



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 12:42 pm BST

PDB ID : 5BPF  
Title : Crystal structure of ADP complexed D-alanine-D-alanine ligase(DDL) from *Yersinia pestis*  
Authors : Tran, H.T.; Kang, L.W.; Hong, M.K.  
Deposited on : 2015-05-28  
Resolution : 2.28 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)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

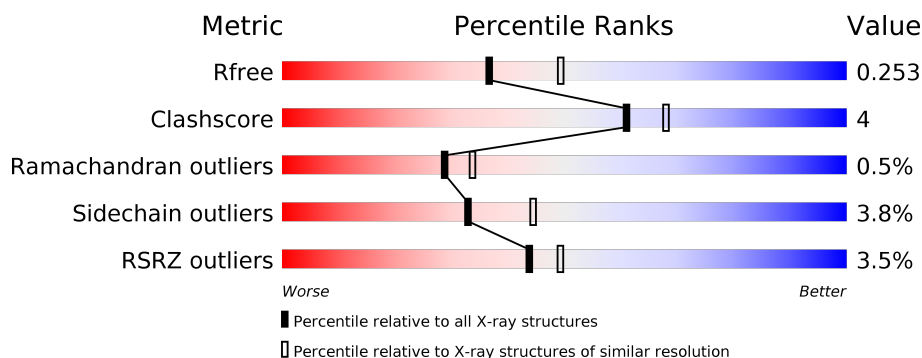
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.28 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))
$R_{free}$	130704	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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 on 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	306	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>%</span> <span>83%</span> <span>12%</span> <span>5%</span> </div> </div>
1	B	306	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>8%</span> <span>83%</span> <span>13%</span> <span>• •</span> </div> </div>
1	C	306	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span></span> <span>91%</span> <span>8%</span> <span>•</span> </div> </div>
1	D	306	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>5%</span> <span>86%</span> <span>10%</span> <span>• •</span> </div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9628 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called D-alanine-D-alanine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	291	Total	C	N	O	S	0	0	0
			2212	1409	368	424	11			
1	B	301	Total	C	N	O	S	0	0	0
			2291	1462	377	441	11			
1	C	306	Total	C	N	O	S	0	0	0
			2332	1487	384	450	11			
1	D	296	Total	C	N	O	S	0	0	0
			2251	1436	373	431	11			

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



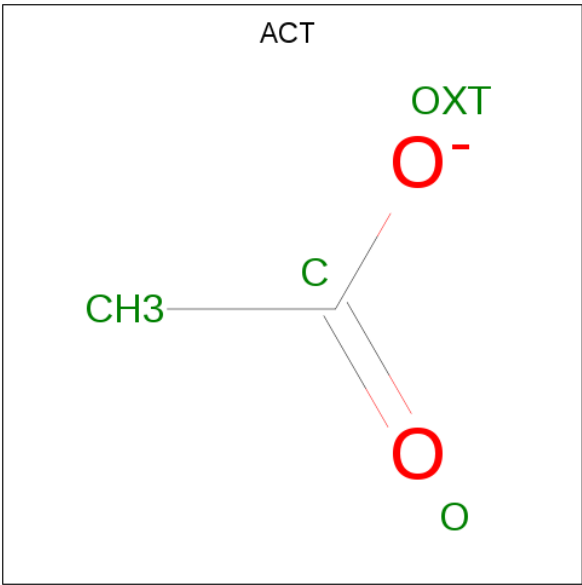
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



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

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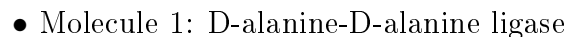
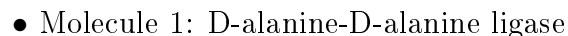
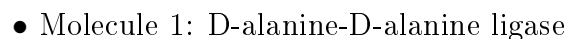
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	110	Total	O	0	0
			110	110		
6	B	81	Total	O	0	0
			81	81		
6	C	149	Total	O	0	0
			149	149		
6	D	70	Total	O	0	0
			70	70		



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







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.87Å 106.47Å 211.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.51 – 2.28 37.51 – 2.28	Depositor EDS
% Data completeness (in resolution range)	100.0 (37.51-2.28) 100.0 (37.51-2.28)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.26 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.186 , 0.253 0.191 , 0.253	Depositor DCC
$R_{free}$ test set	3336 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.2	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 42.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9628	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.96% of the height of the origin peak. No significant pseudotranslation is detected.*

<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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ACT, ADP, NA

