



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:17 AM UTC

PDB ID : 1WBD / pdb_00001wbd
Title : Crystal structure of E. coli DNA mismatch repair enzyme MutS, E38Q 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 : 2.40 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

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

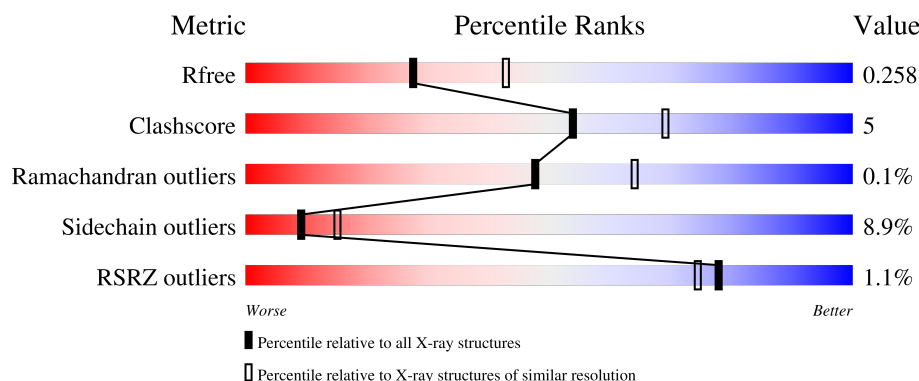
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 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	 81% 16% ..
1	B	800	 % 77% 16% • 6%
2	E	18	 11% 83% 17%
3	F	17	 6% 71% 29%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13160 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	1104	1169	29			
1	B	754	Total	C	N	O	S	0	0	0
			5964	3756	1061	1119	28			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	38	GLN	GLU	engineered mutation	UNP P23909
B	38	GLN	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).



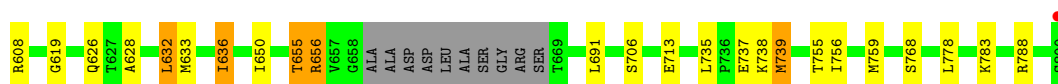
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

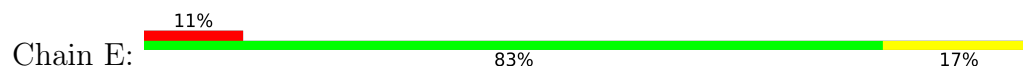
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Mg 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	128	Total O 128 128	0	0
6	B	116	Total O 116 116	0	0
6	E	2	Total O 2 2	0	0
6	F	1	Total O 1 1	0	0



● 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	89.62Å 92.04Å 260.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 20.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.3 (20.00-2.40) 99.2 (20.00-2.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.212 , 0.259 0.215 , 0.258	Depositor DCC
R_{free} test set	1644 reflections (1.94%)	wwPDB-VP
Wilson B-factor (Å ²)	38.9	Xtriage
Anisotropy	0.469	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.015 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13160	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% 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

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	0.87	6/6313 (0.1%)	0.96	5/8544 (0.1%)
1	B	0.83	2/6062 (0.0%)	0.97	4/8199 (0.0%)
2	E	0.52	0/412	1.20	1/634 (0.2%)
3	F	0.50	0/388	1.22	0/598
All	All	0.84	8/13175 (0.1%)	0.99	10/17975 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	624	MET	SD-CE	-7.50	1.60	1.79
1	A	490	MET	SD-CE	6.07	1.94	1.79
1	A	739	MET	SD-CE	5.90	1.94	1.79
1	B	313	MET	SD-CE	5.82	1.94	1.79
1	A	759	MET	SD-CE	5.82	1.94	1.79
1	B	68	MET	SD-CE	5.39	1.93	1.79
1	A	674	MET	SD-CE	5.32	1.92	1.79
1	A	33	MET	SD-CE	5.18	1.92	1.79

