



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 11:05 AM BST

PDB ID : 1OH6  
Title : THE CRYSTAL STRUCTURE OF E. COLI MUTS BINDING TO DNA  
WITH AN A:A MISMATCH  
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Deposited on : 2003-05-23  
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 : 2.13.1  
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

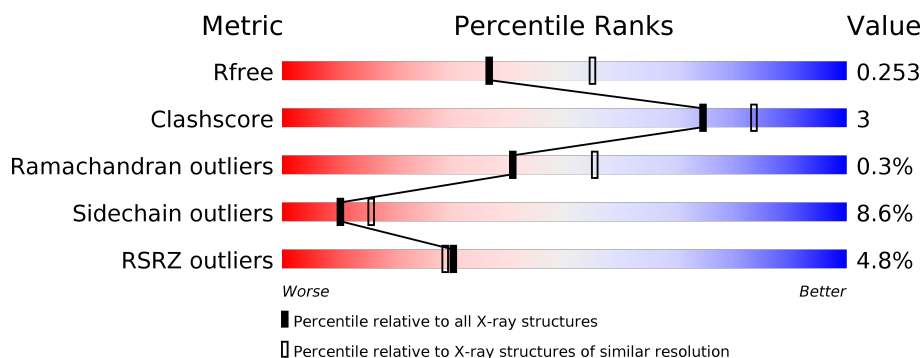
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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>4%</div> <div> <div></div> <div>84%</div> <div>14%</div> <div>••</div> </div> </div>
1	B	800	<div> <div>5%</div> <div> <div></div> <div>77%</div> <div>15%</div> <div>• 6%</div> </div> </div>
2	E	30	<div> <div>17%</div> <div> <div></div> <div>33%</div> <div>20%</div> <div>47%</div> </div> </div>
3	F	30	<div> <div>10%</div> <div> <div></div> <div>30%</div> <div>23%</div> <div>47%</div> </div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13233 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\*AP\*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	16	Total	C	N	O	P	0	0	0
			324	154	65	90	15			

- 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	16	Total	C	N	O	P	0	0	0
			330	156	60	98	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	0	0
			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	0	0
			1	1		

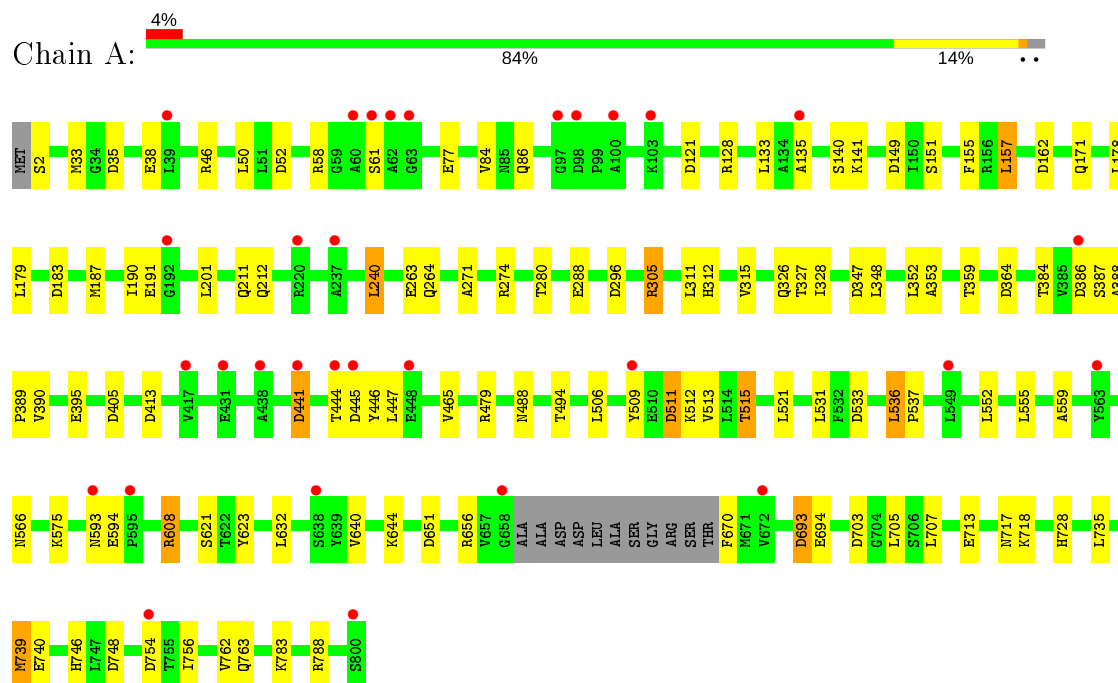
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	202	Total	O	0	0
			202	202		
6	B	170	Total	O	0	0
			170	170		
6	E	4	Total	O	0	0
			4	4		
6	F	4	Total	O	0	0
			4	4		