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	0.81	0/2253	0.84	1/3052 (0.0%)
1	B	0.80	0/2333	0.83	0/3159
1	C	0.84	0/2379	0.93	5/3226 (0.2%)
1	D	0.74	0/2294	0.82	1/3108 (0.0%)
All	All	0.80	0/9259	0.86	7/12545 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	96	ASP	CB-CG-OD1	7.26	124.84	118.30
1	C	96	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	C	255	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	C	255	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	C	259	MET	CG-SD-CE	-5.41	91.54	100.20
1	D	255	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	A	306	ASP	CB-CG-OD2	5.10	122.89	118.30

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	2212	0	2219	20	0
1	B	2291	0	2290	30	0
1	C	2332	0	2323	14	0
1	D	2251	0	2252	17	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	12	0	16	0	0
3	C	6	0	8	0	0
3	D	12	0	16	1	0
4	B	27	0	12	4	0
4	C	27	0	12	0	0
4	D	27	0	12	2	0
5	B	8	0	6	1	0
5	C	8	0	6	0	0
6	A	110	0	0	0	0
6	B	81	0	0	0	0
6	C	149	0	0	0	0
6	D	70	0	0	2	0
All	All	9628	0	9172	82	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (82) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:PRO:HG2	1:B:49:GLN:HG3	1.57	0.85
1:C:214:ALA:O	1:C:221:THR:HG21	1.82	0.79
1:C:119:ARG:NH2	1:C:171:PHE:O	2.22	0.73
1:B:144:LYS:NZ	1:B:180:GLU:OE1	2.20	0.73
1:B:259:MET:HE1	4:B:401:ADP:C4	2.25	0.71
1:A:57:LYS:HD3	1:A:302:LEU:HD11	1.73	0.70
1:D:142:ILE:HD11	1:D:182:TRP:CE3	2.26	0.69
1:A:126:SER:OG	1:A:129:GLU:HG2	1.92	0.69
1:B:259:MET:HE1	4:B:401:ADP:N3	2.07	0.69
1:D:270:GLU:OE1	4:D:401:ADP:O2A	2.15	0.65
1:B:196:GLU:OE1	1:B:290:TYR:OH	2.09	0.63
1:D:119:ARG:O	1:D:123:GLU:HG3	1.97	0.63
1:C:208:VAL:HG23	1:C:209:PHE:CD2	2.33	0.63
1:C:206:PRO:HD3	1:C:221:THR:HB	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:LEU:CD2	1:C:298:VAL:HG13	2.32	0.60
1:D:142:ILE:HD11	1:D:182:TRP:CZ3	2.37	0.59
1:B:169:GLU:O	1:B:170:ALA:HB3	2.03	0.58
1:A:122:PHE:O	1:A:123:GLU:HB2	2.05	0.56
1:B:46:PRO:HG2	1:B:49:GLN:CG	2.32	0.56
1:D:47:VAL:HG12	1:D:75:VAL:HG11	1.88	0.56
1:B:142:ILE:HD11	1:B:182:TRP:HD1	1.72	0.54
1:A:189:THR:HG22	1:A:201:ILE:HB	1.91	0.53
1:B:152:VAL:HG12	1:B:153:GLY:N	2.24	0.53
1:D:142:ILE:HD11	1:D:182:TRP:HE3	1.71	0.53
1:B:118:ASN:H	1:B:121:GLN:NE2	2.06	0.52
1:B:12:THR:H	5:B:403:ACT:H2	1.73	0.52
1:B:207:GLY:O	1:B:208:VAL:HG12	2.10	0.52
1:A:196:GLU:OE1	1:A:300:ARG:NH1	2.43	0.52
1:C:227:SER:OG	1:C:234:GLU:OE2	2.28	0.51
1:A:57:LYS:HD3	1:A:302:LEU:CD1	2.39	0.51
1:B:47:VAL:HG13	1:B:75:VAL:HG11	1.93	0.51
