



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 03:16 PM BST

PDB ID : 1OH5  
Title : THE CRYSTAL STRUCTURE OF E. COLI MUTS BINDING TO DNA  
WITH A C:A MISMATCH  
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Sixma, T.K.  
Deposited on : 2003-05-23  
Resolution : 2.90 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

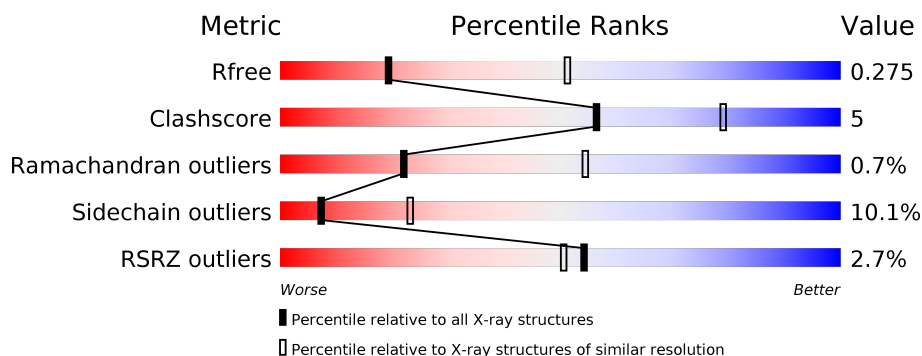
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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>78%</div> <div>18%</div> <div>• •</div> </div>
1	B	800	<div> <div>2%</div> <div>76%</div> <div>16%</div> <div>• 6%</div> </div>
2	E	30	<div> <div>17%</div> <div>30%</div> <div>23%</div> <div>7%</div> <div>40%</div> </div>
3	F	30	<div> <div>7%</div> <div>27%</div> <div>10%</div> <div>20%</div> <div>43%</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12968 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	1103	1170	29			
1	B	754	Total	C	N	O	S	0	0	0
			5964	3756	1060	1120	28			

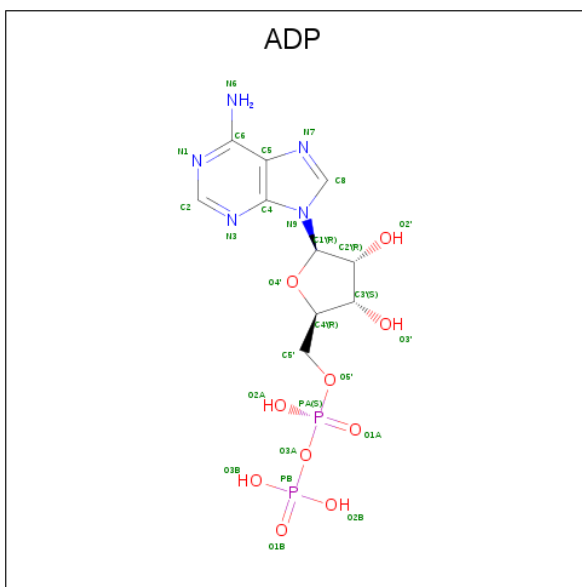
- Molecule 2 is a DNA chain called 5'-D(\*AP\*GP\*CP\*TP\*GP\*CP\*CP\*AP\*CP\*GP \*CP\*A P\*CP\*CP\*AP\*GP\*TP\*GP\*TP\*CP\*AP\*GP\*CP\*GP\*TP \*CP\*CP\*TP\*AP\*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	18	Total	C	N	O	P	0	0	0
			364	173	70	104	17			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	17	Total	C	N	O	P	0	0	0
			348	166	65	101	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

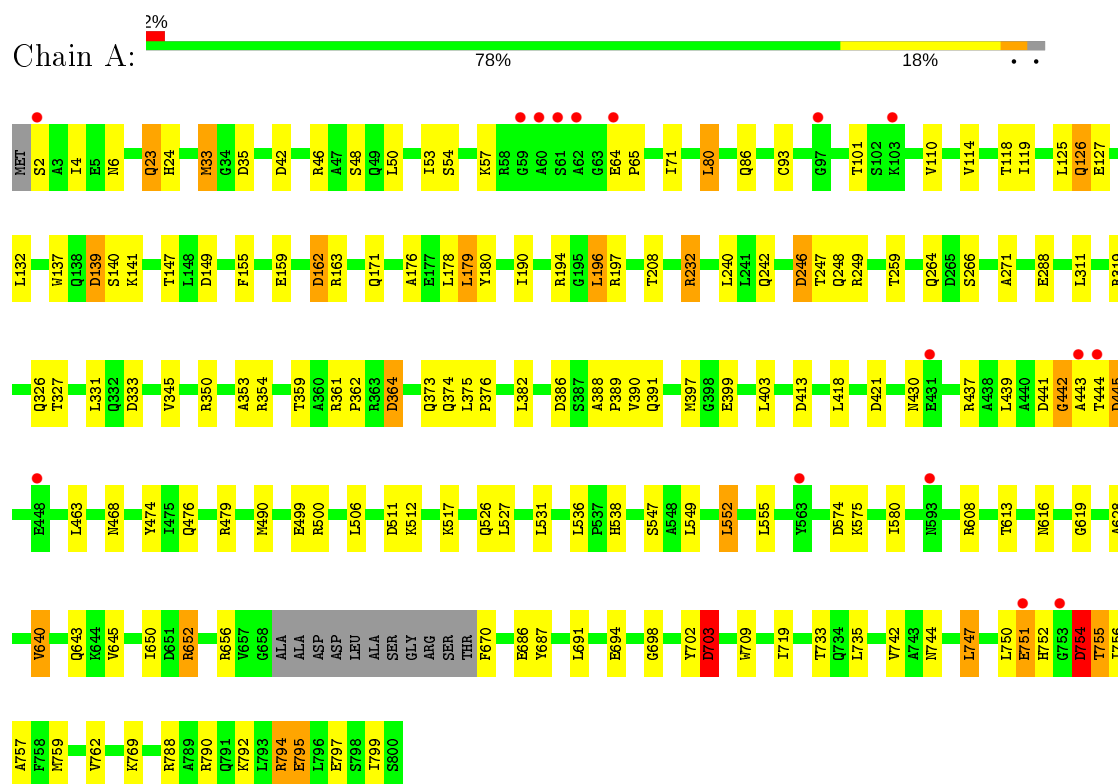
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	31	Total	O		
			31	31	0	0
6	B	26	Total	O		
			26	26	0	0

