



# Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 08:51 pm BST

PDB ID : 1WBD  
Title : Crystal structure of E. coli DNA mismatch repair enzyme MutS, E38Q mutant, in complex with a G.T mismatch  
Authors : Natrajan, G.; Georgijevic, D.; Lebbink, J.H.G.; Winterwerp, H.H.K.; de Wind, N.; Sixma, T.K.  
Deposited on : 2004-10-31  
Resolution : 2.40 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

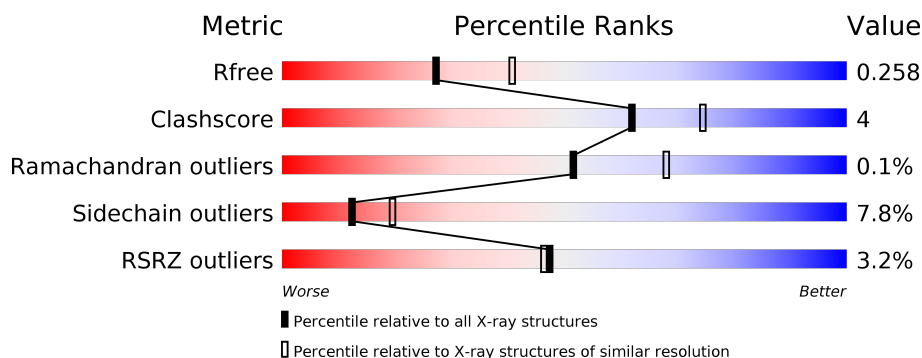
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	800	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>14%</div> <div>• •</div> </div> </div>
1	B	800	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>16%</div> <div>• 6%</div> </div> </div>
2	E	18	<div> <div>22%</div> <div> <div></div> <div>72%</div> <div>22%</div> <div>6%</div> </div> </div>
3	F	17	<div> <div>18%</div> <div> <div></div> <div>47%</div> <div>35%</div> <div>18%</div> </div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13160 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 DNA MISMATCH REPAIR PROTEIN MUTS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	788	Total	C	N	O	S	0	0	0
			6207	3905	1104	1169	29			
1	B	754	Total	C	N	O	S	0	0	0
			5964	3756	1061	1119	28			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	38	GLN	GLU	engineered mutation	UNP P23909
B	38	GLN	GLU	engineered mutation	UNP P23909

- Molecule 2 is a DNA chain called 5'-D(\*AP\*GP\*CP\*TP\*GP\*CP\*CP\*AP\*GP\*GP \*CP\*A P\*CP\*CP\*AP\*GP\*TP\*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	18	Total	C	N	O	P	0	0	0
			367	174	72	104	17			

- Molecule 3 is a DNA chain called 5'-D(\*AP\*CP\*TP\*GP\*GP\*TP\*GP\*CP\*TP\*TP \*GP\*G P\*CP\*AP\*GP\*CP\*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	17	Total	C	N	O	P	0	0	0
			347	166	62	103	16			

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

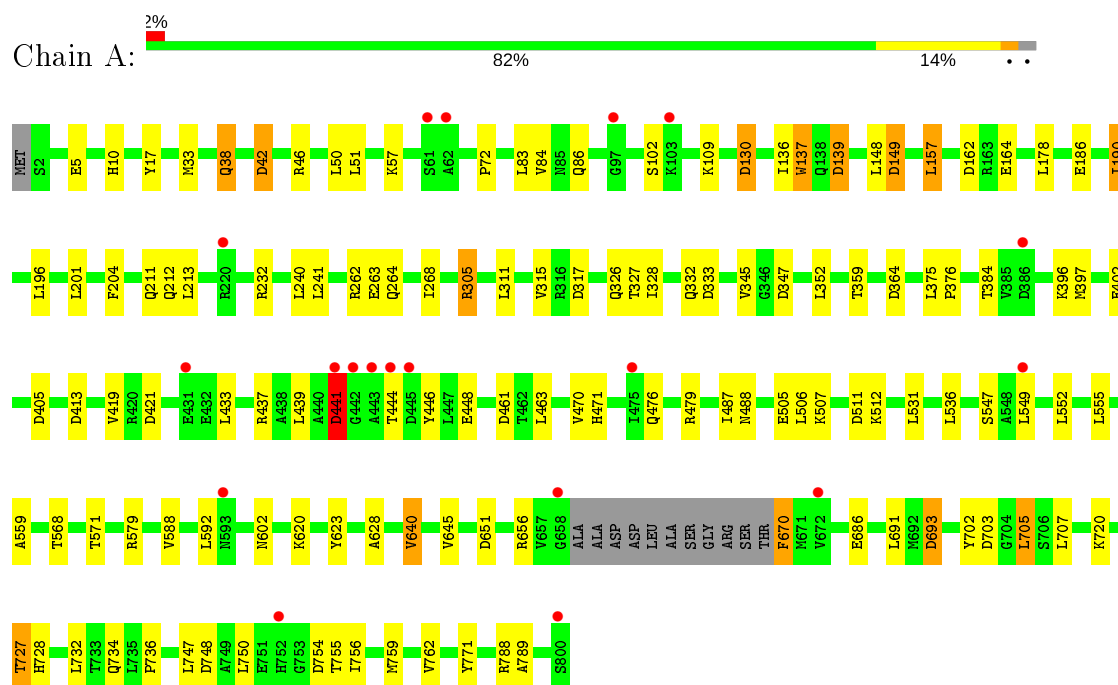
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	128	Total	O		
			128	128	0	0
6	B	116	Total	O		
			116	116	0	0
6	E	2	Total	O		
			2	2	0	0
6	F	1	Total	O		
			1	1	0	0

