



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2024 – 11:27 PM EDT

PDB ID : 6CIB  
Title : The structure of YcaO from Methanopyrus kandleri bound with AMPPCP and Mg<sup>2+</sup>  
Authors : Dong, S.-H.; Nair, S.K.  
Deposited on : 2018-02-23  
Resolution : 2.05 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.

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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
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)	:	2.37.1

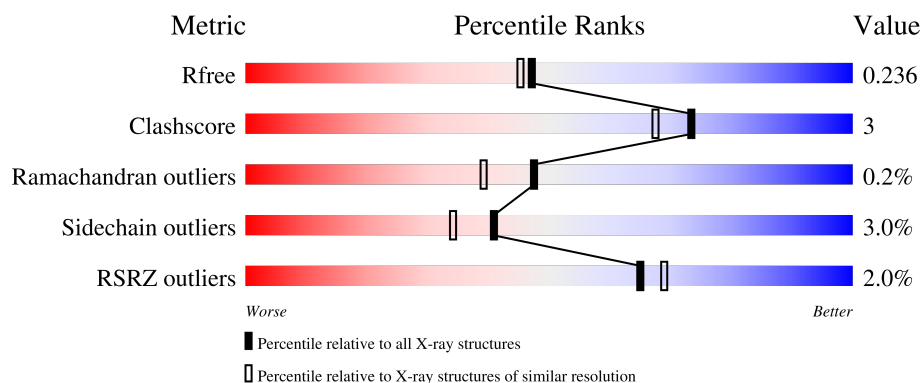
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	377	<div> <div>2%</div> <div>88%</div> <div>7%</div> <div>• •</div> </div>
1	B	377	<div> <div>3%</div> <div>86%</div> <div>8%</div> <div>• •</div> </div>
1	C	377	<div> <div>2%</div> <div>87%</div> <div>8%</div> <div>5%</div> </div>
1	D	377	<div> <div>2%</div> <div>85%</div> <div>10%</div> <div>• 5%</div> </div>
1	E	377	<div> <div>2%</div> <div>83%</div> <div>12%</div> <div>• •</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	377	<div> <div></div> <div>%</div> <div>86%</div> <div>9%</div> <div>..</div> </div>

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	OXM	B	403	-	-	X	-
4	OXM	C	403	-	-	X	-
4	OXM	D	403	-	-	X	-
4	OXM	F	403	-	-	X	-

## 2 Entry composition [i](#)

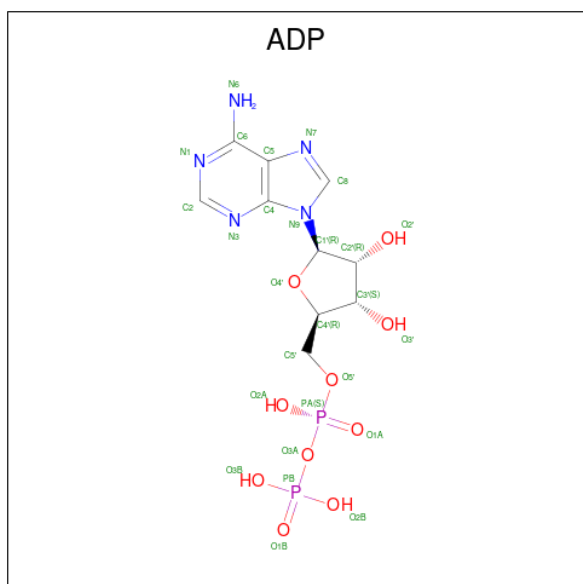
There are 5 unique types of molecules in this entry. The entry contains 19088 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 YcaO.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	363	Total	C	N	O	S	Se	0	0	0
			2902	1824	523	547	1	7			
1	B	364	Total	C	N	O	S	Se	0	0	0
			2908	1828	524	548	1	7			
1	C	360	Total	C	N	O	S	Se	0	0	0
			2878	1808	519	543	1	7			
1	D	360	Total	C	N	O	S	Se	0	0	0
			2878	1809	519	542	1	7			
1	E	361	Total	C	N	O	S	Se	0	0	0
			2889	1816	520	545	1	7			
1	F	362	Total	C	N	O	S	Se	0	0	0
			2891	1816	521	546	1	7			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).

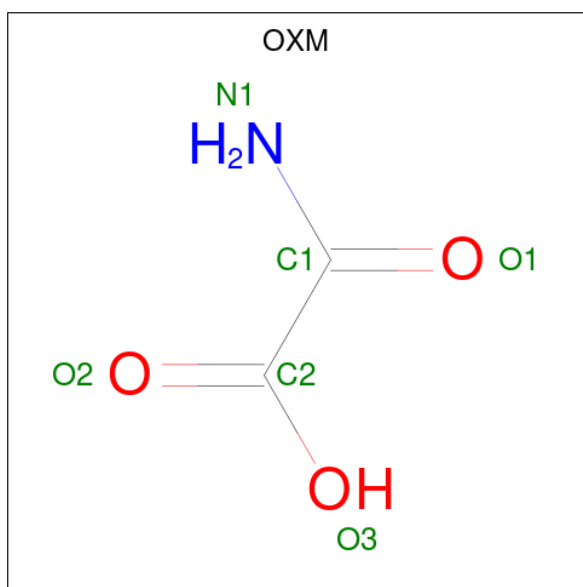


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		

- Molecule 4 is OXAMIC ACID (three-letter code: OXM) (formula: C<sub>2</sub>H<sub>3</sub>NO<sub>3</sub>).



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

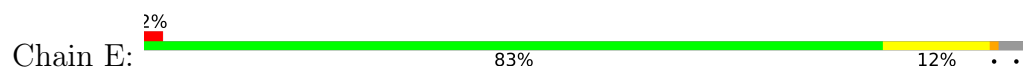
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	254	Total	O	0	0
			254	254		
5	B	292	Total	O	0	0
			292	292		
5	C	205	Total	O	0	0
			205	205		
5	D	200	Total	O	0	0
			200	200		
5	E	283	Total	O	0	0
			283	283		
5	F	304	Total	O	0	0
			304	304		

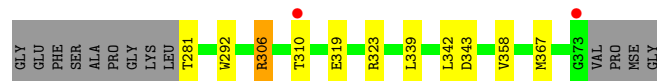
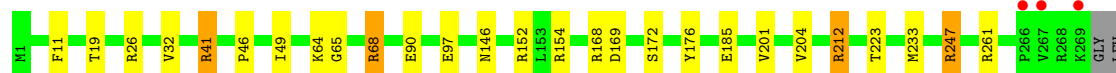
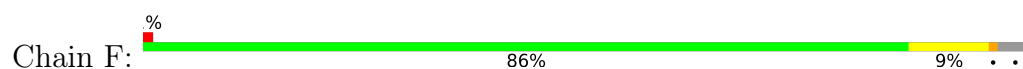




• Molecule 1: YcaO



• Molecule 1: YcaO





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	123.23Å 105.63Å 139.30Å 90.00° 103.64° 90.00°	Depositor
Resolution (Å)	25.00 – 2.05 80.74 – 2.04	Depositor EDS
% Data completeness (in resolution range)	90.8 (25.00-2.05) 90.7 (80.74-2.04)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.47 (at 2.03Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.195 , 0.234 0.198 , 0.236	Depositor DCC
$R_{free}$ test set	9926 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.8	Xtriage
Anisotropy	0.434	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 49.3	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	19088	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.97% 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: MG, OXM, ADP

