



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:47 PM UTC

PDB ID : 3Q10 / pdb_00003q10
Title : Pantoate-beta-alanine ligase from Yersinia pestis
Authors : Osipiuk, J.; Maltseva, N.; Kwon, K.; Anderson, W.F.; Joachimiak, A.; Center
for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2010-12-16
Resolution : 1.83 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

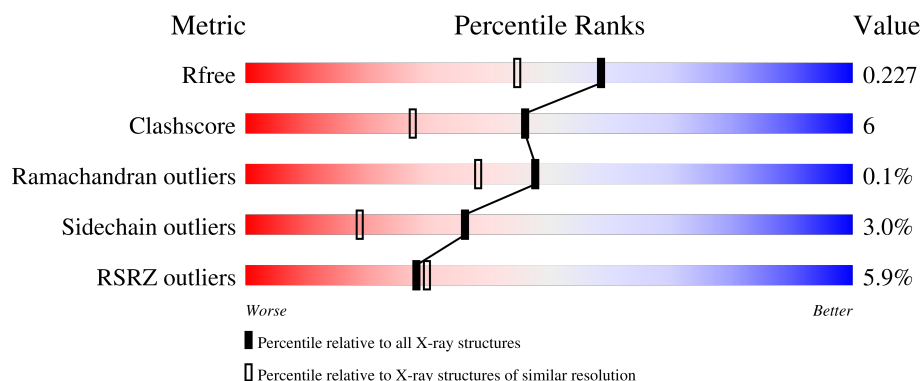
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.83 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	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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	287	% 92% 7%
1	B	287	2% 93% 6%
1	C	287	11% 80% 16%
1	D	287	7% 60% 8% 31%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9440 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.

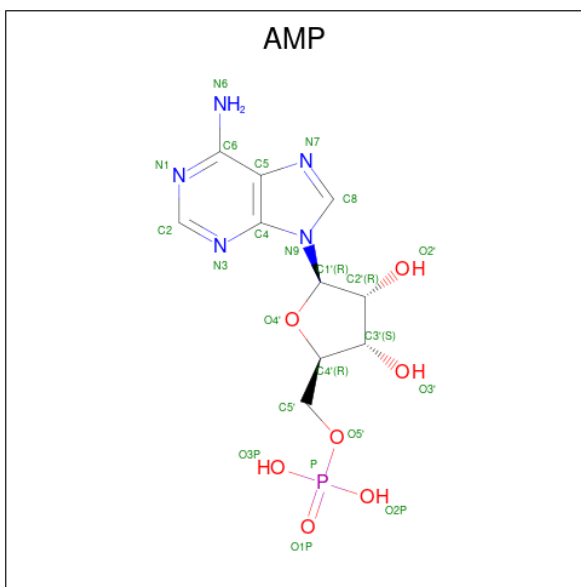
- Molecule 1 is a protein called Pantoate--beta-alanine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	0	20	0
			2361	1504	410	437	10			
1	B	285	Total	C	N	O	S	0	15	0
			2320	1479	400	431	10			
1	C	284	Total	C	N	O	S	0	19	0
			2343	1498	405	429	11			
1	D	198	Total	C	N	O	S	0	5	0
			1590	1015	278	289	8			

There are 12 discrepancies between the modelled and reference sequences:

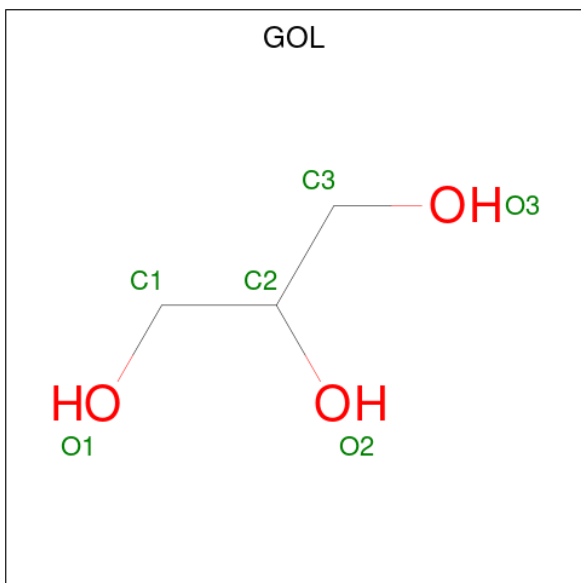
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q8ZBK7
A	-1	ASN	-	expression tag	UNP Q8ZBK7
A	0	ALA	-	expression tag	UNP Q8ZBK7
B	-2	SER	-	expression tag	UNP Q8ZBK7
B	-1	ASN	-	expression tag	UNP Q8ZBK7
B	0	ALA	-	expression tag	UNP Q8ZBK7
C	-2	SER	-	expression tag	UNP Q8ZBK7
C	-1	ASN	-	expression tag	UNP Q8ZBK7
C	0	ALA	-	expression tag	UNP Q8ZBK7
D	-2	SER	-	expression tag	UNP Q8ZBK7
D	-1	ASN	-	expression tag	UNP Q8ZBK7
D	0	ALA	-	expression tag	UNP Q8ZBK7

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



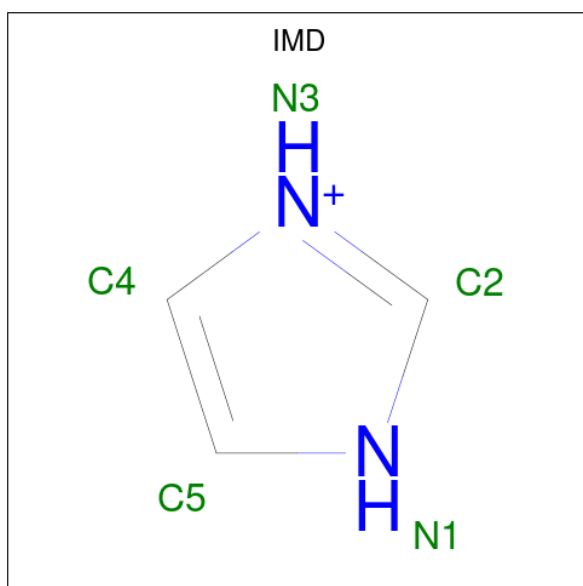
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	D	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is IMIDAZOLE (CCD ID: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			5	3	2		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cl	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	292	Total 292	O 292	0	4
6	B	163	Total 163	O 163	0	0
6	C	196	Total 196	O 196	0	2
6	D	47	Total 47	O 47	0	0

