	0	0
5	G	217	Total O 217 217	0	0
5	H	259	Total O 259 259	0	0

### 3 Residue-property plots


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

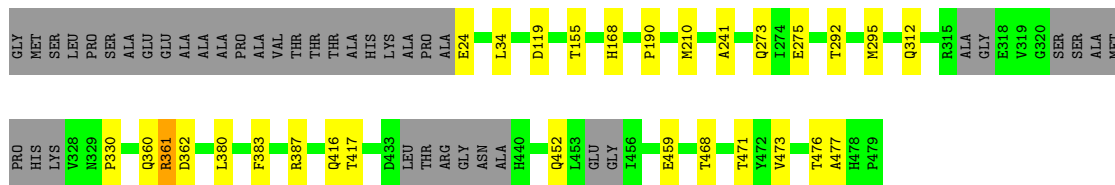
- Molecule 1: Adenylosuccinate lyase

Chain A:  84% 5% 12%




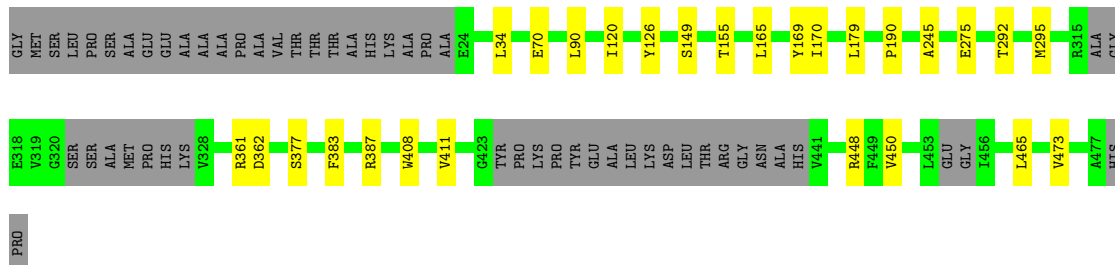
- Molecule 1: Adenylosuccinate lyase

Chain B:  85% 6% 9%




- Molecule 1: Adenylosuccinate lyase

Chain C:  83% 6% 11%



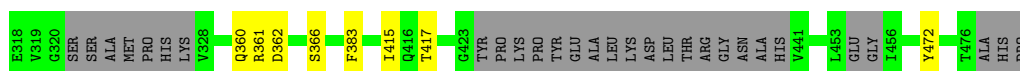
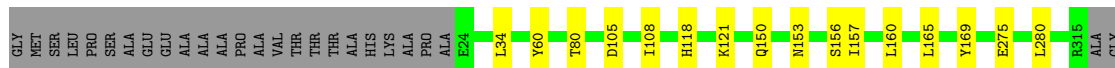
- Molecule 1: Adenylosuccinate lyase

Chain D:  86% 5% 9%



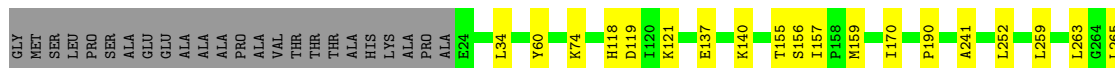
- Molecule 1: Adenylosuccinate lyase

Chain E: 84% 5% 11%



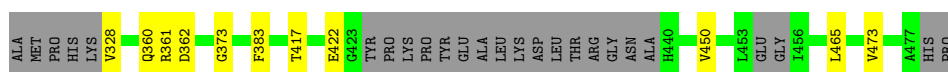
- Molecule 1: Adenylosuccinate lyase

Chain F: 84% 6% 10%



- Molecule 1: Adenylosuccinate lyase

Chain G: 84% 5% 11%



- Molecule 1: Adenylosuccinate lyase

Chain H: 85% 7% 9%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	124.02Å 194.70Å 147.51Å 90.00° 91.31° 90.00°	Depositor
Resolution (Å)	34.98 – 1.90 34.98 – 1.90	Depositor EDS
% Data completeness (in resolution range)	95.7 (34.98-1.90) 89.4 (34.98-1.90)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.94 (at 1.89Å)	Xtrriage
Refinement program	BUSTER-TNT BUSTER 2.10.0, BUSTER 2.10.0	Depositor
R, $R_{free}$	0.218 , 0.253 0.226 , 0.262	Depositor DCC
$R_{free}$ test set	13161 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.5	Xtrriage
Anisotropy	0.309	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 32.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.199 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	29460	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.58 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.4942e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, GOL, SO4

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	0.87	2/3424 (0.1%)	1.23	4/4649 (0.1%)
1	B	0.88	0/3626	1.21	8/4921 (0.2%)
1	C	0.87	1/3460 (0.0%)	1.22	5/4692 (0.1%)
1	D	0.86	2/3585 (0.1%)	1.24	6/4870 (0.1%)
1	E	0.83	0/3442	1.24	7/4673 (0.1%)
1	F	0.87	2/3556 (0.1%)	1.22	7/4827 (0.1%)
1	G	0.86	2/3471 (0.1%)	1.23	8/4710 (0.2%)
1	H	0.85	1/3607 (0.0%)	1.22	7/4900 (0.1%)
All	All	0.86	10/28171 (0.0%)	1.23	52/38242 (0.1%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	342	MET	SD-CE	-10.19	1.54	1.79
1	H	97	THR	CA-C	7.28	1.55	1.52
1	G	170	ILE	CA-C	6.88	1.59	1.52
1	D	374	VAL	CA-CB	5.80	1.57	1.54
1	D	342	MET	SD-CE	-5.74	1.65	1.79
1	C	170	ILE	CA-C	5.72	1.58	1.52
1	G	170	ILE	CA-CB	5.41	1.57	1.54
1	A	46	THR	CA-C	5.16	1.57	1.52
1	A	374	VAL	CA-CB	5.11	1.57	1.54
1	F	374	VAL	CA-C	5.02	1.58	1.52

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	383	PHE	CA-CB-CG	6.37	120.17	113.80
1	F	157	ILE	N-CA-CB	5.94	115.08	110.45
1	C	383	PHE	CA-CB-CG	5.91	119.71	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	362	ASP	N-CA-C	-5.84	101.09	110.14
1	B	119	ASP	CA-CB-CG	5.82	118.42	112.60
1	F	383	PHE	CA-CB-CG	5.81	119.61	113.80
1	E	415	ILE	CA-C-N	5.79	128.04	120.28
1	E	415	ILE	C-N-CA	5.79	128.04	120.28
1	G	383	PHE	CA-CB-CG	5.77	119.57	113.80
1	B	362	ASP	N-CA-C	-5.77	101.20	110.14
1	C	362	ASP	N-CA-C	-5.69	101.32	110.14
1	A	360	GLN	CA-C-N	5.68	132.40	121.54
1	A	360	GLN	C-N-CA	5.68	132.40	121.54
1	B	155	THR	N-CA-C	-5.67	105.46	112.72
1	B	383	PHE	CA-CB-CG	5.57	119.37	113.80
1	G	362	ASP	N-CA-C	-5.53	101.58	110.14
1	F	119	ASP	CA-CB-CG	5.50	118.10	112.60
1	D	373	GLY	CA-C-N	5.50	124.73	120.33
1	D	373	GLY	C-N-CA	5.50	124.73	120.33
1	E	280	LEU	N-CA-C	-5.47	105.39	111.36
1	G	373	GLY	CA-C-N	5.47	124.71	120.33
1	G	373	GLY	C-N-CA	5.47	124.71	120.33
1	F	360	GLN	CA-C-N	5.47	131.98	121.54
1	F	360	GLN	C-N-CA	5.47	131.98	121.54
1	H	362	ASP	N-CA-C	-5.45	101.69	110.14
1	E	383	PHE	CA-CB-CG	5.43	119.23	113.80
1	A	383	PHE	CA-CB-CG	5.41	119.21	113.80
1	E	360	GLN	CA-C-N	5.39	131.84	121.54
1	E	360	GLN	C-N-CA	5.39	131.84	121.54
1	B	476	THR	CA-C-N	5.39	128.04	120.28
1	B	476	THR	C-N-CA	5.39	128.04	120.28
1	F	362	ASP	N-CA-C	-5.34	101.86	110.14
1	G	360	GLN	CA-C-N	5.26	131.59	121.54
1	G	360	GLN	C-N-CA	5.26	131.59	121.54
1	D	362	ASP	N-CA-C	-5.25	102.01	110.14
1	H	457	THR	CA-C-N	5.23	127.72	120.29
1	H	457	THR	C-N-CA	5.23	127.72	120.29
1	F	170	ILE	N-CA-CB	5.21	114.52	110.45
1	B	360	GLN	CA-C-N	5.20	131.47	121.54
1	B	360	GLN	C-N-CA	5.20	131.47	121.54
1	C	448	ARG	CA-C-N	5.19	127.23	120.28
1	C	448	ARG	C-N-CA	5.19	127.23	120.28
1	C	155	THR	N-CA-C	-5.15	106.12	112.72
1	E	362	ASP	N-CA-C	-5.14	102.18	110.14
1	H	119	ASP	CA-CB-CG	5.12	117.72	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	383	PHE	CA-CB-CG	5.09	118.89	113.80
1	D	360	GLN	CA-C-N	5.07	131.22	121.54
1	D	360	GLN	C-N-CA	5.07	131.22	121.54
1	G	169	TYR	CA-C-N	5.07	124.38	120.33
1	G	169	TYR	C-N-CA	5.07	124.38	120.33
1	H	360	GLN	CA-C-N	5.05	131.19	121.54
1	H	360	GLN	C-N-CA	5.05	131.19	121.54

