Full wwPDB X-ray Structure Validation Report ⓘ

Dec 9, 2023 – 10:42 am GMT

PDB ID	:	1WBB
Title	:	Crystal structure of E. coli DNA mismatch repair enzyme MutS, E38A mutant, in complex with a G.T mismatch
Authors	:	Natrajan, G.; Georgijevic, D.; Lebbink, J.H.G.; Winterwerp, H.H.K.; de Wind, N.; Sixma, T.K.
Deposited on	:	2004-10-31
Resolution	:	2.50 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
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)	:	2.36
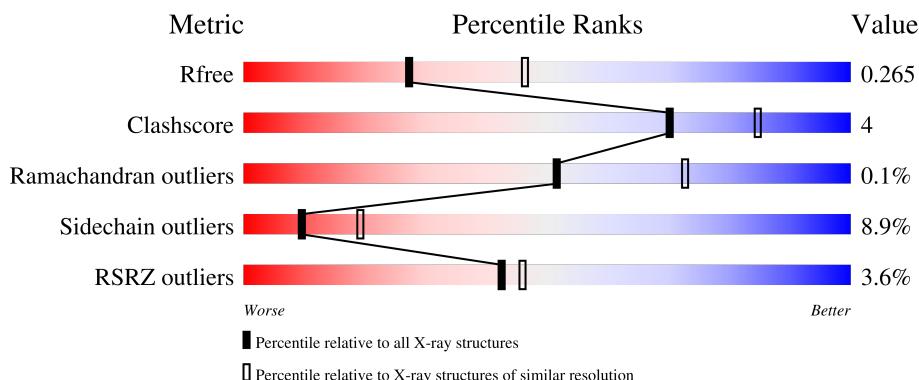
1   Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
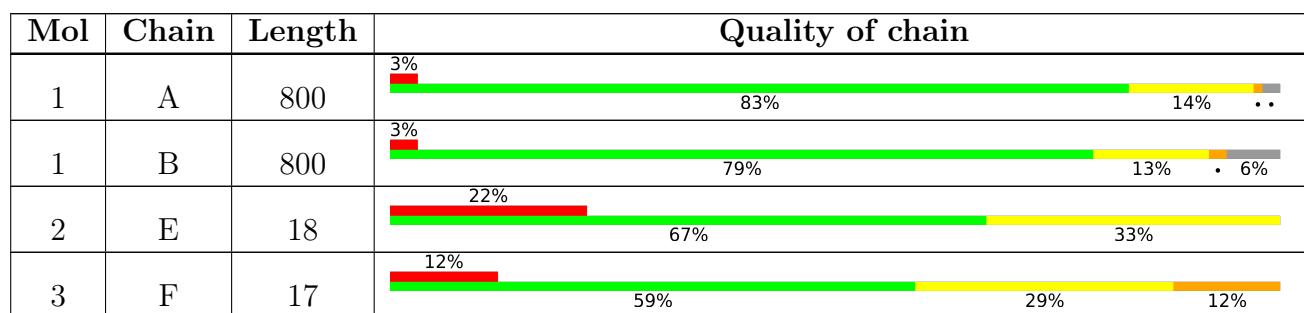
The reported resolution of this entry is 2.50 Å.

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	Percentile Ranks	Value
Rfree		0.265
Clashscore		4
Ramachandran outliers		0.1%
Sidechain outliers		8.9%
RSRZ outliers		3.6%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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% 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	3% / 83% / 14% / ••
1	B	800	3% / 79% / 13% / • / 6%
2	E	18	22% / 67% / 33%
3	F	17	12% / 59% / 29% / 12%

2   Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 13190 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 6203	C 3903	N 1103	O 1168	S 29	0	0	0
1	B	754	Total 5960	C 3754	N 1060	O 1118	S 28	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	38	ALA	GLU	engineered mutation	UNP P23909
B	38	ALA	GLU	engineered mutation	UNP P23909
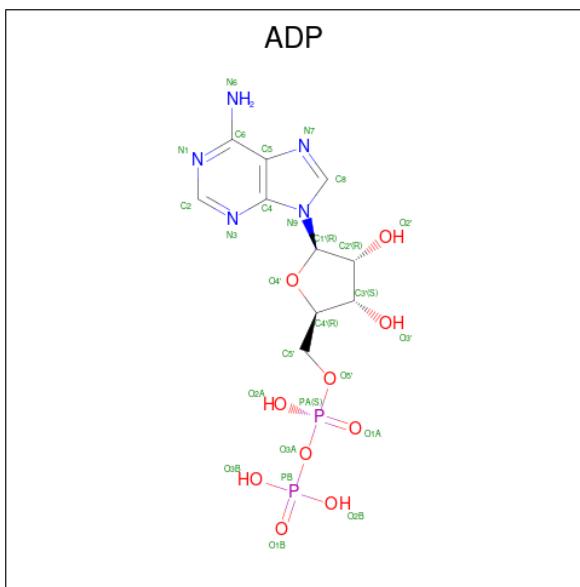
- Molecule 2 is a DNA chain called 5'-D(*AP*GP*CP*TP*GP*CP*CP*AP*GP*GP *CP*AP*CP*CP*AP*GP*TP*G)-3'.

