Full wwPDB X-ray Structure Validation Report (i)

Feb 5, 2024 – 01:21 AM EST

PDB ID	:	1S16
Title	:	Crystal Structure of E. coli Topoisomerase IV ParE 43kDa subunit complexed with ADPNP
Authors	:	Wei, Y.; Gross, C.H.
Deposited on	:	2004-01-05
Resolution	:	2.10 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

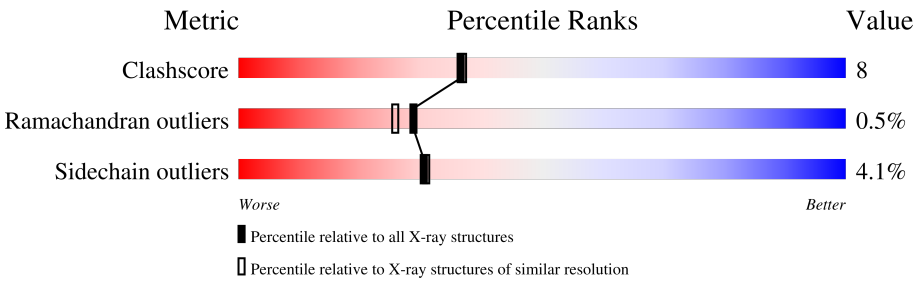
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.10 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))
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)

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 >=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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	390	81% 15% • •
1	B	390	78% 17% • •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6211 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.

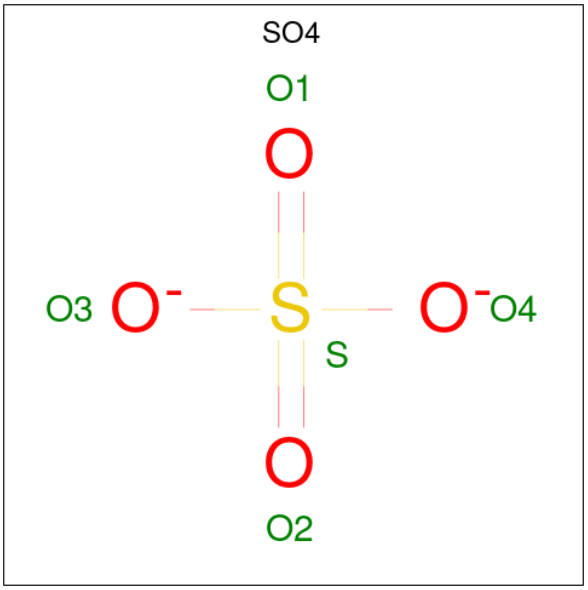
- Molecule 1 is a protein called Topoisomerase IV subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	380	2945	1849	520	562	14	0	0	0
1	B	380	2945	1849	520	562	14	0	0	0

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

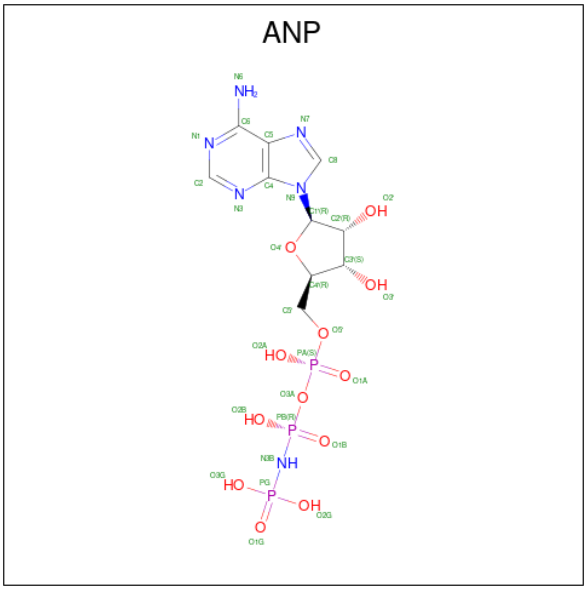
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
2	A	1	1	1	0	0
2	B	1	1	1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
3	A	1	5	4	1	0	0
			Total	O	S		
3	B	1	5	4	1	0	0