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3333	0	3288	8	0
1	B	3522	0	3471	9	0
1	C	3367	0	3322	10	0
1	D	3487	0	3454	10	0
1	E	3347	0	3299	13	0
1	F	3450	0	3429	13	0
1	G	3375	0	3335	8	0
1	H	3490	0	3460	13	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
2	E	23	0	12	0	0
2	F	23	0	12	0	0
2	G	23	0	12	0	0
2	H	23	0	12	0	0
3	C	5	0	0	0	0
3	G	5	0	0	0	0
3	H	5	0	0	0	0
4	E	6	0	8	5	0
5	A	233	0	0	0	0
5	B	244	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	212	0	0	0	0
5	D	265	0	0	1	0
5	E	215	0	0	0	0
5	F	239	0	0	1	0
5	G	217	0	0	0	0
5	H	259	0	0	0	0
All	All	29460	0	27162	75	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 1.

All (75) 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:E:157:ILE:HD11	4:E:501:GOL:H32	1.39	1.05
1:A:244[B]:CYS:HG	1:E:472:TYR:HD2	1.05	0.98
1:H:170:ILE:HD11	1:H:223:LEU:HD23	1.67	0.76
1:E:366:SER:HA	4:E:501:GOL:H12	1.67	0.75
1:E:157:ILE:CD1	4:E:501:GOL:H32	2.18	0.72
1:B:417[B]:THR:HG21	1:F:241:ALA:HB1	1.72	0.71
1:F:259[B]:LEU:HD22	1:F:265:LEU:HB2	1.77	0.66
1:B:241:ALA:HB1	1:F:417[B]:THR:HG21	1.77	0.65
1:F:259[B]:LEU:HD23	1:F:263:LEU:HD12	1.78	0.65
1:D:241:ALA:HB1	1:H:417[B]:THR:HG21	1.79	0.63
1:F:155:THR:HG22	1:F:259[B]:LEU:HD21	1.81	0.62
1:E:118:HIS:HD2	1:E:121:LYS:H	1.48	0.60
1:B:468:THR:H	1:B:471[A]:THR:HG22	1.65	0.60
1:A:59:LYS:HD3	1:A:101:PHE:HB3	1.87	0.57
1:A:241:ALA:HB1	1:E:417[B]:THR:HG21	1.88	0.56
1:H:170:ILE:HD11	1:H:223:LEU:CD2	2.37	0.54
1:D:415:ILE:HG23	1:D:464:LEU:HD22	1.89	0.54
1:G:190:PRO:HB3	1:G:473:VAL:HG11	1.89	0.54
1:H:120:ILE:HG13	1:H:149:SER:HB3	1.90	0.54
1:D:118:HIS:HD2	1:D:121:LYS:H	1.55	0.52
1:E:165:LEU:HA	1:E:169:TYR:HB3	1.92	0.50
1:H:118[A]:HIS:HD2	1:H:121:LYS:H	1.59	0.49
1:F:259[B]:LEU:CD2	1:F:263:LEU:HD12	2.43	0.49
1:E:105:ASP:HA	1:E:108:ILE:HD12	1.95	0.49
1:E:60:TYR:HB3	1:E:156:SER:HB2	1.94	0.49
1:B:190:PRO:HB3	1:B:473:VAL:HG11	1.94	0.49
1:B:210[B]:MET:SD	1:B:477:ALA:HA	2.54	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:190:PRO:HB3	1:F:473:VAL:HG11	1.96	0.48
1:F:342:MET:HE3	1:F:342:MET:HA	1.95	0.48
1:C:377:SER:OG	1:D:34:LEU:HD11	2.13	0.47
1:D:165:LEU:HA	1:D:169:TYR:HB3	1.96	0.47
1:B:312:GLN:HE22	1:B:330:PRO:HA	1.79	0.47
1:H:190:PRO:HB3	1:H:473:VAL:HG11	1.97	0.47
1:H:210[B]:MET:SD	1:H:477:ALA:HA	2.54	0.47
1:H:312:GLN:HE22	1:H:330:PRO:HA	1.80	0.47
1:B:273:GLN:HB3	1:B:361:ARG:HG2	1.97	0.47
1:C:245:ALA:HB2	1:G:417:THR:HG23	1.98	0.46
1:A:168[B]:HIS:HD2	1:A:380:LEU:HD11	1.81	0.45
1:H:175:GLN:HB3	1:H:387:ARG:NH2	2.31	0.45
1:C:165:LEU:HA	1:C:169:TYR:HB3	1.98	0.45
1:C:292:THR:HA	1:C:295:MET:HE3	1.98	0.45
1:G:292:THR:HA	1:G:295:MET:HE3	1.97	0.45
1:E:366:SER:HA	4:E:501:GOL:C1	2.42	0.44
1:A:411:VAL:HB	1:A:467:ILE:HG22	1.99	0.44
1:C:450:VAL:HG11	1:C:465:LEU:HG	1.99	0.44
1:F:252:LEU:HD21	5:F:605:HOH:O	2.18	0.44
1:H:419:LEU:HB3	1:H:424:TYR:HB3	2.00	0.44
1:D:241:ALA:O	1:H:417[A]:THR:HG21	2.17	0.44
1:G:105:ASP:HA	1:G:108:ILE:HD12	2.00	0.43
1:D:118:HIS:CD2	1:D:121:LYS:H	2.36	0.43
1:G:165:LEU:HA	1:G:169:TYR:HB3	2.00	0.43
1:A:165:LEU:HA	1:A:169:TYR:HB3	2.00	0.43
1:E:118:HIS:CD2	1:E:121:LYS:H	2.33	0.43
1:H:408:TRP:O	1:H:411:VAL:HG22	2.18	0.43
1:E:157:ILE:HA	1:E:160:LEU:HG	2.00	0.42
1:C:179:LEU:HD22	1:C:387[B]:ARG:HG3	2.02	0.42
1:E:153:ASN:CG	4:E:501:GOL:H2	2.44	0.42
1:F:60:TYR:HB3	1:F:156[B]:SER:HB2	2.00	0.42
1:C:120:ILE:HG21	1:C:149:SER:HA	2.02	0.42
1:G:63:GLN:HA	1:G:98:PHE:CD2	2.54	0.42
1:B:292:THR:HA	1:B:295:MET:HE3	2.02	0.41
1:C:408:TRP:O	1:C:411:VAL:HG22	2.20	0.41
1:G:450:VAL:HG11	1:G:465:LEU:HG	2.02	0.41
1:A:464:LEU:HA	1:A:467:ILE:HD12	2.03	0.41
1:B:168[B]:HIS:HD2	1:B:380:LEU:HD11	1.85	0.41
1:D:238:ASN:ND2	5:D:852:HOH:O	2.53	0.41
1:F:137:GLU:O	1:F:140:LYS:HG2	2.20	0.41
1:A:155:THR:C	1:A:158:PRO:HD2	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:190:PRO:HB3	1:C:473:VAL:HG11	2.02	0.40
1:F:159:MET:HG3	1:F:265:LEU:HD11	2.03	0.40
1:C:70:GLU:HG3	1:C:90:LEU:HD13	2.04	0.40
1:F:118:HIS:CD2	1:F:121:LYS:H	2.39	0.40
1:D:193:ALA:CB	1:H:236:THR:HG21	2.51	0.40
1:D:408:TRP:O	1:D:411:VAL:HG22	2.20	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	422/480 (88%)	409 (97%)	12 (3%)	1 (0%)	43 36
1	B	444/480 (92%)	422 (95%)	21 (5%)	1 (0%)	43 36
1	C	424/480 (88%)	408 (96%)	15 (4%)	1 (0%)	43 36
1	D	441/480 (92%)	421 (96%)	19 (4%)	1 (0%)	43 36
1	E	424/480 (88%)	408 (96%)	15 (4%)	1 (0%)	43 36
1	F	433/480 (90%)	415 (96%)	17 (4%)	1 (0%)	43 36
1	G	427/480 (89%)	411 (96%)	15 (4%)	1 (0%)	43 36
1	H	442/480 (92%)	422 (96%)	19 (4%)	1 (0%)	43 36
All	All	3457/3840 (90%)	3316 (96%)	133 (4%)	8 (0%)	43 36