1:A:229:LEU:HB2	1:A:234:GLU:HG2	1.93	0.49
3:D:403:GOL:H31	3:D:404:GOL:H11	1.96	0.47
1:D:96:ASP:OD2	1:D:99:ARG:HD2	2.14	0.47
1:A:121:GLN:C	1:A:122:PHE:O	2.52	0.47
1:B:270:GLU:OE2	4:B:401:ADP:O1A	2.33	0.47
1:D:130:LEU:O	1:D:133:CYS:HB2	2.15	0.47
1:A:198:LEU:HB3	1:A:199:PRO:CD	2.43	0.47
1:B:253:TRP:CH2	1:B:275:PRO:HD2	2.50	0.47
1:D:142:ILE:HG13	4:D:401:ADP:C6	2.50	0.47
1:B:127:PRO:HB3	1:B:164:GLN:HG3	1.97	0.47
1:C:305:ALA:O	1:C:306:ASP:HB2	2.16	0.46
1:B:208:VAL:HG13	1:B:209:PHE:N	2.31	0.46
1:C:253:TRP:CH2	1:C:275:PRO:HD2	2.51	0.46
1:B:259:MET:CE	4:B:401:ADP:C4	2.97	0.46
1:D:30:LEU:HD22	1:D:35:ILE:HD13	1.97	0.46
1:A:119:ARG:NH1	1:A:171:PHE:O	2.50	0.45
1:A:198:LEU:HD22	1:A:290:TYR:CD2	2.52	0.44
1:B:168:VAL:C	1:B:169:GLU:O	2.49	0.44
1:A:296:GLN:O	1:A:300:ARG:HG3	2.17	0.44
1:B:169:GLU:O	1:B:170:ALA:CB	2.66	0.44
1:B:112:SER:HB3	1:B:183:LEU:HD11	2.00	0.43
1:D:125:LEU:HG	1:D:129:GLU:CG	2.48	0.43
1:D:147:HIS:HE1	6:D:541:HOH:O	2.01	0.43
1:B:152:VAL:O	1:B:154:MET:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:125:LEU:HG	1:D:129:GLU:HG2	1.99	0.43
1:A:115:VAL:HG13	1:A:137:LEU:HD11	2.00	0.43
1:B:198:LEU:HD22	1:B:290:TYR:CD2	2.54	0.42
1:B:96:ASP:OD2	1:B:99:ARG:HD2	2.19	0.42
1:A:16:ARG:CZ	1:A:43:LYS:HE2	2.49	0.42
1:B:205:PRO:O	1:B:207:GLY:N	2.53	0.42
1:C:130:LEU:HD12	1:C:164:GLN:HE22	1.85	0.42
1:D:260:GLN:HA	1:D:265:HIS:O	2.20	0.42
1:A:49:GLN:HG2	1:A:52:GLU:OE2	2.20	0.42
1:A:122:PHE:O	1:A:124:THR:N	2.49	0.42
1:B:118:ASN:OD1	1:B:118:ASN:N	2.53	0.42
1:B:47:VAL:CG1	1:B:75:VAL:HG11	2.49	0.41
1:B:144:LYS:CE	1:B:180:GLU:OE1	2.68	0.41
1:B:119:ARG:O	1:B:121:GLN:N	2.49	0.41
1:C:182:TRP:CZ3	1:C:184:SER:HA	2.54	0.41
1:D:283:VAL:HB	1:D:284:PRO:HD3	2.01	0.41
1:D:71:THR:HG21	6:D:513:HOH:O	2.20	0.41
1:C:118:ASN:HD22	1:C:118:ASN:C	2.23	0.41
1:A:101:LYS:O	1:A:105:GLN:HG3	2.21	0.41
1:A:198:LEU:HB3	1:A:199:PRO:HD2	2.03	0.41
1:C:182:TRP:CH2	1:C:184:SER:HA	2.56	0.41
1:C:30:LEU:HD21	1:C:298:VAL:HG13	2.03	0.41
1:A:120:GLN:O	1:A:122:PHE:O	2.38	0.41
1:D:45:PHE:CZ	1:D:53:GLN:HG3	2.55	0.41
1:A:261:ASP:OD2	1:A:265:HIS:HD2	2.05	0.40
1:B:170:ALA:HB1	1:B:177:VAL:HG21	2.03	0.40
1:C:130:LEU:O	1:C:131:VAL:C	2.60	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	285/306 (93%)	277 (97%)	7 (2%)	1 (0%)	34	40
1	B	293/306 (96%)	276 (94%)	13 (4%)	4 (1%)	11	10
1	C	304/306 (99%)	297 (98%)	7 (2%)	0	100	100
1	D	290/306 (95%)	277 (96%)	12 (4%)	1 (0%)	41	49
All	All	1172/1224 (96%)	1127 (96%)	39 (3%)	6 (0%)	29	34

