Full wwPDB X-ray Structure Validation Report (i)

Aug 20, 2023 – 11:31 AM EDT

PDB ID	:	2O8F
Title	:	human MutSalpha (MSH2/MSH6) bound to DNA with a single base T insert
Authors	:	Warren, J.J.; Pohlhaus, T.J.; Changela, A.; Modrich, P.L.; Beese, L.S.
Deposited on	:	2006-12-12
Resolution	:	3.25 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 (i) 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 (i)) were used in the production of this report:

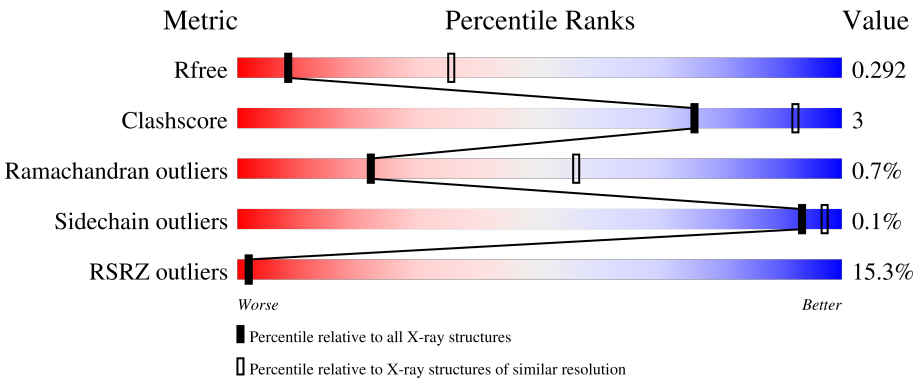
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	E	17	6%; 71%; 24%; 6%
2	F	18	17%; 78%; 11%; 11%
3	A	934	17%; 81%; 8%; 11%
4	B	1022	11%; 83%; 8%; 9%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 14708 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*CP*GP*GP*CP*CP*GP*CP*CP*GP*CP*TP*AP*GP*CP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	E	17	346	163	68	99	16	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	F	18	365	173	67	108	17	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	832	6494	4119	1103	1238	34	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	B	933	7456	4730	1279	1396	51	0	0	0

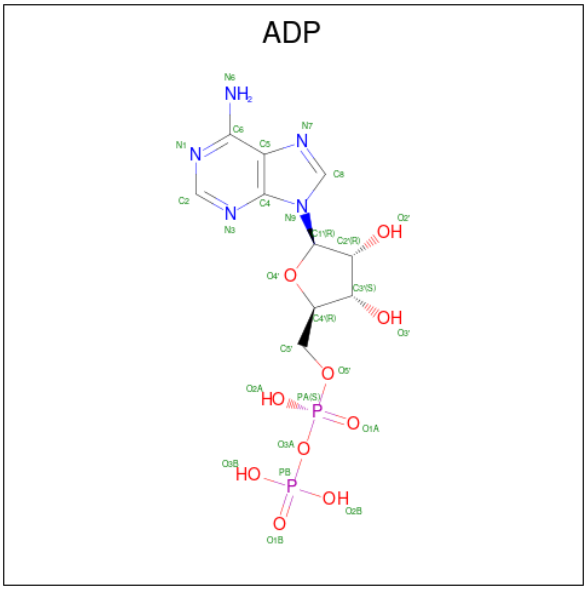
There are 2 discrepancies between the modelled and reference sequences:

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
			Total	Mg		
5	A	1	1	1	0	0

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



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

- Molecule 7 is water.

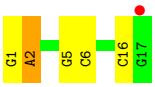
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	E	1	1	1	0	0
			Total	O		
7	A	1	1	1	0	0
			Total	O		
7	B	17	17	17	0	0

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.

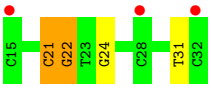
• Molecule 1: 5'-D(*GP*AP*CP*GP*GP*CP*CP*GP*CP*CP*GP*CP*TP*AP*GP*CP*G)-3'

Chain E:



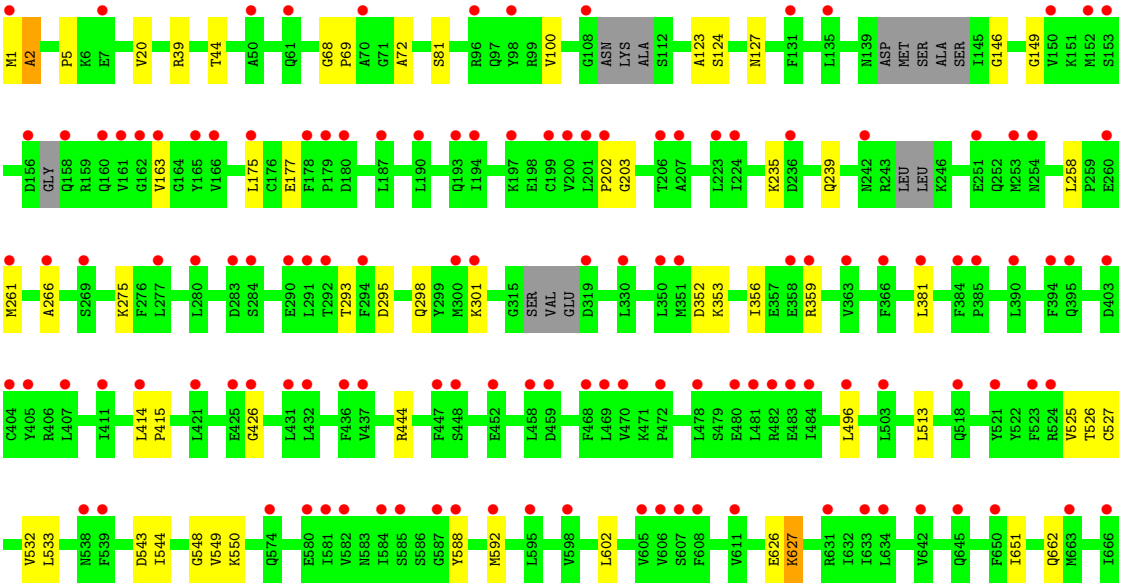
• Molecule 2: 5'-D(*CP*GP*CP*TP*AP*GP*CP*GP*TP*GP*CP*GP*GP*CP*CP*GP*TP*C)-3'

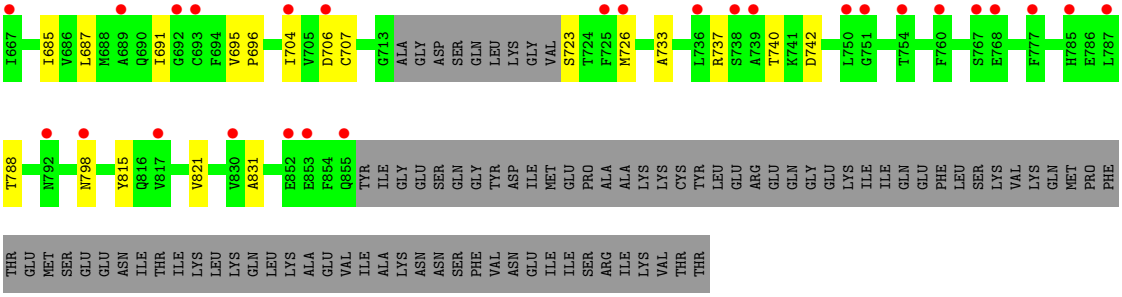
Chain F:



• Molecule 3: DNA mismatch repair protein Msh2

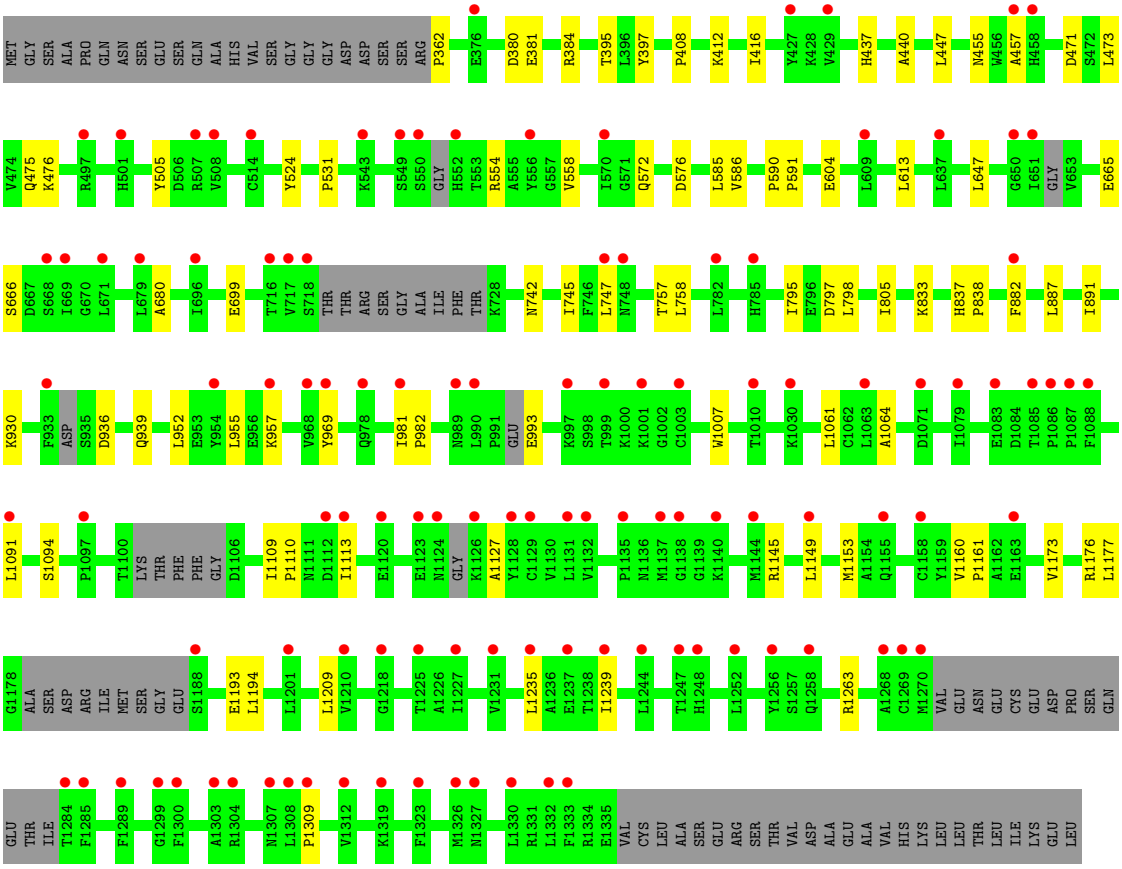
Chain A:





- Molecule 4: DNA mismatch repair protein MSH6

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 3 2	Depositor
Cell constants a, b, c, α, β, γ	259.55Å 259.55Å 259.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.25 82.08 – 3.25	Depositor EDS
% Data completeness (in resolution range)	99.6 (20.00-3.25) 99.5 (82.08-3.25)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	2.47 (at 3.26Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.243 , 0.293 0.250 , 0.292	Depositor DCC
R_{free} test set	2382 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	85.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 136.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	14708	wwPDB-VP
Average B, all atoms (Å^2)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.32% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	E	0.61	0/388	1.32	5/597 (0.8%)
2	F	0.61	0/408	1.46	6/628 (1.0%)
3	A	0.30	0/6595	0.56	0/8898
4	B	0.32	0/7600	0.58	0/10244
All	All	0.33	0/14991	0.65	11/20367 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	22	DG	O3'-P-O5'	-11.73	81.71	104.00
2	F	22	DG	OP1-P-O3'	-7.96	87.68	105.20
2	F	22	DG	OP2-P-O3'	-7.58	88.53	105.20
1	E	2	DA	P-O3'-C3'	7.20	128.34	119.70
1	E	1	DG	P-O3'-C3'	7.11	128.23	119.70
1	E	5	DG	P-O3'-C3'	7.10	128.22	119.70
1	E	6	DC	O4'-C1'-N1	6.83	112.78	108.00
1	E	16	DC	P-O3'-C3'	6.20	127.14	119.70
2	F	21	DC	P-O3'-C3'	5.97	126.86	119.70
2	F	21	DC	O4'-C1'-N1	5.50	111.85	108.00
2	F	24	DG	O4'-C1'-N9	-5.15	104.39	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	346	0	190	1	0
2	F	365	0	203	2	0
3	A	6494	0	6491	43	0
4	B	7456	0	7431	48	0
5	A	1	0	0	0	0
6	A	27	0	12	0	0
7	A	1	0	0	0	0
7	B	17	0	0	0	0
7	E	1	0	0	0	0
All	All	14708	0	14327	90	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 3.