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	229	ASN	N-CA-C	7.09	121.56	112.34
1	B	739	MET	N-CA-C	6.87	119.30	108.79
1	A	487	ILE	CA-C-N	5.87	128.95	120.38
1	A	487	ILE	C-N-CA	5.87	128.95	120.38
1	A	206	ILE	N-CA-C	5.34	116.11	110.72
1	B	619	GLY	N-CA-C	5.34	119.13	112.73
1	B	626	GLN	N-CA-C	-5.31	105.66	111.82
2	E	9	DG	O3'-P-O5'	-5.18	96.24	104.00
1	A	755	THR	N-CA-C	5.14	116.66	108.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	587	VAL	N-CA-C	-5.14	106.67	111.45

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	6207	0	6253	69	0
1	B	5964	0	6020	55	0
2	E	367	0	202	2	0
3	F	347	0	194	4	0
4	A	27	0	12	1	0
5	A	1	0	0	0	0
6	A	128	0	0	13	0
6	B	116	0	0	5	0
6	E	2	0	0	0	0
6	F	1	0	0	0	0
All	All	13160	0	12681	126	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 5.

All (126) 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	1.56	0.86
1:B:327:THR:HG21	1:B:555:LEU:HD13	1.66	0.77
1:A:130:ASP:OD1	6:A:2029:HOH:O	2.03	0.77
1:B:273:THR:HG23	1:B:655:THR:HG23	1.68	0.76
1:A:33:MET:HE2	1:A:38:GLN:HG3	1.67	0.74
1:A:149:ASP:OD2	6:A:2029:HOH:O	2.06	0.72
1:A:327:THR:HG21	1:A:555:LEU:HD13	1.73	0.70
1:B:108:ARG:N	6:B:2007:HOH:O	2.23	0.69
1:B:656:ARG:O	1:B:656:ARG:HG3	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:VAL:HG13	1:B:116:PRO:HA	1.77	0.66
1:A:692:MET:HE3	1:A:695:ILE:HD13	1.79	0.64
1:B:633:MET:O	1:B:636:ILE:HG22	1.98	0.63
1:A:727:THR:HG21	1:A:732:LEU:HD12	1.81	0.63
1:B:151:SER:O	1:B:353:ALA:HB2	1.99	0.63
1:A:359:THR:HG21	6:A:2023:HOH:O	2.00	0.62
1:A:186:GLU:HG2	6:A:2030:HOH:O	2.00	0.62
1:B:51:LEU:HD21	1:B:83:LEU:HG	1.81	0.62
1:B:332:GLN:NE2	1:B:333:ASP:OD1	2.33	0.61
1:A:211:GLN:HE22	1:A:212:GLN:NE2	1.96	0.61
1:B:445:ASP:HB3	6:B:2060:HOH:O	2.02	0.60
1:B:342:LEU:HD11	1:B:552:LEU:HD23	1.84	0.59
1:B:37:TYR:HE2	1:B:76:VAL:HG21	1.67	0.59
1:A:50:LEU:HD22	1:A:86:GLN:OE1	2.05	0.57
1:A:433:LEU:HD21	1:A:437:ARG:NH2	2.20	0.57
1:A:51:LEU:HD21	1:A:83:LEU:HD21	1.86	0.57
1:A:211:GLN:NE2	1:A:212:GLN:NE2	2.53	0.57
1:A:693:ASP:OD2	6:A:2092:HOH:O	2.18	0.55
1:A:396:LYS:NZ	6:A:2064:HOH:O	2.40	0.55
1:B:713:GLU:HA	1:B:739:MET:HE1	1.89	0.55
1:A:623:TYR:CE1	1:A:762:VAL:HG21	2.43	0.54
