



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:44 PM UTC

PDB ID : 2O8C / pdb_00002o8c
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 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

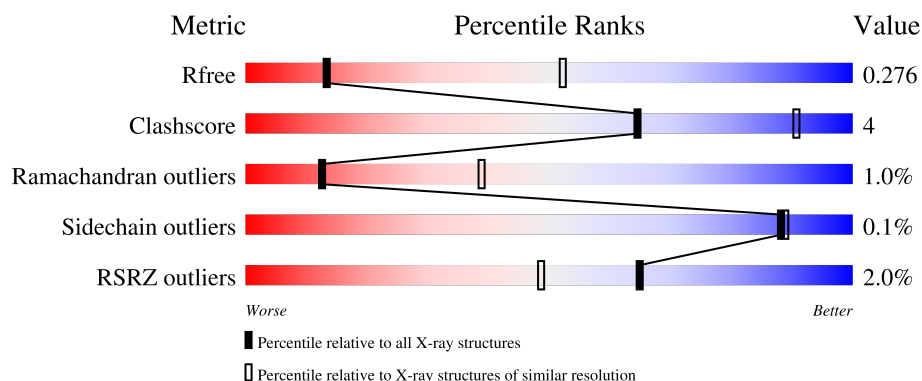
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1047 (3.42-3.34)
Clashscore	190562	1067 (3.42-3.34)
Ramachandran outliers	187476	1056 (3.42-3.34)
Sidechain outliers	187428	1056 (3.42-3.34)
RSRZ outliers	180081	1047 (3.42-3.34)

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	E	15	7% 80% 20%
2	F	15	13% 100%
3	A	934	% 80% 9% 11%
4	B	1022	2% 79% 12% 9%

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*C P*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*G P*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			

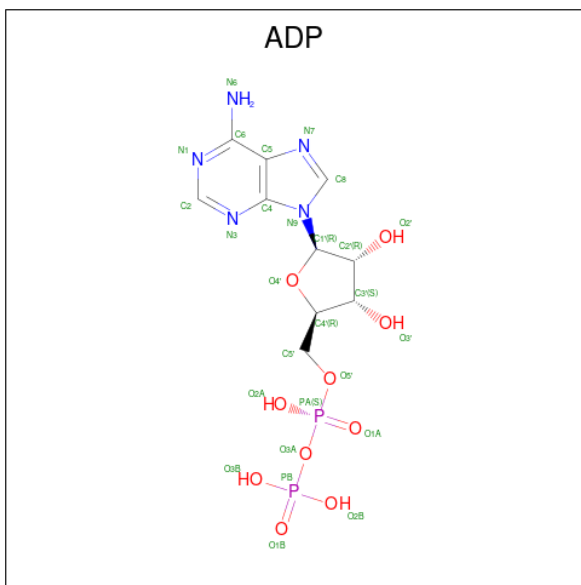
There are 2 discrepancies between the modelled and reference sequences:

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

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

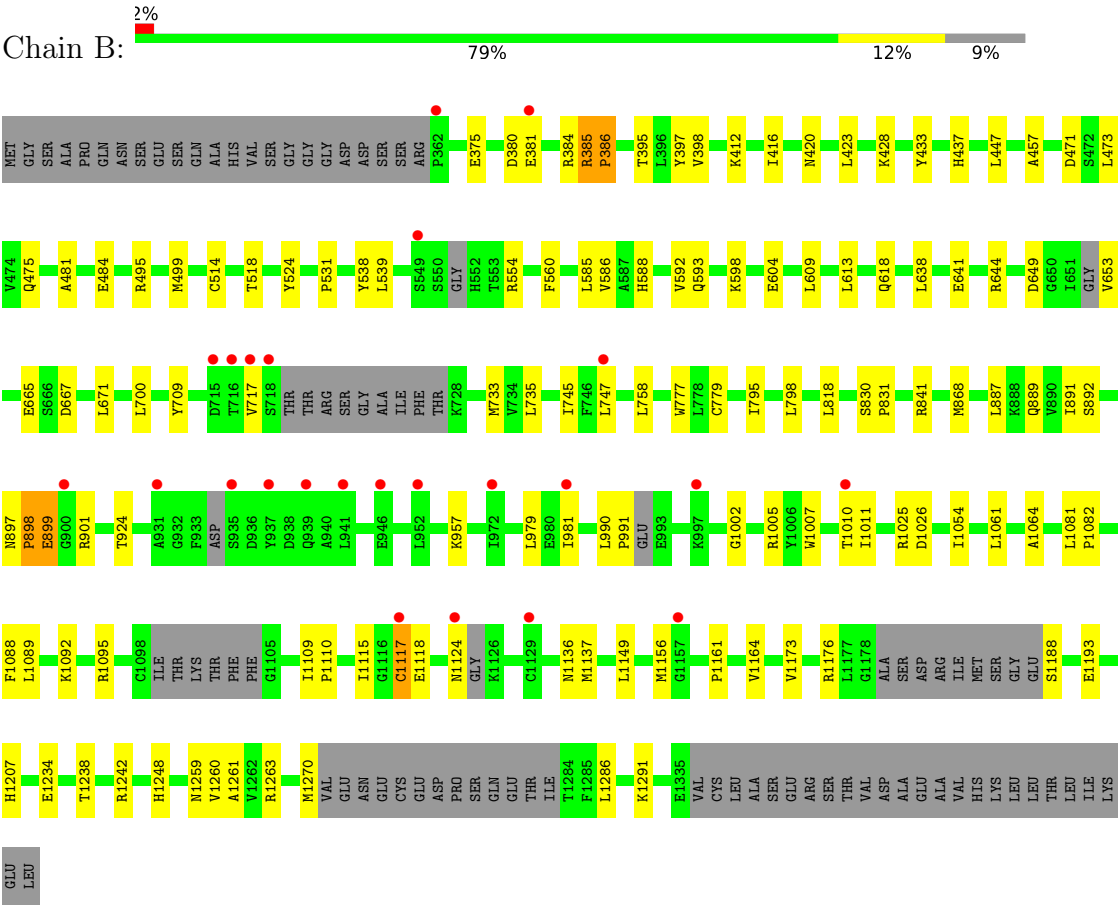
- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	F	1	Total O 1 1	0	0
7	A	1	Total O 1 1	0	0
7	B	20	Total O 20 20	0	0



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 20.00 – 3.37	Depositor EDS
% Data completeness (in resolution range)	99.1 (20.00-3.37) 98.5 (20.00-3.37)	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 (4.98%)	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)	0.28 , 136.0	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	0.89	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 6OG, 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	E	0.19	0/319	0.71	0/488
2	F	0.21	0/338	0.73	0/520
3	A	0.41	0/6539	0.88	11/8828 (0.1%)
4	B	0.42	0/7587	0.93	16/10226 (0.2%)
All	All	0.41	0/14783	0.90	27/20062 (0.1%)

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	787	LEU	N-CA-C	-8.80	102.56	113.38
4	B	665	GLU	N-CA-C	6.99	119.50	111.11
3	A	691	ILE	N-CA-C	-6.85	105.96	113.43
4	B	957	LYS	N-CA-C	-6.67	104.16	112.90
3	A	96	ARG	N-CA-C	6.39	120.69	113.02
4	B	598	LYS	N-CA-C	6.29	118.94	111.33
3	A	435	VAL	N-CA-C	-6.23	107.06	113.10
3	A	617	VAL	CA-C-N	6.06	127.41	119.84
3	A	617	VAL	C-N-CA	6.06	127.41	119.84
3	A	424	HIS	CB-CA-C	-6.04	109.59	116.54
3	A	587	GLY	N-CA-C	-6.00	106.30	115.66
4	B	841	ARG	N-CA-C	-5.97	105.73	114.39
4	B	1011	ILE	N-CA-C	5.59	115.72	110.30
3	A	651	ILE	CA-C-N	5.54	125.48	119.78
3	A	651	ILE	C-N-CA	5.54	125.48	119.78
4	B	398	VAL	CA-C-N	5.48	125.79	119.93
4	B	398	VAL	C-N-CA	5.48	125.79	119.93
4	B	1005	ARG	N-CA-C	5.47	118.36	109.06
4	B	981	ILE	CA-C-N	5.34	125.34	119.89
4	B	981	ILE	C-N-CA	5.34	125.34	119.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	629	GLN	N-CA-C	-5.26	106.70	113.23
4	B	385	ARG	CA-C-N	5.20	126.34	119.84
4	B	385	ARG	C-N-CA	5.20	126.34	119.84
4	B	538	TYR	N-CA-C	5.19	118.47	110.42
4	B	700	LEU	N-CA-C	5.16	116.98	111.36
4	B	924	THR	CB-CA-C	-5.08	109.12	116.54
4	B	1117	CYS	N-CA-C	5.03	116.79	110.91