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	208	VAL
1	B	121	GLN
1	D	219	ASP
1	A	152	VAL
1	B	206	PRO
1	B	127	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	239/251 (95%)	233 (98%)	6 (2%)	47	62
1	B	247/251 (98%)	234 (95%)	13 (5%)	22	29
1	C	251/251 (100%)	244 (97%)	7 (3%)	43	57
1	D	243/251 (97%)	232 (96%)	11 (4%)	27	36
All	All	980/1004 (98%)	943 (96%)	37 (4%)	33	44

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

Mol	Chain	Res	Type
1	A	17	GLU
1	A	46	PRO
1	A	53	GLN
1	A	65	ARG
1	A	120	GLN

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Mol	Chain	Res	Type
1	A	155	SER
1	B	47	VAL
1	B	118	ASN
1	B	119	ARG
1	B	129	GLU
1	B	131	VAL
1	B	133	CYS
1	B	151	SER
1	B	175	SER
1	B	180	GLU
1	B	213	ASP
1	B	217	LEU
1	B	218	SER
1	B	219	ASP
1	C	48	THR
1	C	118	ASN
1	C	120	GLN
1	C	204	GLN
1	C	221	THR
1	C	298	VAL
1	C	303	MET
1	D	1	MET
1	D	19	SER
1	D	24	GLN
1	D	50	LEU
1	D	117	LEU
1	D	125	LEU
1	D	131	VAL
1	D	208	VAL
1	D	220	LYS
1	D	255	ARG
1	D	288	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	GLN
1	A	265	HIS
1	B	105	GLN
1	B	121	GLN
1	C	49	GLN
1	C	118	ASN

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Mol	Chain	Res	Type
1	C	164	GLN
1	C	172	GLN
1	D	24	GLN
1	D	105	GLN
1	D	121	GLN
1	D	147	HIS
1	D	236	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

Of 17 ligands modelled in this entry, 5 are monoatomic - leaving 12 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	$\# Z  > 2$
3	GOL	C	405	-	5,5,5	0.93	0	5,5,5	0.94	0
5	ACT	C	404	-	1,3,3	0.78	0	0,3,3	0.00	-
4	ADP	D	401	-	24,29,29	1.31	4 (16%)	29,45,45	1.26	4 (13%)
5	ACT	B	403	-	1,3,3	3.20	1 (100%)	0,3,3	0.00	-
5	ACT	C	403	-	1,3,3	2.17	1 (100%)	0,3,3	0.00	-
3	GOL	D	403	-	5,5,5	0.60	0	5,5,5	0.93	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GOL	A	403	-	5,5,5	0.80	0	5,5,5	0.64	0
4	ADP	C	401	-	24,29,29	1.27	3 (12%)	29,45,45	1.33	5 (17%)
4	ADP	B	401	-	24,29,29	1.09	1 (4%)	29,45,45	1.54	6 (20%)
5	ACT	B	404	-	1,3,3	0.70	0	0,3,3	0.00	-
3	GOL	D	404	-	5,5,5	0.52	0	5,5,5	0.80	0
3	GOL	A	402	-	5,5,5	0.43	0	5,5,5	0.45	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	C	405	-	-	2/4/4/4	-
4	ADP	D	401	-	-	4/12/32/32	0/3/3/3
3	GOL	D	403	-	-	2/4/4/4	-
3	GOL	A	403	-	-	2/4/4/4	-
4	ADP	C	401	-	-	0/12/32/32	0/3/3/3
4	ADP	B	401	-	-	5/12/32/32	0/3/3/3
3	GOL	D	404	-	-	4/4/4/4	-
3	GOL	A	402	-	-	0/4/4/4	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	401	ADP	C5-C4	3.50	1.50	1.40
5	B	403	ACT	CH3-C	3.20	1.52	1.48
4	B	401	ADP	C5-C4	3.11	1.49	1.40
4	C	401	ADP	C2-N3	3.04	1.37	1.32
4	C	401	ADP	C5-C4	2.77	1.48	1.40
4	D	401	ADP	O4'-C1'	2.42	1.44	1.41
4	D	401	ADP	C2-N3	2.35	1.35	1.32
4	C	401	ADP	C2-N1	2.22	1.38	1.33
5	C	403	ACT	CH3-C	2.17	1.51	1.48
4	D	401	ADP	C4-N3	2.07	1.38	1.35

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	401	ADP	N3-C2-N1	-3.93	122.53	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	401	ADP	N3-C2-N1	-3.40	123.36	128.68
4	B	401	ADP	C2-N1-C6	2.97	123.83	118.75
4	D	401	ADP	C4-C5-N7	-2.75	106.53	109.40
4	C	401	ADP	O3B-PB-O3A	2.70	113.69	104.64
4	B	401	ADP	C3'-C2'-C1'	2.69	105.03	100.98
4	B	401	ADP	C4-C5-N7	-2.46	106.83	109.40
4	C	401	ADP	C4-C5-N7	-2.46	106.84	109.40
4	B	401	ADP	N6-C6-N1	2.44	123.64	118.57
4	C	401	ADP	N3-C2-N1	-2.36	125.00	128.68
4	C	401	ADP	C1'-N9-C4	-2.22	122.74	126.64
4	B	401	ADP	O2B-PB-O3A	2.15	111.86	104.64
4	D	401	ADP	C2-N1-C6	2.07	122.30	118.75
4	C	401	ADP	O2B-PB-O1B	2.06	118.74	110.68
4	D	401	ADP	C3'-C2'-C1'	2.01	104.00	100.98

There are no chirality outliers.