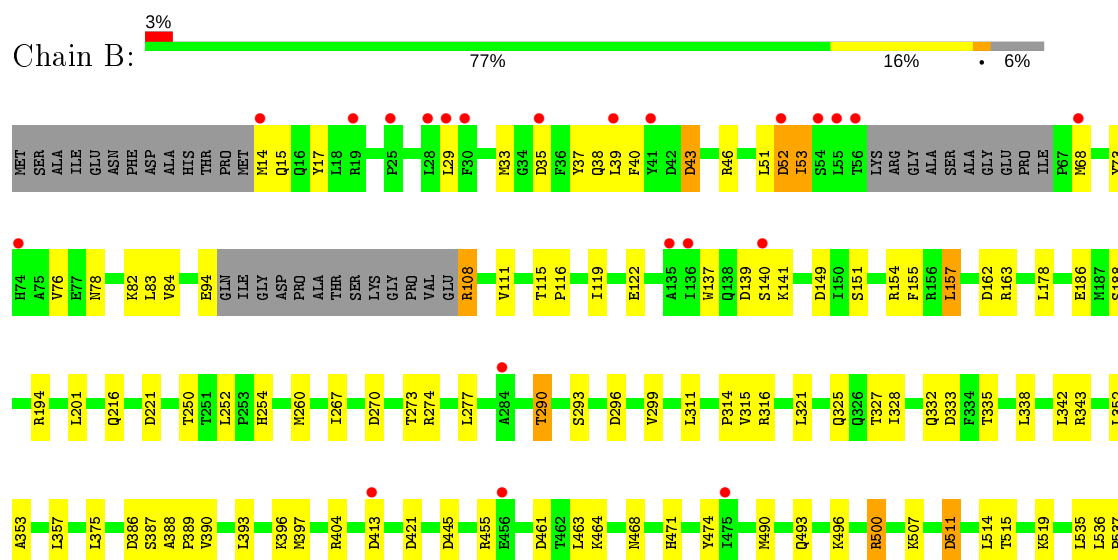
### 3 Residue-property plots [i](#)

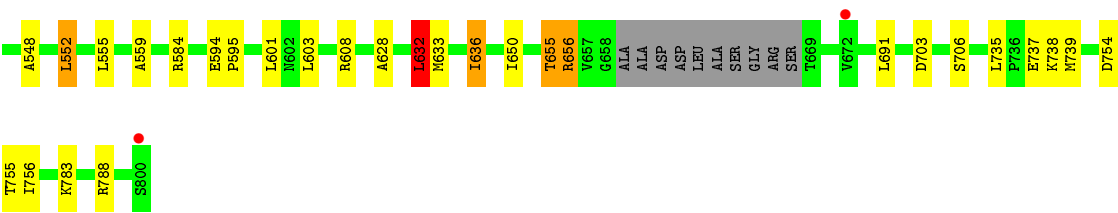
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: DNA MISMATCH REPAIR PROTEIN MUTS



#### • Molecule 1: DNA MISMATCH REPAIR PROTEIN MUTS





● Molecule 2: 5'-D(\*AP\*GP\*CP\*TP\*GP\*CP\*CP\*AP\*GP\*GP \*CP\*AP\*CP\*CP\*AP\*GP\*TP\*G)-3'



● Molecule 3: 5'-D(\*AP\*CP\*TP\*GP\*GP\*TP\*GP\*CP\*TP\*TP \*GP\*GP\*CP\*AP\*GP\*CP\*T)-3',



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.62Å 92.04Å 260.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 19.93 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.3 (20.00-2.40) 99.4 (19.93-2.40)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.74 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.212 , 0.259 0.215 , 0.258	Depositor DCC
$R_{free}$ test set	1644 reflections (1.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.9	Xtriage
Anisotropy	0.469	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 37.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.015 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13160	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% 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: MG, 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	0.65	1/6313 (0.0%)	0.87	24/8544 (0.3%)
1	B	0.62	0/6062	0.84	16/8199 (0.2%)
2	E	1.14	0/412	1.74	4/634 (0.6%)
3	F	1.10	0/388	1.80	12/598 (2.0%)
All	All	0.67	1/13175 (0.0%)	0.95	56/17975 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	703	ASP	CB-CG	-5.18	1.40	1.51

