



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 11, 2021 – 02:15 PM EST

PDB ID : 4ZCF  
Title : Structural basis of asymmetric DNA methylation and ATP-triggered long-range diffusion by EcoP15I  
Authors : Gupta, Y.K.; Chan, S.H.; Xu, S.Y.; Aggarwal, A.K.  
Deposited on : 2015-04-15  
Resolution : 2.60 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 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 : 2.16  
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) : 2.16

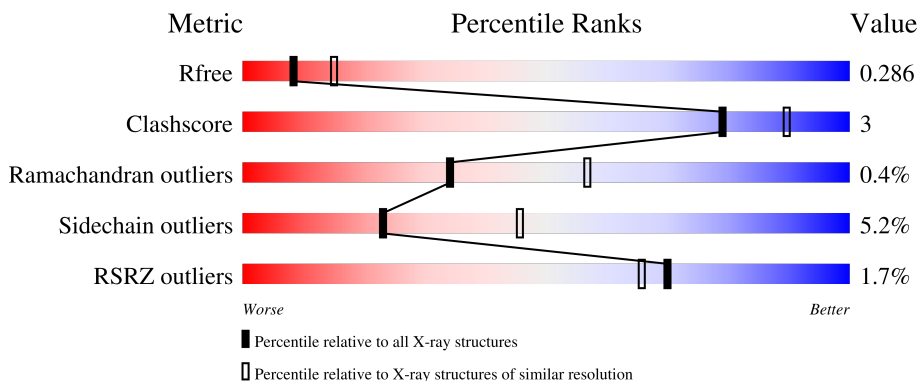
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	644	
1	B	644	
2	C	970	
3	D	20	
4	E	20	

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:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
6	AMP	C	1001	-	-	-	X

## 2 Entry composition i

There are 8 unique types of molecules in this entry. The entry contains 14929 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 Restriction endonuclease EcoP15I, modification subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	616	Total	C	N	O	S	0	0	0
			4833	3096	803	920	14			
1	B	612	Total	C	N	O	S	0	0	0
			4705	3001	784	905	15			

- Molecule 2 is a protein called Restriction endonuclease EcoP15I, restriction subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	627	Total	C	N	O	S	0	0	0
			4452	2848	766	827	11			

- Molecule 3 is a DNA chain called DNA 20-mer ATACAGCAGTAGACTATGAT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	D	20	Total	C	N	O	P	0	0	0
			413	197	79	117	20			

- Molecule 4 is a DNA chain called DNA 20-mer AATCATAGTCTACTGCTGTA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	E	20	Total	C	N	O	P	0	0	0
			405	196	71	119	19			

- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Mn	0	0
			2	2		

- Molecule 6 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>7</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	1	Total	Ca	0	0
			1	1		

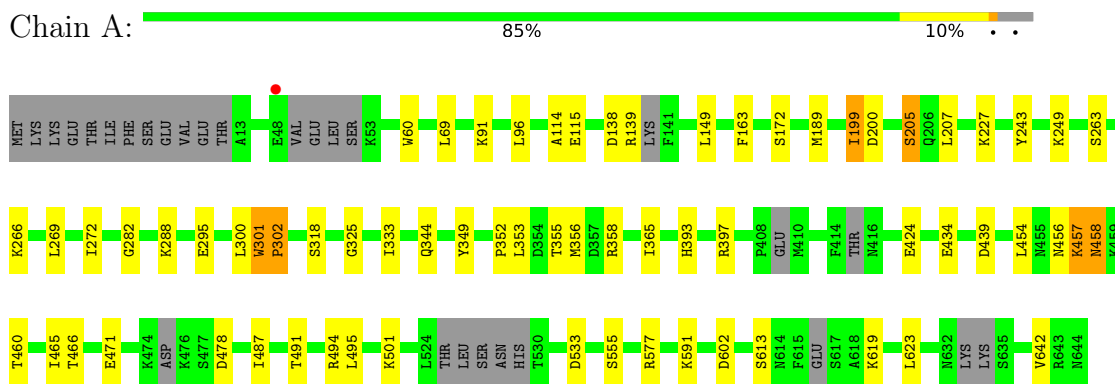
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	43	Total	O	0	0
			43	43		
8	B	36	Total	O	0	0
			36	36		
8	C	4	Total	O	0	0
			4	4		
8	D	7	Total	O	0	0
			7	7		
8	E	5	Total	O	0	0
			5	5		

