



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 06:59 PM UTC

PDB ID : 2O8E / pdb_00002o8e
Title : human MutSalpha (MSH2/MSH6) bound to a G T mispair, with ADP bound to MSH2 only
Authors : Warren, J.J.; Pohlhaus, T.J.; Changela, A.; Modrich, P.L.; Beese, L.S.
Deposited on : 2006-12-12
Resolution : 3.30 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

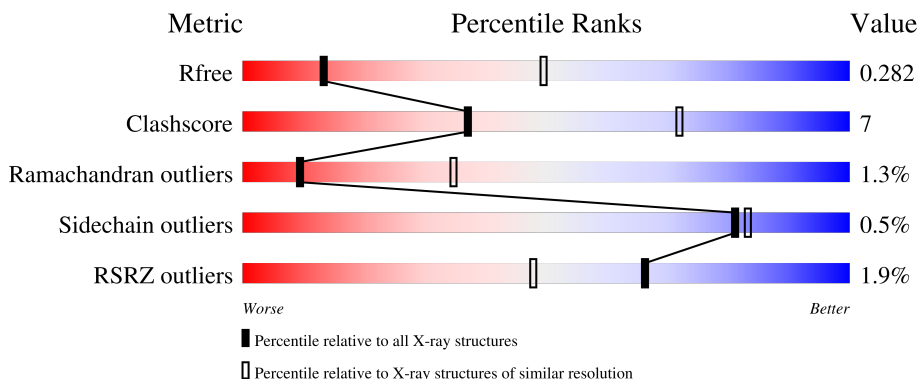
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

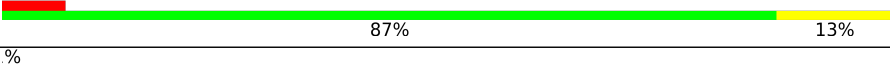
The reported resolution of this entry is 3.30 Å.

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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	
2	F	15	
3	A	934	
4	B	1022	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14587 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*GP*GP*GP*CP*T P*AP*GP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	15	Total	C	N	O	P	0	0	0
			310	146	64	86	14			

- Molecule 2 is a DNA chain called 5'-D(*CP*CP*TP*AP*GP*CP*CP*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
			300	144	51	91	14			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	824	Total	C	N	O	S	0	0	0
			6474	4105	1102	1233	34			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	42	ALA	PHE	engineered mutation	UNP P43246

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	935	Total	C	N	O	S	0	0	0
			7465	4736	1281	1397	51			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	339	MET	-	initiating methionine	UNP P52701

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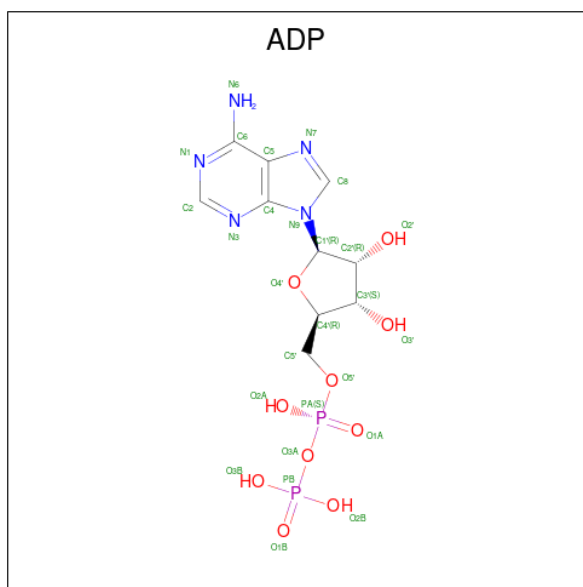
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Chain	Residue	Modelled	Actual	Comment	Reference
B	340	GLY	-	cloning artifact	UNP P52701

- 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

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

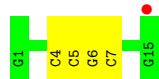
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	10	Total O 10 10	0	0

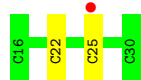
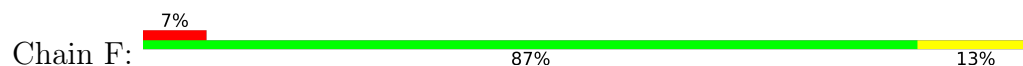
3 Residue-property plots

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.

