



Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2020 – 10:17 pm BST

PDB ID : 2O8C
Title : human MutSalpha (MSH2/MSH6) bound to ADP and an O6-methyl-guanine
T mispair
Authors : Warren, J.J.; Pohlhaus, T.J.; Changela, A.; Modrich, P.L.; Beese, L.S.
Deposited on : 2006-12-12
Resolution : 3.37 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

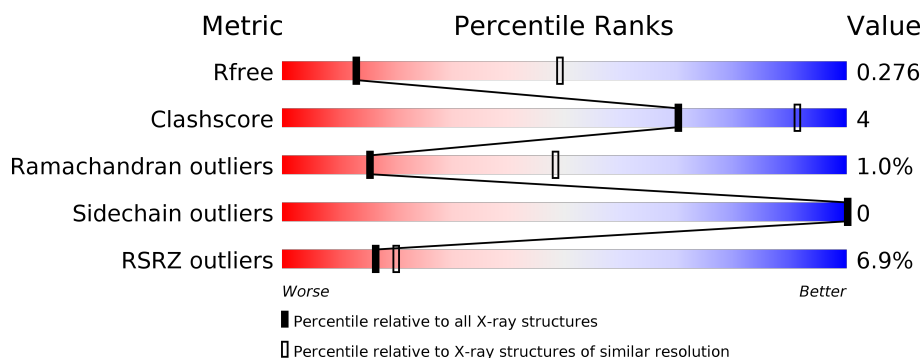
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.37 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1691 (3.46-3.30)
Clashscore	141614	1762 (3.46-3.30)
Ramachandran outliers	138981	1732 (3.46-3.30)
Sidechain outliers	138945	1731 (3.46-3.30)
RSRZ outliers	127900	1635 (3.46-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	E	15	<div> <div>7%</div> <div> <div></div> <div>73%</div> <div>27%</div> </div> </div>
2	F	15	<div> <div></div> <div> <div>93%</div> <div>7%</div> </div> </div>
3	A	934	<div> <div>8%</div> <div> <div></div> <div>81%</div> <div>8%</div> <div>11%</div> </div> </div>
4	B	1022	<div> <div>5%</div> <div> <div></div> <div>81%</div> <div>10%</div> <div>9%</div> </div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14571 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 DNA chain called 5'-D(*GP*AP*AP*CP*CP*GP*CP*(6OG)P*CP*GP*CP*TP*AP*GP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	15	Total	C	N	O	P	0	0	0
			308	146	62	86	14			

- Molecule 2 is a DNA chain called 5'-D(*CP*CP*TP*AP*GP*CP*GP*TP*GP*CP*GP*GP*TP*TP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	15	Total	C	N	O	P	0	0	0
			303	145	53	91	14			

- Molecule 3 is a protein called DNA mismatch repair protein Msh2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	830	Total	C	N	O	S	0	0	0
			6439	4085	1092	1228	34			

- Molecule 4 is a protein called DNA mismatch repair protein MSH6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	932	Total	C	N	O	S	0	0	0
			7443	4721	1277	1394	51			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	339	MET	-	INITIATING METHIONINE	UNP P52701
B	340	GLY	-	CLONING ARTIFACT	UNP P52701

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

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

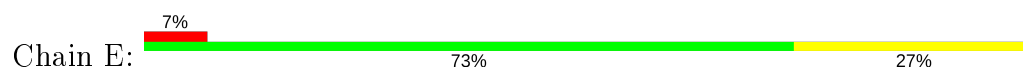
- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

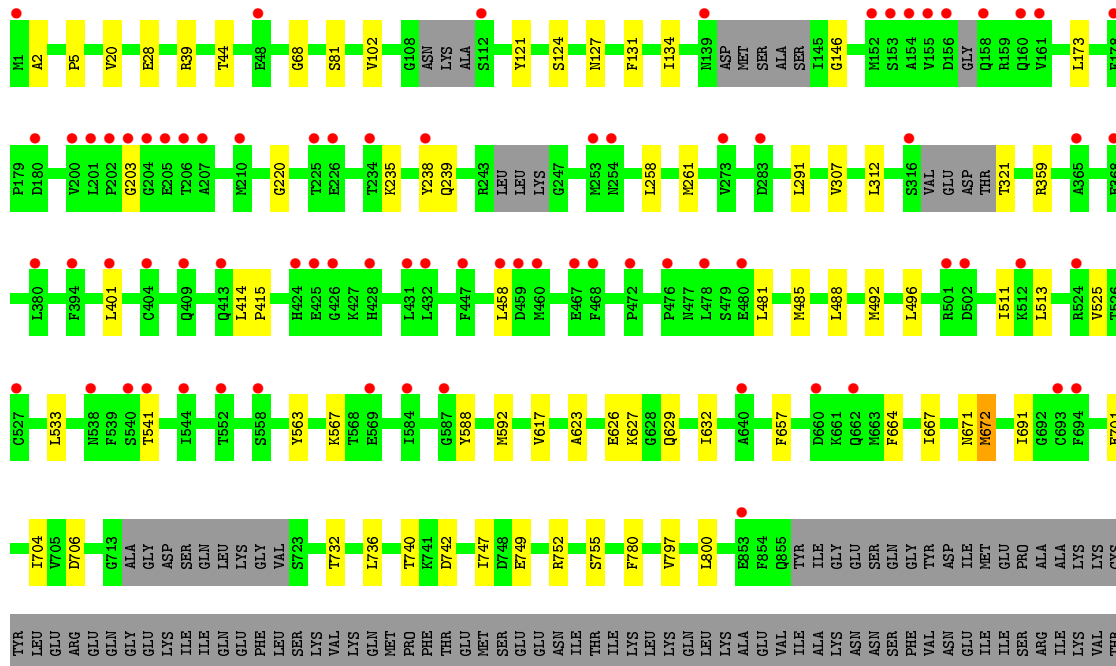
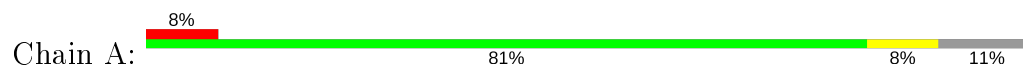
- Molecule 1: 5'-D(*GP*AP*AP*CP*CP*GP*CP*(6OG)P*CP*GP*CP*TP*AP*GP*G)-3',