1:B:290:THR:HG22	1:B:293:SER:H	1.72	0.54
1:A:190:ILE:HG23	1:A:196:LEU:HD11	1.90	0.54
1:A:705:LEU:HD12	1:A:705:LEU:O	2.09	0.53
1:A:305:ARG:NH2	1:A:347:ASP:OD2	2.42	0.53
1:A:211:GLN:NE2	1:A:212:GLN:HE21	2.07	0.52
1:B:601:LEU:HD11	1:B:603:LEU:HG	1.92	0.52
1:A:640:VAL:HG11	1:A:645:VAL:HG21	1.92	0.52
1:A:579:ARG:HG2	1:A:602:ASN:HD22	1.73	0.52
1:A:38:GLN:NE2	1:A:68:MET:HE2	2.25	0.51
1:B:17:TYR:CE2	1:B:29:LEU:HD23	2.45	0.51
1:A:137:TRP:HB3	1:A:204:PHE:CE2	2.45	0.51
1:A:623:TYR:CZ	1:A:762:VAL:HG21	2.45	0.51
1:B:37:TYR:CE2	1:B:76:VAL:HG21	2.46	0.51
1:A:263:GLU:HA	1:A:268:ILE:HD11	1.93	0.51
1:A:328:ILE:HG23	1:A:559:ALA:HA	1.93	0.50
1:B:471:HIS:CE1	1:B:493:GLN:HB2	2.46	0.50
1:A:42:ASP:HB2	6:A:2012:HOH:O	2.10	0.50
1:A:437:ARG:O	1:A:441:ASP:HB2	2.12	0.50
1:A:686:GLU:HG2	1:A:720:LYS:HB2	1.93	0.50
1:B:515:THR:HB	1:B:519:LYS:NZ	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:628:ALA:HB2	1:B:691:LEU:HD11	1.94	0.50
1:A:670:PHE:N	1:A:670:PHE:CD2	2.80	0.49
1:A:13:MET:HE3	1:A:33:MET:SD	2.53	0.49
1:B:321:LEU:O	1:B:325:GLN:HG3	2.13	0.49
1:B:632:LEU:C	1:B:632:LEU:HD12	2.38	0.49
1:B:468:ASN:HD22	2:E:5:DG:H5"	1.78	0.49
1:A:315:VAL:HG12	1:A:317:ASP:H	1.78	0.48
1:B:387:SER:OG	1:B:389:PRO:HD2	2.13	0.48
1:A:750:LEU:HD12	1:A:759:MET:SD	2.53	0.48
1:A:326:GLN:HB3	6:A:2063:HOH:O	2.13	0.48
1:A:5:GLU:HB3	1:A:10:HIS:HE1	1.79	0.48
1:A:17:TYR:CD2	1:A:17:TYR:C	2.92	0.48
1:B:277:LEU:HD21	1:B:655:THR:HG21	1.95	0.48
1:B:388:ALA:N	1:B:389:PRO:CD	2.76	0.47
1:B:157:LEU:C	1:B:157:LEU:HD23	2.39	0.47
1:B:515:THR:HB	1:B:519:LYS:HZ1	1.79	0.47
1:A:463:LEU:HA	1:A:476:GLN:O	2.15	0.47
1:B:474:TYR:CE1	1:B:500:ARG:HD2	2.49	0.47
1:A:213:LEU:HD23	1:A:241:LEU:HD22	1.97	0.47
1:A:693:ASP:CG	6:A:2092:HOH:O	2.59	0.46
1:A:588:VAL:HG13	1:A:592:LEU:HD13	1.97	0.46
1:A:620:LYS:NZ	4:A:1801:ADP:O3B	2.35	0.46
1:A:262:ARG:NH1	6:A:2053:HOH:O	2.47	0.46
1:A:789:ALA:O	1:B:706:SER:HB3	2.16	0.46
1:B:463:LEU:HD23	1:B:464:LYS:N	2.30	0.46
1:B:73:TYR:O	1:B:76:VAL:HG23	2.16	0.46
1:A:359:THR:HG22	1:A:359:THR:O	2.16	0.45
1:A:628:ALA:HB2	1:A:691:LEU:HD11	1.97	0.45
1:B:108:ARG:CA	6:B:2007:HOH:O	2.62	0.45
1:A:136:ILE:HD13	1:A:190:ILE:HD11	1.99	0.45
1:B:375:LEU:HD22	1:B:397:MET:HG2	1.99	0.45