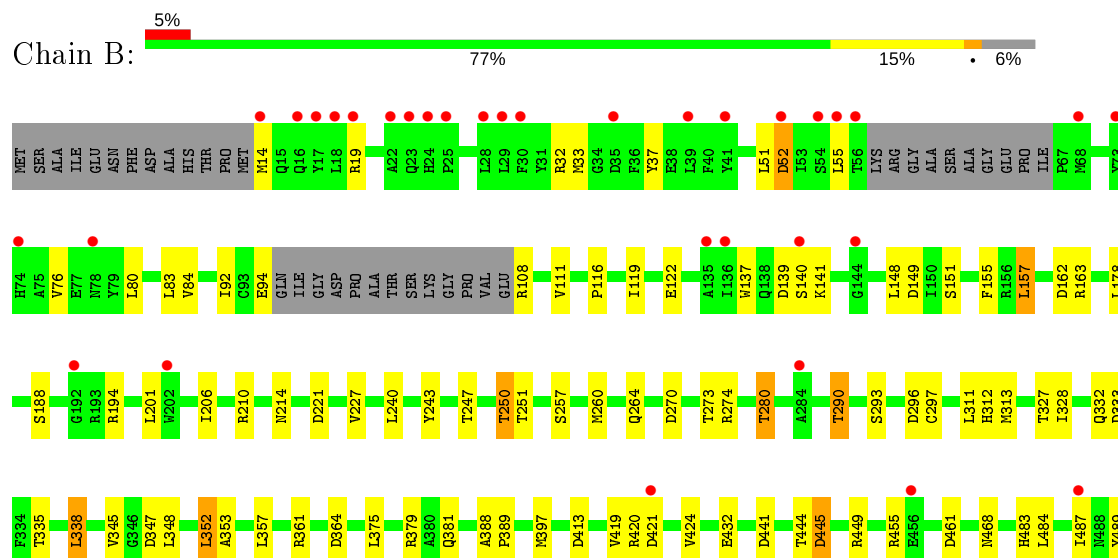
### 3 Residue-property plots [i](#)

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

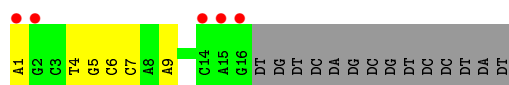


#### • Molecule 1: DNA MISMATCH REPAIR PROTEIN MUTS

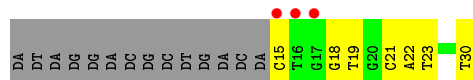
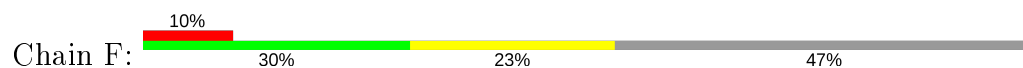




- Molecule 2: 5'-D(\*AP\*GP\*CP\*TP\*GP\*CP\*CP\*AP\*AP\*GP \*CP\*AP\*CP\*CP\*AP\*GP\*TP\*GP\*TP\*CP\*AP\*GP\*CP\*GP\*TP\* CP\*CP\*TP\*AP\*T)-3'



- 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, $\alpha$ , $\beta$ , $\gamma$	89.49Å 91.81Å 260.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.40 21.98 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.2 (15.00-2.40) 98.2 (21.98-2.40)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.46 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.205 , 0.253 0.209 , 0.253	Depositor DCC
$R_{free}$ test set	1609 reflections (1.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.6	Xtriage
Anisotropy	0.554	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 51.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13233	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% 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	0.56	1/6313 (0.0%)	0.82	21/8544 (0.2%)
1	B	0.52	0/6062	0.80	18/8199 (0.2%)
2	E	1.02	0/364	1.61	5/559 (0.9%)
3	F	0.98	0/369	1.68	5/568 (0.9%)
All	All	0.58	1/13108 (0.0%)	0.88	49/17870 (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	-5.30	1.40	1.51