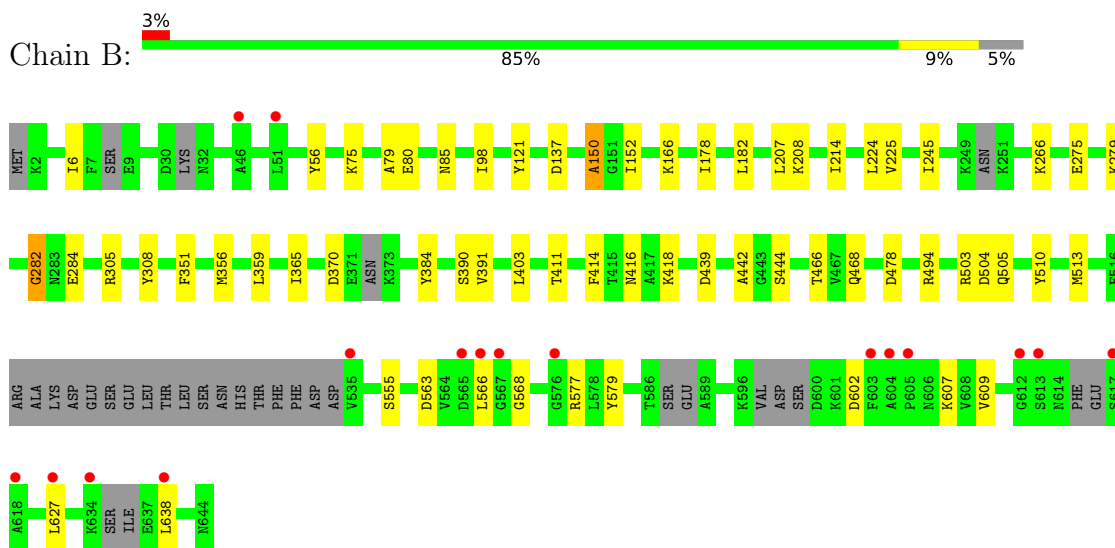
### 3 Residue-property plots [i](#)

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.

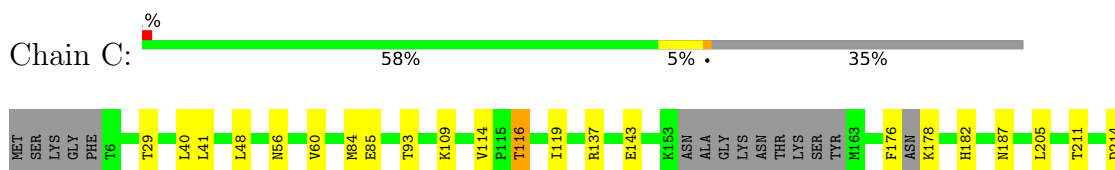
- Molecule 1: Restriction endonuclease EcoP15I, modification subunit