1:B:40:PHE:CE1	1:B:68:MET:HG2	2.52	0.45
1:B:216:GLN:NE2	1:B:252:LEU:O	2.50	0.44
1:B:594:GLU:HG3	1:B:595:PRO:HD2	2.00	0.44
2:E:2:DG:O6	3:F:28:DG:O6	2.35	0.44
1:B:267:ILE:HD12	1:B:314:PRO:HB2	2.00	0.44
1:B:396:LYS:HG2	1:B:548:ALA:HB2	1.99	0.44
3:F:20:DG:H4'	3:F:21:DC:OP1	2.18	0.44
1:A:33:MET:HE2	1:A:38:GLN:CG	2.44	0.43
1:B:328:ILE:HG23	1:B:559:ALA:HA	2.00	0.43
1:A:211:GLN:CD	1:A:212:GLN:HE21	2.25	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:VAL:HB	1:B:343:ARG:HB2	2.00	0.43
3:F:19:DT:C2'	3:F:20:DG:O5'	2.66	0.43
1:A:494:THR:OG1	1:A:499:GLU:OE2	2.20	0.43
1:A:727:THR:HG23	6:A:2103:HOH:O	2.19	0.43
1:A:771:TYR:HA	6:A:2123:HOH:O	2.17	0.43
1:A:38:GLN:CD	1:A:68:MET:HE2	2.44	0.43
1:B:594:GLU:O	1:B:595:PRO:C	2.62	0.43
1:A:72:PRO:HG3	3:F:23:DT:O2	2.18	0.43
1:A:305:ARG:HH22	1:A:347:ASP:CG	2.26	0.43
1:B:240:LEU:C	1:B:240:LEU:HD23	2.43	0.43
1:B:311:LEU:HD23	1:B:636:ILE:HD12	2.00	0.43
1:A:375:LEU:N	1:A:376:PRO:CD	2.82	0.42
1:B:316:ARG:HD3	1:B:650:ILE:O	2.20	0.42
1:A:23:GLN:C	1:A:24:HIS:CD2	2.98	0.42
1:A:352:LEU:HD23	1:A:352:LEU:HA	1.91	0.42
1:A:51:LEU:HD21	1:A:83:LEU:CD2	2.49	0.42
1:B:52:ASP:O	1:B:53:ILE:HG23	2.20	0.42
1:B:154:ARG:HD3	6:B:2019:HOH:O	2.20	0.42
1:B:759:MET:HA	1:B:759:MET:HE3	2.02	0.42
1:A:487:ILE:HD12	1:A:487:ILE:HA	1.91	0.42
1:B:536:LEU:N	1:B:537:PRO:CD	2.82	0.42
1:A:470:VAL:HG12	1:A:471:HIS:CD2	2.55	0.41
1:B:393:LEU:HD13	1:B:552:LEU:HD12	2.02	0.41
1:A:345:VAL:HG11	1:A:549:LEU:HD13	2.02	0.41
1:B:39:LEU:HD23	1:B:43:ASP:HB3	2.01	0.41
1:B:157:LEU:O	1:B:260:MET:HA	2.20	0.41
1:B:387:SER:HB3	1:B:390:VAL:HB	2.02	0.41
1:A:702:TYR:HD1	1:A:705:LEU:HD23	1.85	0.41
1:A:148:LEU:CB	1:A:240:LEU:HD21	2.50	0.41
1:A:196:LEU:C	1:A:197:ARG:HG2	2.45	0.41
1:A:579:ARG:HG2	1:A:602:ASN:ND2	2.35	0.41
1:B:315:VAL:HB	6:B:2034:HOH:O	2.20	0.40
1:A:446:TYR:OH	1:A:505:GLU:HG2	2.22	0.40
1:A:270:ASP:OD1	1:A:273:THR:OG1	2.32	0.40
1:A:359:THR:HG22	6:A:2024:HOH:O	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%)	756 (96%)	28 (4%)	0	100	100
1	B	746/800 (93%)	726 (97%)	19 (2%)	1 (0%)	48	64
All	All	1530/1600 (96%)	1482 (97%)	47 (3%)	1 (0%)	48	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	141	LYS