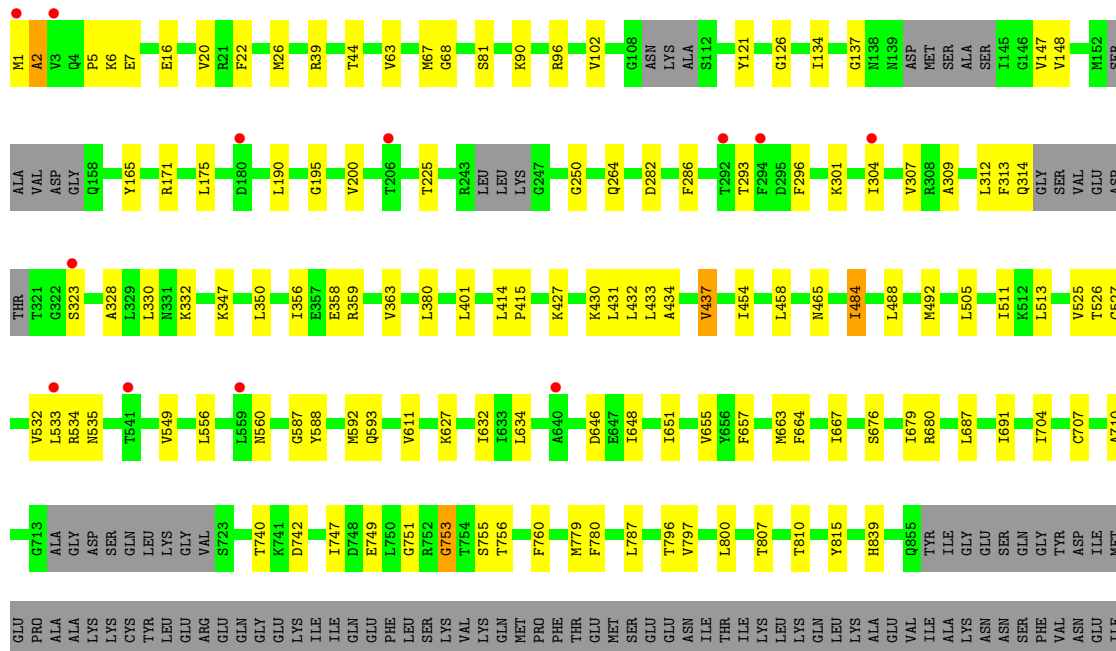
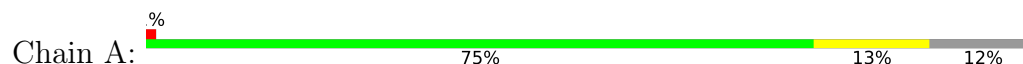
- Molecule 1: 5'-D(*GP*AP*AP*CP*CP*GP*CP*GP*GP*GP*CP*TP*AP*GP*G)-3'

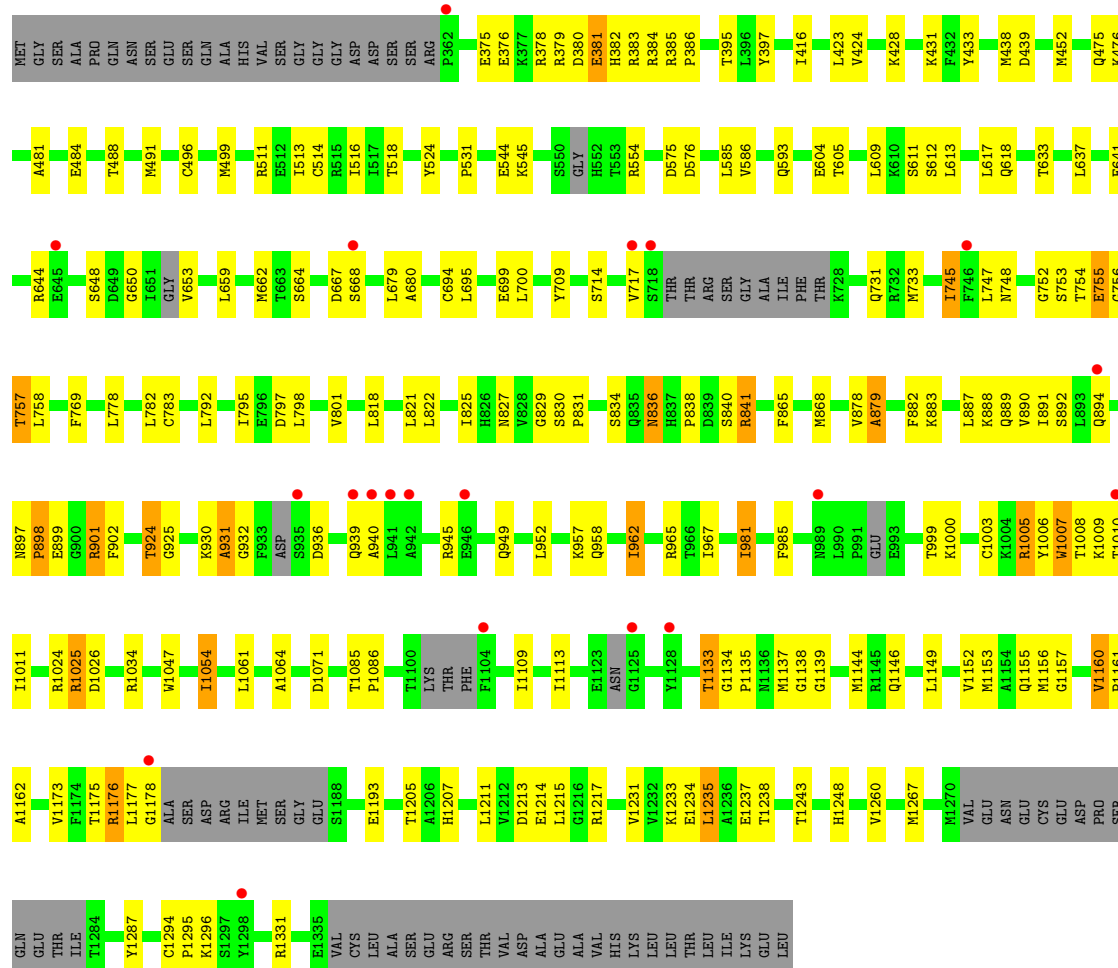


- Molecule 2: 5'-D(*CP*CP*TP*AP*GP*CP*CP*TP*GP*CP*GP*GP*TP*TP*C)-3'



- Molecule 3: DNA mismatch repair protein Msh2





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 3 2	Depositor
Cell constants a, b, c, α , β , γ	257.51Å 257.51Å 257.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.30 20.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	98.5 (20.00-3.30) 97.9 (20.00-3.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.22 (at 3.33Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.253 , 0.291 0.243 , 0.282	Depositor DCC
R_{free} test set	2230 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	91.6	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 133.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	14587	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.45% 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: 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	0.34	0/349	1.09	0/538
2	F	0.29	0/334	0.90	0/513
3	A	0.43	0/6575	0.94	16/8866 (0.2%)
4	B	0.57	0/7609	1.06	26/10254 (0.3%)
All	All	0.50	0/14867	1.01	42/20171 (0.2%)

There are no bond length outliers.