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	0.43	0/2955	0.67	2/3996 (0.1%)
1	B	0.45	0/2960	0.71	5/4004 (0.1%)
1	C	0.42	0/2929	0.66	1/3961 (0.0%)
1	D	0.44	0/2930	0.69	3/3964 (0.1%)
1	E	0.45	0/2940	0.73	5/3975 (0.1%)
1	F	0.46	0/2943	0.70	4/3982 (0.1%)
All	All	0.44	0/17657	0.69	20/23882 (0.1%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	41	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	E	247	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	B	41	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	E	212	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	F	212	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	E	41	ARG	NE-CZ-NH2	-5.63	117.49	120.30
1	E	212	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	D	41	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	D	247	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	F	247	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	C	247	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	D	41	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	B	247	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	A	41	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	B	68	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	B	212	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	A	258	MSE	CG-SE-CE	-5.23	87.39	98.90
1	F	68	ARG	NE-CZ-NH2	-5.19	117.70	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	41	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	E	52	ARG	NE-CZ-NH2	-5.02	117.79	120.30

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	2902	0	2893	18	0
1	B	2908	0	2895	23	0
1	C	2878	0	2862	15	0
1	D	2878	0	2865	20	0
1	E	2889	0	2878	24	0
1	F	2891	0	2871	21	0
2	A	27	0	12	0	0
2	B	27	0	12	0	0
2	C	27	0	12	0	0
2	D	27	0	12	0	0
2	E	27	0	12	0	0
2	F	27	0	12	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	6	0	2	0	0
4	B	6	0	2	4	0
4	C	6	0	2	3	0
4	D	6	0	2	2	0
4	E	6	0	2	1	0
4	F	6	0	2	6	0
5	A	254	0	0	0	0
5	B	292	0	0	1	0
5	C	205	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	200	0	0	1	0
5	E	283	0	0	1	0
5	F	304	0	0	0	0
All	All	19088	0	17348	116	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 3.

All (116) 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:68:ARG:HD2	4:B:403:OXM:O2	1.74	0.86
1:B:243:MSE:SE	5:B:650:HOH:O	2.42	0.86
1:D:243:MSE:HE3	1:D:247:ARG:CZ	2.08	0.83
1:B:238:SER:HB2	1:B:243:MSE:HE2	1.62	0.82
1:C:41:ARG:HH11	4:C:403:OXM:HN2	1.27	0.80
1:B:243:MSE:HE3	1:B:247:ARG:CZ	2.12	0.79
1:F:68:ARG:HH11	4:F:403:OXM:HN1	1.29	0.77
1:E:68:ARG:HD2	4:E:403:OXM:O3	1.85	0.75
1:D:68:ARG:HD2	4:D:403:OXM:O3	1.90	0.72
1:C:367:MSE:HB3	1:E:284:ARG:HH22	1.55	0.72
1:D:238:SER:HB2	1:D:243:MSE:HE2	1.73	0.71
1:A:222:VAL:HG12	1:A:233:MSE:HG2	1.75	0.69
1:C:45:ILE:HD11	1:C:193:LEU:HD11	1.73	0.69
1:C:68:ARG:HD2	4:C:403:OXM:O1	1.94	0.68
1:C:169:ASP:OD2	1:C:212:ARG:HD3	1.94	0.67
1:B:238:SER:CB	1:B:243:MSE:HE2	2.24	0.66
1:B:146:ASN:OD1	1:B:168:ARG:HG3	1.96	0.65
1:F:169:ASP:OD2	1:F:212:ARG:HD3	1.97	0.65
1:E:81:GLU:OE2	1:E:82:ARG:NH1	2.31	0.63
1:D:243:MSE:SE	5:D:553:HOH:O	2.65	0.63
1:F:41:ARG:HH11	4:F:403:OXM:HN2	1.47	0.62
1:D:146:ASN:OD1	1:D:168:ARG:HG3	2.02	0.60
1:B:169:ASP:OD2	1:B:212:ARG:HD3	2.01	0.59
1:E:146:ASN:OD1	1:E:168:ARG:HG3	2.03	0.59
1:E:169:ASP:OD2	1:E:212:ARG:HD3	2.02	0.58
1:A:11:PHE:CE1	1:A:310:THR:HG21	2.39	0.58
1:A:169:ASP:OD2	1:A:212:ARG:HD3	2.03	0.57
1:A:254:GLN:O	1:A:258:MSE:HG2	2.04	0.57
1:A:146:ASN:OD1	1:A:168:ARG:HG3	2.05	0.57
1:D:238:SER:CB	1:D:243:MSE:HE2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:PRO:HG2	1:B:100:LYS:HE3	1.87	0.56
1:B:222:VAL:HG12	1:B:233:MSE:HG2	1.87	0.56
1:F:146:ASN:OD1	1:F:168:ARG:HG3	2.05	0.55
1:D:96:PRO:HG3	1:D:113:TRP:CD1	2.43	0.54
1:C:96:PRO:HG2	1:C:100:LYS:HE3	1.88	0.54
1:D:169:ASP:OD2	1:D:212:ARG:HD3	2.06	0.54
1:A:284:ARG:HD2	1:E:194:ARG:HH22	1.73	0.54
4:B:403:OXM:HN1	1:E:331:LYS:HA	1.73	0.54
1:C:146:ASN:OD1	1:C:168:ARG:HG3	2.08	0.54
1:F:68:ARG:CD	4:F:403:OXM:O1	2.56	0.53
1:B:52:ARG:NH1	1:B:61:HIS:NE2	2.56	0.53
1:A:284:ARG:CD	1:E:194:ARG:HH22	2.22	0.53
1:E:348:ARG:NH1	5:E:503:HOH:O	2.43	0.52
1:E:19:THR:HG23	1:E:152:ARG:HD2	1.91	0.52
1:C:134:HIS:ND1	1:C:143:SER:HB3	2.26	0.51
1:E:26:ARG:HH12	1:E:343:ASP:HB3	1.76	0.50
1:B:224:GLU:HA	1:B:231:MSE:HE2	1.93	0.49
1:F:68:ARG:HD3	4:F:403:OXM:O1	2.12	0.49
1:A:281:THR:HG22	1:A:284:ARG:H	1.77	0.49
1:E:89:GLU:HA	1:E:92:ILE:HD12	1.94	0.49
1:D:319:GLU:O	1:D:323:ARG:HG2	2.13	0.49
1:D:222:VAL:HG12	1:D:233:MSE:HG2	1.95	0.48
1:E:310:THR:HG22	1:E:316:LEU:HD13	1.95	0.48
1:E:61:HIS:CE1	1:E:82:ARG:HG3	2.49	0.48
1:F:46:PRO:HD2	1:F:65:GLY:O	2.14	0.48
1:F:11:PHE:CE1	1:F:310:THR:HG21	2.49	0.48
1:C:369:GLU:O	1:E:283:GLU:HG2	2.14	0.47
1:B:225:ALA:H	1:B:231:MSE:HE3	1.79	0.47
1:F:306:ARG:HH12	1:F:310:THR:HG23	1.79	0.47
1:F:41:ARG:HD3	4:F:403:OXM:HN2	1.79	0.47
1:E:319:GLU:O	1:E:323:ARG:HG2	2.15	0.47
1:C:68:ARG:HH11	4:C:403:OXM:HN1	1.64	0.46
1:B:28:LEU:O	1:B:32:VAL:HB	2.15	0.46
1:C:49:ILE:HD13	1:C:261:ARG:HD2	1.98	0.46
1:A:26:ARG:HH22	1:A:343:ASP:HB3	1.80	0.46
1:D:204:VAL:HG22	1:D:223:THR:HG22	1.98	0.46
1:A:32:VAL:HG23	1:A:342:LEU:HD11	1.98	0.46
1:D:68:ARG:CD	4:D:403:OXM:O3	2.63	0.46
1:B:203:ARG:HB2	1:B:224:GLU:HB2	1.97	0.45
1:A:32:VAL:HG22	1:A:83:ALA:CB	2.46	0.45
1:B:61:HIS:CE1	1:B:82:ARG:HG3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:11:PHE:CE1	1:E:310:THR:HG21	2.52	0.45
1:E:255:GLY:HA2	1:E:258:MSE:HE2	1.98	0.44
1:F:49:ILE:HD13	1:F:261:ARG:HD2	1.99	0.44
1:F:247:ARG:NH2	2:F:401:ADP:O3B	2.50	0.44
1:B:26:ARG:HH12	1:B:343:ASP:HB3	1.83	0.44
1:D:160:GLN:OE1	1:D:247:ARG:NH2	2.50	0.44
1:F:68:ARG:HD2	4:F:403:OXM:O1	2.18	0.44
1:C:179:ILE:O	1:C:181:PRO:HD3	2.17	0.44
1:B:41:ARG:NH1	4:B:403:OXM:HN2	2.16	0.44
1:B:68:ARG:CD	4:B:403:OXM:O2	2.58	0.44
1:C:172:SER:HA	1:C:358:VAL:HG13	2.00	0.44
1:E:222:VAL:HG12	1:E:233:MSE:HG2	1.99	0.43
1:F:176:TYR:CG	1:F:367:MSE:HE3	2.53	0.43
1:C:19:THR:HG23	1:C:152:ARG:HD2	2.00	0.43
1:F:319:GLU:O	1:F:323:ARG:HG2	2.18	0.43
1:C:89:GLU:HA	1:C:92:ILE:HD12	2.01	0.43
1:D:264:GLU:HB2	1:D:266:PRO:HD3	2.01	0.43
1:F:26:ARG:HH12	1:F:343:ASP:HB3	1.83	0.43
1:A:28:LEU:O	1:A:32:VAL:HB	2.18	0.43
1:F:19:THR:HG23	1:F:152:ARG:HD3	2.00	0.42
1:A:281:THR:CG2	1:A:284:ARG:H	2.32	0.42
1:A:46:PRO:HB3	1:A:68:ARG:CZ	2.49	0.42
1:D:310:THR:HG22	1:D:316:LEU:HD13	2.01	0.42
1:A:19:THR:HG23	1:A:152:ARG:HD3	2.01	0.42
1:A:204:VAL:HG22	1:A:223:THR:HG22	2.01	0.42
1:A:229:GLU:H	1:A:229:GLU:CD	2.22	0.41
1:B:32:VAL:HG23	1:B:342:LEU:HD11	2.01	0.41
1:F:172:SER:HA	1:F:358:VAL:HG13	2.01	0.41
1:D:49:ILE:HD13	1:D:261:ARG:HD2	2.02	0.41
1:F:339:LEU:O	1:F:342:LEU:O	2.38	0.41
1:B:32:VAL:HG22	1:B:83:ALA:CB	2.50	0.41
1:E:45:ILE:HD11	1:E:193:LEU:HD11	2.02	0.41
1:D:11:PHE:CE1	1:D:310:THR:HG21	2.56	0.41
1:D:133:PHE:O	1:D:143:SER:OG	2.39	0.41
1:F:204:VAL:HG22	1:F:223:THR:HG22	2.03	0.41
1:D:145:THR:HG22	1:D:145:THR:O	2.20	0.41
1:E:371:PRO:HA	1:E:372:PRO:HD3	1.89	0.41
1:E:176:TYR:CG	1:E:367:MSE:HE3	2.56	0.40
1:F:233:MSE:HE1	1:F:292:TRP:NE1	2.36	0.40
1:A:284:ARG:HD2	1:E:198:GLU:OE1	2.21	0.40
1:B:78:GLU:O	1:B:82:ARG:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:201:VAL:HG22	1:E:225:ALA:HB2	2.03	0.40
1:B:51:ARG:HH12	1:B:53:ARG:NH1	2.18	0.40
1:B:319:GLU:O	1:B:323:ARG:HG2	2.21	0.40
1:D:28:LEU:O	1:D:32:VAL:HB	2.21	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	359/377 (95%)	351 (98%)	7 (2%)	1 (0%)	41	31
1	B	360/377 (96%)	350 (97%)	10 (3%)	0	100	100
1	C	356/377 (94%)	348 (98%)	7 (2%)	1 (0%)	41	31
1	D	356/377 (94%)	344 (97%)	11 (3%)	1 (0%)	41	31
1	E	355/377 (94%)	345 (97%)	10 (3%)	0	100	100
1	F	358/377 (95%)	348 (97%)	9 (2%)	1 (0%)	41	31
All	All	2144/2262 (95%)	2086 (97%)	54 (2%)	4 (0%)	47	39