- Molecule 2: 5'-D(*CP*CP*TP*AP*GP*CP*GP*TP*GP*CP*GP*GP*TP*TP*C)-3'

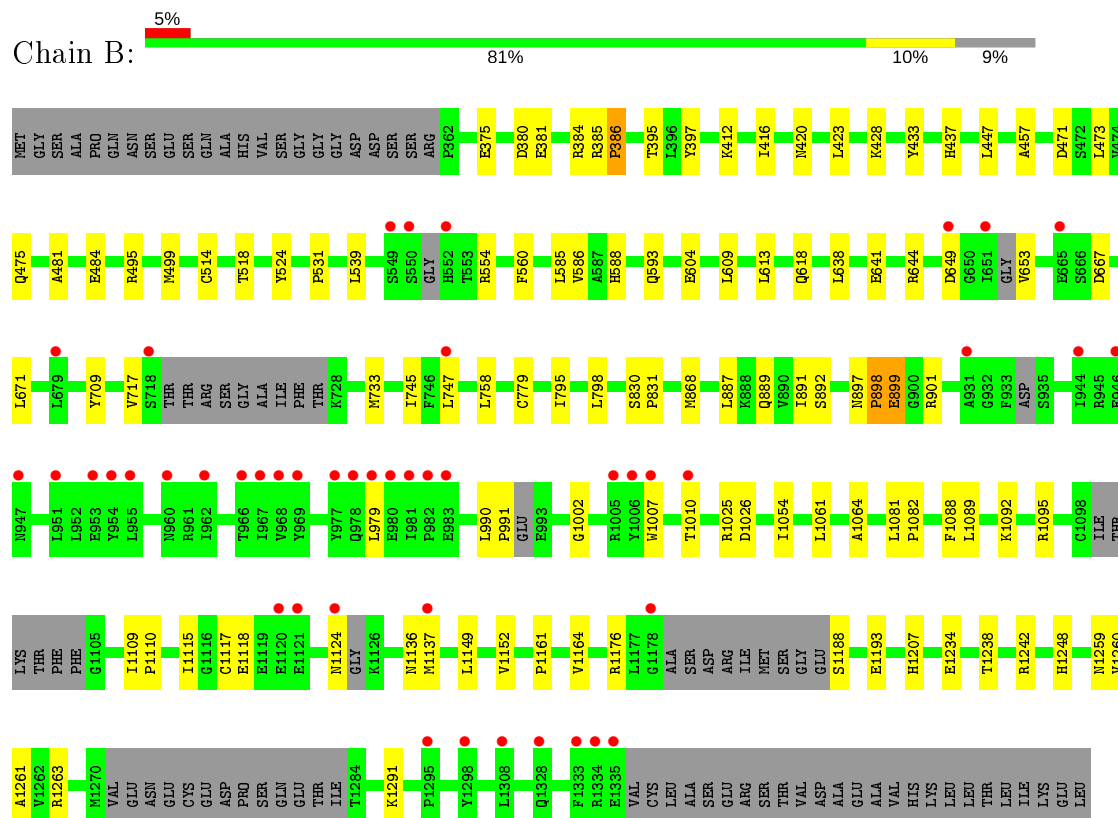


- Molecule 3: DNA mismatch repair protein Msh2



THR

• Molecule 4: DNA mismatch repair protein MSH6



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 3 2	Depositor
Cell constants a, b, c, α , β , γ	259.81Å 259.81Å 259.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.37 48.25 – 3.37	Depositor EDS
% Data completeness (in resolution range)	99.1 (20.00-3.37) 99.1 (48.25-3.37)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	0.20	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 3.40Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.256 , 0.290 0.245 , 0.276	Depositor DCC
R_{free} test set	2133 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	92.3	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 145.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	14571	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% 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: MG, 6OG, 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	E	0.55	0/319	1.18	4/488 (0.8%)
2	F	0.59	0/338	1.23	1/520 (0.2%)
3	A	0.31	0/6539	0.54	0/8828
4	B	0.33	0/7587	0.57	0/10226
All	All	0.33	0/14783	0.61	5/20062 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	4	DC	O4'-C4'-C3'	-8.04	101.18	106.00
2	F	21	DC	P-O3'-C3'	6.36	127.33	119.70
1	E	4	DC	P-O3'-C3'	5.61	126.44	119.70
1	E	14	DG	O4'-C1'-N9	5.58	111.91	108.00
1	E	4	DC	O4'-C1'-N1	5.57	111.90	108.00

