



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:05 AM UTC

PDB ID : 1WBB / pdb_00001wbb
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)

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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

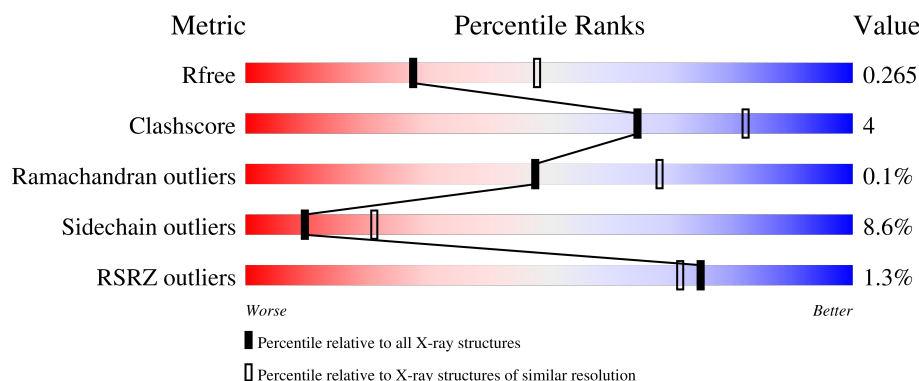
1 Overall quality at a glance

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 $\leq 5\%$. 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	6% 84% 14% ••
1	B	800	79% 13% • 6%
2	E	18	6% 83% 17%
3	F	17	76% 24%

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	C	N	O	S	0	0	0
			6203	3903	1103	1168	29			
1	B	754	Total	C	N	O	S	0	0	0
			5960	3754	1060	1118	28			

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*A P*CP*CP*AP*GP*TP*G)-3'.

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

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

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

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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 (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Mg 1 1	0	0

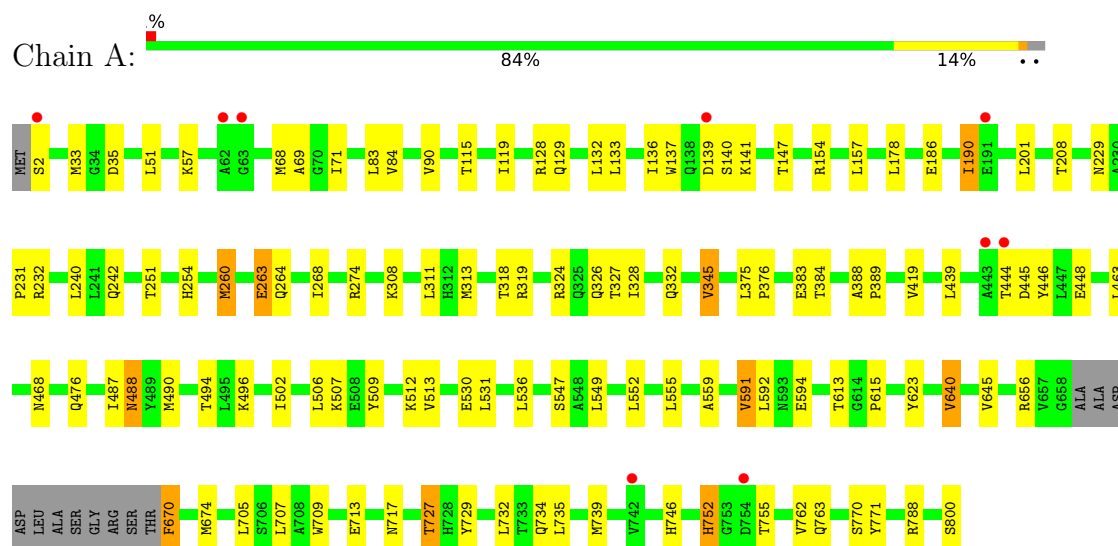
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	138	Total O 138 138	0	0
6	B	136	Total O 136 136	0	0
6	E	4	Total O 4 4	0	0
6	F	7	Total O 7 7	0	0