PRO	LEU	THR	VAL	ASP	SER	GLN	GLN	ALA	V262	I263	A266	A267	TRP	LEU	GLY	LYS	A272	R273	L274	I275	D276	N277	Q278	LEU	VAL	ASP	LEU	ARG	HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	44.81Å 77.24Å 98.46Å 101.33° 94.91° 94.37°	Depositor
Resolution (Å)	33.10 – 1.83 33.10 – 1.83	Depositor EDS
% Data completeness (in resolution range)	96.4 (33.10-1.83) 96.6 (33.10-1.83)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 1.83Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.174 , 0.211 0.188 , 0.227	Depositor DCC
R_{free} test set	5527 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	25.5	Xtriage
Anisotropy	0.714	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9440	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.56% 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, IMD, 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	1.14	2/2461 (0.1%)	0.95	2/3331 (0.1%)
1	B	0.89	0/2404	0.90	0/3260
1	C	1.03	3/2439 (0.1%)	0.93	1/3306 (0.0%)
1	D	0.76	0/1633	0.87	0/2212
All	All	0.98	5/8937 (0.1%)	0.92	3/12109 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	142	GLN	C-O	7.22	1.27	1.23
1	C	92	ALA	CA-CB	6.73	1.62	1.53
1	A	142	GLN	CA-CB	6.59	1.58	1.52
1	A	175	VAL	CA-C	6.01	1.56	1.52
1	C	52	VAL	CA-CB	5.84	1.61	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	141	ILE	CB-CA-C	5.59	115.98	111.06
1	C	182	ASP	N-CA-C	5.41	117.87	111.33
1	A	87	ALA	N-CA-C	-5.10	103.61	110.24