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	E	308	0	170	1	0
2	F	303	0	171	0	0
3	A	6439	0	6410	41	0
4	B	7443	0	7415	74	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	113	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 (113) 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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:359:ARG:NH2	3:A:691:ILE:O	2.28	0.65
4:B:433:TYR:OH	4:B:484:GLU:OE1	2.14	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	0.61
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
4:B:733:MET:HE3	4:B:1173:VAL:HG23	1.86	0.58
3:A:321:THR:O	3:A:321:THR:HG23	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
3:A:679:ILE:HG22	3:A:779:MET:HE2	1.88	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
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
3:A:16:GLU:HG3	3:A:67:MET:HE3	1.89	0.52
4:B:1263:ARG:HH21	4:B:1291:LYS:HD2	1.75	0.52
4:B:777:TRP:HB3	4:B:1156:MET:HE3	1.90	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:641:GLU:HB3	4:B:644:ARG:HG3	1.94	0.50
4:B:818:LEU:HD12	4:B:868:MET:HE3	1.93	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:39:ARG:HE	3:A:44:THR:HG21	1.79	0.48
3:A:258:LEU:HB2	3:A:261:MET:HG2	1.96	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:733:MET:HE3	4:B:1173:VAL:CG2	2.44	0.47
4:B:1270:MET:HE2	4:B:1286:LEU:HD21	1.97	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
4:B:733:MET:HE2	4:B:735:LEU:HD21	1.98	0.45
3:A:1:MET:HE3	4:B:475: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
4:B:990:LEU:HA	4:B:991:PRO:HD3	1.78	0.44
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:1207:HIS:O	4:B:1242:ARG:NH2	2.51	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: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
4:B:1025:ARG:HG3	4:B:1026:ASP:N	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:E:5:DC:H2''	1:E:6:DG:C8	2.55	0.41
4:B:897:ASN:O	4:B:901:ARG:HG3	2.20	0.41
3:A:300:MET:HA	3:A:351:MET:HE2	2.03	0.40
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:HD2	4:B:1176:ARG:HA	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%)	14	41
4	B	912/1022 (89%)	836 (92%)	66 (7%)	10 (1%)	11	37
All	All	1728/1956 (88%)	1572 (91%)	139 (8%)	17 (1%)	12	39

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%)	818 (100%)	1 (0%)	88	89
All	All	1512/1707 (89%)	1511 (100%)	1 (0%)	88	89

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	B	592	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	127	ASN
3	A	285	ASN
3	A	288	GLN
3	A	337	GLN
3	A	518	GLN
3	A	547	ASN
3	A	596	ASN
3	A	629	GLN
3	A	824	GLN
4	B	522	GLN
4	B	534	ASN
4	B	751	ASN
4	B	785	HIS
4	B	949	GLN
4	B	978	GLN
4	B	989	ASN
4	B	1039	ASN
4	B	1048	GLN

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	22,25,26	1.95	3 (13%)	31,36,39	3.66	7 (22%)

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	-	2/9/23/24	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	8	6OG	O6-C6	-6.53	1.25	1.35
1	E	8	6OG	C6-N1	5.23	1.39	1.32
1	E	8	6OG	O6-C	-2.13	1.36	1.42