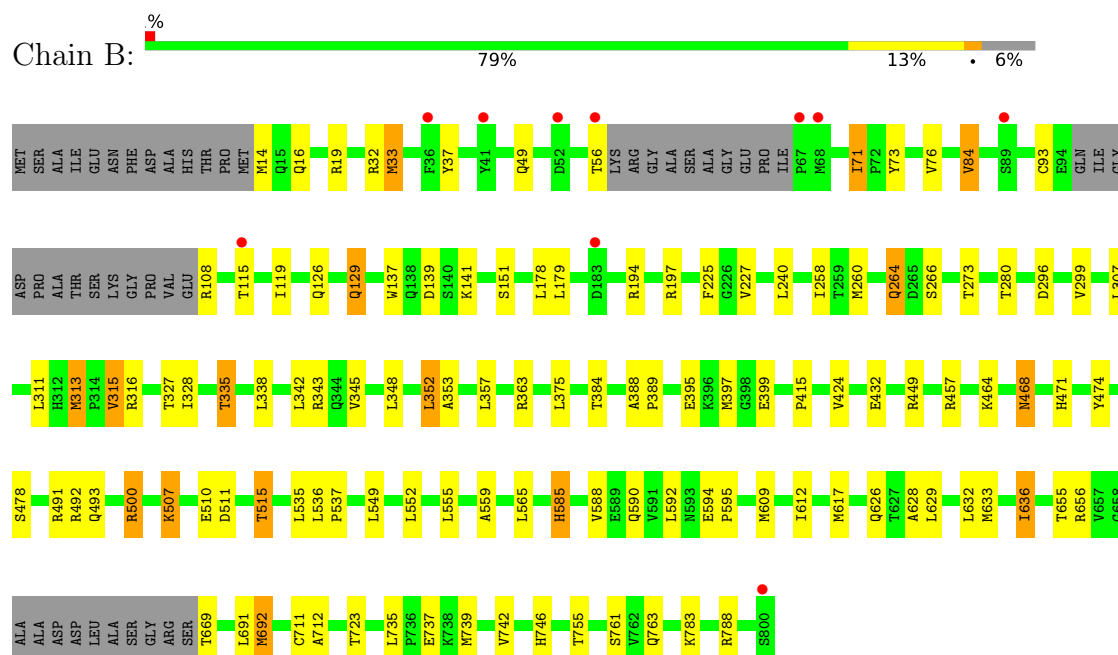
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

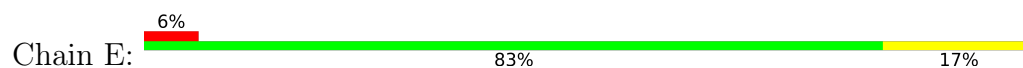
• Molecule 1: DNA MISMATCH REPAIR PROTEIN MUTS



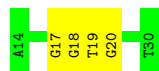
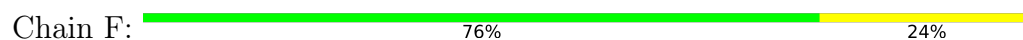
• Molecule 1: DNA MISMATCH REPAIR PROTEIN MUTS



- Molecule 2: 5'-D(*AP*GP*CP*TP*GP*CP*CP*AP*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 20.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.3 (20.00-2.50) 99.0 (20.00-2.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.220 , 0.270 0.222 , 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)	0.33 , 31.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 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	0.64	1/6309 (0.0%)	0.88	3/8539 (0.0%)
1	B	0.65	2/6058 (0.0%)	0.88	2/8194 (0.0%)
2	E	0.39	0/412	1.04	0/634
3	F	0.38	0/388	1.10	0/598
All	All	0.63	3/13167 (0.0%)	0.89	5/17965 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	313	MET	SD-CE	7.00	1.97	1.79
1	B	617	MET	SD-CE	5.26	1.92	1.79
1	A	674	MET	SD-CE	5.12	1.92	1.79

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	229	ASN	N-CA-C	6.02	120.17	112.34
1	B	746	HIS	N-CA-C	5.76	117.29	108.42
1	A	445	ASP	N-CA-C	5.42	116.88	110.97
1	B	415	PRO	O-C-N	5.20	123.59	121.15
1	A	755	THR	N-CA-C	5.20	116.19	108.60