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	2361	0	2445	13	0
1	B	2320	0	2399	15	0
1	C	2343	0	2442	55	0
1	D	1590	0	1627	18	0
2	A	23	0	12	0	0
2	B	23	0	12	0	0
2	C	23	0	12	1	0
2	D	23	0	12	0	0
3	A	6	0	7	0	0
3	B	12	0	16	2	0
3	C	6	0	8	0	0
3	D	6	0	8	0	0
4	A	5	0	5	0	0
5	A	1	0	0	0	0
6	A	292	0	0	3	0
6	B	163	0	0	6	0
6	C	196	0	0	6	0
6	D	47	0	0	1	0
All	All	9440	0	9005	103	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (103) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:215[A]:MET:HE1	1:C:245:ILE:HD13	1.34	1.09
1:C:11[B]:ARG:NH1	1:C:11[B]:ARG:HG2	1.58	1.05
1:C:11[B]:ARG:HG2	1:C:11[B]:ARG:HH11	0.89	1.02
1:C:63[B]:GLU:OE1	1:C:64[B]:ARG:NH2	1.91	1.02
1:B:243:LEU:HD22	1:B:265:MET:HE2	1.42	0.98
1:C:11[B]:ARG:HH11	1:C:11[B]:ARG:CG	1.77	0.97
1:C:203:GLN:HE21	1:C:236:VAL:HG11	1.35	0.91
1:C:215[A]:MET:CE	1:C:245:ILE:HD13	2.03	0.88
2:C:501:AMP:C2	6:C:603:HOH:O	2.29	0.85
1:C:203:GLN:NE2	1:C:236:VAL:HG11	1.91	0.85
1:C:226:LEU:HD11	1:C:245:ILE:HG13	1.63	0.80
1:C:255:THR:HG22	1:C:257:ASP:H	1.46	0.79
1:C:223:ASP:O	1:C:227:GLU:HG3	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:211:LEU:HD21	1:C:215[A]:MET:HE3	1.71	0.73
1:C:18[A]:ARG:HD2	1:C:142:GLN:NE2	2.04	0.72
1:B:243:LEU:HD22	1:B:265:MET:CE	2.16	0.72
1:C:233:LEU:HD23	1:C:238:PHE:HB2	1.74	0.70
1:C:62[B]:PHE:HE2	1:C:68[B]:LEU:CG	2.05	0.70
3:B:605:GOL:H2	6:B:343:HOH:O	1.91	0.69
1:A:195[B]:GLU:HG2	6:A:656:HOH:O	1.93	0.69
1:C:62[B]:PHE:HE2	1:C:68[B]:LEU:CB	2.07	0.67
1:C:62[B]:PHE:CD2	1:C:68[B]:LEU:HB2	2.30	0.67
1:C:62[B]:PHE:CE2	1:C:68[B]:LEU:HB2	2.28	0.67
1:C:57:VAL:CG1	1:C:62[B]:PHE:HZ	2.06	0.67
1:C:57:VAL:HG12	1:C:62[B]:PHE:HZ	1.59	0.65
1:C:62[B]:PHE:CE2	1:C:68[B]:LEU:CB	2.79	0.65
1:B:142:GLN:NE2	6:B:560:HOH:O	2.27	0.65
1:D:112:PRO:O	1:D:113:ALA:HB3	1.98	0.64
1:A:195[B]:GLU:HG3	1:A:196[B]:GLU:OE2	1.98	0.63
1:C:215[A]:MET:HE1	1:C:245:ILE:HG21	1.79	0.62
1:C:233:LEU:HD22	1:C:240:PRO:HB3	1.80	0.62
1:B:265:MET:HE2	1:B:265:MET:HA	1.82	0.61
1:C:62[B]:PHE:HE2	1:C:68[B]:LEU:HG	1.66	0.60
1:B:213:GLU:OE1	6:B:697:HOH:O	2.15	0.59
1:C:226:LEU:HD11	1:C:245:ILE:CG1	2.32	0.58
1:B:243:LEU:HD13	1:B:265:MET:HE1	1.85	0.58
1:D:163:VAL:HG21	1:D:172:ILE:HD11	1.86	0.58
1:A:39[B]:THR:HG21	1:A:178:VAL:HG21	1.86	0.57
1:A:112:PRO:HD2	6:C:366:HOH:O	2.02	0.57
1:A:71:TYR:O	1:A:73[B]:ARG:HD3	2.05	0.57
1:C:208:MET:HA	1:C:265:MET:HE3	1.87	0.57
1:B:105:LYS:O	1:D:161:LYS:NZ	2.37	0.56
1:B:265:MET:CE	1:B:265:MET:HA	2.34	0.56
1:C:43[A]:GLU:OE2	1:C:47:ARG:NE	2.29	0.56
1:C:63[B]:GLU:OE1	1:C:64[B]:ARG:HG3	2.07	0.55
1:A:16[B]:ARG:NE	1:A:20:GLU:OE2	2.41	0.54
1:C:18[A]:ARG:CD	1:C:142:GLN:NE2	2.71	0.54
1:C:211:LEU:CD2	1:C:215[A]:MET:HE3	2.38	0.53
1:C:226:LEU:HD11	1:C:245:ILE:CD1	2.39	0.53
1:D:117:ILE:CG1	1:D:118:LEU:HD13	2.39	0.52
1:C:19:GLN:NE2	6:C:465:HOH:O	2.40	0.52
1:A:226:LEU:HD21	1:A:245:ILE:HG13	1.93	0.51
1:C:57:VAL:HG12	1:C:62[B]:PHE:CZ	2.42	0.50
1:D:117:ILE:HD12	1:D:118:LEU:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:TYR:OH	6:C:520:HOH:O	2.20	0.49
1:B:39[A]:THR:HG21	6:B:527:HOH:O	2.11	0.49
1:D:277:ASN:O	1:D:278:GLN:HB2	2.12	0.49
1:C:226:LEU:CD1	1:C:245:ILE:CD1	2.92	0.48
1:C:236:VAL:O	1:C:236:VAL:HG12	2.14	0.48
1:D:118:LEU:HD12	1:D:118:LEU:N	2.28	0.48
1:D:68:LEU:C	1:D:68:LEU:HD23	2.39	0.47
1:D:112:PRO:O	1:D:113:ALA:CB	2.62	0.47
1:C:63[A]:GLU:H	1:C:63[A]:GLU:CD	2.23	0.47
1:A:96:ALA:O	1:A:100:PRO:HA	2.15	0.47
1:D:117:ILE:HG13	1:D:118:LEU:HD13	1.97	0.47
1:C:11[B]:ARG:NH1	1:C:11[B]:ARG:CG	2.44	0.46
1:B:39[B]:THR:HG21	1:B:178:VAL:HG21	1.96	0.46
1:C:35:GLU:OE2	6:C:639:HOH:O	2.20	0.46
1:D:142:GLN:NE2	6:D:305:HOH:O	2.49	0.46
1:C:208:MET:HA	1:C:265:MET:CE	2.46	0.45
1:C:255:THR:HG22	1:C:257:ASP:N	2.23	0.45
1:C:225:LEU:O	1:C:228:GLU:HB2	2.17	0.44
1:C:182:ASP:OD2	1:C:198:ARG:NH1	2.33	0.44
1:C:219:GLU:HG2	1:C:225:LEU:HD21	1.99	0.44
1:C:160:ARG:NE	6:C:479:HOH:O	2.44	0.43
1:D:117:ILE:CD1	1:D:118:LEU:HD13	2.48	0.43
1:C:239:THR:HB	1:C:268:TRP:HB2	1.98	0.43
1:B:11:ARG:HH12	1:B:142:GLN:HE21	1.65	0.43
1:B:39[A]:THR:HG23	6:B:511:HOH:O	2.19	0.43
1:A:19[A]:GLN:OE1	6:A:572:HOH:O	2.21	0.42
1:A:201:ALA:N	1:A:202:PRO:CD	2.82	0.42
3:B:605:GOL:H31	6:B:664:HOH:O	2.19	0.42
1:D:115:SER:O	1:D:120:GLY:HA3	2.19	0.42
1:D:76:GLN:O	1:D:80[A]:GLU:HG3	2.20	0.42
1:C:62[A]:PHE:HD1	1:C:67:ASP:HB2	1.85	0.42
1:D:53:VAL:HG21	1:D:82:LEU:HD22	2.02	0.42
1:B:235[B]:ARG:HG2	1:B:236:VAL:HG13	2.02	0.42
1:C:114[B]:LEU:HD13	1:C:158:LEU:HA	2.02	0.41
1:D:243:LEU:HD12	1:D:243:LEU:N	2.35	0.41
1:B:211:LEU:HD11	1:B:226:LEU:HD23	2.02	0.41
1:C:119[B]:GLU:OE2	1:C:123:ARG:NH1	2.53	0.41
1:A:39[B]:THR:HG21	6:A:346:HOH:O	2.21	0.41
1:B:259[B]:GLN:NE2	1:B:259[B]:GLN:HA	2.36	0.41
1:C:62[B]:PHE:CE2	1:C:68[B]:LEU:HA	2.56	0.41
1:D:28:PRO:HA	1:D:54:THR:OG1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39[B]:THR:CG2	1:A:178:VAL:HG21	2.50	0.40
1:C:233:LEU:HD23	1:C:238:PHE:CB	2.47	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	302/287 (105%)	297 (98%)	5 (2%)	0	100	100
1	B	298/287 (104%)	293 (98%)	5 (2%)	0	100	100
1	C	301/287 (105%)	294 (98%)	7 (2%)	0	100	100
1	D	195/287 (68%)	190 (97%)	4 (2%)	1 (0%)	24	12
All	All	1096/1148 (96%)	1074 (98%)	21 (2%)	1 (0%)	48	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	113	ALA

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	258/240 (108%)	258 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	253/240 (105%)	246 (97%)	7 (3%)	38	20
1	C	256/240 (107%)	238 (93%)	18 (7%)	14	2
1	D	173/240 (72%)	166 (96%)	7 (4%)	28	11
All	All	940/960 (98%)	908 (97%)	32 (3%)	36	15

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	110[A]	ASP
1	B	110[B]	ASP
1	B	133	ILE
1	B	234	LEU
1	B	239	THR
1	B	242	GLU
1	B	265	MET
1	C	63[A]	GLU
1	C	63[B]	GLU
1	C	66	ASP
1	C	68[A]	LEU
1	C	68[B]	LEU
1	C	110[A]	ASP
1	C	110[B]	ASP
1	C	122	SER
1	C	176	PRO
1	C	189	ARG
1	C	193	LEU
1	C	226	LEU
1	C	232[A]	GLN
1	C	232[B]	GLN
1	C	243[A]	LEU
1	C	243[B]	LEU
1	C	255	THR
1	C	281	ASP
1	D	114	LEU
1	D	118	LEU
1	D	145	VAL
1	D	158	LEU
1	D	177	THR
1	D	243	LEU
1	D	274	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	GLN
1	A	155	GLN
1	B	13	GLN
1	B	32	ASN
1	B	142	GLN
1	B	252	GLN
1	B	260	GLN
1	C	13	GLN
1	C	19	GLN
1	C	203	GLN
1	C	252	GLN
1	C	260	GLN
1	D	13	GLN
1	D	32	ASN
1	D	155	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 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	C	501	-	25,25,25	1.47	3 (12%)	37,38,38	2.20	11 (29%)
3	GOL	C	602	-	5,5,5	0.38	0	5,5,5	0.85	0
3	GOL	D	604	-	5,5,5	0.38	0	5,5,5	0.62	0
4	IMD	A	606	-	5,5,5	0.70	0	5,5,5	0.45	0
2	AMP	D	501	-	25,25,25	1.39	4 (16%)	37,38,38	2.07	11 (29%)
3	GOL	B	605	-	5,5,5	0.48	0	5,5,5	0.54	0
3	GOL	A	601	-	5,5,5	1.00	0	5,5,5	1.27	0
2	AMP	B	501	-	25,25,25	1.33	3 (12%)	37,38,38	1.86	9 (24%)
3	GOL	B	603	-	5,5,5	0.57	0	5,5,5	1.08	1 (20%)
2	AMP	A	501	-	25,25,25	1.53	6 (24%)	37,38,38	1.88	10 (27%)