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	22	DA	O4'-C1'-N9	-8.57	102.00	108.00
1	A	162	ASP	CB-CG-OD2	8.41	125.87	118.30
1	B	461	ASP	CB-CG-OD2	7.83	125.34	118.30
1	A	305	ARG	NE-CZ-NH1	7.74	124.17	120.30
3	F	23	DT	O4'-C1'-N1	-7.21	102.96	108.00
1	A	413	ASP	CB-CG-OD2	6.71	124.34	118.30
1	B	632	LEU	CA-CB-CG	6.61	130.50	115.30
1	A	703	ASP	CB-CG-OD2	6.53	124.18	118.30
1	B	347	ASP	CB-CG-OD2	6.51	124.16	118.30
2	E	9	DA	O3'-P-O5'	-6.37	91.90	104.00
1	B	754	ASP	CB-CG-OD2	6.36	124.02	118.30
3	F	21	DC	O4'-C1'-N1	6.34	112.44	108.00
1	A	364	ASP	CB-CG-OD2	6.14	123.83	118.30
2	E	7	DC	C1'-O4'-C4'	-6.01	104.09	110.10
1	B	553	ASP	CB-CG-OD2	5.97	123.67	118.30
2	E	1	DA	O4'-C1'-N9	5.94	112.16	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	15	DC	O4'-C1'-N1	5.91	112.14	108.00
1	B	52	ASP	CB-CG-OD2	5.88	123.59	118.30
1	B	511	ASP	CB-CG-OD2	5.84	123.56	118.30
1	A	305	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	B	221	ASP	CB-CG-OD2	5.83	123.54	118.30
1	A	748	ASP	CB-CG-OD2	5.75	123.48	118.30
1	A	511	ASP	CB-CG-OD2	5.70	123.43	118.30
1	A	441	ASP	CB-CG-OD2	5.67	123.41	118.30
1	B	764	ASP	CB-CG-OD2	5.62	123.36	118.30
2	E	6	DC	P-O3'-C3'	5.62	126.44	119.70
1	A	121	ASP	CB-CG-OD2	5.58	123.32	118.30
1	B	270	ASP	CB-CG-OD2	5.57	123.32	118.30
1	A	296	ASP	CB-CG-OD2	5.41	123.17	118.30
1	B	421	ASP	CB-CG-OD2	5.35	123.11	118.30
1	A	405	ASP	CB-CG-OD2	5.33	123.09	118.30
1	B	157	LEU	CA-CB-CG	5.33	127.55	115.30
1	B	162	ASP	CB-CG-OD2	5.32	123.08	118.30
1	A	754	ASP	CB-CG-OD2	5.30	123.07	118.30
1	B	149	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	157	LEU	CA-CB-CG	5.16	127.18	115.30
1	A	149	ASP	CB-CG-OD2	5.15	122.94	118.30
1	B	296	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	52	ASP	CB-CG-OD2	5.11	122.89	118.30
1	A	183	ASP	CB-CG-OD2	5.11	122.89	118.30
1	A	693	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	651	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	533	ASP	CB-CG-OD2	5.07	122.86	118.30
1	B	533	ASP	CB-CG-OD2	5.07	122.86	118.30
1	A	445	ASP	CB-CG-OD2	5.06	122.85	118.30
1	B	413	ASP	CB-CG-OD2	5.06	122.85	118.30
2	E	4	DT	O4'-C1'-N1	-5.05	104.46	108.00
1	B	441	ASP	CB-CG-OD2	5.02	122.82	118.30
3	F	30	DT	C5-C4-O4	-5.01	121.39	124.90