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	31	10	6	12	3	0	0
			Total	C	N	O	P		
4	B	1	31	10	6	12	3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	129	129	129	0	0
			Total	O		
5	B	118	118	118	0	0

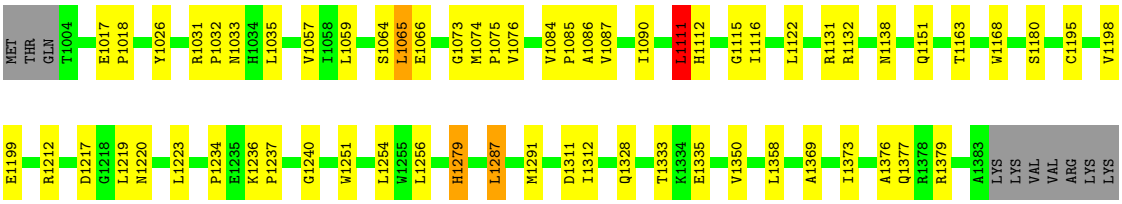
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

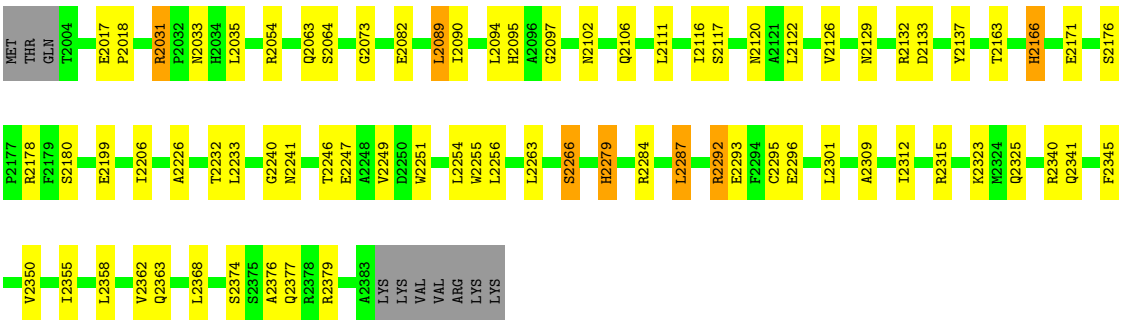
• Molecule 1: Topoisomerase IV subunit B

Chain A: 81% 15% • •



• Molecule 1: Topoisomerase IV subunit B

Chain B: 78% 17% • •



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	94.90Å 120.80Å 136.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10	Depositor
% Data completeness (in resolution range)	96.4 (20.00-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
Refinement program	CNX	Depositor
R, R_{free}	0.224 , 0.240	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6211	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

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: SO4, MG, ANP

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	0.32	0/3004	0.60	0/4080
1	B	0.31	0/3004	0.58	0/4080
All	All	0.31	0/6008	0.59	0/8160

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2945	0	2873	45	0
1	B	2945	0	2873	49	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	31	0	13	1	0
4	B	31	0	13	1	0
5	A	129	0	0	0	0
5	B	118	0	0	2	0
All	All	6211	0	5772	93	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 8.