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

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

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

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	27	10	5	10	2	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
5	A	1	1	1	0	0
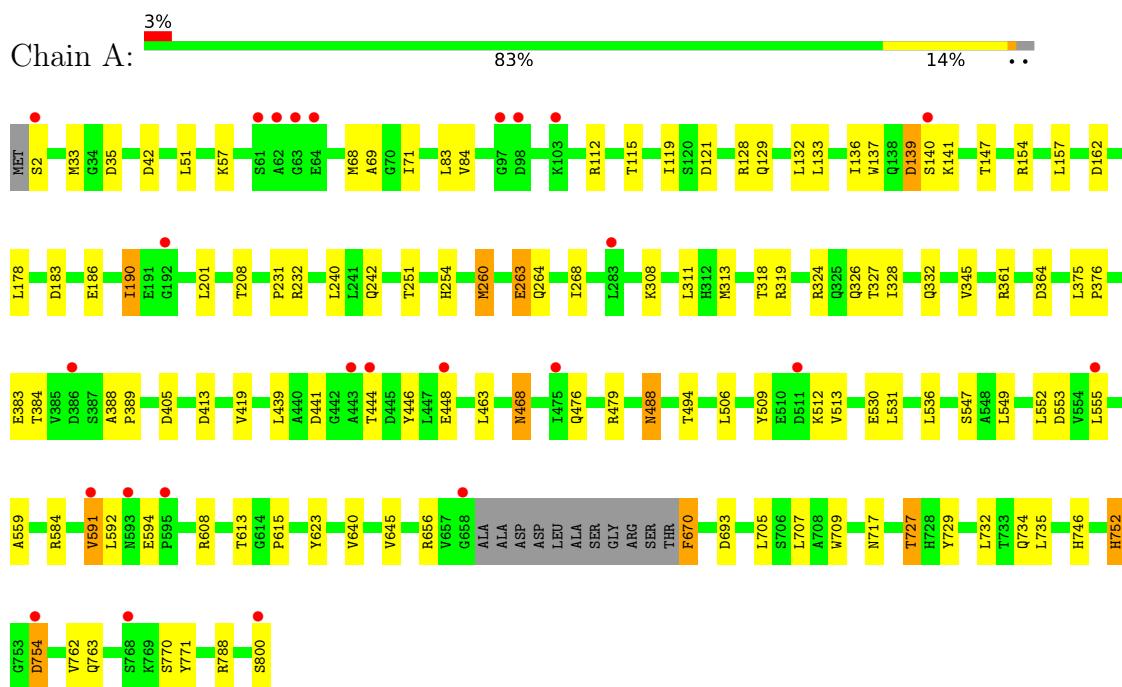
- Molecule 6 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	138	Total 138	O 138	0	0
6	B	136	Total 136	O 136	0	0
6	E	4	Total 4	O 4	0	0
6	F	7	Total 7	O 7	0	0
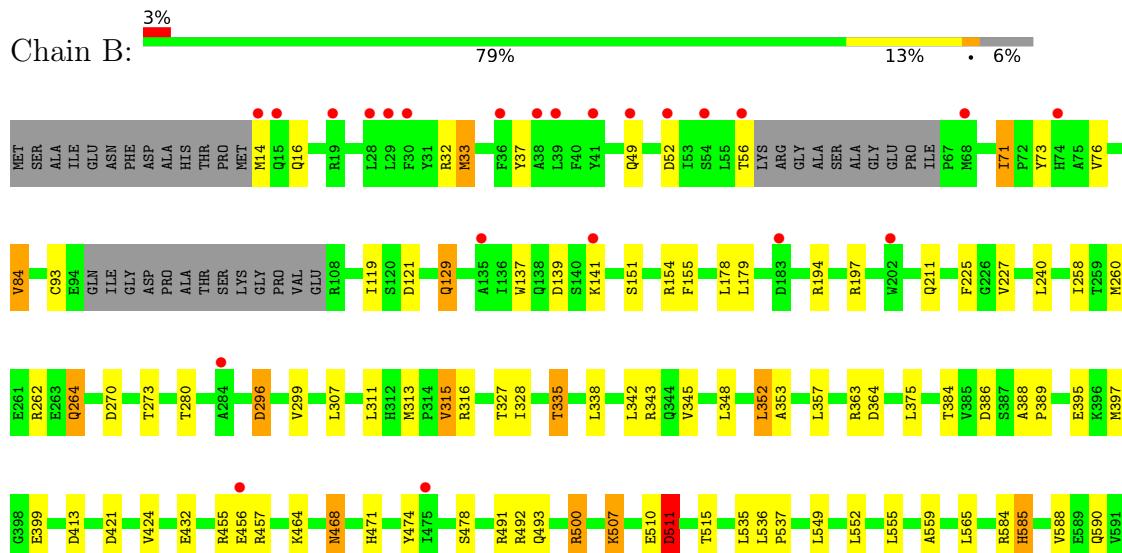
3 Residue-property plots ⓘ