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	6207	0	6251	37	0
1	B	5964	0	6018	45	0
2	E	324	0	179	1	0
3	F	330	0	181	1	0
4	A	27	0	12	0	0
5	A	1	0	0	0	0
6	A	202	0	0	7	0
6	B	170	0	0	3	0
6	E	4	0	0	0	0
6	F	4	0	0	0	0
All	All	13233	0	12641	82	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 (82) 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:633:MET:O	1:B:636:ILE:HG22	1.67	0.95
1:A:359:THR:HG21	6:A:2027:HOH:O	1.80	0.80
1:B:327:THR:HG21	1:B:555:LEU:HD13	1.65	0.79
1:B:511:ASP:O	1:B:515:THR:OG1	2.03	0.75
1:B:151:SER:O	1:B:353:ALA:HB2	1.91	0.71
1:B:328:ILE:HG23	1:B:559:ALA:HA	1.80	0.64
1:A:50:LEU:HD22	1:A:86:GLN:OE1	1.98	0.64
1:A:211:GLN:NE2	6:A:2064:HOH:O	2.32	0.61
1:B:273:THR:HG23	1:B:655:THR:HG23	1.80	0.61
1:B:445:ASP:HB3	6:B:2094:HOH:O	2.00	0.61
1:B:311:LEU:HD23	1:B:636:ILE:HD12	1.83	0.61
1:A:305:ARG:NH2	1:A:347:ASP:OD2	2.34	0.60
1:B:37:TYR:CE2	1:B:76:VAL:HG21	2.35	0.60
1:B:250:THR:HG23	1:B:251:THR:O	2.02	0.60
1:B:290:THR:HG22	1:B:293:SER:H	1.68	0.59
1:A:511:ASP:O	1:A:515:THR:OG1	2.19	0.58
1:A:623:TYR:CE1	1:A:762:VAL:HG21	2.39	0.58
1:B:84:VAL:HG11	1:B:119:ILE:HD13	1.86	0.56
1:B:280:THR:HG1	1:B:312:HIS:HE2	1.52	0.56
1:B:227:VAL:HG12	1:B:260:MET:HB2	1.89	0.55
1:A:728:HIS:H	1:A:728:HIS:CD2	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:375:LEU:O	1:B:379:ARG:HG3	2.07	0.54
1:A:212:GLN:HG2	6:A:2064:HOH:O	2.08	0.54
1:A:327:THR:HG23	1:A:390:VAL:HG22	1.91	0.53
1:A:746:HIS:CE1	1:A:763:GLN:HB2	2.45	0.51
1:A:327:THR:HG21	1:A:555:LEU:HD13	1.93	0.51
1:B:332:GLN:NE2	1:B:333:ASP:OD1	2.43	0.51
1:B:32:ARG:O	1:B:108:ARG:NH2	2.43	0.50
1:B:388:ALA:N	1:B:389:PRO:HD2	2.27	0.49
1:A:280:THR:OG1	1:A:312:HIS:HE1	1.95	0.49
1:B:139:ASP:HB3	1:B:141:LYS:H	1.77	0.49
1:B:628:ALA:HB2	1:B:691:LEU:HD11	1.94	0.49
1:A:509:TYR:O	1:A:513:VAL:HG12	2.13	0.48
1:B:297:CYS:H	1:B:557:ASN:HD21	1.62	0.48
1:B:507:LYS:NZ	1:B:510:GLU:OE1	2.34	0.48
1:B:243:TYR:O	1:B:247:THR:HG23	2.13	0.48
1:B:375:LEU:HD22	1:B:397:MET:HG2	1.95	0.47
1:B:32:ARG:O	1:B:33:MET:HG2	2.14	0.47
1:A:446:TYR:C	1:A:446:TYR:CD1	2.87	0.47