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	C	501	-	-	2/10/26/26	0/3/3/3
3	GOL	C	602	-	-	0/4/4/4	-
3	GOL	D	604	-	-	2/4/4/4	-
4	IMD	A	606	-	-	-	0/1/1/1
2	AMP	D	501	-	-	3/10/26/26	0/3/3/3
3	GOL	B	605	-	-	2/4/4/4	-
3	GOL	A	601	-	-	2/4/4/4	-
2	AMP	B	501	-	-	2/10/26/26	0/3/3/3
3	GOL	B	603	-	-	4/4/4/4	-
2	AMP	A	501	-	-	0/10/26/26	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	AMP	C5-C4	4.54	1.47	1.39
2	D	501	AMP	C5-C4	4.38	1.46	1.39
2	A	501	AMP	C5-C4	3.78	1.45	1.39
2	B	501	AMP	C5-C4	3.57	1.45	1.39
2	C	501	AMP	C5-C6	3.35	1.50	1.41
2	A	501	AMP	C5-N7	-3.03	1.33	1.39
2	B	501	AMP	C8-N7	2.94	1.37	1.31
2	B	501	AMP	C4-N9	-2.71	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	AMP	C8-N7	2.53	1.36	1.31
2	D	501	AMP	C5-C6	2.52	1.48	1.41
2	C	501	AMP	C8-N7	2.50	1.36	1.31
2	A	501	AMP	C4-N9	-2.45	1.32	1.37
2	D	501	AMP	C4-N9	-2.34	1.32	1.37
2	D	501	AMP	C5-N7	-2.29	1.34	1.39
2	A	501	AMP	C2-N1	2.15	1.37	1.33
2	A	501	AMP	P-O3P	-2.01	1.47	1.54

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	AMP	C5-C4-N3	-5.88	118.63	126.72
2	D	501	AMP	C5-C4-N3	-5.08	119.72	126.72
2	C	501	AMP	N3-C4-N9	4.94	135.57	127.17
2	A	501	AMP	C5-C4-N3	-4.76	120.17	126.72
2	B	501	AMP	C4-N9-C8	4.54	110.51	105.74
2	A	501	AMP	N3-C4-N9	4.52	134.85	127.17
2	D	501	AMP	N3-C4-N9	4.50	134.82	127.17
2	D	501	AMP	N3-C2-N1	-4.39	121.94	128.58
2	B	501	AMP	C5-C4-N3	-4.37	120.69	126.72
2	C	501	AMP	C4-C5-N7	-4.10	105.90	110.58
2	C	501	AMP	C5-N7-C8	4.03	109.79	103.45
2	B	501	AMP	N3-C4-N9	3.98	133.93	127.17
2	D	501	AMP	C4-N9-C8	3.89	109.82	105.74
2	D	501	AMP	C2-N3-C4	3.87	121.27	111.83
2	C	501	AMP	C4-N9-C8	3.73	109.66	105.74
2	A	501	AMP	N3-C2-N1	-3.71	122.97	128.58
2	A	501	AMP	C4-N9-C8	3.62	109.54	105.74
2	B	501	AMP	N3-C2-N1	-3.61	123.12	128.58
2	C	501	AMP	C2-N3-C4	3.60	120.64	111.83
2	C	501	AMP	N9-C8-N7	-3.58	108.86	113.94
2	C	501	AMP	N3-C2-N1	-3.50	123.28	128.58
2	A	501	AMP	C2-N3-C4	3.33	119.97	111.83
2	D	501	AMP	C4-C5-N7	-3.23	106.89	110.58
2	B	501	AMP	C2-N3-C4	3.07	119.32	111.83
2	B	501	AMP	N9-C8-N7	-2.79	109.98	113.94
2	D	501	AMP	C5-N7-C8	2.64	107.60	103.45
2	D	501	AMP	N9-C8-N7	-2.61	110.23	113.94
2	A	501	AMP	N9-C8-N7	-2.56	110.30	113.94
2	A	501	AMP	C5-C6-N6	-2.56	116.95	123.29
2	D	501	AMP	C2-N1-C6	2.51	122.85	118.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	AMP	N6-C6-N1	2.43	123.79	118.38
2	D	501	AMP	C6-C5-N7	2.37	136.65	132.09
2	C	501	AMP	O2'-C2'-C1'	2.26	117.88	110.10
2	B	501	AMP	N6-C6-N1	2.25	123.39	118.38
2	B	501	AMP	C4-C5-N7	-2.22	108.05	110.58
2	B	501	AMP	C2-N1-C6	2.18	122.32	118.73
2	A	501	AMP	C4-N9-C1'	-2.15	121.60	126.63
2	C	501	AMP	C6-C5-N7	2.15	136.23	132.09
2	D	501	AMP	O4'-C1'-N9	2.12	112.16	108.09
3	B	603	GOL	C3-C2-C1	-2.09	104.14	111.80
2	C	501	AMP	C2-N1-C6	2.05	122.10	118.73
2	A	501	AMP	O4'-C1'-N9	2.05	112.03	108.09

There are no chirality outliers.