All (93) 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:1376:ALA:HA	1:A:1379:ARG:HH12	1.28	0.97
1:B:2033:ASN:HD21	1:B:2180:SER:H	0.94	0.89
1:A:1033:ASN:HD21	1:A:1180:SER:H	0.91	0.87
1:A:1376:ALA:HA	1:A:1379:ARG:NH1	1.92	0.84
1:A:1033:ASN:HD21	1:A:1180:SER:N	1.76	0.83
1:B:2284:ARG:HD3	1:B:2309:ALA:HB1	1.64	0.80
1:B:2033:ASN:HD21	1:B:2180:SER:N	1.76	0.79
1:B:2033:ASN:ND2	1:B:2180:SER:H	1.77	0.78
1:A:1033:ASN:ND2	1:A:1180:SER:H	1.76	0.77
1:B:2376:ALA:HA	1:B:2379:ARG:HD3	1.69	0.74
1:A:1074:MET:HE2	1:A:1087:VAL:HG13	1.68	0.73
1:A:1333:THR:HG22	1:A:1335:GLU:HG3	1.72	0.70
1:A:1220:ASN:OD1	1:A:1237:PRO:HG2	1.92	0.69
1:B:2232:THR:HG22	1:B:2256:LEU:HD22	1.73	0.69
1:B:2376:ALA:O	1:B:2379:ARG:HG2	1.92	0.69
1:A:1084:VAL:HG13	1:A:1085:PRO:HD2	1.75	0.69
1:A:1195:CYS:O	1:A:1198:VAL:HG12	1.95	0.67
1:B:2256:LEU:O	1:B:2315:ARG:HD3	1.95	0.66
1:A:1291:MET:HE1	1:A:1369:ALA:HA	1.80	0.63
1:A:1111:LEU:HD13	1:A:1112:HIS:CD2	2.34	0.62
1:B:2247:GLU:HG3	1:B:2345:PHE:CZ	2.37	0.60
1:A:1311:ASP:OD1	1:A:1379:ARG:NH1	2.35	0.60
1:A:1076:VAL:HG12	1:A:1087:VAL:HG21	1.83	0.60
1:A:1065:LEU:HD13	1:A:1066:GLU:N	2.17	0.59
1:B:2376:ALA:HA	1:B:2379:ARG:CD	2.31	0.58
1:B:2340:ARG:NH1	1:B:2341:GLN:HE21	2.02	0.58
1:B:2374:SER:HA	1:B:2377:GLN:HE21	1.68	0.58
1:B:2102:ASN:HD21	1:B:2325:GLN:HB3	1.69	0.58
1:A:1138:ASN:HD22	1:A:1151:GLN:HE21	1.53	0.56
1:A:1373:ILE:O	1:A:1377:GLN:HG3	2.05	0.56
1:B:2246:THR:HA	1:B:2325:GLN:NE2	2.21	0.56
1:B:2279:HIS:H	1:B:2279:HIS:CD2	2.24	0.54
1:B:2362:VAL:HG23	1:B:2363:GLN:N	2.23	0.54
1:B:2246:THR:HA	1:B:2325:GLN:HE21	1.72	0.54
1:A:1333:THR:CG2	1:A:1335:GLU:HG3	2.39	0.53
1:B:2064:SER:OG	1:B:2166:HIS:HE1	1.90	0.53
1:A:1090:ILE:HG23	4:A:1500:ANP:H5'1	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2293:GLU:OE1	1:B:2355:ILE:HD13	2.10	0.52
1:B:2241:ASN:HA	1:B:2249:VAL:O	2.10	0.51
1:A:1057:VAL:HG13	1:A:1065:LEU:HD11	1.93	0.50
1:A:1076:VAL:HG12	1:A:1087:VAL:CG2	2.40	0.49
1:A:1131:ARG:O	1:A:1132:ARG:HG3	2.13	0.49
1:B:2292:ARG:O	1:B:2296:GLU:HG3	2.13	0.49
1:A:1287:LEU:HD13	1:A:1350:VAL:CG1	2.44	0.48
1:B:2233:LEU:HG	1:B:2368:LEU:CD2	2.43	0.48
1:B:2031:ARG:HH11	1:B:2031:ARG:HB3	1.79	0.48
1:B:2233:LEU:HG	1:B:2368:LEU:HD21	1.96	0.48
1:B:2312:ILE:C	1:B:2312:ILE:HD12	2.34	0.48