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	8	6OG	O6-C6-C5	12.88	132.71	117.17
1	E	8	6OG	C5-C6-N1	-9.34	110.99	123.49
1	E	8	6OG	C-O6-C6	8.08	124.75	117.20
1	E	8	6OG	C2-N1-C6	7.19	125.96	115.96
1	E	8	6OG	N3-C4-N9	-2.99	123.20	126.99
1	E	8	6OG	C5-C4-N3	2.88	130.21	127.18
1	E	8	6OG	C4-C5-C6	2.75	117.93	115.22

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 oligosaccharides 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	28,29,29	1.49	5 (17%)	43,45,45	1.78	8 (18%)
6	ADP	B	202	5	28,29,29	1.43	4 (14%)	43,45,45	1.83	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
6	ADP	A	936	5	-	1/16/32/32	0/3/3/3
6	ADP	B	202	5	-	1/16/32/32	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	936	ADP	C5-C4	4.91	1.47	1.39
6	B	202	ADP	C5-C4	4.87	1.47	1.39
6	B	202	ADP	C5-C6	2.88	1.49	1.41
6	A	936	ADP	C5-C6	2.80	1.48	1.41
6	A	936	ADP	PA-O3A	2.50	1.62	1.59
6	B	202	ADP	C8-N7	2.47	1.36	1.31
6	A	936	ADP	C5-N7	-2.31	1.34	1.39
6	A	936	ADP	C8-N7	2.29	1.36	1.31
6	B	202	ADP	C5-N7	-2.11	1.35	1.39

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	202	ADP	C5-C4-N3	-5.89	118.61	126.72
6	A	936	ADP	C5-C4-N3	-5.80	118.72	126.72
6	A	936	ADP	N3-C4-N9	4.55	134.90	127.17
6	B	202	ADP	N3-C4-N9	4.52	134.86	127.17
6	B	202	ADP	C2-N3-C4	3.81	121.14	111.83
6	B	202	ADP	C4-C5-N7	-3.63	106.43	110.58
6	A	936	ADP	C2-N3-C4	3.58	120.58	111.83
6	A	936	ADP	C4-C5-N7	-3.48	106.61	110.58
6	B	202	ADP	N3-C2-N1	-3.36	123.50	128.58
6	A	936	ADP	N3-C2-N1	-3.10	123.89	128.58
6	B	202	ADP	C5-N7-C8	2.58	107.51	103.45
6	B	202	ADP	C4-N9-C8	2.43	108.29	105.74
6	A	936	ADP	C5-N7-C8	2.42	107.25	103.45
6	A	936	ADP	C4-N9-C8	2.36	108.21	105.74
6	B	202	ADP	C6-C5-N7	2.33	136.59	132.09
6	A	936	ADP	C3'-C2'-C1'	2.29	105.79	101.46
6	B	202	ADP	C3'-C2'-C1'	2.10	105.43	101.46

There are no chirality outliers.