All (17) torsion outliers are listed below:

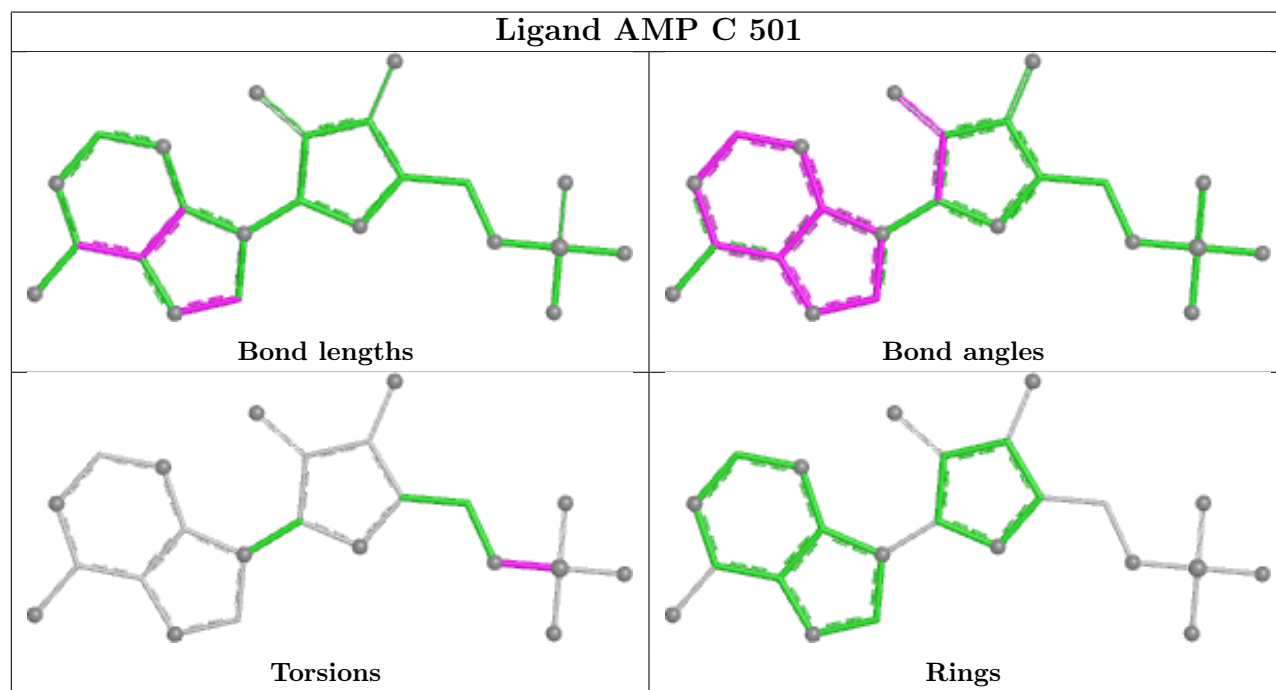
Mol	Chain	Res	Type	Atoms
2	C	501	AMP	C5'-O5'-P-O1P
2	D	501	AMP	C5'-O5'-P-O1P
2	D	501	AMP	C5'-O5'-P-O2P
2	D	501	AMP	C5'-O5'-P-O3P
3	B	603	GOL	O1-C1-C2-C3
3	B	603	GOL	C1-C2-C3-O3
3	B	605	GOL	O1-C1-C2-C3
3	D	604	GOL	C1-C2-C3-O3
3	D	604	GOL	O2-C2-C3-O3
3	A	601	GOL	C1-C2-C3-O3
3	B	603	GOL	O1-C1-C2-O2
3	B	605	GOL	O1-C1-C2-O2
2	B	501	AMP	C5'-O5'-P-O1P
3	B	603	GOL	O2-C2-C3-O3
3	A	601	GOL	O2-C2-C3-O3
2	B	501	AMP	C5'-O5'-P-O2P
2	C	501	AMP	C5'-O5'-P-O2P

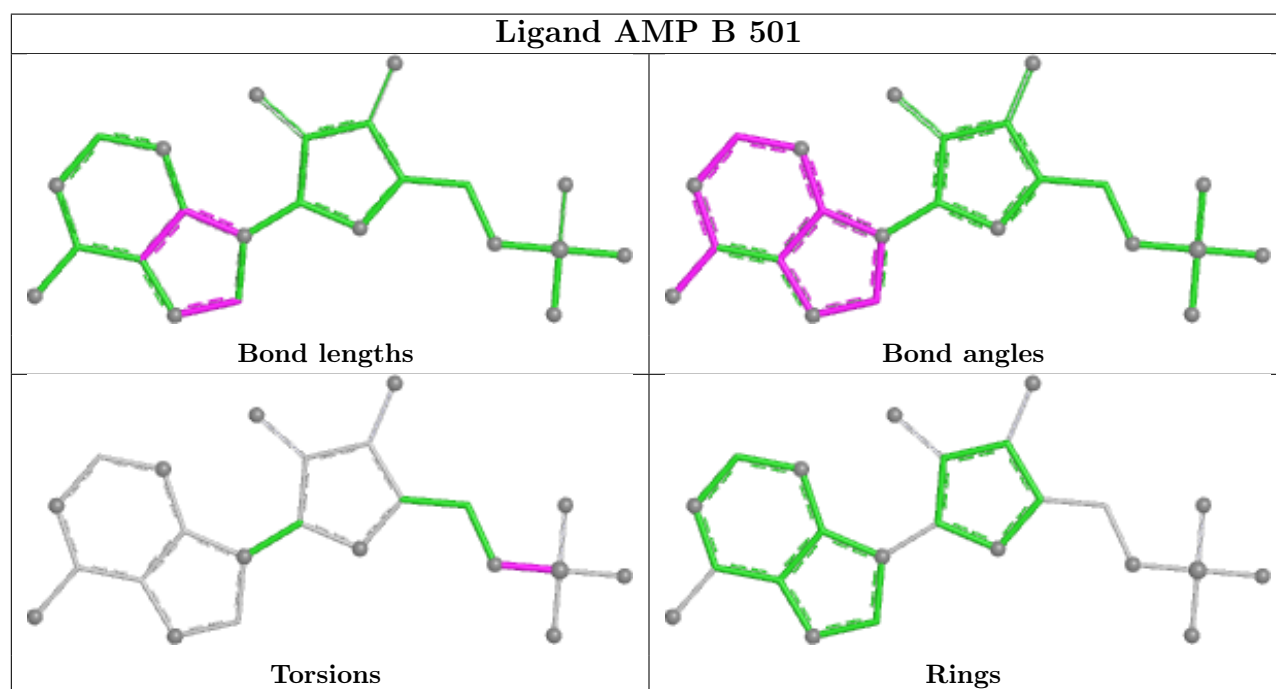
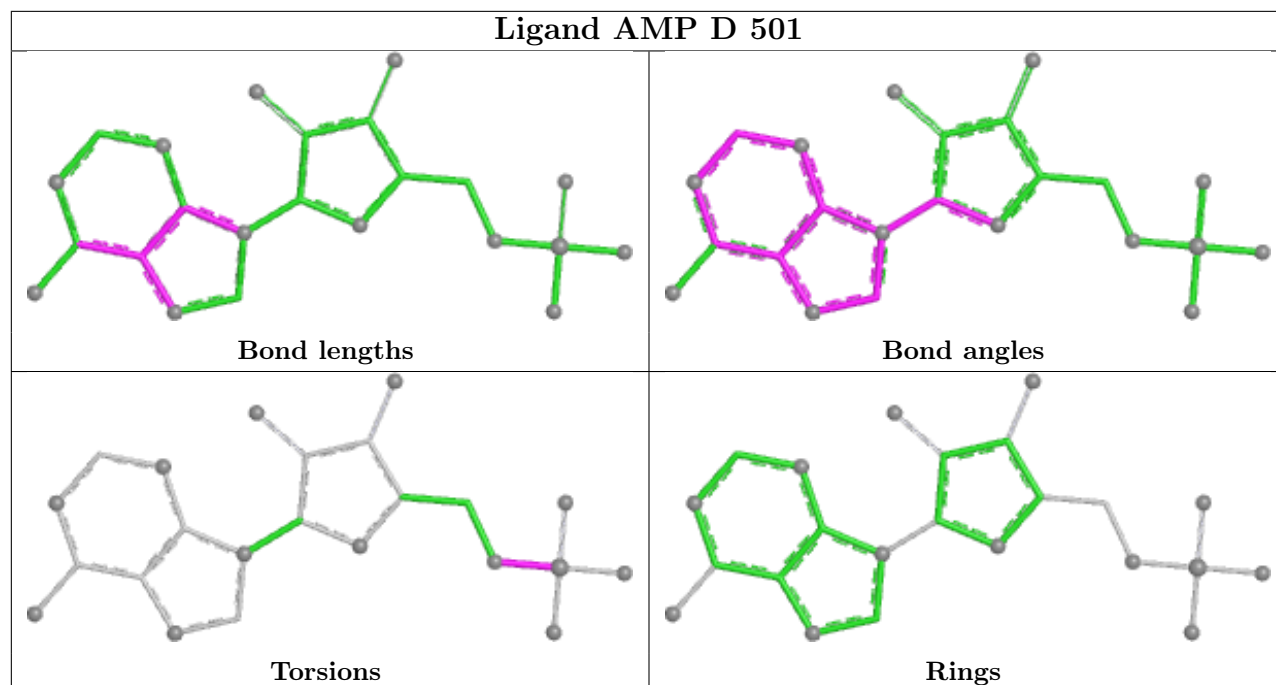
There are no ring outliers.