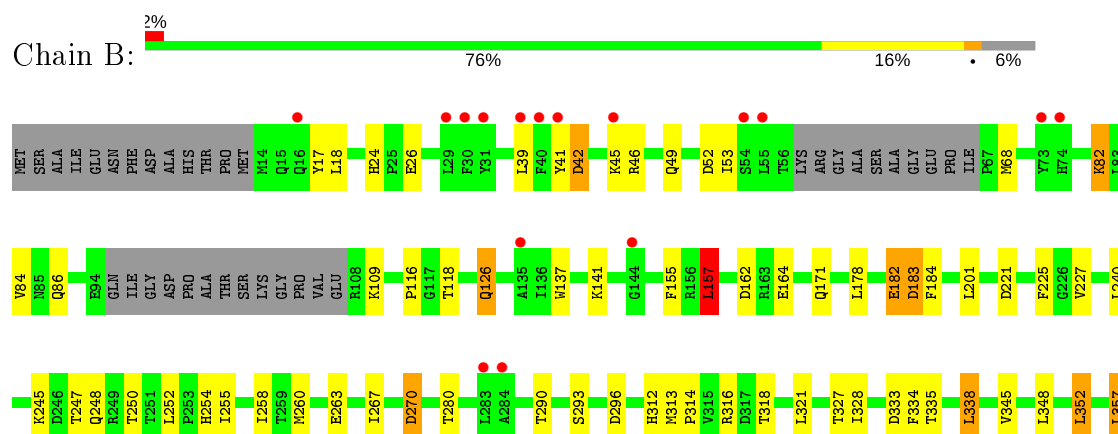
### 3 Residue-property plots [i](#)

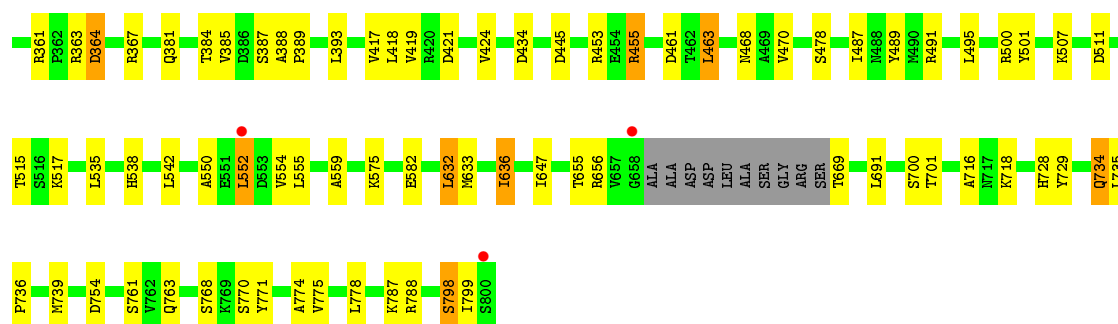
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

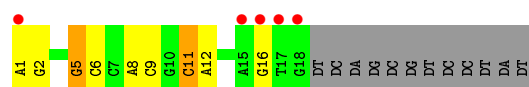
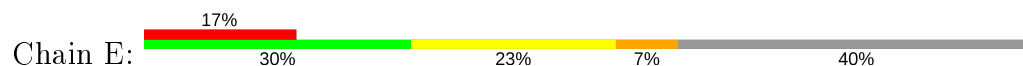


#### • Molecule 1: DNA MISMATCH REPAIR PROTEIN MUTS

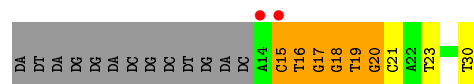




● Molecule 2: 5'-D(\*AP\*GP\*CP\*TP\*GP\*CP\*CP\*AP\*CP\*GP \*CP\*AP\*CP\*CP\*AP\*GP\*TP\*GP\*TP\*CP\*AP\*GP\*CP\*GP\*TP \*CP\*CP\*TP\*AP\*T)-3'