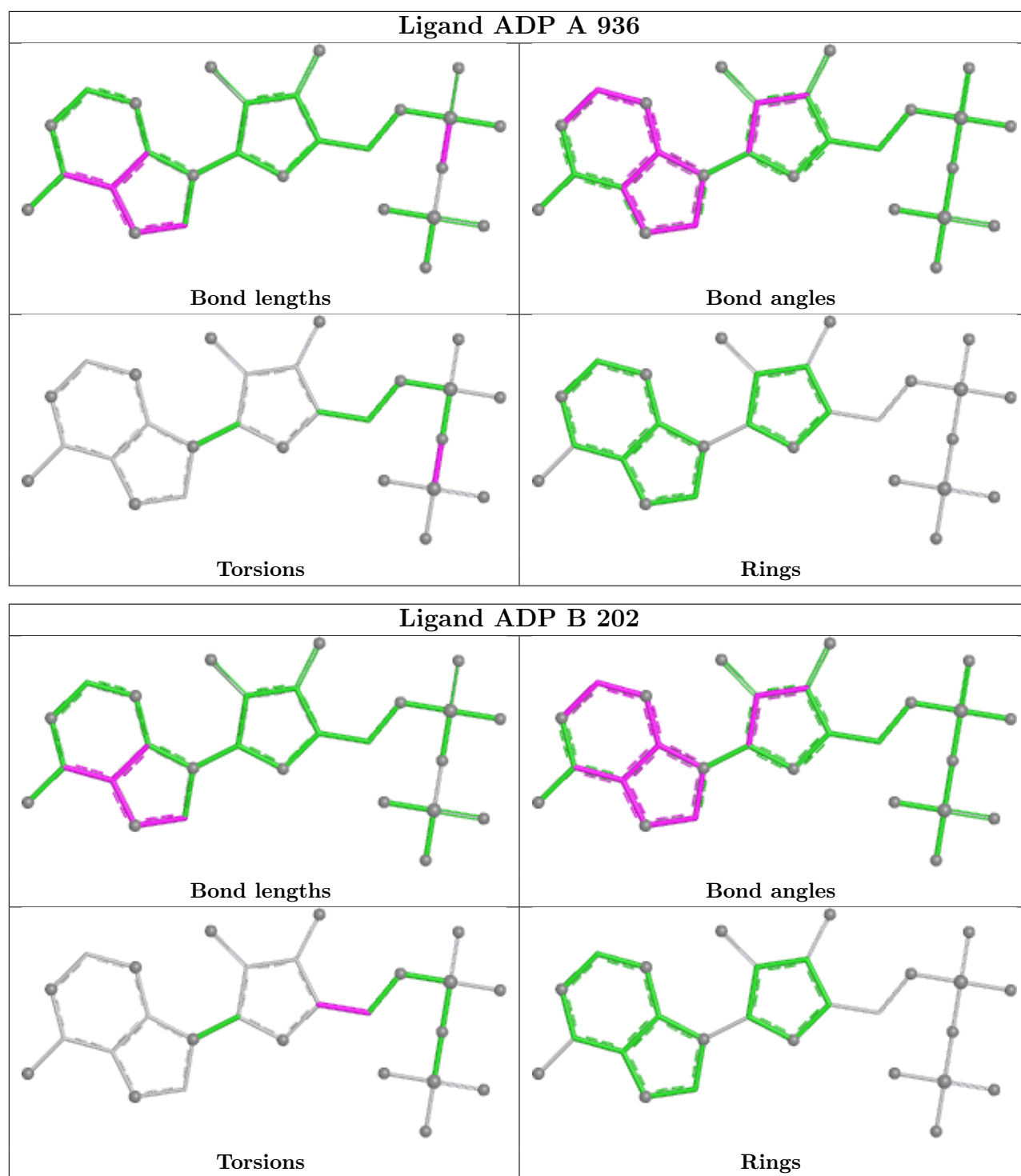
All (2) torsion outliers are listed below:

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

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 ⓘ

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	E	14/15 (93%)	0.97	1 (7%) 22 18	68, 78, 91, 91	0
2	F	15/15 (100%)	0.87	2 (13%) 7 8	65, 72, 89, 91	0
3	A	830/934 (88%)	0.04	9 (1%) 78 64	20, 73, 76, 83	0
4	B	932/1022 (91%)	0.10	24 (2%) 57 42	30, 73, 82, 89	0
All	All	1791/1986 (90%)	0.09	36 (2%) 65 49	20, 73, 80, 91	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	B	939	GLN	5.9
4	B	935	SER	4.4
1	E	15	DG	3.9
3	A	558	SER	3.7
4	B	941	LEU	3.7
3	A	1	MET	3.4
4	B	1010	THR	3.3
4	B	362	PRO	3.2
4	B	931	ALA	3.2
4	B	946	GLU	3.1
4	B	717	VAL	3.0
3	A	587	GLY	2.8
2	F	25	DC	2.7
4	B	1117	CYS	2.7
4	B	1124	ASN	2.7
3	A	559	LEU	2.7
3	A	180	ASP	2.6
4	B	1129	CYS	2.6
4	B	716	THR	2.5
4	B	718	SER	2.4
4	B	747	LEU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	A	548	GLY	2.4
4	B	952	LEU	2.4
4	B	549	SER	2.3
4	B	997	LYS	2.3
4	B	715	ASP	2.3
3	A	304	ILE	2.2
4	B	972	ILE	2.2
4	B	981	ILE	2.2
3	A	785	HIS	2.2
4	B	937	TYR	2.2
2	F	24	DG	2.2
4	B	1157	GLY	2.2
3	A	309	ALA	2.1
4	B	900	GLY	2.1
4	B	381	GLU	2.1