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	E	308	0	170	1	0
2	F	303	0	171	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	6439	0	6410	37	0
4	B	7443	0	7415	68	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	27	0	12	0	0
6	B	27	0	12	0	0
7	A	1	0	0	0	0
7	B	20	0	0	0	0
7	F	1	0	0	0	0
All	All	14571	0	14190	104	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 (104) 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)
4:B:385:ARG:HD2	4:B:386:PRO:HD2	1.66	0.76
4:B:380:ASP:HB2	4:B:384:ARG:H	1.60	0.66
3:A:359:ARG:NH2	3:A:691:ILE:O	2.28	0.65
3:A:5:PRO:HB3	3:A:81:SER:HB3	1.77	0.65
4:B:897:ASN:HB3	4:B:901:ARG:HE	1.62	0.64
4:B:1176:ARG:HE	4:B:1193:GLU:HG3	1.63	0.62
3:A:671:ASN:O	3:A:672:MET:HB2	2.00	0.62
4:B:420:ASN:HB3	4:B:423:LEU:HD12	1.83	0.61
3:A:20:VAL:HG21	3:A:68:GLY:HA2	1.83	0.60
4:B:1007:TRP:HE1	4:B:1010:THR:HB	1.66	0.59
4:B:554:ARG:HH12	4:B:604:GLU:HB2	1.66	0.58
3:A:321:THR:HG23	3:A:321:THR:O	2.03	0.58
3:A:588:TYR:O	3:A:592:MET:HG2	2.02	0.58
4:B:892:SER:O	4:B:901:ARG:HB3	2.03	0.58
4:B:795:ILE:HG23	4:B:1064:ALA:HA	1.85	0.57
4:B:887:LEU:O	4:B:891:ILE:HG12	2.05	0.57
4:B:638:LEU:HD11	4:B:671:LEU:HD12	1.85	0.57
4:B:899:GLU:O	4:B:901:ARG:NH1	2.37	0.57
4:B:423:LEU:HD13	4:B:481:ALA:HB2	1.87	0.56
4:B:380:ASP:O	4:B:397:TYR:HB2	2.05	0.56
4:B:868:MET:HG2	4:B:1054:ILE:HD12	1.87	0.56
4:B:433:TYR:OH	4:B:484:GLU:OE1	2.14	0.56
4:B:1259:ASN:O	4:B:1261:ALA:N	2.35	0.55
4:B:554:ARG:HH22	4:B:604:GLU:HG3	1.72	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1007:TRP:NE1	4:B:1010:THR:HB	2.23	0.54
4:B:471:ASP:O	4:B:475:GLN:HG2	2.07	0.54
4:B:586:VAL:HG11	4:B:613:LEU:HD11	1.90	0.53
4:B:897:ASN:HB3	4:B:901:ARG:NE	2.24	0.52
4:B:1095:ARG:HH21	4:B:1161:PRO:HB3	1.75	0.52
4:B:1263:ARG:HH21	4:B:1291:LYS:HD2	1.75	0.52
4:B:381:GLU:HB2	4:B:395:THR:HB	1.90	0.52
3:A:672:MET:SD	4:B:1188:SER:HB2	2.50	0.51
4:B:889:GLN:HG2	4:B:901:ARG:NH1	2.25	0.51
3:A:488:LEU:O	3:A:492:MET:HG2	2.10	0.51
3:A:664:PHE:HB3	3:A:797:VAL:HA	1.92	0.51
3:A:235:LYS:HB3	3:A:238:TYR:HB2	1.93	0.51
4:B:798:LEU:HD13	4:B:1061:LEU:HD23	1.92	0.50
3:A:755:SER:HA	4:B:1248:HIS:HB3	1.93	0.50
3:A:749:GLU:HG2	3:A:752:ARG:HD2	1.94	0.50
4:B:641:GLU:HB3	4:B:644:ARG:HG3	1.94	0.50
4:B:758:LEU:HD22	4:B:1149:LEU:HD22	1.94	0.50
3:A:732:THR:O	3:A:736:LEU:HB2	2.12	0.49
3:A:496:LEU:HD21	3:A:513:LEU:HB2	1.94	0.49
4:B:412:LYS:HE3	4:B:416:ILE:HD11	1.93	0.49
3:A:307:VAL:HG13	3:A:312:LEU:HB2	1.94	0.49
4:B:524:TYR:CE1	4:B:531:PRO:HA	2.48	0.48
3:A:258:LEU:HB2	3:A:261:MET:HG2	1.96	0.48
3:A:39:ARG:HE	3:A:44:THR:HG21	1.79	0.48
3:A:667:ILE:HG12	3:A:800:LEU:HB2	1.96	0.48