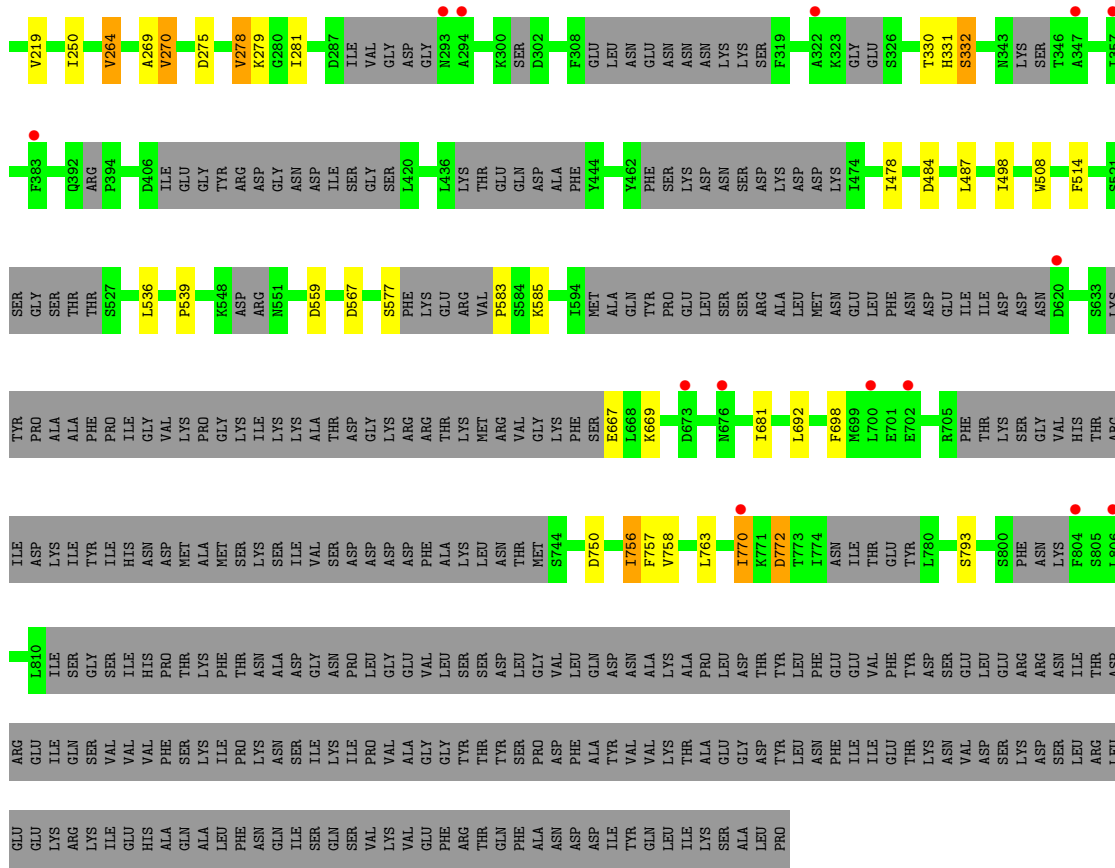


- Molecule 1: Restriction endonuclease EcoP15I, modification subunit



- Molecule 2: Restriction endonuclease EcoP15I, restriction subunit





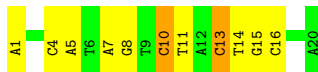
- Molecule 3: DNA 20-mer ATACAGCAGTAGACTATGAT

Chain D: 50% 50%



- Molecule 4: DNA 20-mer AATCATAGTCTACTGCTGTA

Chain E: 45% 45% 10%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.84Å 101.84Å 533.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.60 47.56 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.5 (40.00-2.60) 97.1 (47.56-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.24 (at 2.58Å)	Xtrriage
Refinement program	BUSTER 2.10.0	Depositor
R, $R_{free}$	0.218 , 0.263 0.236 , 0.286	Depositor DCC
$R_{free}$ test set	4328 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	55.9	Xtrriage
Anisotropy	0.299	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 54.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	14929	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.17% 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: AMP, CA, MN

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	0.54	0/4932	0.75	3/6678 (0.0%)
1	B	0.52	0/4798	0.74	0/6509
2	C	0.52	0/4518	0.71	1/6136 (0.0%)
3	D	1.10	0/464	1.96	13/714 (1.8%)
4	E	1.13	1/453 (0.2%)	2.09	19/697 (2.7%)
All	All	0.58	1/15165 (0.0%)	0.88	36/20734 (0.2%)

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	3
1	B	0	3
2	C	0	5
All	All	0	11

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	14	DT	C3'-O3'	-5.26	1.37	1.44

