



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 09:59 PM BST

PDB ID : 6U1H  
Title : Thermus thermophilus D-alanine-D-alanine ligase in complex with ADP, phosphate, Mg<sup>2+</sup> and K<sup>+</sup>  
Authors : Pederick, J.L.; Bruning, J.B.  
Deposited on : 2019-08-15  
Resolution : 2.20 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 : 2.13.1  
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) : 2.13.1

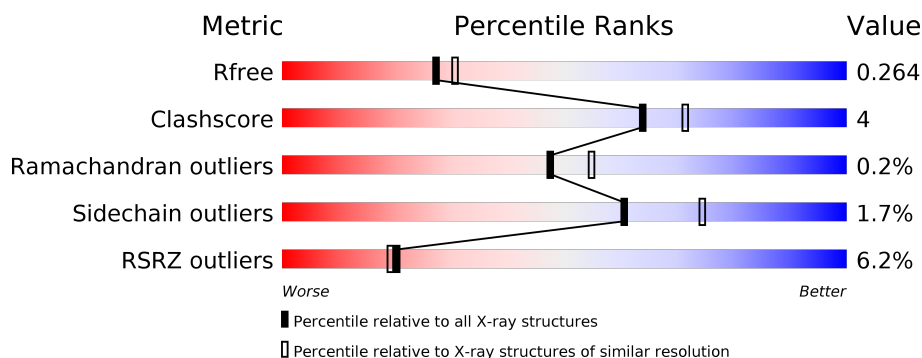
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	327	<div> <div>4%</div> <div> <div></div> <div>91%</div> <div>9%</div> </div> </div>
1	B	327	<div> <div>8%</div> <div> <div></div> <div>86%</div> <div>11%</div> </div> </div>
1	C	327	<div> <div>7%</div> <div> <div></div> <div>85%</div> <div>13%</div> </div> </div>
1	D	327	<div> <div>5%</div> <div> <div></div> <div>80%</div> <div>13%</div> <div>7%</div> </div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9924 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	324	Total	C	N	O	S	0	0	0
			2424	1576	405	438	5			
1	B	318	Total	C	N	O	S	0	1	0
			2365	1536	394	431	4			
1	C	322	Total	C	N	O	S	0	0	0
			2410	1572	393	440	5			
1	D	305	Total	C	N	O	S	0	0	0
			2289	1489	386	409	5			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP Q5SHZ3
A	0	GLU	-	expression tag	UNP Q5SHZ3
A	320	HIS	-	expression tag	UNP Q5SHZ3
A	321	HIS	-	expression tag	UNP Q5SHZ3
A	322	HIS	-	expression tag	UNP Q5SHZ3
A	323	HIS	-	expression tag	UNP Q5SHZ3
A	324	HIS	-	expression tag	UNP Q5SHZ3
A	325	HIS	-	expression tag	UNP Q5SHZ3
B	-1	MET	-	initiating methionine	UNP Q5SHZ3
B	0	GLU	-	expression tag	UNP Q5SHZ3
B	320	HIS	-	expression tag	UNP Q5SHZ3
B	321	HIS	-	expression tag	UNP Q5SHZ3
B	322	HIS	-	expression tag	UNP Q5SHZ3
B	323	HIS	-	expression tag	UNP Q5SHZ3
B	324	HIS	-	expression tag	UNP Q5SHZ3
B	325	HIS	-	expression tag	UNP Q5SHZ3
C	-1	MET	-	initiating methionine	UNP Q5SHZ3
C	0	GLU	-	expression tag	UNP Q5SHZ3
C	320	HIS	-	expression tag	UNP Q5SHZ3
C	321	HIS	-	expression tag	UNP Q5SHZ3
C	322	HIS	-	expression tag	UNP Q5SHZ3

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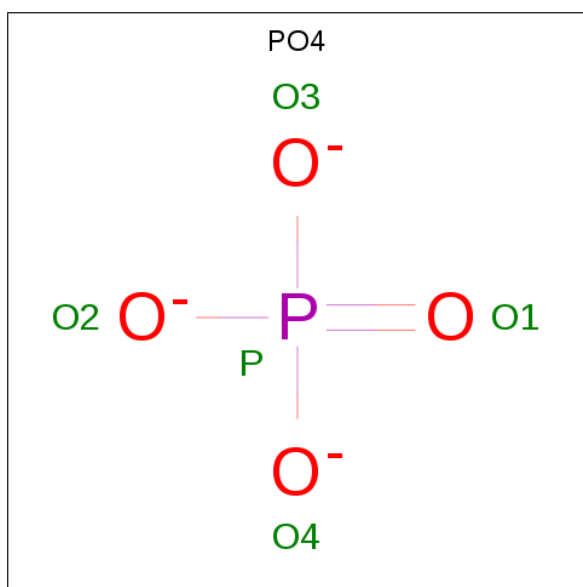
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Chain	Residue	Modelled	Actual	Comment	Reference
C	323	HIS	-	expression tag	UNP Q5SHZ3
C	324	HIS	-	expression tag	UNP Q5SHZ3
C	325	HIS	-	expression tag	UNP Q5SHZ3
D	-1	MET	-	initiating methionine	UNP Q5SHZ3
D	0	GLU	-	expression tag	UNP Q5SHZ3
D	320	HIS	-	expression tag	UNP Q5SHZ3
D	321	HIS	-	expression tag	UNP Q5SHZ3
D	322	HIS	-	expression tag	UNP Q5SHZ3
D	323	HIS	-	expression tag	UNP Q5SHZ3
D	324	HIS	-	expression tag	UNP Q5SHZ3
D	325	HIS	-	expression tag	UNP Q5SHZ3

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).

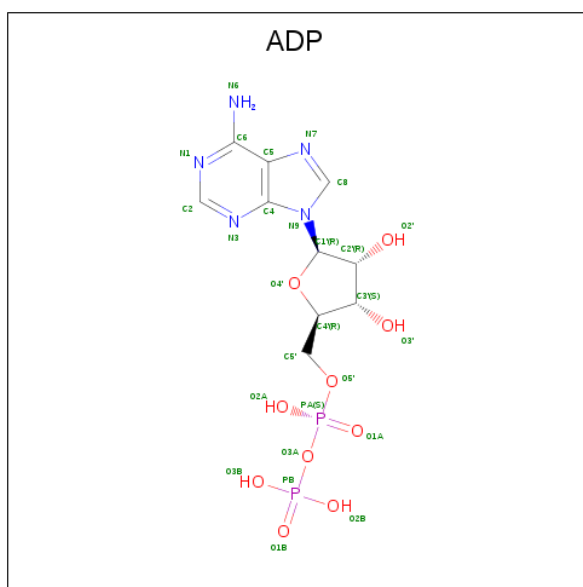


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 5	O 4	P 1	0	0
3	C	1	Total 5	O 4	P 1	0	0

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total K 1 1	0	0
4	C	1	Total K 1 1	0	0

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$ ).