3:A:124:SER:HB2	3:A:127:ASN:HB3	1.96	0.47
4:B:889:GLN:HG2	4:B:901:ARG:HH11	1.79	0.47
4:B:447:LEU:HD21	4:B:473:LEU:HG	1.97	0.46
3:A:632:ILE:HB	3:A:657:PHE:HB2	1.97	0.46
4:B:495:ARG:O	4:B:499:MET:HG2	2.16	0.46
3:A:492:MET:HB3	3:A:513:LEU:HD11	1.98	0.46
3:A:401:LEU:HD11	3:A:458:LEU:HD11	1.98	0.46
4:B:1234:GLU:HG3	4:B:1238:THR:HB	1.97	0.45
3:A:235:LYS:HB2	3:A:239:GLN:HG3	1.98	0.45
3:A:623:ALA:HB3	3:A:701:GLU:HA	1.98	0.45
3:A:626:GLU:HB2	3:A:629:GLN:HB2	1.99	0.44
4:B:889:GLN:HA	4:B:901:ARG:HD3	1.99	0.44
4:B:1092:LYS:HB2	4:B:1164:VAL:HB	2.00	0.44
4:B:1089:LEU:HD23	4:B:1115:ILE:HD12	1.99	0.44
4:B:609:LEU:HB3	4:B:618:GLN:HE21	1.81	0.44
3:A:740:THR:HG23	3:A:742:ASP:H	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:990:LEU:HA	4:B:991:PRO:HD3	1.78	0.44
4:B:1207:HIS:O	4:B:1242:ARG:NH2	2.51	0.43
4:B:518:THR:HG21	4:B:593:GLN:NE2	2.33	0.43
4:B:585:LEU:HD12	4:B:709:TYR:CE2	2.53	0.43
4:B:385:ARG:CD	4:B:386:PRO:HD2	2.44	0.43
4:B:830:SER:HA	4:B:831:PRO:HD3	1.80	0.43
3:A:627:LYS:HA	3:A:704:ILE:HB	2.01	0.43
4:B:1025:ARG:HG3	4:B:1026:ASP:N	2.33	0.43
4:B:428:LYS:HE3	4:B:433:TYR:CZ	2.53	0.43
4:B:437:HIS:HA	4:B:457:ALA:HB3	2.01	0.43
3:A:533:LEU:HD21	3:A:541:THR:HB	2.00	0.43
3:A:563:TYR:HE2	3:A:567:LYS:HE3	1.83	0.42
4:B:588:HIS:CE1	4:B:779:CYS:HB3	2.54	0.42
3:A:414:LEU:N	3:A:415:PRO:HD2	2.35	0.42
4:B:1081:LEU:HA	4:B:1082:PRO:HD3	1.90	0.42
3:A:511:ILE:HG12	3:A:525:VAL:HG22	2.01	0.42
4:B:1136:ASN:O	4:B:1137:MET:HB3	2.19	0.42
4:B:644:ARG:HG2	4:B:653:VAL:HG11	2.01	0.42
3:A:747:ILE:HB	3:A:780:PHE:HD1	1.84	0.42
4:B:1088:PHE:HB2	4:B:1117:CYS:H	1.84	0.42
3:A:131:PHE:HD1	3:A:134:ILE:HD12	1.84	0.42
3:A:173:LEU:HB2	3:A:291:LEU:HD23	2.01	0.42
4:B:898:PRO:O	4:B:899:GLU:HB2	2.18	0.42
4:B:1118:GLU:HG2	4:B:1124:ASN:HB2	2.02	0.41
4:B:889:GLN:O	4:B:901:ARG:HA	2.20	0.41
3:A:102:VAL:HB	3:A:121:TYR:HB2	2.01	0.41
4:B:412:LYS:O	4:B:416:ILE:HG12	2.20	0.41
4:B:484:GLU:HB2	4:B:514:CYS:SG	2.60	0.41
4:B:649:ASP:HB3	4:B:653:VAL:HA	2.01	0.41
4:B:868:MET:CG	4:B:1054:ILE:HD12	2.49	0.41
4:B:733:MET:HE1	4:B:1152:VAL:HG22	2.01	0.41
4:B:897:ASN:O	4:B:901:ARG:HG3	2.20	0.41
1:E:5:DC:H2"	1:E:6:DG:C8	2.55	0.41
3:A:481:LEU:O	3:A:485:MET:HG2	2.21	0.40
3:A:706:ASP:HB2	3:A:742:ASP:HB2	2.03	0.40
4:B:539:LEU:O	4:B:560:PHE:HA	2.21	0.40
4:B:979:LEU:HD11	4:B:1007:TRP:HZ3	1.86	0.40
4:B:1176:ARG:HA	4:B:1176:ARG:HD2	1.78	0.40
4:B:1109:ILE:HA	4:B:1110:PRO:HD3	1.84	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	
3	A	816/934 (87%)	736 (90%)	73 (9%)	7 (1%)	17	51
4	B	912/1022 (89%)	836 (92%)	66 (7%)	10 (1%)	14	46
All	All	1728/1956 (88%)	1572 (91%)	139 (8%)	17 (1%)	15	48