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
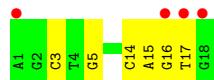
- Molecule 1: DNA MISMATCH REPAIR PROTEIN MUTS
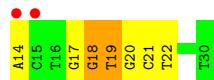
• Molecule 2: 5'-D(*AP*GP*CP*TP*GP*CP*CP*AP*GP*GP *CP*AP*CP*CP*AP*GP*TP* G)-3'

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

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	89.55Å 92.49Å 261.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 19.93 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.3 (20.00-2.50) 99.3 (19.93-2.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.92 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.220 , 0.270 0.221 , 0.265	Depositor DCC
R_{free} test set	1452 reflections (1.93%)	wwPDB-VP
Wilson B-factor (Å^2)	41.0	Xtriage
Anisotropy	0.543	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 33.1	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.018 for k,h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	13190	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: ADP, MG

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	0.47	0/6309	0.77	12/8539 (0.1%)
1	B	0.47	0/6058	0.75	11/8194 (0.1%)
2	E	0.85	0/412	1.49	3/634 (0.5%)
3	F	0.86	0/388	1.65	7/598 (1.2%)
All	All	0.50	0/13167	0.84	33/17965 (0.2%)

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	18	DG	O4'-C4'-C3'	-8.77	100.74	106.00
3	F	14	DA	O4'-C1'-N9	8.15	113.71	108.00
2	E	16	DG	O4'-C1'-N9	7.63	113.34	108.00
2	E	17	DT	O4'-C1'-N1	7.39	113.17	108.00
3	F	22	DT	N3-C2-O2	-7.29	117.93	122.30
1	A	42	ASP	CB-CG-OD2	6.87	124.48	118.30
3	F	21	DC	O4'-C4'-C3'	-6.66	101.83	104.50
1	B	121	ASP	CB-CG-OD2	6.65	124.28	118.30
1	B	270	ASP	CB-CG-OD2	6.58	124.22	118.30
1	B	364	ASP	CB-CG-OD2	6.26	123.94	118.30
1	A	364	ASP	CB-CG-OD2	6.15	123.83	118.30
1	A	413	ASP	CB-CG-OD2	6.03	123.72	118.30
1	A	693	ASP	CB-CG-OD2	6.02	123.72	118.30
1	B	296	ASP	CB-CG-OD2	6.02	123.72	118.30
1	A	121	ASP	CB-CG-OD2	6.01	123.71	118.30
1	A	162	ASP	CB-CG-OD2	5.82	123.54	118.30
1	B	386	ASP	CB-CG-OD2	5.78	123.50	118.30
1	B	413	ASP	CB-CG-OD2	5.70	123.43	118.30
1	B	703	ASP	CB-CG-OD2	5.69	123.42	118.30
1	B	632	LEU	CA-CB-CG	5.57	128.11	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	ASP	CB-CG-OD2	5.48	123.23	118.30
3	F	21	DC	C1'-O4'-C4'	-5.47	104.63	110.10
1	B	511	ASP	CB-CG-OD2	5.40	123.16	118.30
1	A	183	ASP	CB-CG-OD2	5.39	123.15	118.30
2	E	3	DC	P-O3'-C3'	5.35	126.12	119.70
1	B	421	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	405	ASP	CB-CG-OD2	5.20	122.98	118.30
1	B	52	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	441	ASP	CB-CG-OD2	5.11	122.89	118.30
1	A	553	ASP	CB-CG-OD2	5.08	122.88	118.30
3	F	19	DT	C4-C5-C7	5.08	122.05	119.00
3	F	19	DT	C6-C5-C7	-5.07	119.86	122.90
1	A	754	ASP	CB-CG-OD2	5.07	122.86	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6203	0	6250	43	0
1	B	5960	0	6017	48	0
2	E	367	0	202	3	0
3	F	347	0	194	2	0
4	A	27	0	12	0	0
5	A	1	0	0	0	0
6	A	138	0	0	9	0
6	B	136	0	0	4	0
6	E	4	0	0	0	0
6	F	7	0	0	1	0
All	All	13190	0	12675	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 4.