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

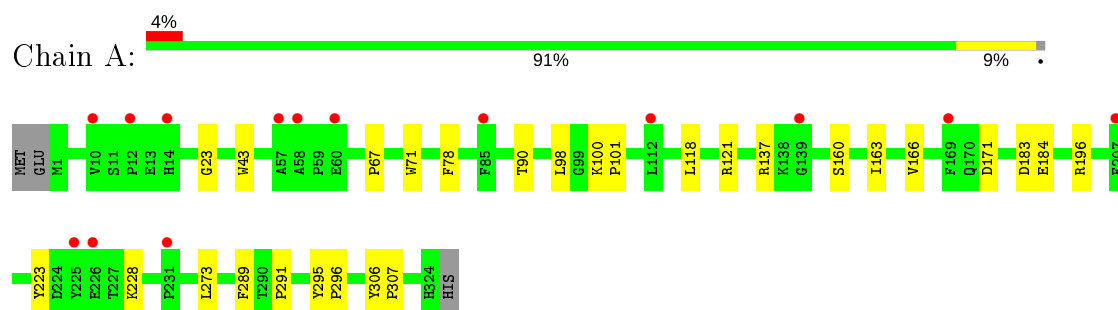
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	93	Total 93	O 93	0	0
6	B	68	Total 68	O 68	0	0
6	C	76	Total 76	O 76	0	0
6	D	74	Total 74	O 74	0	0

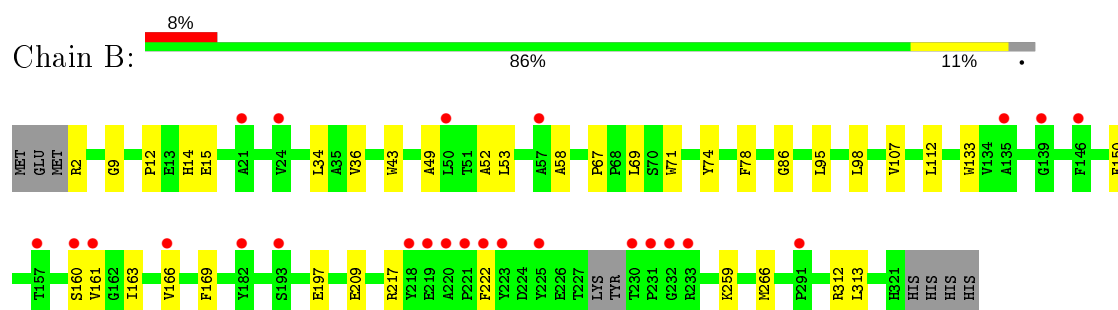
### 3 Residue-property plots [i](#)

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

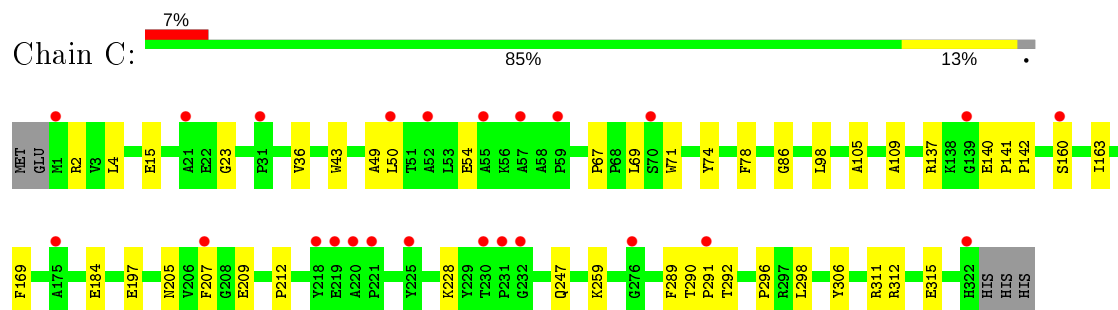
- Molecule 1: D-alanine–D-alanine ligase



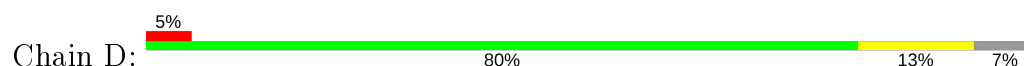
- Molecule 1: D-alanine–D-alanine ligase

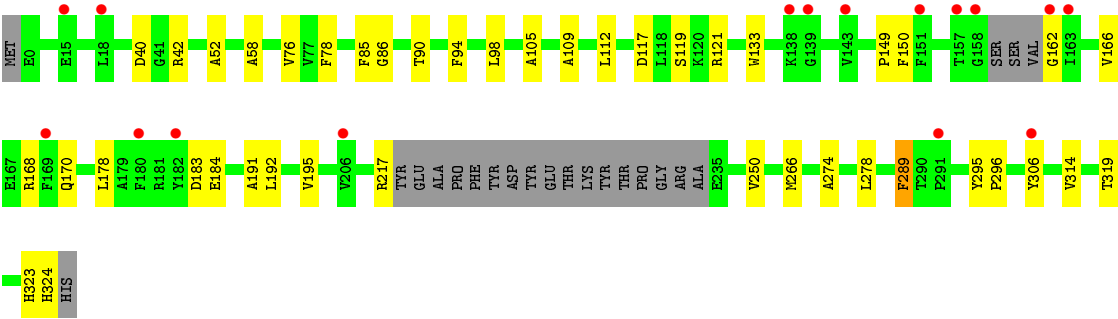


- Molecule 1: D-alanine–D-alanine ligase



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







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.29Å 68.62Å 91.65Å 69.55° 78.97° 66.10°	Depositor
Resolution (Å)	42.43 – 2.20 42.42 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.9 (42.43-2.20) 96.8 (42.42-2.20)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.52 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, $R_{free}$	0.218 , 0.265 0.218 , 0.264	Depositor DCC
$R_{free}$ test set	2916 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.6	Xtriage
Anisotropy	0.447	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 45.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	9924	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 9.97% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, MG, K, 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	0.27	0/2492	0.45	0/3412
1	B	0.26	0/2426	0.45	0/3319
1	C	0.27	0/2478	0.44	0/3395
1	D	0.27	0/2350	0.44	0/3212
All	All	0.27	0/9746	0.45	0/13338

There are no bond length outliers.