● Molecule 3: 5'-D(\*AP\*TP\*AP\*GP\*GP\*AP\*CP\*GP\*CP\*TP \*GP\*AP\*CP\*AP\*CP\*TP\*GP\*GP\*TP\*GP\*CP\*AP\*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, $\alpha$ , $\beta$ , $\gamma$	89.91Å 91.89Å 261.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.90 20.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	93.5 (15.00-2.90) 93.5 (20.00-2.90)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.14 (at 2.88Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.224 , 0.294 0.218 , 0.275	Depositor DCC
$R_{free}$ test set	2251 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	66.0	Xtriage
Anisotropy	0.463	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 41.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.012 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12968	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% 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, 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	0.48	0/6313	0.76	13/8544 (0.2%)
1	B	0.45	0/6062	0.75	14/8199 (0.2%)
2	E	0.82	0/408	1.65	8/627 (1.3%)
3	F	0.99	1/390 (0.3%)	2.02	14/601 (2.3%)
All	All	0.50	1/13173 (0.0%)	0.88	49/17971 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	21	DC	O3'-P	-5.17	1.54	1.61

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	21	DC	O4'-C1'-N1	11.36	115.95	108.00
3	F	19	DT	O4'-C4'-C3'	-9.99	100.01	106.00
2	E	12	DA	O4'-C1'-N9	9.18	114.42	108.00
3	F	15	DC	P-O3'-C3'	8.56	129.97	119.70
3	F	20	DG	O4'-C1'-N9	8.43	113.90	108.00
2	E	9	DC	O4'-C1'-N1	8.37	113.86	108.00
2	E	5	DG	P-O3'-C3'	8.00	129.30	119.70
3	F	21	DC	N1-C1'-C2'	-7.54	98.27	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	333	ASP	CB-CG-OD2	7.30	124.87	118.30
3	F	17	DG	P-O3'-C3'	7.23	128.38	119.70
3	F	23	DT	O4'-C1'-N1	-6.71	103.30	108.00
1	B	364	ASP	CB-CG-OD2	6.66	124.29	118.30
3	F	21	DC	P-O3'-C3'	-6.66	111.71	119.70
1	B	461	ASP	CB-CG-OD2	6.50	124.15	118.30
2	E	11	DC	O4'-C1'-N1	6.28	112.39	108.00
1	A	421	ASP	CB-CG-OD2	6.26	123.94	118.30
1	A	364	ASP	CB-CG-OD2	6.23	123.91	118.30
1	B	754	ASP	CB-CG-OD2	6.17	123.85	118.30
3	F	16	DT	C1'-O4'-C4'	-6.15	103.95	110.10
1	B	270	ASP	CB-CG-OD2	6.07	123.76	118.30
3	F	16	DT	O4'-C4'-C3'	-6.04	102.08	104.50
1	B	157	LEU	CA-CB-CG	5.99	129.08	115.30
3	F	30	DT	O4'-C1'-N1	5.86	112.10	108.00
1	A	139	ASP	CB-CG-OD2	5.85	123.56	118.30
1	A	386	ASP	CB-CG-OD2	5.81	123.53	118.30
1	A	413	ASP	CB-CG-OD2	5.79	123.51	118.30
1	A	445	ASP	CB-CG-OD2	5.77	123.50	118.30
3	F	16	DT	O4'-C1'-N1	5.72	112.00	108.00
1	A	162	ASP	CB-CG-OD2	5.68	123.42	118.30
1	B	296	ASP	CB-CG-OD2	5.63	123.37	118.30
2	E	11	DC	C1'-O4'-C4'	-5.63	104.47	110.10
1	B	42	ASP	CB-CG-OD2	5.56	123.30	118.30
2	E	8	DA	O4'-C1'-N9	-5.51	104.14	108.00
1	A	754	ASP	CB-CG-OD2	5.38	123.15	118.30
3	F	18	DG	O4'-C1'-N9	5.33	111.73	108.00
1	A	246	ASP	CB-CG-OD2	5.29	123.06	118.30
2	E	5	DG	C4'-C3'-C2'	-5.28	98.35	103.10
1	A	42	ASP	CB-CG-OD2	5.25	123.03	118.30
1	A	511	ASP	CB-CG-OD2	5.20	122.98	118.30
1	B	632	LEU	CA-CB-CG	5.16	127.17	115.30
1	A	149	ASP	CB-CG-OD2	5.15	122.94	118.30
1	B	511	ASP	CB-CG-OD2	5.12	122.91	118.30
1	B	221	ASP	CB-CG-OD2	5.10	122.89	118.30
3	F	19	DT	C5'-C4'-O4'	5.09	118.97	109.30
1	A	703	ASP	CB-CG-OD2	5.07	122.86	118.30
1	B	162	ASP	CB-CG-OD2	5.06	122.85	118.30
1	B	434	ASP	CB-CG-OD2	5.05	122.85	118.30
1	B	445	ASP	CB-CG-OD2	5.05	122.84	118.30
2	E	16	DG	P-O3'-C3'	5.02	125.72	119.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	702	TYR	Peptide

## 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	6251	68	0
1	B	5964	0	6018	53	0
2	E	364	0	202	3	0
3	F	348	0	193	7	0
4	A	27	0	12	0	0
5	A	1	0	0	0	0
6	A	31	0	0	1	0
6	B	26	0	0	0	0
All	All	12968	0	12676	127	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 5.