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	841	ARG	N-CA-C	-7.87	103.19	114.12
3	A	787	LEU	N-CA-C	-7.81	103.97	113.97
4	B	965	ARG	N-CA-C	7.69	120.74	111.82
4	B	981	ILE	CA-C-N	6.87	128.43	119.84
4	B	981	ILE	C-N-CA	6.87	128.43	119.84
4	B	879	ALA	N-CA-C	6.87	118.42	111.07
3	A	651	ILE	CA-C-N	6.83	126.59	119.76
3	A	651	ILE	C-N-CA	6.83	126.59	119.76
4	B	756	GLY	N-CA-C	-6.53	97.70	113.18
4	B	836	ASN	N-CA-C	6.43	120.87	112.89
3	A	358	GLU	N-CA-C	-6.43	103.56	111.40
4	B	1005	ARG	N-CA-C	6.33	118.70	109.07
3	A	96	ARG	N-CA-C	6.25	120.37	112.87
4	B	901	ARG	N-CA-C	6.03	119.20	109.79
3	A	710	ALA	N-CA-C	5.99	119.25	108.48
4	B	902	PHE	CA-C-N	5.95	125.89	119.76
4	B	902	PHE	C-N-CA	5.95	125.89	119.76
4	B	381	GLU	N-CA-C	-5.75	105.10	111.71
3	A	587	GLY	N-CA-C	-5.72	106.73	115.66
4	B	957	LYS	N-CA-C	-5.70	104.53	112.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	700	LEU	N-CA-C	5.62	117.40	111.28
3	A	753	GLY	N-CA-C	5.58	115.29	110.21
4	B	755	GLU	N-CA-C	5.56	118.53	109.24
3	A	437	VAL	N-CA-C	-5.53	107.43	112.96
4	B	1025	ARG	N-CA-C	-5.52	105.34	111.36
3	A	380	LEU	N-CA-C	5.52	119.99	112.04
3	A	431	LEU	N-CA-C	-5.40	106.72	113.15
4	B	1138	GLY	N-CA-C	-5.40	106.25	112.73
4	B	757	THR	N-CA-C	5.39	117.64	110.53
3	A	304	ILE	N-CA-C	-5.39	105.01	112.50
3	A	63	VAL	N-CA-C	-5.32	107.63	113.43
4	B	962	ILE	N-CA-C	-5.32	104.31	111.44
4	B	664	SER	N-CA-C	5.15	121.77	110.80
4	B	1160	VAL	CA-C-N	5.13	126.25	119.84
4	B	1160	VAL	C-N-CA	5.13	126.25	119.84
4	B	1295	PRO	N-CA-C	-5.13	101.90	112.47
4	B	424	VAL	N-CA-C	-5.10	100.99	108.54
3	A	484	ILE	N-CA-C	-5.08	105.75	110.53
3	A	264	GLN	N-CA-C	5.06	117.53	111.71
4	B	1139	GLY	N-CA-C	5.04	118.74	112.64
4	B	1294	CYS	N-CA-C	5.03	116.17	109.93
3	A	815	TYR	N-CA-C	5.00	118.97	112.86

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	310	0	168	4	0
2	F	300	0	171	2	0
3	A	6474	0	6500	69	0
4	B	7465	0	7444	137	0
5	A	1	0	0	0	0
6	A	27	0	12	0	0
7	B	10	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	14587	0	14295	205	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 7.