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	361	ARG
1	B	361	ARG
1	C	361	ARG
1	D	361	ARG

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Mol	Chain	Res	Type
1	E	361	ARG
1	F	361	ARG
1	G	361	ARG
1	H	361	ARG

### 5.3.2 Protein sidechains [i](#)

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	350/403 (87%)	346 (99%)	4 (1%)	65 67
1	B	371/403 (92%)	363 (98%)	8 (2%)	45 42
1	C	350/403 (87%)	347 (99%)	3 (1%)	70 73
1	D	370/403 (92%)	363 (98%)	7 (2%)	50 47
1	E	351/403 (87%)	347 (99%)	4 (1%)	65 67
1	F	368/403 (91%)	363 (99%)	5 (1%)	59 59
1	G	353/403 (88%)	348 (99%)	5 (1%)	59 59
1	H	372/403 (92%)	366 (98%)	6 (2%)	55 54
All	All	2885/3224 (90%)	2843 (98%)	42 (2%)	59 56

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	LYS
1	A	275	GLU
1	A	328	VAL
1	A	441	VAL
1	B	24	GLU
1	B	34	LEU
1	B	275	GLU
1	B	387[A]	ARG
1	B	387[B]	ARG
1	B	416	GLN
1	B	452	GLN

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Mol	Chain	Res	Type
1	B	459	GLU
1	C	34	LEU
1	C	126	TYR
1	C	275	GLU
1	D	175	GLN
1	D	252	LEU
1	D	275	GLU
1	D	319	VAL
1	D	328	VAL
1	D	361	ARG
1	D	431	LEU
1	E	34	LEU
1	E	80	THR
1	E	150	GLN
1	E	275	GLU
1	F	34	LEU
1	F	74	LYS
1	F	275	GLU
1	F	451	GLN
1	F	459	GLU
1	G	34	LEU
1	G	92	GLU
1	G	275	GLU
1	G	328	VAL
1	G	422	GLU
1	H	34	LEU
1	H	165[A]	LEU
1	H	165[B]	LEU
1	H	275	GLU
1	H	328	VAL
1	H	431	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	329	ASN
1	B	167	HIS
1	B	198	GLN
1	B	312	GLN
1	B	329	ASN
1	B	462	GLN
1	C	198	GLN

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Mol	Chain	Res	Type
1	C	329	ASN
1	C	339	ASN
1	C	371	ASN
1	C	447	HIS
1	C	462	GLN
1	D	166	HIS
1	D	339	ASN
1	D	371	ASN
1	D	416	GLN
1	D	462	GLN
1	E	198	GLN
1	E	329	ASN
1	F	167	HIS
1	F	329	ASN
1	F	462	GLN
1	G	166	HIS
1	G	175	GLN
1	G	250	ASN
1	G	329	ASN
1	H	167	HIS
1	H	312	GLN
1	H	329	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](#)

12 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
2	AMP	D	501	-	25,25,25	0.13	0	37,38,38	0.51	0
3	SO4	H	502	-	4,4,4	0.30	0	6,6,6	0.24	0
3	SO4	G	502	-	4,4,4	0.28	0	6,6,6	0.09	0
4	GOL	E	501	-	5,5,5	0.11	0	5,5,5	0.51	0
2	AMP	B	501	-	25,25,25	0.38	0	37,38,38	0.48	0
2	AMP	E	502	-	25,25,25	0.22	0	37,38,38	0.45	0
2	AMP	G	501	-	25,25,25	0.29	0	37,38,38	0.42	0
2	AMP	F	501	-	25,25,25	0.17	0	37,38,38	0.40	0
2	AMP	H	501	-	25,25,25	0.19	0	37,38,38	0.45	0
2	AMP	C	501	-	25,25,25	0.36	0	37,38,38	0.45	0
2	AMP	A	501	-	25,25,25	0.32	0	37,38,38	0.57	0
3	SO4	C	502	-	4,4,4	0.35	0	6,6,6	0.11	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	D	501	-	-	2/10/26/26	0/3/3/3
4	GOL	E	501	-	-	0/4/4/4	-
2	AMP	B	501	-	-	4/10/26/26	0/3/3/3
2	AMP	E	502	-	-	2/10/26/26	0/3/3/3
2	AMP	G	501	-	-	3/10/26/26	0/3/3/3
2	AMP	F	501	-	-	4/10/26/26	0/3/3/3
2	AMP	H	501	-	-	2/10/26/26	0/3/3/3
2	AMP	C	501	-	-	2/10/26/26	0/3/3/3
2	AMP	A	501	-	-	2/10/26/26	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:

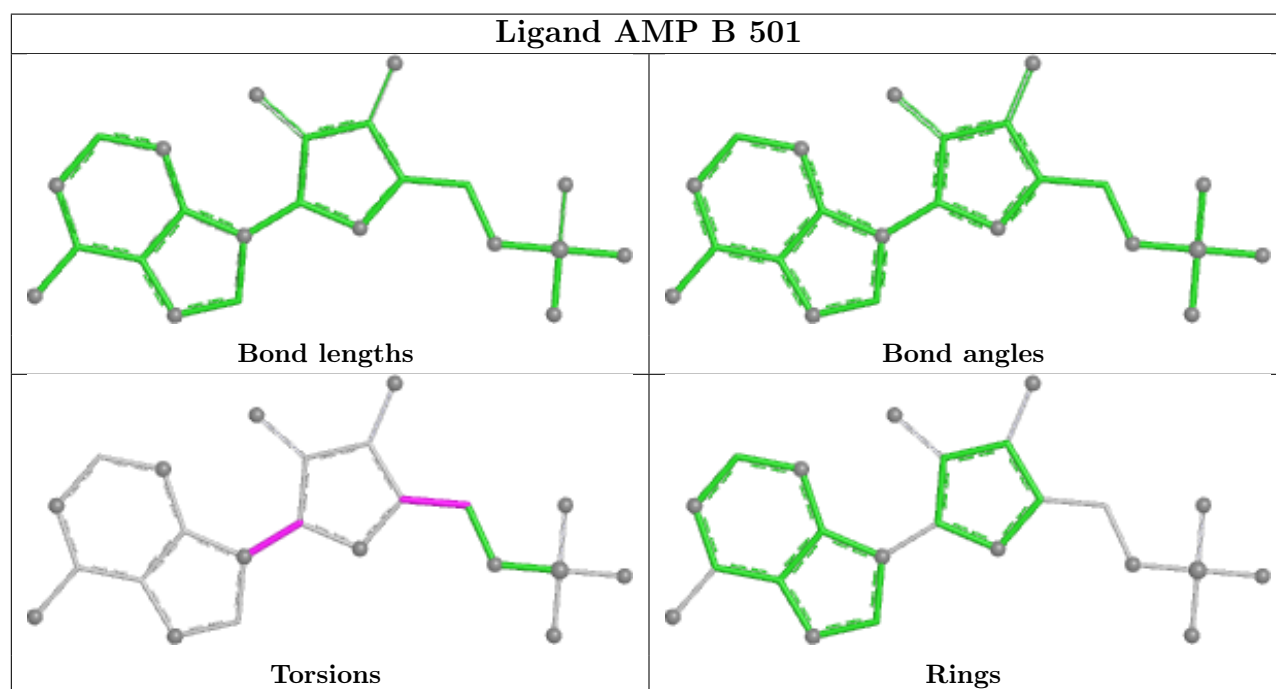
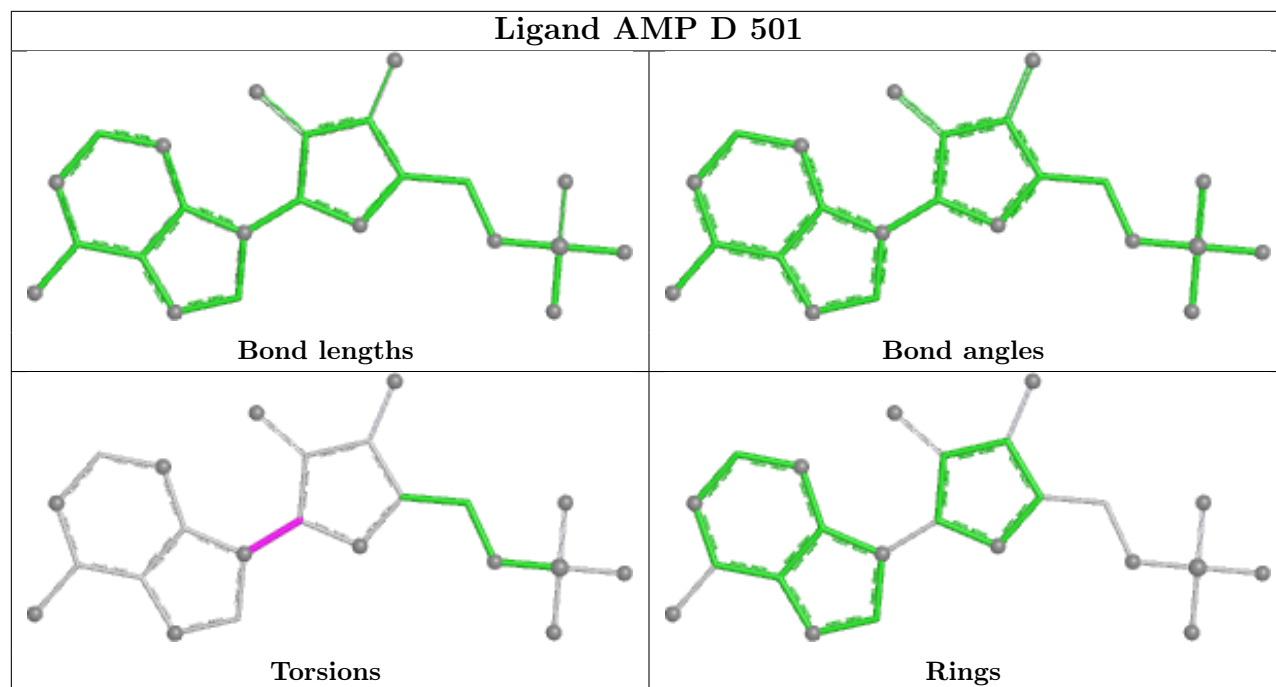
Mol	Chain	Res	Type	Atoms
2	D	501	AMP	C2'-C1'-N9-C8
2	E	502	AMP	C2'-C1'-N9-C8
2	C	501	AMP	C2'-C1'-N9-C8
2	H	501	AMP	C2'-C1'-N9-C8
2	E	502	AMP	C2'-C1'-N9-C4
2	A	501	AMP	C2'-C1'-N9-C8
2	B	501	AMP	C2'-C1'-N9-C8
2	F	501	AMP	C2'-C1'-N9-C8
2	G	501	AMP	C2'-C1'-N9-C8
2	D	501	AMP	C2'-C1'-N9-C4
2	H	501	AMP	C2'-C1'-N9-C4
2	A	501	AMP	C2'-C1'-N9-C4
2	C	501	AMP	C2'-C1'-N9-C4
2	B	501	AMP	C2'-C1'-N9-C4
2	F	501	AMP	C2'-C1'-N9-C4
2	G	501	AMP	C2'-C1'-N9-C4
2	B	501	AMP	O4'-C4'-C5'-O5'
2	F	501	AMP	O4'-C4'-C5'-O5'
2	B	501	AMP	O4'-C1'-N9-C8
2	F	501	AMP	O4'-C1'-N9-C8
2	G	501	AMP	O4'-C1'-N9-C8

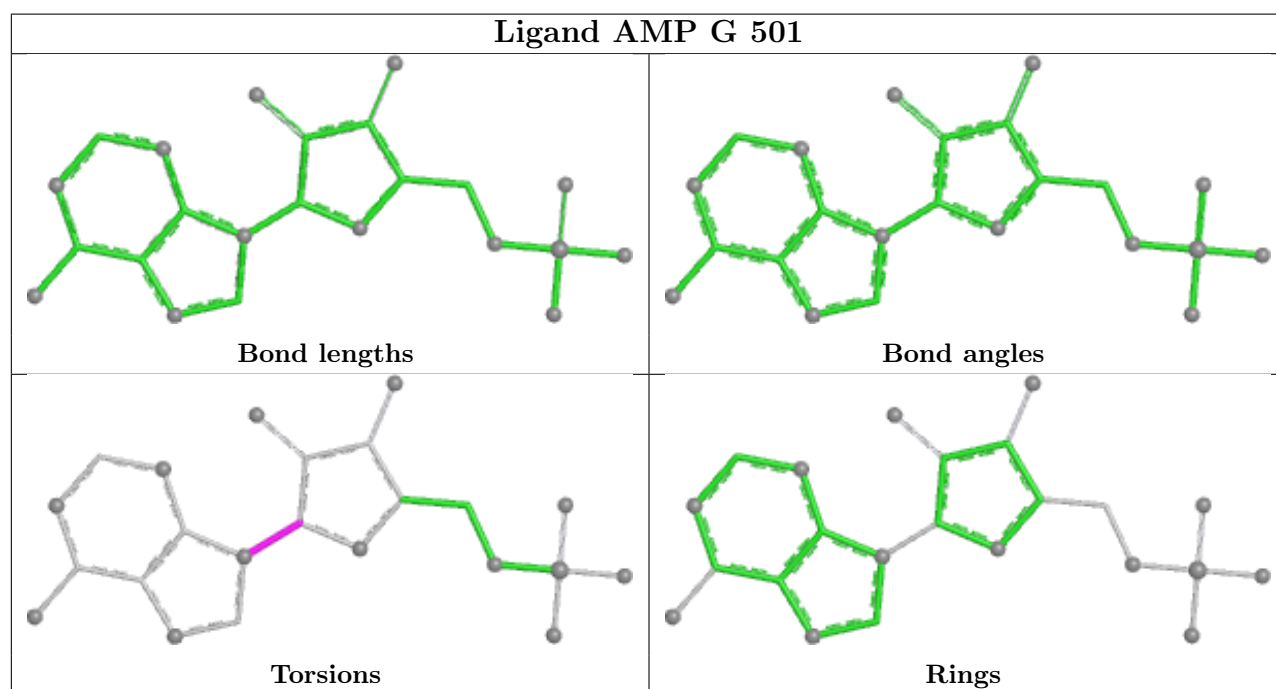
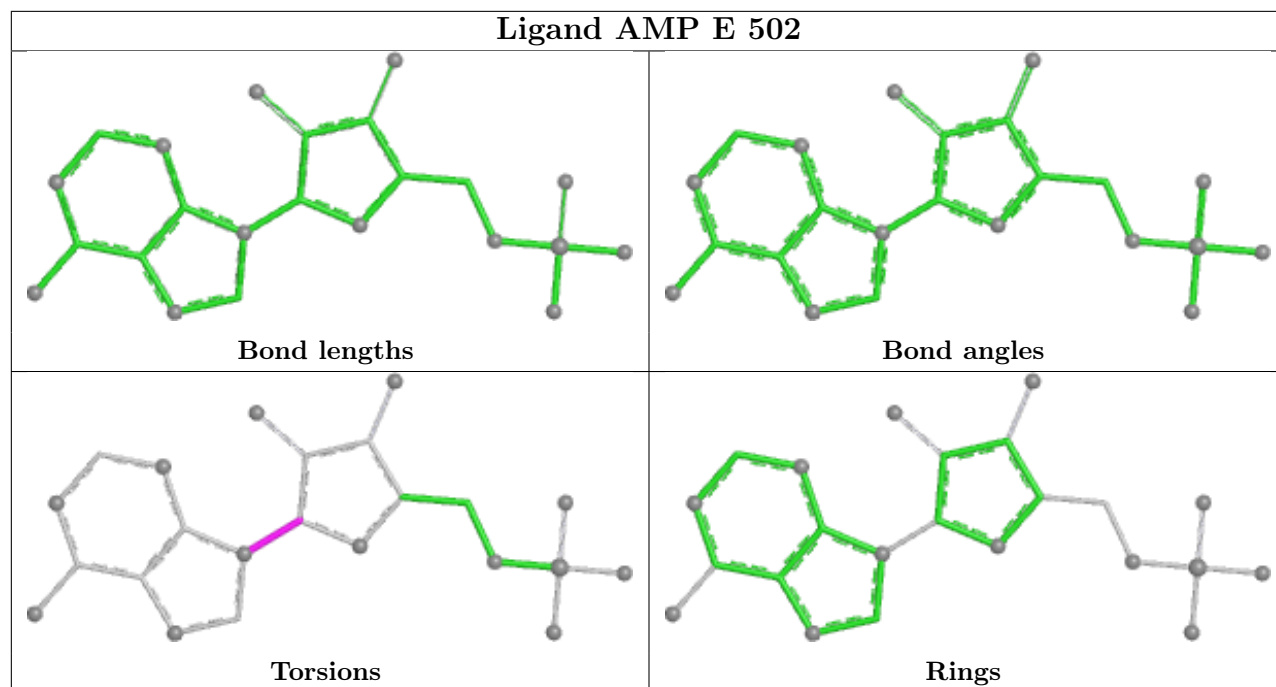
There are no ring outliers.