1:A:621:SER:OG	1:A:693:ASP:OD2	2.33	0.46
1:B:489:TYR:HB3	1:B:501:TYR:CD2	2.50	0.46
1:A:608:ARG:NH2	1:A:740:GLU:OE1	2.48	0.46
1:B:348:LEU:HG	1:B:352:LEU:HD22	1.97	0.46
1:B:51:LEU:HD11	1:B:83:LEU:HD11	1.97	0.46
1:A:171:GLN:HE22	1:A:271:ALA:HA	1.81	0.46
1:B:84:VAL:HG13	1:B:116:PRO:HA	1.98	0.45
1:A:735:LEU:CD2	1:A:739:MET:SD	3.04	0.45
1:A:386:ASP:OD1	1:A:386:ASP:C	2.54	0.45
1:A:305:ARG:HH22	1:A:347:ASP:CG	2.21	0.45
1:A:128:ARG:HD2	6:A:2032:HOH:O	2.16	0.45
1:A:670:PHE:HB3	6:A:2162:HOH:O	2.17	0.44
3:F:18:DG:H2''	3:F:19:DT:H5'	1.98	0.44
1:A:713:GLU:HG2	1:A:739:MET:HE1	2.00	0.44
1:A:328:ILE:HG23	1:A:559:ALA:HA	1.98	0.44
1:B:361:ARG:O	1:B:364:ASP:HB2	2.17	0.44
1:B:571:THR:OG1	1:B:646:GLU:HG2	2.18	0.44
1:B:585:HIS:HE1	6:B:2121:HOH:O	2.01	0.43
1:A:135:ALA:HA	1:A:179:LEU:O	2.17	0.43
1:A:694:GLU:OE2	6:A:2167:HOH:O	2.21	0.43
1:B:338:LEU:HD13	1:B:381:GLN:OE1	2.19	0.43
1:B:388:ALA:N	1:B:389:PRO:CD	2.81	0.43
1:A:632:LEU:C	1:A:632:LEU:HD23	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:585:HIS:HD2	1:B:587:VAL:H	1.66	0.43
1:A:305:ARG:HD2	6:A:2106:HOH:O	2.19	0.42
1:A:171:GLN:NE2	1:A:271:ALA:HA	2.35	0.42
1:A:494:THR:HG21	1:B:491:ARG:HB3	2.00	0.42
1:A:388:ALA:HB3	1:A:389:PRO:HD3	2.01	0.42
1:B:51:LEU:HD21	1:B:83:LEU:HG	2.01	0.42
1:A:133:LEU:HD23	1:A:240:LEU:HD13	2.02	0.41
1:B:585:HIS:CE1	6:B:2121:HOH:O	2.72	0.41
1:B:468:ASN:HB2	2:E:5:DG:H5"	2.01	0.41
1:A:187:MET:O	1:A:191:GLU:HG2	2.20	0.41
1:A:447:LEU:HD22	1:A:465:VAL:HG11	2.02	0.41
1:B:345:VAL:HG11	1:B:549:LEU:HD13	2.02	0.41
1:B:483:HIS:CE1	1:B:484:LEU:HG	2.55	0.41
1:A:348:LEU:O	1:A:352:LEU:HG	2.21	0.41
1:A:536:LEU:N	1:A:537:PRO:CD	2.84	0.41
1:B:210:ARG:O	1:B:214:ASN:ND2	2.54	0.41
1:B:709:TRP:CE3	1:B:732:LEU:HD23	2.56	0.41
1:A:151:SER:HA	1:A:353:ALA:HB1	2.03	0.40
1:B:148:LEU:HB3	1:B:240:LEU:HD21	2.02	0.40
1:B:80:LEU:HA	1:B:80:LEU:HD23	1.93	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	784/800 (98%)	759 (97%)	22 (3%)	3 (0%)	34	48
1	B	746/800 (93%)	724 (97%)	21 (3%)	1 (0%)	51	68
All	All	1530/1600 (96%)	1483 (97%)	43 (3%)	4 (0%)	41	55