There are no bond angle outliers.

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	2424	0	2384	17	0
1	B	2365	0	2331	19	0
1	C	2410	0	2366	24	0
1	D	2289	0	2267	23	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
2	C	2	0	0	0	0
3	A	5	0	0	1	0
3	C	5	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	A	27	0	12	1	0
5	B	27	0	12	2	0
5	C	27	0	12	1	0
5	D	27	0	12	2	0
6	A	93	0	0	2	0
6	B	68	0	0	0	0
6	C	76	0	0	1	0
6	D	74	0	0	1	0
All	All	9924	0	9396	80	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 (80) 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:23:GLY:HA3	1:C:291:PRO:HD3	1.74	0.70
1:B:160:SER:HA	1:B:163:ILE:HD12	1.78	0.64
1:B:12:PRO:HG2	1:B:161:VAL:HG21	1.79	0.64
1:A:90:THR:HG22	1:B:107:VAL:HG21	1.80	0.64
1:C:160:SER:HA	1:C:163:ILE:HD12	1.81	0.63
1:B:197:GLU:OE2	5:B:402:ADP:O2'	2.19	0.60
1:A:71:TRP:CD2	1:A:98:LEU:HD21	2.38	0.58
1:C:15:GLU:N	1:C:15:GLU:OE1	2.35	0.58
1:C:209:GLU:OE1	1:C:312:ARG:NH2	2.34	0.56
1:C:140:GLU:HG2	1:C:141:PRO:HD2	1.86	0.56
1:D:195:VAL:HG21	5:D:401:ADP:H2	1.72	0.55
1:C:2:ARG:HG2	1:C:74:TYR:CD1	2.42	0.55
1:C:137:ARG:NH1	6:C:501:HOH:O	2.32	0.55
1:D:150:PHE:HB2	1:D:166:VAL:HB	1.89	0.55
1:D:217:ARG:NH2	6:D:506:HOH:O	2.38	0.55
1:B:43:TRP:CE3	1:B:67:PRO:HG3	2.42	0.54
1:A:23:GLY:HA3	1:A:291:PRO:HD3	1.90	0.54
1:A:137:ARG:NH1	1:B:259:LYS:HE2	2.23	0.53
1:D:183:ASP:OD1	1:D:184:GLU:N	2.42	0.52
1:D:117:ASP:OD1	1:D:121:ARG:NH1	2.43	0.51
1:C:184:GLU:HG3	1:D:324:HIS:HB3	1.92	0.51
1:C:105:ALA:HB1	1:C:109:ALA:HB3	1.94	0.50
1:D:52:ALA:HB1	1:D:58:ALA:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:311:ARG:O	1:C:315:GLU:HG2	2.13	0.48
1:B:34:LEU:HD22	1:B:53:LEU:HD22	1.95	0.48
1:B:95:LEU:HD23	1:B:98:LEU:HD12	1.94	0.48
1:A:196:ARG:HB2	1:A:273:LEU:HB3	1.95	0.47
1:B:36:VAL:HG23	1:B:49:ALA:HB1	1.97	0.47
1:C:197:GLU:OE1	5:C:405:ADP:O2'	2.30	0.47
1:C:71:TRP:CD2	1:C:98:LEU:HD21	2.50	0.47
1:A:228:LYS:NZ	3:A:403:PO4:O4	2.38	0.47
1:D:117:ASP:O	1:D:121:ARG:HG3	2.15	0.47
1:B:209:GLU:OE2	1:B:312:ARG:NH2	2.36	0.46
1:A:118:LEU:HD23	1:A:121:ARG:HD2	1.98	0.46
1:D:149:PRO:HG2	1:D:191:ALA:HB3	1.97	0.46
1:C:4:LEU:HD21	1:C:69:LEU:HD21	1.98	0.46
1:C:205:ASN:O	1:C:207:PHE:N	2.49	0.45
1:A:160:SER:HA	1:A:163:ILE:HD12	1.99	0.45
1:D:289:PHE:O	1:D:306:TYR:OH	2.26	0.45
1:A:228:LYS:NZ	5:A:405:ADP:O3B	2.50	0.44
1:D:295:TYR:HB3	1:D:296:PRO:HD3	1.99	0.44
1:D:162:GLY:HA2	1:D:178:LEU:HG	2.00	0.44
1:B:52:ALA:HB1	1:B:58:ALA:HB2	2.00	0.44
1:A:166:VAL:HG13	1:A:171:ASP:HB2	2.00	0.44
1:A:306:TYR:HB3	1:A:307:PRO:HD3	2.00	0.44
1:B:9:GLY:O	1:B:14:HIS:ND1	2.50	0.43
1:D:250:VAL:HG22	1:D:278:LEU:HD21	2.00	0.43
1:B:69:LEU:HD23	1:B:71:TRP:CH2	2.53	0.43
1:D:319:THR:O	1:D:323:HIS:HB2	2.18	0.43
1:C:207:PHE:CE1	1:C:259:LYS:HD2	2.53	0.43
1:C:228:LYS:NZ	3:C:403:PO4:O4	2.40	0.43
1:C:50:LEU:O	1:C:54:GLU:HG2	2.19	0.43
1:C:296:PRO:HB3	1:C:306:TYR:HD1	1.84	0.43
1:C:296:PRO:HB3	1:C:306:TYR:CD1	2.54	0.43
1:C:43:TRP:CE3	1:C:67:PRO:HG3	2.54	0.43
1:D:192:LEU:HB3	1:D:274:ALA:HB2	2.01	0.43
1:D:266:MET:SD	1:D:289:PHE:HE2	2.41	0.43
1:A:184:GLU:HG2	6:A:586:HOH:O	2.17	0.42
1:D:94:PHE:CE2	1:D:98:LEU:HD11	2.54	0.42
1:A:100:LYS:HD3	1:A:101:PRO:HD2	2.01	0.42
1:A:137:ARG:NH2	6:A:517:HOH:O	2.52	0.42
1:D:195:VAL:HG21	5:D:401:ADP:C2	2.51	0.42
1:A:43:TRP:CE3	1:A:67:PRO:HG3	2.55	0.42
1:D:112:LEU:O	1:D:119:SER:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:VAL:HG23	1:C:49:ALA:HB1	2.02	0.42
1:B:266:MET:HB3	1:B:313:LEU:HD21	2.00	0.42
1:C:290:THR:HG22	1:C:292:THR:H	1.85	0.42
1:D:85:PHE:HA	1:D:90:THR:OG1	2.20	0.41
1:D:105:ALA:HB1	1:D:109:ALA:HB3	2.02	0.41
1:A:295:TYR:HB3	1:A:296:PRO:HD3	2.02	0.41
1:B:15:GLU:N	1:B:15:GLU:OE1	2.51	0.41
1:B:150:PHE:HB2	1:B:166:VAL:HB	2.03	0.41
1:B:222:PHE:HB2	5:B:402:ADP:H1'	2.01	0.41
1:C:141:PRO:HA	1:C:142:PRO:HD3	1.87	0.41
1:D:76:VAL:HG21	1:D:314:VAL:HG13	2.02	0.41
1:A:183:ASP:OD1	1:A:184:GLU:N	2.54	0.41
1:D:40:ASP:OD2	1:D:42:ARG:HD3	2.21	0.41
1:B:2:ARG:HG2	1:B:74:TYR:CD1	2.56	0.40
1:C:212:PRO:O	1:C:298:LEU:HD22	2.21	0.40
1:B:112:LEU:HA	1:B:112:LEU:HD23	1.92	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	322/327 (98%)	310 (96%)	12 (4%)	0	100	100
1	B	315/327 (96%)	303 (96%)	11 (4%)	1 (0%)	41	46
1	C	320/327 (98%)	311 (97%)	8 (2%)	1 (0%)	41	46
1	D	299/327 (91%)	288 (96%)	10 (3%)	1 (0%)	41	46
All	All	1256/1308 (96%)	1212 (96%)	41 (3%)	3 (0%)	47	55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	86	GLY
1	D	86	GLY
1	C	86	GLY