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	201	VAL
1	D	372	PRO
1	A	201	VAL
1	C	201	VAL

### 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	310/312 (99%)	302 (97%)	8 (3%)	46	39
1	B	310/312 (99%)	301 (97%)	9 (3%)	42	35
1	C	306/312 (98%)	299 (98%)	7 (2%)	50	44
1	D	307/312 (98%)	297 (97%)	10 (3%)	38	31
1	E	309/312 (99%)	296 (96%)	13 (4%)	30	22
1	F	308/312 (99%)	300 (97%)	8 (3%)	46	39
All	All	1850/1872 (99%)	1795 (97%)	55 (3%)	41	34

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	VAL
1	A	64	LYS
1	A	154	ARG
1	A	185	GLU
1	A	280	LEU
1	A	281	THR
1	A	284	ARG
1	A	369	GLU
1	B	32	VAL
1	B	52	ARG
1	B	64	LYS
1	B	93	GLU
1	B	109	GLU
1	B	143	SER
1	B	154	ARG
1	B	194	ARG
1	B	267	VAL
1	C	64	LYS
1	C	93	GLU
1	C	109	GLU
1	C	143	SER
1	C	154	ARG

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Mol	Chain	Res	Type
1	C	194	ARG
1	C	281	THR
1	D	3	ASP
1	D	32	VAL
1	D	64	LYS
1	D	187	HIS
1	D	194	ARG
1	D	263	ILE
1	D	264	GLU
1	D	288	LEU
1	D	290	ARG
1	D	369	GLU
1	E	3	ASP
1	E	32	VAL
1	E	64	LYS
1	E	154	ARG
1	E	178	ARG
1	E	185	GLU
1	E	192	GLU
1	E	194	ARG
1	E	203	ARG
1	E	258	MSE
1	E	264	GLU
1	E	348	ARG
1	E	367	MSE
1	F	32	VAL
1	F	64	LYS
1	F	90	GLU
1	F	97	GLU
1	F	154	ARG
1	F	185	GLU
1	F	281	THR
1	F	306	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 6 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$
2	ADP	C	401	-	24,29,29	1.07	2 (8%)	29,45,45	1.30	2 (6%)
4	OXM	C	403	-	5,5,5	3.30	1 (20%)	4,6,6	1.51	1 (25%)
4	OXM	D	403	-	5,5,5	3.03	1 (20%)	4,6,6	1.00	0
2	ADP	B	401	-	24,29,29	1.15	3 (12%)	29,45,45	1.21	1 (3%)
2	ADP	F	401	-	24,29,29	1.09	3 (12%)	29,45,45	1.33	5 (17%)
4	OXM	F	403	-	5,5,5	3.45	1 (20%)	4,6,6	1.78	2 (50%)
2	ADP	A	401	-	24,29,29	1.10	3 (12%)	29,45,45	1.24	3 (10%)
2	ADP	D	401	-	24,29,29	1.11	3 (12%)	29,45,45	1.19	3 (10%)
4	OXM	E	403	-	5,5,5	3.10	1 (20%)	4,6,6	1.01	0
2	ADP	E	401	-	24,29,29	1.09	3 (12%)	29,45,45	1.29	4 (13%)
4	OXM	B	403	-	5,5,5	3.28	1 (20%)	4,6,6	1.84	2 (50%)
4	OXM	A	403	-	5,5,5	3.14	1 (20%)	4,6,6	1.34	1 (25%)