All (205) 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:1133:THR:HB	4:B:1134:GLY:HA3	1.36	1.07
4:B:554:ARG:HH22	4:B:604:GLU:HG3	1.39	0.85
4:B:1133:THR:HB	4:B:1134:GLY:CA	2.06	0.84
4:B:945:ARG:HD2	4:B:1024:ARG:HH12	1.44	0.82
4:B:1133:THR:CB	4:B:1134:GLY:HA3	2.10	0.82
4:B:868:MET:HG2	4:B:1054:ILE:HD12	1.66	0.76
4:B:380:ASP:HB3	4:B:382:HIS:H	1.51	0.75
4:B:897:ASN:HB3	4:B:901:ARG:HH21	1.53	0.73
4:B:778:LEU:HG	4:B:1156:MET:HE1	1.70	0.72
4:B:733:MET:HE3	4:B:1173:VAL:HG23	1.71	0.72
4:B:795:ILE:HG23	4:B:1064:ALA:HA	1.72	0.71
4:B:699:GLU:HB3	4:B:827:ASN:OD1	1.90	0.71
4:B:385:ARG:HD2	4:B:386:PRO:HD2	1.73	0.70
4:B:544:GLU:OE2	4:B:605:THR:OG1	2.08	0.68
4:B:380:ASP:HB2	4:B:384:ARG:H	1.58	0.68
4:B:897:ASN:HB3	4:B:901:ARG:NH2	2.10	0.66
3:A:525:VAL:HG12	3:A:526:THR:H	1.61	0.66
4:B:930:LYS:H	4:B:930:LYS:HD2	1.61	0.65
4:B:932:GLY:HA2	4:B:936:ASP:H	1.62	0.65
3:A:5:PRO:HB3	3:A:81:SER:HB3	1.78	0.65
4:B:930:LYS:HD2	4:B:930:LYS:N	2.12	0.65
4:B:496:CYS:HA	4:B:499:MET:HG2	1.79	0.65
4:B:1176:ARG:HE	4:B:1193:GLU:HG3	1.61	0.64
4:B:385:ARG:CD	4:B:386:PRO:HD2	2.28	0.64
3:A:430:LYS:HA	3:A:433:LEU:HB2	1.80	0.64
4:B:733:MET:HE3	4:B:1173:VAL:CG2	2.27	0.63
3:A:359:ARG:NH2	3:A:691:ILE:O	2.32	0.63
4:B:888:LYS:O	4:B:892:SER:OG	2.17	0.63
3:A:350:LEU:HB2	3:A:356:ILE:HG12	1.80	0.61
4:B:641:GLU:HB3	4:B:644:ARG:HG3	1.82	0.61
4:B:381:GLU:HB2	4:B:395:THR:HB	1.82	0.61
3:A:39:ARG:HE	3:A:44:THR:HG21	1.66	0.60
4:B:1153:MET:HB3	4:B:1160:VAL:HG12	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:430:LYS:C	3:A:432:LEU:H	2.10	0.60
4:B:1235:LEU:HD21	4:B:1243:THR:HG21	1.84	0.59
1:E:4:DC:H2'	1:E:5:DC:C6	2.38	0.59
4:B:936:ASP:HA	4:B:939:GLN:HB3	1.85	0.58
4:B:1176:ARG:NE	4:B:1193:GLU:HG3	2.18	0.58
4:B:898:PRO:O	4:B:899:GLU:HG3	2.03	0.58
4:B:518:THR:HG21	4:B:593:GLN:NE2	2.19	0.58
4:B:644:ARG:O	4:B:648:SER:HB3	2.04	0.57
4:B:380:ASP:O	4:B:397:TYR:HB2	2.03	0.57
4:B:798:LEU:HD13	4:B:1061:LEU:HD23	1.87	0.57
4:B:747:LEU:HA	4:B:757:THR:HG21	1.86	0.56
3:A:588:TYR:O	3:A:592:MET:HG2	2.06	0.56
3:A:505:LEU:HD12	3:A:511:ILE:HD11	1.87	0.56
4:B:484:GLU:HB2	4:B:514:CYS:SG	2.46	0.56
3:A:309:ALA:O	3:A:680:ARG:HD2	2.07	0.55
4:B:423:LEU:HD13	4:B:481:ALA:HB2	1.88	0.55
4:B:745:ILE:HD11	4:B:1152:VAL:HG21	1.88	0.55
4:B:981:ILE:HD11	4:B:985:PHE:HB2	1.87	0.55
4:B:836:ASN:O	4:B:841:ARG:NH2	2.38	0.55
4:B:1007:TRP:H	4:B:1011:ILE:HD12	1.72	0.55
4:B:585:LEU:HD12	4:B:709:TYR:CE2	2.43	0.54
3:A:414:LEU:N	3:A:415:PRO:HD2	2.23	0.54
4:B:380:ASP:HB2	4:B:384:ARG:N	2.24	0.53
4:B:381:GLU:HB2	4:B:395:THR:CB	2.37	0.53
3:A:634:LEU:HB2	3:A:655:VAL:HB	1.90	0.53
4:B:433:TYR:OH	4:B:484:GLU:OE1	2.24	0.53
4:B:829:GLY:HA2	4:B:1034:ARG:HG2	1.90	0.53
3:A:664:PHE:HB3	3:A:797:VAL:HG22	1.91	0.53
4:B:868:MET:CG	4:B:1054:ILE:HD12	2.38	0.53
3:A:16:GLU:HG3	3:A:67:MET:HE3	1.90	0.52
4:B:585:LEU:C	4:B:585:LEU:HD23	2.34	0.52
4:B:1025:ARG:HG3	4:B:1026:ASP:N	2.22	0.52
4:B:575:ASP:OD1	4:B:576:ASP:N	2.40	0.52
2:F:22:DC:H2''	4:B:452:MET:HE3	1.91	0.52
4:B:496:CYS:HA	4:B:499:MET:CG	2.39	0.52
4:B:887:LEU:O	4:B:891:ILE:HG12	2.10	0.51