All (127) 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:A:703:ASP:OD1	1:B:770:SER:HB2	1.75	0.87
3:F:19:DT:C2'	3:F:20:DG:O5'	2.37	0.73
1:A:180:TYR:CE1	1:A:196:LEU:HD12	2.25	0.71
1:A:698:GLY:HA3	1:A:703:ASP:HB3	1.71	0.71
1:B:328:ILE:HG23	1:B:559:ALA:HA	1.73	0.70
1:A:754:ASP:O	1:A:755:THR:HB	1.90	0.69
1:B:633:MET:O	1:B:636:ILE:HG22	1.92	0.69
1:A:354:ARG:HD2	1:A:364:ASP:OD2	1.93	0.68
1:B:734:GLN:HE21	1:B:734:GLN:HA	1.59	0.67
1:B:327:THR:HG21	1:B:555:LEU:HD13	1.78	0.66
1:B:655:THR:HG22	1:B:691:LEU:HD12	1.76	0.66
3:F:15:DC:H2'	3:F:16:DT:C6	2.30	0.66
1:A:430:ASN:HD22	1:A:527:LEU:HD21	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:656:ARG:O	1:B:656:ARG:HG3	1.97	0.65
1:A:359:THR:HG21	6:A:2007:HOH:O	1.98	0.64
1:A:118:THR:HG21	1:A:247:THR:HG21	1.81	0.63
3:F:18:DG:H2''	3:F:19:DT:O4'	1.98	0.63
1:A:4:ILE:HG22	1:A:6:ASN:HD22	1.62	0.63
1:B:348:LEU:HG	1:B:352:LEU:HD22	1.80	0.63
1:B:248:GLN:HB3	1:B:250:THR:HG22	1.80	0.62
1:A:640:VAL:HG11	1:A:645:VAL:HG21	1.81	0.61
1:B:252:LEU:HD23	1:B:357:LEU:HD11	1.84	0.60
1:A:442:GLY:O	1:A:445:ASP:HB3	2.04	0.58
2:E:1:DA:H2''	2:E:2:DG:O5'	2.03	0.58
1:A:703:ASP:OD1	1:B:770:SER:CB	2.49	0.57
1:A:327:THR:HG21	1:A:555:LEU:HD13	1.87	0.56
1:A:652:ARG:HH11	1:A:652:ARG:HB3	1.69	0.56
1:A:180:TYR:CD1	1:A:196:LEU:HD12	2.40	0.56
1:B:126:GLN:N	1:B:126:GLN:HE21	2.04	0.56
1:A:388:ALA:HB3	1:A:389:PRO:HD3	1.89	0.55
1:B:82:LYS:O	1:B:86:GLN:NE2	2.39	0.55
1:A:50:LEU:HD22	1:A:86:GLN:OE1	2.06	0.55
1:B:771:TYR:O	1:B:775:VAL:HG23	2.07	0.54
1:B:489:TYR:HB3	1:B:501:TYR:CD2	2.44	0.53
1:A:437:ARG:O	1:A:441:ASP:HB2	2.08	0.53
1:A:159:GLU:OE2	1:A:232:ARG:HB2	2.09	0.53
1:B:84:VAL:HG13	1:B:116:PRO:HA	1.92	0.51
1:B:393:LEU:HB3	1:B:552:LEU:CD2	2.40	0.51
1:B:252:LEU:HB3	1:B:255:ILE:HD12	1.91	0.51
1:A:403:LEU:HD21	1:A:538:HIS:CD2	2.46	0.51
1:A:171:GLN:NE2	1:A:271:ALA:HA	2.26	0.51
3:F:15:DC:H2''	3:F:16:DT:OP1	2.11	0.50
1:B:352:LEU:HD11	1:B:542:LEU:HD13	1.94	0.50
1:A:350:ARG:O	1:A:353:ALA:HB3	2.12	0.49
1:A:33:MET:HE1	2:E:11:DC:H5'	1.95	0.49
1:A:345:VAL:HG21	1:A:549:LEU:HD22	1.95	0.49
1:B:118:THR:HG21	1:B:247:THR:HG21	1.95	0.49
1:B:388:ALA:N	1:B:389:PRO:CD	2.76	0.49
1:A:443:ALA:O	1:A:445:ASP:HB2	2.13	0.48
1:A:443:ALA:C	1:A:445:ASP:N	2.67	0.48
1:A:327:THR:HG22	1:A:331:LEU:HD12	1.96	0.48
1:B:455:ARG:HG3	1:B:463:LEU:HB3	1.97	0.47
3:F:19:DT:H2'	3:F:20:DG:O5'	2.13	0.47
1:A:375:LEU:N	1:A:376:PRO:CD	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:799:ILE:HG21	1:B:799:ILE:CG2	2.45	0.47
1:B:126:GLN:CA	1:B:126:GLN:HE21	2.28	0.46
1:A:171:GLN:HE22	1:A:271:ALA:HA	1.79	0.46
1:A:361:ARG:HB3	1:A:362:PRO:HD2	1.97	0.46
3:F:18:DG:H2'	3:F:19:DT:H6	1.81	0.46
1:A:733:THR:O	1:A:744:ASN:ND2	2.47	0.46
1:B:182:GLU:O	1:B:183:ASP:C	2.53	0.46
1:A:430:ASN:ND2	1:A:527:LEU:HD21	2.31	0.45
1:B:774:ALA:O	1:B:778:LEU:HG	2.15	0.45
1:B:280:THR:HG1	1:B:312:HIS:HE2	1.60	0.45