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	13	DC	O4'-C1'-N1	13.64	117.55	108.00
4	E	13	DC	O4'-C4'-C3'	-12.37	98.58	106.00
4	E	1	DA	P-O3'-C3'	10.96	132.85	119.70
4	E	10	DC	O4'-C1'-N1	8.99	114.30	108.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	13	DC	C4'-C3'-C2'	-8.58	95.38	103.10
3	D	13	DA	P-O3'-C3'	8.24	129.59	119.70
3	D	2	DT	C4-C5-C7	8.21	123.92	119.00
3	D	7	DC	P-O5'-C5'	8.03	133.74	120.90
3	D	1	DA	O4'-C1'-N9	7.97	113.58	108.00
3	D	2	DT	C6-C5-C7	-7.93	118.14	122.90
4	E	7	DA	P-O3'-C3'	7.91	129.19	119.70
3	D	11	DA	P-O3'-C3'	7.64	128.87	119.70
4	E	8	DG	P-O3'-C3'	7.49	128.69	119.70
4	E	16	DC	P-O3'-C3'	7.24	128.39	119.70
3	D	5	DA	P-O3'-C3'	7.02	128.12	119.70
4	E	4	DC	P-O3'-C3'	6.92	128.01	119.70
4	E	13	DC	C1'-O4'-C4'	-6.52	103.58	110.10
3	D	7	DC	O4'-C1'-N1	6.38	112.47	108.00
4	E	13	DC	P-O5'-C5'	-6.08	111.17	120.90
3	D	12	DG	C5-C6-O6	-6.08	124.95	128.60
4	E	5	DA	P-O3'-C3'	6.04	126.95	119.70
4	E	14	DT	N3-C2-O2	-5.99	118.71	122.30
4	E	5	DA	N1-C2-N3	-5.96	126.32	129.30
4	E	15	DG	O4'-C1'-N9	5.63	111.94	108.00
2	C	583	PRO	N-CA-CB	5.60	110.02	103.30
3	D	4	DC	P-O3'-C3'	5.42	126.21	119.70
3	D	18	DG	O4'-C1'-N9	5.41	111.78	108.00
1	A	501	LYS	N-CA-C	-5.26	96.80	111.00
4	E	14	DT	C4'-C3'-C2'	5.26	107.83	103.10
1	A	302	PRO	CA-N-CD	-5.21	104.20	111.50
4	E	4	DC	N1-C2-O2	5.21	122.03	118.90
4	E	5	DA	C2-N3-C4	5.19	113.19	110.60
4	E	10	DC	P-O3'-C3'	5.14	125.87	119.70
3	D	20	DT	C4-C5-C7	5.12	122.07	119.00
1	A	301	TRP	C-N-CD	5.06	139.02	128.40
3	D	18	DG	P-O3'-C3'	5.03	125.74	119.70

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	114	ALA	Peptide
1	A	456	ASN	Peptide
1	A	458	ASN	Peptide
1	B	150	ALA	Peptide
1	B	166	LYS	Peptide

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
1	B	282	GLY	Peptide
2	C	330	THR	Peptide
2	C	332	SER	Peptide
2	C	585	LYS	Peptide
2	C	667	GLU	Peptide
2	C	756	ILE	Peptide

## 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	4833	0	4603	25	0
1	B	4705	0	4394	26	0
2	C	4452	0	3830	29	0
3	D	413	0	226	0	0
4	E	405	0	229	3	0
5	A	2	0	0	0	0
6	C	23	0	12	0	0
7	D	1	0	0	0	0
8	A	43	0	0	0	0
8	B	36	0	0	1	0
8	C	4	0	0	0	0
8	D	7	0	0	0	0
8	E	5	0	0	0	0
All	All	14929	0	13294	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 3.

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:A:458:ASN:CB	1:A:460:THR:H	1.82	0.93
1:A:457:LYS:HD2	1:A:457:LYS:O	1.85	0.76
1:B:503:ARG:NH1	1:B:503:ARG:HG3	2.02	0.73
1:B:503:ARG:HH11	1:B:503:ARG:HG3	1.54	0.73