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	0.88	0.14	68,68,69,69	0

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.

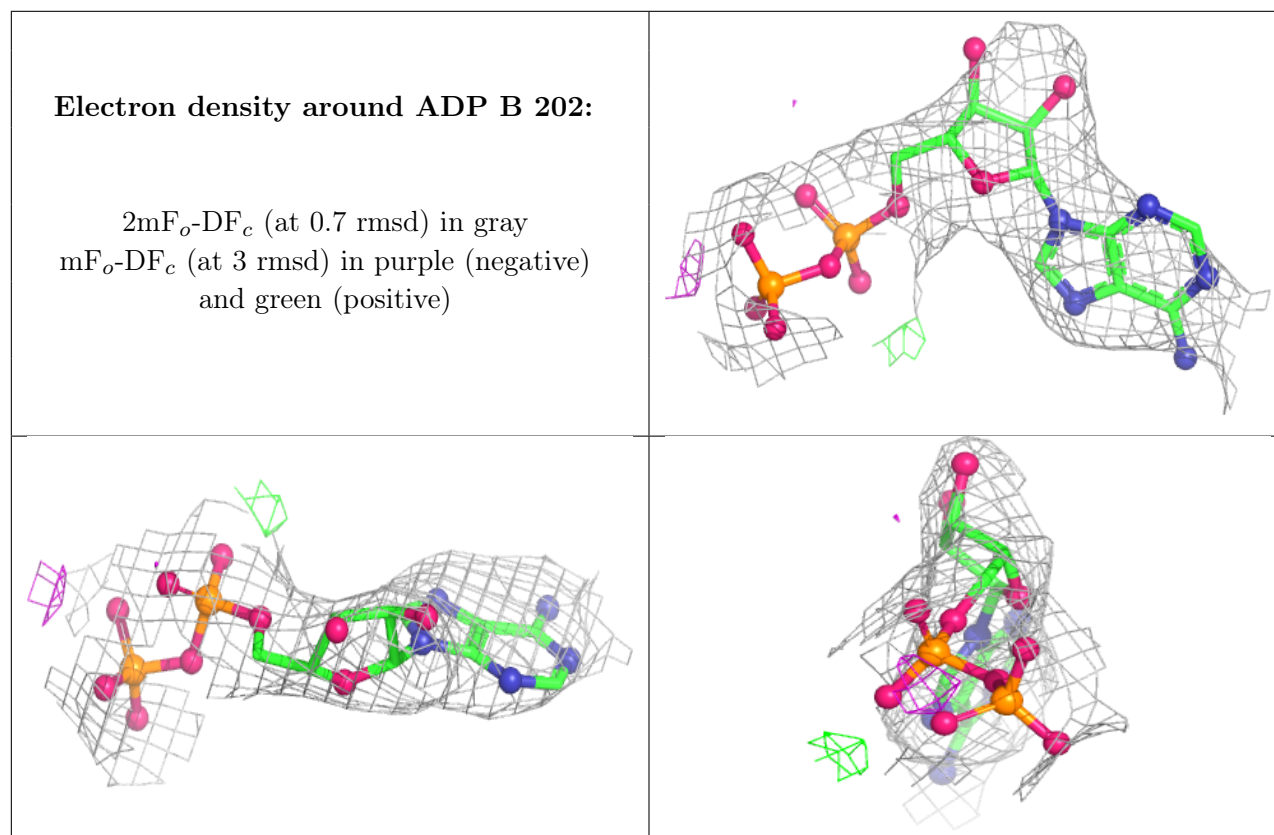
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	ADP	B	202	27/27	0.86	0.09	82,82,83,83	0
5	MG	B	102	1/1	0.94	0.16	58,58,58,58	0