1:A:23:GLN:O	1:A:24:HIS:CG	2.69	0.45
1:A:750:LEU:O	1:A:757:ALA:HB3	2.17	0.45
1:A:48:SER:HB2	1:A:53:ILE:O	2.16	0.45
1:B:328:ILE:HG23	1:B:559:ALA:CA	2.44	0.45
1:B:363:ARG:O	1:B:367:ARG:HG3	2.18	0.44
1:A:552:LEU:HD12	1:A:552:LEU:HA	1.88	0.44
1:A:747:LEU:HD11	1:A:762:VAL:HG22	2.00	0.44
1:A:441:ASP:C	1:A:443:ALA:N	2.70	0.44
1:B:338:LEU:HD13	1:B:381:GLN:OE1	2.16	0.44
1:A:709:TRP:CD1	1:A:709:TRP:C	2.91	0.44
1:B:417:VAL:HG12	1:B:418:LEU:HG	1.99	0.44
1:A:33:MET:HE2	1:A:33:MET:HB3	1.94	0.44
1:A:126:GLN:O	1:A:127:GLU:C	2.55	0.44
1:A:176:ALA:HA	1:A:194:ARG:CZ	2.48	0.44
1:B:393:LEU:HB3	1:B:552:LEU:HD21	1.99	0.44
1:B:728:HIS:CE1	1:B:729:TYR:CZ	3.06	0.43
1:B:52:ASP:O	1:B:53:ILE:HG23	2.19	0.43
1:A:441:ASP:C	1:A:443:ALA:H	2.22	0.43
1:A:686:GLU:HG2	1:A:719:ILE:O	2.18	0.43
1:A:735:LEU:HB3	1:A:742:VAL:HG11	2.00	0.43
1:A:119:ILE:HD12	1:A:125:LEU:HG	1.99	0.43
1:A:628:ALA:HB2	1:A:691:LEU:HD11	2.00	0.43
1:A:619:GLY:CA	1:A:747:LEU:HD22	2.48	0.43
1:A:794:ARG:HA	1:A:797:GLU:HB2	2.00	0.43
1:B:735:LEU:HB2	1:B:736:PRO:HD3	2.00	0.43
1:A:327:THR:HG21	1:A:555:LEU:CD1	2.49	0.43
1:B:225:PHE:HB3	1:B:258:ILE:O	2.19	0.43
1:A:437:ARG:O	1:A:441:ASP:N	2.52	0.42
1:A:463:LEU:HA	1:A:476:GLN:O	2.19	0.42
1:B:468:ASN:HD21	1:B:470:VAL:HB	1.85	0.42
1:A:373:GLN:C	1:A:374:GLN:HE21	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:361:ARG:O	1:B:364:ASP:HB2	2.20	0.42
1:B:318:THR:HA	1:B:321:LEU:HD12	2.00	0.42
1:A:132:LEU:HD13	1:A:147:THR:HB	2.02	0.42
1:A:792:LYS:O	1:A:795:GLU:HB2	2.19	0.42
1:B:550:ALA:O	1:B:554:VAL:HG23	2.20	0.42
1:B:716:ALA:HB3	1:B:739:MET:HE2	2.02	0.42
1:A:650:ILE:HA	1:A:687:TYR:O	2.19	0.42
1:A:752:HIS:HB2	1:A:755:THR:CG2	2.49	0.42
1:A:327:THR:HG23	1:A:390:VAL:HG22	2.02	0.42
1:A:64:GLU:HB3	1:A:65:PRO:HD2	2.02	0.42
1:A:246:ASP:O	1:A:249:ARG:NE	2.52	0.41
1:B:41:TYR:HB3	1:B:42:ASP:H	1.75	0.41
1:B:538:HIS:O	1:B:542:LEU:HG	2.20	0.41
1:B:647:ILE:O	1:B:647:ILE:HG23	2.20	0.41
2:E:5:DG:H1'	2:E:6:DC:C5	2.56	0.41
1:B:507:LYS:HD2	1:B:507:LYS:HA	1.92	0.41
1:B:700:SER:O	1:B:701:THR:C	2.59	0.41
1:B:240:LEU:HD23	1:B:240:LEU:C	2.41	0.41
1:A:80:LEU:HD22	1:A:114:VAL:HG21	2.01	0.41
1:A:179:LEU:HA	1:A:197:ARG:HB2	2.03	0.41
1:A:474:TYR:HB2	1:A:500:ARG:HB3	2.01	0.41
1:A:754:ASP:O	1:A:755:THR:CB	2.64	0.41
1:B:39:LEU:O	1:B:68:MET:HA	2.21	0.41
1:A:375:LEU:HD12	1:A:399:GLU:HA	2.02	0.41
1:B:290:THR:HG22	1:B:293:SER:HB3	2.03	0.41
1:B:157:LEU:HD23	1:B:157:LEU:O	2.21	0.41
1:B:267:ILE:HB	1:B:314:PRO:HG2	2.03	0.41
3:F:17:DG:H2''	3:F:18:DG:H8	1.86	0.41
1:A:93:CYS:HA	1:A:110:VAL:HA	2.03	0.40
1:B:227:VAL:HG12	1:B:260:MET:HB2	2.03	0.40
1:B:334:PHE:CE1	1:B:385:VAL:HG22	2.57	0.40
1:A:382:LEU:O	1:A:391:GLN:NE2	2.54	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%)	732 (93%)	45 (6%)	7 (1%)	17	48
1	B	746/800 (93%)	700 (94%)	42 (6%)	4 (0%)	29	61
All	All	1530/1600 (96%)	1432 (94%)	87 (6%)	11 (1%)	22	54