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:757:PHE:HD1	2:C:757:PHE:H	1.39	0.69
4:E:10:DC:H2"	4:E:11:DT:H71	1.80	0.63
1:B:150:ALA:HB3	1:B:152:ILE:HG12	1.79	0.63
1:A:458:ASN:CB	1:A:460:THR:N	2.60	0.62
2:C:56:ASN:O	2:C:60:VAL:HG23	2.01	0.61
2:C:116:THR:HG22	2:C:119:ILE:H	1.66	0.61
1:B:207:LEU:HD23	1:B:245:ILE:HD12	1.84	0.58
2:C:756:ILE:HD12	2:C:758:VAL:HG13	1.85	0.58
2:C:84:MET:CE	2:C:93:THR:HG21	2.33	0.58
2:C:270:VAL:HG13	2:C:577:SER:OG	2.04	0.57
2:C:757:PHE:CD1	2:C:757:PHE:N	2.73	0.57
1:B:359:LEU:HB2	1:B:365:ILE:HD11	1.87	0.56
1:A:355:THR:HG23	1:A:358:ARG:HH21	1.73	0.54
1:B:182:LEU:HB2	1:B:214:ILE:HD13	1.90	0.54
2:C:85:GLU:HG2	2:C:269:ALA:HB2	1.90	0.53
2:C:84:MET:HE3	2:C:93:THR:HG21	1.91	0.53
1:B:442:ALA:HB3	1:B:468:GLN:HB2	1.91	0.52
2:C:498:ILE:HG21	2:C:508:TRP:CH2	2.45	0.52
1:B:356:MET:HE3	1:B:365:ILE:HD13	1.92	0.52
1:A:115:GLU:HB3	1:A:189:MET:O	2.09	0.52
2:C:211:THR:HG22	2:C:214:ASP:H	1.74	0.52
1:B:577:ARG:HG2	1:B:607:LYS:HB3	1.91	0.51
1:B:579:TYR:HA	1:B:609:VAL:O	2.10	0.51
2:C:281:ILE:HD11	2:C:536:LEU:HD21	1.94	0.50
1:A:96:LEU:HD12	1:A:465:ILE:HG12	1.94	0.49
1:B:121:TYR:OH	1:B:418:LYS:HD2	2.13	0.49
2:C:770:ILE:HG23	2:C:772:ASP:HB2	1.93	0.49
2:C:137:ARG:HD3	2:C:143:GLU:OE2	2.12	0.49
2:C:278:VAL:HG13	2:C:536:LEU:HD22	1.94	0.48
1:A:333:ILE:HD12	1:A:349:TYR:CZ	2.48	0.48
2:C:279:LYS:HE3	2:C:539:PRO:HD3	1.95	0.48
2:C:514:PHE:CZ	2:C:539:PRO:HG3	2.48	0.48
2:C:756:ILE:HD11	2:C:763:LEU:HD21	1.96	0.47
1:B:503:ARG:CG	1:B:503:ARG:HH11	2.21	0.47
1:A:356:MET:HE1	1:A:365:ILE:HG13	1.97	0.47
1:A:227:LYS:HG2	1:A:393:HIS:ND1	2.30	0.46
1:A:471:GLU:O	1:A:487:ILE:HG12	2.15	0.46
2:C:484:ASP:HA	2:C:487:LEU:HD12	1.96	0.46
1:B:98:ILE:HG12	1:B:510:TYR:HB2	1.97	0.46
1:A:491:THR:O	1:A:495:LEU:HD13	2.16	0.46
1:A:356:MET:HE3	1:A:365:ILE:HD11	1.97	0.45

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:681:ILE:HD12	2:C:681:ILE:H	1.80	0.45
1:B:80:GLU:HG2	1:B:85:ASN:HD22	1.82	0.45
2:C:278:VAL:HG22	2:C:536:LEU:HB3	1.99	0.45
1:B:439:ASP:O	1:B:466:THR:HA	2.17	0.44
1:B:79:ALA:HB2	1:B:513:MET:HG3	1.99	0.44
1:A:301:TRP:CG	1:A:302:PRO:HA	2.52	0.44
2:C:84:MET:HE1	2:C:93:THR:HG21	1.98	0.44
2:C:514:PHE:HZ	2:C:539:PRO:HG3	1.82	0.44
2:C:758:VAL:HG22	2:C:763:LEU:HG	2.00	0.44
1:A:439:ASP:HB3	1:A:466:THR:HG22	2.00	0.44
1:A:199:ILE:HG12	1:A:207:LEU:HD23	2.01	0.43
1:B:225:VAL:HG22	1:B:391:VAL:HG13	1.99	0.43
1:B:266:LYS:HD2	1:B:384:TYR:HB3	1.99	0.43
2:C:114:VAL:O	2:C:187:ASN:HA	2.19	0.43
2:C:756:ILE:CD1	2:C:758:VAL:HG13	2.49	0.43
1:A:199:ILE:HD12	1:A:243:TYR:HB2	1.99	0.43
1:A:269:LEU:HD11	1:A:300:LEU:HD22	2.00	0.43
1:B:403:LEU:HD21	1:B:414:PHE:HD2	1.85	0.42
1:A:454:LEU:O	1:A:457:LYS:O	2.38	0.41
1:A:439:ASP:O	1:A:466:THR:HA	2.19	0.41
1:A:205:SER:OG	1:B:208:LYS:HG2	2.20	0.41
1:B:305:ARG:HB2	8:B:730:HOH:O	2.19	0.41
1:B:6:ILE:HG13	1:B:6:ILE:O	2.20	0.41
1:A:263:SER:HB2	1:A:266:LYS:HB3	2.03	0.41
1:B:414:PHE:CZ	1:B:444:SER:HA	2.55	0.41
1:A:149:LEU:HD22	2:C:176:PHE:HE1	1.85	0.41
1:A:352:PRO:HD3	4:E:13:DC:OP2	2.21	0.41
2:C:60:VAL:HG11	2:C:264:VAL:HG22	2.03	0.41
1:A:138:ASP:CG	1:A:139:ARG:H	2.24	0.41
4:E:10:DC:H2''	4:E:11:DT:C7	2.49	0.41
2:C:109:LYS:HG2	2:C:182:HIS:HB2	2.02	0.40
1:A:60:TRP:HB2	1:A:172:SER:HB3	2.02	0.40
1:B:282:GLY:HA2	1:B:284:GLU:N	2.35	0.40
1:B:224:LEU:HD23	1:B:390:SER:HA	2.03	0.40
1:B:359:LEU:HB2	1:B:365:ILE:CD1	2.52	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	598/644 (93%)	569 (95%)	26 (4%)	3 (0%)	29	52
1	B	592/644 (92%)	558 (94%)	33 (6%)	1 (0%)	47	71
2	C	587/970 (60%)	558 (95%)	26 (4%)	3 (0%)	29	52
All	All	1777/2258 (79%)	1685 (95%)	85 (5%)	7 (0%)	34	57