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	17	DT	O4'-C1'-N1	10.99	115.70	108.00
1	B	270	ASP	CB-CG-OD2	8.31	125.78	118.30
3	F	23	DT	O4'-C1'-N1	-8.05	102.37	108.00
3	F	15	DC	O4'-C1'-N1	7.72	113.40	108.00
3	F	18	DG	O4'-C4'-C3'	-7.39	101.55	104.50
1	A	305	ARG	NE-CZ-NH1	7.29	123.95	120.30
1	A	693	ASP	CB-CG-OD2	7.17	124.75	118.30
1	A	413	ASP	CB-CG-OD2	6.96	124.57	118.30
2	E	7	DC	O4'-C1'-N1	-6.92	103.16	108.00
1	A	754	ASP	CB-CG-OD2	6.82	124.44	118.30
1	A	42	ASP	CB-CG-OD2	6.78	124.40	118.30
3	F	19	DT	C4'-C3'-C2'	-6.71	97.06	103.10
1	A	703	ASP	CB-CG-OD2	6.51	124.16	118.30
1	A	305	ARG	NE-CZ-NH2	-6.47	117.06	120.30
3	F	22	DT	O4'-C1'-N1	-6.36	103.55	108.00
1	B	461	ASP	CB-CG-OD2	6.35	124.02	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	333	ASP	CB-CG-OD2	6.29	123.97	118.30
1	A	364	ASP	CB-CG-OD2	6.19	123.87	118.30
1	A	511	ASP	CB-CG-OD2	6.18	123.86	118.30
1	B	421	ASP	CB-CG-OD2	6.13	123.81	118.30
1	B	754	ASP	CB-CG-OD2	6.11	123.80	118.30
1	A	405	ASP	CB-CG-OD2	6.07	123.76	118.30
1	A	651	ASP	CB-CG-OD2	6.03	123.73	118.30
1	B	632	LEU	CA-CB-CG	5.89	128.84	115.30
1	B	386	ASP	CB-CG-OD2	5.84	123.55	118.30
3	F	19	DT	O4'-C1'-N1	5.79	112.05	108.00
1	B	221	ASP	CB-CG-OD2	5.70	123.43	118.30
1	A	421	ASP	CB-CG-OD2	5.68	123.41	118.30
1	B	52	ASP	CB-CG-OD2	5.68	123.41	118.30
3	F	14	DA	O4'-C1'-N9	5.67	111.97	108.00
1	B	35	ASP	CB-CG-OD2	5.66	123.40	118.30
1	A	149	ASP	CB-CG-OD2	5.66	123.39	118.30
1	B	149	ASP	CB-CG-OD2	5.62	123.36	118.30
3	F	19	DT	P-O3'-C3'	5.61	126.43	119.70
1	A	162	ASP	CB-CG-OD2	5.59	123.33	118.30
3	F	22	DT	N3-C2-O2	-5.59	118.94	122.30
1	A	703	ASP	CB-CG-OD1	-5.57	113.29	118.30
1	A	130	ASP	CB-CG-OD2	5.52	123.27	118.30
3	F	14	DA	O4'-C4'-C3'	-5.51	102.30	104.50
1	A	748	ASP	CB-CG-OD2	5.49	123.24	118.30
1	A	157	LEU	CA-CB-CG	5.43	127.80	115.30
1	B	296	ASP	CB-CG-OD2	5.42	123.18	118.30
3	F	21	DC	O4'-C1'-N1	-5.42	104.20	108.00
1	A	461	ASP	CB-CG-OD2	5.38	123.14	118.30
1	A	232	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	A	747	LEU	CA-CB-CG	-5.32	103.06	115.30
1	B	703	ASP	CB-CG-OD2	5.17	122.95	118.30
1	B	413	ASP	CB-CG-OD2	5.17	122.95	118.30
1	B	43	ASP	CB-CG-OD2	5.17	122.95	118.30
3	F	15	DC	O4'-C1'-C2'	-5.15	101.78	105.90
2	E	1	DA	O4'-C1'-N9	5.14	111.60	108.00
2	E	2	DG	O4'-C1'-N9	5.12	111.59	108.00
1	A	139	ASP	CB-CG-OD2	5.10	122.89	118.30
1	B	162	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	441	ASP	CB-CG-OD2	5.04	122.84	118.30
1	B	511	ASP	CB-CG-OD2	5.03	122.83	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	6207	0	6253	57	0
1	B	5964	0	6020	53	0
2	E	367	0	202	2	0
3	F	347	0	194	4	0
4	A	27	0	12	1	0
5	A	1	0	0	0	0
6	A	128	0	0	12	0