All (90) 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)
3:A:39:ARG:HE	3:A:44:THR:HG21	1.52	0.74
4:B:936:ASP:HA	4:B:939:GLN:HB3	1.70	0.73
4:B:747:LEU:HA	4:B:757:THR:HG21	1.70	0.73
4:B:554:ARG:HH22	4:B:604:GLU:HG3	1.55	0.72
4:B:699:GLU:HG2	4:B:833:LYS:HD2	1.75	0.67
4:B:993:GLU:HB3	4:B:1007:TRP:HD1	1.62	0.65
3:A:175:LEU:H	3:A:293:THR:HG21	1.63	0.64
3:A:588:TYR:O	3:A:592:MET:HG2	1.98	0.63
4:B:380:ASP:HB2	4:B:384:ARG:H	1.64	0.62
3:A:627:LYS:HA	3:A:704:ILE:HB	1.80	0.62
3:A:651:ILE:HD12	3:A:815:TYR:HB2	1.83	0.61
4:B:1176:ARG:HE	4:B:1193:GLU:HG3	1.66	0.61
4:B:797:ASP:HB3	4:B:882:PHE:CD1	2.37	0.60
3:A:359:ARG:NH2	3:A:691:ILE:O	2.34	0.59
3:A:20:VAL:HG21	3:A:68:GLY:HA2	1.84	0.59
4:B:380:ASP:O	4:B:397:TYR:HB2	2.02	0.58
3:A:301:LYS:HB2	3:A:707:CYS:HB3	1.86	0.57
4:B:798:LEU:HD13	4:B:1061:LEU:HD23	1.85	0.57
4:B:437:HIS:HA	4:B:457:ALA:HB3	1.86	0.57
3:A:5:PRO:HB3	3:A:81:SER:HB3	1.86	0.57
3:A:175:LEU:HB2	3:A:266:ALA:HB1	1.87	0.56
3:A:415:PRO:HB3	3:A:444:ARG:HE	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:527:CYS:HB2	3:A:548:GLY:HA2	1.88	0.55
4:B:758:LEU:HD22	4:B:1149:LEU:HD22	1.89	0.54
4:B:1173:VAL:HG22	4:B:1209:LEU:HB3	1.91	0.53
3:A:740:THR:HG23	3:A:742:ASP:H	1.75	0.52
4:B:795:ILE:HG23	4:B:1064:ALA:HA	1.91	0.52
3:A:543:ASP:HB3	3:A:550:LYS:HD2	1.92	0.51
4:B:1149:LEU:O	4:B:1153:MET:HG2	2.11	0.51
4:B:981:ILE:HD12	4:B:982:PRO:HD2	1.94	0.50
4:B:412:LYS:O	4:B:416:ILE:HG12	2.11	0.50
4:B:447:LEU:HD21	4:B:473:LEU:HG	1.94	0.49
3:A:525:VAL:C	3:A:527:CYS:H	2.16	0.49
4:B:952:LEU:HD23	4:B:955:LEU:HD12	1.92	0.49
3:A:124:SER:HB2	3:A:127:ASN:HB3	1.95	0.49
3:A:100:VAL:HB	3:A:123:ALA:HB3	1.95	0.49
4:B:742:ASN:HB3	4:B:1177:LEU:HD12	1.94	0.49
3:A:381:LEU:HD21	3:A:602:LEU:HD22	1.94	0.49
1:E:2:DA:H61	2:F:31:DT:H3	1.60	0.48
3:A:788:THR:HG21	3:A:821:VAL:HG21	1.95	0.48
3:A:177:GLU:HG3	3:A:266:ALA:HB2	1.96	0.47
4:B:665:GLU:HG3	4:B:666:SER:H	1.79	0.47
4:B:798:LEU:HB3	4:B:805:ILE:HD11	1.97	0.47
3:A:258:LEU:H	3:A:261:MET:HB2	1.80	0.47
3:A:295:ASP:HB3	3:A:298:GLN:HG3	1.96	0.47
3:A:544:ILE:HG12	3:A:549:VAL:HG13	1.97	0.47
4:B:957:LYS:HE3	4:B:969:TYR:CD2	2.50	0.47
4:B:440:ALA:HB3	4:B:457:ALA:HB1	1.97	0.46
4:B:1127:ALA:HB1	4:B:1263:ARG:HD2	1.96	0.46
4:B:471:ASP:O	4:B:475:GLN:HG2	2.16	0.45
3:A:695:VAL:HA	3:A:696:PRO:HD3	1.86	0.45
3:A:39:ARG:HE	3:A:44:THR:CG2	2.27	0.44
3:A:175:LEU:N	3:A:293:THR:HG21	2.31	0.44
3:A:69:PRO:HG2	3:A:72:ALA:HB3	1.99	0.44
3:A:235:LYS:HB2	3:A:239:GLN:HG3	1.98	0.44
4:B:524:TYR:CE1	4:B:531:PRO:HA	2.53	0.44
3:A:733:ALA:O	3:A:737:ARG:HG2	2.17	0.44
3:A:687:LEU:O	3:A:691:ILE:HG13	2.18	0.43
4:B:586:VAL:HG11	4:B:613:LEU:HD11	1.99	0.43
4:B:837:HIS:HA	4:B:838:PRO:HD3	1.87	0.43
3:A:1:MET:H2	4:B:476:LYS:HG3	1.83	0.43
4:B:381:GLU:HB2	4:B:395:THR:HB	2.00	0.43
4:B:993:GLU:HB3	4:B:1007:TRP:CD1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2:ALA:H	4:B:476:LYS:HE2	1.84	0.43
3:A:831:ALA:HA	4:B:1194:LEU:HD13	1.99	0.43
4:B:408:PRO:HA	4:B:505:TYR:HD1	1.84	0.43
4:B:1091:LEU:HB3	4:B:1094:SER:HB3	2.00	0.43
3:A:353:LYS:HE2	3:A:626:GLU:HG2	2.01	0.42
3:A:352:ASP:O	3:A:356:ILE:HG13	2.19	0.42
3:A:662:GLN:OE1	3:A:798:ASN:HB2	2.19	0.42
4:B:590:PRO:HA	4:B:591:PRO:HD3	1.81	0.42
3:A:723:SER:HB2	3:A:726:MET:H	1.85	0.42
4:B:887:LEU:O	4:B:891:ILE:HG12	2.18	0.42
3:A:414:LEU:N	3:A:415:PRO:HD2	2.34	0.42
3:A:496:LEU:HB2	3:A:513:LEU:HD12	2.01	0.42
4:B:1091:LEU:HB2	4:B:1113:ILE:HB	2.02	0.42
4:B:572:GLN:HB2	4:B:680:ALA:HB2	2.01	0.42
4:B:742:ASN:O	4:B:1145:ARG:NH1	2.53	0.42
4:B:362:PRO:HG2	4:B:455:ASN:HA	2.02	0.42
4:B:1160:VAL:HA	4:B:1161:PRO:HD3	1.88	0.42
4:B:554:ARG:NH2	4:B:604:GLU:HG3	2.29	0.41
4:B:1109:ILE:HA	4:B:1110:PRO:HD3	1.91	0.41
4:B:1235:LEU:HD23	4:B:1239:ILE:HD12	2.03	0.41
4:B:797:ASP:HB3	4:B:882:PHE:HD1	1.84	0.41
4:B:558:VAL:HG21	4:B:585:LEU:HD11	2.03	0.41
3:A:685:ILE:HG12	3:A:696:PRO:HD2	2.04	0.40
3:A:706:ASP:HB2	3:A:742:ASP:HB2	2.03	0.40
2:F:21:DC:H4'	2:F:22:DG:OP1	2.21	0.40
3:A:235:LYS:HE2	3:A:275:LYS:HE3	2.03	0.40
3:A:149:GLY:O	3:A:163:VAL:HA	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	818/934 (88%)	723 (88%)	86 (10%)	9 (1%)	14	46
4	B	913/1022 (89%)	830 (91%)	80 (9%)	3 (0%)	41	72
All	All	1731/1956 (88%)	1553 (90%)	166 (10%)	12 (1%)	22	56