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	ADP	C	401	-	-	1/12/32/32	0/3/3/3
4	OXM	C	403	-	-	0/3/4/4	-
4	OXM	D	403	-	-	0/3/4/4	-
2	ADP	B	401	-	-	1/12/32/32	0/3/3/3
2	ADP	F	401	-	-	1/12/32/32	0/3/3/3
4	OXM	F	403	-	-	0/3/4/4	-
2	ADP	A	401	-	-	2/12/32/32	0/3/3/3
2	ADP	D	401	-	-	1/12/32/32	0/3/3/3
4	OXM	E	403	-	-	0/3/4/4	-
2	ADP	E	401	-	-	1/12/32/32	0/3/3/3
4	OXM	B	403	-	-	0/3/4/4	-
4	OXM	A	403	-	-	0/3/4/4	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	403	OXM	C1-C2	-7.36	1.46	1.55
4	B	403	OXM	C1-C2	-7.05	1.46	1.55
4	C	403	OXM	C1-C2	-7.00	1.46	1.55
4	A	403	OXM	C1-C2	-6.74	1.46	1.55
4	E	403	OXM	C1-C2	-6.47	1.47	1.55
4	D	403	OXM	C1-C2	-6.41	1.47	1.55
2	D	401	ADP	C5-C4	2.80	1.48	1.40
2	B	401	ADP	C5-C4	2.75	1.48	1.40
2	E	401	ADP	C5-C4	2.69	1.48	1.40
2	C	401	ADP	C5-C4	2.65	1.48	1.40
2	E	401	ADP	O4'-C1'	2.63	1.44	1.41
2	F	401	ADP	C5-C4	2.56	1.47	1.40
2	F	401	ADP	O4'-C1'	2.55	1.44	1.41
2	D	401	ADP	O4'-C1'	2.52	1.44	1.41
2	A	401	ADP	C5-C4	2.52	1.47	1.40
2	B	401	ADP	C2-N3	2.51	1.36	1.32
2	C	401	ADP	C2-N3	2.48	1.36	1.32
2	B	401	ADP	O4'-C1'	2.41	1.44	1.41
2	A	401	ADP	O4'-C1'	2.37	1.44	1.41
2	D	401	ADP	C2-N3	2.36	1.35	1.32
2	A	401	ADP	C2-N3	2.24	1.35	1.32
2	E	401	ADP	C2-N3	2.13	1.35	1.32
2	F	401	ADP	C2-N3	2.11	1.35	1.32

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	401	ADP	N3-C2-N1	-3.72	122.87	128.68
2	A	401	ADP	N3-C2-N1	-3.64	122.98	128.68
2	B	401	ADP	N3-C2-N1	-3.62	123.01	128.68
2	E	401	ADP	N3-C2-N1	-3.58	123.08	128.68
2	C	401	ADP	N3-C2-N1	-3.55	123.12	128.68
2	D	401	ADP	N3-C2-N1	-3.36	123.42	128.68
4	B	403	OXM	O3-C2-C1	2.79	120.29	113.84
4	F	403	OXM	O3-C2-C1	2.73	120.14	113.84
2	C	401	ADP	C4-C5-N7	-2.66	106.63	109.40
2	D	401	ADP	C4-C5-N7	-2.49	106.80	109.40
2	E	401	ADP	O3B-PB-O2B	2.45	116.99	107.64
4	B	403	OXM	O2-C2-C1	-2.36	116.81	122.06
4	C	403	OXM	O3-C2-C1	2.35	119.28	113.84
2	F	401	ADP	C2-N1-C6	2.34	122.75	118.75
2	E	401	ADP	C2-N1-C6	2.26	122.63	118.75
2	D	401	ADP	C2-N1-C6	2.26	122.62	118.75
2	A	401	ADP	C4-C5-N7	-2.25	107.05	109.40
4	F	403	OXM	O2-C2-C1	-2.21	117.13	122.06
4	A	403	OXM	O3-C2-C1	2.19	118.91	113.84
2	A	401	ADP	C2-N1-C6	2.15	122.44	118.75
2	F	401	ADP	O3A-PB-O1B	-2.10	99.52	111.19
2	F	401	ADP	C4-C5-N7	-2.06	107.25	109.40
2	E	401	ADP	C4-C5-N7	-2.06	107.26	109.40
2	F	401	ADP	N6-C6-N1	2.01	122.75	118.57

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	ADP	PB-O3A-PA-O5'
2	E	401	ADP	PB-O3A-PA-O5'
2	B	401	ADP	PB-O3A-PA-O5'
2	D	401	ADP	PB-O3A-PA-O5'
2	F	401	ADP	PB-O3A-PA-O5'
2	A	401	ADP	C5'-O5'-PA-O3A
2	C	401	ADP	C5'-O5'-PA-O3A

There are no ring outliers.

6 monomers are involved in 17 short contacts:

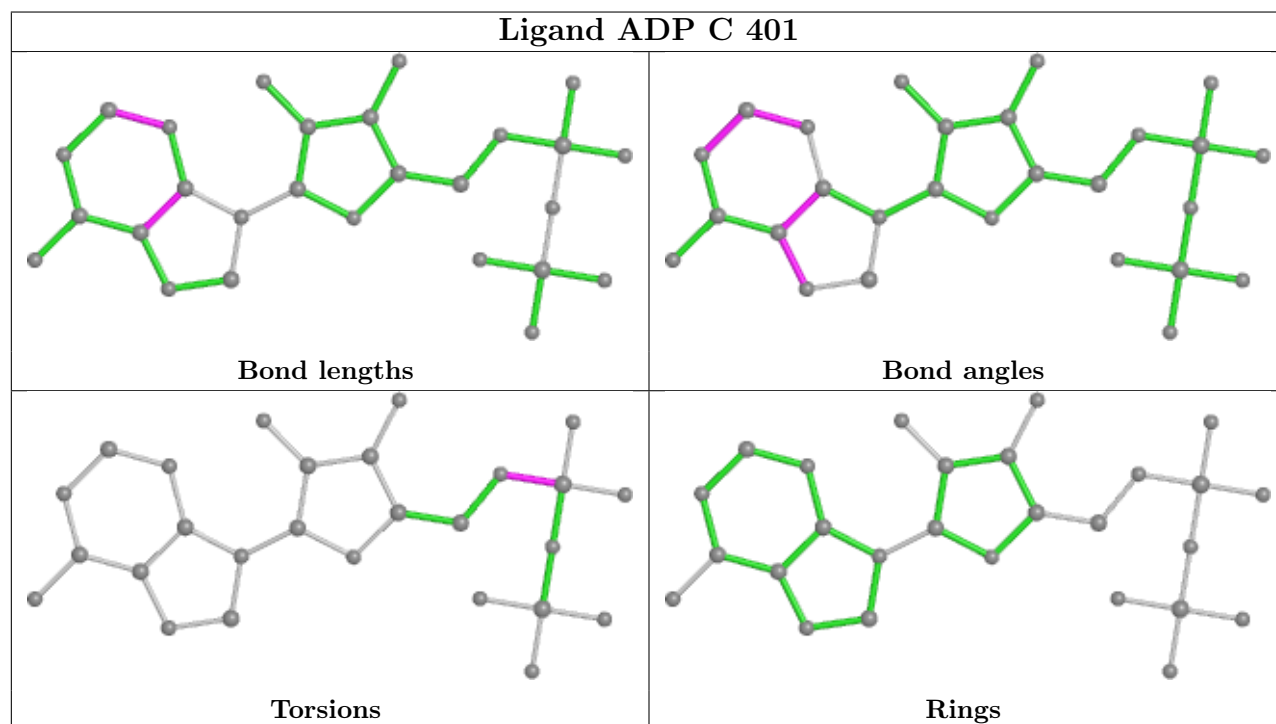
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	403	OXM	3	0