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:B:327:THR:HG21	1:B:555:LEU:HD13	1.62	0.80
1:B:315:VAL:HG23	6:B:2038:HOH:O	1.85	0.77
1:B:633:MET:O	1:B:636:ILE:HG22	1.87	0.74
1:B:311:LEU:HD23	1:B:636:ILE:HD12	1.69	0.72
1:A:727:THR:HG22	1:A:729:TYR:H	1.58	0.69
1:A:345:VAL:HG11	1:A:549:LEU:HD13	1.74	0.69
1:B:655:THR:HG22	1:B:691:LEU:HD12	1.75	0.69
1:B:328:ILE:HG23	1:B:559:ALA:HA	1.76	0.68
1:B:471:HIS:HE1	1:B:493:GLN:HB2	1.60	0.66
1:B:264:GLN:HE21	1:B:264:GLN:H	1.44	0.65
1:B:656:ARG:O	1:B:656:ARG:HG3	1.97	0.63
1:B:342:LEU:HD11	1:B:552:LEU:HD23	1.81	0.62
1:B:735:LEU:HD22	1:B:739:MET:CE	2.31	0.61
1:A:136:ILE:HD13	1:A:190:ILE:HD11	1.84	0.58
1:B:335:THR:HG23	6:B:2050:HOH:O	2.04	0.58
1:A:623:TYR:CE1	1:A:762:VAL:HG21	2.39	0.57
1:B:507:LYS:NZ	1:B:510:GLU:OE1	2.31	0.56
1:B:628:ALA:HB2	1:B:691:LEU:HD11	1.86	0.56
1:A:133:LEU:HG	1:A:240:LEU:HD11	1.88	0.55
1:A:128:ARG:O	1:A:308:LYS:NZ	2.41	0.53
1:A:591:VAL:HG22	1:A:591:VAL:O	2.08	0.53
1:B:468:ASN:HD21	2:E:5:DG:H5"	1.74	0.53
1:A:186:GLU:HG2	6:A:2030:HOH:O	2.09	0.53
1:B:588:VAL:HG13	1:B:592:LEU:HD12	1.91	0.52
1:B:474:TYR:CE1	1:B:500:ARG:HD2	2.44	0.52
1:A:328:ILE:HG23	1:A:559:ALA:HA	1.92	0.51
2:E:14:DC:H2"	2:E:15:DA:C8	2.47	0.50
1:B:299:VAL:HG12	1:B:343:ARG:NH1	2.27	0.50
1:B:37:TYR:HE2	1:B:76:VAL:HG21	1.76	0.49
1:B:585:HIS:CD2	1:B:588:VAL:HG23	2.46	0.49
1:A:752:HIS:CD2	1:A:752:HIS:N	2.81	0.49
1:A:327:THR:HG21	1:A:555:LEU:HD13	1.95	0.49
1:A:463:LEU:HA	1:A:476:GLN:O	2.11	0.49
1:A:530:GLU:HB3	6:A:2092:HOH:O	2.12	0.49
1:B:511:ASP:O	1:B:515:THR:OG1	2.25	0.49
1:B:735:LEU:HD22	1:B:739:MET:HE2	1.94	0.49
1:A:115:THR:O	1:A:119:ILE:HG23	2.13	0.48
1:B:73:TYR:O	1:B:76:VAL:HG23	2.13	0.48
1:A:2:SER:CB	6:A:2002:HOH:O	2.60	0.48
1:A:468:ASN:HB3	6:F:2006:HOH:O	2.14	0.48
1:B:468:ASN:ND2	2:E:5:DG:H5"	2.29	0.48
1:B:71:ILE:HG13	1:B:71:ILE:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:PHE:HB3	1:B:258:ILE:O	2.15	0.47
1:A:231:PRO:HD2	6:A:2037:HOH:O	2.15	0.47
1:B:37:TYR:CE2	1:B:76:VAL:HG21	2.49	0.47
1:B:363:ARG:HB2	6:B:2066:HOH:O	2.13	0.47
1:A:709:TRP:HE3	1:A:732:LEU:HD23	1.79	0.47
1:B:179:LEU:HD23	1:B:197:ARG:HB2	1.97	0.47
1:B:536:LEU:N	1:B:537:PRO:CD	2.77	0.46