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	533	LEU
3	A	526	THR
3	A	627	LYS
3	A	2	ALA
4	B	930	LYS
4	B	1309	PRO
3	A	426	GLY
3	A	146	GLY
3	A	532	VAL
4	B	745	ILE
3	A	203	GLY
3	A	202	PRO

5.3.2 Protein sidechains (i)

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	704/808 (87%)	704 (100%)	0	100	100
4	B	821/899 (91%)	819 (100%)	2 (0%)	93	96
All	All	1525/1707 (89%)	1523 (100%)	2 (0%)	93	97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	B	576	ASP
4	B	647	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such

sidechains are listed below:

Mol	Chain	Res	Type
3	A	798	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 monosaccharides 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	$\#\|Z\| > 2$
6	ADP	A	936	5	24,29,29	1.03	1 (4%)	29,45,45	1.32	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	-	5/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	936	ADP	C5-C4	2.64	1.47	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	936	ADP	N3-C2-N1	-3.29	123.54	128.68
6	A	936	ADP	PA-O3A-PB	-3.15	122.03	132.83
6	A	936	ADP	C4-C5-N7	-2.51	106.78	109.40
6	A	936	ADP	C3'-C2'-C1'	2.49	104.72	100.98

There are no chirality outliers.

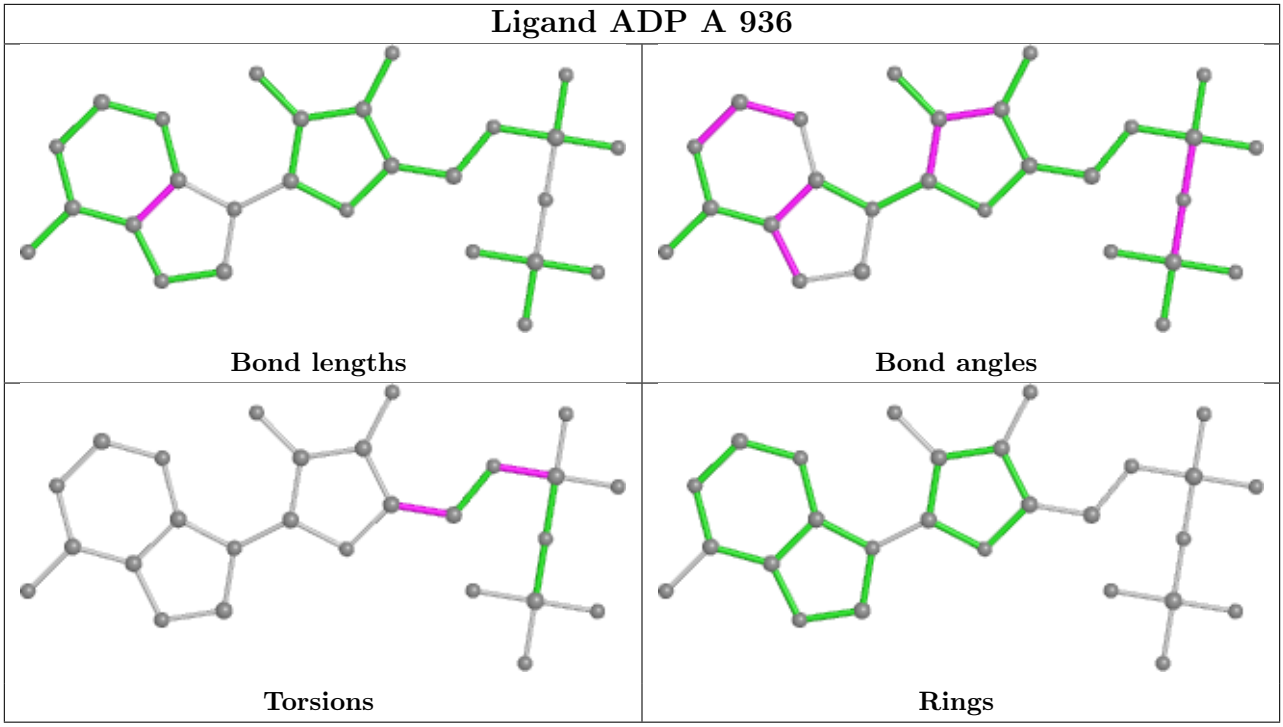
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	936	ADP	C5'-O5'-PA-O2A
6	A	936	ADP	C5'-O5'-PA-O3A
6	A	936	ADP	O4'-C4'-C5'-O5'
6	A	936	ADP	C5'-O5'-PA-O1A
6	A	936	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	17/17 (100%)	0.69	1 (5%)	22	21	105, 113, 127, 132	0
2	F	18/18 (100%)	1.06	3 (16%)	1	1	102, 112, 118, 118	0
3	A	832/934 (89%)	1.07	158 (18%)	1	1	38, 111, 114, 120	0
4	B	933/1022 (91%)	0.84	114 (12%)	4	4	38, 110, 121, 126	0
All	All	1800/1991 (90%)	0.95	276 (15%)	2	2	38, 111, 118, 132	0

All (276) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	B	550	SER	11.0
3	A	153	SER	8.8
3	A	426	GLY	7.1
4	B	1308	LEU	6.8
3	A	366	PHE	6.6
3	A	206	THR	6.3
3	A	152	MET	6.0
4	B	1330	LEU	5.8
4	B	1285	PHE	5.8
3	A	284	SER	5.4
4	B	1269	CYS	5.4
3	A	131	PHE	5.4
3	A	166	VAL	5.3
3	A	692	GLY	5.3
3	A	291	LEU	5.3
3	A	852	GLU	5.2
4	B	651	ILE	5.1
3	A	469	LEU	5.1
1	E	17	DG	5.0
3	A	161	VAL	4.9
3	A	395	GLN	4.8