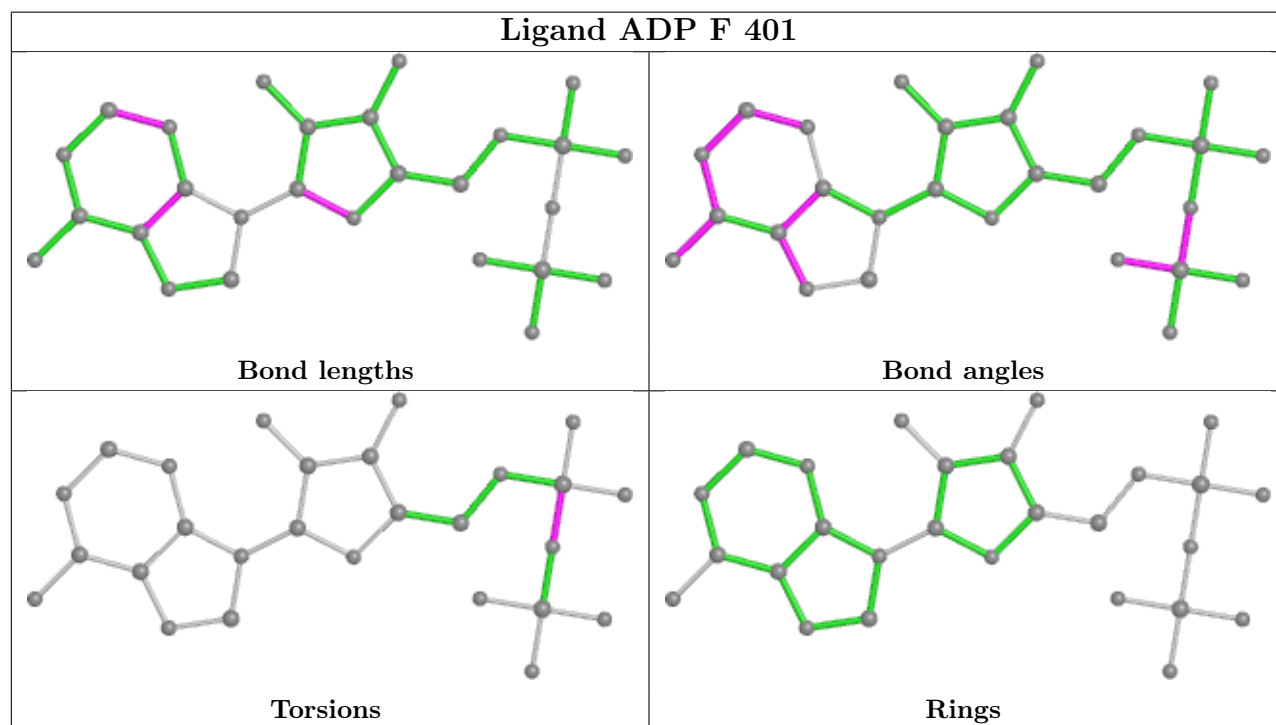
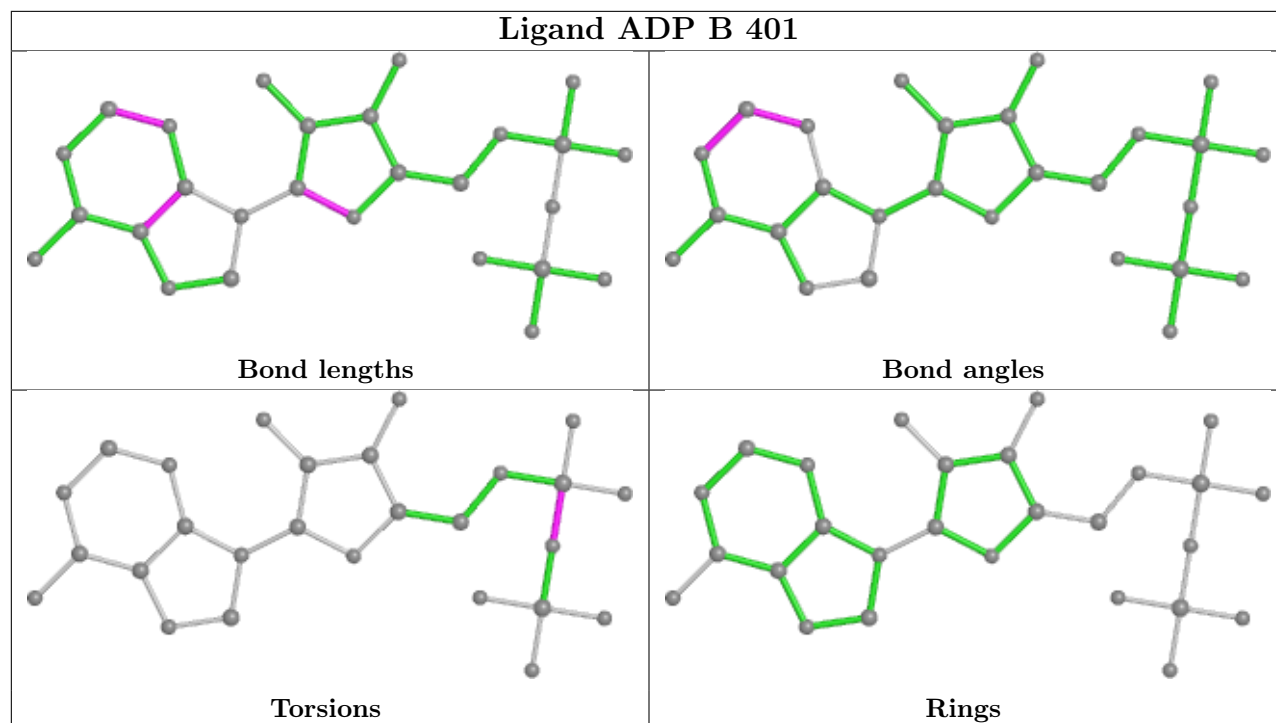
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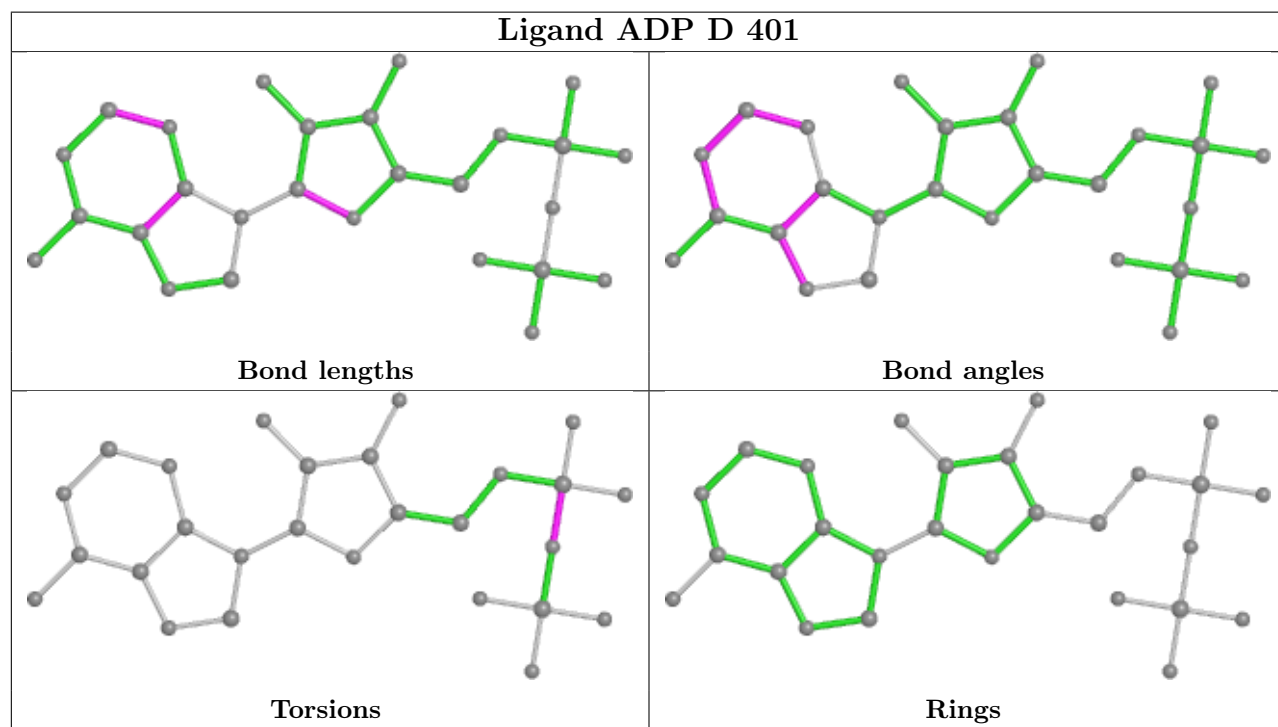
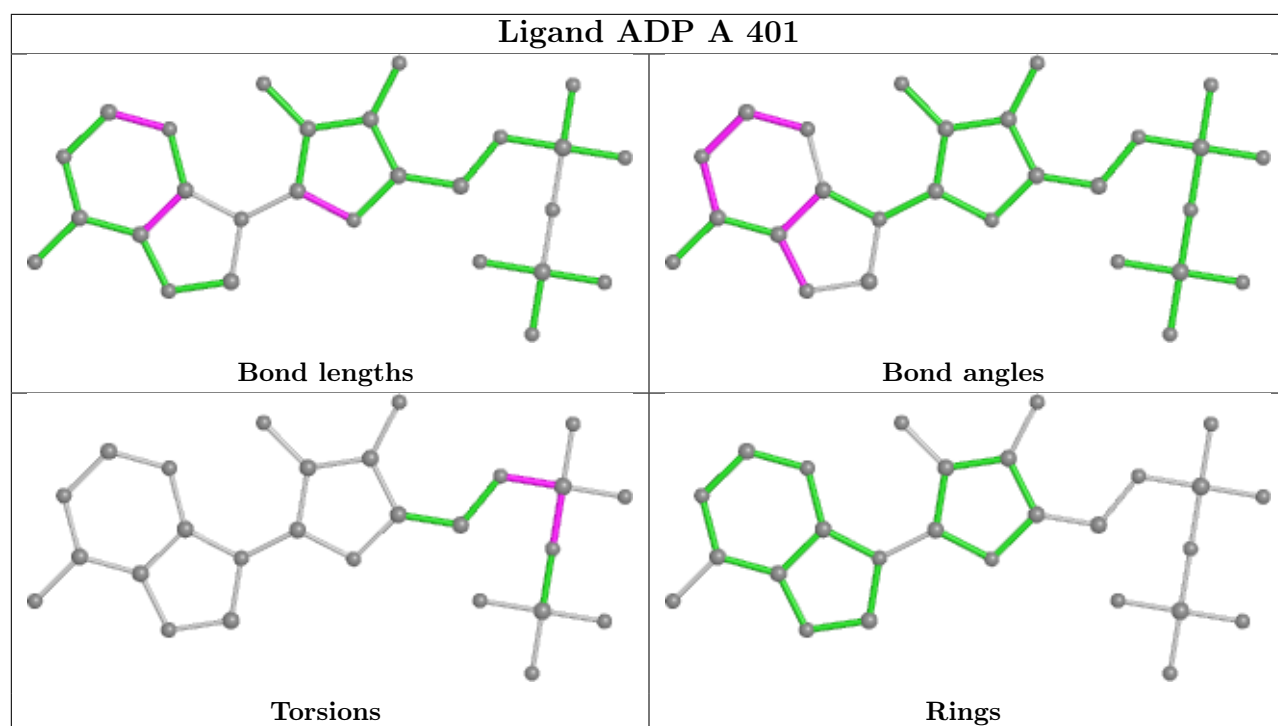
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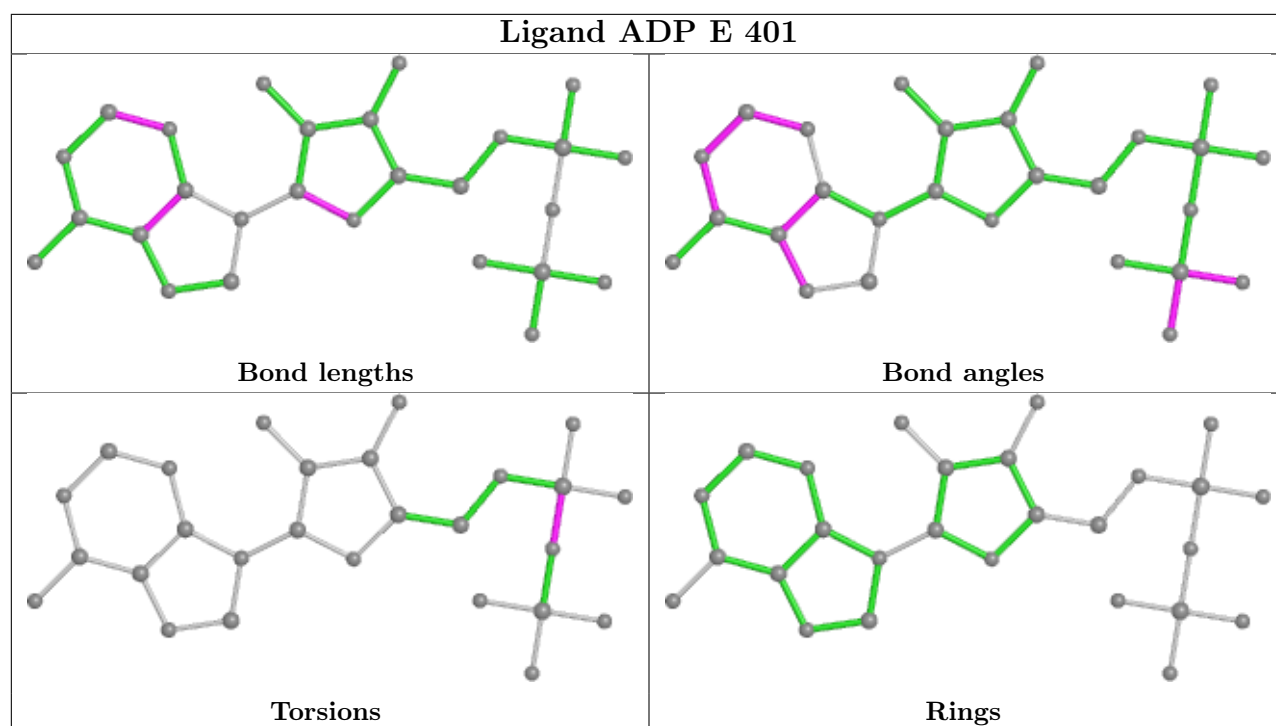
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	403	OXM	2	0
2	F	401	ADP	1	0
4	F	403	OXM	6	0
4	E	403	OXM	1	0
4	B	403	OXM	4	0