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	703	ASP
1	A	751	GLU
1	B	798	SER
1	A	754	ASP
1	A	755	THR
1	B	183	ASP
1	B	582	GLU
1	A	444	THR
1	B	184	PHE
1	A	442	GLY
1	A	756	ILE

### 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%)	585 (89%)	71 (11%)	6	20
1	B	631/664 (95%)	572 (91%)	59 (9%)	8	26
All	All	1287/1328 (97%)	1157 (90%)	130 (10%)	7	23

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER

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Mol	Chain	Res	Type
1	A	23	GLN
1	A	33	MET
1	A	35	ASP
1	A	46	ARG
1	A	54	SER
1	A	57	LYS
1	A	71	ILE
1	A	80	LEU
1	A	101	THR
1	A	126	GLN
1	A	137	TRP
1	A	139	ASP
1	A	140	SER
1	A	141	LYS
1	A	155	PHE
1	A	162	ASP
1	A	163	ARG
1	A	178	LEU
1	A	179	LEU
1	A	190	ILE
1	A	196	LEU
1	A	208	THR
1	A	232	ARG
1	A	240	LEU
1	A	242	GLN
1	A	248	GLN
1	A	259	THR
1	A	264	GLN
1	A	266	SER
1	A	288	GLU
1	A	311	LEU
1	A	319	ARG
1	A	326	GLN
1	A	333	ASP
1	A	397	MET
1	A	418	LEU
1	A	439	LEU
1	A	468	ASN
1	A	479	ARG
1	A	490	MET
1	A	499	GLU
1	A	506	LEU

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Mol	Chain	Res	Type
1	A	512	LYS
1	A	517	LYS
1	A	526	GLN
1	A	531	LEU
1	A	536	LEU
1	A	547	SER
1	A	552	LEU
1	A	574	ASP
1	A	575	LYS
1	A	580	ILE
1	A	608	ARG
1	A	613	THR
1	A	616	ASN
1	A	640	VAL
1	A	643	GLN
1	A	652	ARG
1	A	656	ARG
1	A	670	PHE
1	A	694	GLU
1	A	703	ASP
1	A	747	LEU
1	A	751	GLU
1	A	759	MET
1	A	769	LYS
1	A	788	ARG
1	A	790	ARG
1	A	794	ARG
1	A	795	GLU
1	B	17	TYR
1	B	18	LEU
1	B	24	HIS
1	B	26	GLU
1	B	45	LYS
1	B	46	ARG
1	B	49	GLN
1	B	82	LYS
1	B	109	LYS
1	B	126	GLN
1	B	137	TRP
1	B	141	LYS
1	B	155	PHE
1	B	157	LEU

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Mol	Chain	Res	Type
1	B	164	GLU
1	B	171	GLN
1	B	178	LEU
1	B	182	GLU
1	B	201	LEU
1	B	245	LYS
1	B	254	HIS
1	B	263	GLU
1	B	270	ASP
1	B	313	MET
1	B	316	ARG
1	B	335	THR
1	B	338	LEU
1	B	345	VAL
1	B	352	LEU
1	B	357	LEU
1	B	384	THR
1	B	387	SER
1	B	419	VAL
1	B	421	ASP
1	B	424	VAL
1	B	453	ARG
1	B	455	ARG
1	B	463	LEU
1	B	478	SER
1	B	487	ILE
1	B	491	ARG
1	B	495	LEU
1	B	500	ARG
1	B	515	THR
1	B	517	LYS
1	B	535	LEU
1	B	552	LEU
1	B	575	LYS
1	B	632	LEU
1	B	636	ILE
1	B	669	THR
1	B	718	LYS
1	B	734	GLN
1	B	761	SER
1	B	763	GLN
1	B	768	SER