All (19) torsion outliers are listed below:

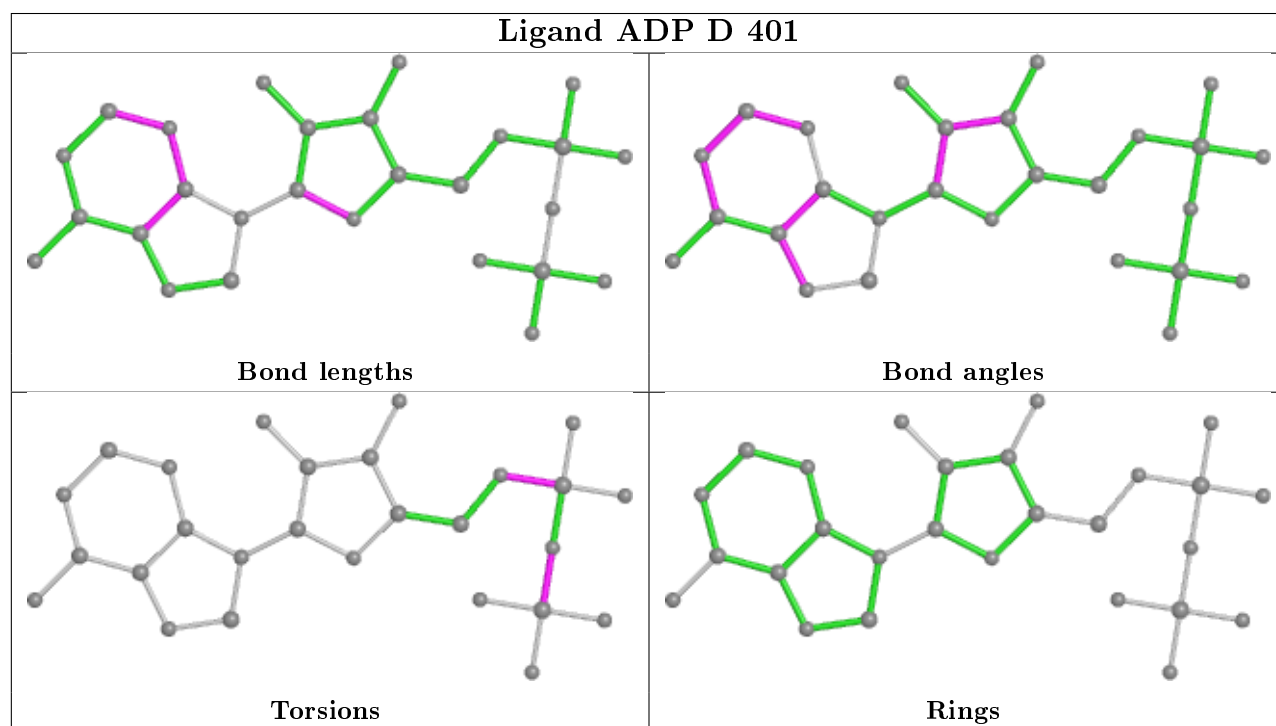
Mol	Chain	Res	Type	Atoms
3	D	403	GOL	O1-C1-C2-C3
4	B	401	ADP	PA-O3A-PB-O2B
3	D	404	GOL	C1-C2-C3-O3
4	D	401	ADP	C5'-O5'-PA-O3A
3	C	405	GOL	C1-C2-C3-O3
3	A	403	GOL	C1-C2-C3-O3
3	D	404	GOL	O1-C1-C2-C3
3	C	405	GOL	O2-C2-C3-O3
3	A	403	GOL	O2-C2-C3-O3
3	D	404	GOL	O1-C1-C2-O2
4	D	401	ADP	PA-O3A-PB-O1B
4	B	401	ADP	PA-O3A-PB-O3B
3	D	403	GOL	C1-C2-C3-O3
4	D	401	ADP	C5'-O5'-PA-O2A
3	D	404	GOL	O2-C2-C3-O3
4	B	401	ADP	PB-O3A-PA-O5'
4	D	401	ADP	C5'-O5'-PA-O1A
4	B	401	ADP	C3'-C4'-C5'-O5'
4	B	401	ADP	PA-O3A-PB-O1B