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	LYS
2	C	332	SER
2	C	331	HIS
2	C	669	LYS
1	A	282	GLY
1	B	568	GLY
1	A	325	GLY

### 5.3.2 Protein sidechains [i](#)

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	502/580 (87%)	475 (95%)	27 (5%)	22	44
1	B	478/580 (82%)	457 (96%)	21 (4%)	28	53
2	C	377/876 (43%)	355 (94%)	22 (6%)	20	40
All	All	1357/2036 (67%)	1287 (95%)	70 (5%)	23	46

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	LEU
1	A	163	PHE
1	A	199	ILE
1	A	200	ASP
1	A	205	SER
1	A	249	LYS
1	A	272	ILE
1	A	288	LYS
1	A	295	GLU
1	A	318	SER
1	A	344	GLN
1	A	353	LEU
1	A	397	ARG
1	A	424	GLU
1	A	434	GLU
1	A	457	LYS
1	A	478	ASP
1	A	494	ARG
1	A	533	ASP
1	A	555	SER
1	A	577	ARG
1	A	591	LYS
1	A	602	ASP
1	A	613	SER
1	A	619	LYS
1	A	623	LEU
1	A	642	VAL
1	B	56	TYR
1	B	75	LYS
1	B	137	ASP
1	B	178	ILE
1	B	275	GLU
1	B	279	LYS
1	B	308	TYR
1	B	351	PHE
1	B	370	ASP
1	B	411	THR
1	B	416	ASN
1	B	478	ASP
1	B	494	ARG
1	B	504	ASP
1	B	505	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	555	SER
1	B	563	ASP
1	B	566	LEU
1	B	602	ASP
1	B	627	LEU
1	B	638	LEU
2	C	29	THR
2	C	40	LEU
2	C	41	LEU
2	C	48	LEU
2	C	116	THR
2	C	178	LYS
2	C	205	LEU
2	C	219	VAL
2	C	250	ILE
2	C	264	VAL
2	C	270	VAL
2	C	275	ASP
2	C	278	VAL
2	C	478	ILE
2	C	559	ASP
2	C	567	ASP
2	C	692	LEU
2	C	698	PHE
2	C	750	ASP
2	C	770	ILE
2	C	772	ASP
2	C	793	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	386	GLN

### 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 4 ligands modelled in this entry, 3 are 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
6	AMP	C	1001	-	22,25,25	1.50	5 (22%)	25,38,38	1.97	7 (28%)

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
6	AMP	C	1001	-	-	4/6/26/26	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1001	AMP	O4'-C1'	3.63	1.46	1.41
6	C	1001	AMP	C2'-C1'	-2.56	1.49	1.53
6	C	1001	AMP	C5-C4	2.49	1.47	1.40
6	C	1001	AMP	C6-N6	2.27	1.42	1.34
6	C	1001	AMP	C5-N7	2.10	1.47	1.39

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1001	AMP	C4-C5-N7	-4.15	105.08	109.40
6	C	1001	AMP	N3-C2-N1	-3.98	122.46	128.68
6	C	1001	AMP	O2P-P-O5'	3.60	116.31	106.73
6	C	1001	AMP	C3'-C2'-C1'	3.16	105.73	100.98
6	C	1001	AMP	O5'-P-O1P	2.80	114.34	106.47
6	C	1001	AMP	C1'-N9-C4	-2.74	121.83	126.64
6	C	1001	AMP	O3P-P-O5'	2.41	113.14	106.73

There are no chirality outliers.