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%)	602 (92%)	54 (8%)	10	18
1	B	631/664 (95%)	570 (90%)	61 (10%)	8	12
All	All	1287/1328 (97%)	1172 (91%)	115 (9%)	9	15

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	46	ARG
1	A	57	LYS
1	A	84	VAL
1	A	102	SER

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Mol	Chain	Res	Type
1	A	137	TRP
1	A	139	ASP
1	A	150	ILE
1	A	157	LEU
1	A	164	GLU
1	A	178	LEU
1	A	190	ILE
1	A	232	ARG
1	A	264	GLN
1	A	274	ARG
1	A	311	LEU
1	A	326	GLN
1	A	332	GLN
1	A	384	THR
1	A	397	MET
1	A	402	GLU
1	A	419	VAL
1	A	439	LEU
1	A	444	THR
1	A	448	GLU
1	A	479	ARG
1	A	487	ILE
1	A	488	ASN
1	A	506	LEU
1	A	507	LYS
1	A	512	LYS
1	A	526	GLN
1	A	531	LEU
1	A	536	LEU
1	A	547	SER
1	A	552	LEU
1	A	568	THR
1	A	571	THR
1	A	575	LYS
1	A	591	VAL
1	A	640	VAL
1	A	656	ARG
1	A	670	PHE
1	A	672	VAL
1	A	705	LEU
1	A	707	LEU
1	A	727	THR

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Mol	Chain	Res	Type
1	A	728	HIS
1	A	734	GLN
1	A	735	LEU
1	A	736	PRO
1	A	755	THR
1	A	756	ILE
1	A	770	SER
1	B	14	MET
1	B	33	MET
1	B	38	GLN
1	B	46	ARG
1	B	53	ILE
1	B	78	ASN
1	B	94	GLU
1	B	108	ARG
1	B	111	VAL
1	B	115	THR
1	B	119	ILE
1	B	122	GLU
1	B	137	TRP
1	B	139	ASP
1	B	140	SER
1	B	156	ARG
1	B	157	LEU
1	B	163	ARG
1	B	178	LEU
1	B	186	GLU
1	B	188	SER
1	B	201	LEU
1	B	206	ILE
1	B	250	THR
1	B	289	ASN
1	B	290	THR
1	B	335	THR
1	B	338	LEU
1	B	352	LEU
1	B	357	LEU
1	B	404	ARG
1	B	408	GLU
1	B	421	ASP
1	B	424	VAL
1	B	464	LYS

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Mol	Chain	Res	Type
1	B	490	MET
1	B	491	ARG
1	B	492	ARG
1	B	496	LYS
1	B	500	ARG
1	B	507	LYS
1	B	511	ASP
1	B	514	LEU
1	B	535	LEU
1	B	552	LEU
1	B	573	ILE
1	B	575	LYS
1	B	591	VAL
1	B	608	ARG
1	B	632	LEU
1	B	636	ILE
1	B	655	THR
1	B	656	ARG
1	B	737	GLU
1	B	738	LYS
1	B	755	THR
1	B	756	ILE
1	B	768	SER
1	B	778	LEU
1	B	783	LYS
1	B	788	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	ASN
1	A	85	ASN
1	A	126	GLN
1	A	211	GLN
1	A	212	GLN
1	A	264	GLN
1	A	430	ASN
1	A	481	GLN
1	A	538	HIS
1	A	566	ASN
1	A	602	ASN
1	A	616	ASN