1:A:1026:TYR:HH	1:B:2095:HIS:HE2	1.60	0.47
1:A:1017:GLU:N	1:A:1018:PRO:HD2	2.29	0.47
1:A:1075:PRO:O	1:A:1086:ALA:HB3	2.15	0.47
1:A:1279:HIS:H	1:A:1279:HIS:CD2	2.30	0.47
1:B:2171:GLU:H	1:B:2171:GLU:CD	2.19	0.47
1:B:2255:TRP:C	1:B:2256:LEU:HD23	2.35	0.47
1:B:2017:GLU:N	1:B:2018:PRO:HD2	2.29	0.46
1:B:2279:HIS:H	1:B:2279:HIS:HD2	1.64	0.46
1:B:2226:ALA:CB	1:B:2263:LEU:HD22	2.47	0.45
1:B:2063:GLN:NE2	1:B:2206:ILE:HD13	2.32	0.45
1:A:1199:GLU:CD	1:A:1212:ARG:HE	2.20	0.45
1:A:1223:LEU:HD23	1:A:1237:PRO:HB3	1.99	0.44
1:B:2287:LEU:HD13	1:B:2350:VAL:HG11	1.99	0.44
1:A:1240:GLY:HA3	1:A:1251:TRP:CZ2	2.53	0.44
1:A:1090:ILE:HG22	1:A:1116:ILE:HG21	2.00	0.44
1:A:1312:ILE:C	1:A:1312:ILE:HD12	2.38	0.44
1:B:2240:GLY:HA3	1:B:2251:TRP:CZ2	2.53	0.44
1:B:2090:ILE:HG22	1:B:2116:ILE:HG21	1.99	0.44
1:B:2295:CYS:HB3	1:B:2301:LEU:HD13	1.99	0.44
1:A:1084:VAL:CG1	1:A:1085:PRO:HD2	2.46	0.43
1:A:1031:ARG:HD3	1:A:1033:ASN:ND2	2.33	0.43
1:B:2082:GLU:HG3	1:B:2089:LEU:HD21	2.00	0.43
1:B:2102:ASN:HD21	1:B:2325:GLN:CB	2.31	0.43
1:B:2266:SER:HB2	5:B:3012:HOH:O	2.17	0.43
1:B:2279:HIS:CD2	1:B:2279:HIS:N	2.86	0.43
1:A:1234:PRO:HG2	1:A:1236:LYS:O	2.19	0.43
1:A:1073:GLY:HA2	1:A:1163:THR:OG1	2.19	0.42
1:B:2018:PRO:HG2	1:B:2094:LEU:HD11	2.02	0.42
1:B:2246:THR:HG22	1:B:2325:GLN:NE2	2.35	0.42
1:A:1333:THR:HG22	1:A:1335:GLU:CG	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2073:GLY:HA2	1:B:2163:THR:OG1	2.20	0.41
1:A:1064:SER:HB3	1:A:1168:TRP:CD1	2.55	0.41
1:A:1279:HIS:CD2	1:A:1279:HIS:N	2.89	0.41
1:B:2176:SER:OG	1:B:2178:ARG:HG2	2.20	0.41
1:A:1291:MET:CE	1:A:1369:ALA:HA	2.49	0.41
1:A:1379:ARG:NH1	1:A:1379:ARG:HB3	2.35	0.41
1:B:2120:ASN:HA	1:B:2126:VAL:HG21	2.02	0.41
1:A:1219:LEU:HD23	1:A:1219:LEU:HA	1.77	0.41
1:B:2097:GLY:HA2	4:B:2500:ANP:H4'	2.02	0.41
1:B:2129:ASN:HA	1:B:2137:TYR:O	2.20	0.41
1:B:2284:ARG:HD3	1:B:2309:ALA:CB	2.41	0.41
1:A:1328:GLN:HG3	5:B:3017:HOH:O	2.20	0.40
1:B:2054:ARG:HG3	1:B:2199:GLU:O	2.21	0.40
1:A:1031:ARG:HB2	1:A:1032:PRO:HD2	2.04	0.40
1:A:1111:LEU:N	1:A:1111:LEU:HD12	2.37	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	378/390 (97%)	368 (97%)	7 (2%)	3 (1%)	19 15
1	B	378/390 (97%)	365 (97%)	12 (3%)	1 (0%)	41 41
All	All	756/780 (97%)	733 (97%)	19 (2%)	4 (0%)	29 26