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	6203	0	6250	45	0
1	B	5960	0	6017	52	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	99	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 (99) 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:735:LEU:HD22	1:B:739:MET:HE2	1.51	0.90
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: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:735:LEU:HD22	1:B:739:MET:CE	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:488:ASN:C	1:A:488:ASN:HD22	2.20	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:713:GLU:HG2	1:A:739:MET:HE3	1.93	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: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: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:739:MET:HE3	1:B:742:VAL:HG21	1.96	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:240:LEU:C	1:B:240:LEU:HD23	2.40	0.47
1:B:71:ILE:HG13	1:B:71:ILE:O	2.14	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:B:32:ARG:C	1:B:33:MET:HG2	2.40	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:446:TYR:CD1	1:A:446:TYR:C	2.94	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:B:692:MET:HE3	1:B:692:MET:HB3	1.84	0.45
1:B:585:HIS:CE1	1:B:629:LEU:CD1	3.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:68:MET:HG2	1:A:69:ALA:N	2.31	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:609:MET:HE2	1:B:723:THR:HG21	2.02	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: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
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:490:MET:HE3	1:A:502:ILE:HG23	2.03	0.41
1:B:711:CYS:O	1:B:712:ALA:C	2.64	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%)	36	55
1	B	746/800 (93%)	722 (97%)	24 (3%)	0	100	100
All	All	1530/1600 (96%)	1473 (96%)	55 (4%)	2 (0%)	48	68

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%)	9	21
1	B	630/663 (95%)	576 (91%)	54 (9%)	10	21
All	All	1285/1326 (97%)	1174 (91%)	111 (9%)	10	21

All (111) 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

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Mol	Chain	Res	Type
1	A	90	VAL
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	274	ARG
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	345	VAL
1	A	383	GLU
1	A	384	THR
1	A	419	VAL
1	A	439	LEU
1	A	448	GLU
1	A	487	ILE
1	A	488	ASN
1	A	496	LYS
1	A	506	LEU
1	A	507	LYS
1	A	512	LYS
1	A	531	LEU
1	A	536	LEU
1	A	547	SER
1	A	552	LEU
1	A	591	VAL
1	A	594	GLU
1	A	613	THR
1	A	640	VAL
1	A	656	ARG

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Mol	Chain	Res	Type
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	770	SER
1	A	788	ARG
1	A	800	SER
1	B	16	GLN
1	B	19	ARG
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	108	ARG
1	B	115	THR
1	B	126	GLN
1	B	129	GLN
1	B	137	TRP
1	B	139	ASP
1	B	141	LYS
1	B	178	LEU
1	B	194	ARG
1	B	264	GLN
1	B	266	SER
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

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Mol	Chain	Res	Type
1	B	432	GLU
1	B	449	ARG
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	515	THR
1	B	535	LEU
1	B	585	HIS
1	B	612	ILE
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	788	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	229	ASN
1	A	381	GLN
1	A	391	GLN
1	A	488	ASN
1	A	497	ASN
1	A	526	GLN
1	A	566	ASN
1	A	590	GLN
1	A	683	ASN
1	A	714	ASN
1	A	760	HIS
1	B	78	ASN
1	B	129	GLN
1	B	216	GLN

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Mol	Chain	Res	Type
1	B	264	GLN
1	B	289	ASN
1	B	332	GLN
1	B	373	GLN
1	B	468	ASN
1	B	471	HIS
1	B	483	HIS
1	B	626	GLN
1	B	717	ASN

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 oligosaccharides 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	28,29,29	1.13	3 (10%)	43,45,45	1.74	9 (20%)

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	-	3/16/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1801	ADP	C2-N1	2.56	1.38	1.33
4	A	1801	ADP	C2-N3	2.55	1.38	1.33
4	A	1801	ADP	C8-N7	2.08	1.35	1.31

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1801	ADP	N3-C2-N1	-5.97	119.55	128.58
4	A	1801	ADP	C5-C4-N3	-3.89	121.36	126.72
4	A	1801	ADP	N9-C8-N7	-3.54	108.91	113.94
4	A	1801	ADP	C2-N3-C4	3.26	119.81	111.83
4	A	1801	ADP	C5-N7-C8	2.93	108.05	103.45
4	A	1801	ADP	N3-C4-N9	2.37	131.20	127.17
4	A	1801	ADP	O4'-C1'-N9	2.30	112.51	108.09
4	A	1801	ADP	C3'-C2'-C1'	2.07	105.38	101.46
4	A	1801	ADP	C4-C5-N7	-2.06	108.23	110.58

There are no chirality outliers.