1:A:670:PHE:CD2	1:A:670:PHE:N	2.83	0.46
1:A:51:LEU:HD21	1:A:83:LEU:HD21	1.98	0.46
3:F:17:DG:H1'	3:F:18:DG:C8	2.51	0.45
1:A:133:LEU:HG	1:A:240:LEU:CD1	2.46	0.45
1:B:388:ALA:HB3	1:B:389:PRO:HD3	1.97	0.45
1:A:488:ASN:HD22	1:A:488:ASN:C	2.20	0.45
1:A:68:MET:HG2	1:A:69:ALA:N	2.31	0.45
1:B:585:HIS:CE1	1:B:629:LEU:CD1	3.00	0.44
1:A:345:VAL:HG11	1:A:549:LEU:CD1	2.45	0.44
1:A:727:THR:HG23	6:A:2116:HOH:O	2.16	0.44
1:A:640:VAL:HG11	1:A:645:VAL:HG21	2.00	0.44
1:B:227:VAL:HG12	1:B:260:MET:HB2	1.99	0.44
1:A:139:ASP:HB2	1:A:232:ARG:NH1	2.33	0.44
1:A:2:SER:HB2	6:A:2002:HOH:O	2.18	0.43
1:B:375:LEU:HD22	1:B:397:MET:HG2	1.99	0.43
1:A:132:LEU:HD13	1:A:147:THR:HB	2.01	0.43
1:B:585:HIS:HB2	1:B:626:GLN:HB3	2.00	0.43
1:A:2:SER:HB3	6:A:2002:HOH:O	2.18	0.43
1:A:251:THR:HG22	6:A:2060:HOH:O	2.19	0.43
1:A:388:ALA:N	1:A:389:PRO:CD	2.82	0.43
1:A:157:LEU:HD22	1:A:260:MET:HG3	2.01	0.43
1:B:565:LEU:HD22	1:B:590:GLN:NE2	2.34	0.43
1:A:509:TYR:CZ	1:A:513:VAL:HG21	2.54	0.42
1:B:84:VAL:HG11	1:B:119:ILE:HD13	2.01	0.42
1:B:240:LEU:C	1:B:240:LEU:HD23	2.40	0.42
1:B:129:GLN:HE21	1:B:129:GLN:HB3	1.67	0.42
1:A:375:LEU:HB2	1:A:376:PRO:HD3	2.02	0.42
1:A:263:GLU:CB	1:A:268:ILE:HD11	2.49	0.42
1:B:151:SER:O	1:B:353:ALA:HB2	2.20	0.42
1:B:32:ARG:C	1:B:33:MET:HG2	2.40	0.42
1:A:746:HIS:CE1	1:A:763:GLN:HB2	2.56	0.41
1:A:324:ARG:O	1:A:328:ILE:HD12	2.19	0.41
1:A:494:THR:HG21	1:B:491:ARG:HB3	2.03	0.41
1:A:84:VAL:HG21	1:A:119:ILE:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:ARG:NH1	6:A:2034:HOH:O	2.53	0.41
1:A:615:PRO:HB3	1:A:771:TYR:HB2	2.02	0.41
1:B:345:VAL:HG11	1:B:549:LEU:HD13	2.01	0.41
1:B:594:GLU:HG3	1:B:595:PRO:HD2	2.02	0.41
1:B:296:ASP:HB2	1:B:307:LEU:HD23	2.02	0.41
1:A:446:TYR:CD1	1:A:446:TYR:C	2.94	0.41
1:B:273:THR:HG23	1:B:655:THR:HG23	2.03	0.40
1:B:14:MET:N	6:B:2001:HOH:O	2.55	0.40
1:B:348:LEU:HG	1:B:352:LEU:HD22	2.03	0.40
3:F:19:DT:H2"	3:F:20:DG:O5'	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	784/800 (98%)	751 (96%)	31 (4%)	2 (0%)	41	61
1	B	746/800 (93%)	722 (97%)	24 (3%)	0	100	100
All	All	1530/1600 (96%)	1473 (96%)	55 (4%)	2 (0%)	51	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	444	THR
1	A	592	LEU