6	B	116	0	0	6	0
6	E	2	0	0	0	0
6	F	1	0	0	0	0
All	All	13160	0	12681	112	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 (112) 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:327:THR:HG21	1:B:555:LEU:HD13	1.66	0.77
1:A:130:ASP:OD1	6:A:2029:HOH:O	2.03	0.77
1:B:273:THR:HG23	1:B:655:THR:HG23	1.68	0.76
1:A:149:ASP:OD2	6:A:2029:HOH:O	2.06	0.72
1:A:327:THR:HG21	1:A:555:LEU:HD13	1.73	0.70
1:B:108:ARG:N	6:B:2007:HOH:O	2.23	0.69
1:B:656:ARG:O	1:B:656:ARG:HG3	1.94	0.68
1:B:84:VAL:HG13	1:B:116:PRO:HA	1.77	0.66
1:B:633:MET:O	1:B:636:ILE:HG22	1.98	0.63
1:A:727:THR:HG21	1:A:732:LEU:HD12	1.81	0.63
1:B:151:SER:O	1:B:353:ALA:HB2	1.99	0.63
1:A:359:THR:HG21	6:A:2023:HOH:O	2.00	0.62
1:A:186:GLU:HG2	6:A:2030:HOH:O	2.00	0.62
1:B:51:LEU:HD21	1:B:83:LEU:HG	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:GLN:NE2	1:B:333:ASP:OD1	2.33	0.61
1:A:211:GLN:HE22	1:A:212:GLN:NE2	1.96	0.61
1:B:445:ASP:HB3	6:B:2060:HOH:O	2.02	0.60
1:B:342:LEU:HD11	1:B:552:LEU:HD23	1.84	0.59
1:B:37:TYR:HE2	1:B:76:VAL:HG21	1.67	0.59
1:A:433:LEU:HD21	1:A:437:ARG:NH2	2.20	0.57
1:A:50:LEU:HD22	1:A:86:GLN:OE1	2.05	0.57
1:A:211:GLN:NE2	1:A:212:GLN:NE2	2.53	0.57
1:A:51:LEU:HD21	1:A:83:LEU:HD21	1.86	0.57
1:A:693:ASP:OD2	6:A:2092:HOH:O	2.18	0.55
1:A:396:LYS:NZ	6:A:2064:HOH:O	2.40	0.55
1:A:623:TYR:CE1	1:A:762:VAL:HG21	2.43	0.54
1:B:290:THR:HG22	1:B:293:SER:H	1.72	0.54
1:A:190:ILE:HG23	1:A:196:LEU:HD11	1.90	0.54
1:A:705:LEU:HD12	1:A:705:LEU:O	2.09	0.53
1:A:305:ARG:NH2	1:A:347:ASP:OD2	2.42	0.53
1:B:735:LEU:HD22	1:B:739:MET:CE	2.39	0.52
1:A:211:GLN:NE2	1:A:212:GLN:HE21	2.07	0.52
1:B:601:LEU:HD11	1:B:603:LEU:HG	1.92	0.52
1:A:640:VAL:HG11	1:A:645:VAL:HG21	1.92	0.52
1:A:579:ARG:HG2	1:A:602:ASN:HD22	1.73	0.52
1:B:17:TYR:CE2	1:B:29:LEU:HD23	2.45	0.51
1:A:137:TRP:HB3	1:A:204:PHE:CE2	2.45	0.51
1:A:623:TYR:CZ	1:A:762:VAL:HG21	2.45	0.51
1:B:37:TYR:CE2	1:B:76:VAL:HG21	2.46	0.51
1:A:263:GLU:HA	1:A:268:ILE:HD11	1.93	0.51
1:A:328:ILE:HG23	1:A:559:ALA:HA	1.93	0.50
1:B:471:HIS:CE1	1:B:493:GLN:HB2	2.46	0.50
1:A:42:ASP:HB2	6:A:2012:HOH:O	2.10	0.50
1:A:437:ARG:O	1:A:441:ASP:HB2	2.12	0.50
1:A:686:GLU:HG2	1:A:720:LYS:HB2	1.93	0.50
1:B:515:THR:HB	1:B:519:LYS:NZ	2.27	0.50
1:B:628:ALA:HB2	1:B:691:LEU:HD11	1.94	0.50
1:A:670:PHE:N	1:A:670:PHE:CD2	2.80	0.49
1:B:321:LEU:O	1:B:325:GLN:HG3	2.13	0.49
1:B:468:ASN:HD22	2:E:5:DG:H5"	1.78	0.49
1:A:315:VAL:HG12	1:A:317:ASP:H	1.78	0.48
1:B:387:SER:OG	1:B:389:PRO:HD2	2.13	0.48
1:A:750:LEU:HD12	1:A:759:MET:SD	2.53	0.48
1:A:326:GLN:HB3	6:A:2063:HOH:O	2.13	0.48
1:A:5:GLU:HB3	1:A:10:HIS:HE1	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:LEU:HD21	1:B:655:THR:HG21	1.95	0.48