All (3) torsion outliers are listed below:

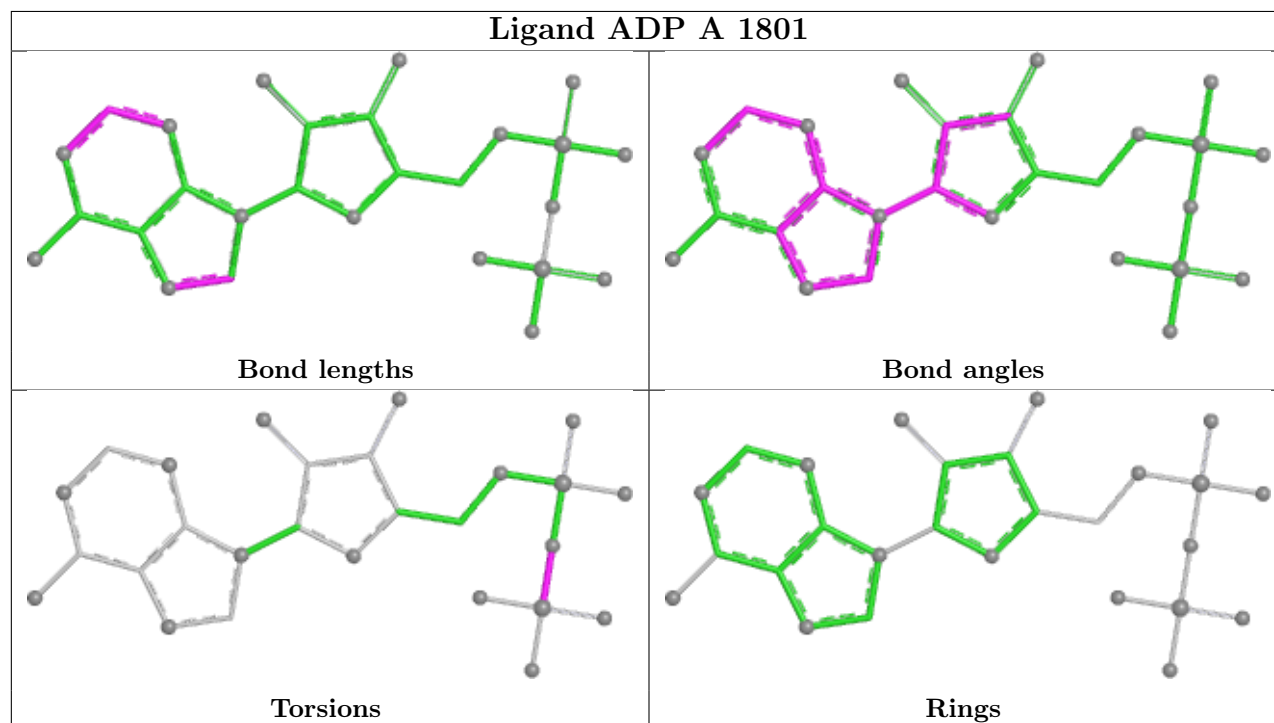
Mol	Chain	Res	Type	Atoms
4	A	1801	ADP	PA-O3A-PB-O2B
4	A	1801	ADP	PA-O3A-PB-O3B
4	A	1801	ADP	PA-O3A-PB-O1B

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 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, 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%)	-0.20	9 (1%) 78 75	9, 18, 25, 40	0
1	B	754/800 (94%)	-0.16	10 (1%) 75 71	8, 18, 24, 32	0
2	E	18/18 (100%)	-0.27	1 (5%) 30 26	10, 17, 34, 35	0
3	F	17/17 (100%)	-0.30	0 100 100	9, 18, 31, 36	0
All	All	1577/1635 (96%)	-0.19	20 (1%) 75 71	8, 18, 25, 40	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	444	THR	4.2
1	A	2	SER	4.2
1	B	183	ASP	3.6
1	A	443	ALA	3.4
1	B	67	PRO	3.1
1	B	41	TYR	3.0
1	A	62	ALA	2.9
1	A	754	ASP	2.8
1	A	742	VAL	2.7
1	B	115	THR	2.7
1	B	800	SER	2.6
1	B	36	PHE	2.4
1	A	191	GLU	2.4
1	B	68	MET	2.4
2	E	18	DG	2.3
1	A	139	ASP	2.3
1	B	56	THR	2.3
1	B	52	ASP	2.2
1	B	89	SER	2.1
1	A	63	GLY	2.1