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Mol	Chain	Res	Type
1	A	682	HIS
1	A	717	ASN
1	A	791	GLN
1	B	38	GLN
1	B	126	GLN
1	B	211	GLN
1	B	242	GLN
1	B	289	ASN
1	B	370	HIS
1	B	374	GLN
1	B	468	ASN
1	B	471	HIS
1	B	717	ASN
1	B	734	GLN
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 oligosaccharides 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	28,29,29	1.28	3 (10%)	43,45,45	1.75	8 (18%)

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	-	4/16/32/32	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-N3	3.04	1.39	1.33
4	A	1801	ADP	C2-N1	2.66	1.38	1.33
4	A	1801	ADP	C5-N7	-2.57	1.34	1.39

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1801	ADP	N3-C2-N1	-5.09	120.88	128.58
4	A	1801	ADP	C5-C4-N3	-3.99	121.22	126.72
4	A	1801	ADP	N9-C8-N7	-3.56	108.88	113.94
4	A	1801	ADP	C5-N7-C8	3.36	108.73	103.45
4	A	1801	ADP	O4'-C1'-N9	3.14	114.13	108.09
4	A	1801	ADP	C2-N3-C4	3.02	119.21	111.83
4	A	1801	ADP	N3-C4-N9	2.89	132.09	127.17
4	A	1801	ADP	O2B-PB-O3A	2.10	111.67	104.64

There are no chirality outliers.

All (4) torsion outliers are listed below:

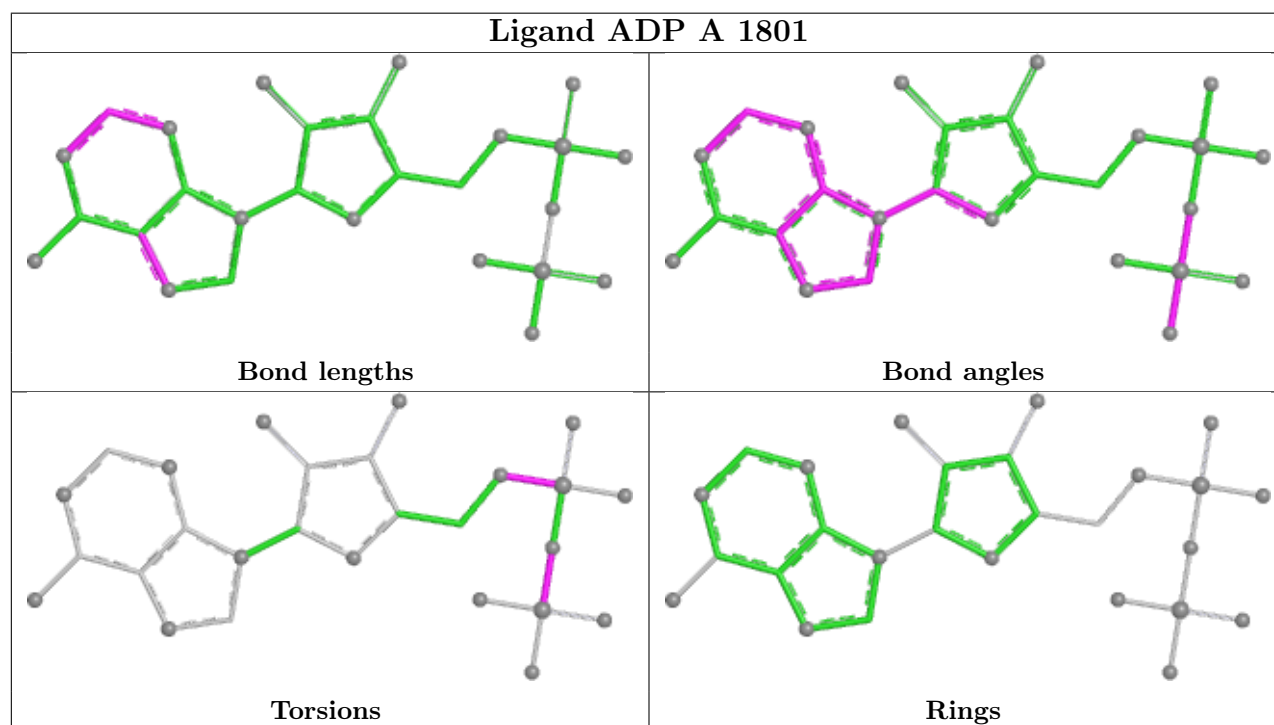
Mol	Chain	Res	Type	Atoms
4	A	1801	ADP	PA-O3A-PB-O2B
4	A	1801	ADP	PA-O3A-PB-O3B
4	A	1801	ADP	C5'-O5'-PA-O1A
4	A	1801	ADP	PA-O3A-PB-O1B