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1217	ASP
1	B	2111	LEU
1	A	1111	LEU

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Mol	Chain	Res	Type
1	A	1115	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	314/327 (96%)	304 (97%)	10 (3%)	39	41
1	B	314/327 (96%)	298 (95%)	16 (5%)	24	22
All	All	628/654 (96%)	602 (96%)	26 (4%)	30	31

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1035	LEU
1	A	1059	LEU
1	A	1065	LEU
1	A	1111	LEU
1	A	1122	LEU
1	A	1254	LEU
1	A	1256	LEU
1	A	1279	HIS
1	A	1287	LEU
1	A	1358	LEU
1	B	2031	ARG
1	B	2035	LEU
1	B	2089	LEU
1	B	2106	GLN
1	B	2117	SER
1	B	2122	LEU
1	B	2132	ARG
1	B	2133	ASP
1	B	2166	HIS
1	B	2254	LEU
1	B	2266	SER
1	B	2279	HIS

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Mol	Chain	Res	Type
1	B	2287	LEU
1	B	2292	ARG
1	B	2323	LYS
1	B	2358	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1006	ASN
1	A	1033	ASN
1	A	1138	ASN
1	A	1216	GLN
1	A	1275	GLN
1	A	1279	HIS
1	A	1285	GLN
1	A	1332	GLN
1	A	1359	ASN
1	A	1361	ASN
1	A	1363	GLN
1	B	2006	ASN
1	B	2033	ASN
1	B	2034	HIS
1	B	2051	HIS
1	B	2102	ASN
1	B	2138	ASN
1	B	2151	GLN
1	B	2166	HIS
1	B	2207	ASN
1	B	2220	ASN
1	B	2275	GLN
1	B	2279	HIS
1	B	2281	ASN
1	B	2325	GLN
1	B	2328	GLN
1	B	2341	GLN
1	B	2359	ASN
1	B	2360	GLN
1	B	2361	ASN
1	B	2363	GLN
1	B	2377	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	ANP	B	2500	2	29,33,33	1.90	7 (24%)	31,52,52	1.92	7 (22%)
4	ANP	A	1500	2	29,33,33	2.09	7 (24%)	31,52,52	1.75	4 (12%)
3	SO4	B	2502	-	4,4,4	0.34	0	6,6,6	0.27	0
3	SO4	A	1502	-	4,4,4	0.38	0	6,6,6	0.13	0

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	ANP	A	1500	2	-	0/14/38/38	0/3/3/3
4	ANP	B	2500	2	-	1/14/38/38	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1500	ANP	C4-N3	5.47	1.43	1.35
4	B	2500	ANP	C4-N3	5.31	1.43	1.35
4	A	1500	ANP	PG-O1G	4.85	1.53	1.46
4	A	1500	ANP	C2-N3	4.49	1.39	1.32
4	B	2500	ANP	C2-N3	3.66	1.38	1.32
4	B	2500	ANP	C5-C4	3.57	1.50	1.40
4	A	1500	ANP	C5-C4	3.39	1.49	1.40
4	B	2500	ANP	PG-O1G	3.27	1.51	1.46
4	B	2500	ANP	C2-N1	2.99	1.39	1.33
4	A	1500	ANP	C2-N1	2.83	1.39	1.33
4	A	1500	ANP	PG-O3G	-2.69	1.49	1.56
4	A	1500	ANP	PB-O1B	2.54	1.50	1.46
4	B	2500	ANP	O4'-C1'	2.21	1.44	1.41
4	B	2500	ANP	PG-N3B	-2.15	1.57	1.63

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	2500	ANP	N3-C2-N1	-6.77	118.09	128.68
4	A	1500	ANP	N3-C2-N1	-6.62	118.33	128.68
4	B	2500	ANP	C2-N1-C6	4.67	126.74	118.75
4	A	1500	ANP	C2-N1-C6	4.45	126.37	118.75
4	B	2500	ANP	O1B-PB-N3B	-2.76	107.70	111.77
4	A	1500	ANP	O3A-PB-N3B	2.55	113.67	106.59
4	B	2500	ANP	C3'-C2'-C1'	-2.46	97.27	100.98
4	B	2500	ANP	O3G-PG-O1G	-2.30	107.67	113.45
4	B	2500	ANP	O2G-PG-O1G	-2.17	107.99	113.45
4	B	2500	ANP	O4'-C1'-C2'	2.05	109.93	106.93
4	A	1500	ANP	O3G-PG-O1G	-2.01	108.40	113.45