4:B:890:VAL:HG23	4:B:891:ILE:HG23	1.92	0.51
4:B:1234:GLU:HG3	4:B:1238:THR:HB	1.92	0.51
1:E:7:DC:H2''	4:B:431:LYS:HD2	1.92	0.51
4:B:782:LEU:O	4:B:1155:GLN:NE2	2.40	0.51
4:B:586:VAL:HG11	4:B:613:LEU:HD11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:897:ASN:O	4:B:901:ARG:NE	2.44	0.51
3:A:20:VAL:HG21	3:A:68:GLY:HA2	1.93	0.51
3:A:755:SER:HA	4:B:1248:HIS:HB3	1.92	0.51
4:B:899:GLU:O	4:B:901:ARG:NH1	2.44	0.51
4:B:1175:THR:HG22	4:B:1211:LEU:HD12	1.93	0.51
4:B:609:LEU:HB3	4:B:618:GLN:HE21	1.76	0.50
4:B:889:GLN:HA	4:B:901:ARG:HD3	1.92	0.50
4:B:633:THR:O	4:B:637:LEU:HG	2.12	0.50
4:B:488:THR:OG1	4:B:491:MET:HG3	2.12	0.50
4:B:545:LYS:HE3	4:B:679:LEU:HD21	1.93	0.50
4:B:516:ILE:HB	4:B:694:CYS:HA	1.92	0.50
4:B:754:THR:C	4:B:755:GLU:HG3	2.36	0.50
4:B:1085:THR:HB	4:B:1086:PRO:HD2	1.93	0.49
4:B:949:GLN:HA	4:B:952:LEU:HB3	1.94	0.49
3:A:687:LEU:O	3:A:691:ILE:HG13	2.12	0.49
3:A:90:LYS:NZ	3:A:134:ILE:O	2.45	0.49
4:B:1109:ILE:HD12	4:B:1287:TYR:HB2	1.93	0.49
3:A:330:LEU:HA	3:A:611:VAL:HG21	1.93	0.49
3:A:511:ILE:HG12	3:A:525:VAL:HG22	1.95	0.48
3:A:359:ARG:O	3:A:363:VAL:HG23	2.14	0.48
3:A:740:THR:HG23	3:A:742:ASP:H	1.78	0.48
4:B:428:LYS:HD2	4:B:484:GLU:OE2	2.14	0.48
3:A:454:ILE:HG23	3:A:458:LEU:HD13	1.96	0.48
3:A:307:VAL:HG22	3:A:312:LEU:HD12	1.97	0.47
4:B:958:GLN:O	4:B:962:ILE:HG13	2.14	0.47
4:B:1215:LEU:HD21	4:B:1231:VAL:HG21	1.96	0.47
3:A:646:ASP:HB3	3:A:648:ILE:HG13	1.97	0.47
4:B:644:ARG:HG2	4:B:653:VAL:HG11	1.96	0.47
4:B:801:VAL:HG21	4:B:878:VAL:HG21	1.97	0.47
3:A:401:LEU:HD11	3:A:458:LEU:HD11	1.95	0.47
3:A:839:HIS:NE2	4:B:1234:GLU:OE1	2.47	0.47
4:B:1137:MET:SD	4:B:1267:MET:HG2	2.54	0.47
4:B:1176:ARG:O	4:B:1176:ARG:HG3	2.14	0.47
4:B:1233:LYS:O	4:B:1237:GLU:HB3	2.14	0.47
3:A:1:MET:HE3	4:B:475:GLN:HG3	1.95	0.47
3:A:679:ILE:HG22	3:A:779:MET:HE2	1.97	0.47
3:A:328:ALA:O	3:A:332:LYS:NZ	2.44	0.46
1:E:5:DC:H2'	1:E:6:DG:C8	2.50	0.46
4:B:662:MET:HE1	4:B:680:ALA:HB3	1.97	0.46
4:B:838:PRO:C	4:B:840:SER:H	2.22	0.46
3:A:126:GLY:HA3	3:A:147:VAL:HG23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:756:THR:O	3:A:760:PHE:HB3	2.15	0.46
4:B:524:TYR:CE1	4:B:531:PRO:HA	2.50	0.46
3:A:556:LEU:HD23	3:A:560:ASN:HB2	1.98	0.46
4:B:792:LEU:HG	4:B:1157:GLY:HA2	1.96	0.46
4:B:1175:THR:HB	4:B:1177:LEU:HG	1.98	0.46
4:B:611:SER:OG	4:B:612:SER:N	2.45	0.46
4:B:797:ASP:HB3	4:B:882:PHE:CD1	2.51	0.46
3:A:200:VAL:HA	3:A:225:THR:O	2.16	0.46
3:A:667:ILE:HG12	3:A:800:LEU:HB2	1.97	0.45
4:B:1113:ILE:HD11	4:B:1146:GLN:HE21	1.80	0.45
3:A:430:LYS:C	3:A:432:LEU:N	2.74	0.45
3:A:313:PHE:HZ	3:A:347:LYS:HG3	1.82	0.45
4:B:1214:GLU:OE1	4:B:1217:ARG:HD3	2.16	0.45
3:A:307:VAL:HG13	3:A:312:LEU:HB2	1.99	0.45
4:B:936:ASP:O	4:B:940:ALA:N	2.44	0.45
4:B:830:SER:HA	4:B:831:PRO:HD3	1.83	0.45
4:B:930:LYS:H	4:B:930:LYS:CD	2.27	0.44
4:B:484:GLU:O	4:B:511:ARG:HA	2.17	0.44
4:B:1008:THR:C	4:B:1010:THR:N	2.75	0.44
4:B:1008:THR:C	4:B:1010:THR:H	2.25	0.44
3:A:7:GLU:CD	3:A:7:GLU:H	2.26	0.44
3:A:22:PHE:O	3:A:26:MET:HG3	2.18	0.44
3:A:663:MET:HB2	3:A:796:THR:HB	2.00	0.44
4:B:818:LEU:HD12	4:B:868:MET:HE3	2.00	0.44