1:B:388:ALA:N	1:B:389:PRO:CD	2.76	0.47
1:B:82:LYS:NZ	6:B:2005:HOH:O	2.45	0.47
1:A:463:LEU:HA	1:A:476:GLN:O	2.15	0.47
1:B:474:TYR:CE1	1:B:500:ARG:HD2	2.49	0.47
1:A:213:LEU:HD23	1:A:241:LEU:HD22	1.97	0.47
1:A:588:VAL:HG13	1:A:592:LEU:HD13	1.97	0.46
1:A:620:LYS:NZ	4:A:1801:ADP:O3B	2.35	0.46
1:A:262:ARG:NH1	6:A:2053:HOH:O	2.47	0.46
1:A:789:ALA:O	1:B:706:SER:HB3	2.16	0.46
1:B:463:LEU:HD23	1:B:464:LYS:N	2.30	0.46
1:B:73:TYR:O	1:B:76:VAL:HG23	2.16	0.46
1:A:359:THR:O	1:A:359:THR:HG22	2.16	0.45
1:A:628:ALA:HB2	1:A:691:LEU:HD11	1.97	0.45
1:B:108:ARG:CA	6:B:2007:HOH:O	2.62	0.45
1:A:136:ILE:HD13	1:A:190:ILE:HD11	1.99	0.45
1:B:375:LEU:HD22	1:B:397:MET:HG2	1.99	0.45
1:B:40:PHE:CE1	1:B:68:MET:HG2	2.52	0.45
1:B:216:GLN:NE2	1:B:252:LEU:O	2.50	0.44
1:B:594:GLU:HG3	1:B:595:PRO:HD2	2.00	0.44
1:B:632:LEU:HD12	1:B:632:LEU:C	2.38	0.44
2:E:2:DG:O6	3:F:28:DG:O6	2.35	0.44
1:B:267:ILE:HD12	1:B:314:PRO:HB2	2.00	0.44
1:B:396:LYS:HG2	1:B:548:ALA:HB2	1.99	0.44
3:F:20:DG:H4'	3:F:21:DC:OP1	2.18	0.44
1:B:328:ILE:HG23	1:B:559:ALA:HA	2.00	0.43
1:B:299:VAL:HB	1:B:343:ARG:HB2	2.00	0.43
1:B:735:LEU:HD22	1:B:739:MET:HE2	2.00	0.43
3:F:19:DT:C2'	3:F:20:DG:O5'	2.66	0.43
1:A:727:THR:HG23	6:A:2103:HOH:O	2.19	0.43
1:A:17:TYR:CD2	1:A:17:TYR:C	2.92	0.43
1:A:771:TYR:HA	6:A:2123:HOH:O	2.17	0.43
1:A:72:PRO:HG3	3:F:23:DT:O2	2.18	0.43
1:B:311:LEU:HD23	1:B:636:ILE:HD12	2.00	0.43
1:B:157:LEU:C	1:B:157:LEU:HD23	2.39	0.42
1:A:375:LEU:N	1:A:376:PRO:CD	2.82	0.42
1:B:316:ARG:HD3	1:B:650:ILE:O	2.20	0.42
1:A:352:LEU:HA	1:A:352:LEU:HD23	1.91	0.42
1:A:51:LEU:HD21	1:A:83:LEU:CD2	2.49	0.42
1:B:154:ARG:HD3	6:B:2019:HOH:O	2.20	0.42
1:B:52:ASP:O	1:B:53:ILE:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:ILE:HD12	1:A:487:ILE:HA	1.91	0.42
1:B:536:LEU:N	1:B:537:PRO:CD	2.82	0.42
1:B:735:LEU:HD22	1:B:739:MET:HE1	2.01	0.42
1:A:470:VAL:HG12	1:A:471:HIS:CD2	2.55	0.41
1:B:393:LEU:HD13	1:B:552:LEU:HD12	2.02	0.41
1:A:345:VAL:HG11	1:A:549:LEU:HD13	2.02	0.41
1:B:157:LEU:O	1:B:260:MET:HA	2.20	0.41
1:B:39:LEU:HD23	1:B:43:ASP:HB3	2.01	0.41
1:B:387:SER:HB3	1:B:390:VAL:HB	2.02	0.41
1:A:702:TYR:HD1	1:A:705:LEU:HD23	1.85	0.41
1:A:148:LEU:CB	1:A:240:LEU:HD21	2.50	0.41
1:A:579:ARG:HG2	1:A:602:ASN:ND2	2.35	0.41
1:A:33:MET:CE	1:A:38:GLN:HG3	2.51	0.40
1:B:315:VAL:HB	6:B:2034:HOH:O	2.20	0.40
1:A:446:TYR:OH	1:A:505:GLU:HG2	2.22	0.40
1:A:359:THR:HG22	6:A:2024:HOH:O	2.22	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	784/800 (98%)	756 (96%)	28 (4%)	0	100	100
1	B	746/800 (93%)	726 (97%)	19 (2%)	1 (0%)	51	68
All	All	1530/1600 (96%)	1482 (97%)	47 (3%)	1 (0%)	51	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	141	LYS