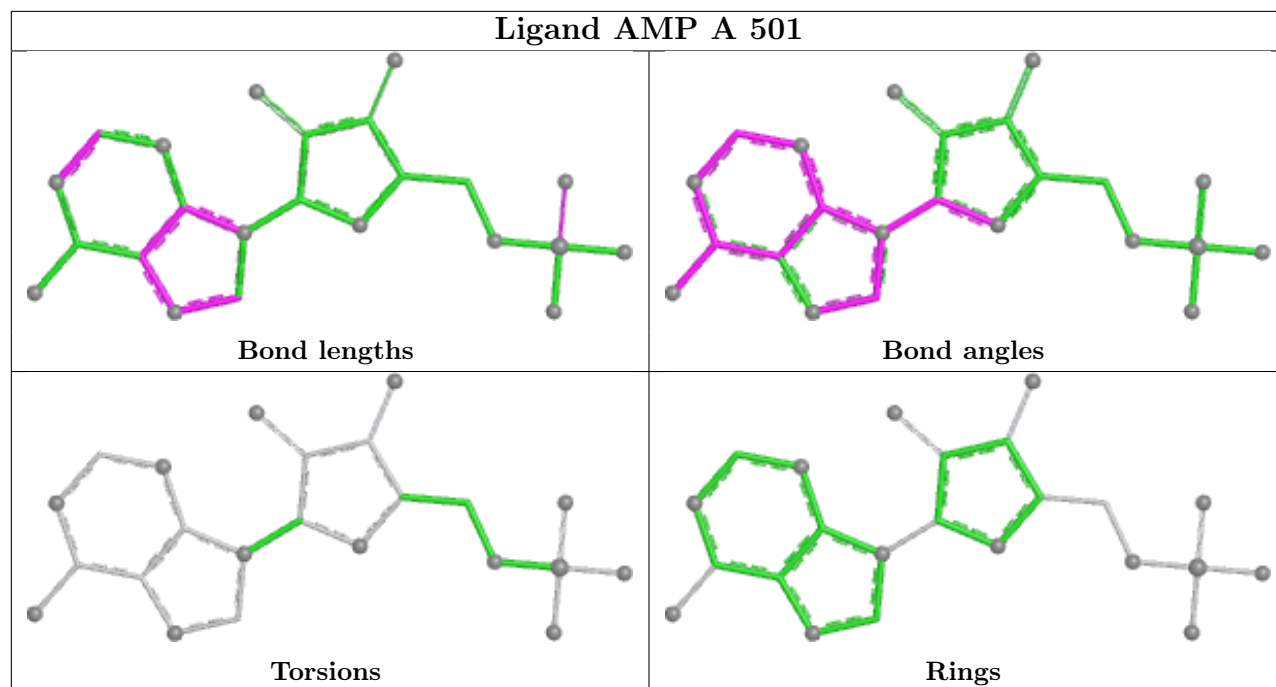
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	AMP	1	0
3	B	605	GOL	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	285/287 (99%)	-0.41	4 (1%) 73 81	9, 23, 37, 46	20 (7%)
1	B	285/287 (99%)	0.18	6 (2%) 63 71	14, 36, 59, 71	15 (5%)
1	C	284/287 (98%)	0.40	32 (11%) 10 10	13, 30, 71, 83	19 (6%)
1	D	198/287 (68%)	0.64	20 (10%) 12 13	24, 45, 95, 113	5 (2%)
All	All	1052/1148 (91%)	0.16	62 (5%) 28 30	9, 32, 68, 113	59 (5%)