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, 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	356/377 (94%)	-0.05	6 (1%) 70 73	23, 35, 63, 113	0
1	B	357/377 (94%)	-0.05	11 (3%) 49 53	22, 34, 67, 100	0
1	C	353/377 (93%)	0.01	6 (1%) 70 73	26, 40, 67, 97	0
1	D	353/377 (93%)	0.02	8 (2%) 60 64	23, 39, 72, 107	0
1	E	354/377 (93%)	0.07	7 (1%) 65 69	22, 33, 59, 115	0
1	F	355/377 (94%)	0.04	5 (1%) 75 78	21, 31, 61, 89	0
All	All	2128/2262 (94%)	0.01	43 (2%) 65 69	21, 35, 66, 115	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	266	PRO	9.3
1	E	266	PRO	8.6
1	E	373	GLY	6.6
1	E	372	PRO	6.0
1	E	267	VAL	5.4
1	F	373	GLY	5.1
1	B	268	ARG	5.1
1	C	279	LYS	4.9
1	D	264	GLU	4.5
1	A	373	GLY	4.4
1	D	265	SER	4.3
1	D	266	PRO	4.2
1	B	267	VAL	3.7
1	E	265	SER	3.6
1	F	269	LYS	3.4
1	C	278	GLY	3.4
1	A	372	PRO	3.3
1	F	266	PRO	3.3
1	F	310	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	310	THR	3.3
1	B	107	ARG	3.2
1	C	280	LEU	3.2
1	D	280	LEU	3.2
1	B	269	LYS	3.1
1	B	373	GLY	3.1
1	B	97	GLU	3.0
1	A	265	SER	3.0
1	F	267	VAL	2.8
1	B	266	PRO	2.8
1	A	310	THR	2.7
1	B	372	PRO	2.7
1	D	227	ARG	2.6
1	D	373	GLY	2.5
1	C	343	ASP	2.4
1	E	310	THR	2.4
1	E	340	GLU	2.3
1	B	111	ARG	2.3
1	A	277	PRO	2.3
1	B	310	THR	2.3
1	C	341	ASN	2.3
1	C	111	ARG	2.2
1	D	288	LEU	2.1
1	B	343	ASP	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