### 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	245/264 (93%)	242 (99%)	3 (1%)	71	83
1	B	238/264 (90%)	234 (98%)	4 (2%)	60	74
1	C	244/264 (92%)	240 (98%)	4 (2%)	62	76
1	D	232/264 (88%)	227 (98%)	5 (2%)	52	65
All	All	959/1056 (91%)	943 (98%)	16 (2%)	60	74

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	PHE
1	A	223	TYR
1	A	289	PHE
1	B	78	PHE
1	B	133	TRP
1	B	169	PHE
1	B	217	ARG
1	C	78	PHE
1	C	169	PHE
1	C	247	GLN
1	C	289	PHE
1	D	78	PHE
1	D	133	TRP
1	D	168	ARG
1	D	170	GLN
1	D	289	PHE

Some 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 ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 7 are monoatomic - leaving 6 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	PO4	A	403	2	4,4,4	0.87	0	6,6,6	0.50	0
5	ADP	D	401	-	24,29,29	0.98	1 (4%)	29,45,45	1.27	4 (13%)
5	ADP	A	405	2	24,29,29	0.97	1 (4%)	29,45,45	1.31	4 (13%)
3	PO4	C	403	2	4,4,4	0.85	0	6,6,6	0.52	0
5	ADP	C	405	2	24,29,29	0.98	1 (4%)	29,45,45	1.32	4 (13%)
5	ADP	B	402	2	24,29,29	0.97	1 (4%)	29,45,45	1.35	4 (13%)

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
5	ADP	A	405	2	-	0/12/32/32	0/3/3/3
5	ADP	C	405	2	-	0/12/32/32	0/3/3/3
5	ADP	D	401	-	-	1/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ADP	B	402	2	-	0/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	401	ADP	C5-C4	2.52	1.47	1.40
5	A	405	ADP	C5-C4	2.46	1.47	1.40
5	B	402	ADP	C5-C4	2.45	1.47	1.40
5	C	405	ADP	C5-C4	2.45	1.47	1.40

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	405	ADP	N3-C2-N1	-3.20	123.68	128.68
5	C	405	ADP	N3-C2-N1	-3.16	123.75	128.68
5	B	402	ADP	N3-C2-N1	-3.11	123.81	128.68
5	B	402	ADP	PA-O3A-PB	-3.09	122.21	132.83
5	D	401	ADP	N3-C2-N1	-2.88	124.17	128.68
5	C	405	ADP	PA-O3A-PB	-2.87	122.98	132.83
5	C	405	ADP	C3'-C2'-C1'	2.83	105.23	100.98
5	A	405	ADP	C4-C5-N7	-2.72	106.57	109.40
5	D	401	ADP	PA-O3A-PB	-2.71	123.52	132.83
5	A	405	ADP	PA-O3A-PB	-2.71	123.53	132.83
5	B	402	ADP	C4-C5-N7	-2.70	106.59	109.40
5	D	401	ADP	C4-C5-N7	-2.60	106.69	109.40
5	B	402	ADP	C3'-C2'-C1'	2.34	104.51	100.98
5	A	405	ADP	C3'-C2'-C1'	2.24	104.36	100.98
5	C	405	ADP	C4-C5-N7	-2.20	107.11	109.40
5	D	401	ADP	C3'-C2'-C1'	2.16	104.23	100.98