### 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	656/664 (99%)	609 (93%)	47 (7%)	14	23
1	B	631/664 (95%)	577 (91%)	54 (9%)	10	16
All	All	1287/1328 (97%)	1186 (92%)	101 (8%)	12	19

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	46	ARG
1	A	57	LYS
1	A	84	VAL
1	A	102	SER
1	A	109	LYS
1	A	137	TRP
1	A	139	ASP
1	A	157	LEU
1	A	164	GLU
1	A	178	LEU
1	A	190	ILE
1	A	201	LEU
1	A	264	GLN
1	A	311	LEU
1	A	332	GLN
1	A	384	THR
1	A	397	MET
1	A	402	GLU
1	A	419	VAL
1	A	439	LEU
1	A	441	ASP
1	A	444	THR
1	A	448	GLU
1	A	479	ARG
1	A	488	ASN
1	A	506	LEU

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Mol	Chain	Res	Type
1	A	507	LYS
1	A	512	LYS
1	A	531	LEU
1	A	536	LEU
1	A	547	SER
1	A	552	LEU
1	A	568	THR
1	A	571	THR
1	A	640	VAL
1	A	656	ARG
1	A	670	PHE
1	A	705	LEU
1	A	707	LEU
1	A	727	THR
1	A	728	HIS
1	A	734	GLN
1	A	736	PRO
1	A	755	THR
1	A	756	ILE
1	A	788	ARG
1	B	14	MET
1	B	15	GLN
1	B	33	MET
1	B	38	GLN
1	B	46	ARG
1	B	53	ILE
1	B	78	ASN
1	B	94	GLU
1	B	108	ARG
1	B	111	VAL
1	B	115	THR
1	B	119	ILE
1	B	122	GLU
1	B	137	TRP
1	B	139	ASP
1	B	140	SER
1	B	155	PHE
1	B	157	LEU
1	B	163	ARG
1	B	178	LEU
1	B	186	GLU
1	B	188	SER

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Mol	Chain	Res	Type
1	B	194	ARG
1	B	201	LEU
1	B	250	THR
1	B	254	HIS
1	B	274	ARG
1	B	290	THR
1	B	335	THR
1	B	338	LEU
1	B	352	LEU
1	B	357	LEU
1	B	404	ARG
1	B	455	ARG
1	B	490	MET
1	B	496	LYS
1	B	500	ARG
1	B	507	LYS
1	B	511	ASP
1	B	514	LEU
1	B	535	LEU
1	B	552	LEU
1	B	584	ARG
1	B	608	ARG
1	B	632	LEU
1	B	636	ILE
1	B	655	THR
1	B	656	ARG
1	B	737	GLU
1	B	738	LYS
1	B	755	THR
1	B	756	ILE
1	B	783	LYS
1	B	788	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	ASN
1	A	171	GLN
1	A	212	GLN
1	A	242	GLN
1	A	566	ASN
1	A	590	GLN

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Mol	Chain	Res	Type
1	A	602	ASN
1	A	682	HIS
1	A	717	ASN
1	B	38	GLN
1	B	289	ASN
1	B	344	GLN
1	B	370	HIS
1	B	468	ASN
1	B	471	HIS
1	B	717	ASN
1	B	791	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\# Z  > 2$
4	ADP	A	1801	5	24,29,29	1.33	2 (8%)	29,45,45	1.37	3 (10%)

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
4	ADP	A	1801	5	-	3/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1801	ADP	C2-N3	4.49	1.39	1.32
4	A	1801	ADP	C2-N1	2.56	1.38	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1801	ADP	N3-C2-N1	-4.99	120.88	128.68
4	A	1801	ADP	PA-O3A-PB	-2.21	125.24	132.83
4	A	1801	ADP	O2B-PB-O3A	2.10	111.67	104.64