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	594	GLU
1	A	441	ASP
1	A	387	SER
1	B	420	ARG

### 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%)	605 (92%)	51 (8%)	12	19
1	B	631/664 (95%)	571 (90%)	60 (10%)	8	12
All	All	1287/1328 (97%)	1176 (91%)	111 (9%)	10	16

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	33	MET
1	A	35	ASP
1	A	38	GLU
1	A	46	ARG
1	A	58	ARG
1	A	61	SER
1	A	77	GLU
1	A	84	VAL
1	A	140	SER
1	A	141	LYS
1	A	155	PHE
1	A	157	LEU
1	A	178	LEU
1	A	190	ILE
1	A	201	LEU
1	A	240	LEU
1	A	263	GLU
1	A	264	GLN
1	A	274	ARG

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Mol	Chain	Res	Type
1	A	288	GLU
1	A	311	LEU
1	A	315	VAL
1	A	326	GLN
1	A	384	THR
1	A	395	GLU
1	A	444	THR
1	A	479	ARG
1	A	488	ASN
1	A	506	LEU
1	A	512	LYS
1	A	515	THR
1	A	521	LEU
1	A	531	LEU
1	A	536	LEU
1	A	552	LEU
1	A	566	ASN
1	A	575	LYS
1	A	593	ASN
1	A	608	ARG
1	A	640	VAL
1	A	644	LYS
1	A	656	ARG
1	A	705	LEU
1	A	707	LEU
1	A	717	ASN
1	A	718	LYS
1	A	739	MET
1	A	756	ILE
1	A	783	LYS
1	A	788	ARG
1	B	14	MET
1	B	19	ARG
1	B	52	ASP
1	B	55	LEU
1	B	92	ILE
1	B	94	GLU
1	B	111	VAL
1	B	122	GLU
1	B	137	TRP
1	B	140	SER
1	B	155	PHE

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Mol	Chain	Res	Type
1	B	157	LEU
1	B	163	ARG
1	B	178	LEU
1	B	188	SER
1	B	194	ARG
1	B	201	LEU
1	B	206	ILE
1	B	250	THR
1	B	257	SER
1	B	264	GLN
1	B	274	ARG
1	B	280	THR
1	B	290	THR
1	B	313	MET
1	B	335	THR
1	B	338	LEU
1	B	352	LEU
1	B	357	LEU
1	B	419	VAL
1	B	424	VAL
1	B	432	GLU
1	B	444	THR
1	B	445	ASP
1	B	449	ARG
1	B	455	ARG
1	B	487	ILE
1	B	497	ASN
1	B	500	ARG
1	B	507	LYS
1	B	514	LEU
1	B	515	THR
1	B	521	LEU
1	B	523	LEU
1	B	530	GLU
1	B	535	LEU
1	B	575	LYS
1	B	584	ARG
1	B	632	LEU
1	B	636	ILE
1	B	655	THR
1	B	718	LYS
1	B	737	GLU

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Mol	Chain	Res	Type
1	B	754	ASP
1	B	755	THR
1	B	756	ILE
1	B	763	GLN
1	B	784	GLU
1	B	788	ARG
1	B	800	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	49	GLN
1	A	78	ASN
1	A	171	GLN
1	A	312	HIS
1	A	488	ASN
1	A	566	ASN
1	A	602	ASN
1	A	643	GLN
1	A	717	ASN
1	A	728	HIS
1	A	746	HIS
1	B	16	GLN
1	B	86	GLN
1	B	344	GLN
1	B	497	ASN
1	B	557	ASN
1	B	585	HIS
1	B	717	ASN

### 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 [i](#)

There are no monosaccharides 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	1.13	2 (8%)	29,45,45	1.70	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	-	1/12/32/32	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	4.08	1.38	1.32
4	A	1801	ADP	C2-N1	2.44	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	-5.64	119.87	128.68
4	A	1801	ADP	C3'-C2'-C1'	3.75	106.63	100.98
4	A	1801	ADP	O3B-PB-O3A	2.82	114.08	104.64
4	A	1801	ADP	PA-O3A-PB	-2.58	123.98	132.83

There are no chirality outliers.