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	401	ADP	PB-O3A-PA-O2A

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	403	PO4	1	0

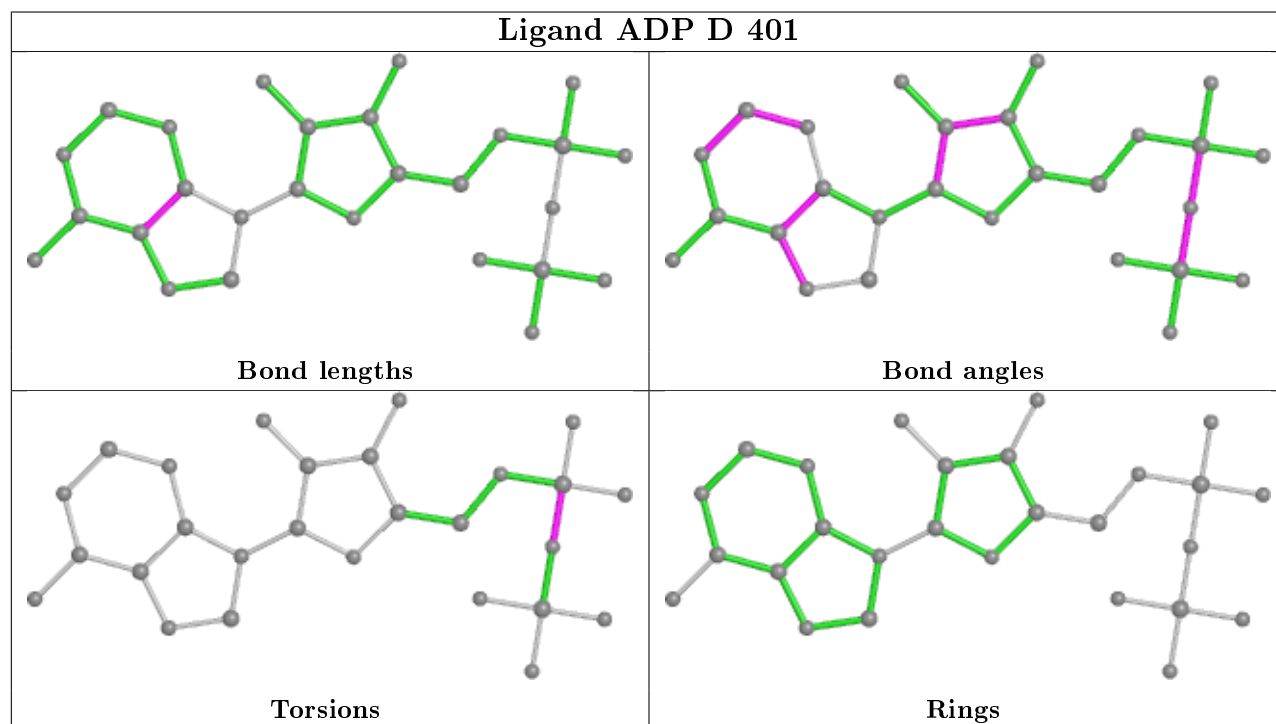
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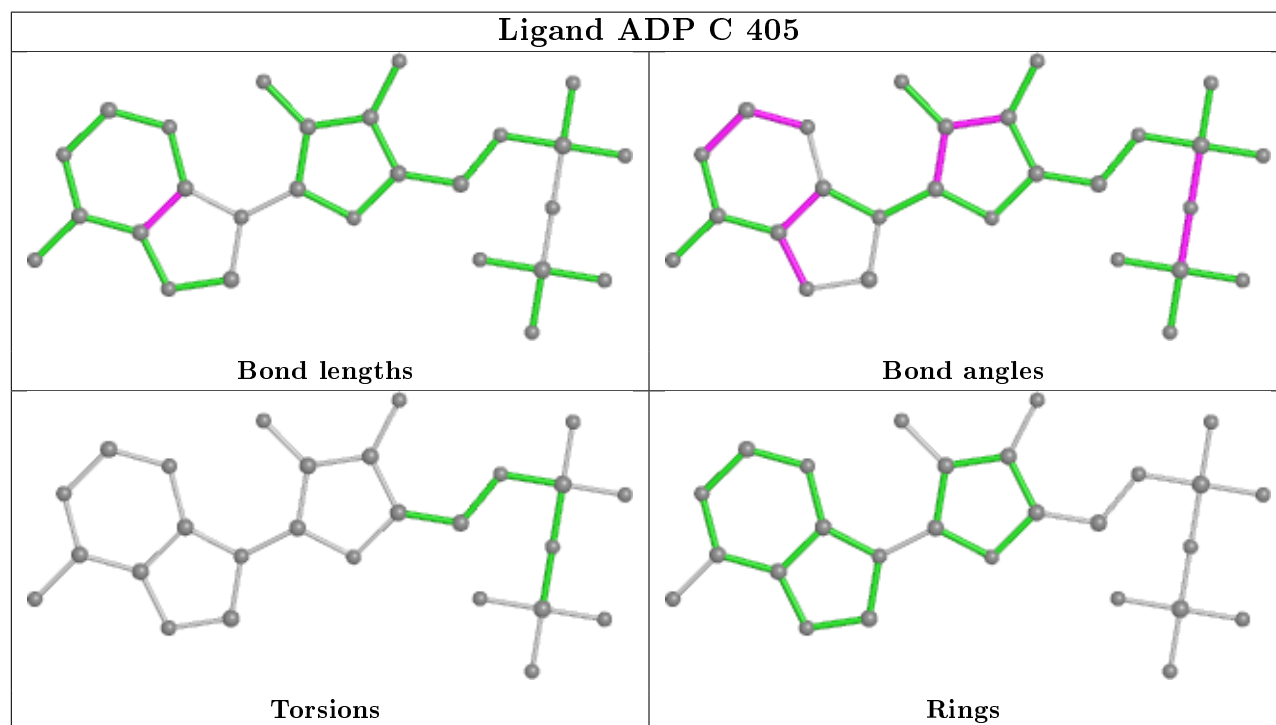
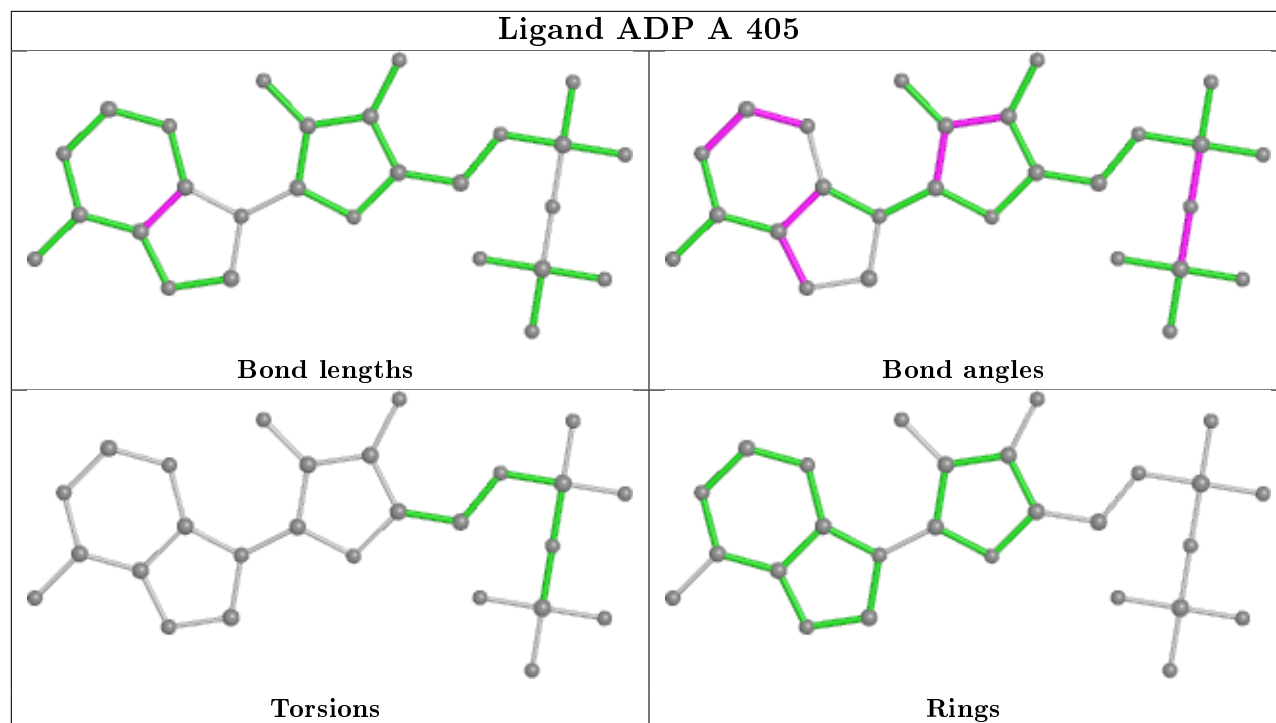