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Mol	Chain	Res	Type	RSRZ
4	B	954	TYR	4.8
4	B	1284	THR	4.7
3	A	587	GLY	4.7
4	B	669	ILE	4.7
3	A	202	PRO	4.7
2	F	15	DC	4.6
3	A	421	LEU	4.6
4	B	716	THR	4.6
3	A	693	CYS	4.6
3	A	319	ASP	4.5
3	A	292	THR	4.5
3	A	706	ASP	4.5
3	A	798	ASN	4.5
4	B	717	VAL	4.4
3	A	480	GLU	4.3
3	A	236	ASP	4.3
4	B	997	LYS	4.2
3	A	750	LEU	4.1
4	B	1309	PRO	4.1
3	A	242	ASN	4.1
4	B	552	HIS	4.0
4	B	1235	LEU	4.0
4	B	1087	PRO	4.0
3	A	156	ASP	3.9
3	A	726	MET	3.9
3	A	478	LEU	3.9
4	B	1137	MET	3.9
4	B	1085	THR	3.9
3	A	390	LEU	3.9
3	A	574	GLN	3.8
3	A	108	GLY	3.8
3	A	384	PHE	3.8
3	A	330	LEU	3.7
3	A	598	VAL	3.7
3	A	608	PHE	3.7
4	B	1323	PHE	3.7
4	B	1303	ALA	3.7
4	B	1135	PRO	3.7
3	A	767	SER	3.7
4	B	1300	PHE	3.7
3	A	1	MET	3.6
4	B	1131	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
4	B	1138	GLY	3.6
3	A	394	PHE	3.5
3	A	582	VAL	3.5
3	A	585	SER	3.5
4	B	1129	CYS	3.5
3	A	436	PHE	3.5
3	A	350	LEU	3.5
4	B	989	ASN	3.5
4	B	747	LEU	3.5
3	A	179	PRO	3.4
4	B	1120	GLU	3.4
3	A	197	LYS	3.4
3	A	736	LEU	3.4
4	B	679	LEU	3.4
4	B	508	VAL	3.4
4	B	1091	LEU	3.4
3	A	704	ILE	3.4
3	A	754	THR	3.3
4	B	1332	LEU	3.3
3	A	254	ASN	3.3
3	A	483	GLU	3.3
3	A	175	LEU	3.3
3	A	404	CYS	3.3
3	A	431	LEU	3.3
4	B	637	LEU	3.3
3	A	224	ILE	3.3
3	A	458	LEU	3.2
4	B	556	TYR	3.2
3	A	201	LEU	3.2
3	A	269	SER	3.2
3	A	751	GLY	3.2
3	A	830	VAL	3.2
4	B	1248	HIS	3.2
3	A	251	GLU	3.1
3	A	363	VAL	3.1
3	A	452	GLU	3.1
3	A	459	ASP	3.1
3	A	414	LEU	3.1
3	A	425	GLU	3.1
3	A	817	VAL	3.1
3	A	785	HIS	3.1
4	B	543	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
3	A	777	PHE	3.0
4	B	1132	VAL	3.0
3	A	787	LEU	3.0
2	F	32	DC	3.0
4	B	1268	ALA	3.0
3	A	738	SER	3.0
4	B	507	ARG	3.0
2	F	28	DC	3.0
4	B	1327	ASN	3.0
3	A	768	GLU	3.0
3	A	437	VAL	2.9
4	B	1270	MET	2.9
4	B	1299	GLY	2.9
4	B	981	ILE	2.9
4	B	1252	LEU	2.9
3	A	180	ASP	2.9
3	A	187	LEU	2.9
3	A	359	ARG	2.9
3	A	158	GLN	2.8
3	A	689	ALA	2.8
4	B	990	LEU	2.8
4	B	501	HIS	2.8
4	B	1128	TYR	2.8
3	A	468	PHE	2.8
4	B	1113	ILE	2.8
4	B	1086	PRO	2.8
3	A	150	VAL	2.8
3	A	725	PHE	2.8
3	A	518	GLN	2.8
4	B	1258	GLN	2.8
3	A	223	LEU	2.8
4	B	1304	ARG	2.8
4	B	1312	VAL	2.8
4	B	1144	MET	2.7
4	B	1001	LYS	2.7
3	A	163	VAL	2.7
3	A	667	ILE	2.7
3	A	190	LEU	2.7
3	A	351	MET	2.7
4	B	933	PHE	2.7
4	B	1149	LEU	2.7
4	B	1231	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
3	A	484	ILE	2.7
3	A	666	ILE	2.7