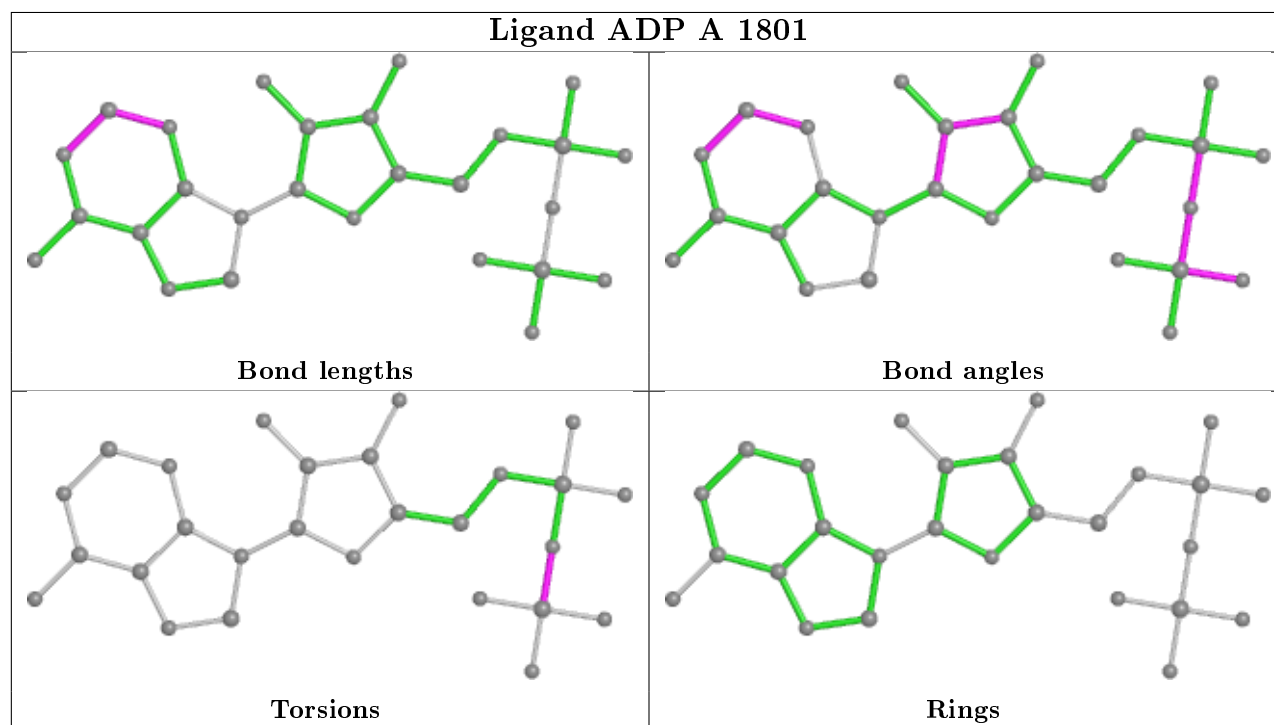
All (1) torsion outliers are listed below:

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

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 ⓘ

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%)	0.01	31 (3%) 39 38	3, 18, 26, 39	0
1	B	754/800 (94%)	0.10	37 (4%) 29 28	8, 18, 25, 34	0
2	E	16/30 (53%)	0.73	5 (31%) 0 0	9, 20, 36, 45	0
3	F	16/30 (53%)	0.55	3 (18%) 1 1	12, 18, 36, 38	0
All	All	1574/1660 (94%)	0.07	76 (4%) 30 29	3, 18, 26, 45	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	74	HIS	5.3
2	E	1	DA	5.0
1	A	593	ASN	4.9
2	E	16	DG	4.9
1	B	56	THR	4.7
1	B	25	PRO	4.6
1	A	62	ALA	4.5
1	B	54	SER	4.5
1	B	19	ARG	4.4
1	A	444	THR	4.4
1	A	103	LYS	4.3
3	F	15	DC	4.2
1	B	35	ASP	4.1
1	B	78	ASN	3.9
1	B	512	LYS	3.8
1	B	55	LEU	3.8
1	B	41	TYR	3.7
1	A	61	SER	3.7
1	A	63	GLY	3.6
1	B	14	MET	3.6
1	A	441	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
3	F	16	DT	3.5
1	B	22	ALA	3.4
1	A	672	VAL	3.3
1	B	52	ASP	3.3
1	A	549	LEU	3.3
1	A	800	SER	3.3
2	E	15	DA	3.2
1	A	509	TYR	3.2
1	B	73	TYR	3.1
1	B	456	GLU	3.1
2	E	2	DG	2.9
1	B	284	ALA	2.9
1	B	18	LEU	2.8
1	A	220	ARG	2.8
1	A	658	GLY	2.8
1	B	29	LEU	2.8
1	B	28	LEU	2.8
1	A	754	ASP	2.8
1	B	202	TRP	2.7
1	B	16	GLN	2.7
1	B	17	TYR	2.7
1	A	135	ALA	2.7
1	A	563	TYR	2.6
1	A	386	ASP	2.6
1	A	237	ALA	2.6
1	A	100	ALA	2.6
1	B	135	ALA	2.5
1	B	140	SER	2.5
1	A	448	GLU	2.5
1	B	800	SER	2.5
1	A	60	ALA	2.5
2	E	14	DC	2.4
1	A	595	PRO	2.4
1	B	593	ASN	2.4
1	B	421	ASP	2.4
1	A	98	ASP	2.3
1	A	445	ASP	2.3
1	B	487	ILE	2.3
1	A	438	ALA	2.3
1	B	690	VAL	2.3
1	A	97	GLY	2.3
1	B	144	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	68	MET	2.3
1	B	39	LEU	2.2
1	B	136	ILE	2.2
1	B	30	PHE	2.2
1	B	192	GLY	2.1
1	B	24	HIS	2.1
3	F	17	DG	2.1
1	A	417	VAL	2.1
1	B	23	GLN	2.1
1	A	39	LEU	2.1
1	A	192	GLY	2.1
1	A	431	GLU	2.0
1	A	638	SER	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](#)