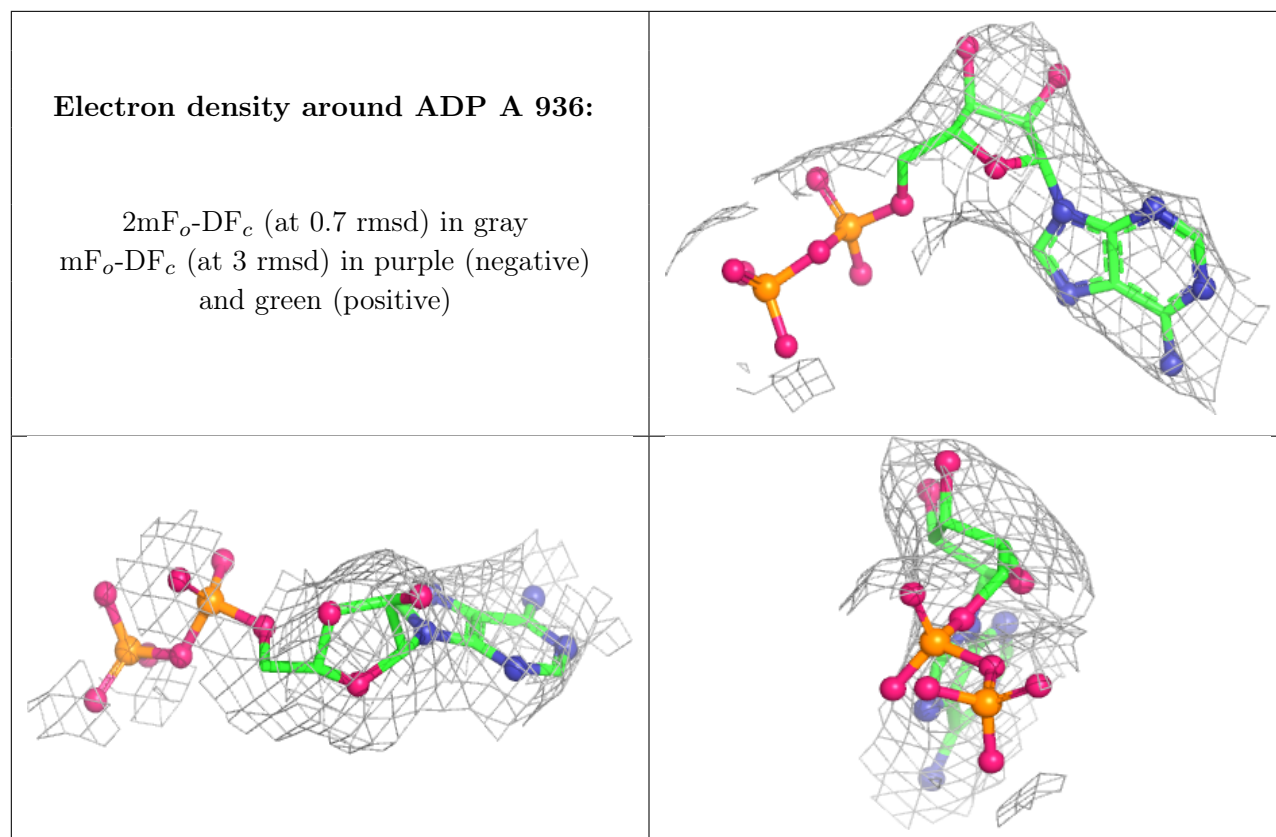
Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	ADP	A	936	27/27	0.94	0.08	70,70,75,75	0
5	MG	A	935	1/1	0.94	0.05	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.