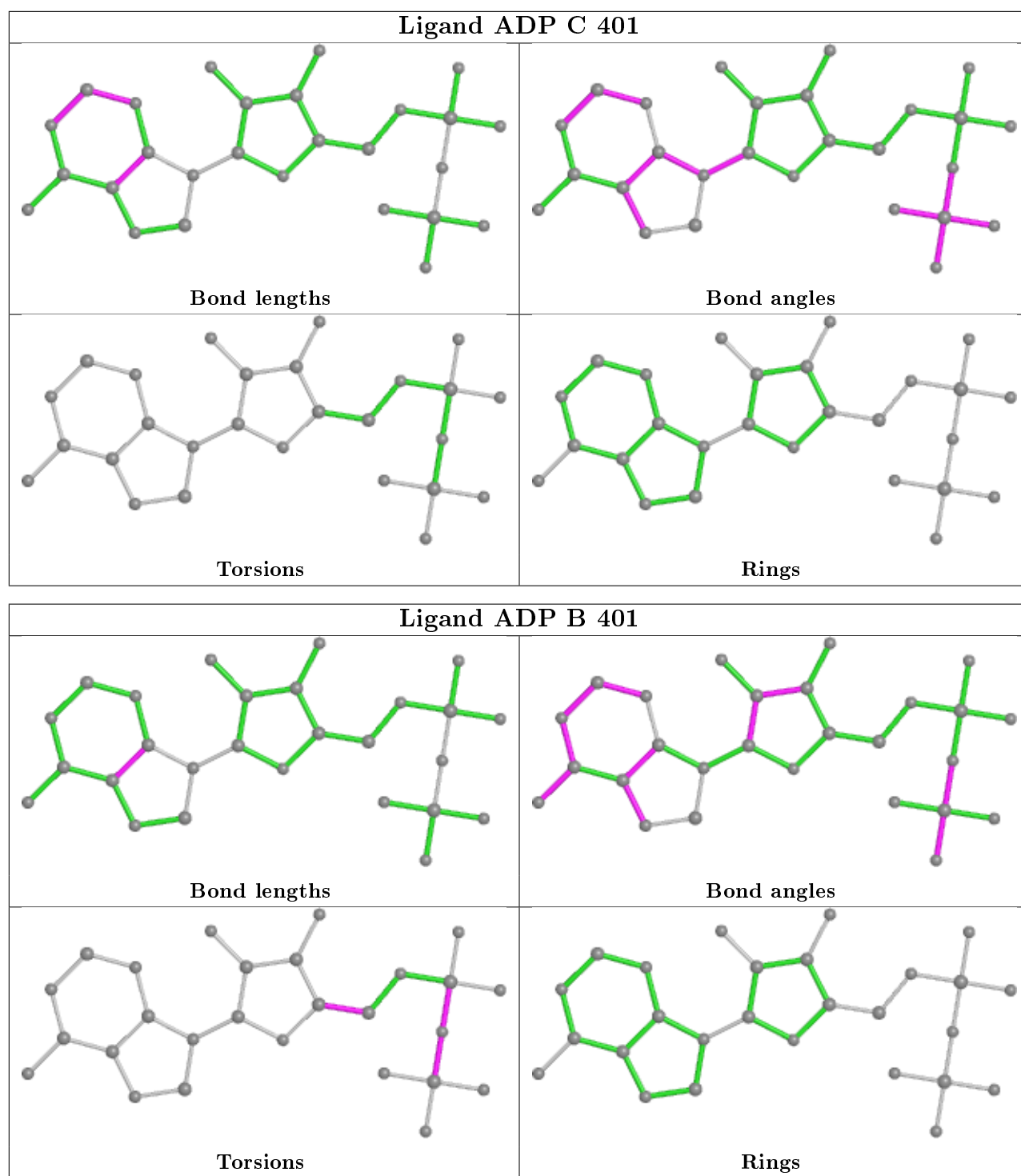
There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	401	ADP	2	0
5	B	403	ACT	1	0
3	D	403	GOL	1	0
4	B	401	ADP	4	0
3	D	404	GOL	1	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 ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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, 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	291/306 (95%)	-0.26	2 (0%) 87 90	16, 29, 61, 83	0
1	B	301/306 (98%)	0.15	23 (7%) 13 17	16, 31, 90, 118	0
1	C	306/306 (100%)	-0.37	1 (0%) 94 95	18, 27, 49, 70	0
1	D	296/306 (96%)	-0.02	16 (5%) 25 31	20, 38, 71, 92	0
All	All	1194/1224 (97%)	-0.13	42 (3%) 44 49	16, 31, 72, 118	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	217	LEU	8.4
1	B	170	ALA	6.3
1	B	219	ASP	6.2
1	B	212	TYR	6.2
1	B	213	ASP	5.9
1	A	151	SER	5.5
1	B	120	GLN	5.1
1	B	125	LEU	5.1
1	B	171	PHE	4.0
1	B	129	GLU	3.7
1	B	214	ALA	3.5
1	B	169	GLU	3.5
1	B	172	GLN	3.5
1	D	129	GLU	3.4
1	D	219	ASP	3.4
1	D	280	HIS	3.3
1	B	168	VAL	3.2
1	D	218	SER	3.1
1	D	220	LYS	3.1
1	D	206	PRO	3.0
1	B	207	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	231	ASP	2.9
1	B	165	LYS	2.8
1	D	165	LYS	2.7
1	D	125	LEU	2.7
1	B	124	THR	2.6
1	D	168	VAL	2.6
1	B	166	ALA	2.5
1	B	122	PHE	2.5
1	D	166	ALA	2.5
1	D	124	THR	2.4
1	D	207	GLY	2.4
1	B	130	LEU	2.4
1	B	163	LEU	2.3
1	C	124	THR	2.3
1	D	128	GLU	2.3
1	B	128	GLU	2.2
1	B	117	LEU	2.2
1	B	153	GLY	2.2
1	D	135	ALA	2.1
1	A	280	HIS	2.1
1	D	120	GLN	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 carbohydrates 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, 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.