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1801	ADP	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 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%)	-0.35	4 (0%) 87 85	2, 16, 25, 38	0
1	B	754/800 (94%)	-0.21	11 (1%) 72 68	8, 16, 24, 34	0
2	E	18/18 (100%)	0.03	2 (11%) 10 7	9, 17, 96, 109	0
3	F	17/17 (100%)	-0.38	1 (5%) 28 24	8, 15, 59, 95	0
All	All	1577/1635 (96%)	-0.28	18 (1%) 78 74	2, 16, 25, 109	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	18	DG	3.9
1	A	444	THR	3.6
1	B	800	SER	3.6
1	B	115	THR	3.3
1	B	89	SER	3.2
3	F	14	DA	3.1
1	B	68	MET	2.9
1	B	54	SER	2.8
1	A	742	VAL	2.7
1	B	14	MET	2.6
1	A	754	ASP	2.3
1	B	52	ASP	2.3
1	B	41	TYR	2.3
2	E	17	DT	2.3
1	B	56	THR	2.3
1	A	62	ALA	2.2
1	B	74	HIS	2.1
1	B	67	PRO	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

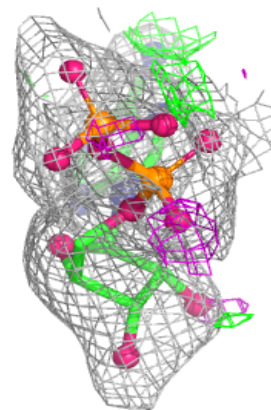
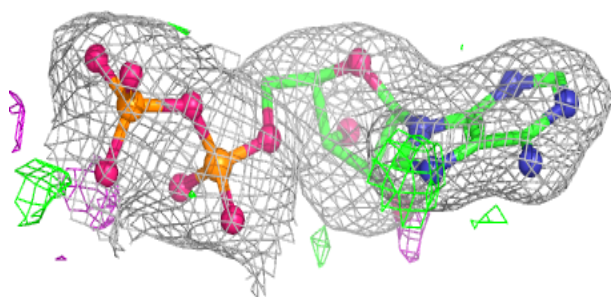
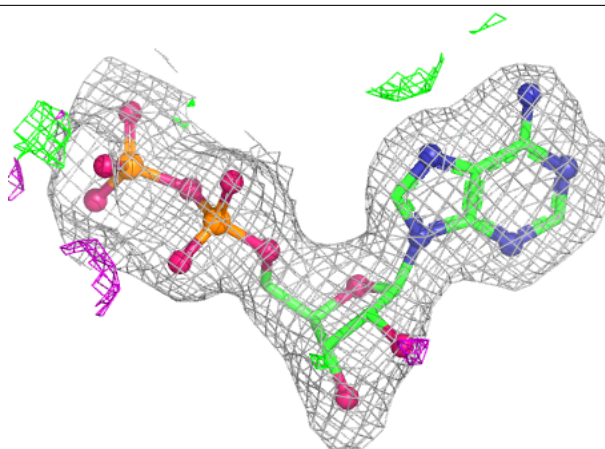
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
5	MG	A	1802	1/1	0.91	0.07	18,18,18,18	0
4	ADP	A	1801	27/27	0.97	0.06	5,13,16,20	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:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.