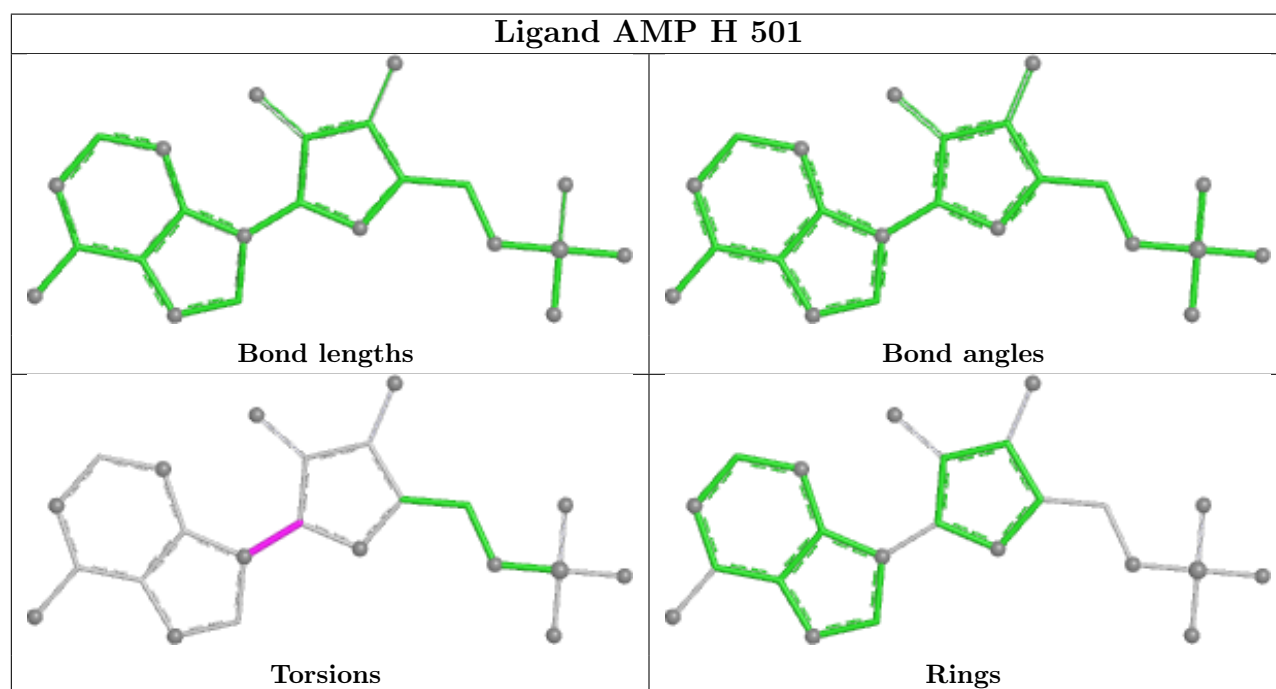
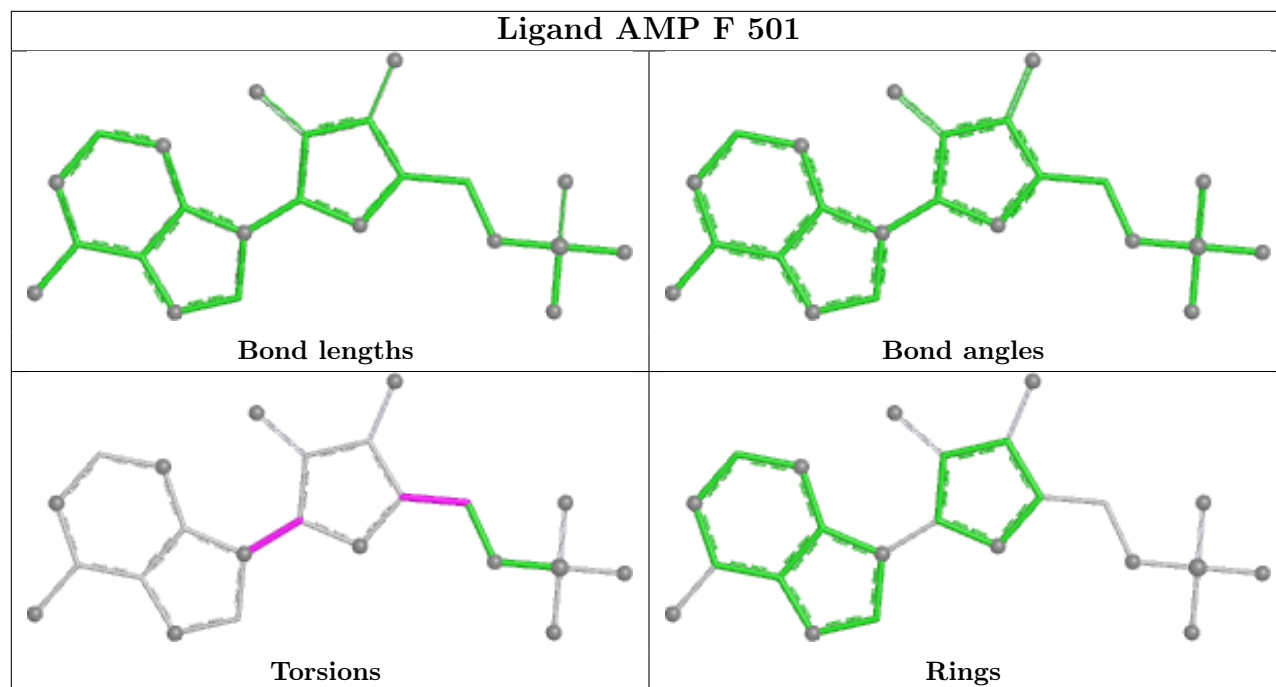
1 monomer is involved in 5 short contacts:

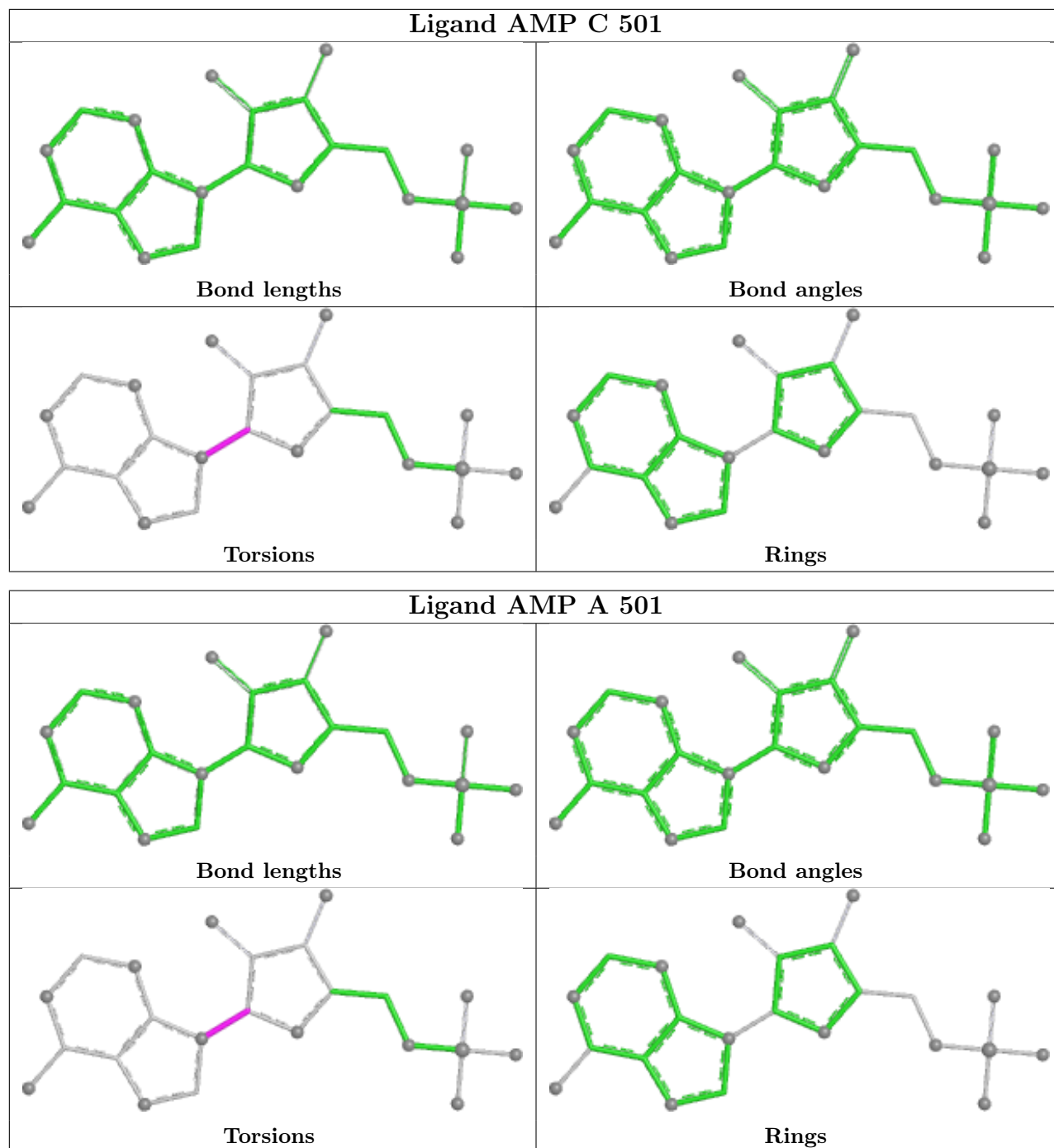
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	501	GOL	5	0

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	424/480 (88%)	-1.00	0 100 100	8, 17, 43, 83	8 (1%)
1	B	439/480 (91%)	-1.06	0 100 100	4, 16, 40, 75	15 (3%)
1	C	426/480 (88%)	-0.95	0 100 100	8, 18, 47, 75	8 (1%)
1	D	439/480 (91%)	-1.07	0 100 100	6, 16, 38, 64	9 (2%)
1	E	425/480 (88%)	-0.94	0 100 100	9, 19, 46, 74	9 (2%)
1	F	431/480 (89%)	-1.02	0 100 100	8, 17, 38, 81	12 (2%)
1	G	427/480 (88%)	-0.94	0 100 100	8, 19, 43, 77	9 (2%)
1	H	438/480 (91%)	-1.04	0 100 100	8, 16, 39, 72	14 (3%)
All	All	3449/3840 (89%)	-1.00	0 100 100	4, 17, 43, 83	84 (2%)

There are no RSRZ outliers to report.

### 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](#)

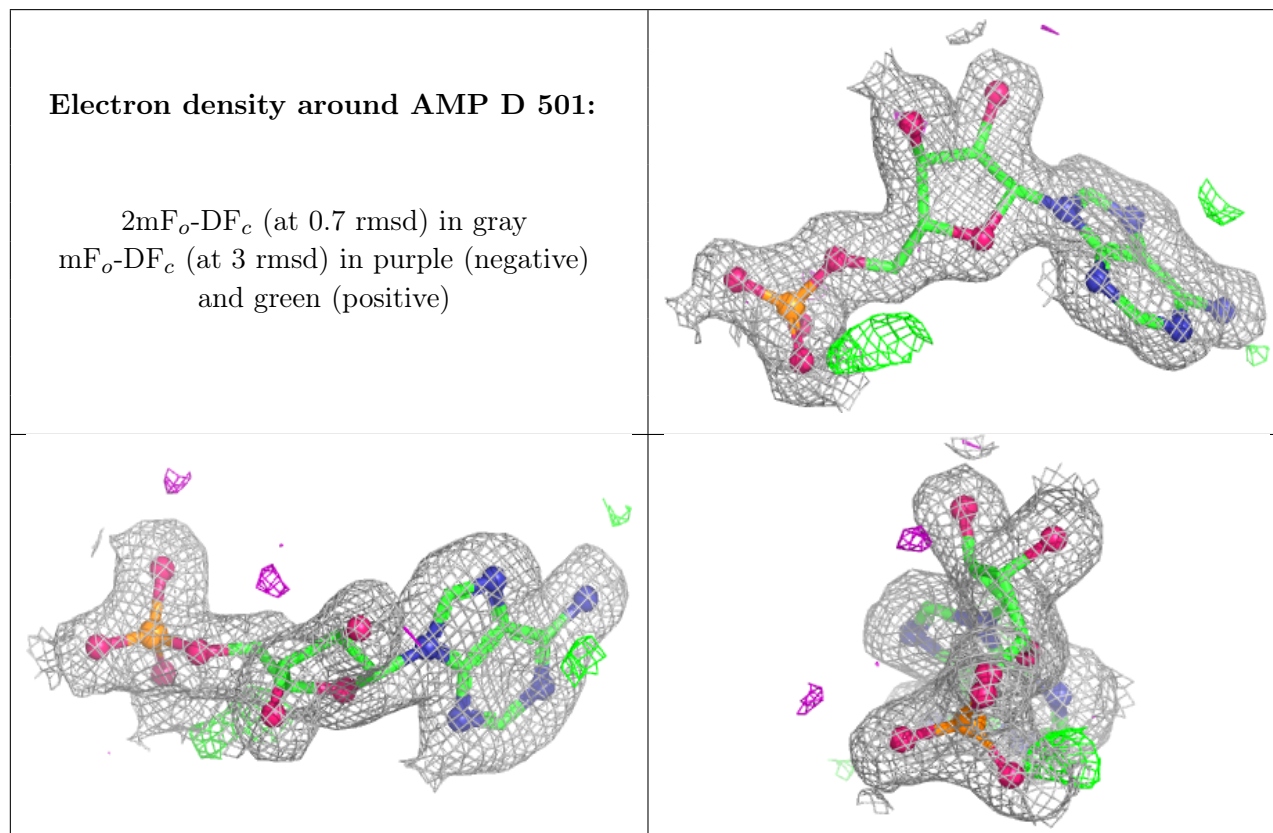
There are no oligosaccharides in this entry.