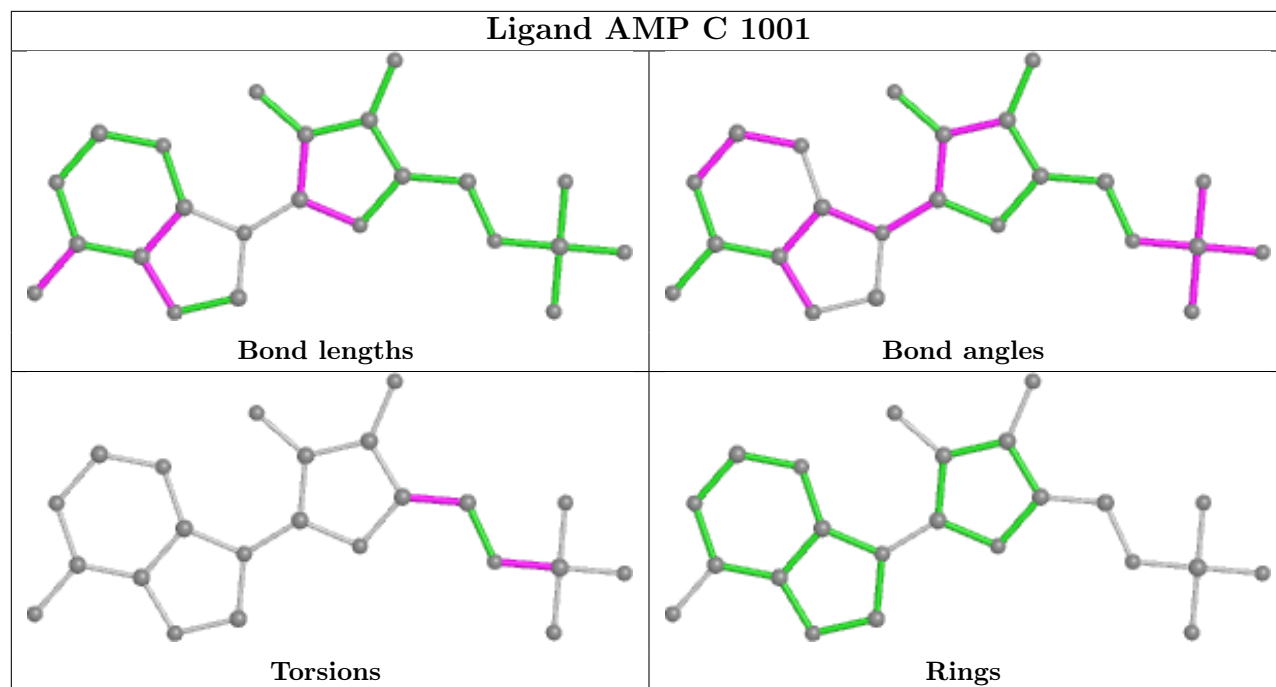
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	1001	AMP	C5'-O5'-P-O1P
6	C	1001	AMP	C5'-O5'-P-O2P
6	C	1001	AMP	C5'-O5'-P-O3P
6	C	1001	AMP	O4'-C4'-C5'-O5'

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 [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	616/644 (95%)	-0.38	1 (0%) 95 95	27, 51, 80, 101	0
1	B	612/644 (95%)	-0.13	17 (2%) 53 46	29, 55, 101, 124	0
2	C	627/970 (64%)	-0.07	14 (2%) 62 56	40, 71, 99, 111	0
3	D	20/20 (100%)	-0.54	0 100 100	34, 49, 73, 73	0
4	E	20/20 (100%)	-0.58	0 100 100	32, 48, 74, 87	0
All	All	1895/2298 (82%)	-0.20	32 (1%) 70 66	27, 59, 97, 124	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	627	LEU	5.1
1	B	638	LEU	3.9
1	B	576	GLY	3.5
2	C	620	ASP	3.4
2	C	293	ASN	3.4
1	B	603	PHE	3.3
1	B	46	ALA	3.2
1	B	605	PRO	3.2
2	C	294	ALA	3.1
1	B	618	ALA	2.9
1	B	566	LEU	2.8
1	B	567	GLY	2.6
2	C	770	ILE	2.6
2	C	676	ASN	2.6
2	C	700	LEU	2.6
1	A	48	GLU	2.5
1	B	565	ASP	2.5
1	B	617	SER	2.4
2	C	673	ASP	2.4
2	C	383	PHE	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	604	ALA	2.3
1	B	634	LYS	2.3
1	B	612	GLY	2.2
1	B	535	VAL	2.2
2	C	702	GLU	2.2
2	C	806	LEU	2.1
2	C	322	ALA	2.1
2	C	347	ALA	2.1
1	B	51	LEU	2.1
2	C	804	PHE	2.1
1	B	613	SER	2.1
2	C	357	ILE	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](#)