3:A:632:ILE:HB	3:A:657:PHE:HB2	1.99	0.44
3:A:175:LEU:H	3:A:293:THR:HG21	1.83	0.44
4:B:967:ILE:HG12	4:B:981:ILE:HB	1.99	0.43
3:A:532:VAL:O	3:A:533:LEU:HB2	2.18	0.43
3:A:484:ILE:O	3:A:488:LEU:HG	2.18	0.43
3:A:1:MET:O	3:A:2:ALA:HB3	2.19	0.43
3:A:301:LYS:HB2	3:A:707:CYS:HB3	2.01	0.43
3:A:427:LYS:HA	3:A:430:LYS:HB2	2.00	0.43
3:A:807:THR:HB	3:A:810:THR:HB	2.01	0.43
4:B:659:LEU:HD23	4:B:662:MET:HG3	2.01	0.43
3:A:39:ARG:HE	3:A:44:THR:CG2	2.30	0.43
4:B:822:LEU:HD23	4:B:822:LEU:HA	1.88	0.43
3:A:313:PHE:CZ	3:A:347:LYS:HG3	2.54	0.43
4:B:865:PHE:CZ	4:B:1047:TRP:HB3	2.54	0.43
3:A:434:ALA:HA	3:A:437:VAL:HB	1.99	0.43
3:A:492:MET:HE3	3:A:513:LEU:HD11	2.00	0.43
4:B:375:GLU:HG2	4:B:378:ARG:CZ	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:924:THR:HB	4:B:925:GLY:H	1.59	0.43
4:B:667:ASP:CG	4:B:668:SER:H	2.25	0.43
3:A:1:MET:H2	4:B:476:LYS:HE2	1.84	0.42
4:B:379:ARG:HD3	4:B:383:ARG:O	2.18	0.42
4:B:748:ASN:H	4:B:757:THR:HG21	1.84	0.42
4:B:879:ALA:HA	4:B:882:PHE:CD2	2.54	0.42
4:B:999:THR:OG1	4:B:1000:LYS:N	2.51	0.42
4:B:376:GLU:H	4:B:376:GLU:HG3	1.59	0.42
4:B:438:MET:CG	4:B:439:ASP:H	2.33	0.42
4:B:731:GLN:HB2	4:B:783:CYS:SG	2.59	0.42
4:B:758:LEU:HD22	4:B:1149:LEU:HD22	2.02	0.42
4:B:897:ASN:O	4:B:901:ARG:CZ	2.68	0.42
3:A:747:ILE:HB	3:A:780:PHE:HD1	1.83	0.42
3:A:751:GLY:C	3:A:753:GLY:H	2.28	0.42
4:B:882:PHE:CE2	4:B:891:ILE:HD11	2.54	0.42
3:A:556:LEU:O	3:A:560:ASN:N	2.50	0.42
4:B:518:THR:HG21	4:B:593:GLN:CD	2.45	0.42
4:B:769:PHE:HE1	4:B:1054:ILE:HG22	1.84	0.42
3:A:148:VAL:HG12	3:A:165:TYR:HB3	2.02	0.42
3:A:313:PHE:O	3:A:314:GLN:HG3	2.19	0.42
4:B:695:LEU:HA	4:B:695:LEU:HD23	1.73	0.42
3:A:190:LEU:HD11	3:A:296:PHE:HB2	2.01	0.42
4:B:416:ILE:HG23	4:B:513:ILE:HD11	2.01	0.42
4:B:1160:VAL:C	4:B:1162:ALA:H	2.28	0.42
3:A:282:ASP:HB2	3:A:286:PHE:CE2	2.54	0.41
4:B:1177:LEU:HA	4:B:1213:ASP:HB3	2.02	0.41
3:A:102:VAL:HB	3:A:121:TYR:HB2	2.02	0.41
4:B:694:CYS:O	4:B:695:LEU:HB2	2.21	0.41
4:B:797:ASP:CG	4:B:883:LYS:H	2.28	0.41
4:B:378:ARG:HD3	7:B:47:HOH:O	2.19	0.41
4:B:428:LYS:HE3	4:B:433:TYR:CZ	2.55	0.41
3:A:430:LYS:HG2	3:A:433:LEU:HB2	2.02	0.41
3:A:527:CYS:HA	3:A:549:VAL:HG23	2.02	0.41
4:B:931:ALA:C	4:B:936:ASP:HB3	2.46	0.41
4:B:1003:CYS:SG	4:B:1005:ARG:NH1	2.93	0.41
4:B:1177:LEU:O	4:B:1178:GLY:C	2.64	0.41
4:B:894:GLN:H	4:B:894:GLN:CD	2.28	0.41
4:B:1144:MET:O	4:B:1211:LEU:HD13	2.21	0.41
4:B:821:LEU:O	4:B:825:ILE:HG13	2.21	0.41
4:B:1008:THR:O	4:B:1010:THR:N	2.54	0.41
3:A:627:LYS:HA	3:A:704:ILE:HB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1205:THR:C	4:B:1207:HIS:H	2.28	0.41
3:A:534:ARG:HG3	3:A:535:ASN:H	1.86	0.41
4:B:514:CYS:C	4:B:695:LEU:HD12	2.47	0.40
4:B:593:GLN:HG3	4:B:617:LEU:HB2	2.02	0.40
1:E:5:DC:C2'	1:E:6:DG:C8	3.04	0.40
2:F:25:DC:O5'	3:A:6:LYS:HD3	2.20	0.40
3:A:171:ARG:HE	3:A:593:GLN:HE22	1.68	0.40
3:A:676:SER:O	3:A:680:ARG:HG3	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	
3	A	810/934 (87%)	725 (90%)	78 (10%)	7 (1%)	14	43
4	B	915/1022 (90%)	813 (89%)	86 (9%)	16 (2%)	7	30
All	All	1725/1956 (88%)	1538 (89%)	164 (10%)	23 (1%)	9	35