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1801	ADP	PA-O3A-PB-O2B
4	A	1801	ADP	PA-O3A-PB-O3B
4	A	1801	ADP	PA-O3A-PB-O1B

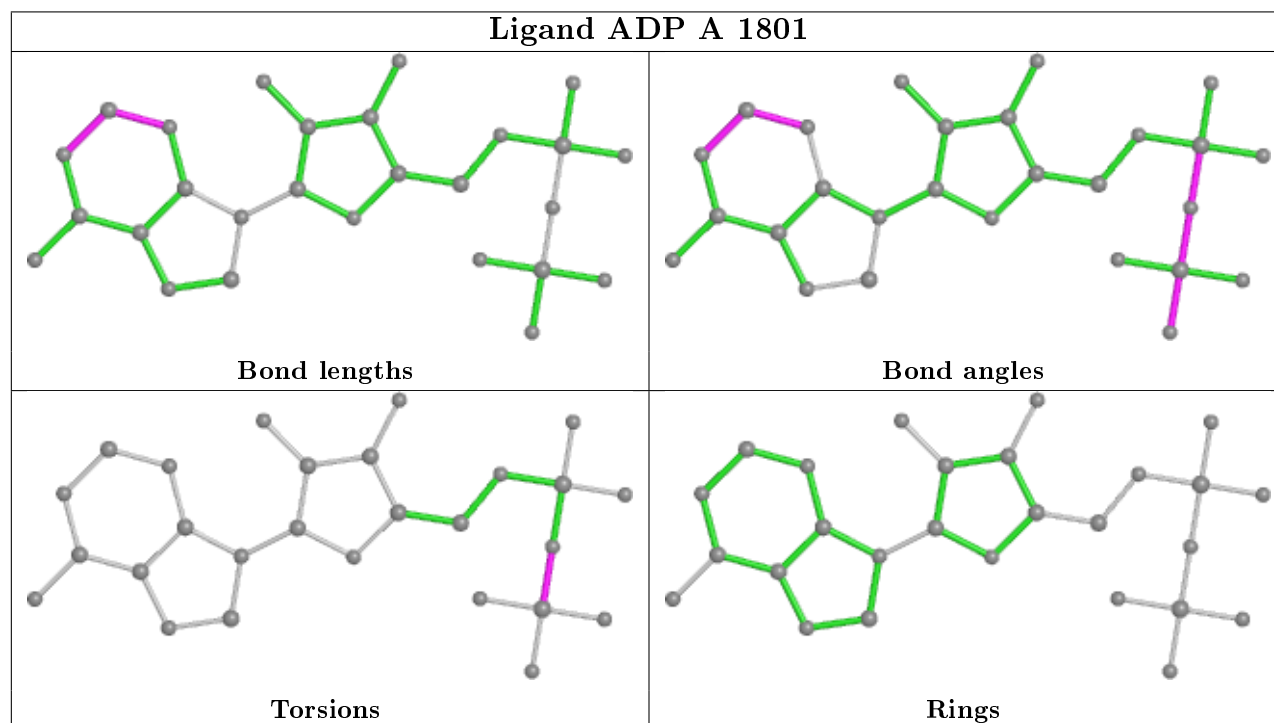
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1801	ADP	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 [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	788/800 (98%)	-0.05	19 (2%) 59 57	2, 16, 25, 38	0
1	B	754/800 (94%)	0.02	24 (3%) 47 46	8, 16, 24, 34	0
2	E	18/18 (100%)	0.57	4 (22%) 0 0	9, 17, 96, 109	0
3	F	17/17 (100%)	0.22	3 (17%) 1 1	8, 15, 59, 95	0
All	All	1577/1635 (96%)	-0.01	50 (3%) 47 46	2, 16, 25, 109	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	444	THR	7.5
2	E	18	DG	5.7
3	F	14	DA	4.6
1	A	62	ALA	4.4
2	E	17	DT	4.0
1	B	800	SER	3.9
1	A	441	ASP	3.9
1	B	74	HIS	3.8
2	E	1	DA	3.8
1	B	29	LEU	3.8
1	A	61	SER	3.6
1	A	800	SER	3.5
1	B	25	PRO	3.5
1	B	56	THR	3.3
1	B	456	GLU	3.2
2	E	16	DG	3.2
1	A	658	GLY	3.2
1	B	140	SER	3.1
1	A	443	ALA	3.1
1	B	54	SER	3.1
1	B	28	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	14	MET	3.0
1	A	103	LYS	3.0
1	A	475	ILE	2.9
1	B	52	ASP	2.9
1	A	593	ASN	2.8
1	B	35	ASP	2.8
1	B	68	MET	2.7
1	A	220	ARG	2.6
1	B	39	LEU	2.6
1	B	135	ALA	2.6
1	B	30	PHE	2.6
3	F	15	DC	2.5
1	A	549	LEU	2.5
1	A	752	HIS	2.5
1	B	413	ASP	2.5
1	B	136	ILE	2.5
1	A	445	ASP	2.5
1	A	672	VAL	2.4
1	A	386	ASP	2.4
1	B	475	ILE	2.4
1	B	19	ARG	2.4
1	A	97	GLY	2.3
1	B	672	VAL	2.3
1	A	442	GLY	2.3
1	B	284	ALA	2.3
1	B	41	TYR	2.1
1	A	431	GLU	2.1
1	B	55	LEU	2.0
3	F	16	DT	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 ⓘ