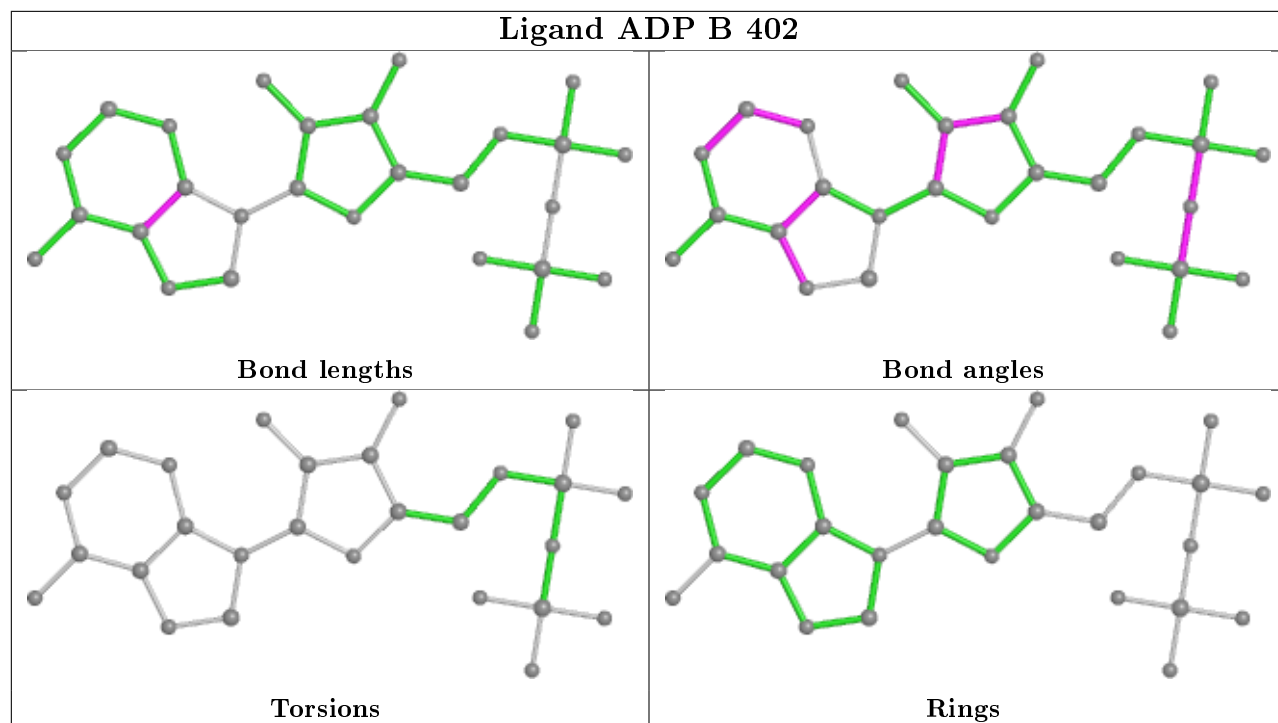
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	401	ADP	2	0
5	A	405	ADP	1	0
3	C	403	PO4	1	0
5	C	405	ADP	1	0
5	B	402	ADP	2	0

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, 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	324/327 (99%)	0.25	14 (4%) 35 33	20, 33, 53, 70	0
1	B	318/327 (97%)	0.40	25 (7%) 12 11	20, 36, 57, 85	0
1	C	322/327 (98%)	0.46	24 (7%) 14 13	22, 39, 58, 65	0
1	D	305/327 (93%)	0.34	16 (5%) 27 26	21, 36, 54, 68	0
All	All	1269/1308 (97%)	0.36	79 (6%) 20 19	20, 36, 57, 85	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1	MET	4.9
1	D	139	GLY	4.7
1	B	21	ALA	4.5
1	A	225	TYR	4.5
1	D	157	THR	4.4
1	D	180	PHE	4.4
1	B	220	ALA	4.4
1	B	232	GLY	4.4
1	D	291	PRO	4.4
1	C	207	PHE	4.2
1	A	169	PHE	4.2
1	A	57	ALA	4.0
1	B	221	PRO	3.9
1	C	139	GLY	3.8
1	D	163	ILE	3.7
1	A	139	GLY	3.7
1	B	146	PHE	3.7
1	A	226	GLU	3.6
1	C	225	TYR	3.6
1	D	158	GLY	3.5
1	A	207	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	151	PHE	3.4
1	A	112	LEU	3.4
1	B	231	PRO	3.3
1	C	218	TYR	3.3
1	B	225	TYR	3.2
1	C	21	ALA	3.2
1	B	160	SER	3.1
1	D	162	GLY	3.1
1	C	160	SER	3.1
1	D	169	PHE	3.0
1	C	57	ALA	2.9
1	A	14	HIS	2.9
1	B	291	PRO	2.9
1	A	12	PRO	2.8
1	A	231	PRO	2.8
1	D	182	TYR	2.8
1	B	57	ALA	2.7
1	B	24	VAL	2.7
1	A	58	ALA	2.7
1	C	220	ALA	2.7
1	B	233	ARG	2.7
1	C	59	PRO	2.6
1	D	18	LEU	2.6
1	C	70	SER	2.6
1	B	219	GLU	2.6
1	C	175	ALA	2.5
1	B	218	TYR	2.5
1	C	221	PRO	2.5
1	C	55	ALA	2.4
1	A	85	PHE	2.4
1	C	230	THR	2.4
1	C	276	GLY	2.4
1	C	52	ALA	2.4
1	C	231	PRO	2.4
1	B	157	THR	2.4
1	D	143	VAL	2.4
1	B	50	LEU	2.4
1	C	291	PRO	2.4
1	B	193	SER	2.4
1	C	322	HIS	2.3
1	B	139	GLY	2.3
1	C	31	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	135	ALA	2.3
1	D	206	VAL	2.3
1	B	161	VAL	2.3
1	B	223	TYR	2.2
1	A	10	VAL	2.2
1	B	222	PHE	2.2
1	C	219	GLU	2.2
1	B	230	THR	2.2
1	B	182	TYR	2.2
1	B	166	VAL	2.1
1	D	15	GLU	2.1
1	D	138	LYS	2.1
1	C	232	GLY	2.1
1	C	50	LEU	2.1
1	A	60	GLU	2.0
1	D	306	TYR	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.