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	2500	ANP	C5'-O5'-PA-O1A

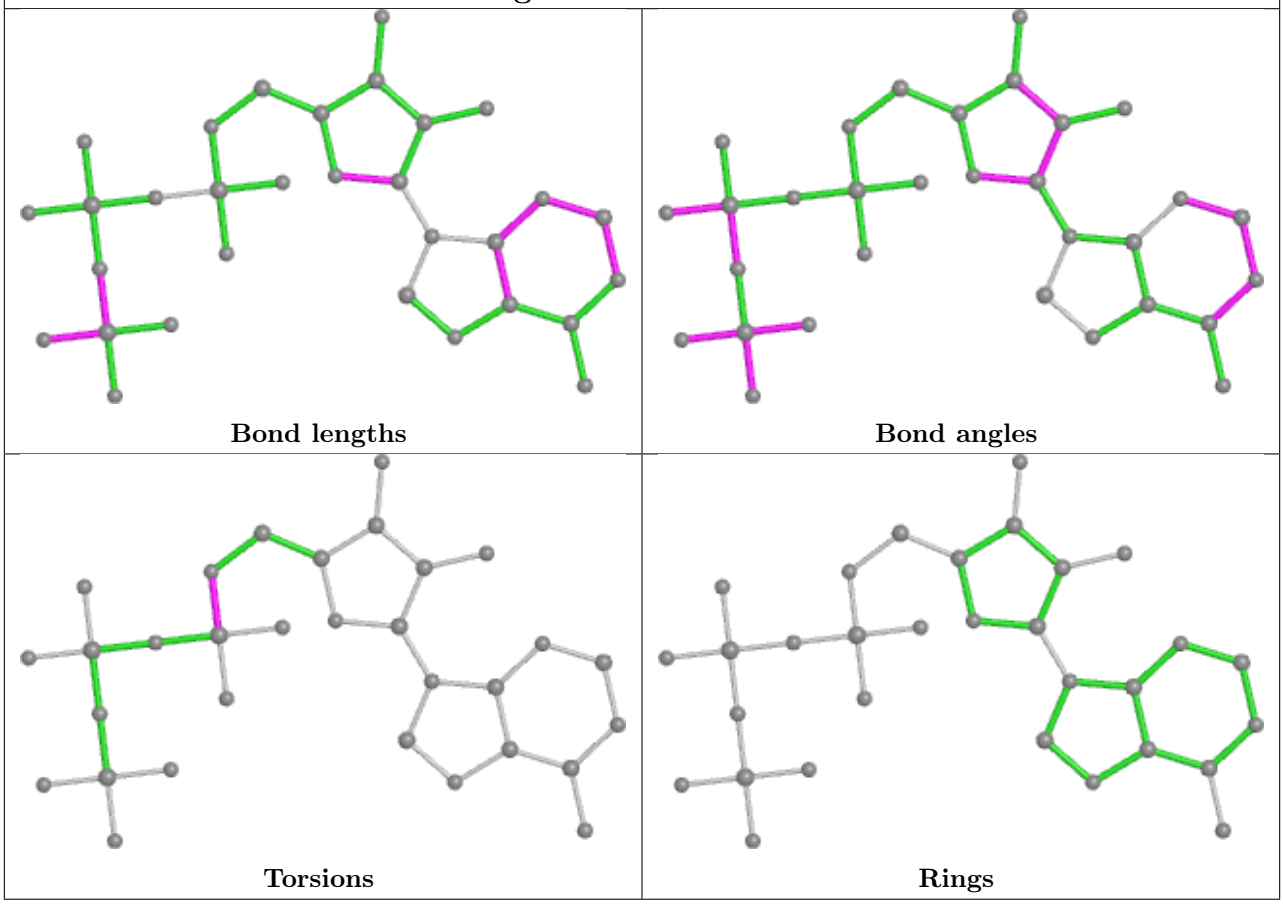
There are no ring outliers.