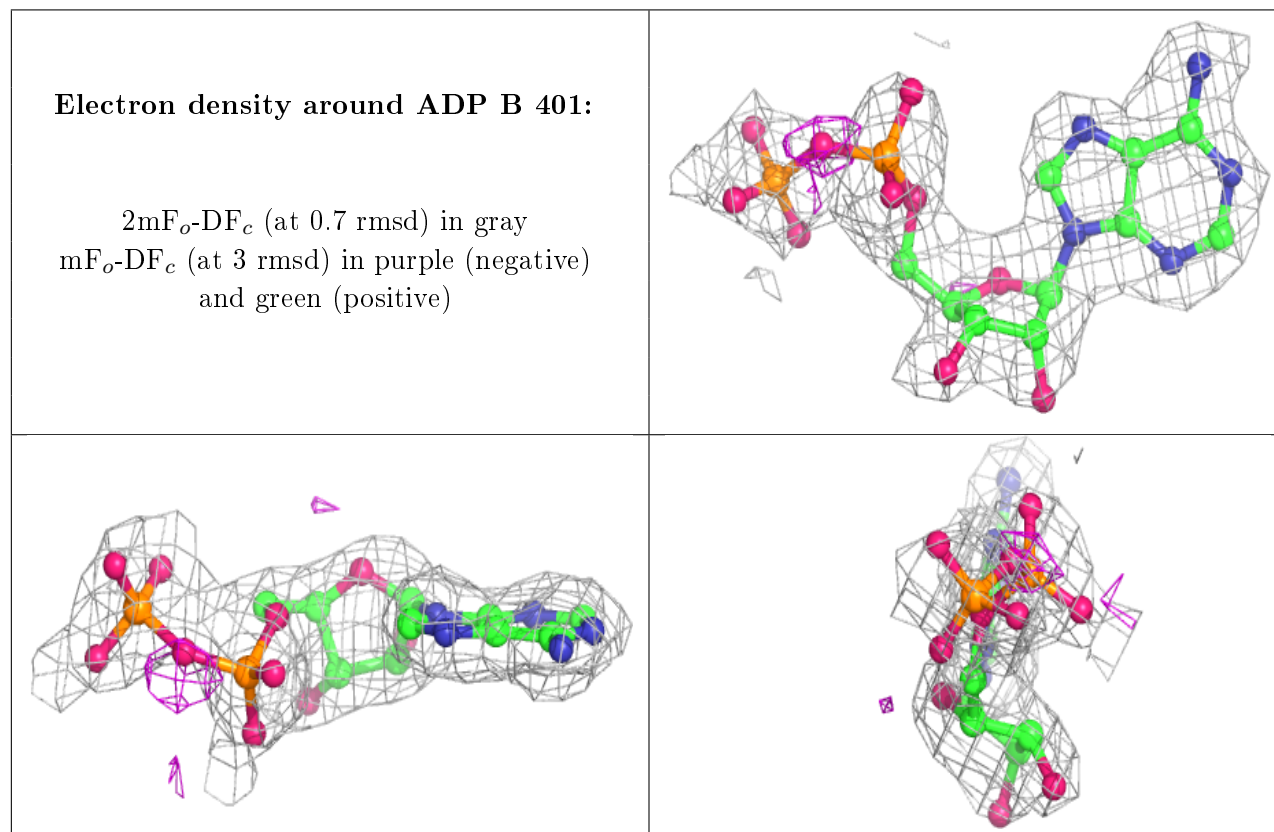
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	ACT	C	404	4/4	0.81	0.16	53,55,57,63	0
5	ACT	B	403	4/4	0.84	0.16	36,44,46,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	A	403	6/6	0.84	0.22	30,45,46,47	0
4	ADP	B	401	27/27	0.84	0.17	49,59,107,109	0
3	GOL	C	405	6/6	0.87	0.15	35,45,51,51	0
5	ACT	B	404	4/4	0.88	0.20	51,57,58,64	0
3	GOL	A	402	6/6	0.89	0.12	48,61,63,63	0
3	GOL	D	403	6/6	0.90	0.13	37,44,45,50	0
4	ADP	D	401	27/27	0.91	0.14	43,52,89,96	0
2	NA	D	402	1/1	0.91	0.09	23,23,23,23	0
3	GOL	D	404	6/6	0.92	0.13	32,41,44,44	0
2	NA	A	404	1/1	0.94	0.18	28,28,28,28	0
4	ADP	C	401	27/27	0.97	0.10	26,30,69,71	0
5	ACT	C	403	4/4	0.97	0.11	34,34,35,36	0
2	NA	A	401	1/1	0.98	0.15	19,19,19,19	0
2	NA	C	402	1/1	0.98	0.09	21,21,21,21	0
2	NA	B	402	1/1	0.98	0.09	17,17,17,17	0