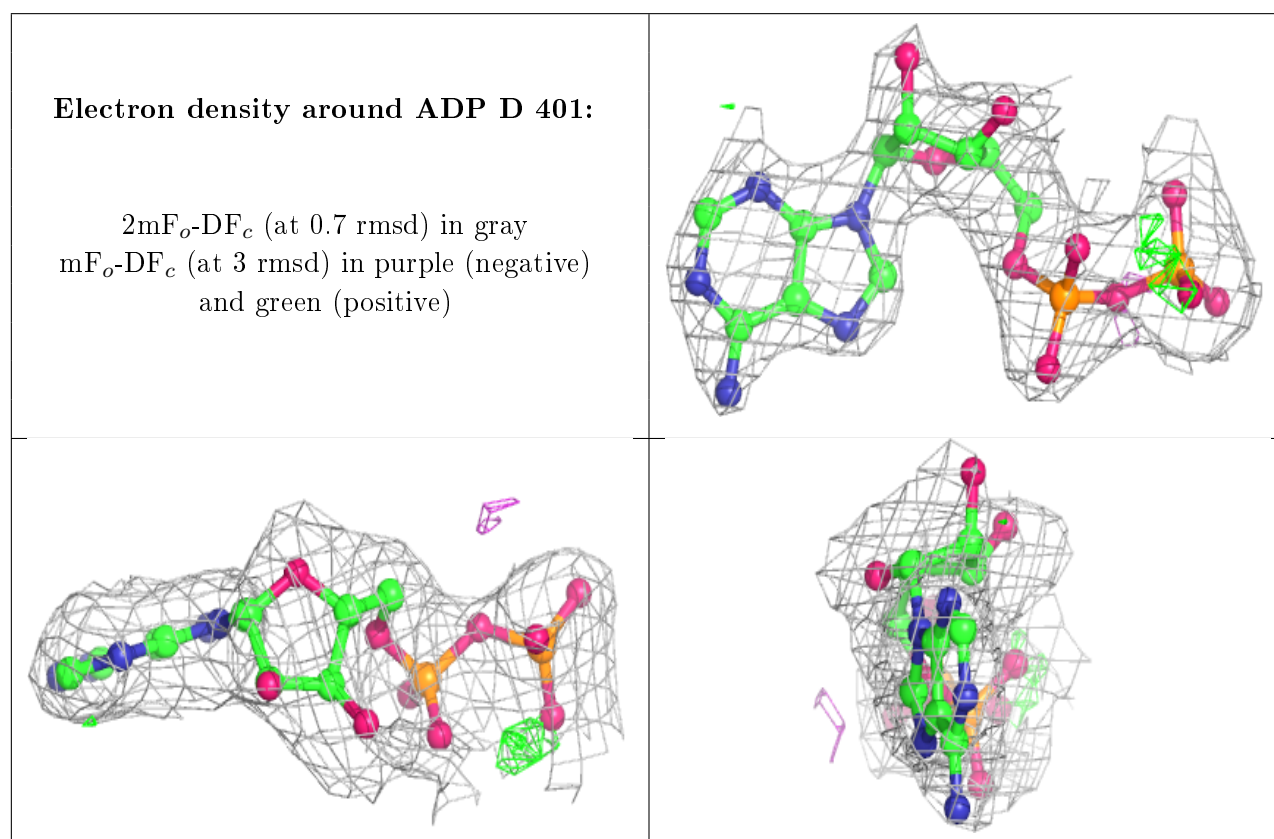
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	C	401	1/1	0.91	0.05	38,38,38,38	0
5	ADP	D	401	27/27	0.93	0.16	38,46,58,59	0
3	PO4	A	403	5/5	0.93	0.12	27,28,30,33	5
5	ADP	B	402	27/27	0.94	0.15	28,35,44,48	0
2	MG	C	402	1/1	0.95	0.07	40,40,40,40	0
5	ADP	A	405	27/27	0.96	0.12	22,31,37,41	0
5	ADP	C	405	27/27	0.96	0.11	27,32,39,42	0

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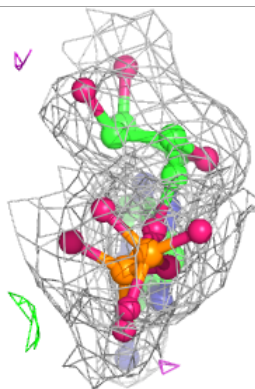
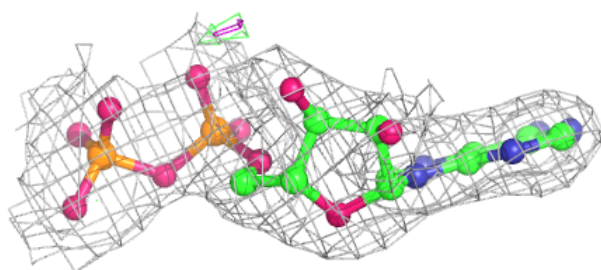
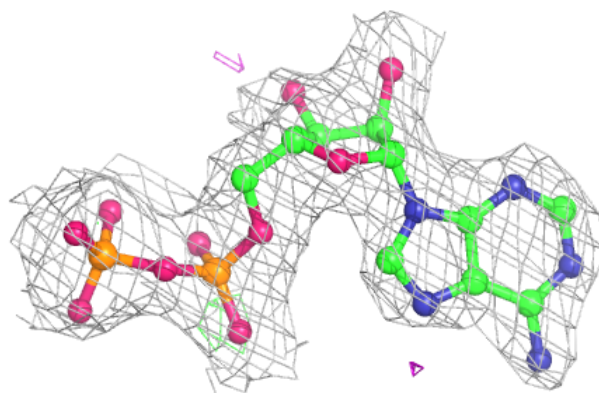
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	B	401	1/1	0.97	0.11	44,44,44,44	0
4	K	A	404	1/1	0.97	0.07	27,27,27,27	1
3	PO4	C	403	5/5	0.97	0.07	25,34,41,43	5
2	MG	A	402	1/1	0.98	0.04	29,29,29,29	0
2	MG	A	401	1/1	0.98	0.04	32,32,32,32	1
4	K	C	404	1/1	0.99	0.08	29,29,29,29	1