### 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, 95<sup>th</sup> 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.

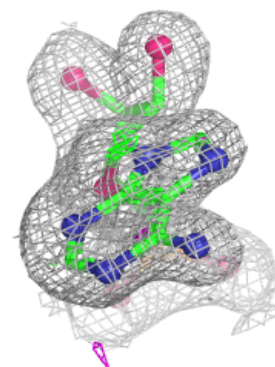
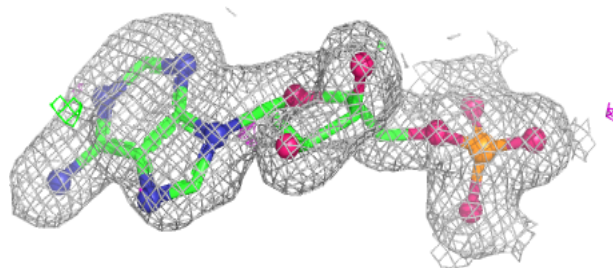
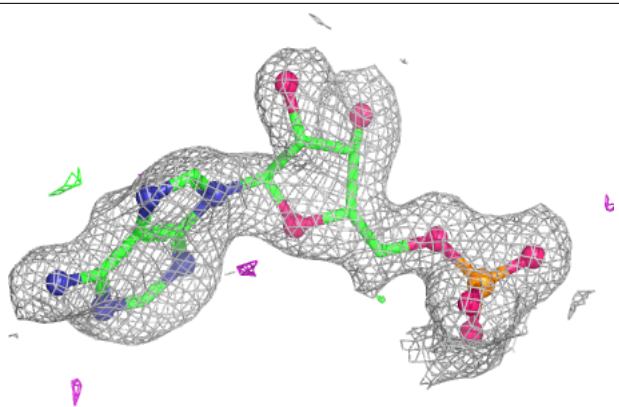
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SO4	G	502	5/5	0.98	0.05	30,34,36,38	0
3	SO4	H	502	5/5	0.98	0.05	44,47,48,48	0
4	GOL	E	501	6/6	0.98	0.06	26,27,30,31	0
2	AMP	D	501	23/23	0.99	0.03	10,17,19,20	0
2	AMP	E	502	23/23	0.99	0.04	15,22,23,24	0
2	AMP	F	501	23/23	0.99	0.03	14,19,22,23	0
2	AMP	G	501	23/23	0.99	0.03	11,15,19,20	0
2	AMP	H	501	23/23	0.99	0.03	11,18,20,21	0
3	SO4	C	502	5/5	0.99	0.06	29,30,32,32	0
2	AMP	A	501	23/23	0.99	0.03	8,14,16,17	0
2	AMP	B	501	23/23	0.99	0.03	8,16,19,19	0
2	AMP	C	501	23/23	0.99	0.03	8,14,18,20	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.

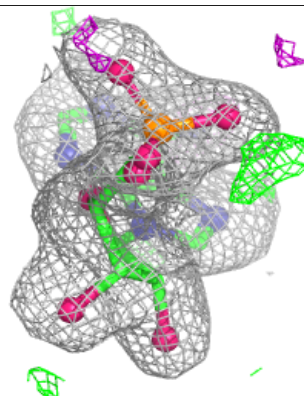
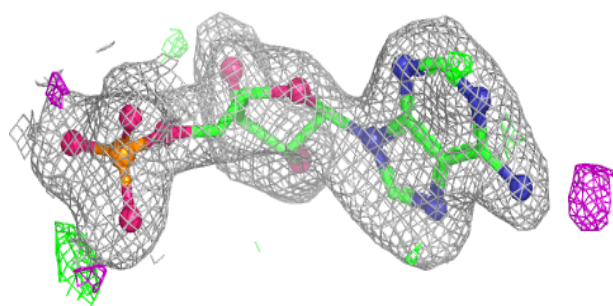
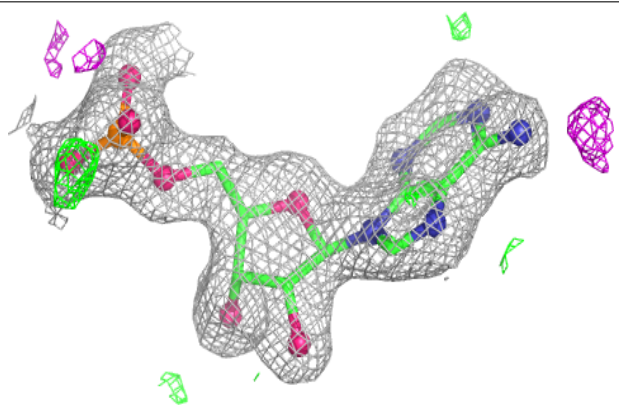


**Electron density around AMP E 502:**

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

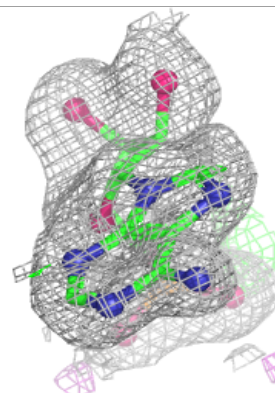
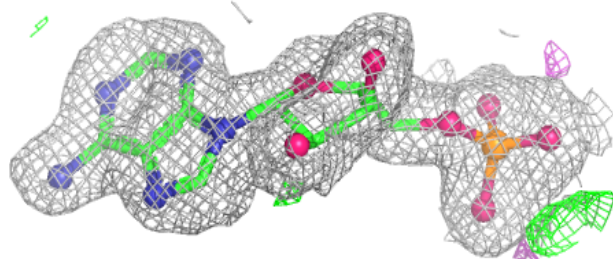
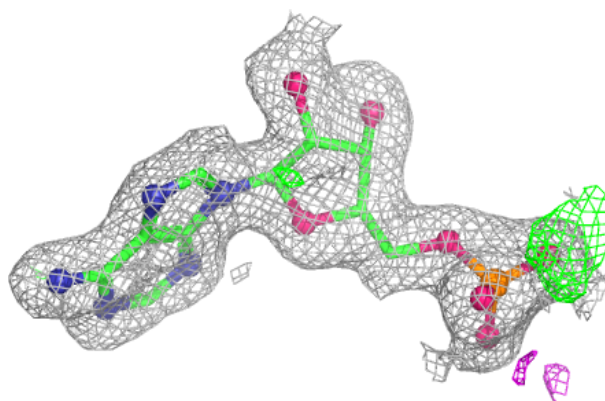
**Electron density around AMP F 501:**