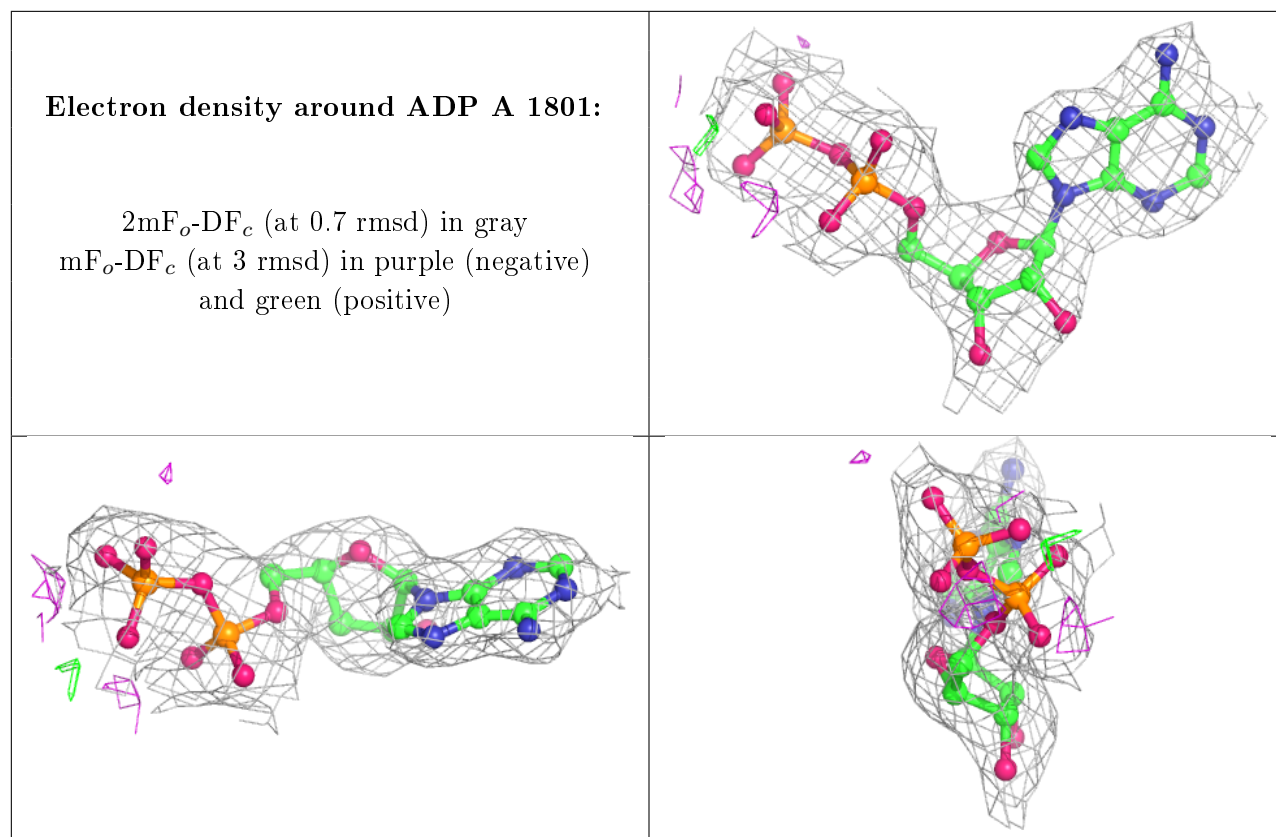
There are no monosaccharides in this entry.

## 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
5	MG	A	1802	1/1	0.83	0.12	12,12,12,12	0
4	ADP	A	1801	27/27	0.98	0.10	13,20,22,25	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.