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	146	GLY
3	A	28	GLU
4	B	667	ASP
4	B	898	PRO
3	A	672	MET
4	B	745	ILE
4	B	747	LEU
4	B	899	GLU
3	A	2	ALA
3	A	220	GLY
4	B	375	GLU
4	B	386	PRO
4	B	1260	VAL
3	A	203	GLY
3	A	617	VAL
4	B	717	VAL
4	B	1002	GLY

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	
3	A	693/808 (86%)	693 (100%)	0	100	100
4	B	819/899 (91%)	819 (100%)	0	100	100
All	All	1512/1707 (89%)	1512 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	377	GLN
4	B	534	ASN
4	B	989	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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	$\# Z > 2$
1	6OG	E	8	1,2	18,25,26	1.44	2 (11%)	20,36,39	3.51	5 (25%)

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
1	6OG	E	8	1,2	-	2/5/23/24	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	8	6OG	C6-N1	4.69	1.39	1.31
1	E	8	6OG	C8-N7	-2.10	1.31	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	8	6OG	O6-C6-C5	11.68	132.71	116.01
1	E	8	6OG	C5-C6-N1	-6.44	110.99	123.26
1	E	8	6OG	C2-N1-C6	6.15	125.96	116.08
1	E	8	6OG	C2-N3-C4	-3.63	111.21	115.36
1	E	8	6OG	N3-C2-N1	-2.63	123.71	127.22

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	E	8	6OG	N1-C6-O6-C
1	E	8	6OG	C5-C6-O6-C

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\# Z > 2$
6	ADP	A	936	5	24,29,29	1.00	1 (4%)	29,45,45	1.40	4 (13%)
6	ADP	B	202	5	24,29,29	0.98	1 (4%)	29,45,45	1.46	4 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ADP	A	936	5	-	1/12/32/32	0/3/3/3
6	ADP	B	202	5	-	2/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	936	ADP	C5-C4	2.61	1.47	1.40
6	B	202	ADP	C5-C4	2.59	1.47	1.40

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	202	ADP	PA-O3A-PB	-3.74	119.98	132.83
6	B	202	ADP	N3-C2-N1	-3.32	123.50	128.68
6	A	936	ADP	C3'-C2'-C1'	3.20	105.79	100.98
6	A	936	ADP	N3-C2-N1	-3.07	123.89	128.68
6	A	936	ADP	PA-O3A-PB	-2.99	122.56	132.83
6	B	202	ADP	C3'-C2'-C1'	2.96	105.43	100.98
6	B	202	ADP	C4-C5-N7	-2.85	106.43	109.40
6	A	936	ADP	C4-C5-N7	-2.68	106.61	109.40

There are no chirality outliers.

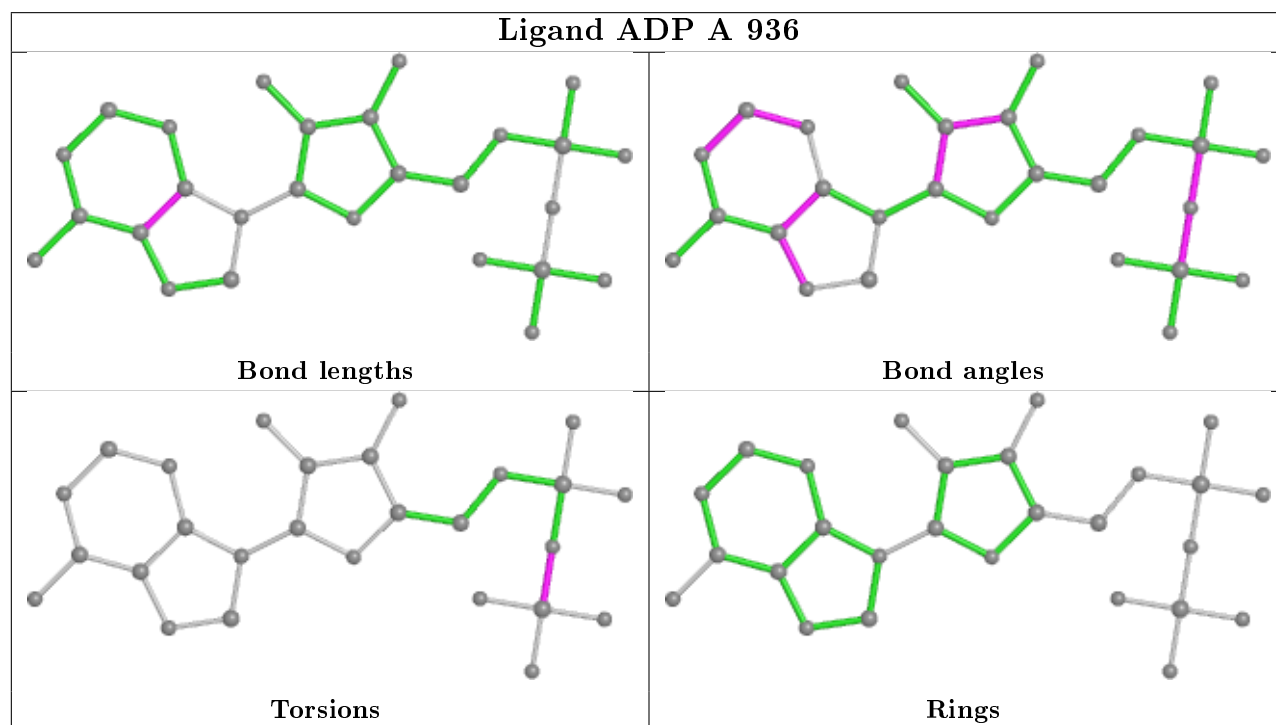
All (3) torsion outliers are listed below:

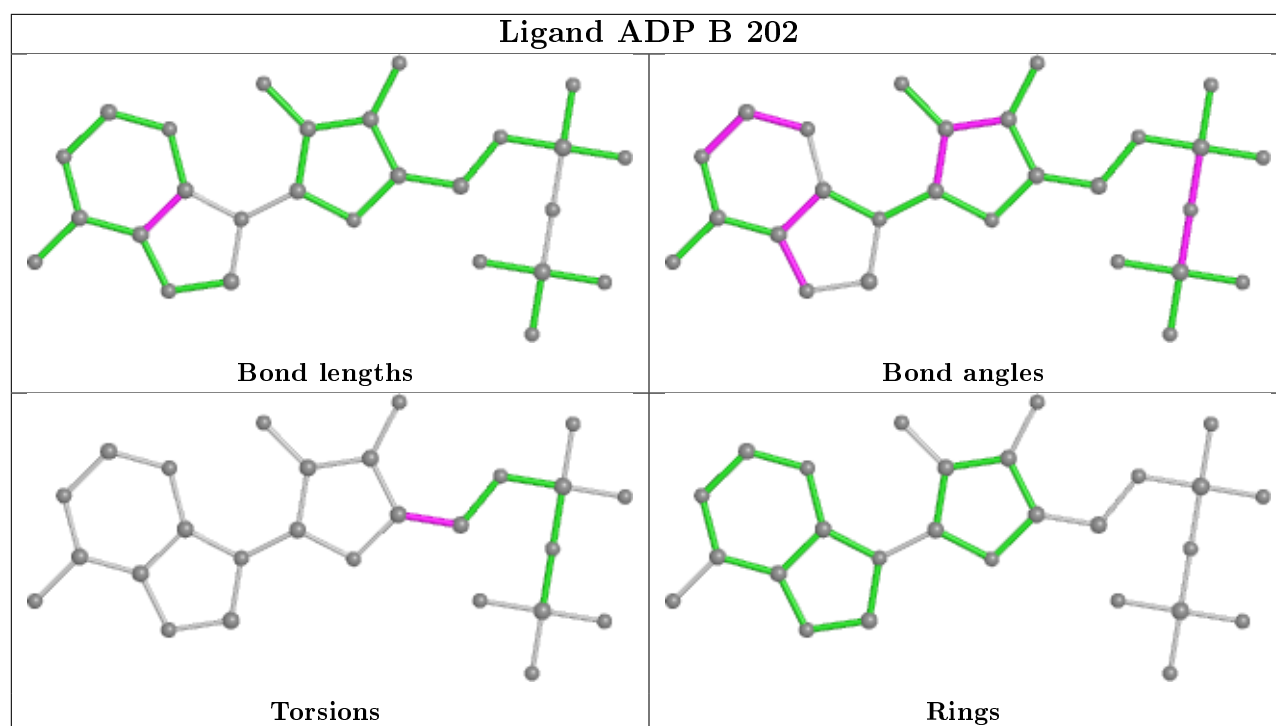
Mol	Chain	Res	Type	Atoms
6	B	202	ADP	O4'-C4'-C5'-O5'
6	A	936	ADP	PA-O3A-PB-O3B
6	B	202	ADP	C3'-C4'-C5'-O5'