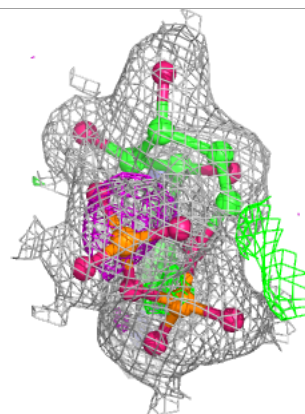
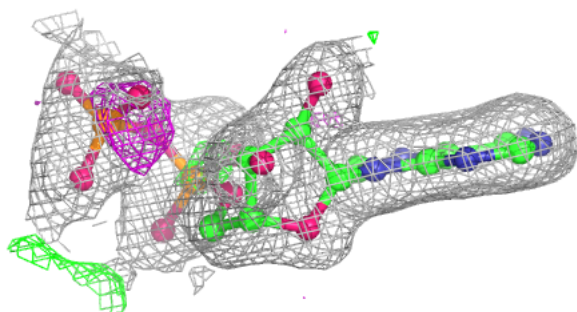
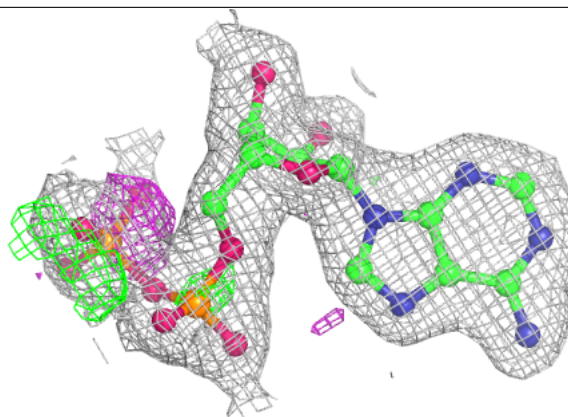
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	MG	E	402	1/1	0.89	0.10	43,43,43,43	0
3	MG	B	402	1/1	0.92	0.14	47,47,47,47	0
3	MG	F	402	1/1	0.92	0.08	41,41,41,41	0
3	MG	C	402	1/1	0.94	0.06	47,47,47,47	0
4	OXM	C	403	6/6	0.94	0.16	44,45,46,48	0
4	OXM	D	403	6/6	0.94	0.24	38,40,42,43	0
3	MG	D	402	1/1	0.95	0.13	42,42,42,42	0
2	ADP	D	401	27/27	0.96	0.14	28,31,50,53	0
4	OXM	B	403	6/6	0.96	0.10	24,27,28,28	0
2	ADP	E	401	27/27	0.97	0.12	25,27,48,53	0
2	ADP	F	401	27/27	0.97	0.12	28,31,45,48	0
4	OXM	A	403	6/6	0.97	0.10	31,34,35,35	0
2	ADP	B	401	27/27	0.97	0.11	26,27,44,49	0
2	ADP	C	401	27/27	0.97	0.13	30,35,52,56	0
2	ADP	A	401	27/27	0.97	0.12	28,30,47,51	0
4	OXM	F	403	6/6	0.97	0.14	34,37,38,39	0
4	OXM	E	403	6/6	0.98	0.10	29,30,31,31	0
3	MG	A	402	1/1	0.98	0.07	40,40,40,40	0

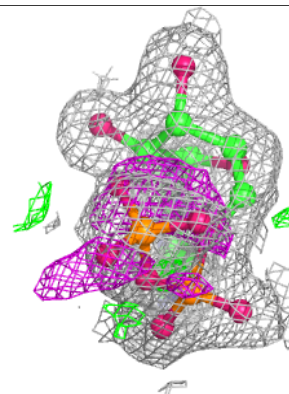
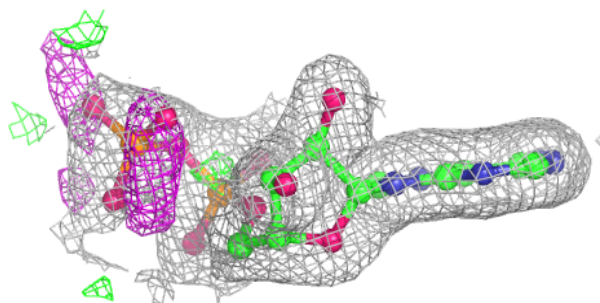
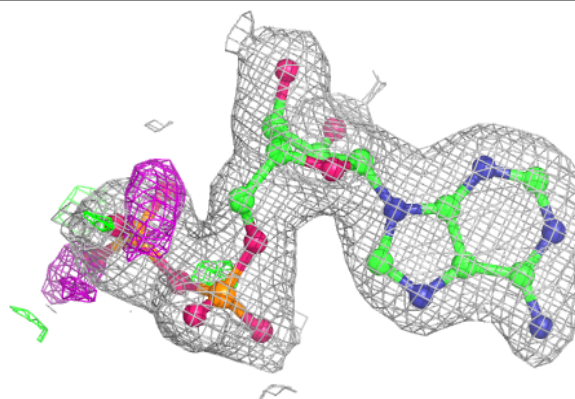
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