4	B	514	CYS	2.7
3	A	470	VAL	2.7
4	B	1003	CYS	2.7
3	A	194	ILE	2.7
3	A	482	ARG	2.6
4	B	1307	ASN	2.6
4	B	1126	LYS	2.6
3	A	50	ALA	2.6
3	A	301	LYS	2.6
3	A	448	SER	2.6
3	A	381	LEU	2.6
3	A	294	PHE	2.6
3	A	588	TYR	2.6
3	A	283	ASP	2.6
3	A	260	GLU	2.5
3	A	538	ASN	2.5
4	B	1218	GLY	2.5
4	B	1326	MET	2.5
4	B	1333	PHE	2.5
3	A	496	LEU	2.5
3	A	592	MET	2.5
3	A	207	ALA	2.5
3	A	135	LEU	2.5
3	A	634	LEU	2.5
4	B	1289	PHE	2.5
4	B	549	SER	2.5
3	A	631	ARG	2.5
3	A	405	TYR	2.5
3	A	266	ALA	2.5
3	A	760	PHE	2.5
4	B	1155	GLN	2.5
4	B	1158	CYS	2.4
4	B	978	GLN	2.4
3	A	253	MET	2.4
3	A	61	GLN	2.4
4	B	1237	GLU	2.4
4	B	1227	ILE	2.4
4	B	1247	THR	2.4
3	A	523	PHE	2.4
4	B	1079	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
3	A	200	VAL	2.4
3	A	300	MET	2.4
3	A	584	ILE	2.4
3	A	358	GLU	2.4
3	A	411	ILE	2.4
4	B	1140	LYS	2.4
3	A	178	PHE	2.4
3	A	739	ALA	2.4
4	B	957	LYS	2.4
4	B	1256	TYR	2.4
3	A	407	LEU	2.4
4	B	1063	LEU	2.4
3	A	447	PHE	2.4
4	B	668	SER	2.4
3	A	642	VAL	2.3
3	A	595	LEU	2.3
4	B	696	ILE	2.3
4	B	1010	THR	2.3
4	B	1239	ILE	2.3
3	A	472	PRO	2.3
4	B	497	ARG	2.3
4	B	882	PHE	2.3
3	A	580	GLU	2.3
4	B	376	GLU	2.3
4	B	609	LEU	2.3
3	A	261	MET	2.3
4	B	718	SER	2.3
3	A	524	ARG	2.3
3	A	162	GLY	2.3
3	A	199	CYS	2.3
3	A	280	LEU	2.2
3	A	432	LEU	2.2
3	A	581	ILE	2.2
4	B	570	ILE	2.2
4	B	1225	THR	2.2
4	B	1244	LEU	2.2
3	A	96	ARG	2.2
4	B	427	TYR	2.2
4	B	650	GLY	2.2
3	A	792	ASN	2.2
4	B	1124	ASN	2.2
4	B	1083	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
3	A	605	VAL	2.2
3	A	606	VAL	2.2
4	B	1088	PHE	2.2
3	A	290	GLU	2.2
3	A	403	ASP	2.2
3	A	607	SER	2.1
3	A	539	PHE	2.1
3	A	165	TYR	2.1
3	A	521	TYR	2.1
4	B	1123	GLU	2.1
3	A	663	MET	2.1
4	B	1188	SER	2.1
3	A	503	LEU	2.1
4	B	1112	ASP	2.1
3	A	160	GLN	2.1
3	A	193	GLN	2.1
3	A	611	VAL	2.1
3	A	633	ILE	2.1
4	B	968	VAL	2.1
4	B	1210	VAL	2.1
4	B	785	HIS	2.1
3	A	855	GLN	2.1
4	B	969	TYR	2.1
4	B	1071	ASP	2.1
3	A	650	PHE	2.1
4	B	748	ASN	2.1
3	A	98	TYR	2.1
3	A	481	LEU	2.1
3	A	385	PRO	2.1
4	B	457	ALA	2.1
4	B	1097	PRO	2.1
3	A	277	LEU	2.1
4	B	671	LEU	2.1
3	A	645	GLN	2.0
4	B	1030	LYS	2.0
3	A	70	ALA	2.0
4	B	458	HIS	2.0
4	B	782	LEU	2.0
3	A	7	GLU	2.0
4	B	1163	GLU	2.0
4	B	429	VAL	2.0
4	B	1201	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
3	A	853	GLU	2.0
4	B	999	THR	2.0
4	B	1319	LYS	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 monosaccharides in this entry.