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	E	14/15 (93%)	0.63	1 (7%) 16 19	68, 78, 91, 91	0
2	F	15/15 (100%)	0.34	0 100 100	65, 72, 89, 91	0
3	A	830/934 (88%)	0.63	76 (9%) 9 11	20, 73, 76, 83	0
4	B	932/1022 (91%)	0.39	46 (4%) 29 33	30, 73, 82, 89	0
All	All	1791/1986 (90%)	0.51	123 (6%) 16 20	20, 73, 80, 91	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	206	THR	7.6
4	B	968	VAL	6.5
1	E	15	DG	6.2
4	B	954	TYR	5.8
3	A	541	THR	5.2
3	A	558	SER	4.9
4	B	980	GLU	4.7
3	A	202	PRO	4.6
4	B	1124	ASN	4.6
3	A	693	CYS	4.5
3	A	139	ASN	4.4
4	B	549	SER	4.1
3	A	180	ASP	4.0
3	A	467	GLU	4.0
3	A	154	ALA	4.0
3	A	587	GLY	3.8
4	B	982	PRO	3.8
3	A	201	LEU	3.8
3	A	394	PHE	3.8
3	A	640	ALA	3.7
3	A	428	HIS	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	A	156	ASP	3.7
3	A	207	ALA	3.6
3	A	426	GLY	3.6
4	B	979	LEU	3.5
3	A	112	SER	3.4
4	B	1010	THR	3.4
3	A	432	LEU	3.3
3	A	205	GLU	3.3
3	A	210	MET	3.3
3	A	153	SER	3.3
4	B	969	TYR	3.3
4	B	981	ILE	3.3
3	A	225	THR	3.2
3	A	1	MET	3.2
3	A	527	CYS	3.2
4	B	1007	TRP	3.2
3	A	501	ARG	3.1
4	B	552	HIS	3.1
4	B	1334	ARG	3.1
3	A	253	MET	3.1
3	A	458	LEU	3.1
4	B	651	ILE	3.0
3	A	584	ILE	3.0
3	A	552	THR	3.0
4	B	967	ILE	3.0
4	B	1335	GLU	2.9
3	A	447	PHE	2.9
4	B	1120	GLU	2.9
3	A	502	ASP	2.8
3	A	203	GLY	2.8
3	A	155	VAL	2.8
3	A	480	GLU	2.8
3	A	413	GLN	2.8
3	A	425	GLU	2.8
4	B	944	ILE	2.7
3	A	200	VAL	2.7
3	A	538	ASN	2.7
4	B	1006	TYR	2.7
3	A	283	ASP	2.7
3	A	424	HIS	2.7
3	A	472	PRO	2.6
3	A	694	PHE	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	A	569	GLU	2.6
3	A	404	CYS	2.6
3	A	524	ARG	2.6
4	B	747	LEU	2.6
3	A	234	THR	2.6
4	B	951	LEU	2.6
3	A	662	GLN	2.6
3	A	316	SER	2.6
4	B	665	GLU	2.6
3	A	204	GLY	2.6
4	B	955	LEU	2.6
3	A	660	ASP	2.5
4	B	550	SER	2.5
3	A	161	VAL	2.5
4	B	946	GLU	2.5
3	A	468	PHE	2.5
4	B	1121	GLU	2.5
4	B	718	SER	2.4
4	B	1298	TYR	2.4
4	B	977	TYR	2.4
4	B	649	ASP	2.4
3	A	238	TYR	2.4
3	A	409	GLN	2.4
3	A	853	GLU	2.4
3	A	459	ASP	2.3
3	A	48	GLU	2.3
3	A	160	GLN	2.3
4	B	966	THR	2.3
4	B	983	GLU	2.3
3	A	158	GLN	2.3
4	B	931	ALA	2.3
3	A	152	MET	2.3
4	B	947	ASN	2.3
4	B	1328	GLN	2.3
3	A	544	ILE	2.3
4	B	1295	PRO	2.3
4	B	1178	GLY	2.2
3	A	460	MET	2.2
4	B	1005	ARG	2.2
3	A	478	LEU	2.2
3	A	540	SER	2.2
3	A	401	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	A	431	LEU	2.2
3	A	273	VAL	2.1
4	B	1308	LEU	2.1
3	A	365	ALA	2.1
4	B	962	ILE	2.1
4	B	978	GLN	2.1
4	B	960	ASN	2.1
4	B	1137	MET	2.1
3	A	476	PRO	2.1
3	A	380	LEU	2.1
3	A	178	PHE	2.1
3	A	512	LYS	2.0
3	A	226	GLU	2.0
4	B	1333	PHE	2.0
4	B	679	LEU	2.0
3	A	254	ASN	2.0
3	A	368	GLU	2.0
4	B	953	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
1	6OG	E	8	23/24	0.91	0.27	68,68,69,69	0

6.3 Carbohydrates [i](#)

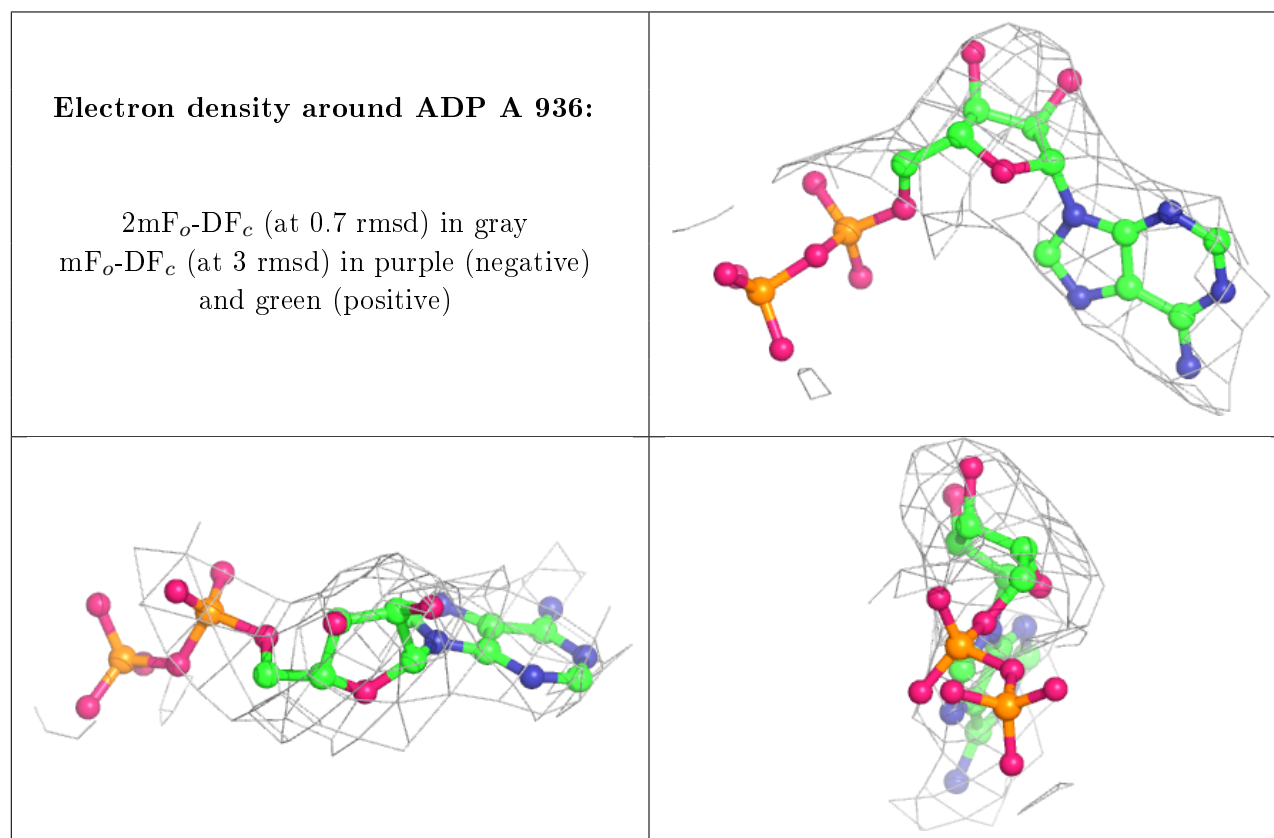
There are no carbohydrates in this entry.