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

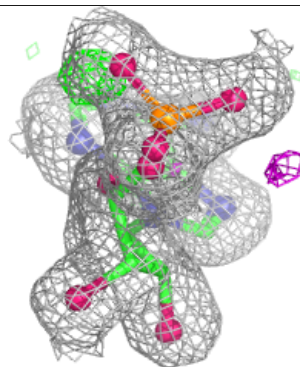
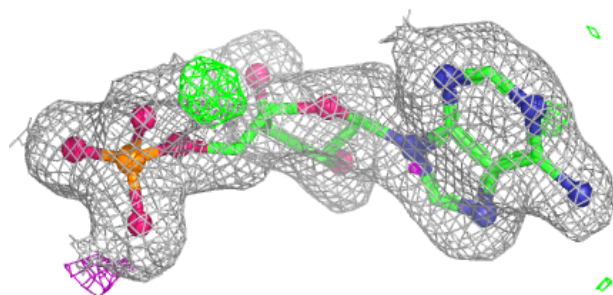
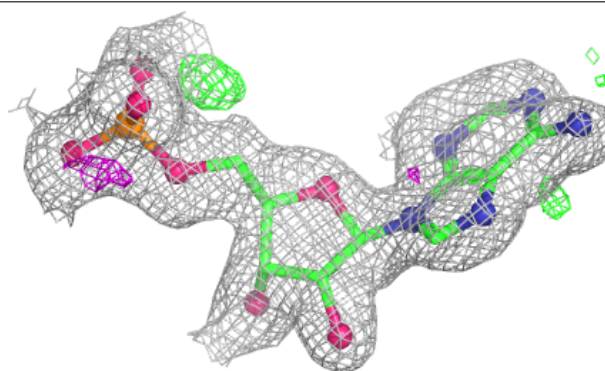


**Electron density around AMP G 501:**

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

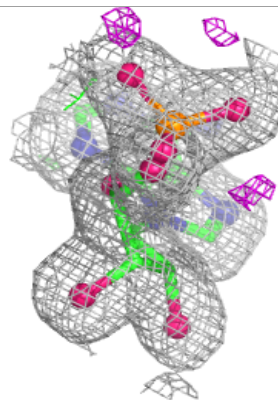
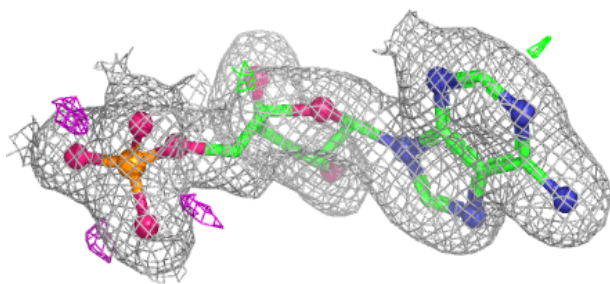
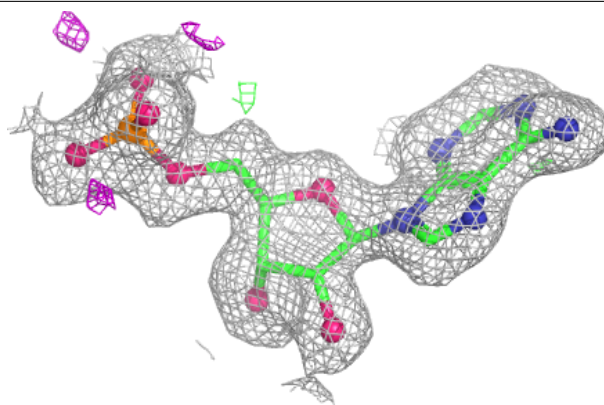
**Electron density around AMP H 501:**

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

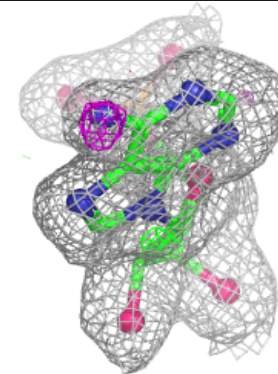
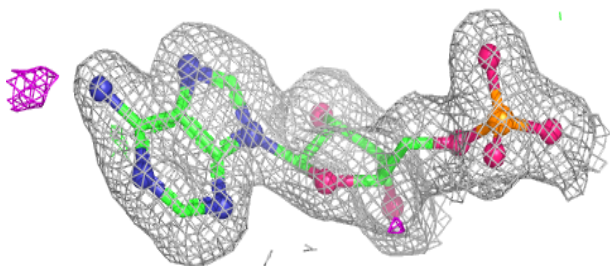
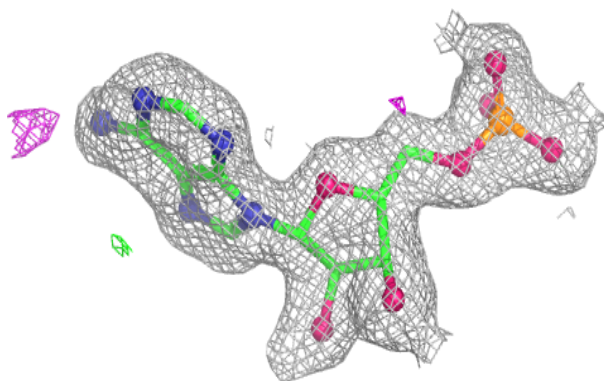


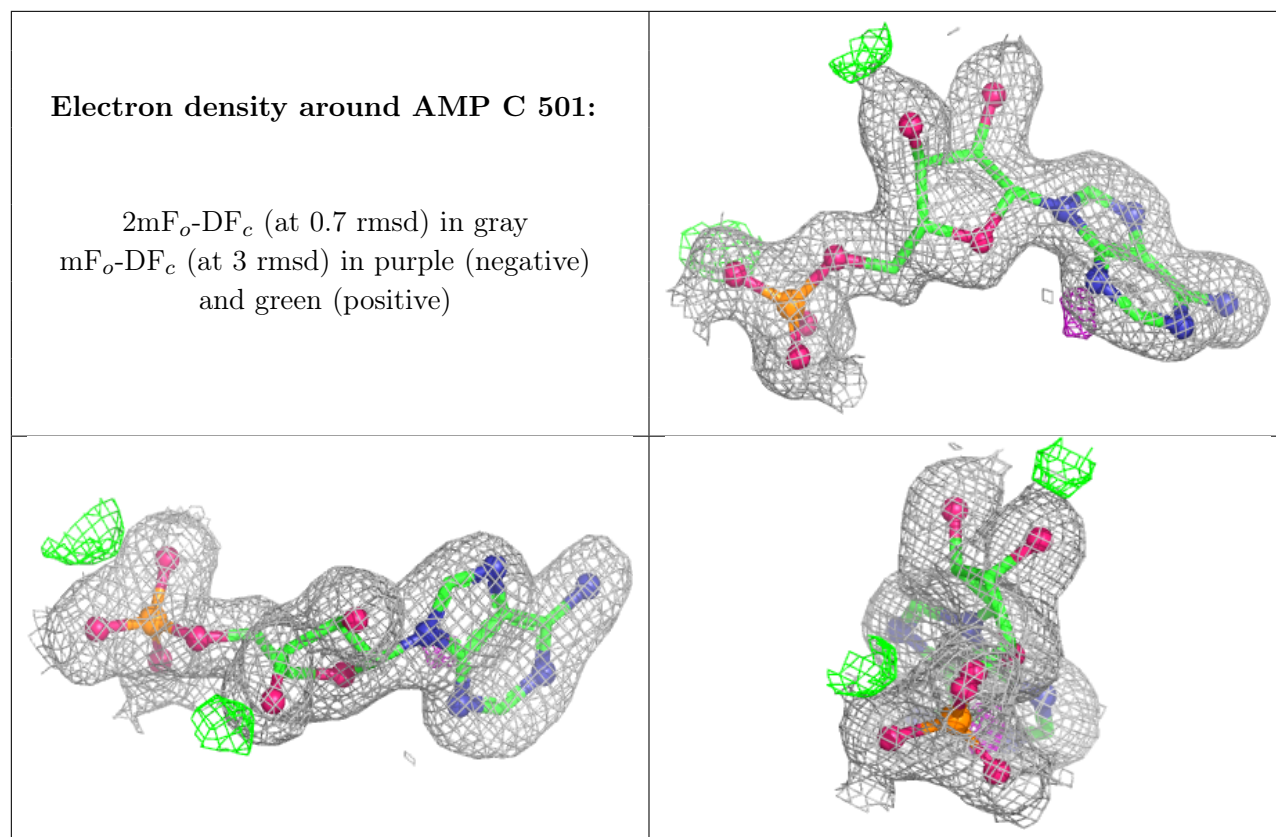
**Electron density around AMP A 501:**

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

**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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.