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	B	753	SER
3	A	749	GLU
4	B	650	GLY
4	B	834	SER
4	B	931	ALA
4	B	1009	LYS
4	B	1161	PRO
4	B	714	SER
4	B	752	GLY
4	B	1296	LYS

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Mol	Chain	Res	Type
3	A	137	GLY
4	B	745	ILE
3	A	2	ALA
3	A	465	ASN
4	B	898	PRO
4	B	1133	THR
3	A	323	SER
4	B	1135	PRO
4	B	1331	ARG
3	A	250	GLY
4	B	717	VAL
4	B	1260	VAL
3	A	195	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	707/807 (88%)	707 (100%)	0	100	100
4	B	821/899 (91%)	814 (99%)	7 (1%)	70	78
All	All	1528/1706 (90%)	1521 (100%)	7 (0%)	81	83

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	B	924	THR
4	B	1006	TYR
4	B	1007	TRP
4	B	1054	ILE
4	B	1071	ASP
4	B	1176	ARG
4	B	1235	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	105	ASN
3	A	285	ASN
3	A	288	GLN
3	A	395	GLN
3	A	545	GLN
3	A	629	GLN
3	A	690	GLN
3	A	824	GLN
4	B	367	HIS
4	B	475	GLN
4	B	522	GLN
4	B	593	GLN
4	B	835	GLN
4	B	989	ASN
4	B	1065	ASN
4	B	1317	HIS

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
6	ADP	A	936	5	28,29,29	1.41	4 (14%)	43,45,45	1.88	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	-	4/16/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	936	ADP	C5-C4	4.66	1.47	1.39
6	A	936	ADP	C5-C6	2.71	1.48	1.41
6	A	936	ADP	C5-N7	-2.38	1.34	1.39
6	A	936	ADP	C8-N7	2.37	1.36	1.31

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	936	ADP	C5-C4-N3	-5.96	118.51	126.72
6	A	936	ADP	N3-C4-N9	4.69	135.14	127.17
6	A	936	ADP	C2-N3-C4	3.80	121.12	111.83
6	A	936	ADP	C4-C5-N7	-3.50	106.58	110.58
6	A	936	ADP	N3-C2-N1	-3.46	123.35	128.58
6	A	936	ADP	C5-N7-C8	2.58	107.50	103.45
6	A	936	ADP	C4-N9-C8	2.50	108.36	105.74
6	A	936	ADP	C3'-C2'-C1'	2.34	105.89	101.46
6	A	936	ADP	C6-C5-N7	2.07	136.08	132.09

There are no chirality outliers.

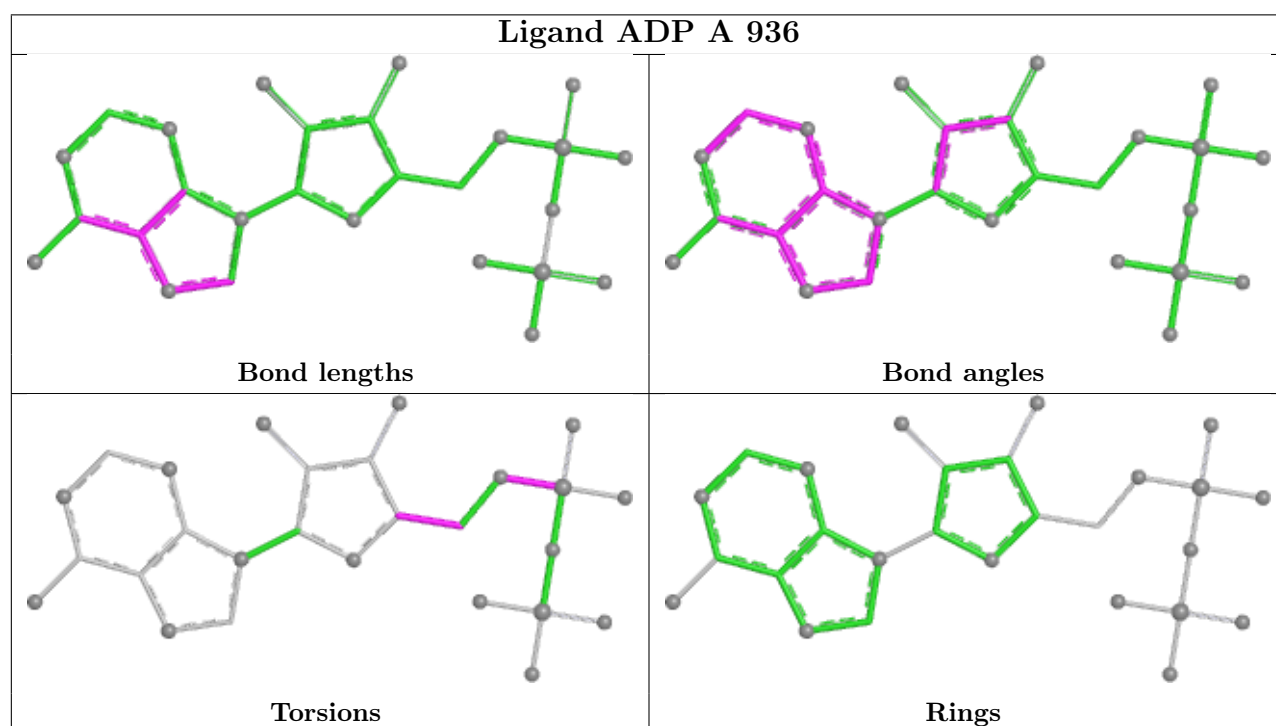
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	936	ADP	C5'-O5'-PA-O1A
6	A	936	ADP	C5'-O5'-PA-O3A
6	A	936	ADP	O4'-C4'-C5'-O5'
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 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	15/15 (100%)	0.66	1 (6%) 24 16	93, 101, 115, 116	0
2	F	15/15 (100%)	0.70	1 (6%) 24 16	90, 100, 119, 123	0
3	A	824/934 (88%)	0.15	12 (1%) 72 53	95, 103, 108, 113	0
4	B	935/1022 (91%)	0.17	20 (2%) 63 44	37, 102, 116, 122	0
All	All	1789/1986 (90%)	0.17	34 (1%) 66 48	37, 103, 114, 123	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	B	935	SER	5.3
4	B	946	GLU	4.8
4	B	939	GLN	4.5
4	B	989	ASN	4.3
4	B	1298	TYR	3.9
4	B	717	VAL	3.6
3	A	533	LEU	3.4
3	A	1	MET	3.1
1	E	15	DG	3.0
4	B	1128	TYR	3.0
3	A	180	ASP	3.0
3	A	292	THR	2.9
4	B	668	SER	2.9
4	B	940	ALA	2.8
4	B	942	ALA	2.7
3	A	304	ILE	2.6
4	B	645	GLU	2.6
4	B	718	SER	2.6
3	A	640	ALA	2.6
3	A	323	SER	2.5
4	B	746	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
4	B	894	GLN	2.4
4	B	362	PRO	2.4
3	A	206	THR	2.3
4	B	1178	GLY	2.3
3	A	559	LEU	2.3
3	A	3	VAL	2.3
4	B	1125	GLY	2.2
3	A	294	PHE	2.2
4	B	1010	THR	2.1
3	A	541	THR	2.1
4	B	1104	PHE	2.0
2	F	25	DC	2.0
4	B	941	LEU	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](#)