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Mol	Chain	Res	Type
1	B	787	LYS
1	B	788	ARG
1	B	798	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	23	GLN
1	A	74	HIS
1	A	171	GLN
1	A	211	GLN
1	A	242	GLN
1	A	248	GLN
1	A	312	HIS
1	A	526	GLN
1	A	538	HIS
1	A	643	GLN
1	B	86	GLN
1	B	126	GLN
1	B	171	GLN
1	B	242	GLN
1	B	339	GLN
1	B	344	GLN
1	B	370	HIS
1	B	590	GLN
1	B	717	ASN
1	B	734	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

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	1.17	2 (8%)	29,45,45	1.83	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
4	ADP	A	1801	5	-	4/12/32/32	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	3.96	1.38	1.32
4	A	1801	ADP	C2-N1	2.49	1.38	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1801	ADP	N3-C2-N1	-5.76	119.67	128.68
4	A	1801	ADP	PA-O3A-PB	-5.48	114.03	132.83
4	A	1801	ADP	O3B-PB-O3A	3.46	116.22	104.64
4	A	1801	ADP	C3'-C2'-C1'	2.95	105.42	100.98

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1801	ADP	PA-O3A-PB-O2B
4	A	1801	ADP	O4'-C4'-C5'-O5'

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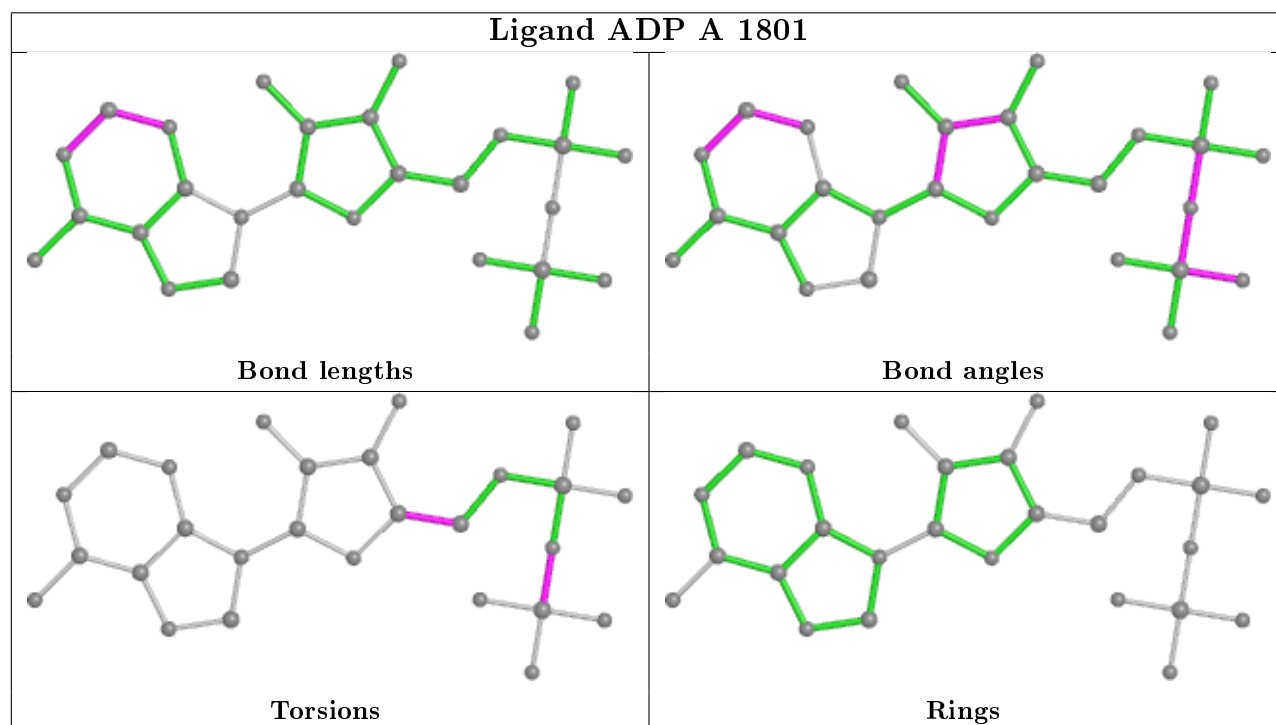
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Mol	Chain	Res	Type	Atoms
4	A	1801	ADP	C3'-C4'-C5'-O5'
4	A	1801	ADP	PA-O3A-PB-O3B

There are no ring outliers.

No monomer is involved in short contacts.