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	236	VAL	5.0
1	C	267	ALA	4.8
1	C	268	TRP	4.7
1	C	69	ALA	4.6
1	D	274	LEU	4.3
1	D	263	ILE	4.3
1	D	245	ILE	4.2
1	D	272	ALA	4.2
1	C	234	LEU	4.2
1	C	233	LEU	4.0
1	D	240	PRO	3.9
1	C	230	ALA	3.9
1	C	256	VAL	3.8
1	C	238	PHE	3.7
1	D	267	ALA	3.6
1	D	262	VAL	3.6
1	D	177	THR	3.6
1	C	239	THR	3.5
1	B	66	ASP	3.4
1	C	192	TYR	3.3
1	C	270	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	284	HIS	3.2
1	D	275	ILE	3.1
1	C	272	ALA	3.1
1	C	226	LEU	2.8
1	D	278	GLN	2.8
1	C	269	LEU	2.8
1	A	284[A]	HIS	2.7
1	C	231	ALA	2.7
1	D	266	ALA	2.7
1	C	224	ALA	2.6
1	D	72	PRO	2.5
1	D	244	PHE	2.5
1	C	229	ALA	2.5
1	C	218	GLY	2.4
1	C	200	ILE	2.4
1	B	217	LEU	2.4
1	C	194	THR	2.4
1	C	193	LEU	2.4
1	D	243	LEU	2.4
1	C	235	ARG	2.3
1	B	113	ALA	2.3
1	B	235[A]	ARG	2.3
1	C	196	GLU	2.3
1	C	225	LEU	2.3
1	D	48	ALA	2.3
1	A	66	ASP	2.3
1	A	0	ALA	2.2
1	C	237	GLY	2.2
1	C	221	GLN	2.2
1	C	195	GLU	2.2
1	C	282	LEU	2.2
1	D	70[A]	HIS	2.2
1	A	283	ARG	2.2
1	D	246	ARG	2.2
1	D	0	ALA	2.2
1	D	277	ASN	2.1
1	B	71	TYR	2.1
1	D	118	LEU	2.1
1	C	275	ILE	2.0
1	C	271	LYS	2.0
1	C	191	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

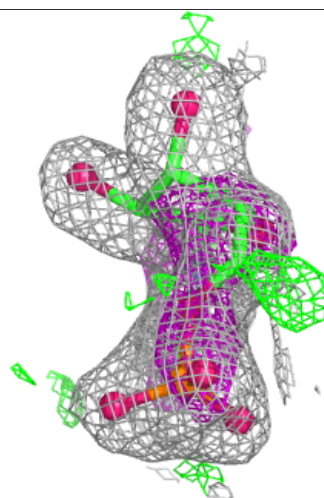
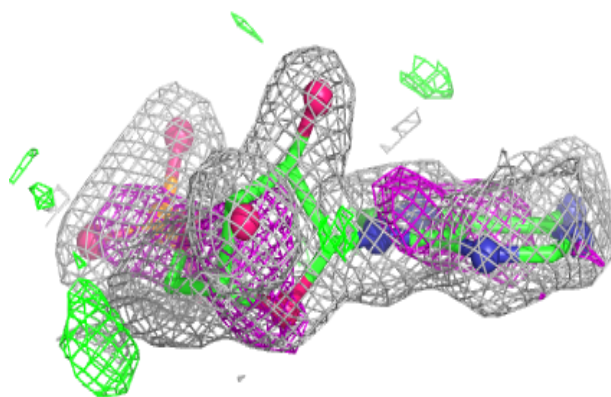
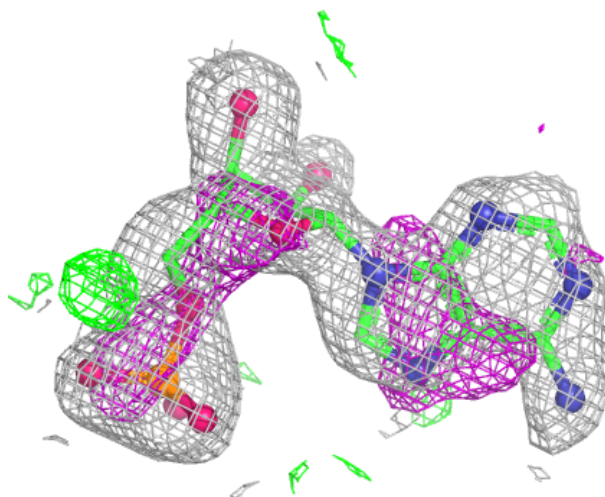
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	B	605	6/6	0.65	0.16	72,74,74,74	0
4	IMD	A	606	5/5	0.84	0.17	70,70,71,71	0
3	GOL	B	603	6/6	0.86	0.15	52,53,55,58	0
2	AMP	C	501	23/23	0.86	0.11	25,40,47,48	0
2	AMP	D	501	23/23	0.86	0.11	56,67,72,75	0
3	GOL	D	604	6/6	0.91	0.15	50,65,69,70	0
3	GOL	C	602	6/6	0.91	0.10	25,36,38,43	0
3	GOL	A	601	6/6	0.94	0.11	25,35,39,45	0
2	AMP	B	501	23/23	0.95	0.07	29,36,46,50	0
2	AMP	A	501	23/23	0.97	0.05	14,21,27,28	0
5	CL	A	607	1/1	0.99	0.07	32,32,32,32	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.

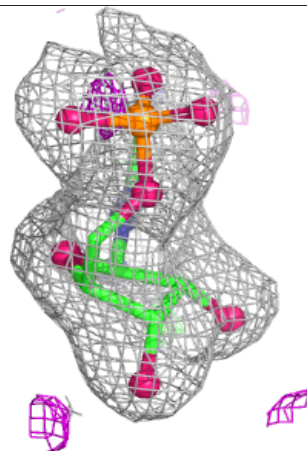
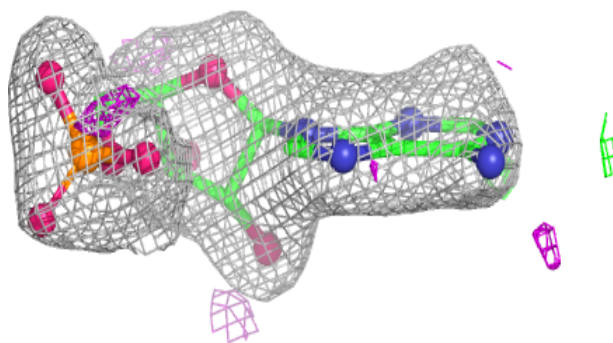
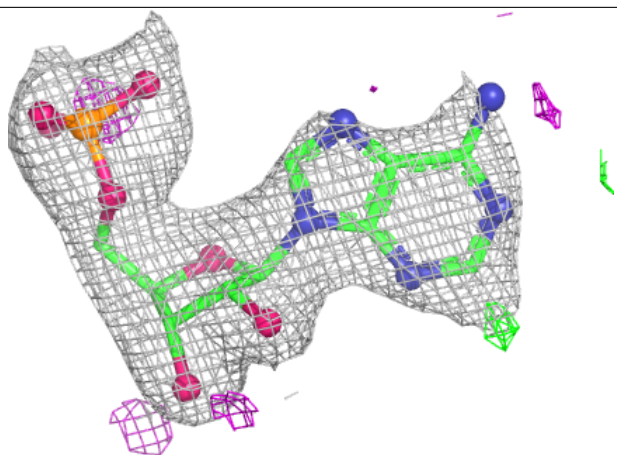
Electron density around AMP C 501:

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



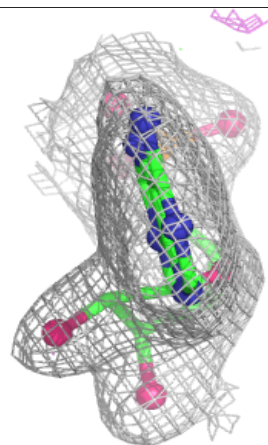
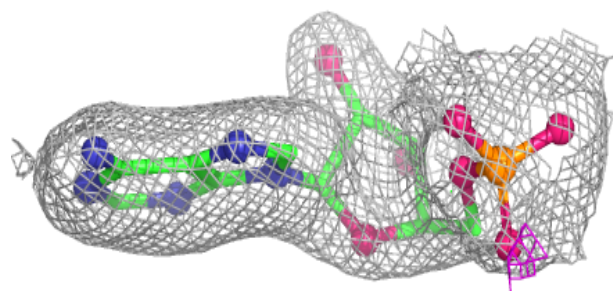
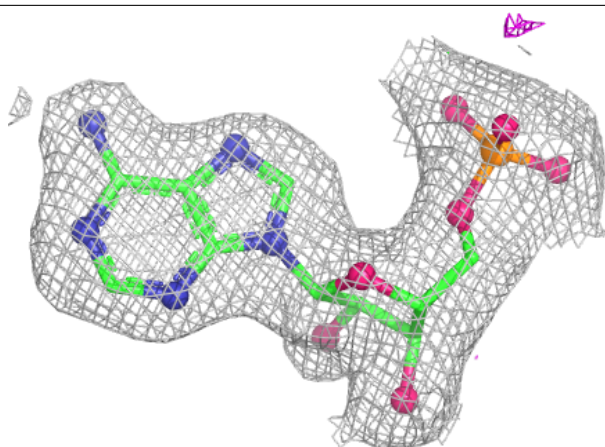
Electron density around AMP D 501:

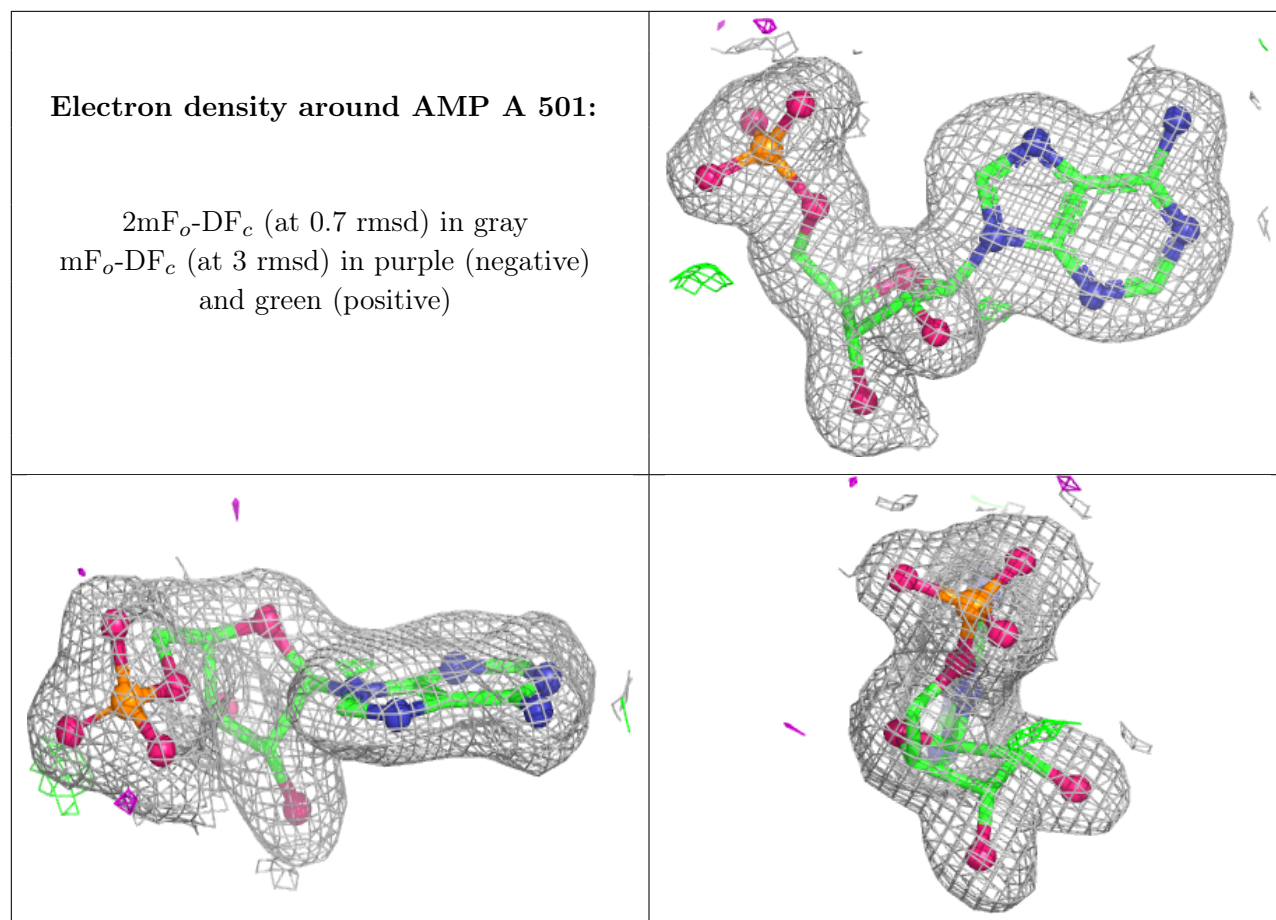
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around AMP 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 ⓘ

There are no such residues in this entry.