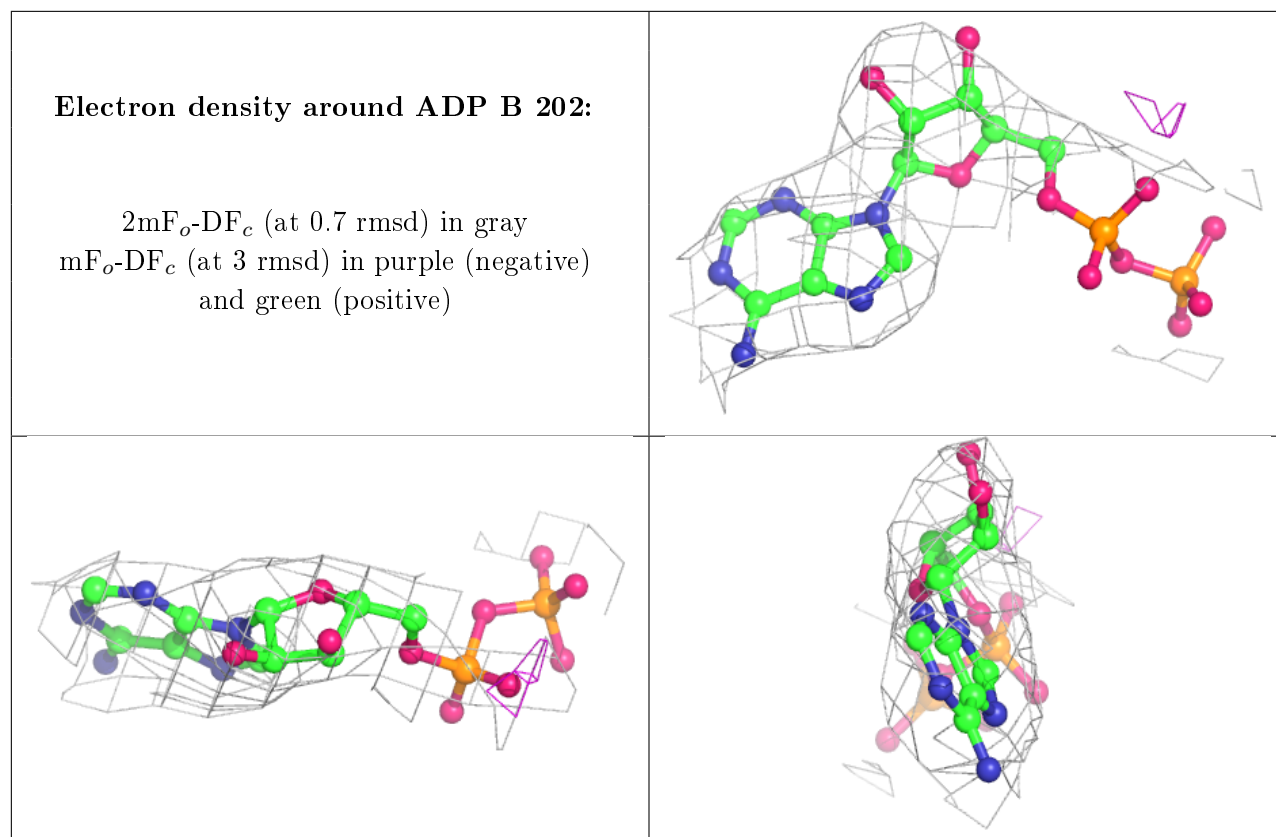
6.4 Ligands [i](#)

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(\AA^2)	Q<0.9
6	ADP	A	936	27/27	0.89	0.23	70,70,75,75	0
6	ADP	B	202	27/27	0.90	0.19	82,82,83,83	0
5	MG	B	102	1/1	0.96	0.09	58,58,58,58	0
5	MG	A	935	1/1	0.97	0.30	73,73,73,73	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.