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

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%)	-0.09	16 (2%) 65 63	25, 38, 45, 54	0
1	B	754/800 (94%)	-0.07	19 (2%) 57 55	29, 39, 44, 49	0
2	E	18/30 (60%)	0.83	5 (27%) 0 0	27, 35, 49, 59	0
3	F	17/30 (56%)	0.31	2 (11%) 4 3	29, 38, 52, 52	0
All	All	1577/1660 (95%)	-0.07	42 (2%) 54 50	25, 39, 45, 59	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	18	DG	5.9
1	A	2	SER	4.9
2	E	16	DG	4.7
1	A	444	THR	4.2
1	B	74	HIS	4.1
1	B	54	SER	4.0
2	E	1	DA	3.8
1	B	16	GLN	3.8
1	B	55	LEU	3.4
3	F	14	DA	3.4
1	A	60	ALA	3.3
2	E	17	DT	3.1
1	A	103	LYS	3.1
1	B	284	ALA	2.9
1	A	59	GLY	2.7
1	A	61	SER	2.7
1	B	658	GLY	2.7
1	B	39	LEU	2.7
1	B	31	TYR	2.6
1	A	751	GLU	2.6
1	B	41	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	62	ALA	2.6
1	B	40	PHE	2.5
1	A	431	GLU	2.5
1	B	283	LEU	2.4
1	A	64	GLU	2.3
1	A	448	GLU	2.3
1	A	563	TYR	2.3
2	E	15	DA	2.3
1	A	593	ASN	2.3
1	B	45	LYS	2.3
1	A	97	GLY	2.3
1	B	800	SER	2.2
1	B	73	TYR	2.2
1	B	552	LEU	2.2
1	B	30	PHE	2.2
1	B	144	GLY	2.2
1	A	443	ALA	2.1
1	A	753	GLY	2.1
1	B	135	ALA	2.0
1	B	29	LEU	2.0
3	F	15	DC	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 ⓘ

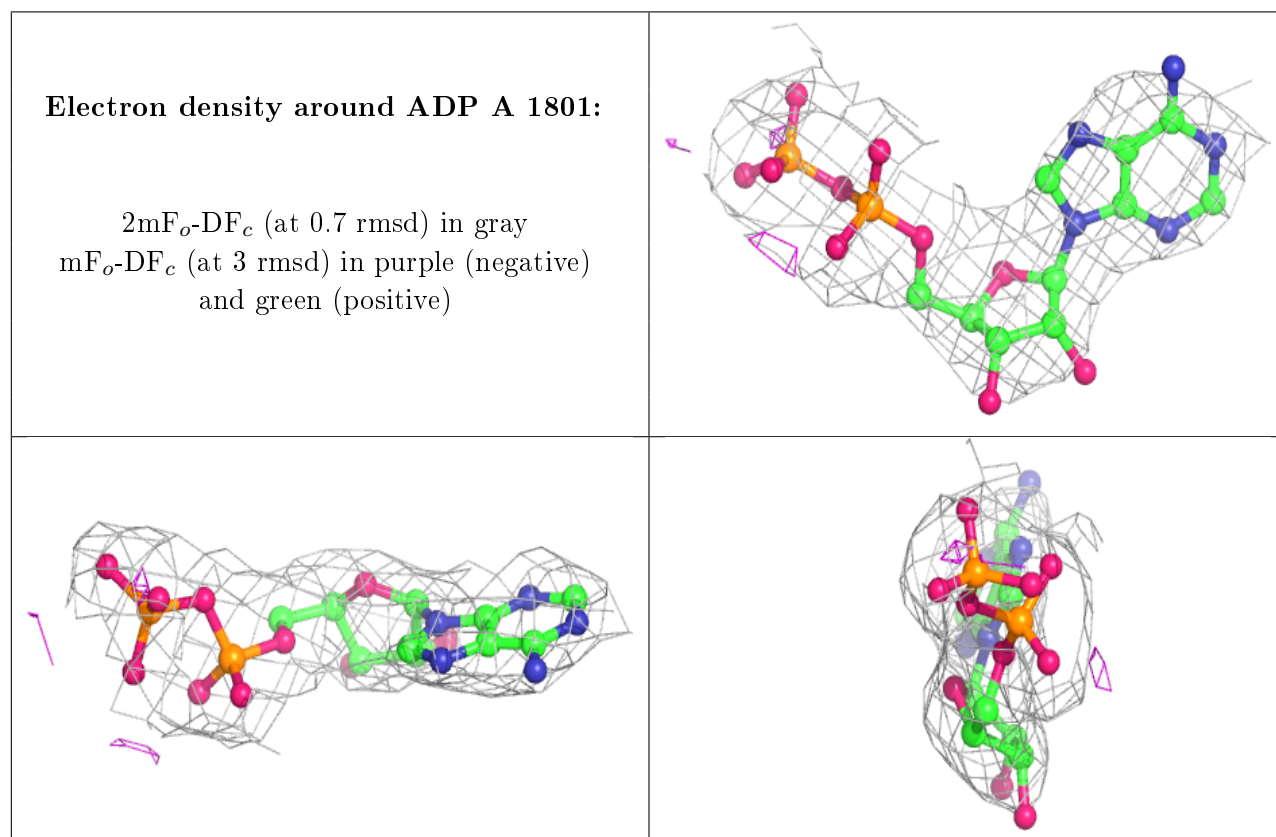
There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	MG	A	1802	1/1	0.43	0.11	26,26,26,26	0
4	ADP	A	1801	27/27	0.95	0.14	32,39,40,41	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.