6.4 Ligands (i)

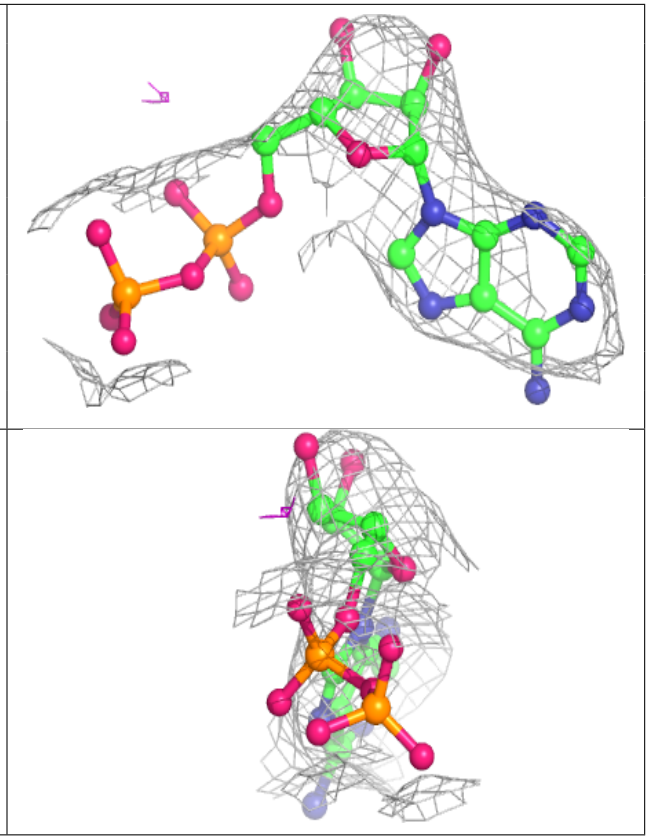
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MG	A	935	1/1	0.95	0.24	92,92,92,92	0
6	ADP	A	936	27/27	0.95	0.22	110,110,111,111	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 936:

$2mF_o$-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.