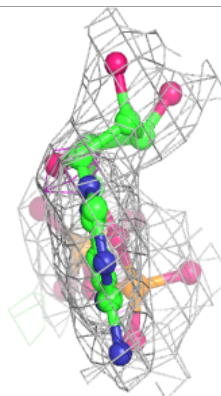
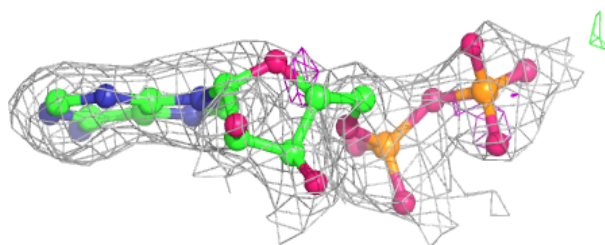
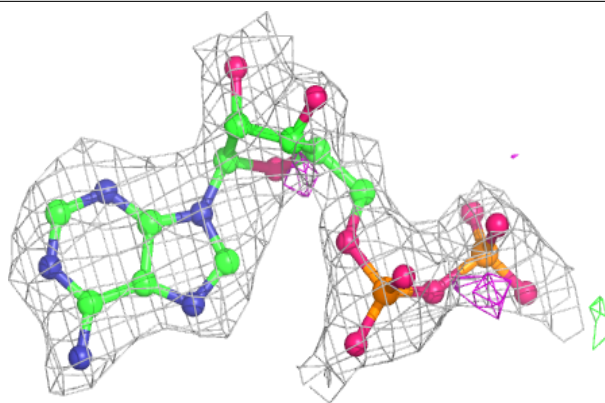
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



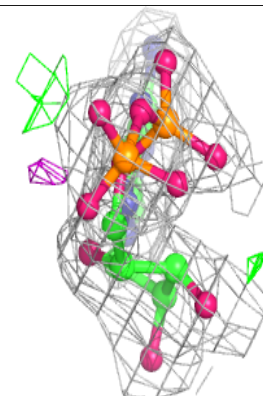
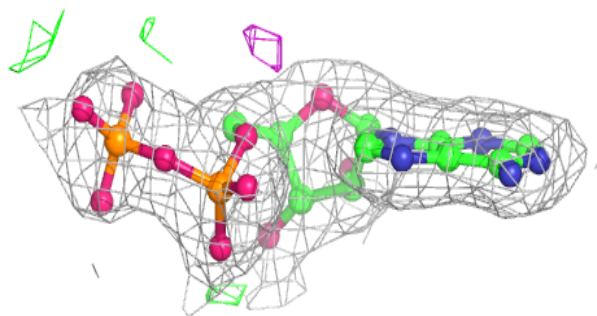
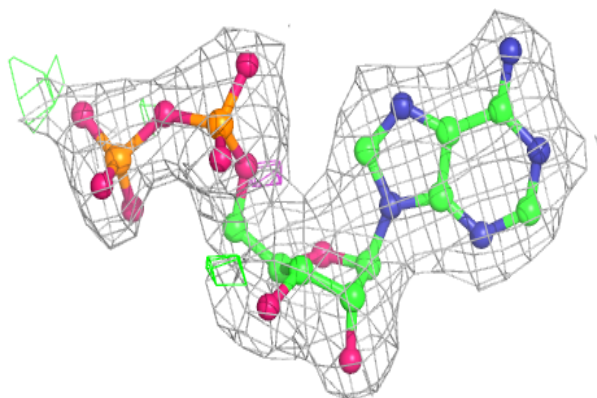


**Electron density around ADP D 401:**

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

**Electron density around ADP C 401:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.