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	655/663 (99%)	598 (91%)	57 (9%)	10	20
1	B	630/663 (95%)	573 (91%)	57 (9%)	9	19
All	All	1285/1326 (97%)	1171 (91%)	114 (9%)	9	19

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	MET
1	A	35	ASP
1	A	57	LYS
1	A	71	ILE
1	A	112	ARG
1	A	129	GLN
1	A	137	TRP
1	A	140	SER
1	A	141	LYS
1	A	178	LEU
1	A	190	ILE
1	A	201	LEU
1	A	208	THR
1	A	242	GLN
1	A	254	HIS
1	A	260	MET
1	A	263	GLU
1	A	264	GLN
1	A	311	LEU
1	A	313	MET
1	A	318	THR
1	A	319	ARG
1	A	326	GLN
1	A	332	GLN
1	A	361	ARG
1	A	383	GLU
1	A	384	THR
1	A	419	VAL
1	A	439	LEU
1	A	448	GLU
1	A	468	ASN
1	A	479	ARG
1	A	488	ASN

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Mol	Chain	Res	Type
1	A	506	LEU
1	A	512	LYS
1	A	531	LEU
1	A	536	LEU
1	A	547	SER
1	A	552	LEU
1	A	584	ARG
1	A	591	VAL
1	A	594	GLU
1	A	608	ARG
1	A	613	THR
1	A	656	ARG
1	A	670	PHE
1	A	705	LEU
1	A	707	LEU
1	A	717	ASN
1	A	727	THR
1	A	734	GLN
1	A	735	LEU
1	A	752	HIS
1	A	754	ASP
1	A	770	SER
1	A	788	ARG
1	A	800	SER
1	B	16	GLN
1	B	33	MET
1	B	49	GLN
1	B	56	THR
1	B	71	ILE
1	B	84	VAL
1	B	93	CYS
1	B	129	GLN
1	B	137	TRP
1	B	139	ASP
1	B	141	LYS
1	B	154	ARG
1	B	155	PHE
1	B	178	LEU
1	B	194	ARG
1	B	211	GLN
1	B	262	ARG
1	B	264	GLN

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Mol	Chain	Res	Type
1	B	280	THR
1	B	313	MET
1	B	315	VAL
1	B	316	ARG
1	B	335	THR
1	B	338	LEU
1	B	352	LEU
1	B	357	LEU
1	B	384	THR
1	B	395	GLU
1	B	399	GLU
1	B	424	VAL
1	B	432	GLU
1	B	455	ARG
1	B	456	GLU
1	B	457	ARG
1	B	464	LYS
1	B	468	ASN
1	B	478	SER
1	B	492	ARG
1	B	500	ARG
1	B	507	LYS
1	B	511	ASP
1	B	535	LEU
1	B	584	ARG
1	B	585	HIS
1	B	632	LEU
1	B	636	ILE
1	B	669	THR
1	B	692	MET
1	B	737	GLU
1	B	755	THR
1	B	761	SER
1	B	763	GLN
1	B	783	LYS
1	B	787	LYS
1	B	788	ARG
1	B	794	ARG
1	B	800	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	HIS
1	A	49	GLN
1	A	229	ASN
1	A	344	GLN
1	A	752	HIS
1	B	74	HIS
1	B	129	GLN
1	B	264	GLN
1	B	281	GLN
1	B	332	GLN
1	B	468	ASN
1	B	471	HIS
1	B	714	ASN
1	B	717	ASN
1	B	791	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	1.24	2 (8%)	29,45,45	1.52	3 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	A	1801	5	-	3/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1801	ADP	C2-N3	3.95	1.38	1.32
4	A	1801	ADP	C2-N1	2.46	1.38	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1801	ADP	N3-C2-N1	-5.84	119.55	128.68
4	A	1801	ADP	PA-O3A-PB	-3.05	122.35	132.83
4	A	1801	ADP	C3'-C2'-C1'	2.92	105.38	100.98

There are no chirality outliers.