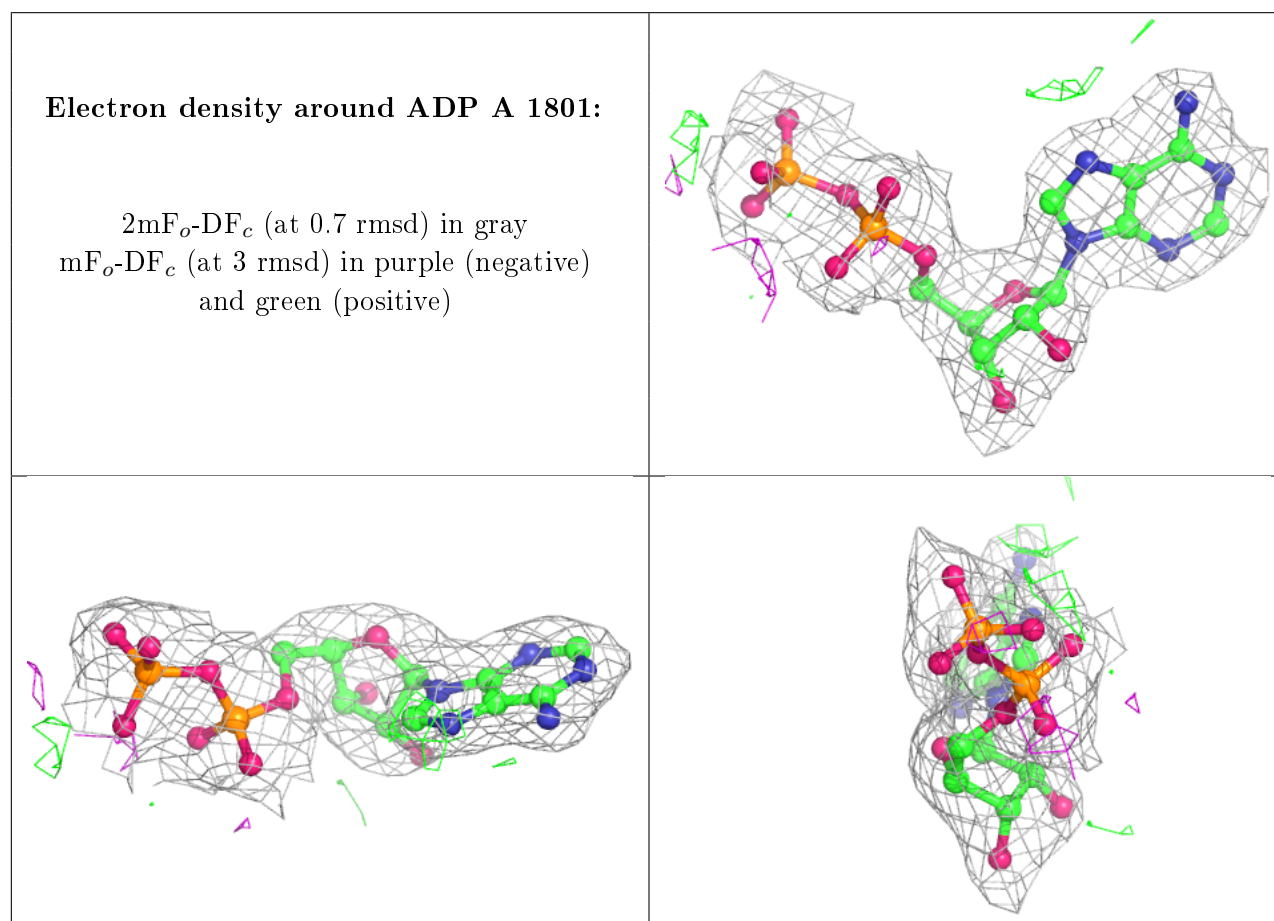
There are no carbohydrates in this entry.

## 6.4 Ligands [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
5	MG	A	1802	1/1	0.57	0.10	18,18,18,18	0
4	ADP	A	1801	27/27	0.97	0.10	5,13,16,20	0

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.