2 monomers are involved in 2 short contacts:

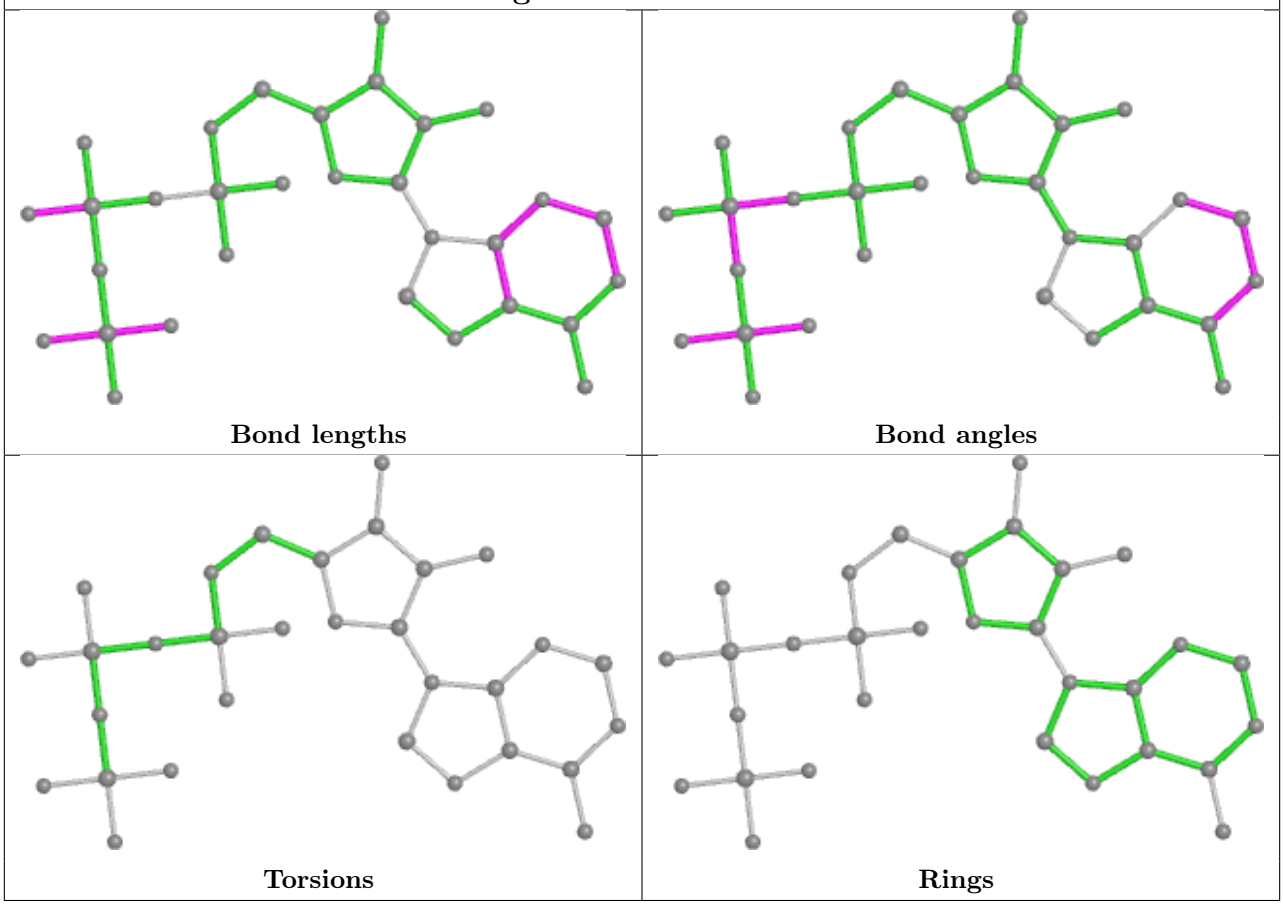
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2500	ANP	1	0
4	A	1500	ANP	1	0

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 then 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.

Ligand ANP B 2500



Ligand ANP A 1500



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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.