All (3) torsion outliers are listed below:
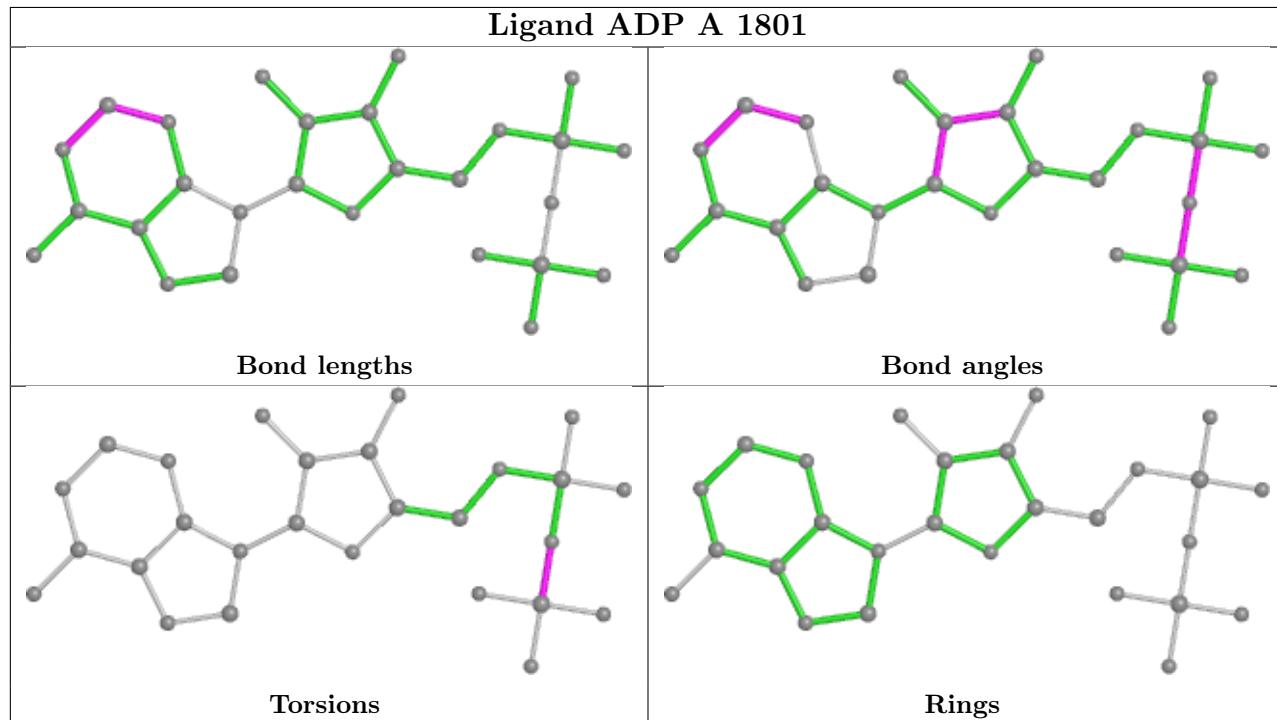
Mol	Chain	Res	Type	Atoms
4	A	1801	ADP	PA-O3A-PB-O2B
4	A	1801	ADP	PA-O3A-PB-O3B
4	A	1801	ADP	PA-O3A-PB-O1B

There are no ring outliers.

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 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 ADP A 1801