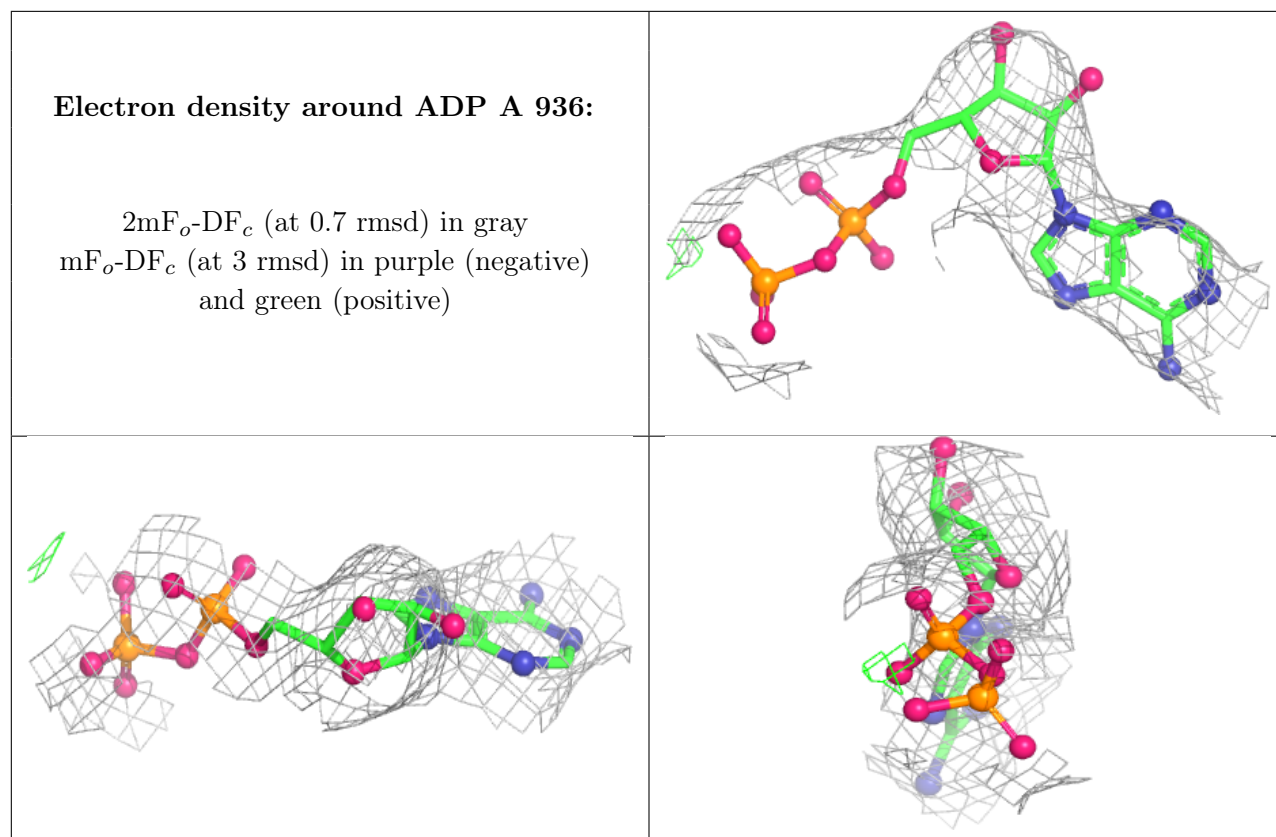
There are no oligosaccharides in this entry.

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	935	1/1	0.79	0.20	79,79,79,79	0
6	ADP	A	936	27/27	0.96	0.06	97,98,100,100	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.