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.

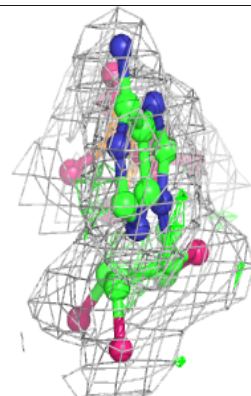
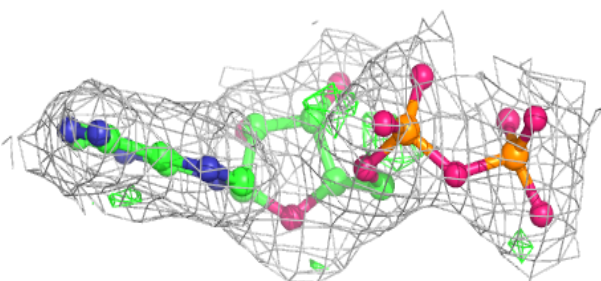
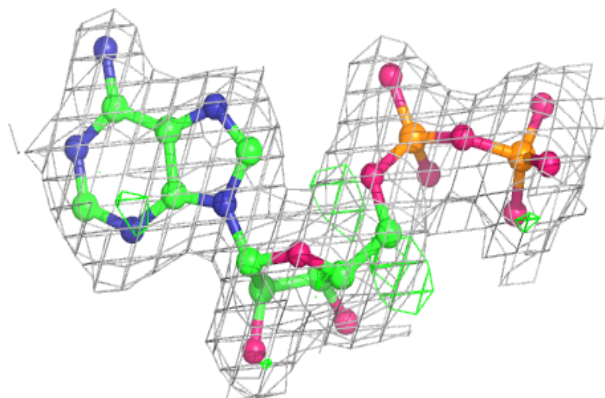


**Electron density around ADP B 402:**

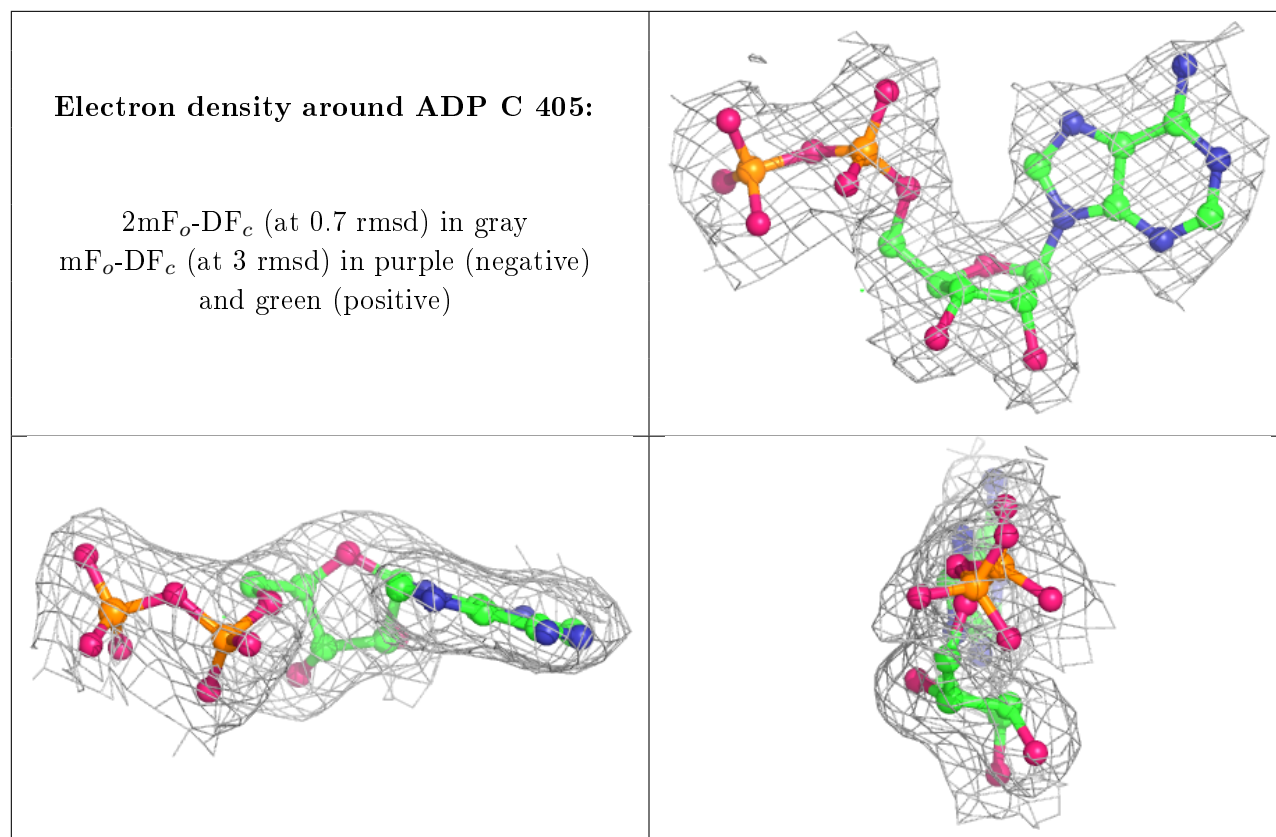
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around ADP A 405:**

$2mF_o-DF_c$  (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.