Bond lengths

Bond angles

Torsions

Rings

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, 95th 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^2)	Q<0.9
1	A	788/800 (98%)	0.09	25 (3%)	47	51	9, 18, 25, 40	0
1	B	754/800 (94%)	0.05	25 (3%)	46	50	8, 18, 24, 32	0
2	E	18/18 (100%)	0.52	4 (22%)	0	0	10, 17, 34, 35	0
3	F	17/17 (100%)	0.20	2 (11%)	4	4	9, 18, 31, 36	0
All	All	1577/1635 (96%)	0.08	56 (3%)	42	46	8, 18, 25, 40	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	444	THR	7.1
2	E	18	DG	5.5
1	A	443	ALA	4.8
3	F	14	DA	4.8
1	A	2	SER	4.7
1	A	63	GLY	4.5
1	B	52	ASP	4.3
1	B	183	ASP	4.3
1	A	62	ALA	4.3
1	A	754	ASP	4.0
1	A	61	SER	3.7
1	B	456	GLU	3.4
1	B	29	LEU	3.4
1	A	800	SER	3.4
1	B	41	TYR	3.3
1	B	19	ARG	3.2
2	E	1	DA	3.2
1	B	39	LEU	3.1
1	A	593	ASN	3.1
2	E	16	DG	3.0
1	B	135	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
2	E	17	DT	2.9
1	A	591	VAL	2.8
1	B	800	SER	2.8
1	A	475	ILE	2.8
1	A	98	ASP	2.8
1	B	68	MET	2.8
1	B	15	GLN	2.7
1	B	56	THR	2.7
1	B	30	PHE	2.7
1	A	283	LEU	2.7
1	B	74	HIS	2.6
1	A	97	GLY	2.6
1	A	658	GLY	2.6
1	B	38	ALA	2.6
1	A	140	SER	2.6
1	A	768	SER	2.6
1	A	103	LYS	2.5
1	A	64	GLU	2.5
1	B	202	TRP	2.5
1	B	28	LEU	2.4
1	A	448	GLU	2.4
1	B	36	PHE	2.4
1	B	14	MET	2.4
1	B	54	SER	2.3
1	B	284	ALA	2.2
1	A	192	GLY	2.2
1	A	555	LEU	2.2
1	B	475	ILE	2.1
1	B	49	GLN	2.1
1	A	511	ASP	2.1
1	A	595	PRO	2.1
1	B	738	LYS	2.1
3	F	15	DC	2.0
1	A	386	ASP	2.0
1	B	141	LYS	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 ⓘ
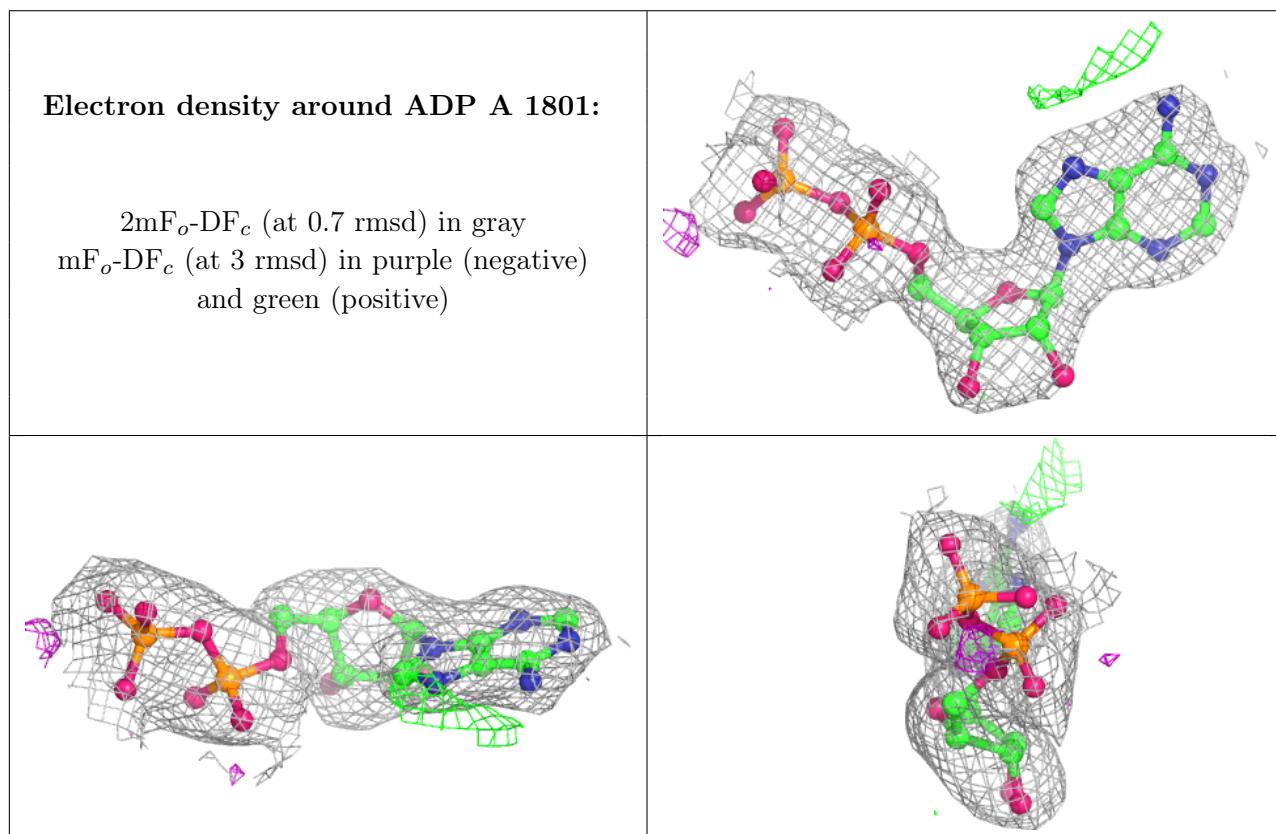
There are no monosaccharides in this entry.

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, 95th 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^2)	Q<0.9
5	MG	A	1802	1/1	0.89	0.07	18,18,18,18	0
4	ADP	A	1801	27/27	0.97	0.10	11,17,19,23	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.

Electron density around ADP A 1801:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

6.5 Other polymers ⓘ

There are no such residues in this entry.