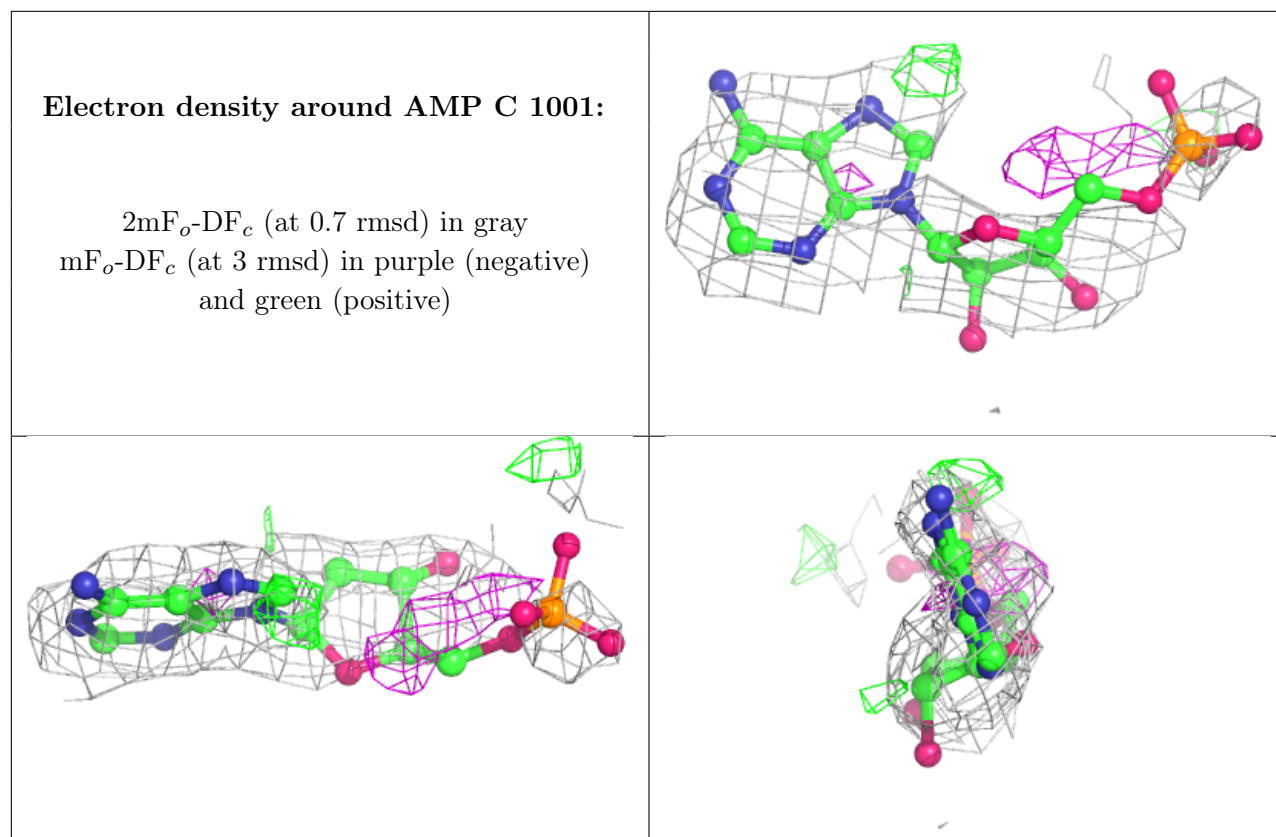
There are no monosaccharides in this entry.

## 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(Å <sup>2</sup> )	Q<0.9
6	AMP	C	1001	23/23	0.54	0.43	128,133,149,150	0
5	MN	A	701	1/1	0.83	0.24	113,113,113,113	0
5	MN	A	702	1/1	0.96	0.29	75,75,75,75	0
7	CA	D	101	1/1	0.97	0.19	31,31,31,31	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.