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](#)

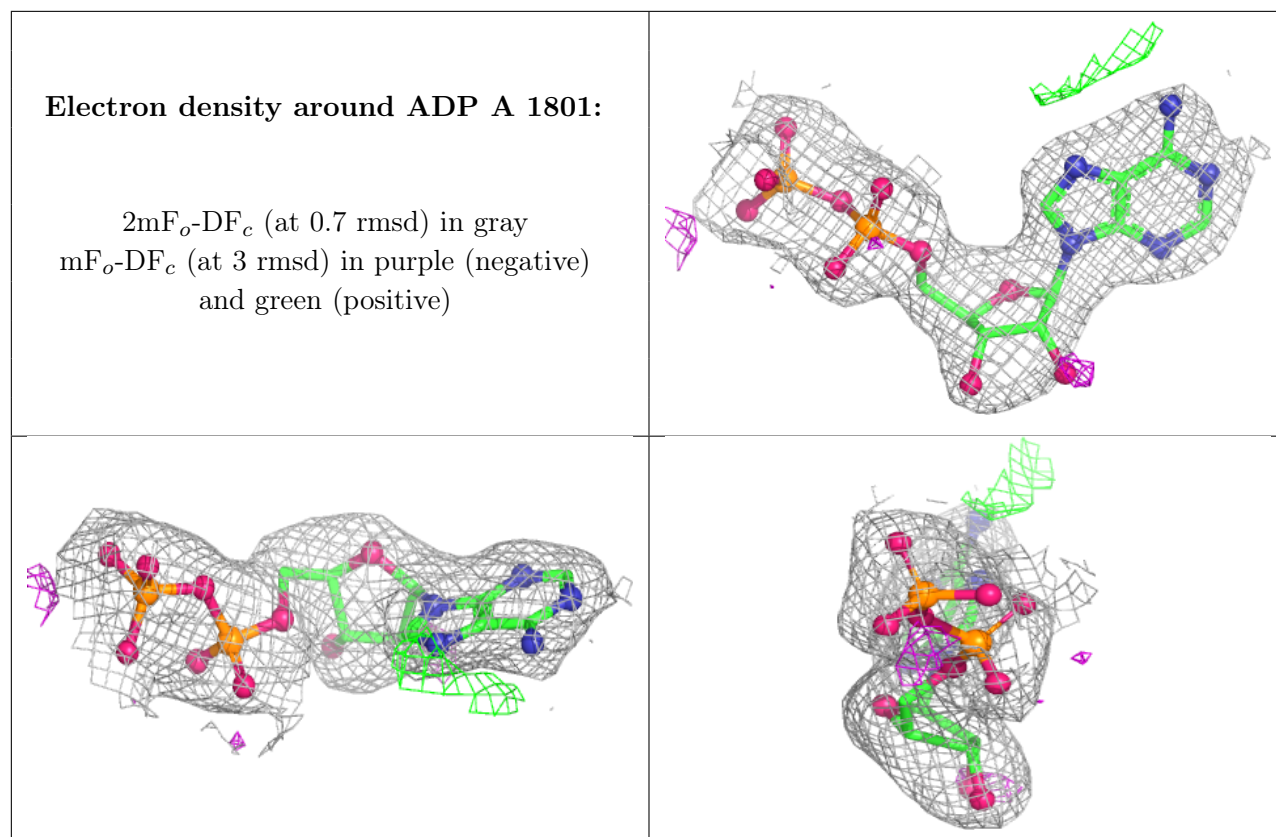
There are no oligosaccharides in this entry.

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, 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($\text{\AA}^2$)	Q<0.9
4	ADP	A	1801	27/27	0.97	0.06	11,17,19,23	0
5	MG	A	1802	1/1	0.97	0.05	18,18,18,18	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.