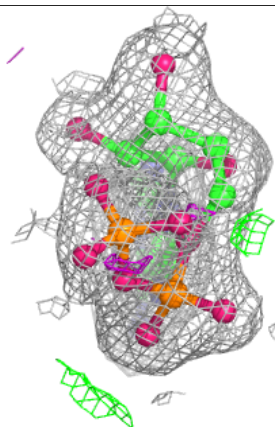
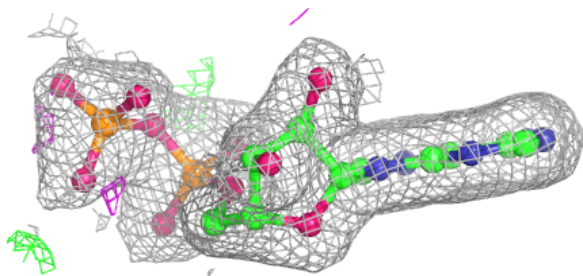
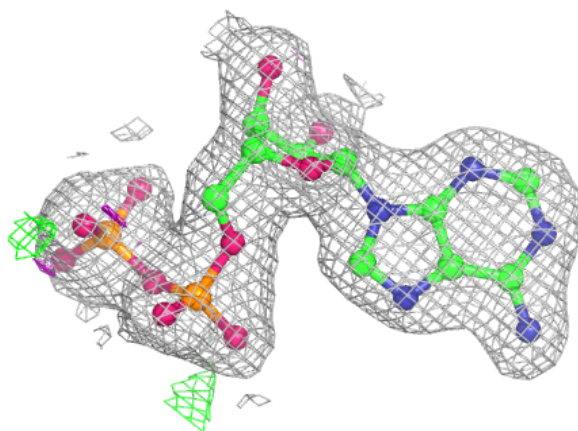
**Electron density around ADP E 401:**

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

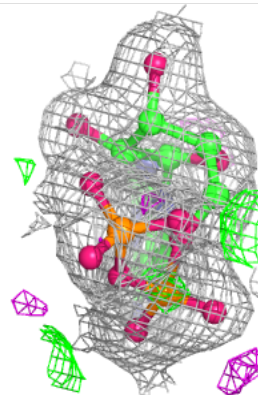
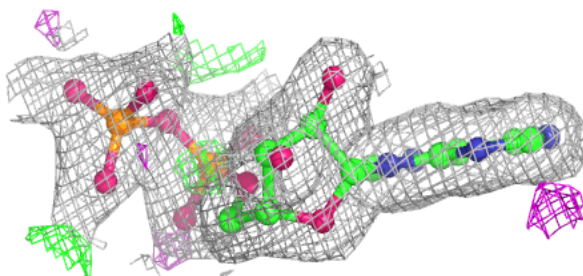
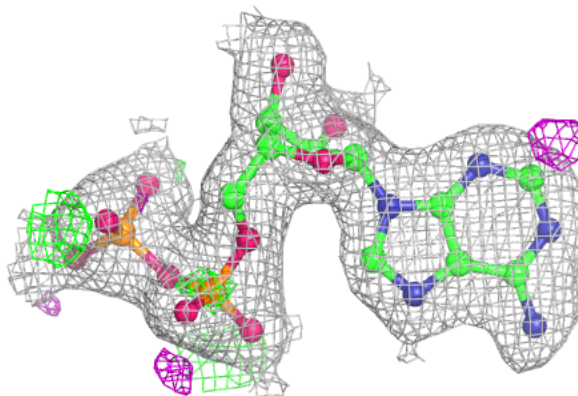


**Electron density around ADP F 401:**

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

**Electron density around ADP B 401:**

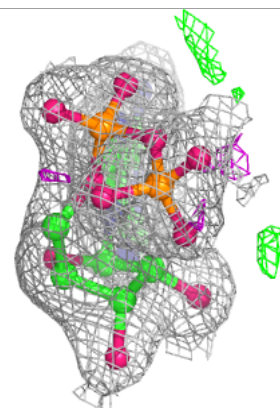
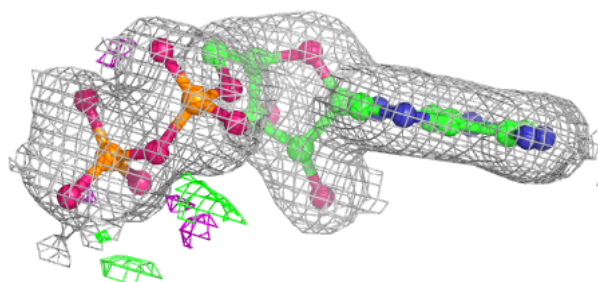
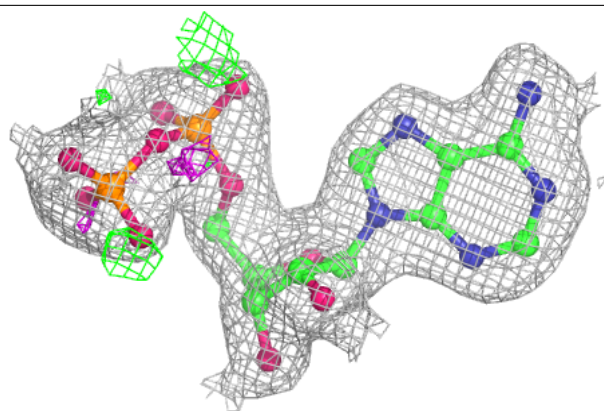
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



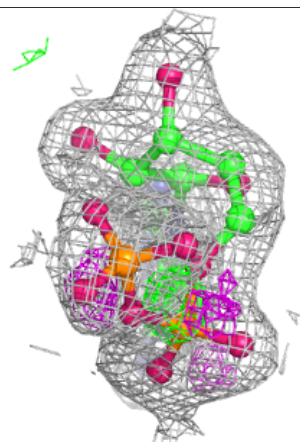
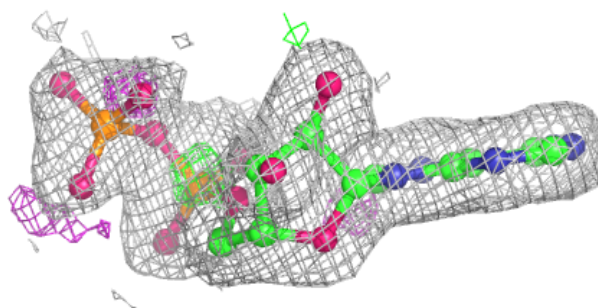
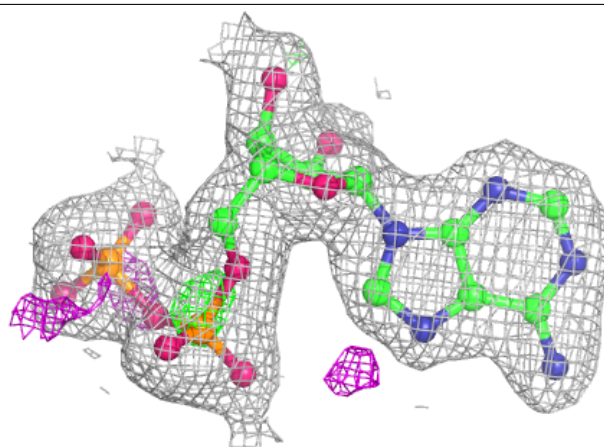


**Electron density around ADP C 401:**

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

**Electron density around ADP A 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.